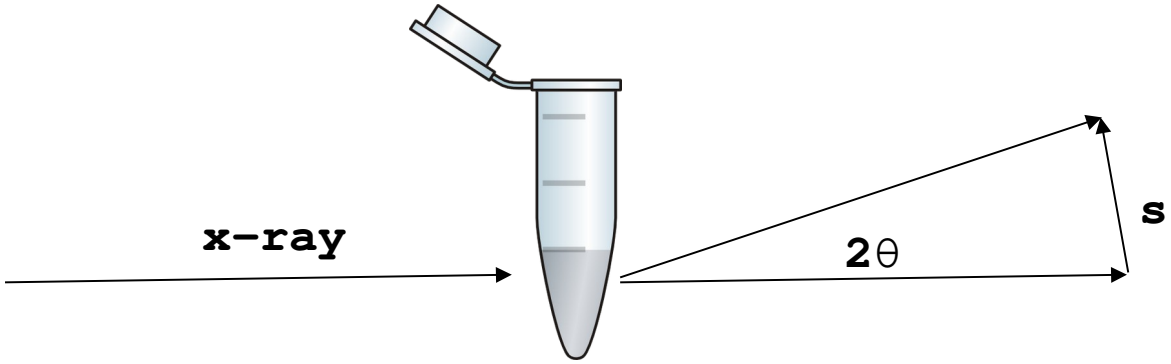
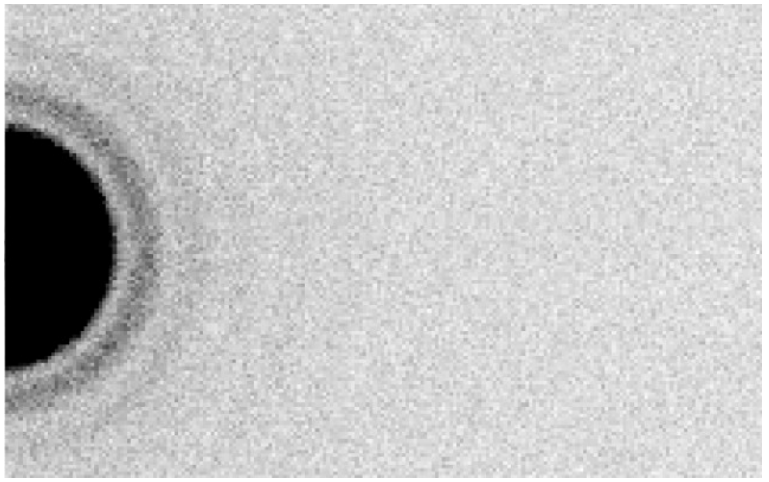
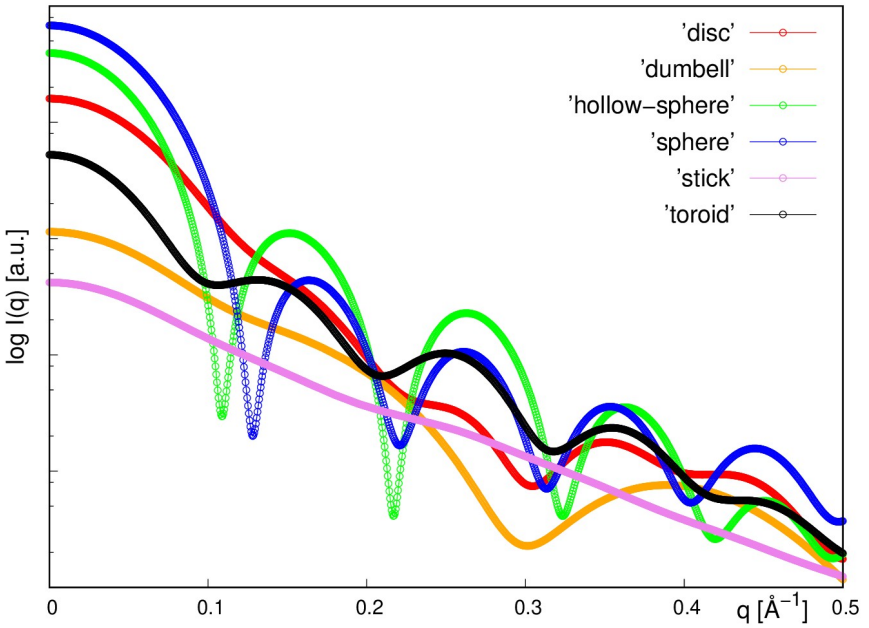


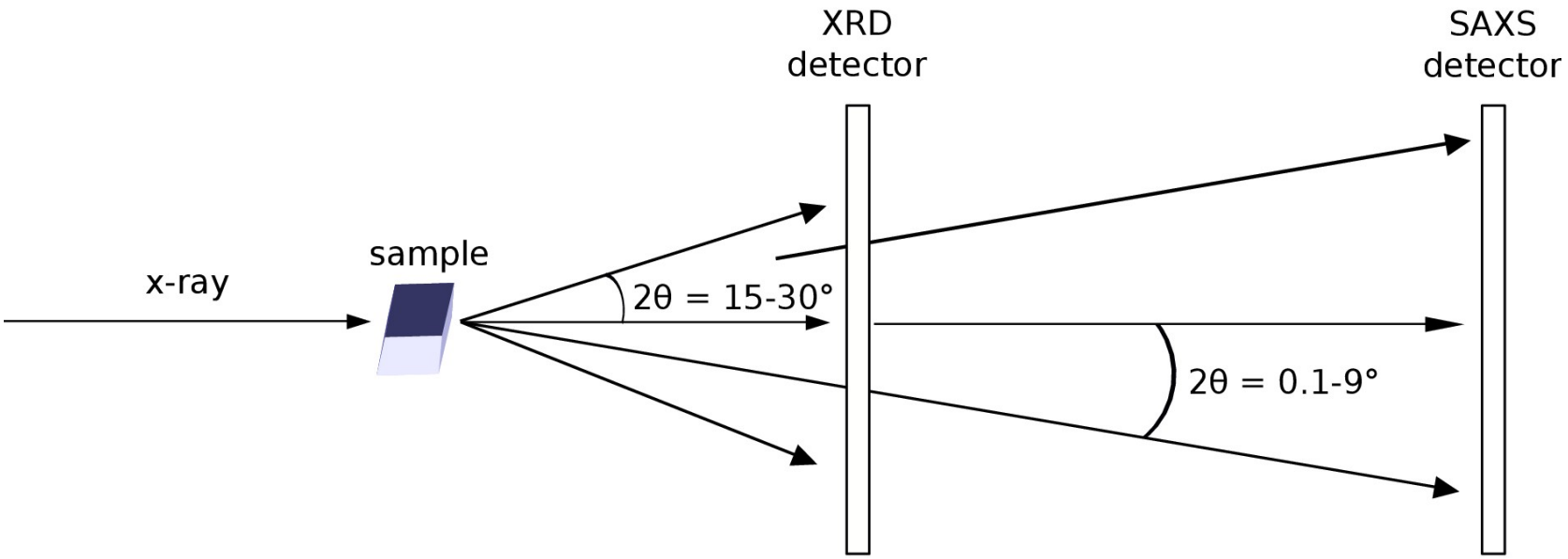


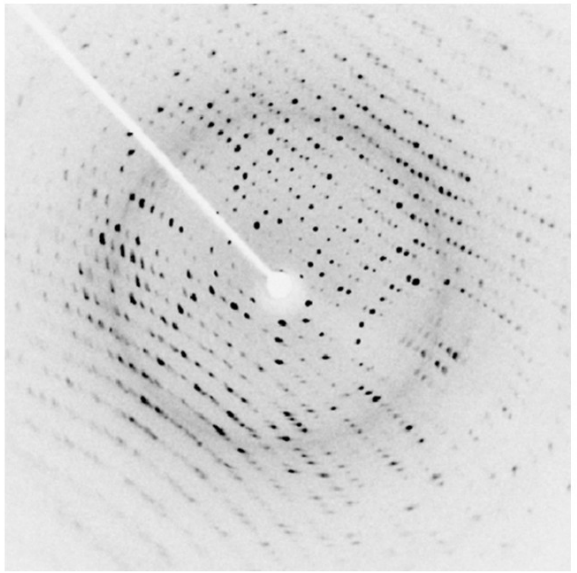
- size (Rg, Dmax, volume)
- folding state, compactness
- overal shape ~30 Å resolution

- oligomeric state
- quaternary structure
- flexible systems

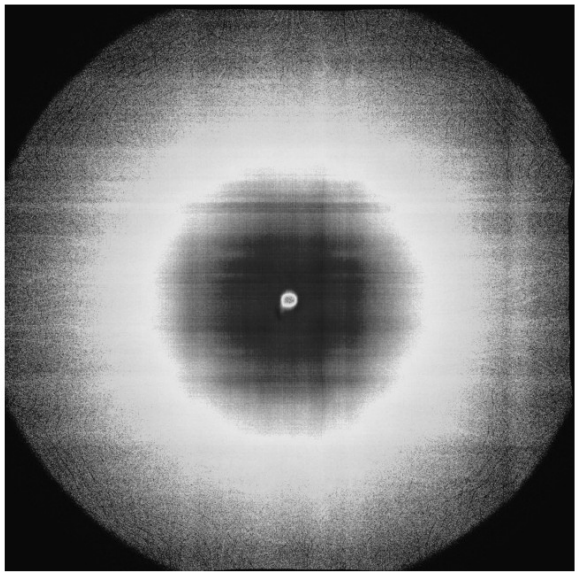


Experimental setup XRD vs SAXS

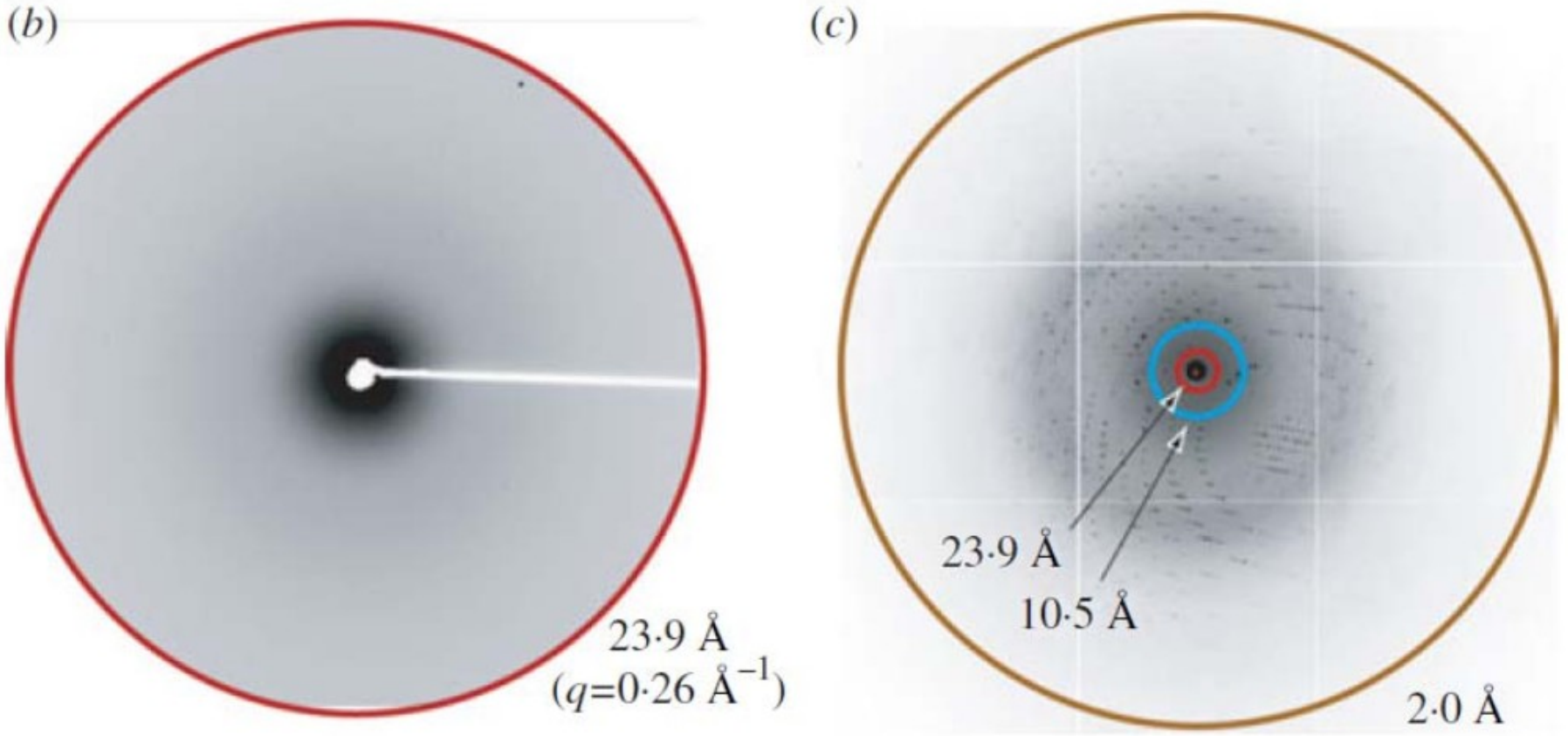




XRD detector image
diffarction spots

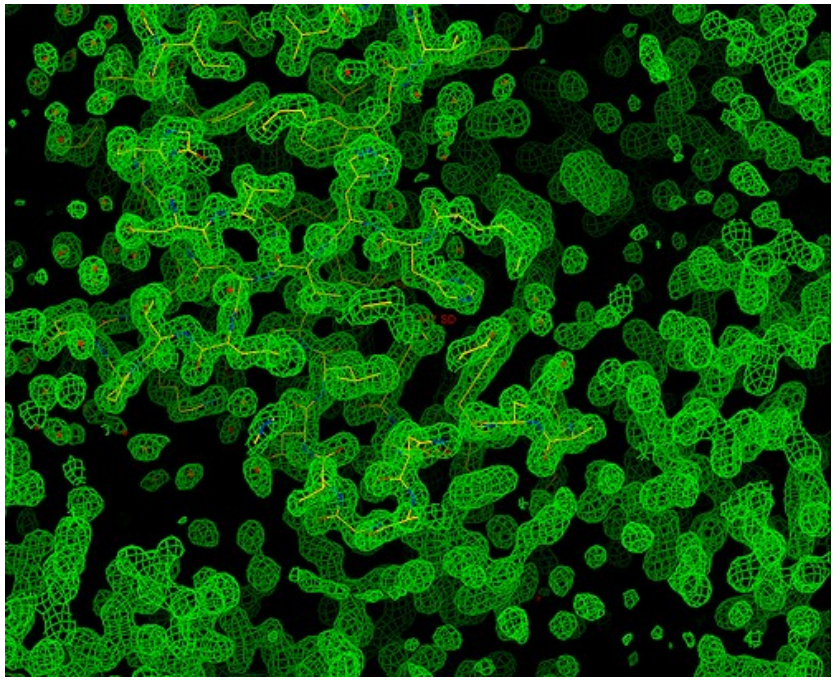


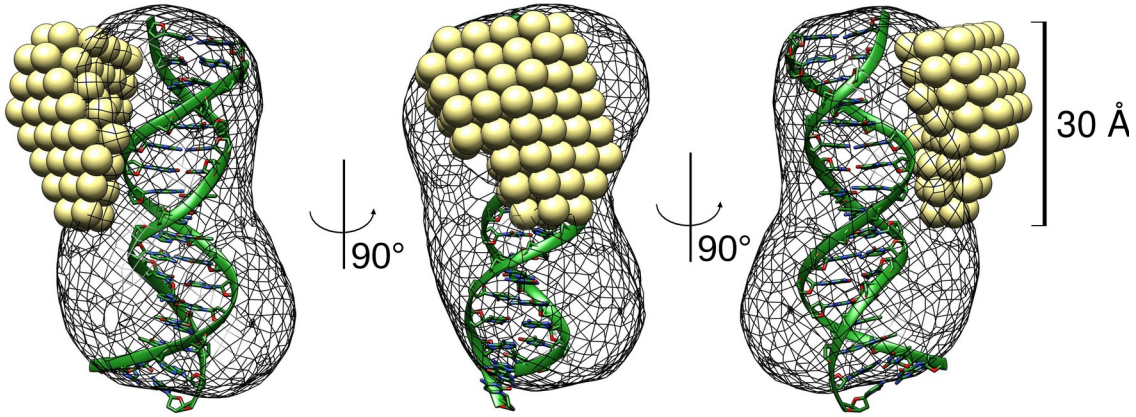
SAXS detector image
x-ray scattering



Putnam et al. (2007) *Quart. Rev. Biophys.* **40**(3), 191-285.

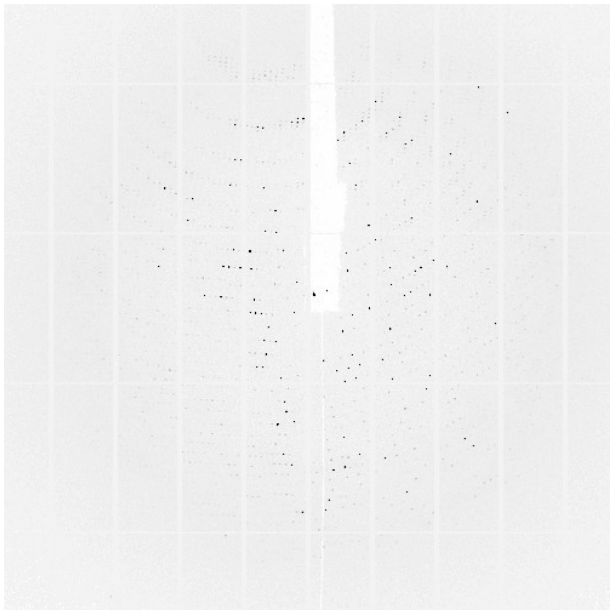
Output structure XRD vs SAXS



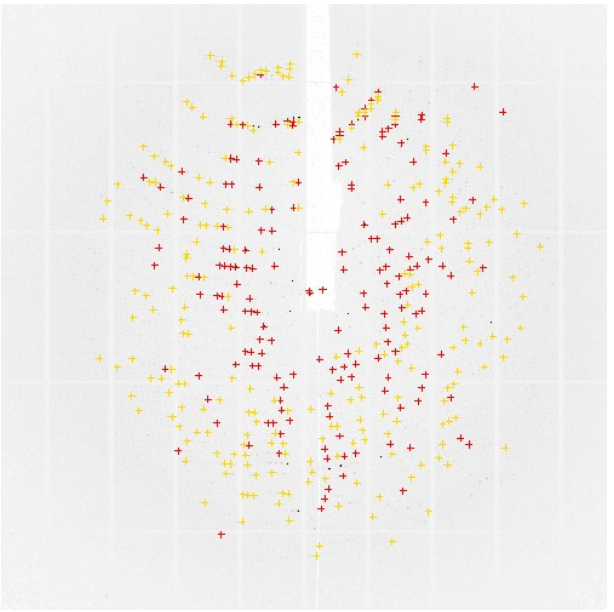


XRD – data reduction

Set of diffraction images



indexing



Space group determination

Space group	P 61 2 2
Space group confidence	S (spacegroup is known)
Cell	177.54 177.54 203.64 90 90 120
Resolution low	48.33
Resolution high	2.832
Number of lattices	1
Number of reflections	398868
Number of datasets	1

indexing integration

Reduced data – intensities with h, k, l indices

	h	k	l	Orig. H	Orig. K	Orig. L	M/ISYM	BATCH	I	SIGI	FRACTIONCALC	XDET	YDET	ROT	LP	FLAG
1	0	0	5	0	0	5	1	706	0,45	0,34	1,00	1248,00	1285,20	70,50	0,01	0
2	0	0	6	0	0	6	1	710	11780,00	315,60	1,00	1260,90	1281,00	70,93	0,01	0
3	0	0	7	0	0	7	1	714	-0,17	0,52	1,00	1273,90	1276,90	71,36	0,01	0
4	0	0	13	0	0	13	1	740	0,54	0,98	1,00	1351,80	1252,00	73,93	0,02	0
5	0	0	14	0	0	14	1	744	1,26	1,08	1,00	1364,80	1247,90	74,35	0,02	0
6	0	0	15	0	0	15	1	748	3,08	1,15	1,00	1377,80	1243,80	74,78	0,02	0
7	0	0	16	0	0	16	1	753	-0,63	1,18	1,00	1390,90	1239,70	75,21	0,02	0
8	0	0	17	0	0	17	1	757	-0,12	1,25	1,00	1403,90	1235,60	75,64	0,03	0
9	0	0	18	0	0	18	1	761	157,10	5,16	1,00	1417,00	1231,50	76,07	0,03	0
10	0	0	19	0	0	19	1	766	1,74	1,48	1,00	1430,10	1227,50	76,51	0,03	0
11	0	0	20	0	0	20	1	770	3,40	1,58	1,00	1443,20	1223,40	76,94	0,03	0
12	0	0	21	0	0	21	1	774	2,61	1,65	1,00	1456,30	1219,30	77,37	0,03	0
13	0	0	21	0	0	-21	2	595	-0,20	1,56	0,79	910,30	1393,30	59,46	0,03	0
14	0	0	22	0	0	22	1	779	13,00	2,00	1,00	1469,50	1215,30	77,80	0,03	0
15	0	0	22	0	0	-22	2	591	10,20	1,68	1,00	897,20	1397,40	59,03	0,03	0
16	0	0	23	0	0	-23	2	587	6,14	1,68	1,00	884,00	1401,50	58,60	0,04	0
17	0	0	24	0	0	24	1	787	17610,00	472,70	1,00	1495,80	1207,20	78,67	0,04	0
18	0	0	24	0	0	-24	2	582	17080,00	458,50	1,00	870,90	1405,60	58,17	0,04	0
19	0	0	25	0	0	25	1	792	1,56	1,96	1,00	1509,10	1203,20	79,10	0,04	0
20	0	0	25	0	0	-25	2	578	-2,49	1,81	1,00	857,70	1409,60	57,73	0,04	0
21	0	0	26	0	0	26	1	796	1,20	2,02	0,89	1522,30	1199,20	79,54	0,04	0
22	0	0	26	0	0	-26	2	574	-1,04	1,93	1,00	844,40	1413,70	57,30	0,04	0
23	0	0	27	0	0	-27	2	569	-0,63	1,98	1,00	831,20	1417,70	56,87	0,04	0
24	0	0	28	0	0	-28	2	565	2,69	2,06	1,00	817,90	1421,80	56,43	0,04	0
25	0	0	29	0	0	-29	2	561	-0,08	2,09	1,00	804,70	1425,80	56,00	0,04	0
26	0	0	30	0	0	-30	2	556	3668,00	99,62	1,00	791,30	1429,80	55,56	0,05	0
27	0	0	31	0	0	-31	2	552	-0,04	2,20	1,00	778,00	1433,80	55,13	0,05	0
28	0	0	32	0	0	-32	2	547	0,58	2,33	1,00	764,60	1437,70	54,69	0,05	0

XRD – outputs

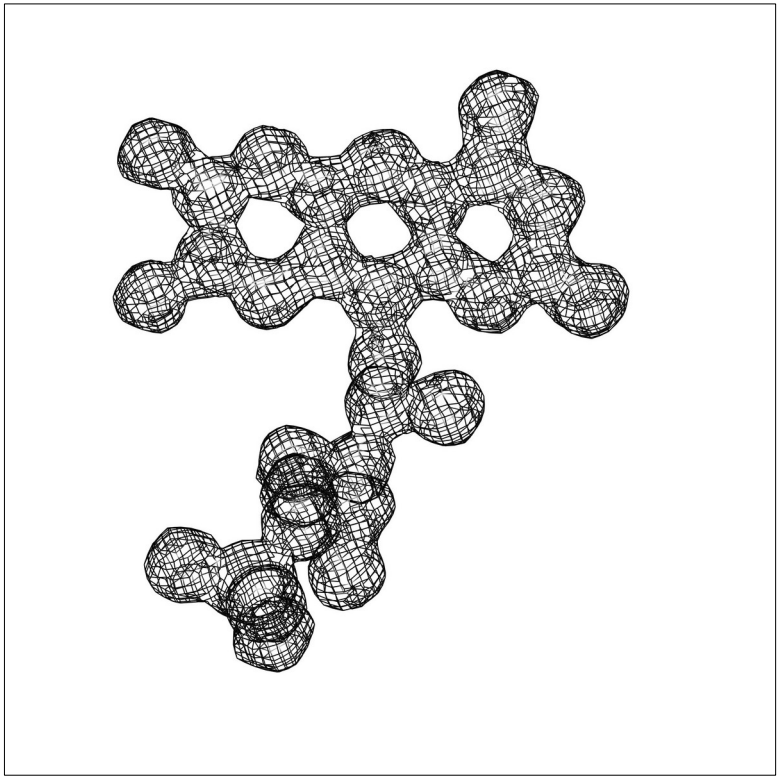
xrd intensities ~10^5 reflexions, reciprocal space, indices *h, k, l*

	h	k	l	Orig. H	Orig. K	Orig. L	M/ISYM	BATCH	I	SIGI	FRACTIONCALC	XDET	YDET	ROT	LP	FLAG
1	0	0	5	0	0	5	1	706	0,45	0,34	1,00	1248,00	1285,20	70,50	0,01	0
2	0	0	6	0	0	6	1	710	11780,00	315,60	1,00	1260,90	1281,00	70,93	0,01	0
3	0	0	7	0	0	7	1	714	-0,17	0,52	1,00	1273,90	1276,90	71,36	0,01	0
4	0	0	13	0	0	13	1	740	0,54	0,98	1,00	1351,80	1252,00	73,93	0,02	0
5	0	0	14	0	0	14	1	744	1,26	1,08	1,00	1364,80	1247,90	74,35	0,02	0
6	0	0	15	0	0	15	1	748	3,08	1,15	1,00	1377,80	1243,80	74,78	0,02	0
7	0	0	16	0	0	16	1	753	-0,63	1,18	1,00	1390,90	1239,70	75,21	0,02	0
8	0	0	17	0	0	17	1	757	-0,12	1,25	1,00	1403,90	1235,60	75,64	0,03	0
9	0	0	18	0	0	18	1	761	157,10	5,16	1,00	1417,00	1231,50	76,07	0,03	0
10	0	0	19	0	0	19	1	766	1,74	1,48	1,00	1430,10	1227,50	76,51	0,03	0
11	0	0	20	0	0	20	1	770	3,40	1,58	1,00	1443,20	1223,40	76,94	0,03	0
12	0	0	21	0	0	21	1	774	2,61	1,65	1,00	1456,30	1219,30	77,37	0,03	0
13	0	0	21	0	0	-21	2	595	-0,20	1,56	0,79	910,30	1393,30	59,46	0,03	0
14	0	0	22	0	0	22	1	779	13,00	2,00	1,00	1469,50	1215,30	77,80	0,03	0
15	0	0	22	0	0	-22	2	591	10,20	1,68	1,00	897,20	1397,40	59,03	0,03	0
16	0	0	23	0	0	-23	2	587	6,14	1,68	1,00	884,00	1401,50	58,60	0,04	0
17	0	0	24	0	0	24	1	787	17610,00	472,70	1,00	1495,80	1207,20	78,67	0,04	0
18	0	0	24	0	0	-24	2	582	17080,00	458,50	1,00	870,90	1405,60	58,17	0,04	0
19	0	0	25	0	0	25	1	792	1,56	1,96	1,00	1509,10	1203,20	79,10	0,04	0
20	0	0	25	0	0	-25	2	578	-2,49	1,81	1,00	857,70	1409,60	57,73	0,04	0
21	0	0	26	0	0	26	1	796	1,20	2,02	0,89	1522,30	1199,20	79,54	0,04	0
22	0	0	26	0	0	-26	2	574	-1,04	1,93	1,00	844,40	1413,70	57,30	0,04	0
23	0	0	27	0	0	-27	2	569	-0,63	1,98	1,00	831,20	1417,70	56,87	0,04	0
24	0	0	28	0	0	-28	2	565	2,69	2,06	1,00	817,90	1421,80	56,43	0,04	0
25	0	0	29	0	0	-29	2	561	-0,08	2,09	1,00	804,70	1425,80	56,00	0,04	0
26	0	0	30	0	0	-30	2	556	3668,00	99,62	1,00	791,30	1429,80	55,56	0,05	0
27	0	0	31	0	0	-31	2	552	-0,04	2,20	1,00	778,00	1433,80	55,13	0,05	0
28	0	0	32	0	0	-32	2	547	0,58	2,33	1,00	764,60	1437,70	54,69	0,05	0
29	0	0	33	0	0	-33	2	543	0,79	2,38	1,00	751,20	1441,70	54,25	0,05	0
30	0	0	34	0	0	-34	2	539	2,15	2,44	1,00	737,80	1445,70	53,82	0,05	0
31	0	0	35	0	0	-35	2	534	1,52	2,54	1,00	724,30	1449,60	53,38	0,05	0
32	0	0	36	0	0	-36	2	530	531,30	16,14	1,00	710,90	1453,50	52,94	0,06	0
33	0	0	37	0	0	-37	2	526	0,98	2,68	1,00	697,30	1457,40	52,50	0,06	0
34	0	0	38	0	0	-38	2	521	-0,53	2,85	1,00	683,80	1461,30	52,05	0,06	0
35	0	0	39	0	0	-39	2	517	-4,92	3,00	0,95	670,20	1465,10	51,61	0,06	0
36	0	0	45	0	0	-45	2	490	2,37	3,73	1,00	587,80	1487,90	48,93	0,07	0

Phase problem

Fourier transform

Electron density map



XRD – outputs

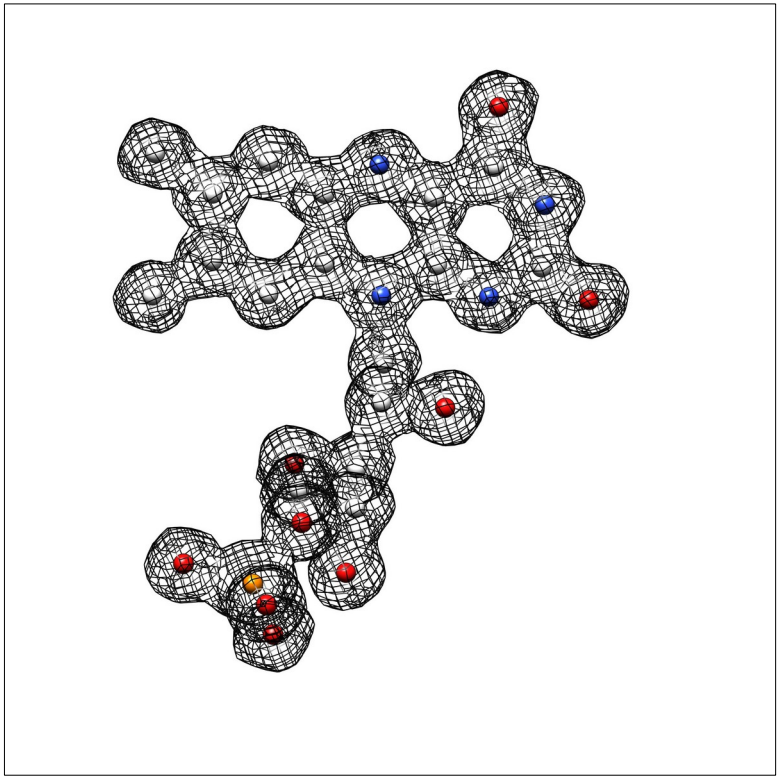
xrd intensities ~10^5 reflexions, reciprocal space, indices *h, k, l*

	h	k	l	Orig. H	Orig. K	Orig. L	M/ISYM	BATCH	I	SIGI	FRACTIONCALC	XDET	YDET	ROT	LP	FLAG
1	0	0	5	0	0	5	1	706	0,45	0,34	1,00	1248,00	1285,20	70,50	0,01	0
2	0	0	6	0	0	6	1	710	11780,00	315,60	1,00	1260,90	1281,00	70,93	0,01	0
3	0	0	7	0	0	7	1	714	-0,17	0,52	1,00	1273,90	1276,90	71,36	0,01	0
4	0	0	13	0	0	13	1	740	0,54	0,98	1,00	1351,80	1252,00	73,93	0,02	0
5	0	0	14	0	0	14	1	744	1,26	1,08	1,00	1364,80	1247,90	74,35	0,02	0
6	0	0	15	0	0	15	1	748	3,08	1,15	1,00	1377,80	1243,80	74,78	0,02	0
7	0	0	16	0	0	16	1	753	-0,63	1,18	1,00	1390,90	1239,70	75,21	0,02	0
8	0	0	17	0	0	17	1	757	-0,12	1,25	1,00	1403,90	1235,60	75,64	0,03	0
9	0	0	18	0	0	18	1	761	157,10	5,16	1,00	1417,00	1231,50	76,07	0,03	0
10	0	0	19	0	0	19	1	766	1,74	1,48	1,00	1430,10	1227,50	76,51	0,03	0
11	0	0	20	0	0	20	1	770	3,40	1,58	1,00	1443,20	1223,40	76,94	0,03	0
12	0	0	21	0	0	21	1	774	2,61	1,65	1,00	1456,30	1219,30	77,37	0,03	0
13	0	0	21	0	0	-21	2	595	-0,20	1,56	0,79	910,30	1393,30	59,46	0,03	0
14	0	0	22	0	0	22	1	779	13,00	2,00	1,00	1469,50	1215,30	77,80	0,03	0
15	0	0	22	0	0	-22	2	591	10,20	1,68	1,00	897,20	1397,40	59,03	0,03	0
16	0	0	23	0	0	-23	2	587	6,14	1,68	1,00	884,00	1401,50	58,60	0,04	0
17	0	0	24	0	0	24	1	787	17610,00	472,70	1,00	1495,80	1207,20	78,67	0,04	0
18	0	0	24	0	0	-24	2	582	17080,00	458,50	1,00	870,90	1405,60	58,17	0,04	0
19	0	0	25	0	0	25	1	792	1,56	1,96	1,00	1509,10	1203,20	79,10	0,04	0
20	0	0	25	0	0	-25	2	578	-2,49	1,81	1,00	857,70	1409,60	57,73	0,04	0
21	0	0	26	0	0	26	1	796	1,20	2,02	0,89	1522,30	1199,20	79,54	0,04	0
22	0	0	26	0	0	-26	2	574	-1,04	1,93	1,00	844,40	1413,70	57,30	0,04	0
23	0	0	27	0	0	-27	2	569	-0,63	1,98	1,00	831,20	1417,70	56,87	0,04	0
24	0	0	28	0	0	-28	2	565	2,69	2,06	1,00	817,90	1421,80	56,43	0,04	0
25	0	0	29	0	0	-29	2	561	-0,08	2,09	1,00	804,70	1425,80	56,00	0,04	0
26	0	0	30	0	0	-30	2	556	3668,00	99,62	1,00	791,30	1429,80	55,56	0,05	0
27	0	0	31	0	0	-31	2	552	-0,04	2,20	1,00	778,00	1433,80	55,13	0,05	0
28	0	0	32	0	0	-32	2	547	0,58	2,33	1,00	764,60	1437,70	54,69	0,05	0
29	0	0	33	0	0	-33	2	543	0,79	2,38	1,00	751,20	1441,70	54,25	0,05	0
30	0	0	34	0	0	-34	2	539	2,15	2,44	1,00	737,80	1445,70	53,82	0,05	0
31	0	0	35	0	0	-35	2	534	1,52	2,54	1,00	724,30	1449,60	53,38	0,05	0
32	0	0	36	0	0	-36	2	530	531,30	16,14	1,00	710,90	1453,50	52,94	0,06	0
33	0	0	37	0	0	-37	2	526	0,98	2,68	1,00	697,30	1457,40	52,50	0,06	0
34	0	0	38	0	0	-38	2	521	-0,53	2,85	1,00	683,80	1461,30	52,05	0,06	0
35	0	0	39	0	0	-39	2	517	-4,92	3,00	0,95	670,20	1465,10	51,61	0,06	0
36	0	0	45	0	0	-45	2	490	2,37	3,73	1,00	587,80	1487,90	48,93	0,07	0

Phase problem

Fourier transform

Electron density map
Atom coordinates

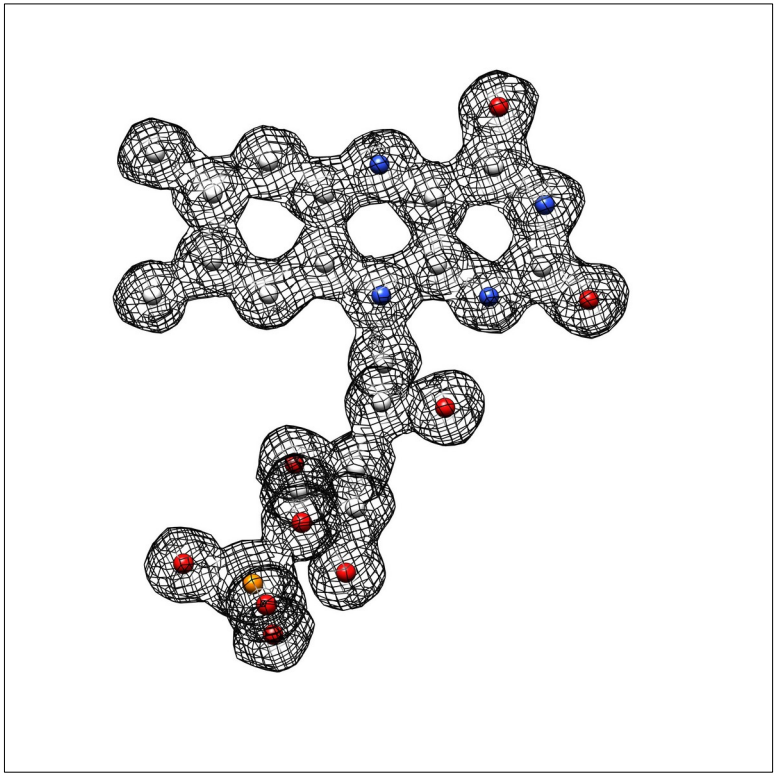


XRD – output

Structure with high resolution

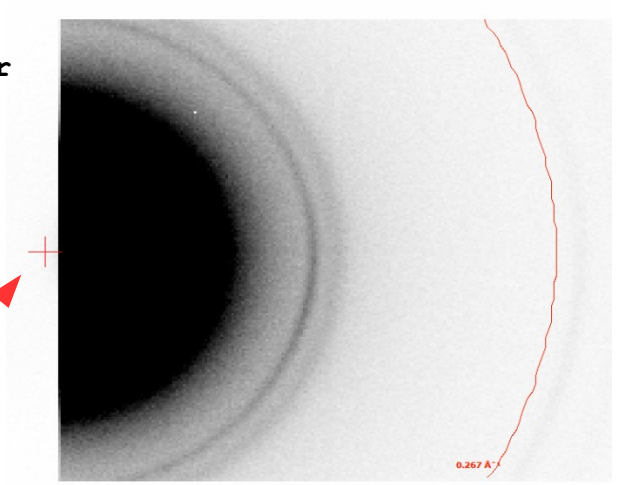
3D coordinates,
PDB format, in real space x, y, z

HETATM	2968	C9A	FNR B 201	18.093	-4.814	66.786	1.00	7.49	C
HETATM	2969	N10	FNR B 201	18.926	-4.246	67.742	1.00	7.31	N
HETATM	2970	CAA	FNR B 201	20.263	-4.072	67.478	1.00	7.09	C
HETATM	2971	N1	FNR B 201	21.001	-3.377	68.290	1.00	7.03	N
HETATM	2972	C2	FNR B 201	22.260	-3.219	68.029	1.00	7.67	C
HETATM	2973	O2	FNR B 201	22.895	-2.495	68.786	1.00	8.20	O
HETATM	2974	N3	FNR B 201	22.832	-3.652	66.907	1.00	7.06	N
HETATM	2975	C4	FNR B 201	22.174	-4.394	65.997	1.00	6.83	C
HETATM	2976	O4	FNR B 201	22.762	-4.851	64.973	1.00	6.36	O
HETATM	2977	C4A	FNR B 201	20.769	-4.664	66.266	1.00	6.92	C
HETATM	2978	N5	FNR B 201	19.988	-5.342	65.408	1.00	7.47	N
HETATM	2979	C5A	FNR B 201	18.678	-5.408	65.569	1.00	7.59	C
HETATM	2980	C6	FNR B 201	17.856	-5.955	64.611	1.00	7.52	C
HETATM	2981	C7	FNR B 201	16.502	-5.982	64.805	1.00	7.90	C
HETATM	2982	C7M	FNR B 201	15.729	-6.554	63.669	1.00	8.29	C
HETATM	2983	C8	FNR B 201	15.929	-5.414	65.987	1.00	8.03	C
HETATM	2984	C8M	FNR B 201	14.454	-5.501	66.238	1.00	8.78	C
HETATM	2985	C9	FNR B 201	16.734	-4.854	66.964	1.00	7.60	C
HETATM	2986	C1'	FNR B 201	18.395	-3.681	68.980	1.00	7.22	C
HETATM	2987	C2'	FNR B 201	18.023	-2.264	68.917	1.00	7.07	C
HETATM	2988	O2'	FNR B 201	19.202	-1.525	69.187	1.00	6.83	O
HETATM	2989	C3'	FNR B 201	16.991	-1.922	69.974	1.00	7.10	C
HETATM	2990	O3'	FNR B 201	15.809	-2.741	69.803	1.00	7.23	O
HETATM	2991	C4'	FNR B 201	16.644	-0.457	69.874	1.00	7.17	C
HETATM	2992	O4'	FNR B 201	15.924	-0.152	71.082	1.00	7.78	O
HETATM	2993	C5'	FNR B 201	15.746	-0.178	68.686	1.00	6.50	C
HETATM	2994	O5'	FNR B 201	15.556	1.235	68.495	1.00	6.21	O
HETATM	2995	P	FNR B 201	14.156	1.902	68.939	1.00	5.78	P
HETATM	2996	O1P	FNR B 201	14.298	3.344	68.517	1.00	5.61	O
HETATM	2997	O2P	FNR B 201	13.020	1.211	68.280	1.00	5.79	O
HETATM	2998	O3P	FNR B 201	14.088	1.723	70.433	1.00	6.03	O



SAXS – isotropic scattering -> radial averaging

Image from detector

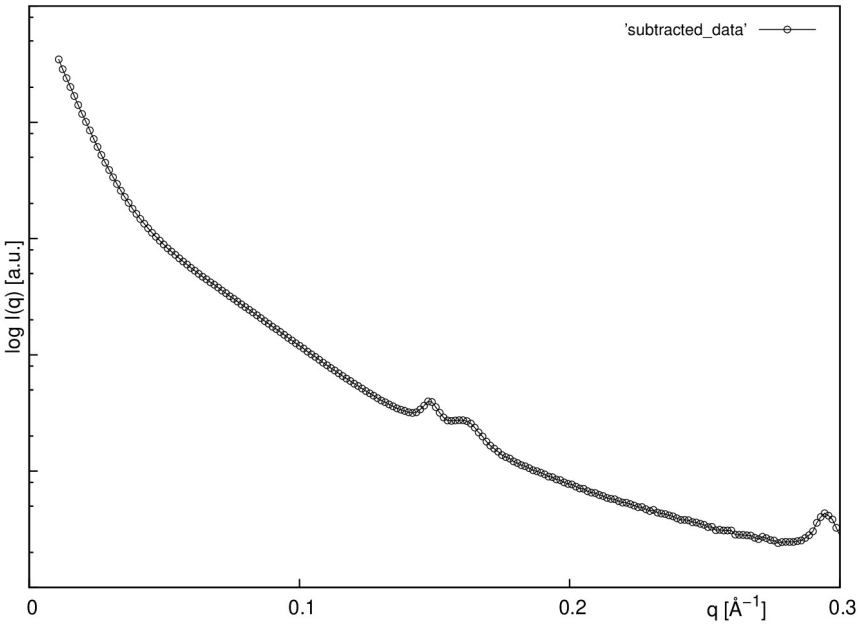


Beam center position

SAXS curve – txt file

S	I	SD
0.0166627	0.973409	0.0105135
0.0181009	0.949327	0.00825875
0.019539	0.926431	0.00710475
0.0209772	0.903951	0.00601258
0.0224154	0.874771	0.00508973
0.0238536	0.852858	0.00497113
0.0252918	0.814447	0.00488254
0.0267299	0.786807	0.00621834
0.0281681	0.764362	0.00503159
0.0296063	0.728444	0.00473319
0.0310445	0.715133	0.00407554
0.0324826	0.689458	0.00290202
0.0339208	0.673741	0.00323363
0.035359	0.643885	0.00306539
0.0367972	0.62527	0.00308635
0.0382354	0.607309	0.00260789
0.0396735	0.577026	0.00250923
0.0411117	0.559098	0.00284009
0.0425499	0.539921	0.00270961
0.0439881	0.517847	0.00237405
0.0454262	0.498033	0.00242969
0.0468644	0.479202	0.00216011
0.0483026	0.46049	0.00254124
0.0497408	0.442897	0.00241848
0.051179	0.430697	0.00202251
0.0526171	0.410743	0.00230559
0.0540553	0.396025	0.00210054
0.0554935	0.380624	0.00223789
0.0569317	0.362036	0.00205874
0.0583698	0.351014	0.002059
0.059808	0.336265	0.00196403
0.0612462	0.324684	0.00208857
0.0626844	0.311476	0.00170515
0.0641225	0.299744	0.00185129
0.0655607	0.290324	0.00174539
0.0669989	0.276878	0.00176257
0.0684371	0.267973	0.00167985
0.0698753	0.255922	0.00181061
0.0713134	0.245727	0.00178832

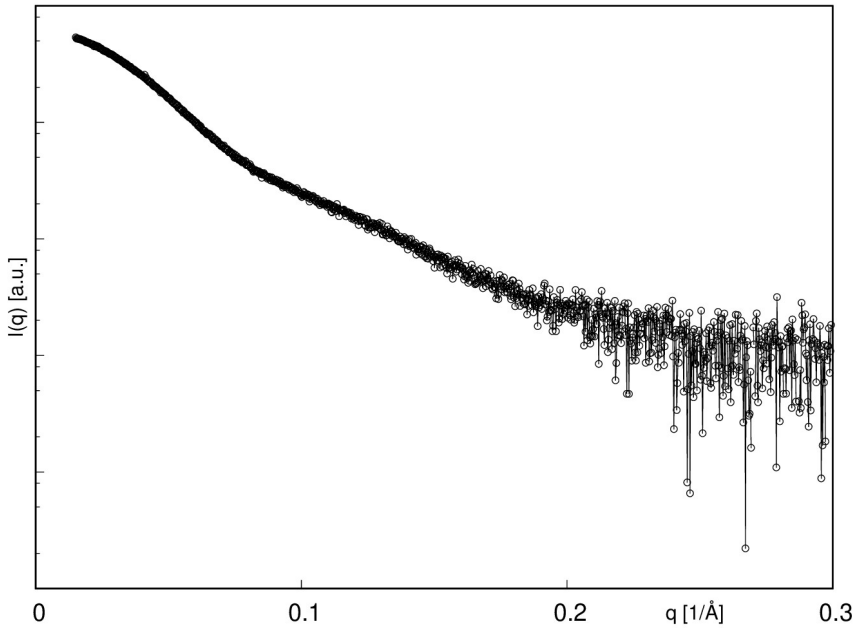
Radialy averaged data – SAXS curve



SAXS - output

Low resolution structure

SAXS data

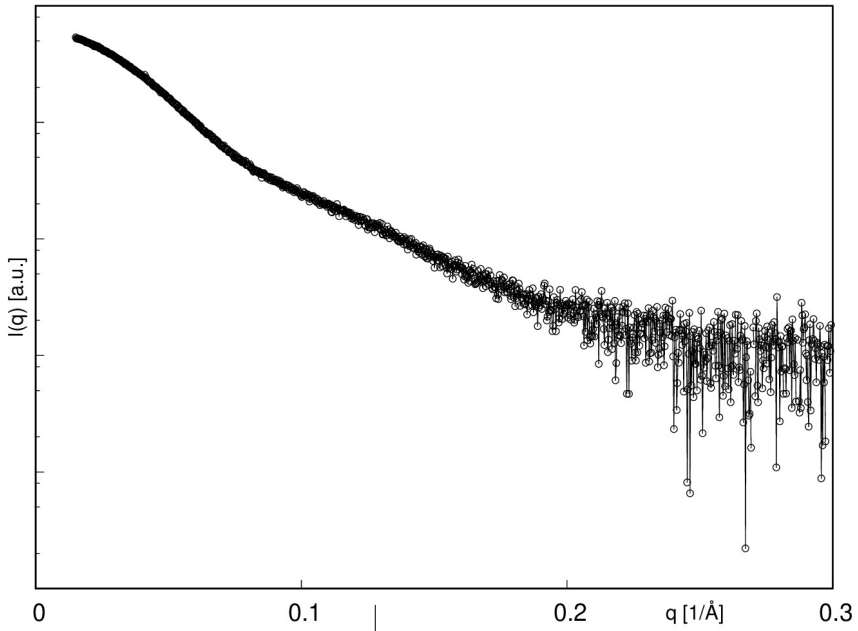


Data-collection parameters	
Instrument	BioSAXS-1000 (Rigaku)
Wavelength [Å]	1.5418
q range [Å^-1]	0.0095 - 0.65
Exposure time [min]	60
Temperature [°C]	4
Concentration [mg ml^-1]	5.0
Structural parameters	
Rg [Å] (from Guinier)	18.163
Rg [Å] (from P(r)	18.85
Dmax [Å]	62.21
Porod volume estimate [Å^3]	15417
MW theoretical [kDa]	9.4
MW porod [kDa]	9.4
MW dammin [kDa]	10.5

SAXS - output

Low resolution structure

SAXS data



SAXS table

Data-collection parameters	
Instrument	BioSAXS-1000 (Rigaku)
Wavelength [Å]	1.5418
q range [Å^-1]	0.0095 - 0.65
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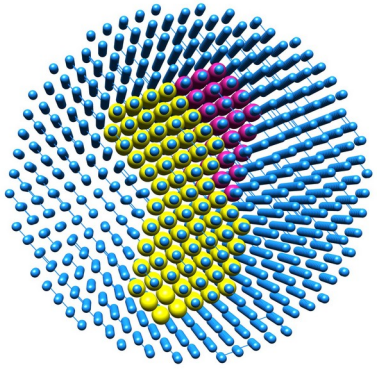
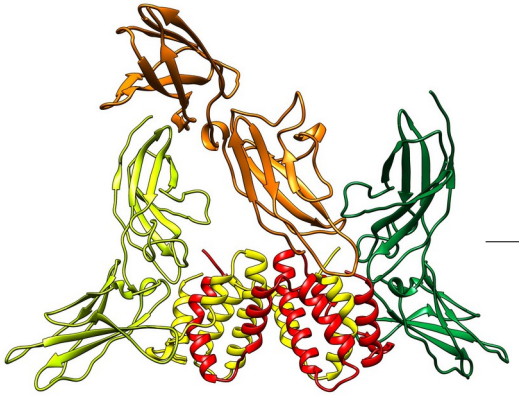
Dmax [Å]	62.21
Porod volume estimate [Å^3]	15417
MW theoretical [kDa]	9.4
MW porod [kDa]	9.4
MW dammin [kDa]	10.5

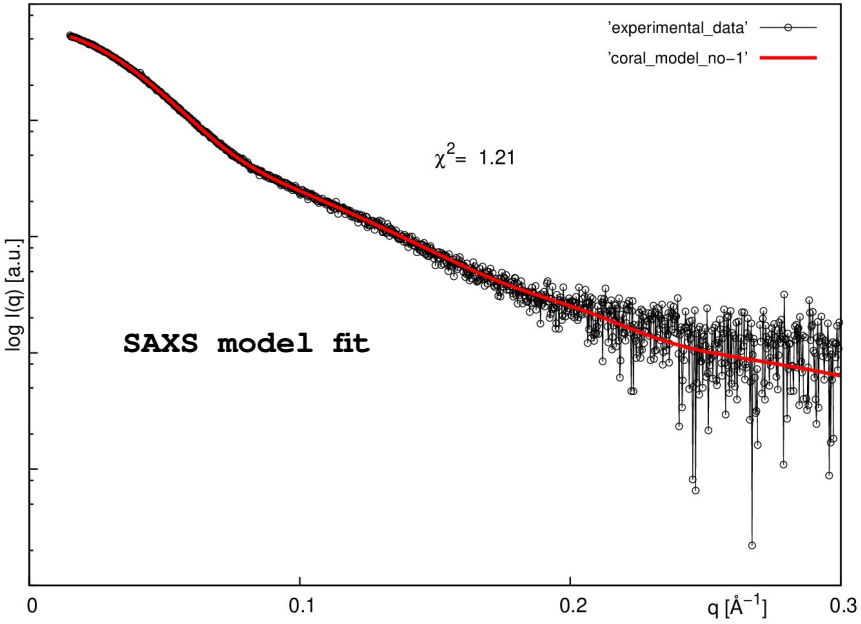
reconstruction



***Ab initio* modeling**

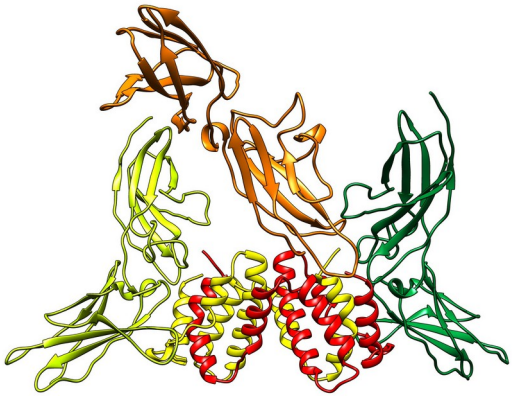


Rigid body modeling



SAXS - output

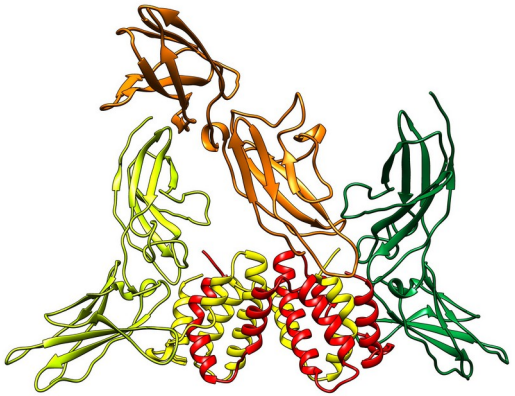
Low resolution structure

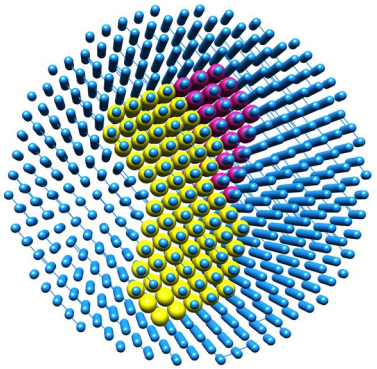


```
ATOM      1  N   ILE A   4     -36.360  17.558  21.748  1.00 20.00
ATOM      2  CA  ILE A   4     -36.096  16.392  22.585  1.00 20.00
ATOM      3  C   ILE A   4     -35.687  16.837  23.988  1.00 20.00
ATOM      4  O   ILE A   4     -34.781  17.649  24.159  1.00 20.00
ATOM      5  CB  ILE A   4     -35.027  15.488  21.933  1.00 20.00
ATOM      6  CG1 ILE A   4     -35.563  14.881  20.645  1.00 20.00
ATOM      7  CG2 ILE A   4     -34.584  14.383  22.884  1.00 20.00
ATOM      8  CD1 ILE A   4     -34.500  14.135  19.847  1.00 20.00
ATOM      9  N   GLY A   5     -36.348  16.278  25.000  1.00 20.00
ATOM     10  CA  GLY A   5     -36.166  16.769  26.356  1.00 20.00
ATOM     11  C   GLY A   5     -34.790  16.441  26.907  1.00 20.00
ATOM     12  O   GLY A   5     -34.256  15.350  26.703  1.00 20.00
ATOM     13  N   THR A   6     -34.216  17.399  27.635  1.00 20.00
ATOM     14  CA  THR A   6     -32.917  17.203  28.259  1.00 20.00
ATOM     15  C   THR A   6     -33.002  16.952  29.758  1.00 20.00
ATOM     16  O   THR A   6     -31.999  16.560  30.359  1.00 20.00
ATOM     17  CB  THR A   6     -32.014  18.421  28.013  1.00 20.00
ATOM     18  CG2 THR A   6     -31.912  18.722  26.539  1.00 20.00
ATOM     19  OG1 THR A   6     -32.570  19.559  28.685  1.00 20.00
ATOM     20  N   GLY A   7     -34.162  17.186  30.377  1.00 20.00
ATOM     21  CA  GLY A   7     -34.280  17.005  31.806  1.00 20.00
ATOM     22  C   GLY A   7     -34.519  15.562  32.194  1.00 20.00
ATOM     23  O   GLY A   7     -34.870  14.716  31.368  1.00 20.00
ATOM     24  N   PHE A   8     -34.320  15.295  33.486  1.00 20.00
ATOM     25  CA  PHE A   8     -34.561  13.987  34.094  1.00 20.00
ATOM     26  C   PHE A   8     -35.542  14.179  35.247  1.00 20.00
ATOM     27  O   PHE A   8     -35.138  14.249  36.417  1.00 20.00
```

SAXS – output

Low resolution structure





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ATOM      1  N   ILE A   4     -36.360  17.558  21.748  1.00 20.00
ATOM      2  CA  ILE A   4     -36.096  16.392  22.585  1.00 20.00
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ATOM      4  O   ILE A   4     -34.781  17.649  24.159  1.00 20.00
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ATOM      6  CG1 ILE A   4     -35.563  14.881  20.645  1.00 20.00
ATOM      7  CG2 ILE A   4     -34.584  14.383  22.884  1.00 20.00
ATOM      8  CD1 ILE A   4     -34.500  14.135  19.847  1.00 20.00
ATOM      9  N   GLY A   5     -36.348  16.278  25.000  1.00 20.00
ATOM     10  CA  GLY A   5     -36.166  16.769  26.356  1.00 20.00
ATOM     11  C   GLY A   5     -34.790  16.441  26.907  1.00 20.00
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ATOM     18  CG2 THR A   6     -31.912  18.722  26.539  1.00 20.00
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ATOM     24  N   PHE A   8     -34.320  15.295  33.486  1.00 20.00
ATOM     25  CA  PHE A   8     -34.561  13.987  34.094  1.00 20.00
ATOM     26  C   PHE A   8     -35.542  14.179  35.247  1.00 20.00
ATOM     27  O   PHE A   8     -35.138  14.249  36.417  1.00 20.00
```

```
ATOM      1  CA  ASP     1       0.778  -0.275  -0.227  1.00 20.00
ATOM      2  CA  ASP     1      -7.972   1.475  12.148  1.00 20.00
ATOM      3  CA  ASP     1       9.528  -5.525 -12.601  1.00 20.00
ATOM      4  CA  ASP     1      13.028  -5.525 -12.601  1.00 20.00
ATOM      5  CA  ASP     1      -0.972  15.475   7.198  1.00 20.00
ATOM      6  CA  ASP     1      11.278   6.725  14.623  1.00 20.00
ATOM      7  CA  ASP     1       9.528   8.475  12.148  1.00 20.00
ATOM      8  CA  ASP     1     -14.972   1.475  -2.701  1.00 20.00
ATOM      9  CA  ASP     1      -6.222  -0.275  14.623  1.00 20.00
ATOM     10  CA  ASP     2      11.278  -3.775 -15.076  1.00 20.00
ATOM     11  CA  ASP     2       2.528  -2.025   2.248  1.00 20.00
ATOM     12  CA  ASP     2       2.528  15.475   7.198  1.00 20.00
ATOM     13  CA  ASP     2      -6.222   3.225  14.623  1.00 20.00
ATOM     14  CA  ASP     2      11.278  13.725  -5.176  1.00 20.00
ATOM     15  CA  ASP     2       0.778  17.225   4.723  1.00 20.00
ATOM     16  CA  ASP     2     -14.972   4.975  -2.701  1.00 20.00
ATOM     17  CA  ASP     2     -16.721   3.225  -0.227  1.00 20.00
ATOM     18  CA  ASP     2       7.778  -3.775 -15.076  1.00 20.00
ATOM     19  CA  ASP     2      16.529   4.975  -2.701  1.00 20.00
ATOM     20  CA  ASP     3       0.778  13.725   4.723  1.00 20.00
ATOM     21  CA  ASP     3      -7.972   1.475  17.098  1.00 20.00
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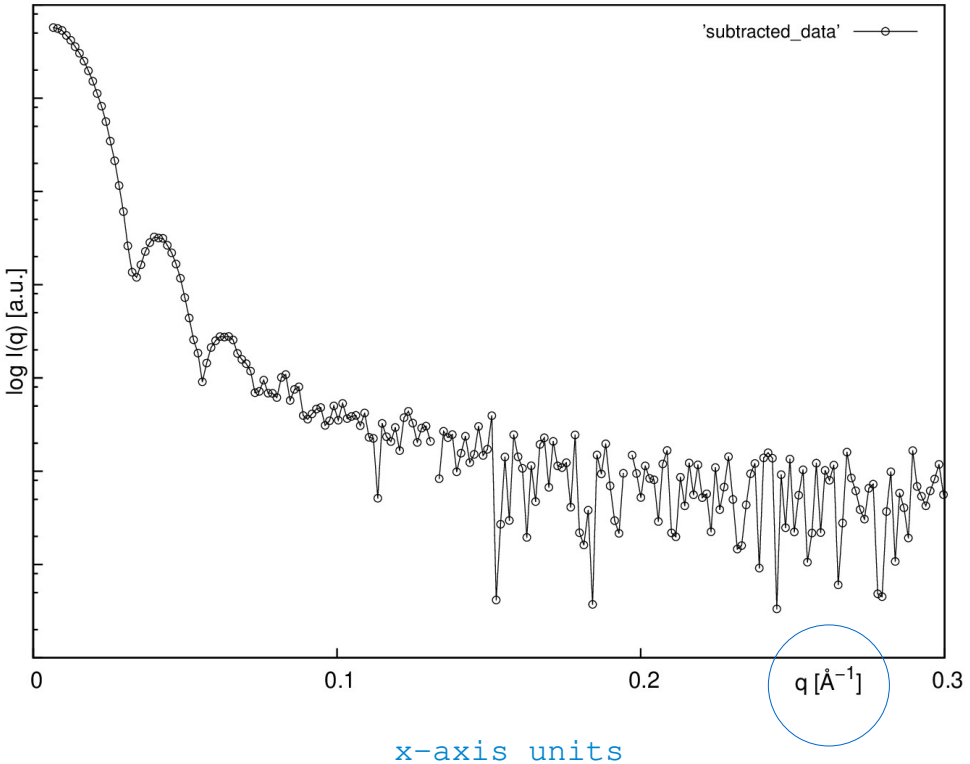
ATOM     23  CA  ASP     3      -2.722  13.725   4.723  1.00 20.00
ATOM     24  CA  ASP     3      11.278  -7.275 -15.076  1.00 20.00
ATOM     25  CA  ASP     3       9.528  -9.025 -12.601  1.00 20.00
ATOM     26  CA  ASP     3     -13.222   3.225  -0.227  1.00 20.00
```

SAXS curve – SAXS data

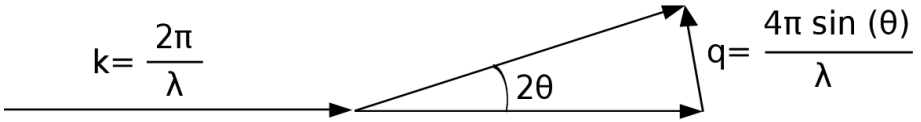
averaged data – SAXS profil



x-axis units

scattering vector, momentum transfer: s = q [nm $^{-1}$; Å $^{-1}$]

$$k = \frac{2\pi}{\lambda}$$



$$q = \frac{4\pi \sin(\theta)}{\lambda}$$

SAXS – application

Sample: solution of proteins, nucleic acids, and complexes

1. **size**
2. **shape**
3. **homogenous vs. aggregated sample**
4. **folded vs. flexible protein**
5. **oligomeric state (mixtures)**
6. **interaction, quarternary structure**
7. **modeling of flexible systems**

SAXS – advantages

1. sample preparation
2. in solution – close to „natural conditions“
3. usefull before and after molecular structure is known
4. time consumption
5. not limited by size or flexibility (almost)

SAXS – disadvantages

1. low resolution
2. non unambiguous interpretation

SAXS – resolution

1. Bragg`s

$q_{min} = 0.006\ Å^{-1} \sim d = 1000\ Å$

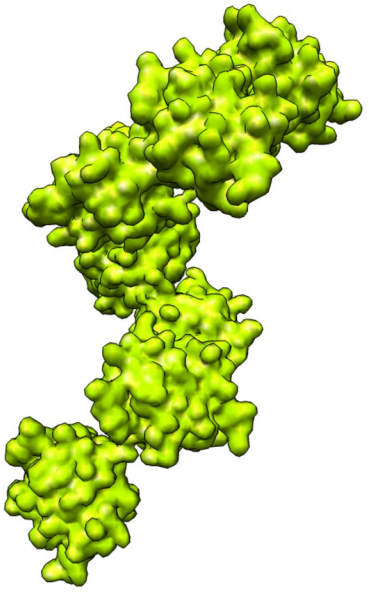
$q_{max} = 0.6\ Å^{-1} \sim d = 10\ Å$

$$d = \frac{2\pi}{q}$$

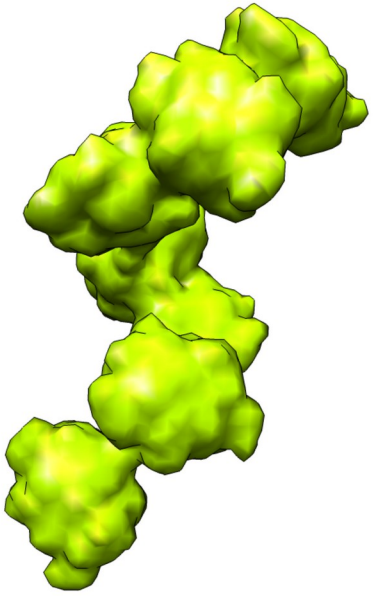
2. Efective

„low resolution structure“ 20–30 Å

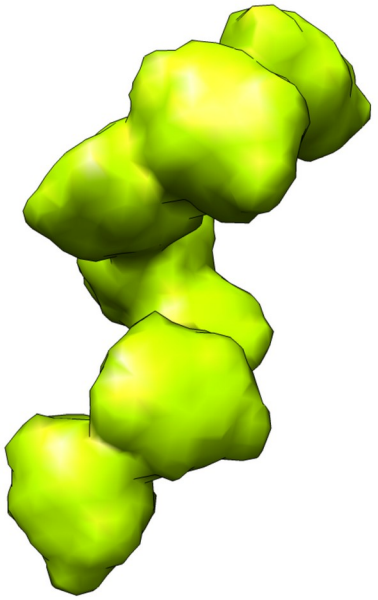
crystal structure
ribbon model



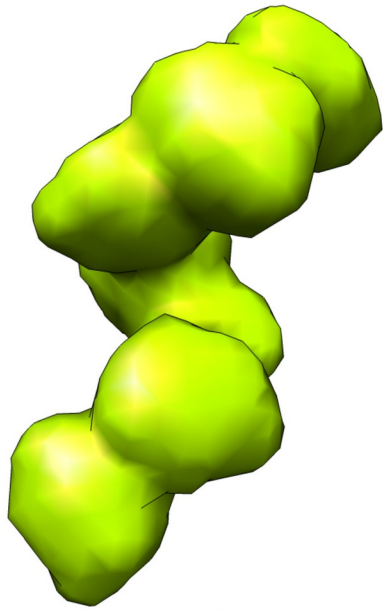
5Å



10Å



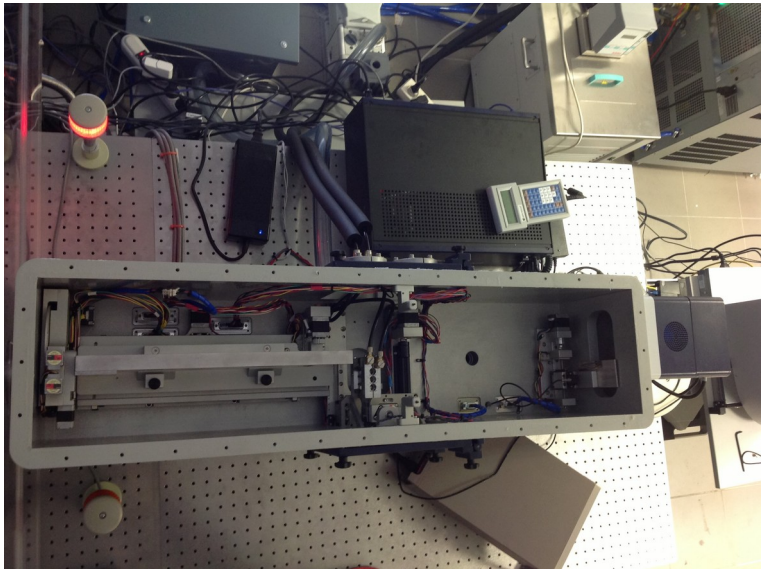
15Å



20Å

SAXS – experiment – home source

- rotating anode
- point focus
- colimation: 2D Kratky
- Pilatus 100K
- temperature range –30 to +65°C



SAXS – experiment – home source

Data-collection parameters	
Instrument	BioSAXS-1000 (Rigaku)
Wavelength [Å]	1.5418
q range [Å^-1]	0.0095 - 0.65
Exposure time [min]	60
Temperature [°C]	4
Concentration [mg ml^-1]	5.0
Structural parameters	
Rg [Å] (from Guinier)	
Rg [Å] (from P(r)	
Dmax [Å]	
Porod volume estimate [Å^3]	
MW theoretical [kDa]	9.4
MW porod [kDa]	
MW dammin [kDa]	

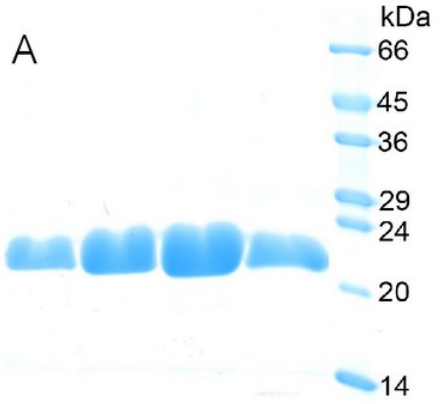
SAXS – experiment – sample

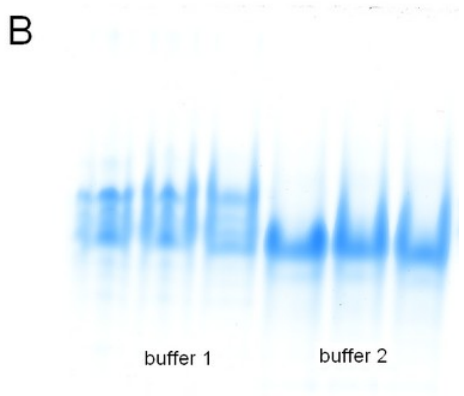
Sample quality:
- pure as possible
- monodisperse
- free of aggregation

SAXS – experiment – sample

Sample quality:
- pure as possible
- monodisperse
- free of aggregation

Quality control:
- native gels
- DLS

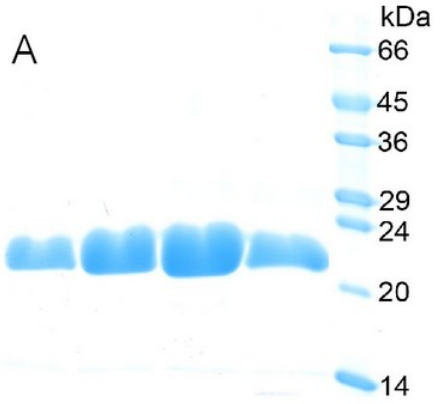


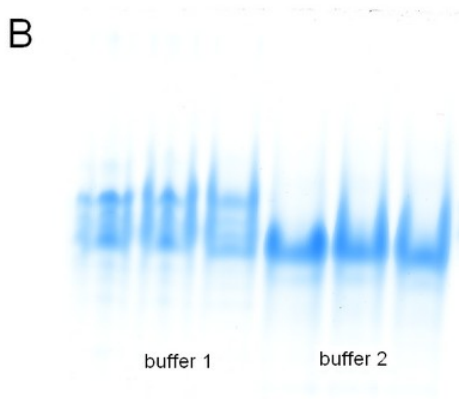


SAXS – experiment – sample

Sample quality:
- pure as possible
- monodisperse
- free of aggregation

Quality control:
- native gels
- DLS



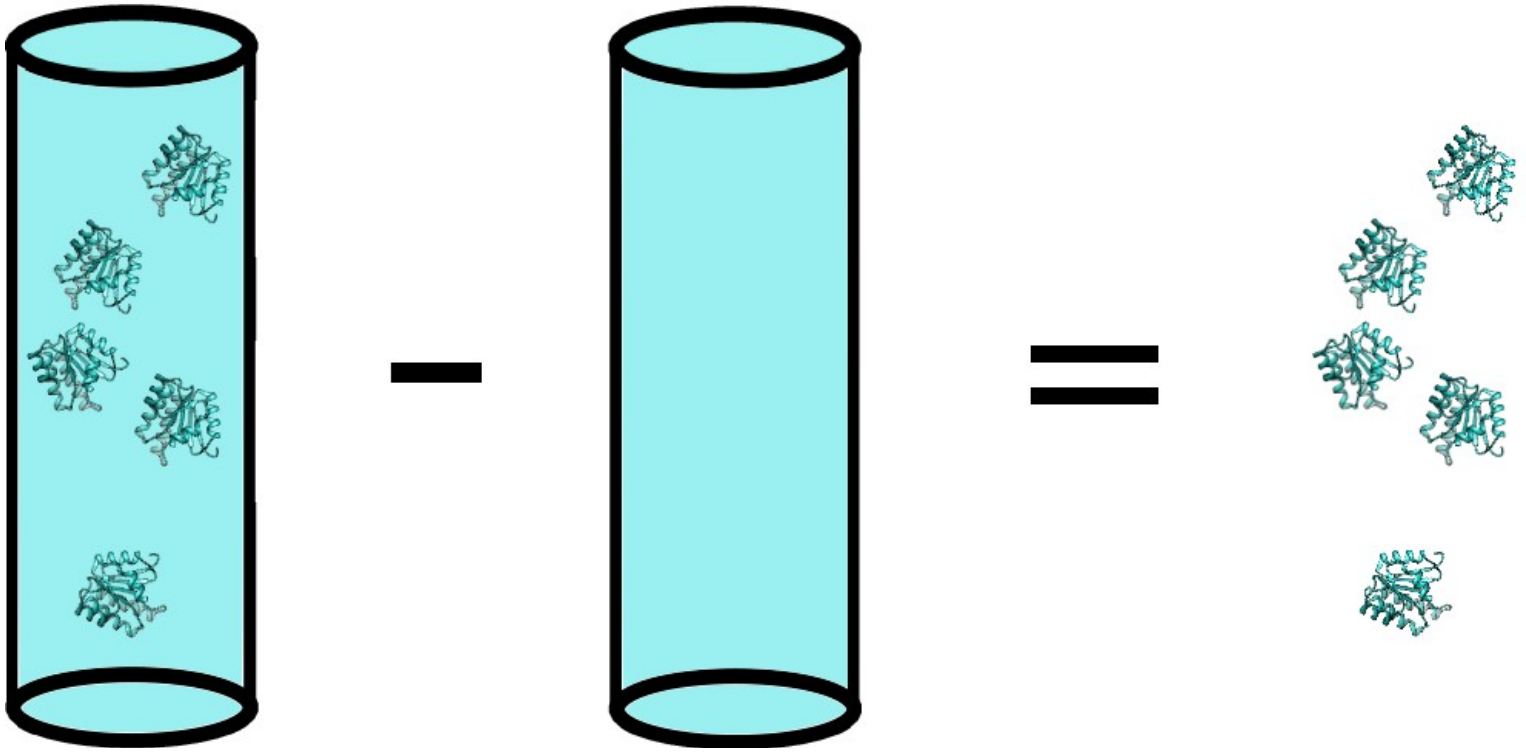


Sample volume and concentration:
- ~25 microL
- concentration series 10; 5; 2.5 mg/ml

Forward scattering intensity is proportional to size (number of electrons):
15 kDa protein needs 2.0 mg/ml
300 kDa protein …… 0.1 mg/ml

=> Aggregates ruins meaningful data interpretation

SAXS – subtraction



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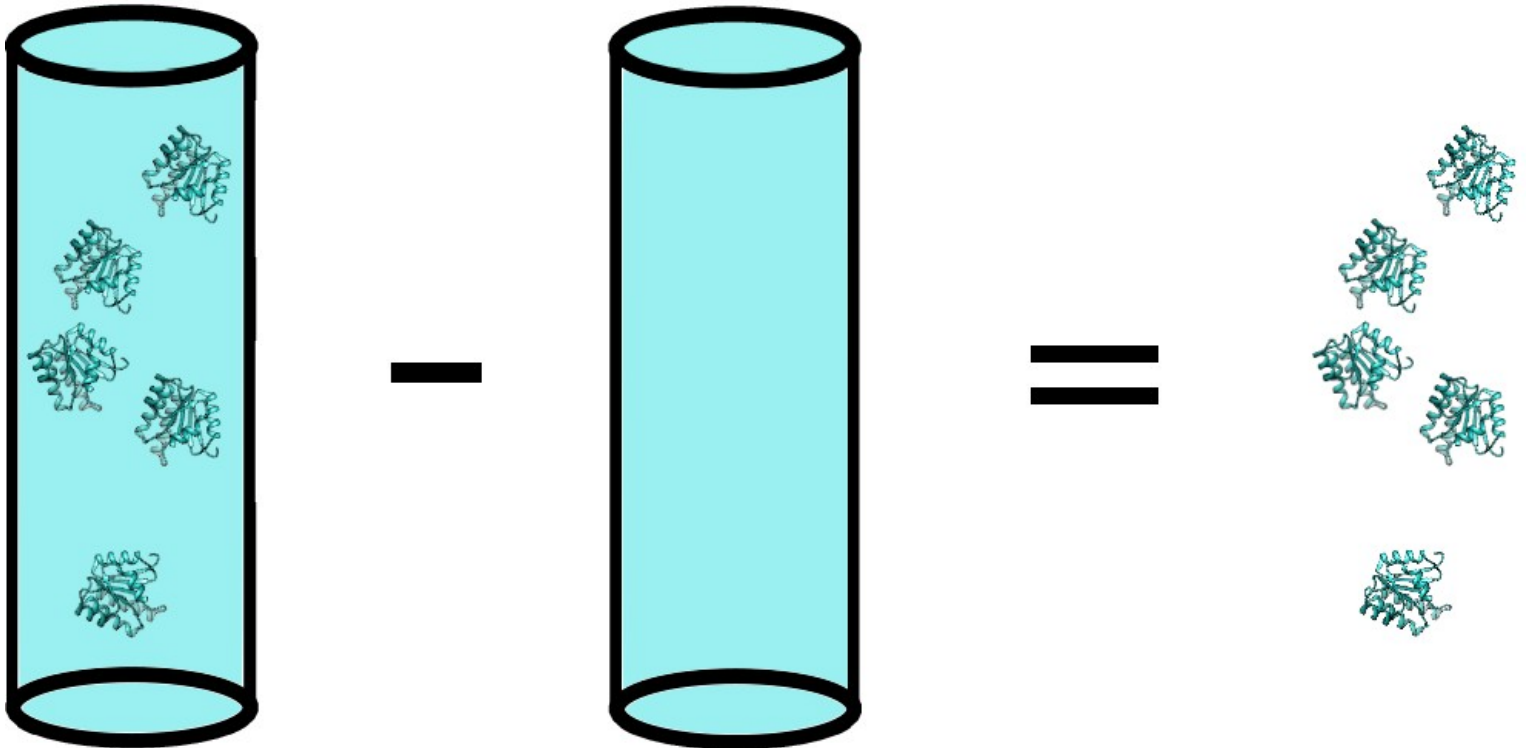
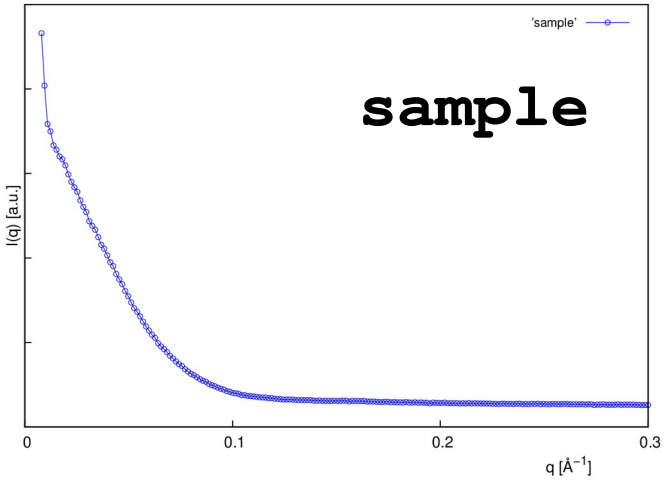
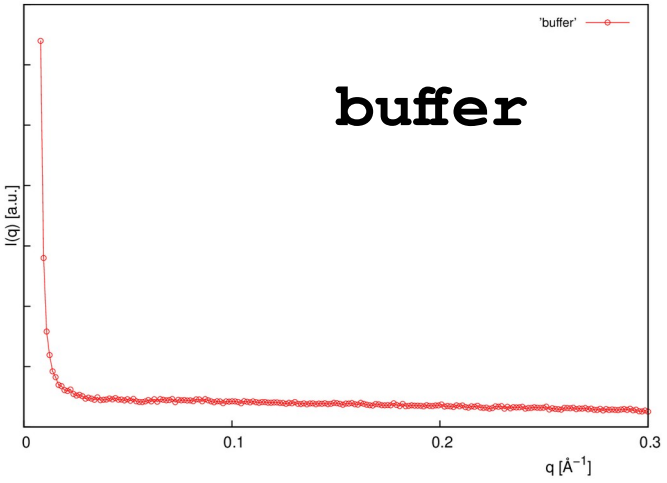
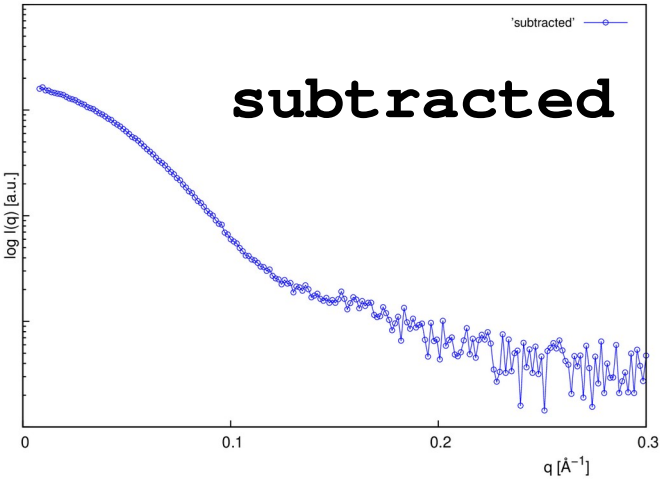




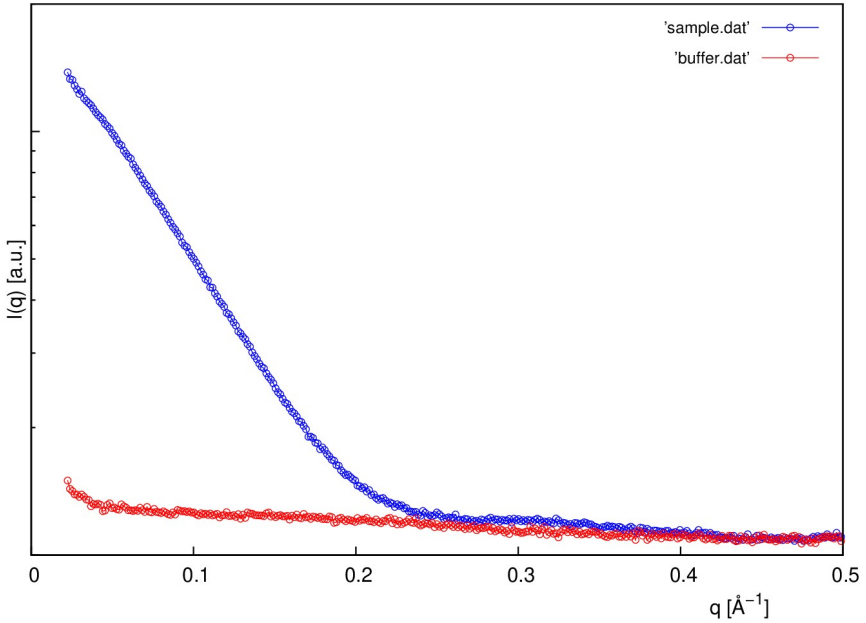




SAXS – buffer

Buffer requirements:
- identical to last step of purification (dialysis)
- salt < 1 M
- glycerol < 5% v/v
- detergents < CMC

Matching buffer = no oversubtraction or undersubtraction



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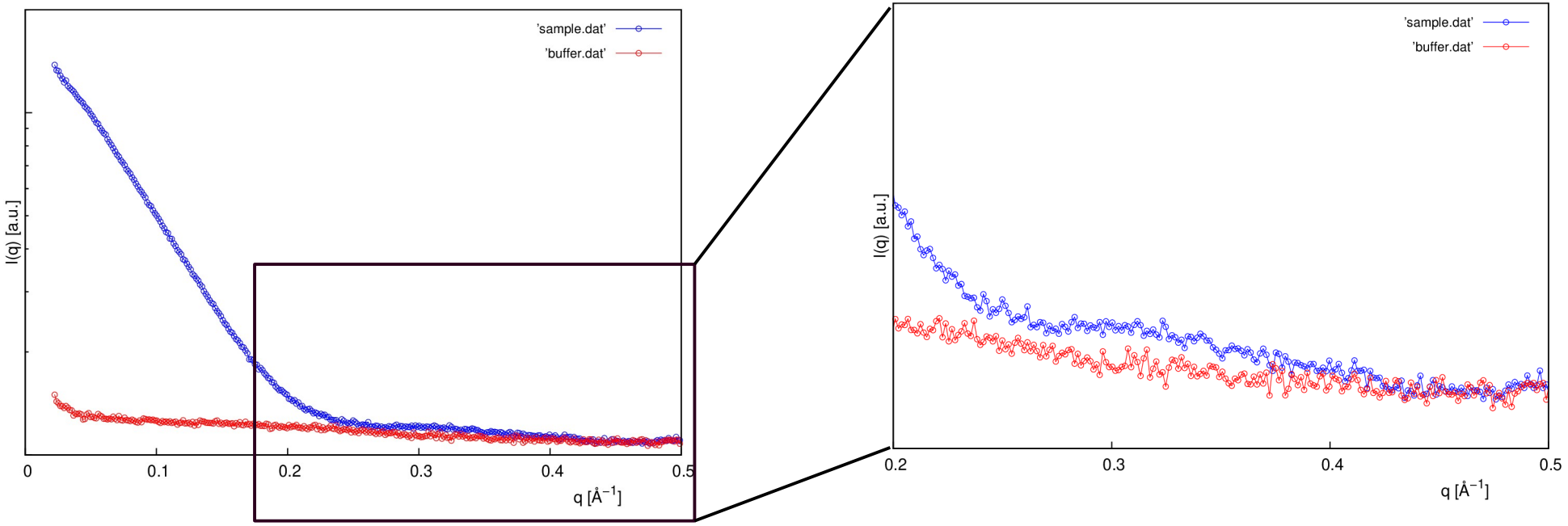

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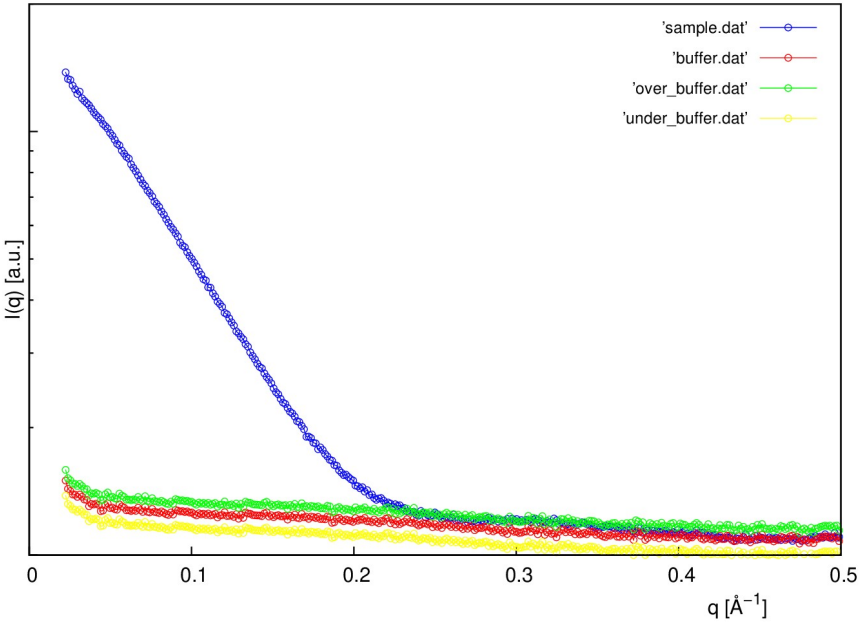

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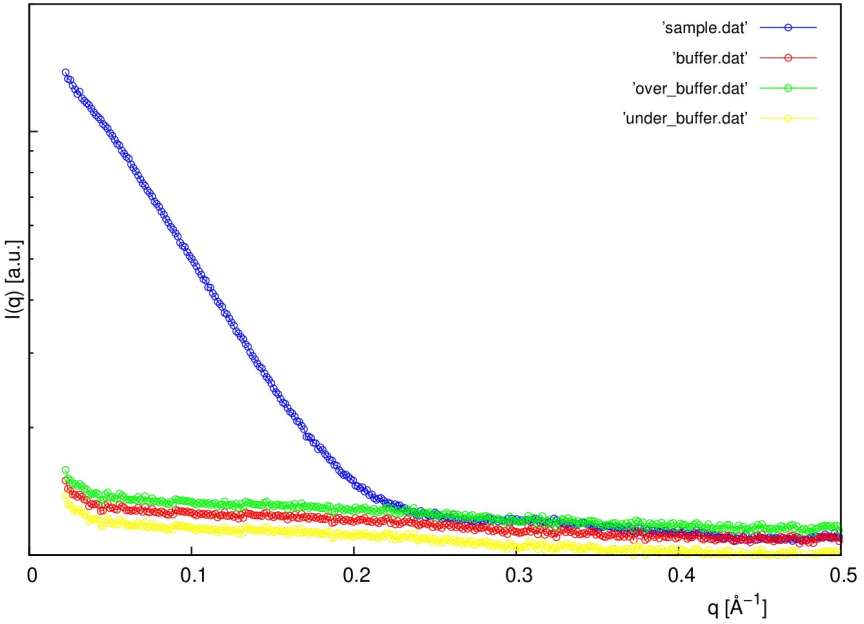

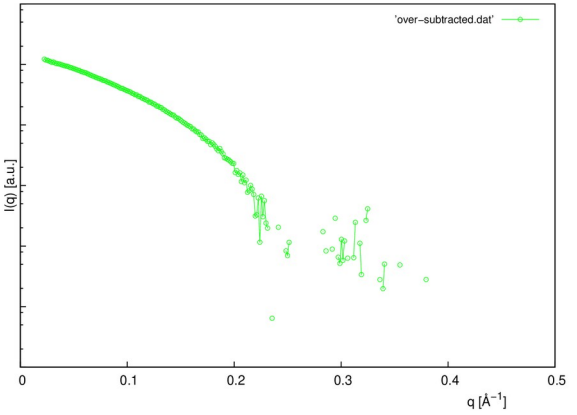

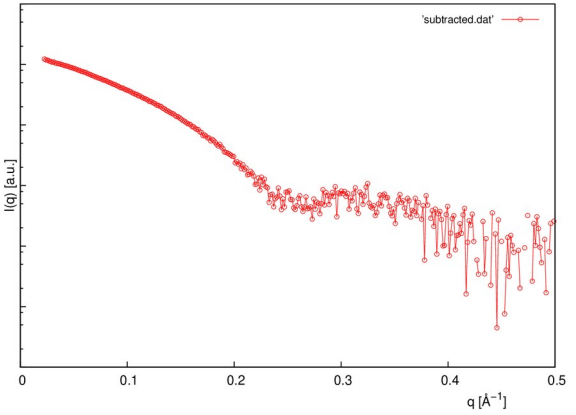

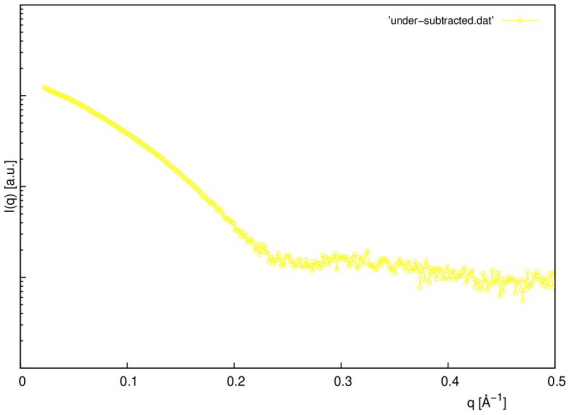

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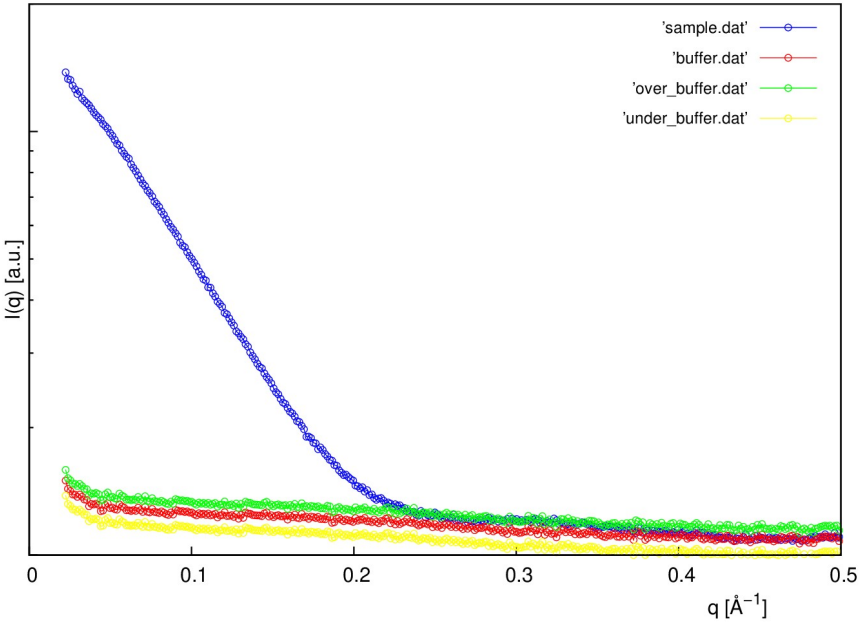
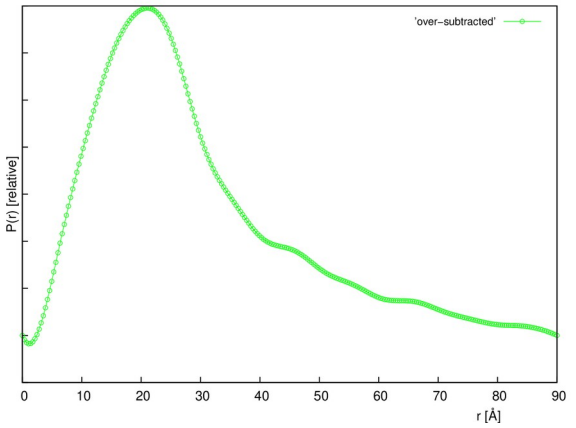
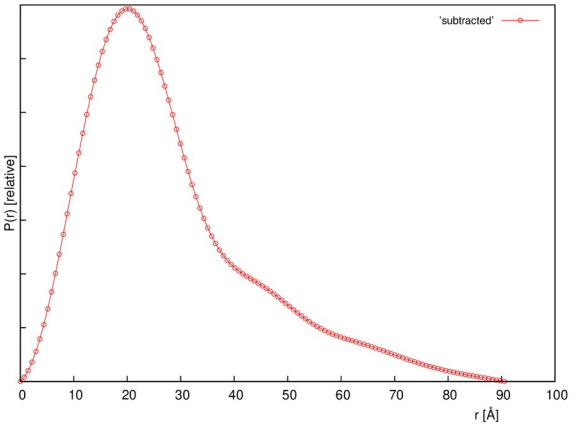
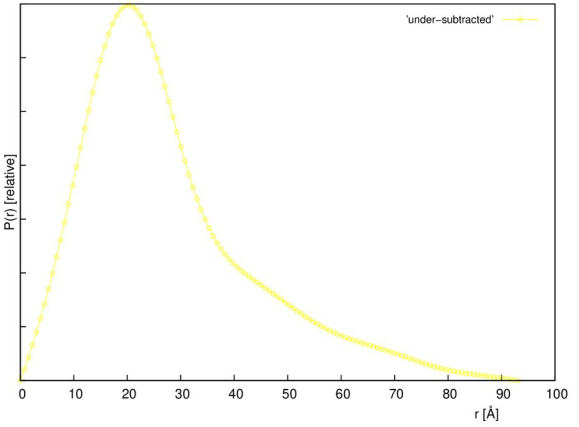
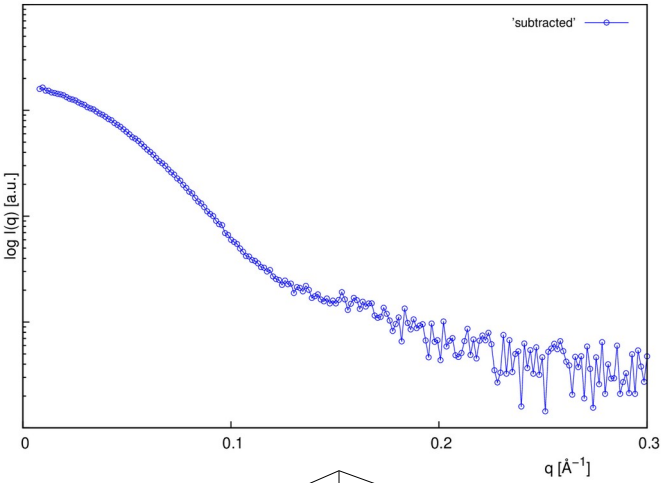




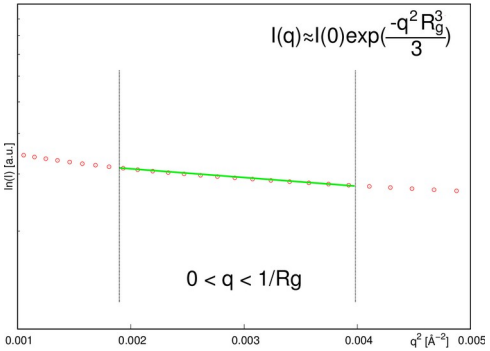




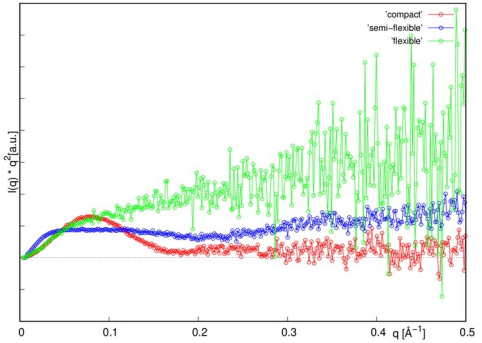
Subtracted SAXS data



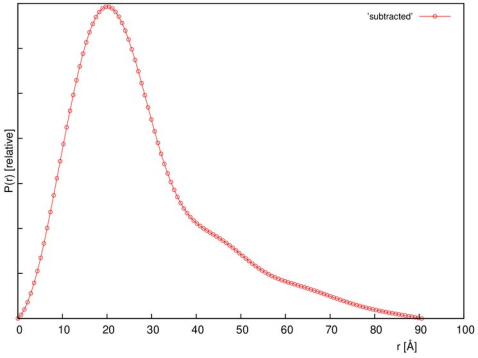
Guinier plot



Kratky plot



P(r) Pair distance distribution function



Guinier plot

- analysis of very low angle
- slope of decay proportional to size (Rg)

$$K = \frac{R_g^2}{3}$$

- Rg = radius of gyration

$$R_g = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(r_i - r_{cm})^2}$$

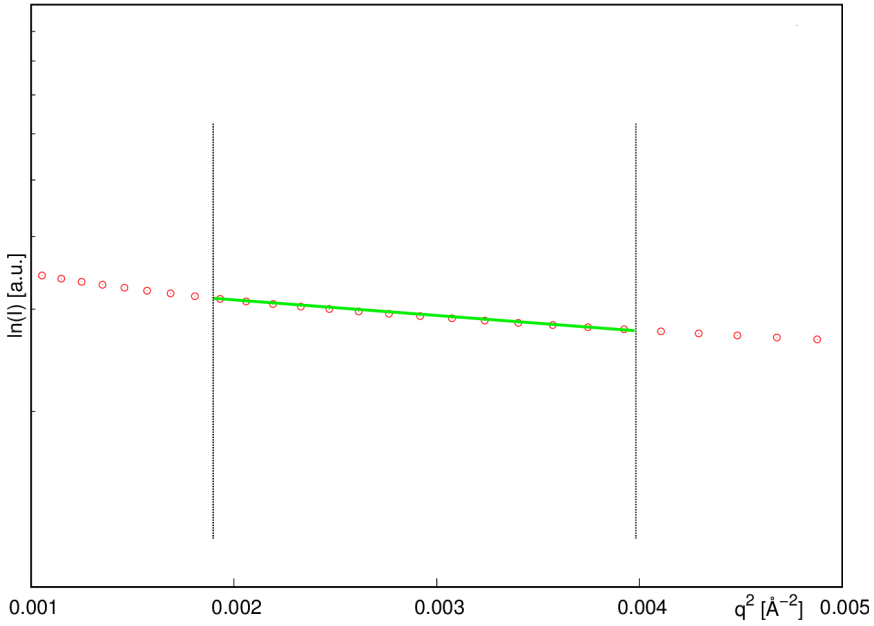
- aggregation/repulsion detection

$$\ln[I(q)] \simeq \ln[I(0)]\exp\left(\frac{-R_g^2 q^2}{3}\right)$$

Valid in:

$$0 < R_g q < 1.2$$

$$0 < R_g q < \frac{1}{R_g}$$



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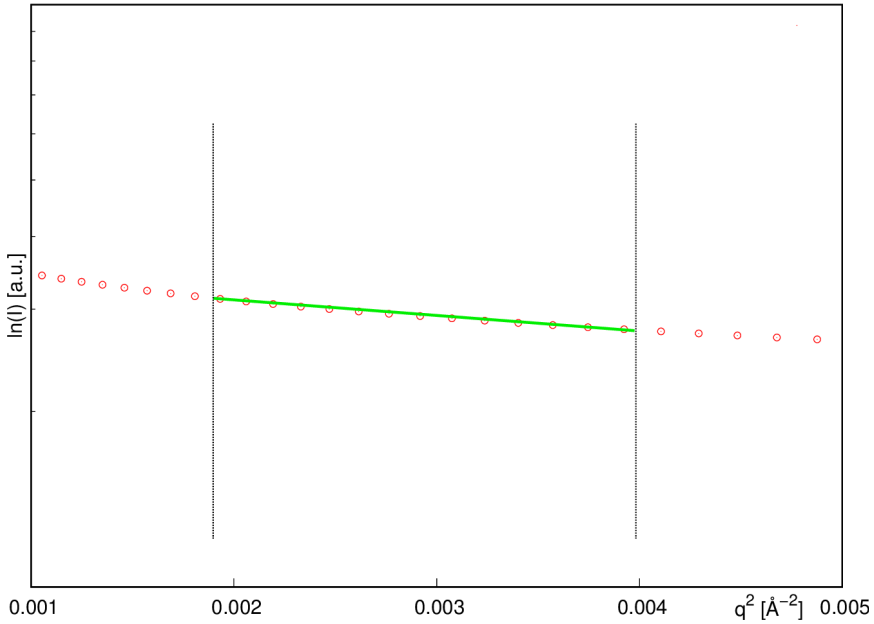

Data-collection parameters	
Instrument	BioSAXS-1000 (Rigaku)
Wavelength [Å]	1.5418
q range [Å^-1]	0.0095 - 0.65
Exposure time [min]	60
Temperature [°C]	4
Concentration [mg ml^-1]	5.0
Structural parameters	
Rg [Å] (from Guinier)	18.163
Rg [Å] (from P(r)	
Dmax [Å]	
Porod volume estimate [Å^3]	
MW theoretical [kDa]	9.4
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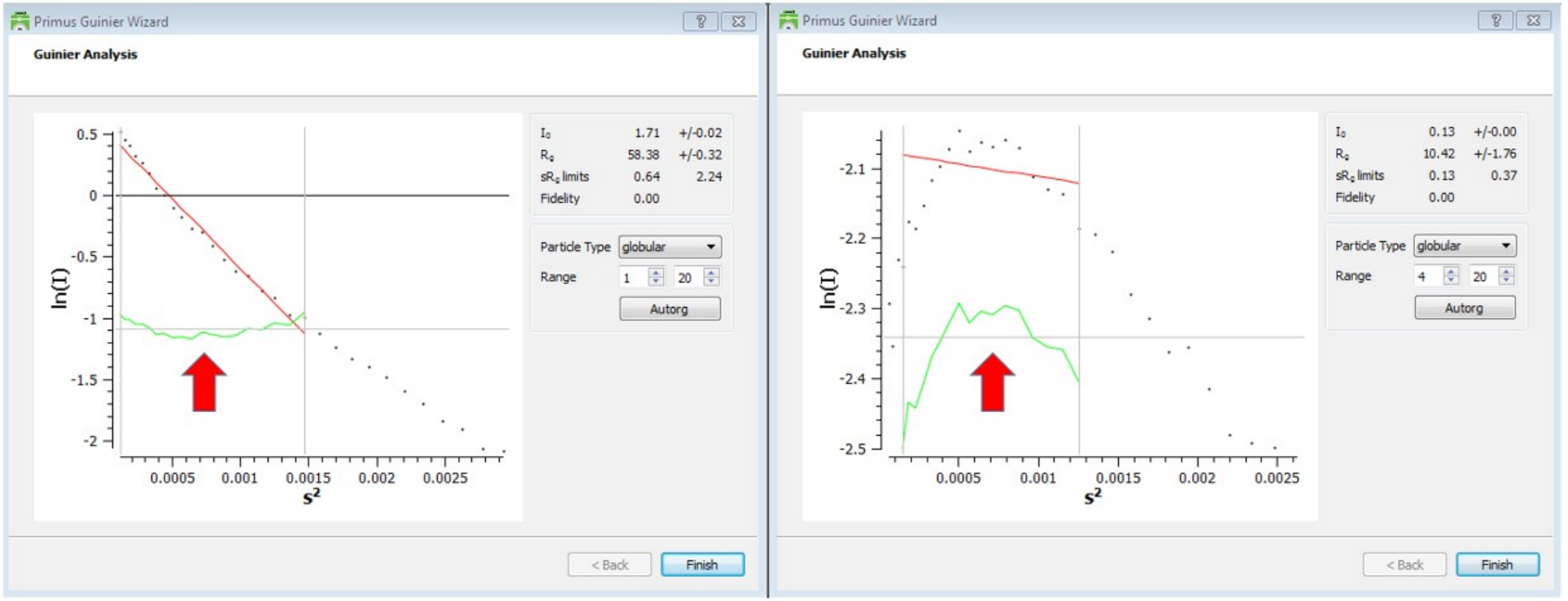
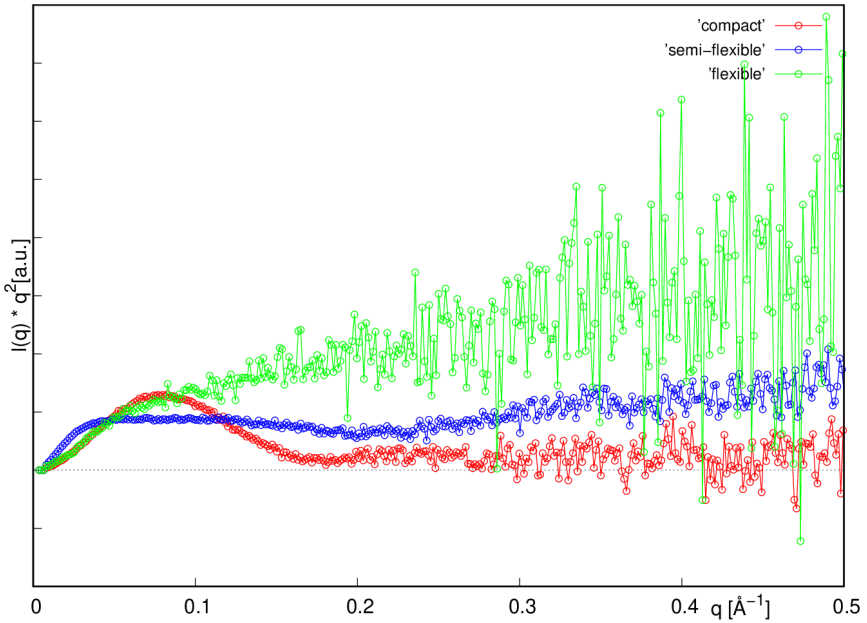


Kratky plot

Chain compactness

- slope of decay of intensity in „Kratky“ region
- compact well folded chains have clear minima
- dependent on data quality (subtraction)



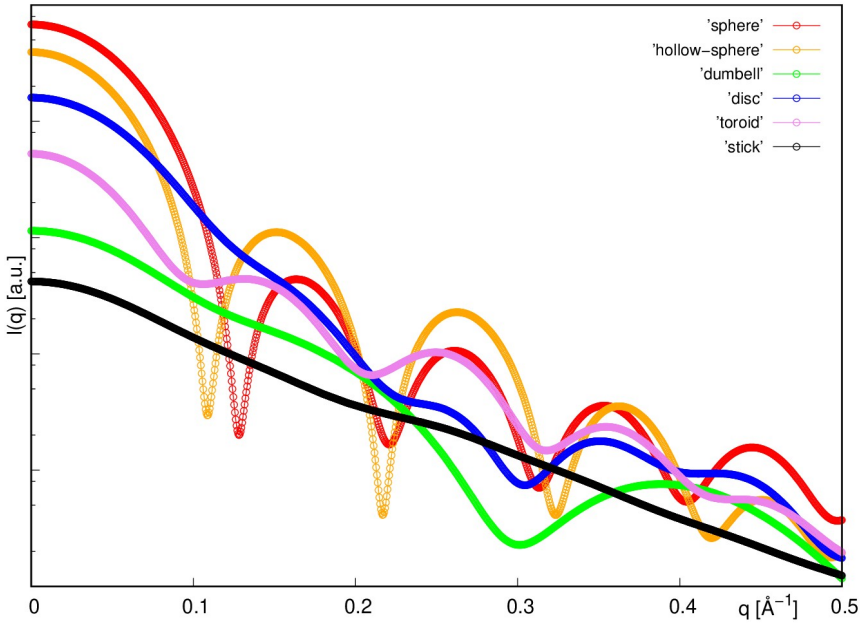
Pair distance distribution function
P (r)

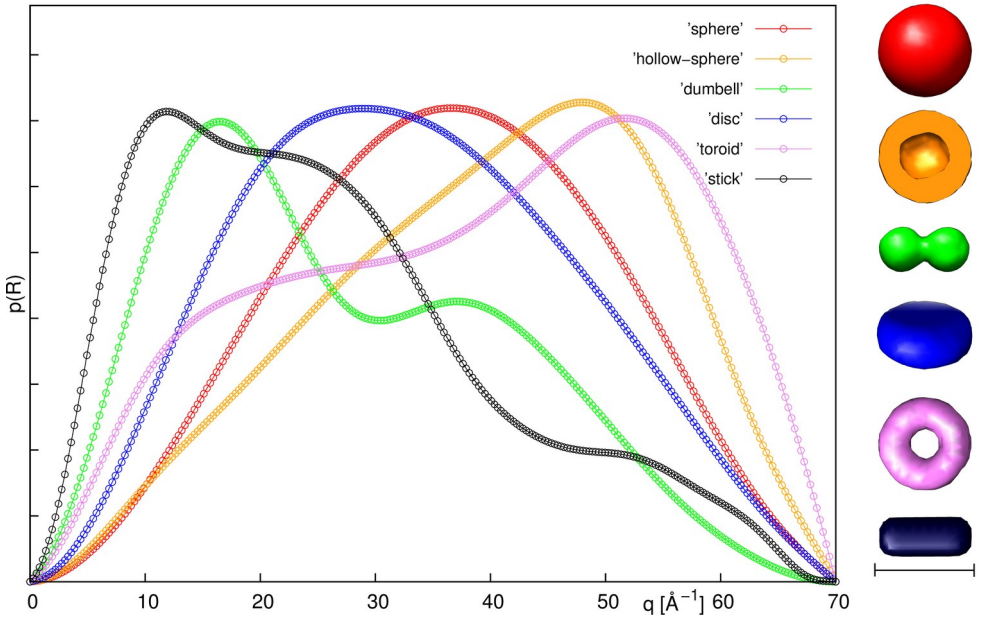
- indirect Fourier transform of scattered intensity
- GNOM – Svergun's perceptual criteria (smoothness, systematic deviation, …)

- distances of all pairs of points (electrons) of the particle (weighted)

$$p(r)=\gamma(r)\pi r^2$$

$$I(q)=4\pi\int_0^{Dmax} p(r)\frac{\sin(qr)}{qr}dr \quad \longleftrightarrow \quad p(r)=\frac{r^2}{2\pi^2}\int_0^{\infty} q^2 I(q)\frac{\sin(qr)}{qr}dq$$





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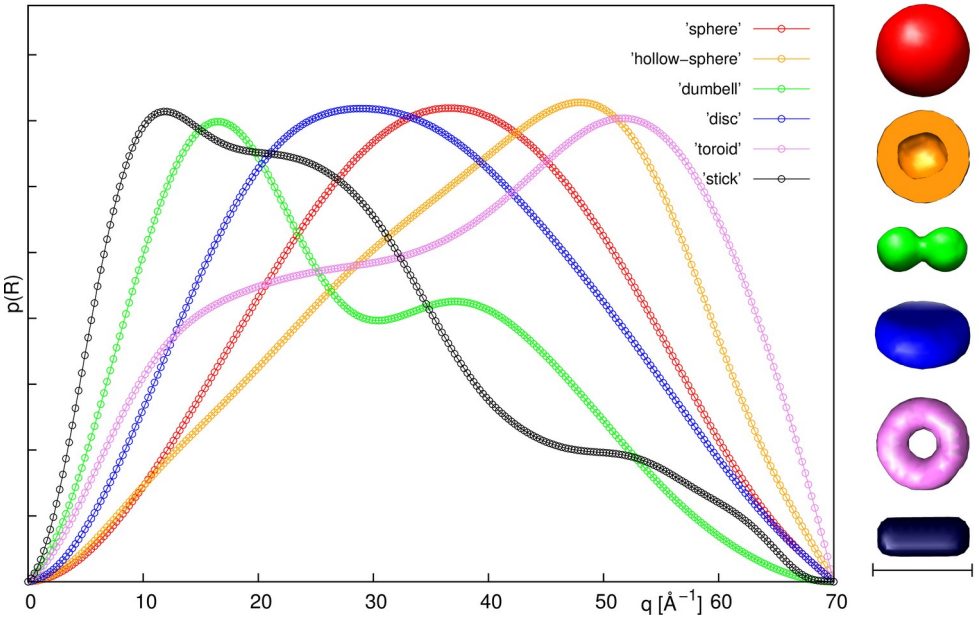
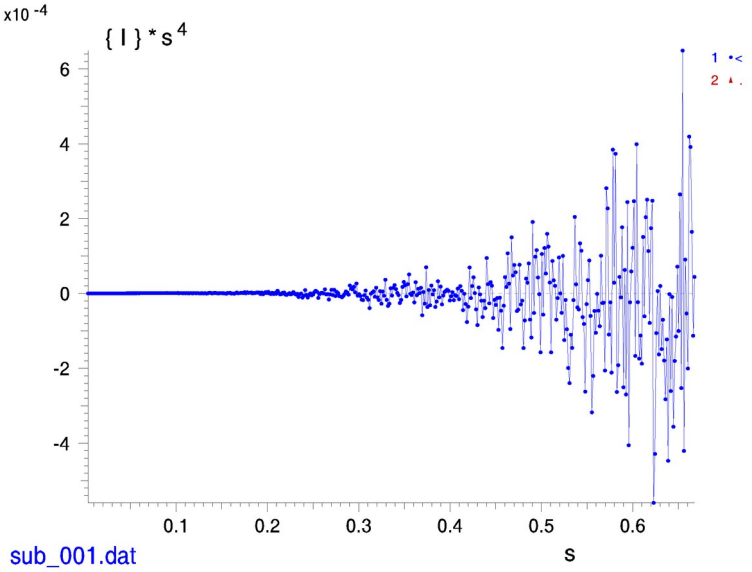


Porod volume

- applicable for folded macromolecules
- Porod's law – intensity decay $I(q)=q^{-4}$
- Porod's invariant

$$Q=\int_0^{\infty} q^2[I(q)-K]dq$$

$$V_p=\frac{2\pi^2 I(0)}{Q}$$



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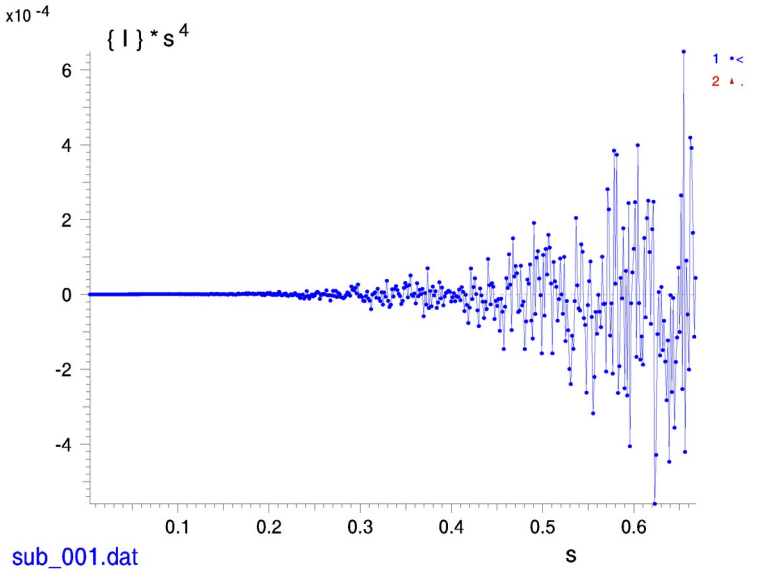
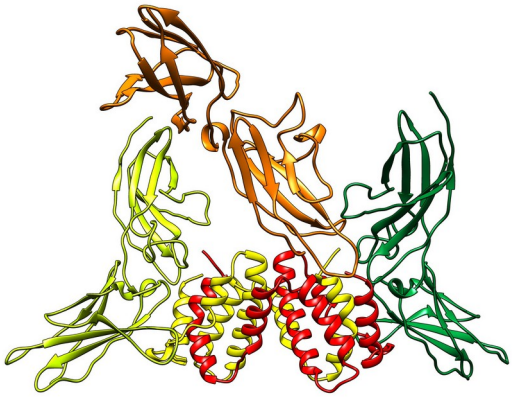


MW magic number for proteins = 0.625

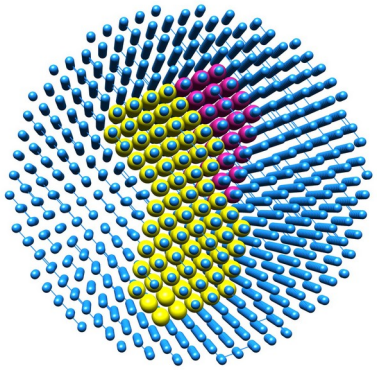
$$V_p[Å^3]*0.625=MW[Da]$$

SAXS – theoretical scattering

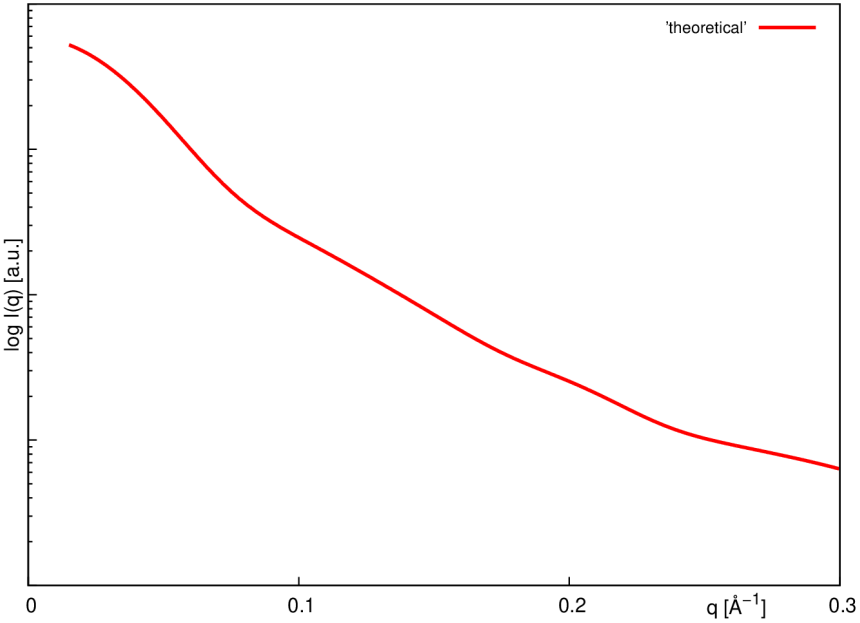
Debye's formula



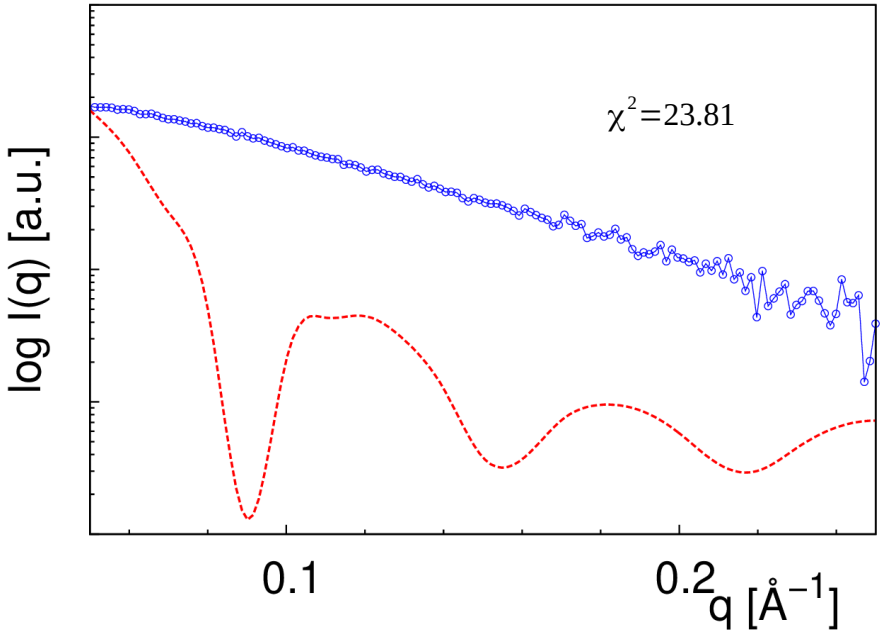
PDB coordinates



$$I(q)=\sum_{i=1}^{N_{sph}} F_i^2(q)+2\sum_{i=1}^{N_{sph}-1}\sum_{j=i+1}^{N_{sph}} F_i(q)F_j(q)\frac{\sin(qr_{ij})}{qr_{ij}}$$



SAXS – modeling



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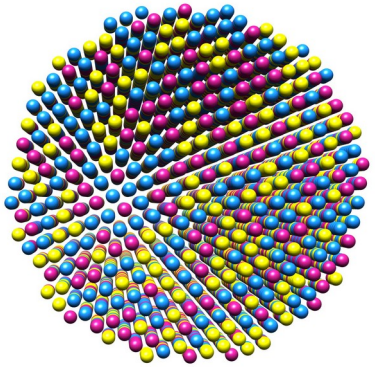
Debye's formula

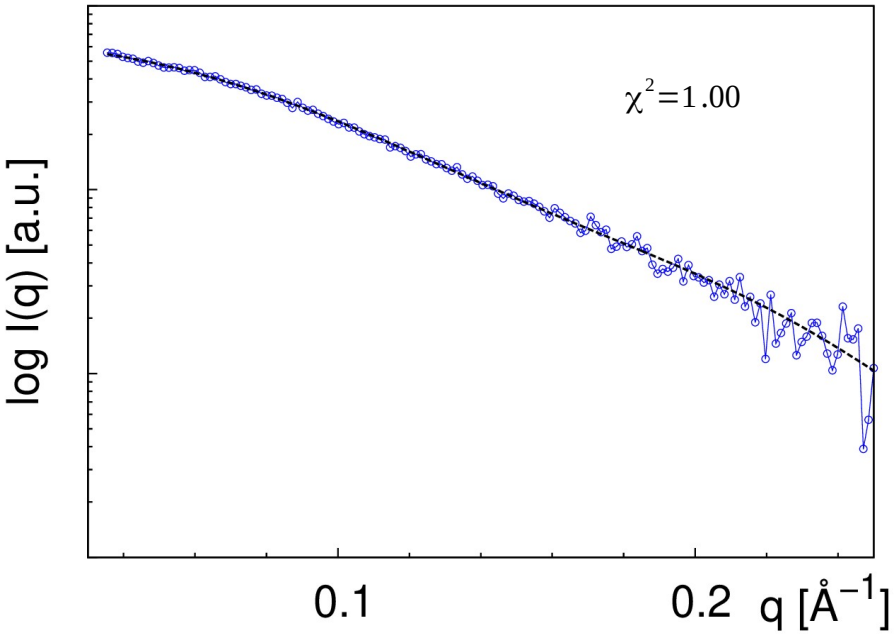
$$\chi^2=\frac{1}{N_p}\sum_{k=1}^{N_p}\left[\frac{I_{\exp}(q_k)-c\,.\,I_{calc}(q_k)}{\sigma_k}\right]^2$$

Quality of fit



initial model
(ab initio, rigid body)

SAXS – modeling



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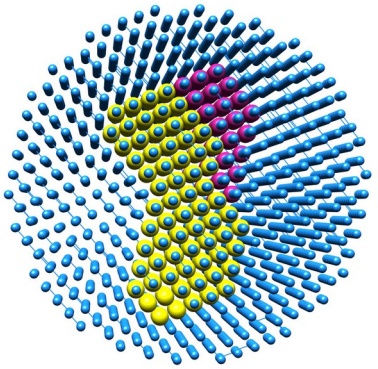

final model
(ab initio, rigid body)

SAXS software

- **ATSAS (Svergun group)**
- **SCATTER (Rambo group)**

- **http://smallangle.org/content/Software#Model-Fitting**

ATSAS software

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

EMBL Biological Small Angle Scattering

Home > ATSAS software

- Group members
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  - CORAL
  - CRYSOL
  - CRYSON
  - DAMAVER
  - DAMMIF
  - DAMMIN
  - DATtools
  - EOM
  - GASBOR
  - GLOBSYMM
  - GNOM
  - MASSHA
  - MIXTURE
  - MONSA
  - OLIGOMER
  - PEAK
  - PRIMUS
  - SASFLOW
  - SASREF
  - SREFLEX
  - SUPCOMB
  - Manuals
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- Facilities
- Courses
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Data analysis software ATSAS 2.8.0

A program suite for small-angle scattering data analysis from biological macromolecules

Data processing
PRIMUS - manipulations with experimental 1D SAS data
GNOM - indirect transform program that evaluates the particle distance distribution function p(r)
Data manipulation and analysis tools - AUTORG, ALMERGE, DATGNOM, DATPOROD etc.

***Ab initio* methods**
DAMMIN - *ab initio* shape determination using a dummy atom model
DAMMIF - rapid shape determination
GASBOR - reconstruction of a protein structure by a chain-like ensemble of dummy residues
MONSA - shape determination using a multiphase dummy atom model

Rigid body modelling
SASREF - modelling of multisubunit complexes
BUNCH - modelling of multidomain proteins against multiple data sets
CORAL - modelling of multidomain protein complexes against multiple data sets
MASSHA - interactive modelling of atomic structures and shape analysis
GLOBSYMM - rigid body modelling of symmetric oligomers

Mixtures and flexible systems
OLIGOMER - volume fractions of mixtures with known scattering intensities from the components
MIXTURE - modelling of multicomponent systems
EOM - Ensemble Optimization Method for flexible proteins
SREFLEX - flexible refinement of high-resolution models combining SAXS and NMA

PDB oriented tools
CRYSOL - X-ray scattering patterns from known hi-res structures
CRYSON - neutron scattering patterns from known hi-res structures
SUPCOMB - superimposes one 3D structure onto another
DAMAVER - align *ab initio* models, select the most typical one

Manuals

If you use ATSAS please cite:

Petoukhov, M.V., Franke, D., Shkumatov, A.V., Tria, G., Kikhney, A.G., Gajda, M., Gorba, C., Mertens, H.D.T., Konarev, P.V. and Svergun, D.I. (2012)
New developments in the ATSAS program package for small-angle scattering data analysis
J. Appl. Cryst. 45, 342-350 © International Union of Crystallography DOI

Last modified: October 8. 2015

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Small Angle X-ray Scattering Initiative for Europe :: Forum

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General	
	Announcements Courses and workshops, new software releases
	SAS Hardware/Instrumentation Detectors, sample changers, home sources, nanomanipulation tools, add-ons (Raman spectrometer, HPLC), gas phase scattering etc.
	SAS Experiment Design Plan your small angle X-ray or neutron scattering measurements
	Literature Books and reviews on small angle scattering. Discussions and criticism on recent SAXS papers.
	Feedback Suggestions for new topics to discuss, questions on the use of the Forum
ATSAS	
	FAQ Frequently Asked Questions about ATSAS small-angle scattering analysis program package
	ATSAS Package in General ATSAS for Linux and Mac, general installation issues, ATSAS online etc.
	Primary Data Processing Interactive and automated data processing tools (PRIMUS, GNOM, AUTORG). Scattering from simple bodies (BODIES), peak analysis (PEAK), data plotting (SASPLOT) etc.
	Ab Initio Shape Determination Ab initio modelling: DAMMIF, DAMMIN, GASBOR, MONSA
	Rigid Body Modelling Interactive modelling (MASSHA, SASpy) and global minimization programs (SASREF, BUNCH, CORAL, GLOBSYMM)
	Mixtures and Flexible Systems Linear (OLIGOMER), and non-linear (MIXTURE) analysis, singular value decomposition (SVDPLOT), addition of missing fragments (BUNCH, CORAL), analysis of flexible systems (EOM/RAN models (SREFLEX)
	Working with Models Calculation of SAXS and SANS profiles (CRYSOL, CRYSON), superposition of models (SUPCOMB, DAMAVER, DAMCLUST), database DARA
Other Software	
	SAXS & SANS Software Small angle scattering software (except ATSAS)

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ATSAS software

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

EMBL Biological Small Angle Scattering

Home > ATSAS software

- Group members
- ATSAS software
  - Download
  - BUNCH
  - CORAL
  - CRYSOL
  - CRYSON
  - DAMAVER
  - DAMMIF
  - DAMMIN
  - DATtools
  - EOM
  - GASBOR
  - GLOBSYMM
  - GNOM
  - MASSHA
  - MIXTURE
  - MONSA
  - OLIGOMER
  - PEAK
  - PRIMUS
  - SASFLOW
  - SASREF
  - SREFLEX
  - SUPCOMB
  - Manuals
- Web services
- Facilities
- Courses
- Contact us

Data analysis software ATSAS 2.8.0

A program suite for small-angle scattering data analysis from biological

Data processing

PRIMUS - manipulations with experimental 1D SAS data
GNOM - indirect transform program that evaluates the particle distance distribution functio
Data manipulation and analysis tools - AUTORG, ALMERGE, DATGNOM, DATPOROD et

***Ab initio* methods**

DAMMIN - *ab initio* shape determination using a dummy atom model
DAMMIF - rapid shape determination
GASBOR - reconstruction of a protein structure by a chain-like ensemble of dummy residu
MONSA - shape determination using a multiphase dummy atom model

Rigid body modelling

SASREF - modelling of multisubunit complexes
BUNCH - modelling of multidomain proteins against multiple data sets
CORAL - modelling of multidomain protein complexes against multiple data sets
MASSHA - interactive modelling of atomic structures and shape analysis
GLOBSYMM - rigid body modelling of symmetric oligomers

Mixtures and flexible systems

OLIGOMER - volume fractions of mixtures with known scattering intensities from the components
MIXTURE - modelling of multicomponent systems
EOM - Ensemble Optimization Method for flexible proteins
SREFLEX - flexible refinement of high-resolution models combining SAXS and NMA

PDB oriented tools

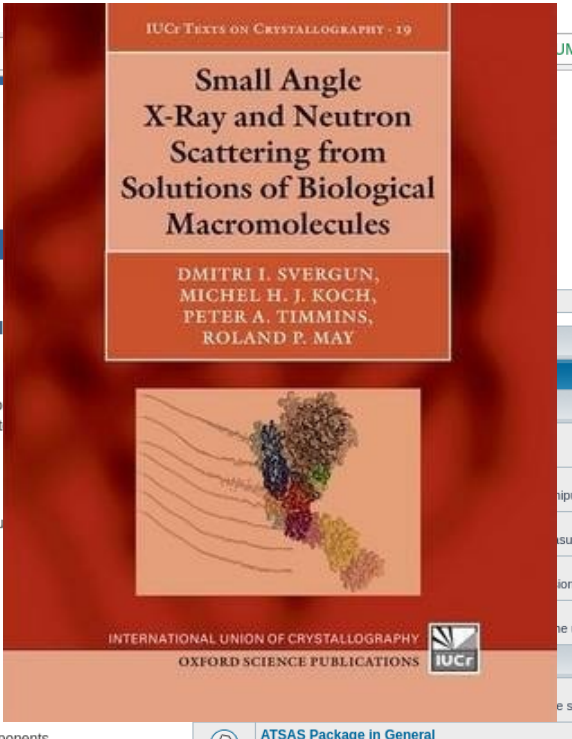
CRYSOL - X-ray scattering patterns from known hi-res structures
CRYSON - neutron scattering patterns from known hi-res structures
SUPCOMB - superimposes one 3D structure onto another
DAMAVER - align *ab initio* models, select the most typical one

Manuals

If you use ATSAS please cite:

Petoukhov, M.V., Franke, D., Shkumatov, A.V., Tria, G., Kikhney, A.G., Gajda, M., Gorba, C., Mertens, H.D.T., Konarev, P.V. and Svergun, D.I. (2012)
New developments in the ATSAS program package for small-angle scattering data analysis
J. Appl. Cryst. 45, 342-350 © International Union of Crystallography DOI

Last modified: October 8. 2015



UM FÜR MOLEKULARBIOLOGIE [DE] | https://www.saxier.org/forum/

SAXS
Small Angle X-ray Scattering Initiative for Europe :: Forum

Forum

...nipulation tools, add-ons (Raman spectrometer, HPLC), gas phase scattering etc.

...asurements

...ions and criticism on recent SAXS papers.

...he use of the Forum

...e scattering analysis program package

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Small angle scattering software (except ATSAS)

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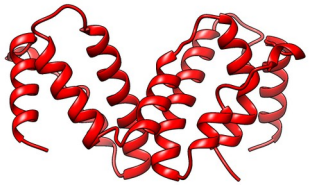
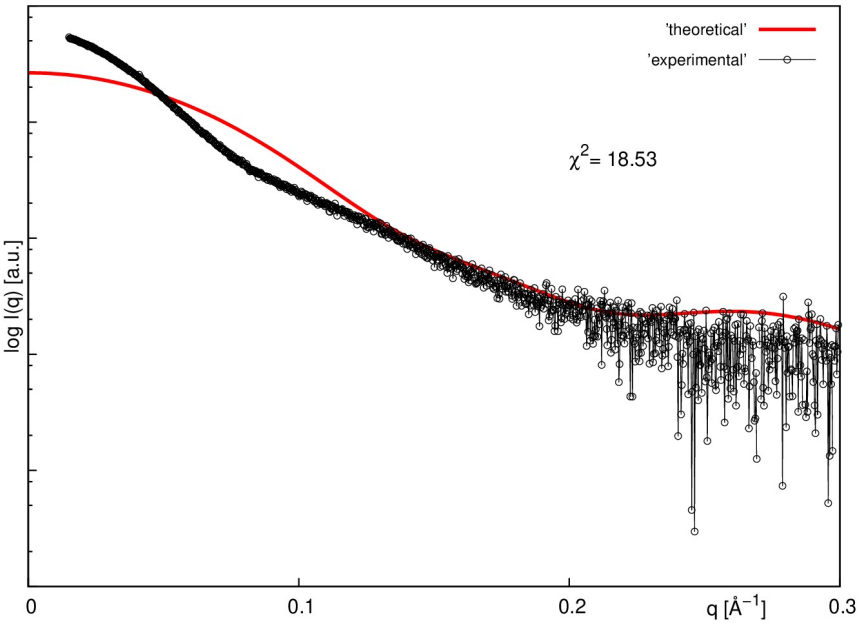
Board index

SAXS – theoretical scattering
CRYSOL

- evaluation of solution scattering of known atomic structure
- fitting to experimental data
- validation tool





https://www.embl-hamburg.de/biosaxs/reprints/crysol_1995.pdf

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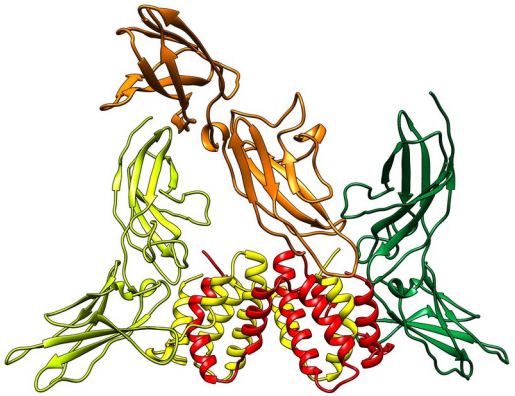

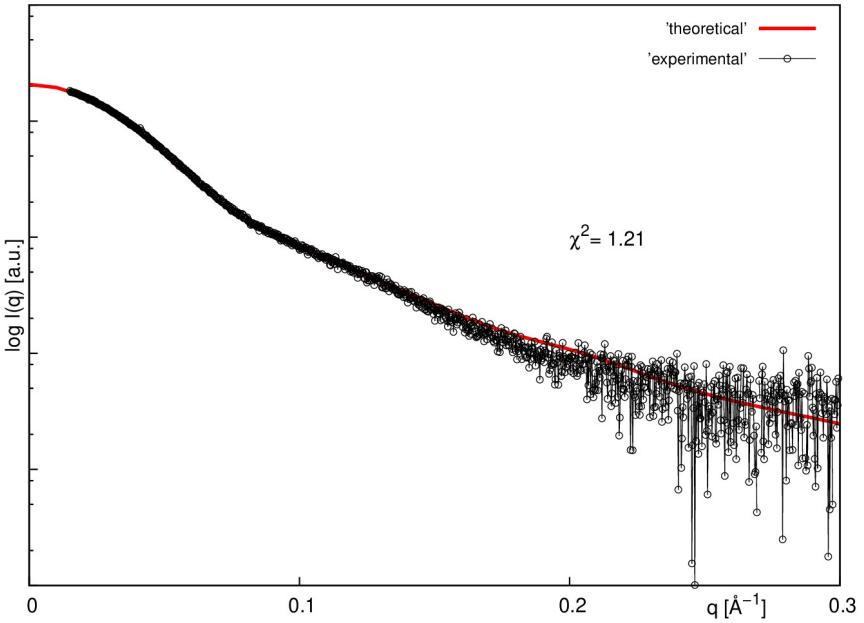

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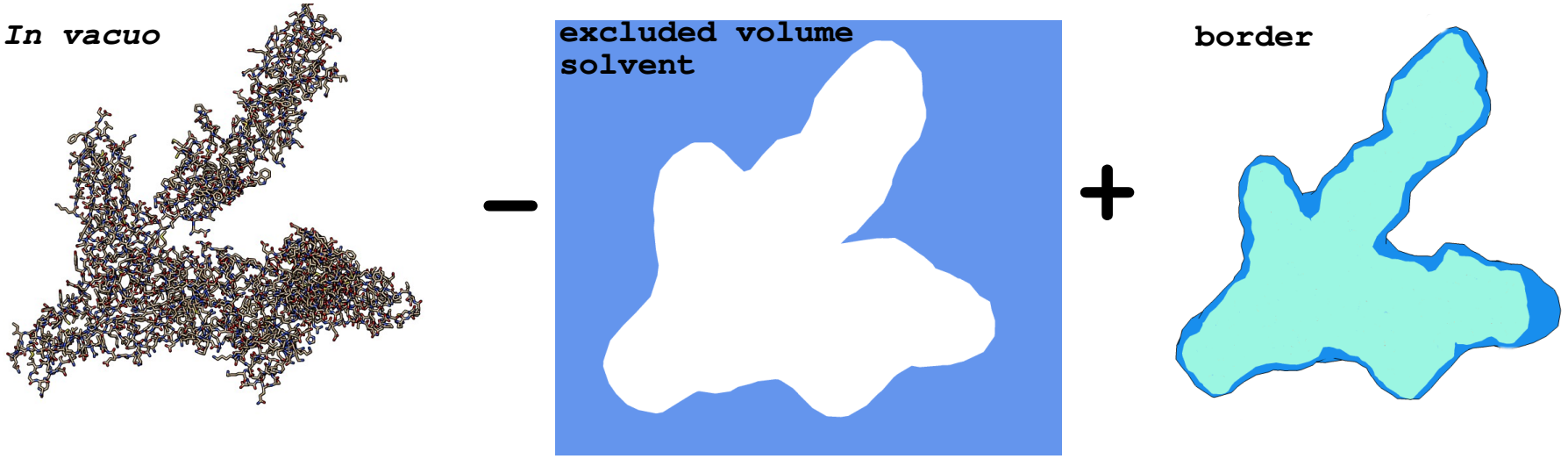

$$I(q)=\langle|A_a(q)-\rho_s A_s(q)+\delta\rho_b A_b(q)|^2\rangle_\Omega$$

https://www.embl-hamburg.de/biosaxs/reprints/crysol_1995.pdf

SAXS – theoretical scattering
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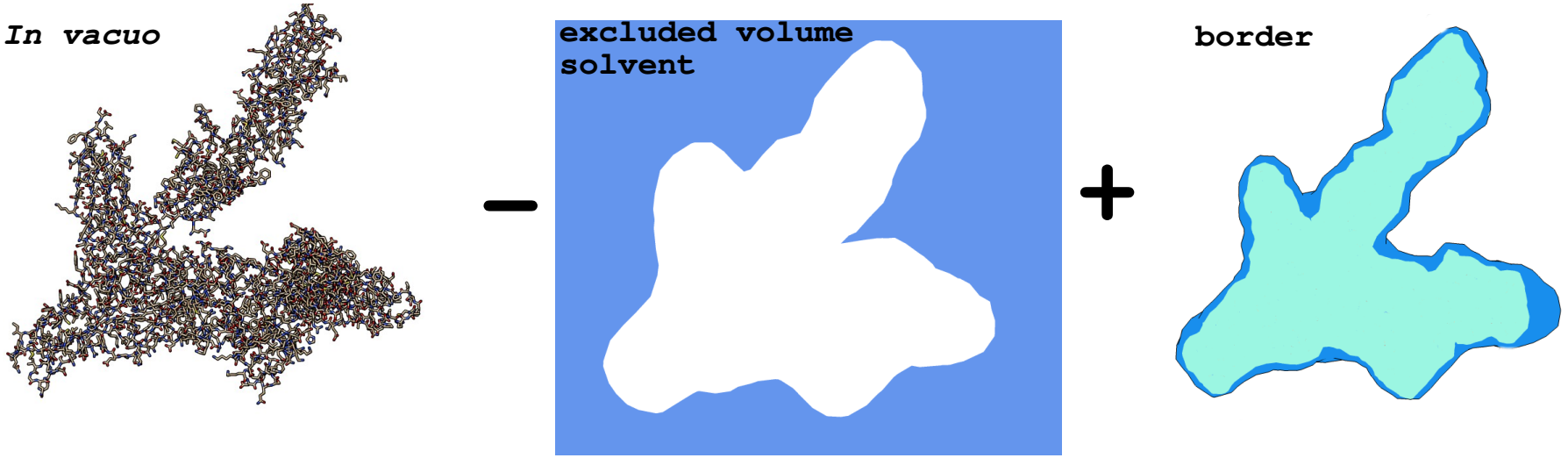
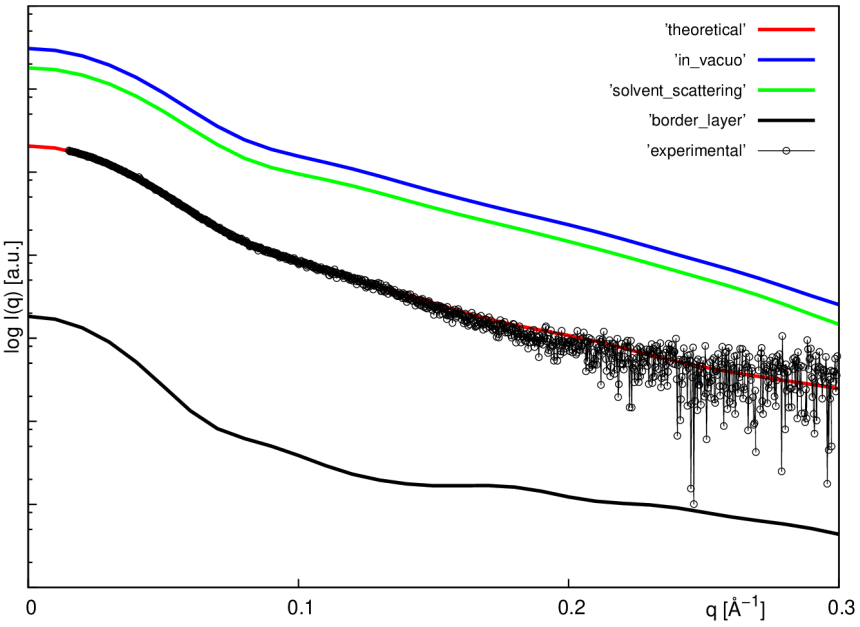


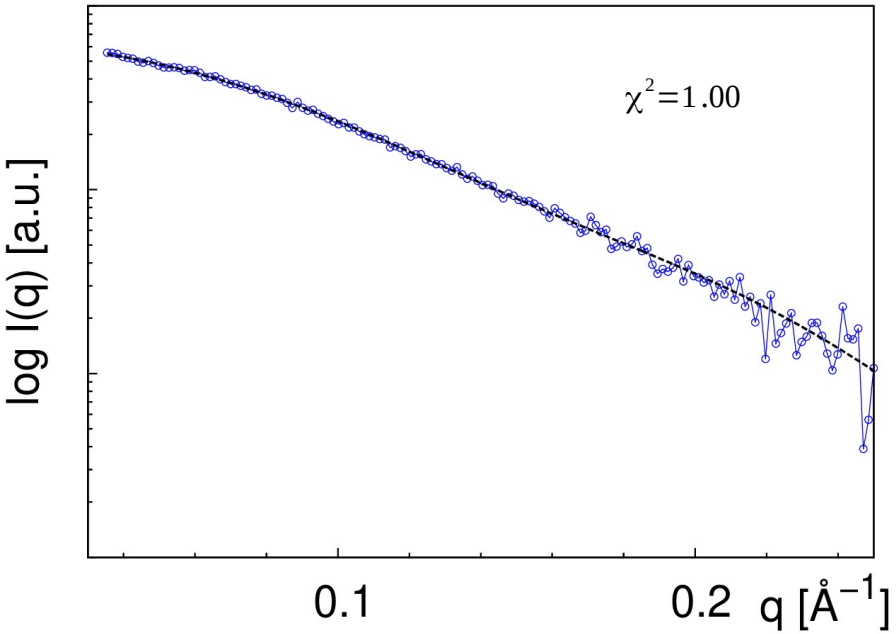
$$I(q) = \langle |A_a(q) - \rho_s A_s(q) + \delta \rho_b A_b(q)|^2 \rangle_\Omega$$

$$\chi^2 = \frac{1}{N_p} \sum_{k=1}^{N_p} \left[\frac{I_{\exp}(q_k) - c \, . \, I_{calc}(q_k, r_{0,} \delta\rho)}{\sigma_k} \right]^2$$



https://www.embl-hamburg.de/biosaxs/reprints/crysol_1995.pdf

SAXS – modeling

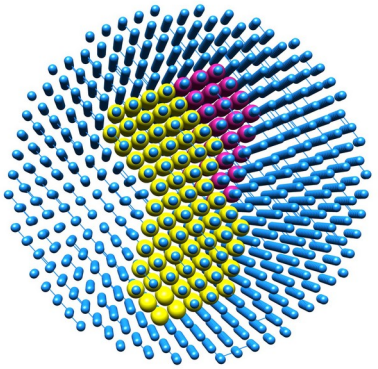


$$I(q)=\sum_{i=1}^{N_{sph}} F_i^2(q)+2\sum_{i=1}^{N_{sph}-1}\sum_{j=i+1}^{N_{sph}} F_i(q)F_j(q)\frac{\sin(qr_{ij})}{qr_{ij}}$$

Debye's formula

$$\chi^2=\frac{1}{N_p}\sum_{k=1}^{N_p}\left[\frac{I_{\exp}(q_k)-c.I_{calc}(q_k)}{\sigma_k}\right]^2$$

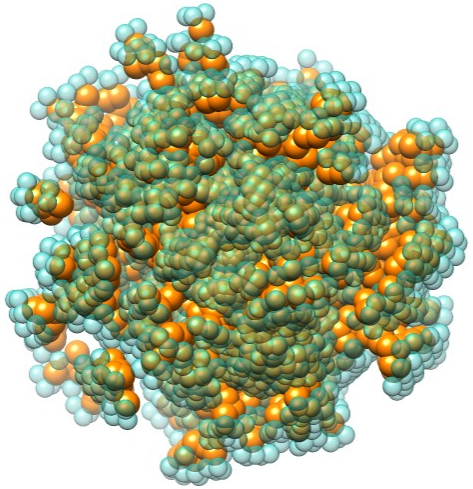
Quality of fit



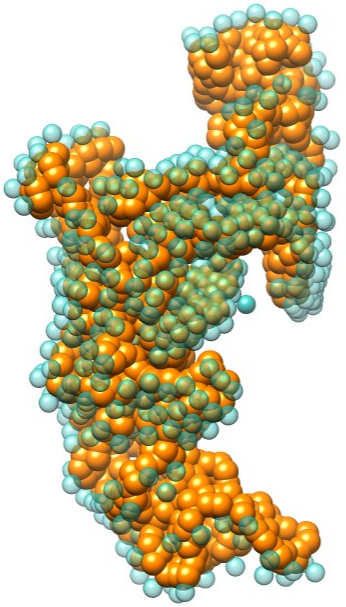
final model
(ab initio, rigid body)

Ab initio modeling
dummy residues – *GASBOR*

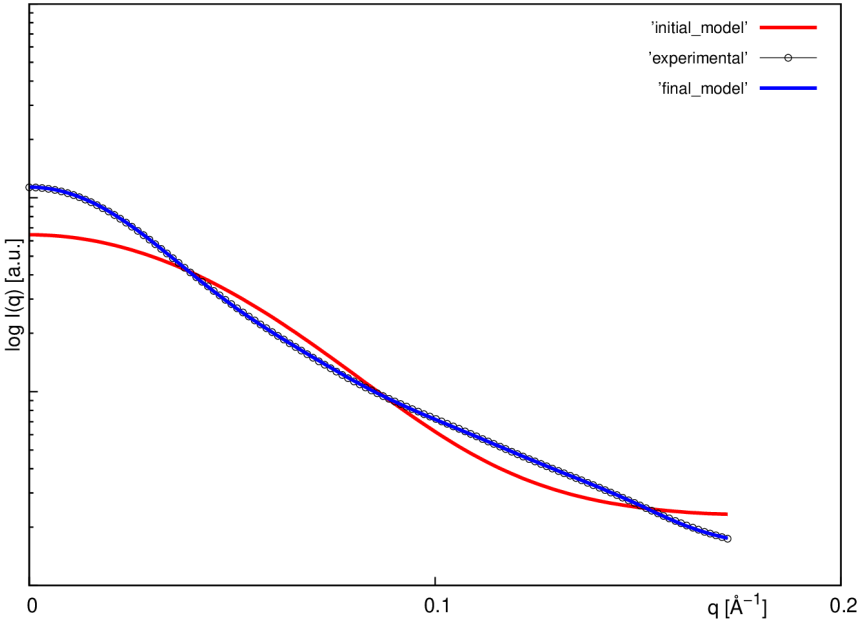
- low resolution shape reconstruction
- dummy residues: spheres with electron density as average AA resudue
- distance constrain 3.8 Å as approx. Cα–Cα position
- fixed number of dummy residues (protein sequence)



initial model

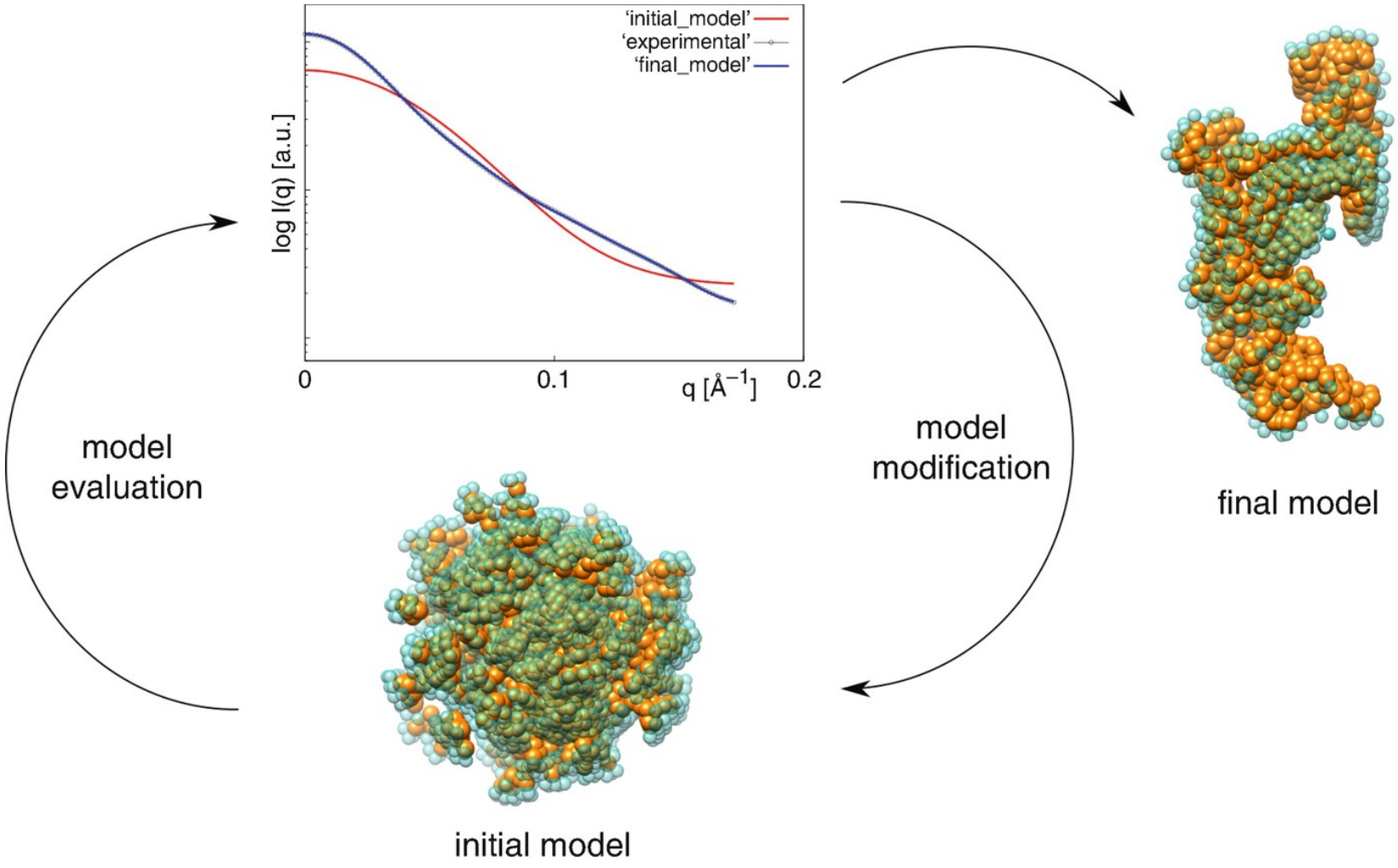


final model



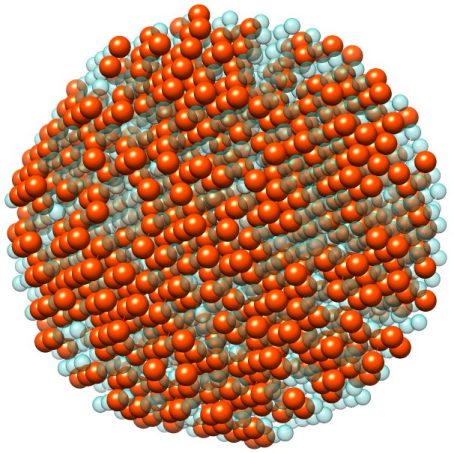
- simulated annealing method to minimize goal function: $f(x)=\chi^2+\sum \alpha P(x)$
- penalties: bond length, hidtogram distances, peripherial, discontiguity

Ab initio modeling
dummy residues – *GASBOR*



Ab initio modeling
dummy atoms – *DAMMIN*

- low resolution shape reconstruction
- dummy atoms – densely packed spheres (beads)
- search volume ~ Dmax, radius of beads << Dmax
- two phases: solute (protein) and solvent (water)



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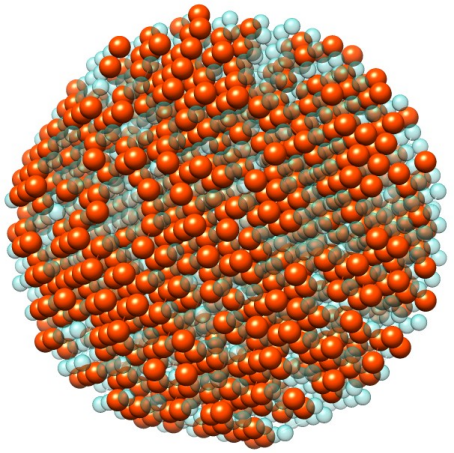

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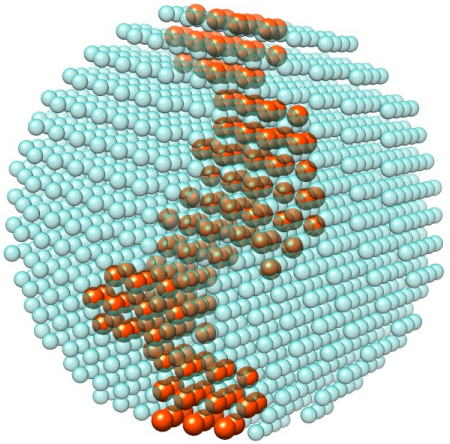
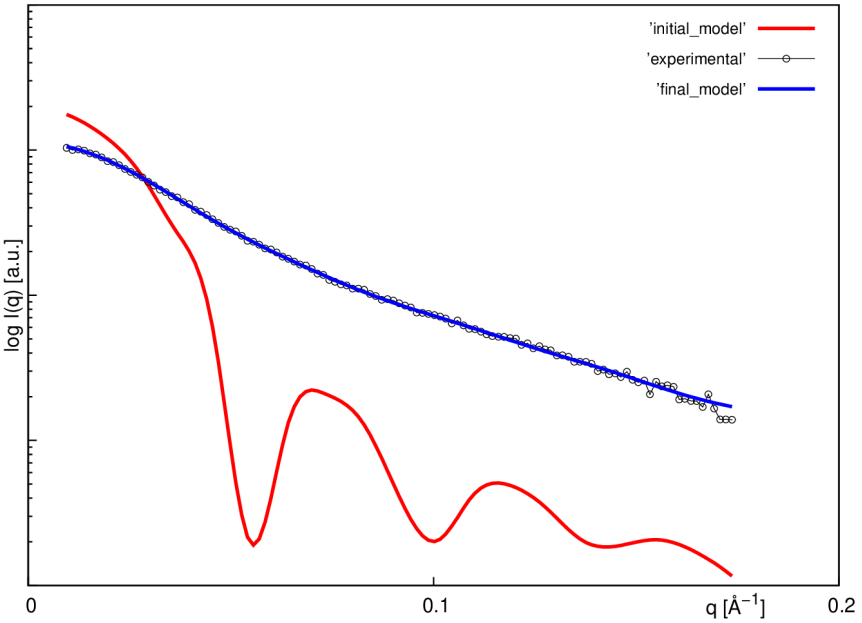


final model



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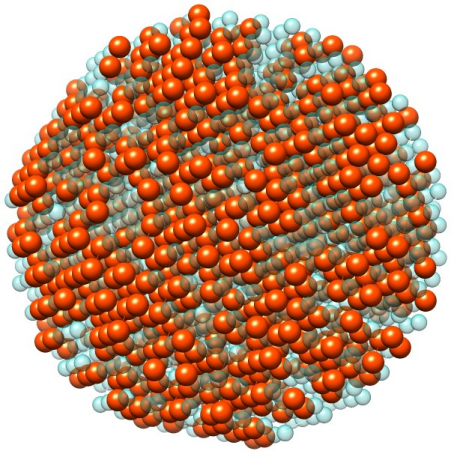

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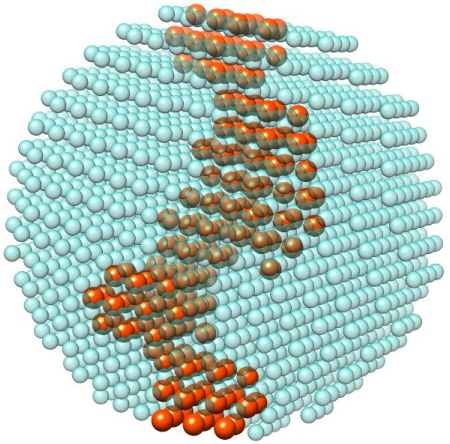

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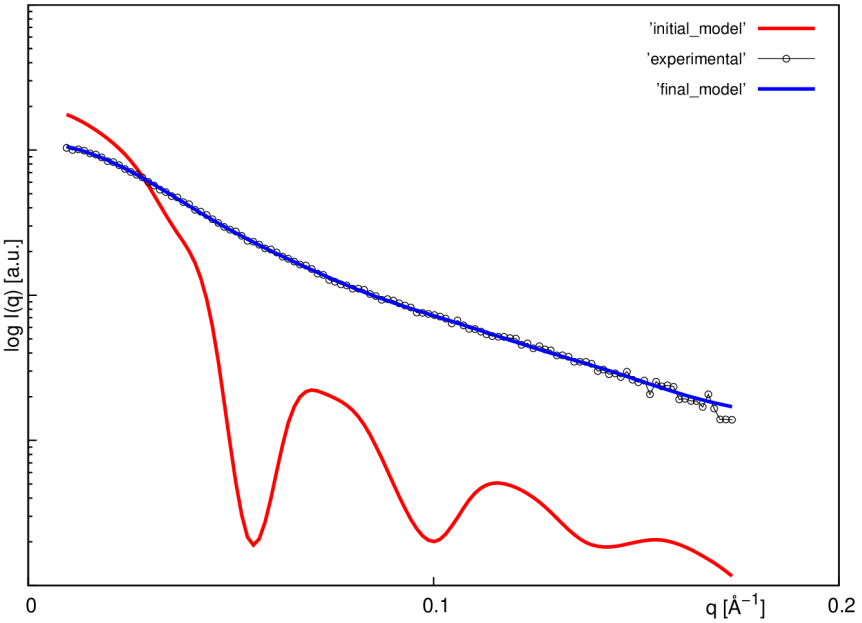
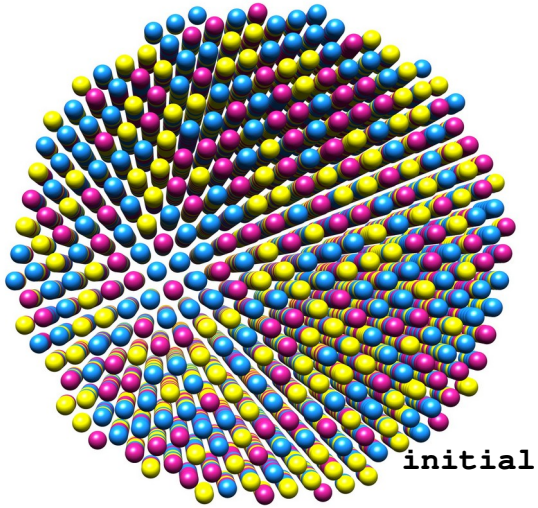


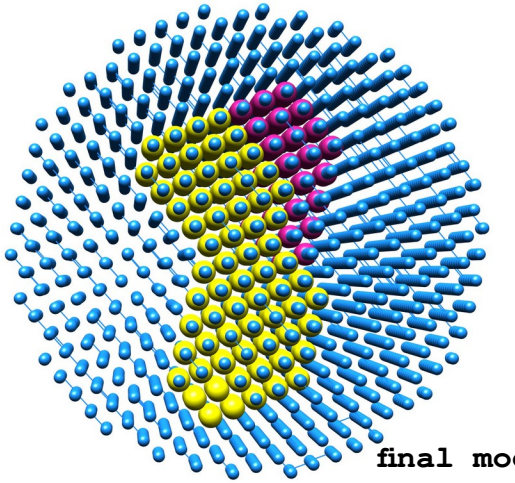
- simulated annealing method to minimize goal function: $f(x)=\chi^2+\sum \alpha P(x)$
- penalties: loosenes, disconnectivity, peripherial

Ab initio multi-phase modeling
dummy atoms – *MONSA*

- low resolution shape reconstruction
- dummy atoms – densely packed spheres (beads)
- search volume ~ Dmax, radius of beads << Dmax
- up to 4 phases: protein–protein complexes, protein::nucleic acid complexes



initial model



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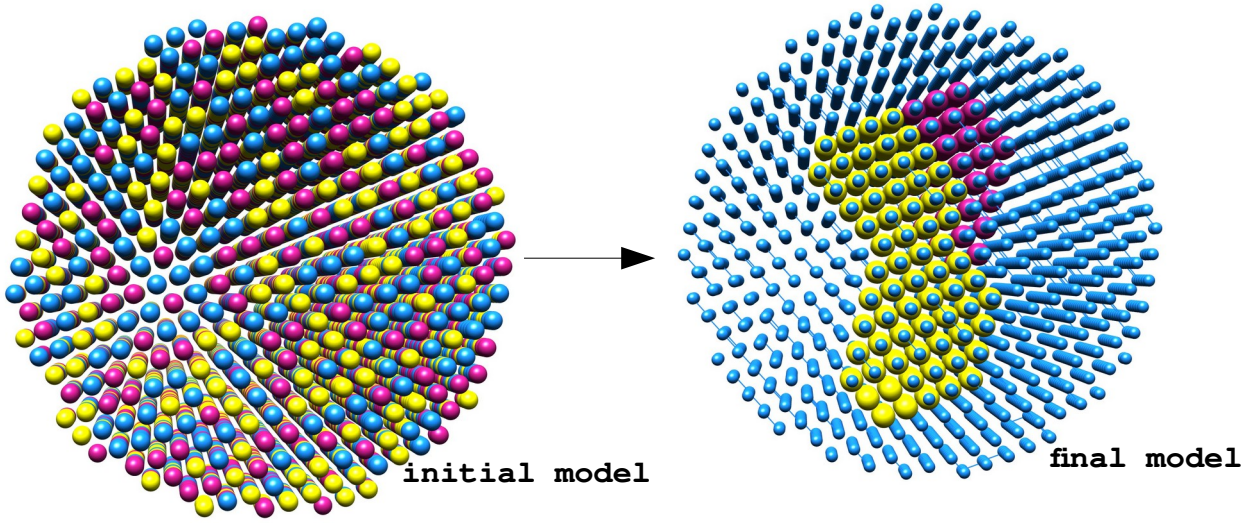
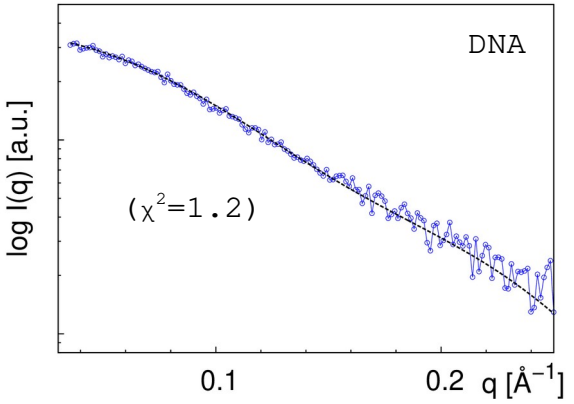
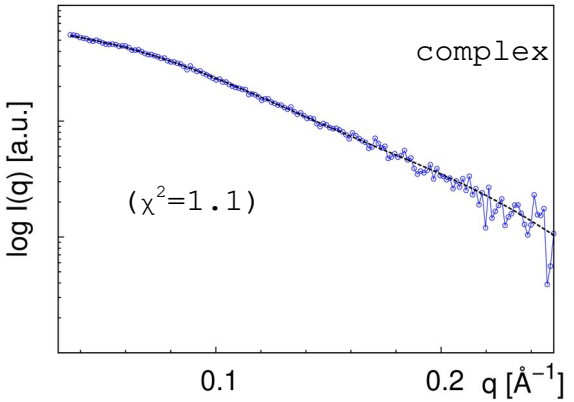
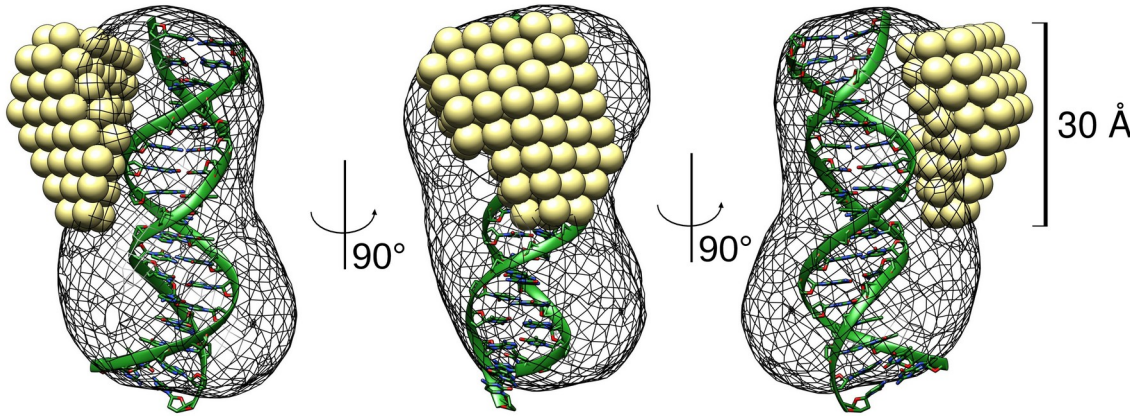


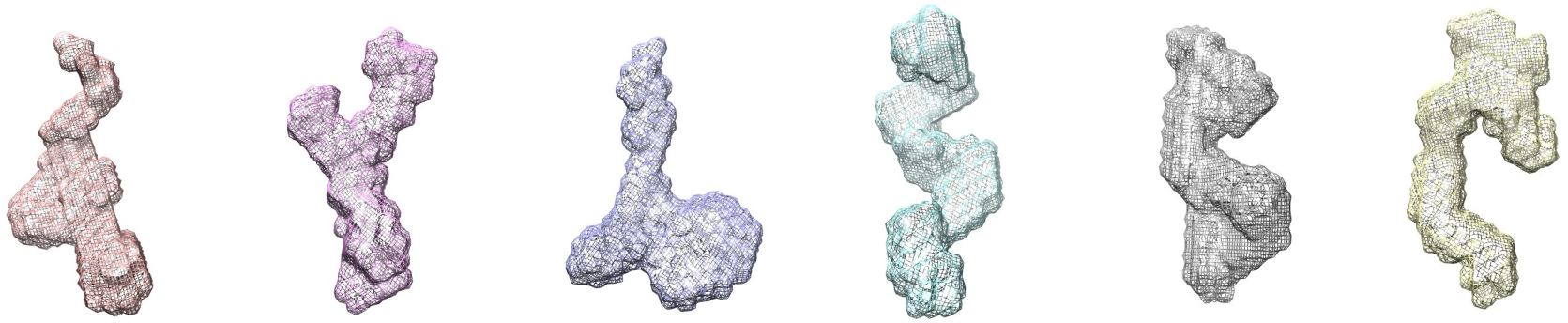




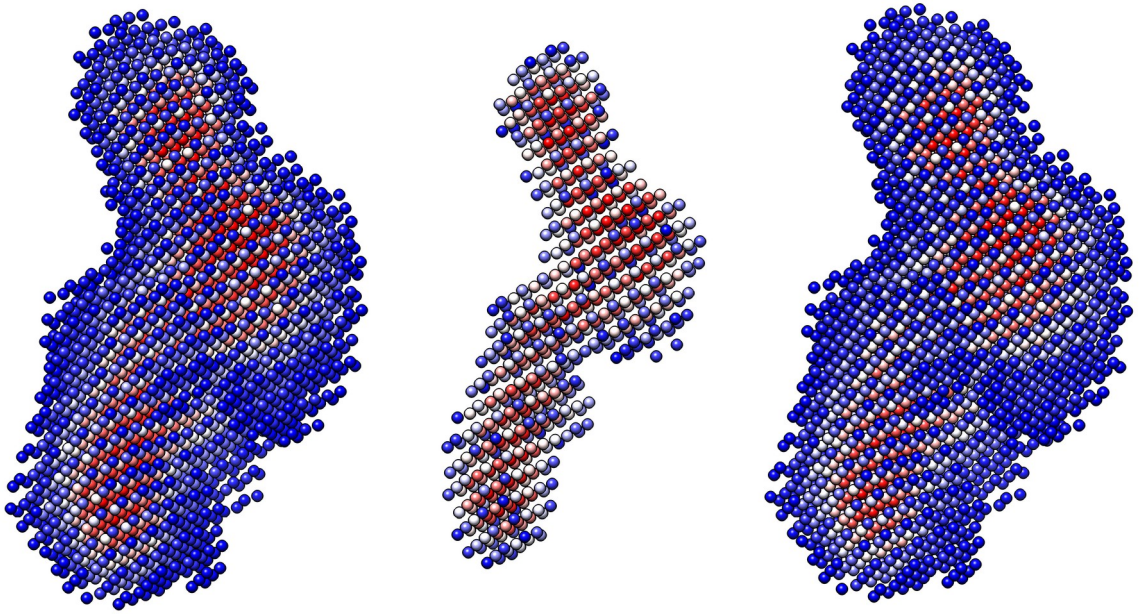


Ab initio modeling refinement

- mutiple runs of ab initio reconstruction give different results
- refinement: alignment, averaging, clustering, most typical model
- dummy atoms/res. with highest ‚occupancy' used as starting structure



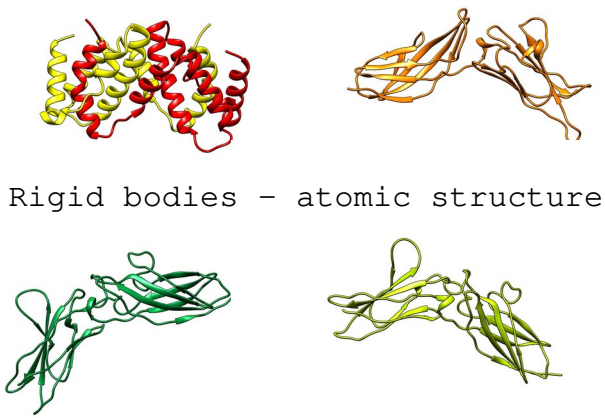
Recommendation	NSD	File
Include	0.735	dammif3.pdb
Include	0.739	dammif1.pdb
Include	0.739	dammif8.pdb
Include	0.740	dammif4.pdb
Include	0.750	dammif9.pdb
Include	0.752	dammif7.pdb
Include	0.754	dammif10.pdb
Include	0.756	dammif6.pdb
Include	0.756	dammif2.pdb
Discard	0.851	dammif5.pdb



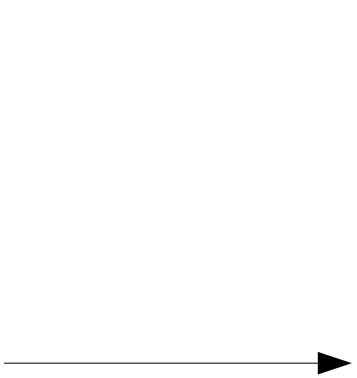
damaver damfilt damstart

Rigid body modeling
CORAL

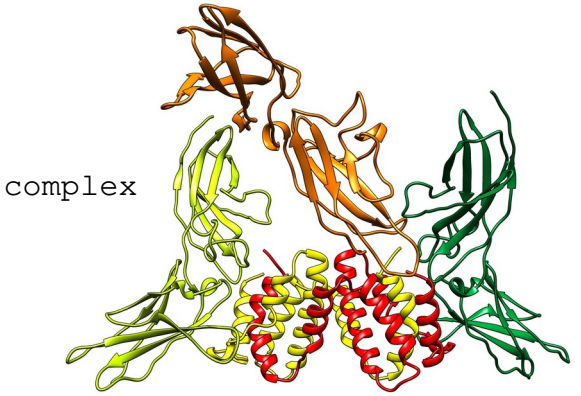
- **Complexes with Random Loops**
- **translation and rotation search**
- **library of random loops composed of dummy residues (5–100AA)**
- **contact constrains, if known**
- **penalties: clashes, shift, contacts**



Rigid bodies – atomic structures



complex



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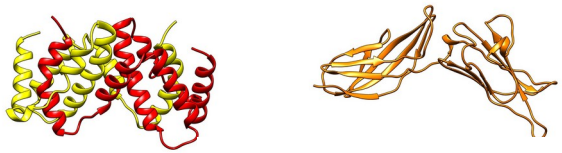
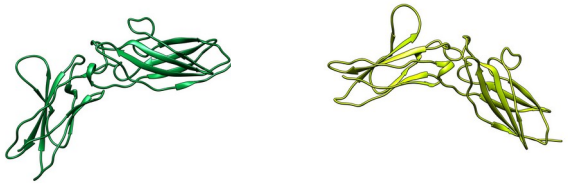
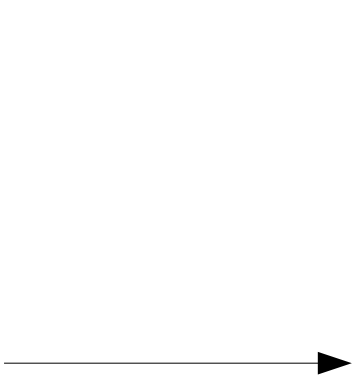


Rigid bodies – atomic structures





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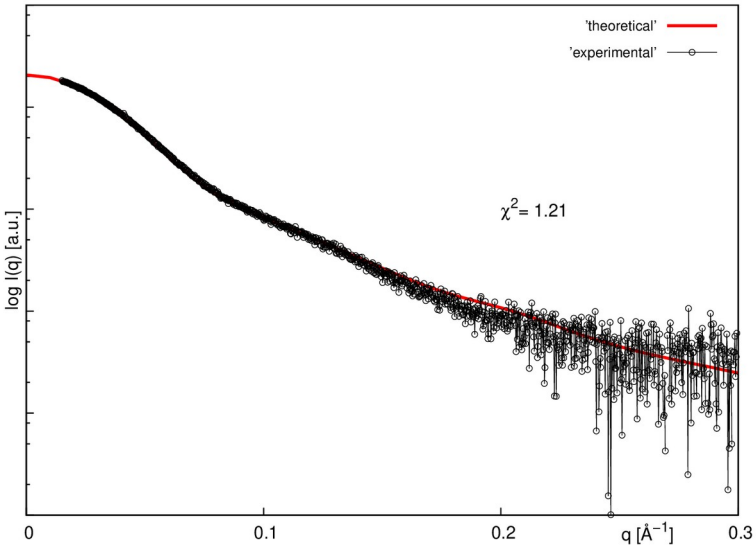


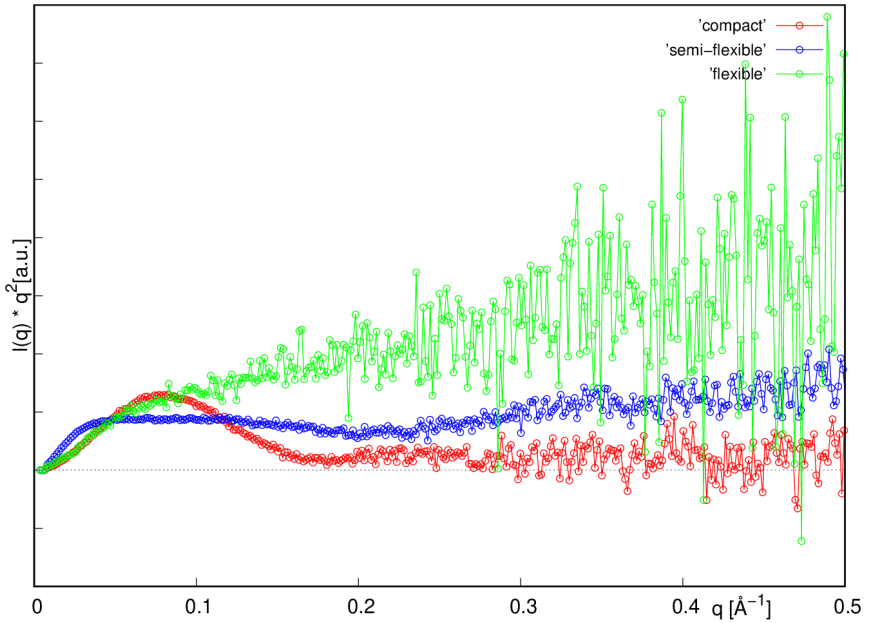
Simulated annealing
Aim: find vector of M variables minimizing a function f(x)

1. start from random configuration x at high temperature T
2. make a small random modification of configuration x → x`
   and compute the difference Δ=f(x`)–F(x)
3. if Δ>0, accept it with probability $e^{-\Delta/T}$
4. make another step from previous configuration
   if previous step was rejected
   or from new configuration, if was accepted
5. repeat 2–4 many times, then decrease the temperature
6. continue the cooling until no improvement is observed

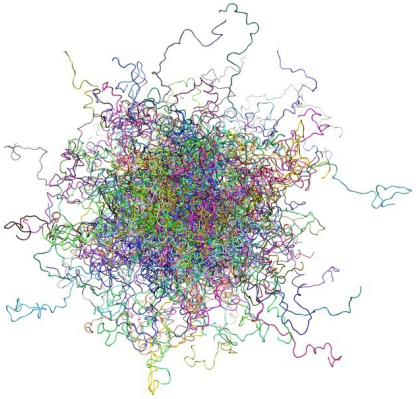
Flexible systems

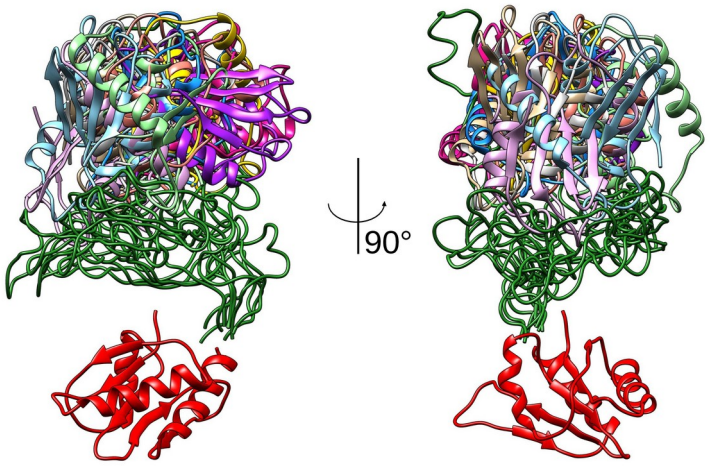
Conformational polydispersity
Fully or partialy unstructured chains

- conformational polydispersity
- fully/partialy unstructured chains
- ensemble modeling (selection)

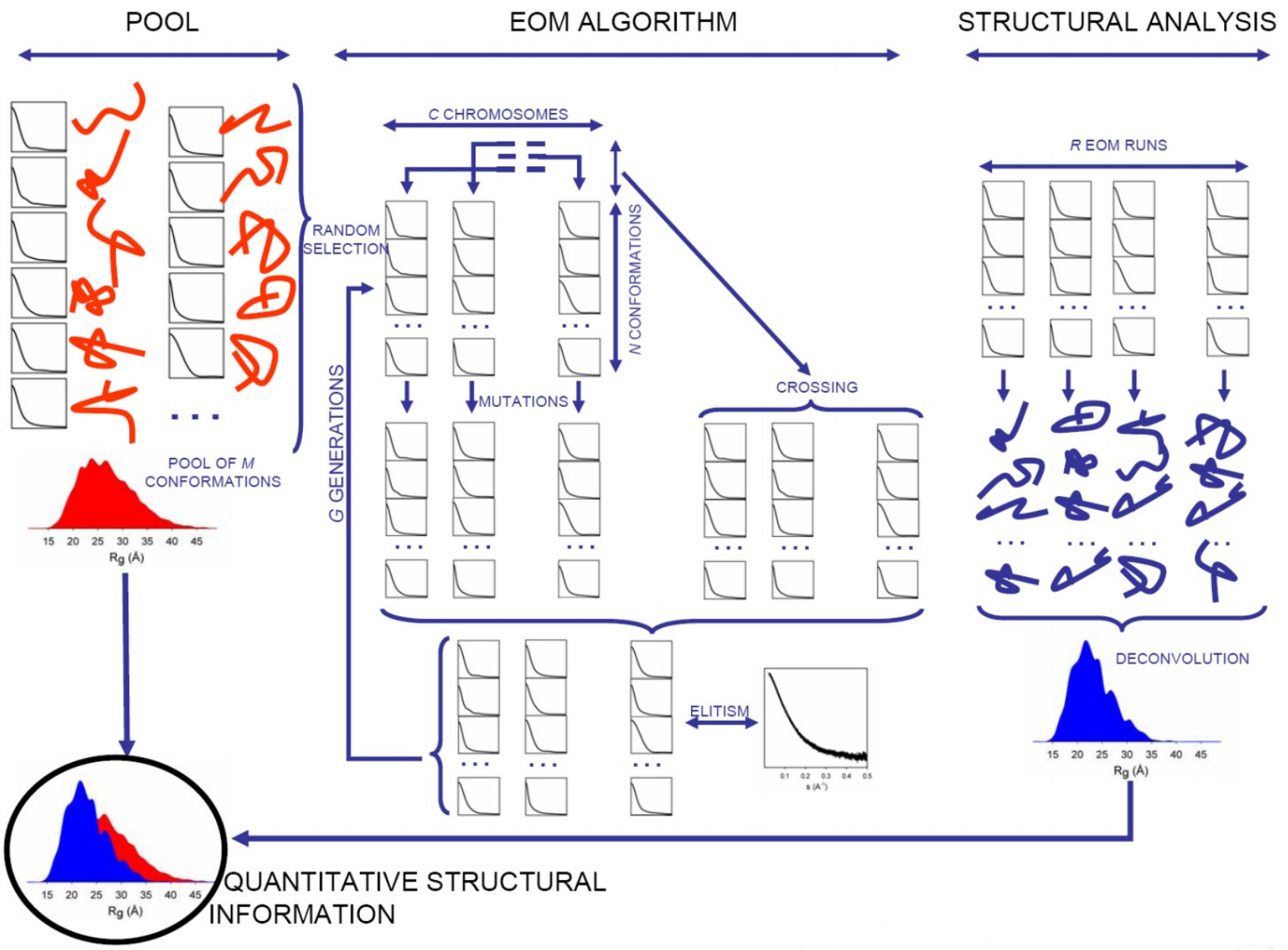


-multidomain proteins with flexible linkers, IDPs





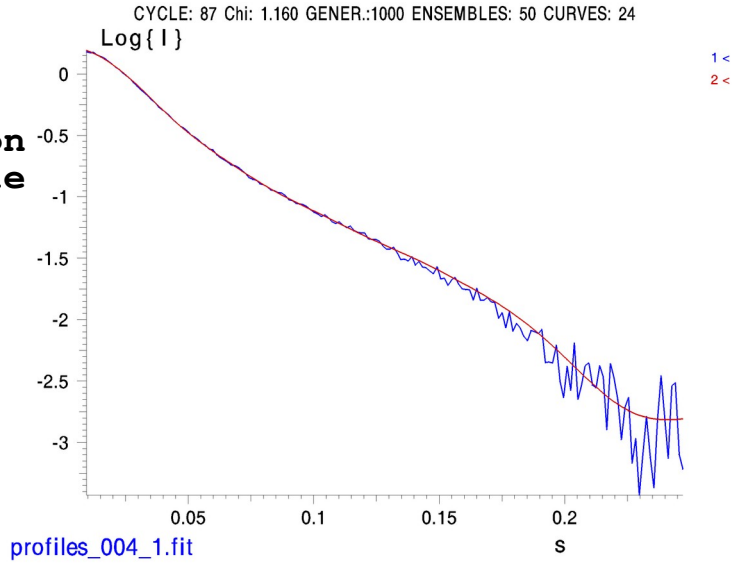
Ensemble modeling
EOM



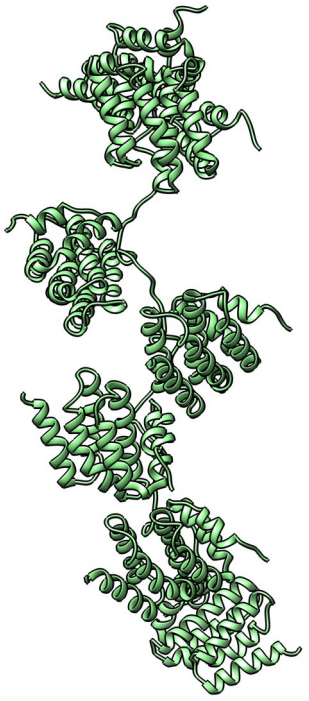
https://www.embl-hamburg.de/biosaxs/eom.html

Ensemble modeling
EOM

- ensemble representation of possible flexibility
- model conformations not necessarily exists in solution
- Rg and Dmax distribution of pool and selected ensemble



37%



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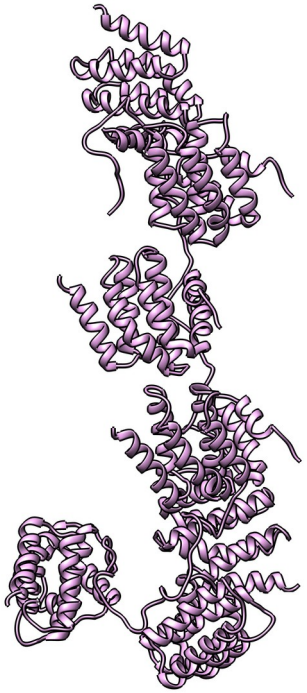

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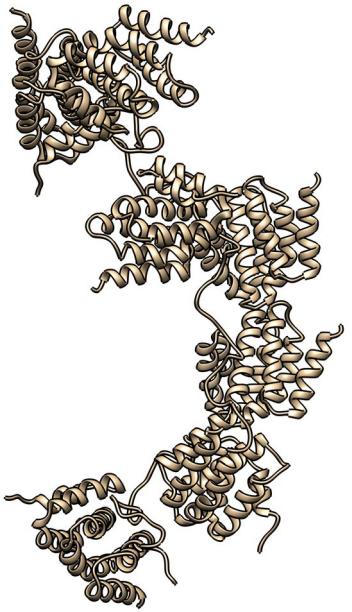

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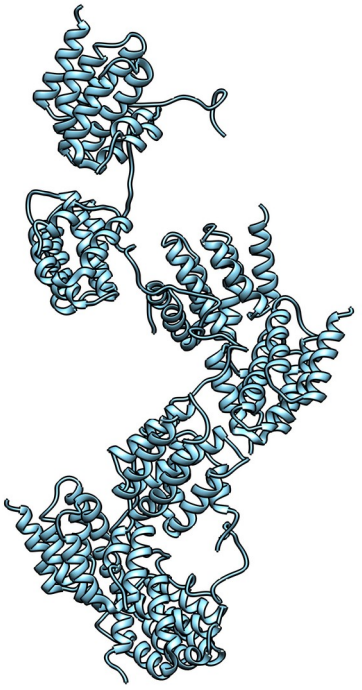
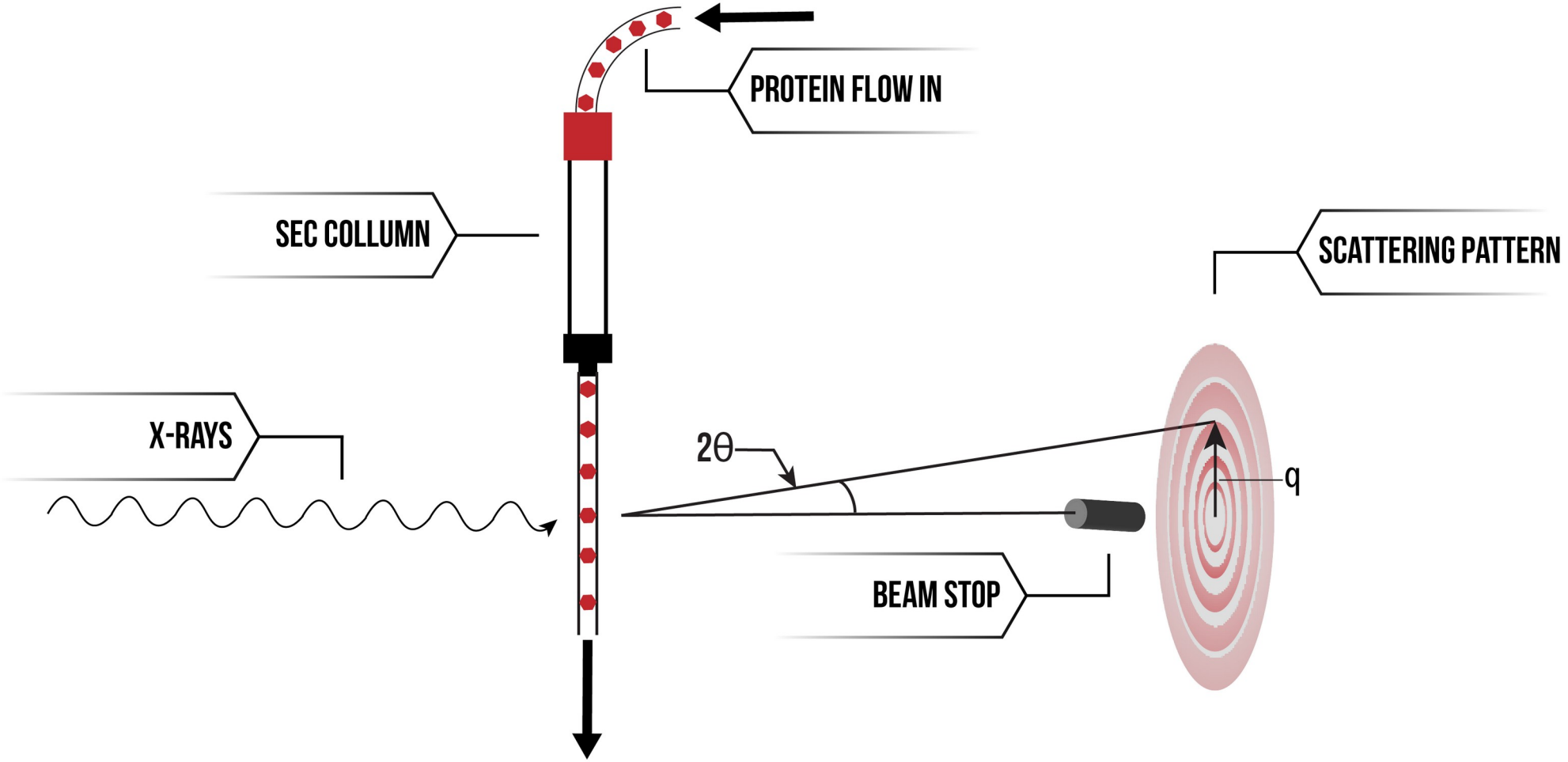
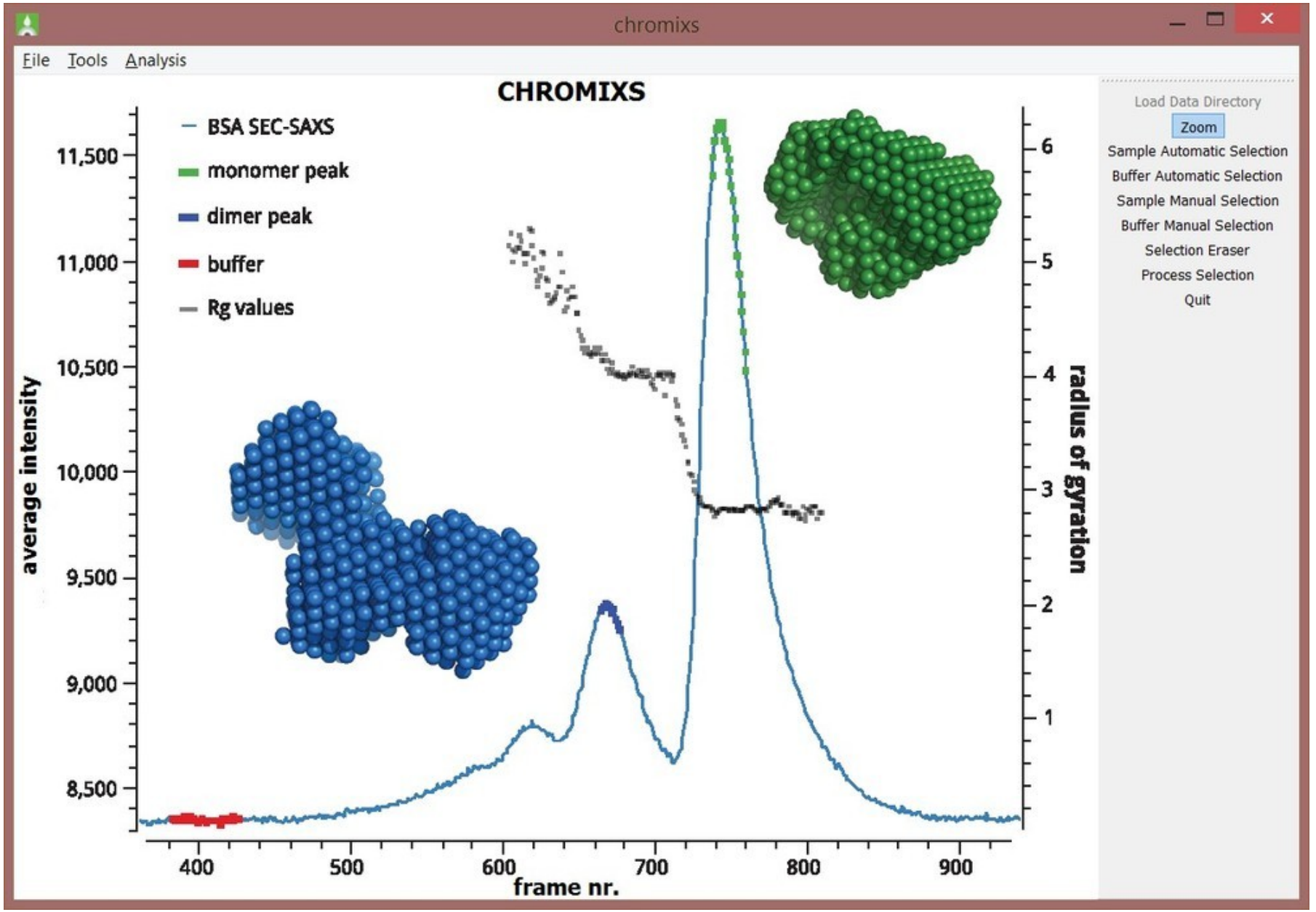


SEC–SAXS


PROTEIN FLOW IN
SEC COLLUMN
SCATTERING PATTERN
X-RAYS
2θ
q
BEAM STOP


chromixs
File
Tools
Analysis
CHROMIXS
BSA SEC-SAXS
monomer peak
dimer peak
buffer
Rg values
average intensity
radius of gyration
frame nr.
11,500
11,000
10,500
10,000
9,500
9,000
8,500
6
5
4
3
2
1
400
500
600
700
800
900
Load Data Directory
Zoom
Sample Automatic Selection
Buffer Automatic Selection
Sample Manual Selection
Buffer Manual Selection
Selection Eraser
Process Selection
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Contact us

Data analysis software ATSAS 2.8.0

A program suite for small-angle scattering data analysis from biological macromolecules

Data processing

PRIMUS - manipulations with experimental 1D SAS data
GNOM - indirect transform program that evaluates the particle distance distribution function p(r)
Data manipulation and analysis tools - AUTORG, ALMERGE, DATGNOM, DATPOROD etc.

Ab initio methods

DAMMIN - *ab initio* shape determination using a dummy atom model
DAMMIF - rapid shape determination
GASBOR - reconstruction of a protein structure by a chain-like ensemble of dummy residues
MONSA - shape determination using a multiphase dummy atom model

Rigid body modelling

SASREF - modelling of multisubunit complexes
BUNCH - modelling of multidomain proteins against multiple data sets
CORAL - modelling of multidomain protein complexes against multiple data sets
MASSHA - interactive modelling of atomic structures and shape analysis
GLOBSYMM - rigid body modelling of symmetric oligomers

Mixtures and flexible systems

OLIGOMER - volume fractions of mixtures with known scattering intensities from the components
MIXTURE - modelling of multicomponent systems
EOM - Ensemble Optimization Method for flexible proteins
SREFLEX - flexible refinement of high-resolution models combining SAXS and NMA

PDB oriented tools

CRYSOL - X-ray scattering patterns from known hi-res structures
CRYSON - neutron scattering patterns from known hi-res structures
SUPCOMB - superimposes one 3D structure onto another
DAMAVER - align *ab initio* models, select the most typical one

Manuals

If you use ATSAS please cite:

Petoukhov, M.V., Franke, D., Shkumatov, A.V., Tria, G., Kikhney, A.G., Gajda, M., Gorba, C., Mertens, H.D.T., Konarev, P.V. and Svergun, D.I. (2012)
New developments in the ATSAS program package for small-angle scattering data analysis

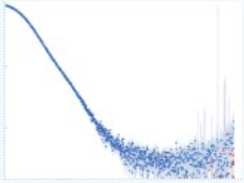
Curated repository for small angle scattering data and models

Small angle scattering (SAS) of X-ray and neutrons provides structural information on biological macromolecules in solution at a resolution of 1-2 nm.
SASBDB is a fully searchable curated repository of freely accessible and downloadable experimental data, which are deposited together with the relevant experimental conditions, sample details, derived models and their fits to the data.

SASBDB currently contains:
1262 experimental data sets
1892 models
428 experimental data sets on hold
565 models on hold

Recent depositions:

SASDGB6 – Resistance to inhibitors of cholinesterase 8 homolog A (Ric8A) miniGi complex



Sample: Resistance to inhibitors of cholinesterase 8 homolog A monomer, 56 kDa *Bos taurus* protein
MiniGi monomer, 25 kDa *synthetic construct* protein

Buffer: 20 mM Tris, 150 mM KCl, 5 % glycerol, 1 mM TCEP, pH: 8

Experiment: SAXS data collected at BioCAT 18ID, Advanced Photon Source (APS), Argonne National Laboratory on 2018 Oct 27

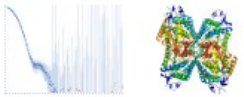
$R_g^{Guinier}$ 3.2 nm
D_{max} 10.7 nm

Large-scale conformational rearrangement of the α5-helix of Gα subunits in complex with the guanine nucleotide exchange factor Ric8A. *J Biol Chem* (2019)
Srivastava D, Artemyev NO

SASDG76 – Inhibitor of apopt

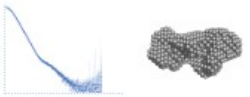
Flexible Tethering of ASPP Prot

SASDGJ4 – Human alpha-am



Structural Analysis of Pathogen

SASDFB6 – The periplasmica



Protease-associated import syst

SASDDR3 – Yeast tRNA Nm34

Structure of tRNA methyltransfe

SASDFL5 – Plasmodium falci

Structural studies of the Hsp70/

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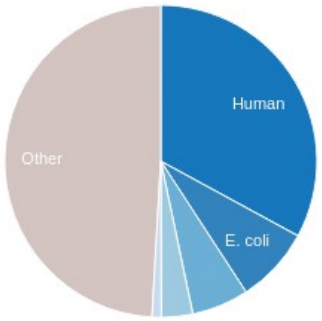
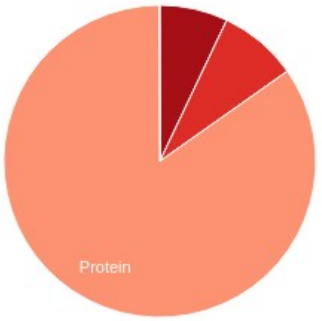
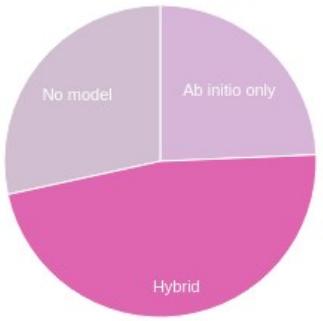


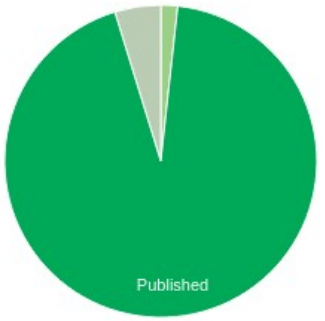
Organism



Macromolecule type



Model type



Dissemination type

To cite SASBDB refer to: Valentini E, Kikhney AG, Previtali G, Jeffries CM, Svergun DI. SASBDB, a repository for biological small-angle scattering data. Nucleic Acids Res. 2015 Jan 28;43:D357-63.

Combination of SAXS and Protein Painting Discloses the Three-Dimensional Organization of the Bacterial Cysteine Synthase Complex, a Potential Target for Enhancers of Antibiotic Action

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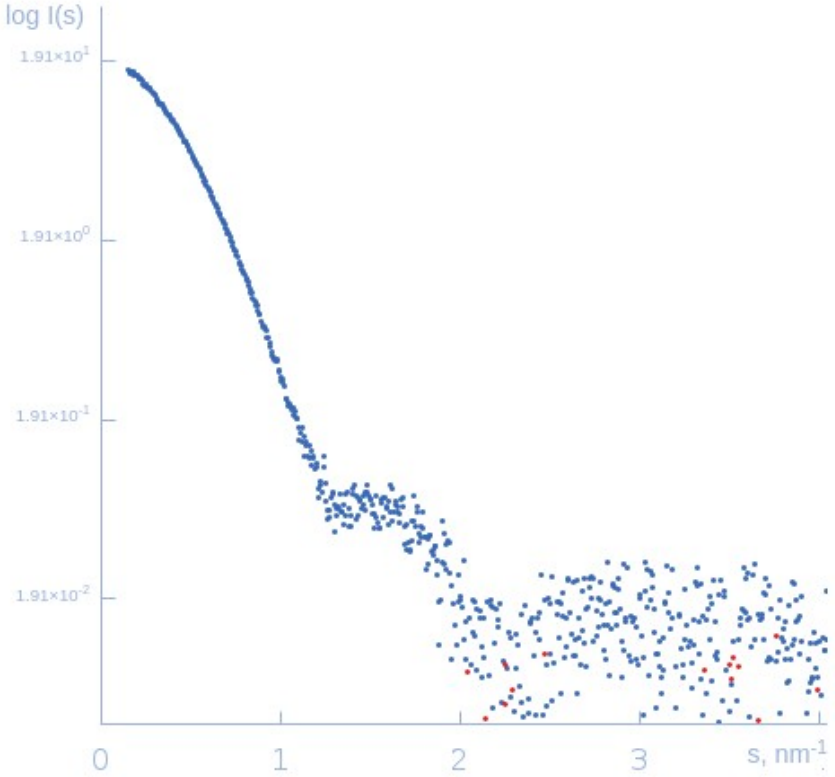
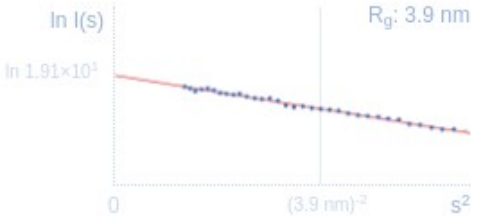
Rosa B, Marchetti M, Paredi G, **Amenitsch H**, Franko N, Benoni R, Giabbai B, De Marino M, Mozzarelli A, Ronda L, Storici P, Campanini B, Bettati S, *International Journal of Molecular Sciences* 20(20):5219 (2019) DOI

SASDGW6 – Serine acetyltransferase

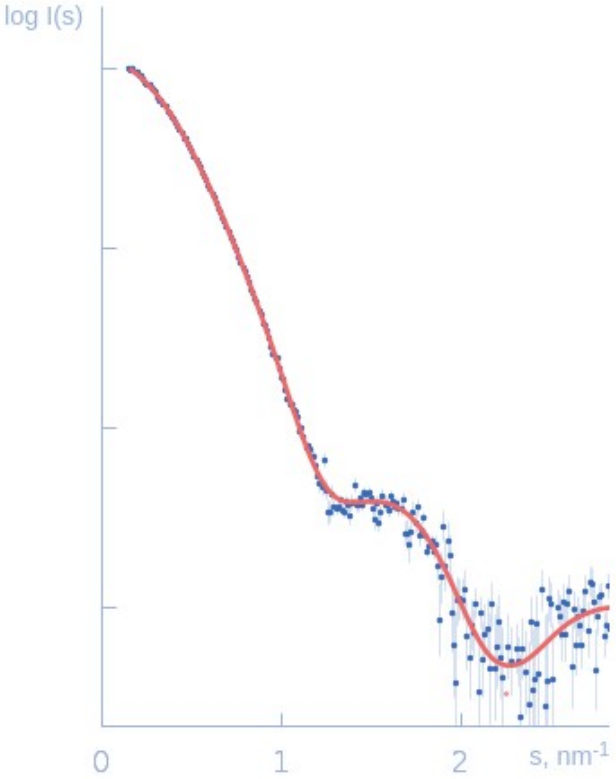
Serine acetyltransferase

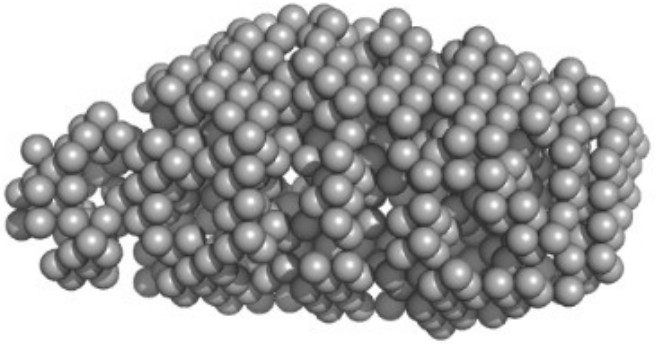


$MW^{experimental}$	189	kDa
$MW^{expected}$	177	kDa
V^{Porod}	280	nm^3



Fits and models





Synchrotron SAXS data from solutions of serine acetyltransferase in 20 mM sodium phosphate, 85 mM NaCl, 2 mM EDTA, 10 mM 2-MCE, pH 7.5 were collected on the Austrian SAXS beamline 5.2L beam line at the ELETTRA - Sincrotrone Trieste storage ring (Trieste, Italy) using a Dectris / Pilatus3 1M detector at a wavelength of λ = 0.154 nm (I(s) vs s, where s = 4πsinθ/λ, and 2θ is the scattering angle). Solute concentrations ranging between 0.5 and 1.5 mg/ml were measured at 20°C. 12 successive 10 second frames were collected. The data were normalized to the intensity of the transmitted beam and radially averaged; the scattering of the solvent-blank was subtracted. The low angle data collected at lower concentration were merged with the highest concentration high angle data to yield the final composite scattering curve.

Serine acetyltransferase (CysE)

Mol. type	Protein
Organism	*Escherichia coli K-12*
Olig. state	Hexamer
Mon. MW	29.4 kDa

UniProt	P0A9D4 (2-273)
Sequence	FASTA

Structure and dynamics of the RNAPII CTDsome with Rtt103.
Jasnovidova O, **Klumpler T**, Kubicek K, Kalynych S, Plevka P, Stefl R, *Proc Natl Acad Sci U S A* 114(42):11133-11138 (2017) Europe PMC

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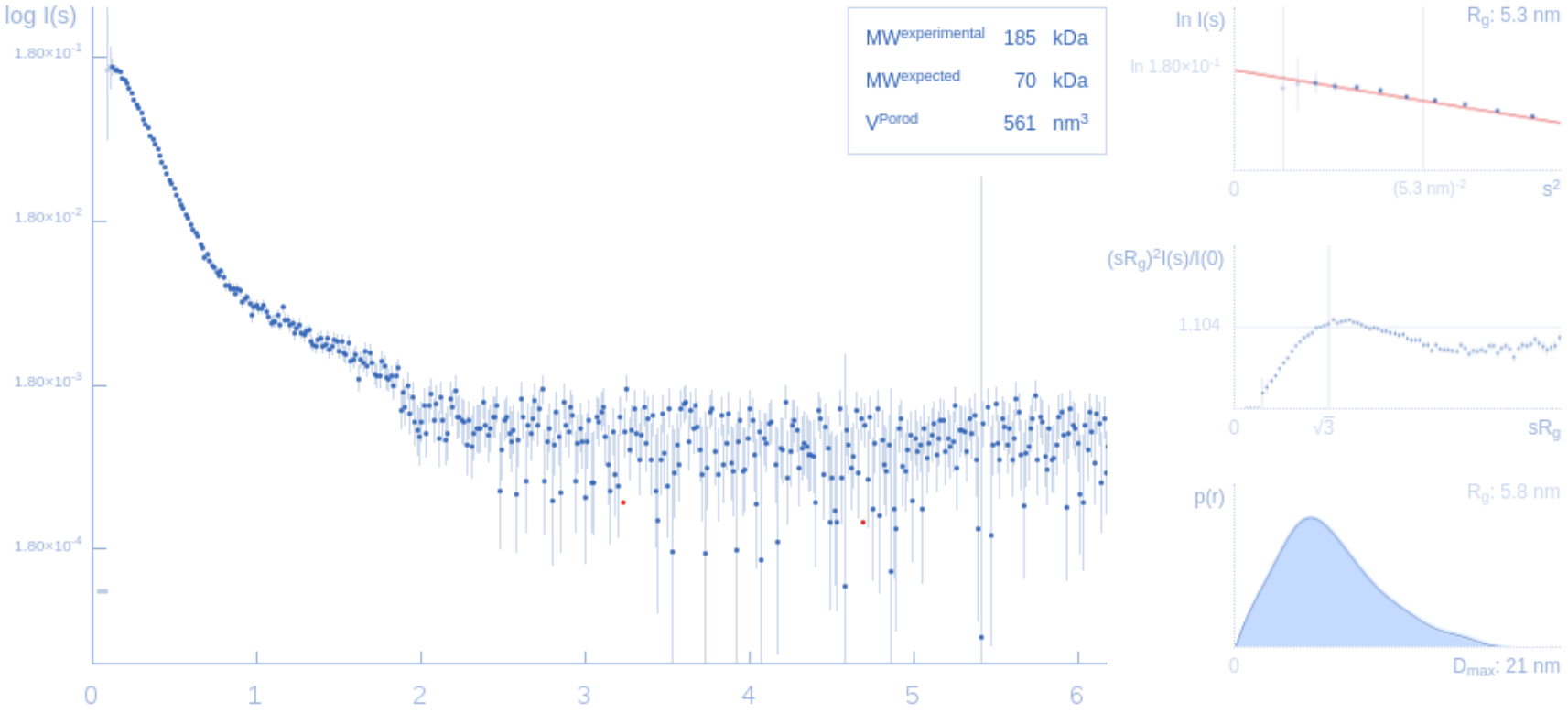
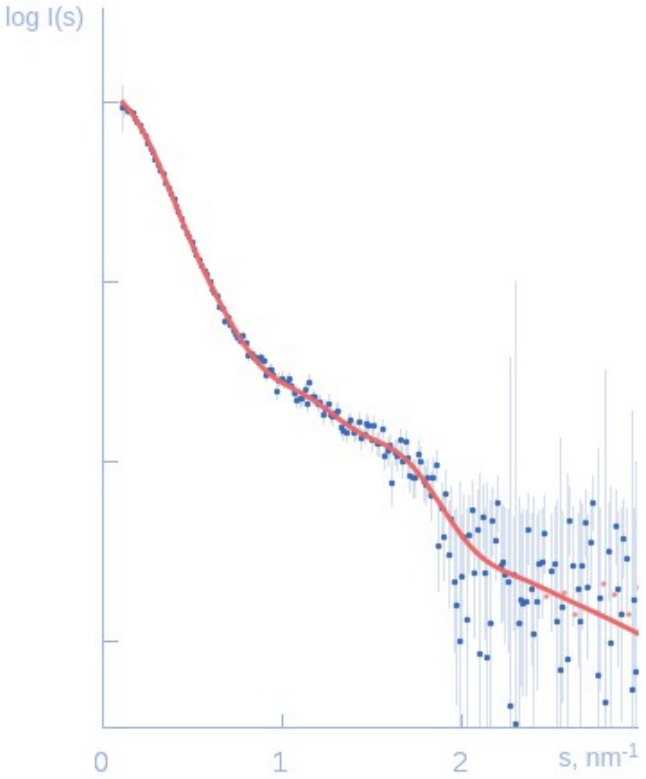
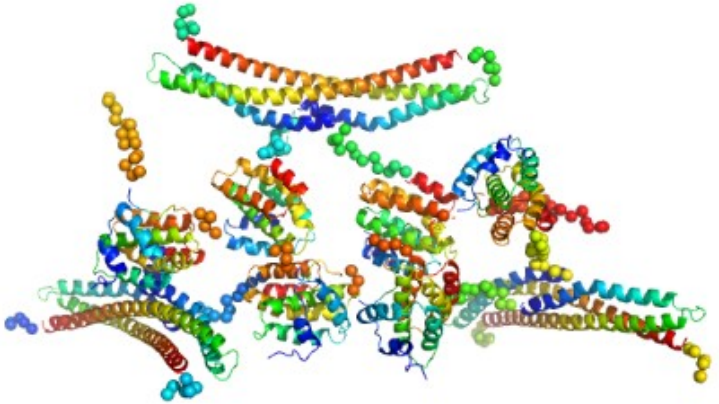
SASDCZ2 – Yeast CTDsome: transcription termination factor Rtt103p/C-terminal domain of DNA-directed RNA polymerase II subunit RPB1 (Rtt103 1-246-phospho-mimetic complex)

Regulator of Ty1 transposition protein 103
DNA-directed RNA polymerase II subunit RPB1







SAXS data from solutions of Rtt103 1-246-phospho-mimetic complex in 25 mM KH2PO4, 300 mM KCl, 10 mM β-mercaptoethanol, pH 6.5 were collected using a BioSAXS-1000 instrument at CEITEC (Brno, Czech Republic) equipped with a Pilatus 100K detector at a sample-detector distance of 0.5 m and at a wavelength of λ = 0.154 nm (I(s) vs s, where s = 4πsinθ/λ and 2θ is the scattering angle). Five successive 3600 second frames were collected at a sample temperature of 4°C. The data were normalized to the intensity of the transmitted beam and radially averaged and the corresponding scattering from the solvent-blank was subtracted to produce the scattering profile displayed in this entry.

Regulator of Ty1 transposition protein 103

Mol. type	Protein
Organism	*Saccharomyces cerevisiae (strain ATCC 204508 / S288c)*
Olig. state	Dimer
Mon. MW	28.6 kDa

bioSAXS – summary

With good quality SAXS data:

1. model independent:	**integral structural parameters: Rg, Dmax, Vporod**
	agregation, folding/flexibility
	overal shape *ab initio*
2. model dependent:	**validation of molecular structures (XRD, NMR, molecular dynamics, docking)**
	oligomeric state, mixtures
	quaternary structere
	missing parts in XRD structures
	study of flexible systems