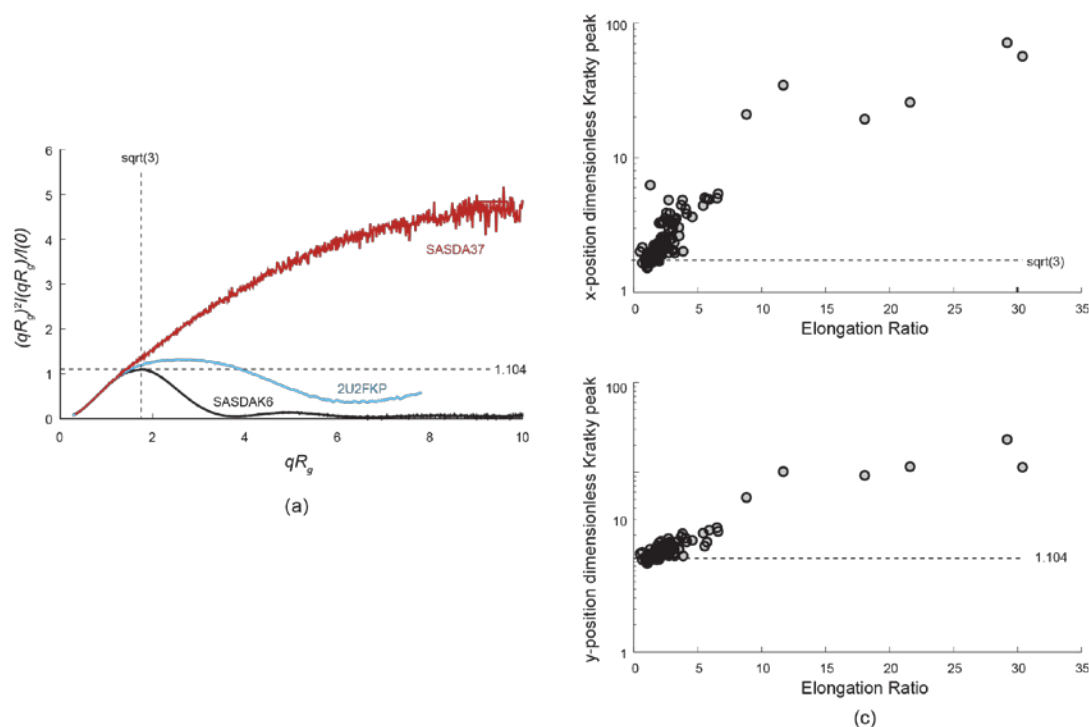JOURNAL OF
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Supporting information for article:

Guinier Peak Analysis for Visual and Automated Inspection of Small Angle X-ray Scattering Data

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Supplementary Figure 1. The ER value correlates with the peak position in dimensionless Kratky plots. (a) The dimensionless Kratky plot (Durand *et al.*, 2010; Receveur-Brechot & Durand, 2012) has a peak at *(sqrt(3), 1.104)* for compact, symmetric scatterers, such as SASDAK6 (*Streptomyces rubiginosus* xylose isomerase). Deviations from this position indicate either flexibility or asymmetry, such as with 2U2FKP (human U2AF65 RRM1-RRM3). Extended scatterers, such as SASDA37 (*Staphlococcus aureus* surface protein G, SasG construct containing repeats G51-G52), do not have a peak. Datasets are from the BIOSIS and SASBDB databases. **(b)** The x-positions of dimensionless Kratky peaks calculated for datasets in the BIOISIS and SASBDB databases were near the theoretical value (dashed line) for symmetric particles (ER near 1) and increased as the ER value increased. **(c)** Similar trends are observed for the y-positions of dimensionless Kratky peaks calculated for the datasets in BIOISIS and SASBDB.
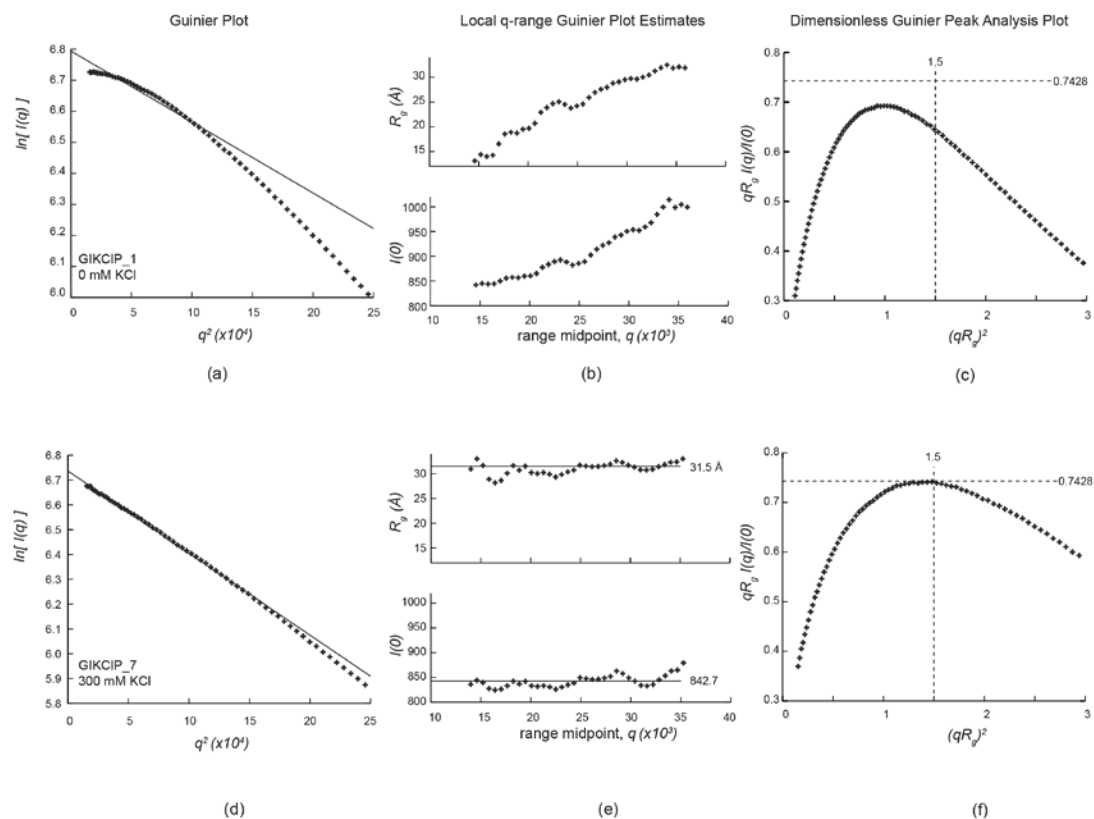
Supplementary Figure 2. Glucose isomerase data with interparticle repulsion was an outlier in the dimensionless GPA plots. Scattering data from *Streptomyces rubiginesis* glucose isomerase (BIOISIS dataset GIKCIP) contains data collected at 0 mM KCl (panels a-c) and at 300 mM KCl (panels d-f). **(a)** At low salt, the scattering showed evidence of interparticle repulsion due to the concave-down behaviour of the scattering in the Guinier plot. **(b)** Estimates of R_g and $I(0)$ based on local q-ranges containing six adjacent points within the Guinier region showed a continuous increase in R_g and $I(0)$ as the center of the q-range considered increased. **(c)** The Guinier peak in the dimensionless GPA plot was an outlier for the 0 mM KCl data. **(d)** At high salt, glucose isomerase had a linear Guinier region. **(e)** Local q-range estimates of R_g and $I(0)$ from the Guinier plot were consistent with each other and the global fit for the high salt data. **(f)** The dimensionless GPA plot revealed that the peak for the high salt data was very near to the theoretical position.
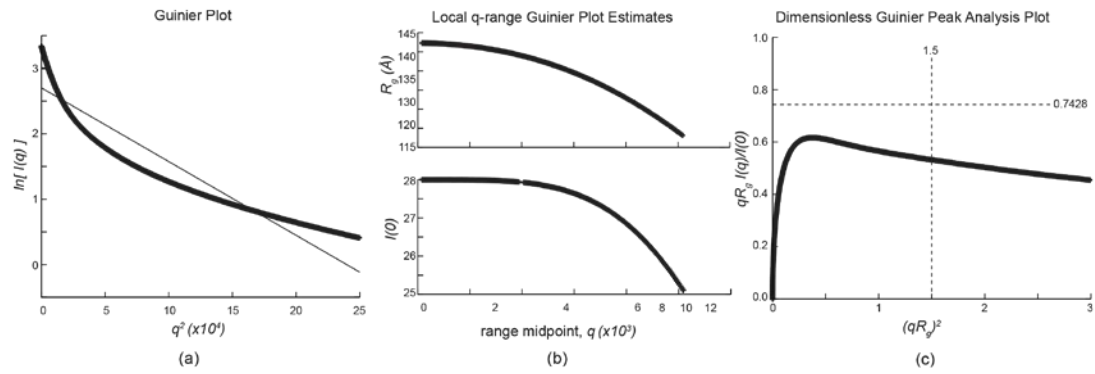
Supplementary Figure 3. Scattering from a continuous distribution of spheres was an outlier in the dimensionless GPA plot. **(a)** The Guinier plot of a calculated scattering continuous distribution of spheres of radii from 30 Å to 300 Å (R_g 23.6 Å to 236 Å) revealed a concave upward distribution in the Guinier plot. **(b)** Estimates of R_g and $I(0)$ using 6 point q-ranges within the Guinier region decreased as the midpoint of the q-range increased. **(c)** The Guinier peak was a clear outlier in the dimensionless GPA plot.
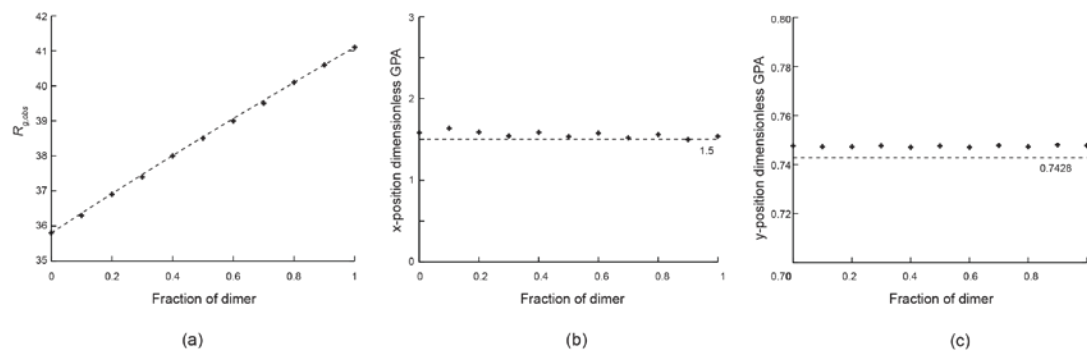
Supplementary Figure 4. Scattering from theoretical mixtures of monomers and dimers were not outliers in dimensionless GPA plots. (a) Theoretical mixtures of monomers and dimers calculated from the structure of *Thermus aquaticus* MutS (PDBid 1fw6, (Junop *et al.*, 2001)) using CRYSOL (Petoukhov *et al.*, 2012) give observed R_g values (crosses) that z-averages of the monomer and dimer R_g values. **(b)** The x-position of the Guinier peak in dimensionless GPA was insensitive to the dimer fraction. **(c)** The y-position of the Guinier peak in dimensionless GPA was insensitive to the dimer fraction.

Guinier Plot

Dimensionless Guinier Peak Analysis Plot

(a)

(b)

(c)

(d)
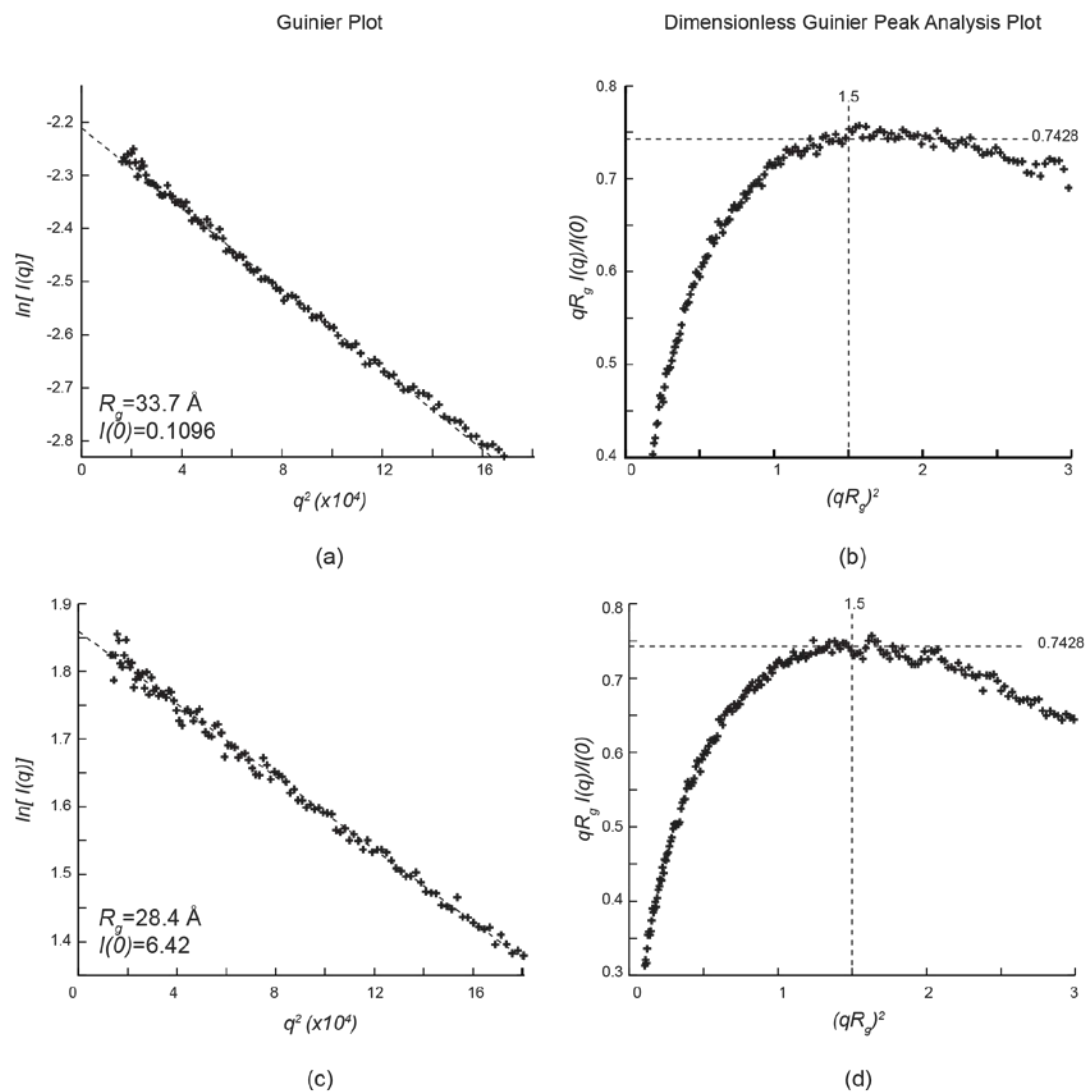
Supplementary Figure 5. Scattering from bovine serum albumin (BSA) containing aggregation was not flagged as an outlier in GPA analysis. BSA containing some aggregates (panels a and b) and BSA purified by size-exclusion chromatography (panels c and d) were analysed by SAXS. **(a)** The aggregated BSA had a linear Guinier region in the Guinier plot with an R_g=33.7 Å. **(b)** The Guinier peak in dimensionless GPA analysis was near the theoretical position. **(c)** BSA which had aggregates removed by size-exclusion chromatography also had a linear Guinier region with a lower R_g=28.4 Å. **(d)** The Guinier peak for the size-selected BSA was also near the theoretical position.
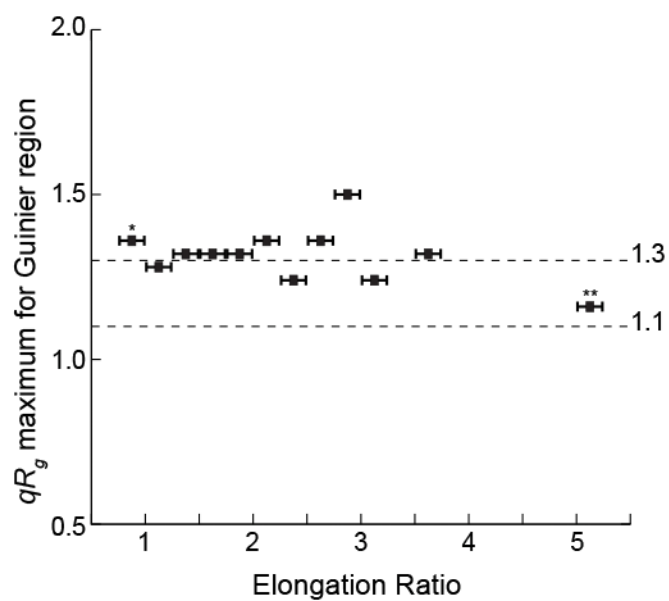
Supplementary Figure 6. Maximum qR_g range for the Guinier approximation as a function of ER. After binning datasets based on the ER, the qR_g maximum where the Guinier approximation held was determined (Supplementary Figures 2-4). The standard "rule-of-thumb" maxima of 1.3 (for globular scatterers) and 1.1 (for extended scatterers) are shown as dashed lines. The value shown in the 0.75-1.0 bind correspond to all datasets with ER values less than 1 (asterisk), and the value shown in the 5.0-5.25 bin correspond to all datasets with ER values greater than 5 (double asterisk).

Supplementary Table 1. List of scattering curves from database sources and parameters (Excel spreadsheet).

Cluster	Sample	Database	Rg, Angstroms (reported)	I(0) (reported)	Dmax, Angstroms (reported)	Fixed Rg/I(0)	Rg, Angstroms (used)	I(0) (used)	Peak (qRg)**2	Peak qRgI(q)/I(0)	Elongation Ratio	Guinier Peak Outlier	Notes
1	SASDA82	SASBDB	67.5	356	128.0	No	67.5	356	1.6625	0.742652	0.4935	No	
1	SASDAQ5	SASBDB	61.8	580240	155.0	Yes (0.84, 0.81)	86.4	884000	1.6440	0.744834	0.6739	No	
2	MNME2P	BIOISIS	37.2	39.8	138.0	Yes (1.54, 0.000005)	39.4	0.000264	1.7248	0.756392	1.1433	No	
2	APSODP	BIOISIS	20.5	20.5	65.0	Yes (1.24, 15.7)	20.7	438.1	1.2658	0.739752	1.3371	No	
2	SASDAL2	SASBDB	25.0	37	78.0	No	25.0	37	1.774051	0.761184	1.3639	Yes	
2	SASDB52	SASBDB	27.0	795	810.0	No	27.0	795	1.6987	0.753837	1.6106	No	
2	SASDB72	SASBDB	24.0	623	750.0	No	24.0	623	1.4314	0.768532	1.3982	Yes	Noisy high-resolution data required truncation before Guinier Peak Analysis
2	SASDAA8	SASBDB	18.7	87.52	50.0	No	18.7	87.52	1.3154	0.743641	1.1519	No	
2	SASDA78	SASBDB	20.6	119.52	60.0	No	20.6	119.52	1.6685	0.746632	1.2167	No	
2	SASDA92	SASBDB	41.0	222	109.0	No	41.0	222	1.6869	0.738675	1.2276	No	
2	SASDAQ2	SASBDB	13.6	7.41	49.0	No	13.6	7.41	1.5596	0.738478	1.2102	No	
2	LYSOZP_1	BIOISIS	15.6	57	49.0	No	15.6	57	1.5091	0.749424	1.1461	No	
2	1NADHP	BIOISIS	23.1	701	96.0	No	23.1	701	1.5919	0.748508	1.3288	No	
2	MRERAP	BIOISIS	41.6	9.5	130.0	No	41.6	9.5	1.631885	0.749555	1.0517	No	
2	HRCC1P_1	BIOISIS	25.1	61.2	80.0	No	25.1	61.2	1.624485	0.740717	1.3354	No	
2	1XYNTP_1	BIOISIS	16.7	133	43.0	No	16.7	133	1.4799	0.736812	1.1242	No	

2	SASDAX2	SASBDB	39.0	10.2	110.0	No	39.0	10.2	1.4133	0.742768	1.0252	No	
2	SASDAK6	SASBDB	34.0	165.24	97.4	No	34.0	165.24	1.5255	0.741098	1.0918	No	
2	1TSPHP	BIOISIS	16.7	4039	58.0	No	16.7	4039	1.6113	0.74614	1.2401	No	
2	AT5GHP	BIOISIS	21.2	0.03	74.0	No Yes (1.38, 0.78)	21.7	0.0325	1.4458	0.736922	1.4249	No	Evidence of intermolecular repulsion
2	SASDAX6	SASBDB	15.3	14.8	50.0	No	15.3	14.8	1.509618	0.743307	1.3696	No	
2	1PORHP	BIOISIS	37.3	1102	133.0	No	37.3	1102	1.4696	0.744158	1.2948	No	
2	SASDA96	SASBDB	15.0	779.5	47.9	No	15.0	779.5	1.4307	0.743226	1.1778	No	
2	SASDA52	SASBDB	31.6	76.55	89.3	No	31.6	76.55	1.4812	0.742807	1.0545	No	
2	SASDAU4	SASBDB	22.0	36.7	70.0	Yes (1.38, 0.72)	22.0	36.7	1.537475	0.741475	1.0642	No	
2	1RBDGP	BIOISIS	11.0	1404	29.0	Yes (1.46, 0.77)	10.4	1410	1.304	0.729319	1.0726	No	Sample defeated automated heuristic for identifying Guinier peak position
2	SASDA97	SASBDB	39.5	1380.54	105.0	No	39.5	1380.54	1.3831	0.738385	0.9115	No	
2	SASDAK4	SASBDB	36.1	1.658	100.0	No	36.1	1.658	1.5056	0.743784	1.2265	No	
2	1PYR1P_1	BIOISIS	22.7	38.1	68.0	No	22.7	38.1	1.4616	0.739404	1.2397	No	
2	SASDAA6	SASBDB	28.0	521.4	84.2	No	28.0	521.4	1.4738	0.742526	1.3094	No	
2	SASDAH2	SASBDB	16.5	10.7	50.0	No	16.5	10.7	1.4169	0.743769	1.3646	No	
2	SASDAK2	SASBDB	16.4	10.6	50.0	No	16.4	10.6	1.3998	0.746175	1.1607	No	
2	SASDAC2	SASBDB	14.7	12.4	40.0	No	14.7	12.4	1.3949	0.745069	0.9952	No	
2	SASDAG2	SASBDB	14.5	12.29	40.0	No	14.5	12.29	1.3572	0.741611	1.0575	No	
2	BASODP	BIOISIS	14.6	50	43.0	No	14.6	50	1.3631	0.756417	1.0705	No	
2	1GINTP_1	BIOISIS	33.4	372	96.0	No	33.4	372	1.4571	0.741787	1.1056	No	
2	SASDAB2	SASBDB	13.0	7.46	35.0	No	13.0	7.46	1.433555	0.74042	0.9509	No	
2	1SPXGP	BIOISIS	22.1	4540.2	80.0	No	22.1	4540.2	1.4470	0.733447	0.9587	No	
2	SASDAB6	SASBDB	32.1	3733.8	91.0	No	32.1	3733.8	1.4682	0.741553	0.9947	No	
2	2SAMRR_1	BIOISIS	22.9	138	76.0	No	22.9	138	1.4835	0.748462	1.5118	No	
2	SASDA35	SASBDB	25.0	45.524	85.0	No	25.0	45.524	1.625724	0.745803	1.7104	No	

2	SASDAN3	SASBDB	47.0	10500	155.0	Yes (1.84, 0.78)	43.6	10300	1.5790	0.741906	1.4125	No	Noisy high-resolution data required truncation before Guinier Peak Analysis
2	1TLSRR	BIOISIS	30.9	244	108.0	No	30.9	244	1.5149	0.743021	1.2330	No	
2	SPNexP	BIOISIS	36.1	212	123.0	Yes (1.49, 0.76)	35.2	216	1.4113	0.729042	1.2791	No	
2	SASDAR6	SASBDB	56.7	188.32	179.0	No	56.7	188.32	1.6712	0.743945	1.4737	No	
2	SS30SX	BIOISIS	69.7	17800	231.0	No	69.7	17800	1.4594	0.741264	1.8138	No	
2	SASDAS5	SASBDB	26.0	1032000	80.0	No	26.0	1032000	1.3068	0.729728	1.3970	No	Sample defeated automated heuristic for identifying Guinier peak position
2	NTNH6P	BIOISIS	39.5	1719.5	131.0	No	39.5	1719.5	1.4119	0.742183	1.5207	No	
2	SASDAB7	SASBDB	33.7	0.05529	107.0	No	33.7	0.05529	1.4972	0.737327	1.2548	No	
2	NTNH8P	BIOISIS	39.7	1717.6	127.0	No	39.7	1717.6	1.5158	0.744404	1.6670	No	
2	SASDA45	SASBDB	54.0	26.8	1650.0	No	54.0	26.8	1.5895	0.746588	1.6478	No	
2	MNME3P	BIOISIS	37.4	691	136.0	No	37.4	691	1.4773	0.729075	1.0902	No	
2	MNME1P	BIOISIS	38.6	39.8	139.0	No	38.6	39.8	1.5619	0.744014	1.0414	No	Sample defeated automated heuristic for identifying Guinier peak position
2	SASDAV3	SASBDB	29.0	150.448	100.0	No	29.0	150.448	1.6353	0.747757	1.5035	No	
2	ST2ILP	BIOISIS	28.9	226	100.0	No	28.9	226	1.4865	0.742256	1.9956	No	
2	SASDAC9	SASBDB	38.7	4298	164.0	No	38.7	4298	1.4691	0.742514	1.4479	No	
2	SASDA32	SASBDB	29.2	59.3	93.0	No	29.2	59.3	1.4894	0.747321	1.2568	No	
2	SASDA68	SASBDB	36.4	389.27	105.0	No	36.4	389.27	1.586519	0.745135	1.2416	No	
2	SASDAM4	SASBDB	43.0	113	150.0	No	43.0	113	1.5124	0.748305	1.0723	No	
2	SASDA62	SASBDB	42.1	164.38	127.0	No	42.1	164.38	1.3748	0.740794	1.0540	No	
2	SASDAR5	SASBDB	26.0	123	80.0	No	26.0	123	1.4458	0.754706	1.3669	No	
2	SASDAX4	SASBDB	28.0	62.3	94.0	No	28.0	62.3	1.448187	0.740658	1.3543	No	
2	SASDA55	SASBDB	39.9	0.501	126.0	No	39.9	0.501	1.3056	0.729798	1.3970	No	
2	SASDAL4	SASBDB	41.4	1.771	140.0	No	41.4	1.771	1.623549	0.742397	1.1181	No	

2	SASDB62	SASBDB	25.0	717	900.0	No	25.0	717	1.3474	0.732413	1.5992	No	Noisy high-resolution data required truncation before Guinier Peak Analysis
2	SASDAS3	SASBDB	19.2	41.5	60.0	No	19.2	41.5	1.512319	0.740467	1.4656	No	
2	SASDAN2	SASBDB	15.8	13.5	50.0	No	15.8	13.5	1.4931	0.742121	1.2934	No	
2	SASDAR2	SASBDB	16.0	13.65	50.0	No	16.0	13.65	1.5311	0.743298	1.4384	No	
2	SASDA75	SASBDB	47.0	0.471	145.0	No	47.0	0.471	1.457558	0.731574	1.1232	No	
2	2HYPOP	BIOISIS	35.6	92.58	110.0	No	35.6	92.58	1.4962	0.739943	1.5482	No	
2	ZGDWKP	BIOISIS	29.5	2.274	79.0	No	29.5	2.274	1.5540	0.746958	1.8074	No	
2	GIKClP_1	BIOISIS	26.6	892.7	97.0	No	26.6	892.7	0.9895	0.69315	1.0567	**Yes**	Intermolecular repulsion
2	GNaClP_1	BIOISIS	26.4	908.3	97.0	No	26.4	908.3	1.006675	0.693971	1.0567	**Yes**	Intermolecular repulsion
2	LNaClP_1	BIOISIS	13.2	53.5	48.0	No	13.2	53.5	1.228378	0.707721	1.1461	**Yes**	Intermolecular repulsion
2	LYKClP_1	BIOISIS	13.2	51.1	49.0	No	13.2	51.1	1.271802	0.708862	1.1461	**Yes**	Intermolecular repulsion
2	SASDAD5	SASBDB	85.5	4070	280.0	No	85.5	4070	1.4180	0.752408	0.8695	No	
2	SASDAJ6	SASBDB	52.0	144	170.0	No Yes (1.51, 0.72)	52.3	140	1.5262	0.748841	0.9162	No	
2	SASDAJ4	SASBDB	38.0	1.15	110.0	No	38.0	1.15	1.4501	0.73496	0.6721	No	
2	SASDAF4	SASBDB	36.0	91.2	120.0	No	36.0	91.2	1.5089	0.744933	1.9862	No	
3	1ASRDP	BIOISIS	19.2	61.94	80.0	No	19.2	61.94	1.694879	0.737418	1.4880	No	
3	SASDA58	SASBDB	26.2	2964	106.0	No	26.2	2964	1.537948	0.746376	1.7406	No	
3	1FERHP	BIOISIS	30.9	1233	101.0	No	30.9	1233	1.663098	0.743909	1.9735	No	Noisy data in the Guinier region ~qRg = 1.5
3	MnmG1P	BIOISIS	42.3	0	139.0	No Yes (n/a, n/a)	42.2	0.000193	1.4025	0.739381	1.7649	No	
3	SASDA27	SASBDB	35.1	156.8	119.3	No	35.1	156.8	1.6464	0.757837	1.4804	No	
3	SASDAV6	SASBDB	32.0	68	109.0	No	32.0	68	1.5754	0.760273	1.7272	No	
3	SASDAG5	SASBDB	32.0	130	112.0	No Yes (1.63, 0.77)	31.8	133	1.6102	0.743314	1.5913	No	
3	SASDAZ6	SASBDB	31.1	88.44	108.7	No	31.1	88.44	1.5701	0.747027	1.5744	No	
3	SASDAD8	SASBDB	26.4	0.188	111.0	No	26.4	0.188	1.6453	0.746845	1.8524	No	

3	SASDAJ5	SASBDB	24.0	40.26	76.0	No	24.0	40.26	1.4521	0.740452	1.4325	No	Noisy low-resolution data requiring truncation
3	SASDAV4	SASBDB	25.0	39.2	85.0	No	25.0	39.2	1.5098	0.73028	1.5523	No	Noisy low-resolution data requiring truncation
3	SASDAW4	SASBDB	24.0	44.9	83.0	No	24.0	44.9	1.5961	0.75296	1.3260	No	
3	SASDAA2	SASBDB	37.8	82.8	110.0	No	37.8	82.8	1.913996	0.739959	1.5669	No	
3	SASDA98	SASBDB	78.6	2510.92	240.0	No	78.6	2510.92	1.6469	0.743533	1.6469	No	
3	SASDAQ4	SASBDB	58.5	87600	230.0	No	58.5	87600	1.7095	0.744691	1.6145	No	
3	SASDA72	SASBDB	32.4	93.43	144.0	No	32.4	93.43	1.6926	0.750993	1.6307	No	
3	SASDAW6	SASBDB	18.7	17.2	64.0	No Yes (1.73, 0.77)	18.3	17.2	1.6614	0.751258	1.9022	No	
3	SASDAN5	SASBDB	21.4	5.2	85.0	Yes (1.43, 0.70)	23.6	5.26	1.7427	0.764818	2.4577	**Yes**	
3	SASDAD4	SASBDB	51.0	280	190.0	No	51.0	280	1.567348	0.772554	1.7253	**Yes**	Sample defeated automated heuristic for identifying Guinier peak position
3	SASDAR3	SASBDB	22.7	16.7	77.0	No	22.7	16.7	1.8747	0.7608	1.7470	No	
3	SASDAZ5	SASBDB	39.0	3638	135.0	No	39.0	3638	1.529431	0.761691	2.1253	**Yes**	Sample defeated automated heuristic for identifying Guinier peak position
3	MnmG2X	BIOISIS	45.3	41	158.0	No	45.3	41	1.8292	0.755605	2.3114	No	
3	SASDAA5	SASBDB	40.0	45.63	145.0	No	40.0	45.63	1.65288	0.773147	2.4053	**Yes**	
3	SASDAV5	SASBDB	40.0	45.31	135.0	No	40.0	45.31	1.913541	0.768707	2.0589	**Yes**	Noisy high-resolution data required truncation before Guinier Peak Analysis
3	RPADCP	BIOISIS	38.8	327.39	171.0	No	38.8	327.39	1.8405	0.751463	2.2612	No	
3	SASDAW3	SASBDB	38.0	211.49	140.0	No	38.0	211.49	1.7140	0.740194	1.9017	No	
3	1TPHER	BIOISIS	24.3	71.2	98.0	No	24.3	71.2	1.7104	0.758461	2.2193	No	
3	SASDA85	SASBDB	49.0	109.38	174.0	No	49.0	109.38	1.538108	0.733432	2.0958	No	
3	SASDAY5	SASBDB	33.0	71.09	135.0	No	33.0	71.09	1.495454	0.740075	2.6408	No	
3	1ATPHP	BIOISIS	80.0	983	300.0	No	80.0	983	1.5344	0.733233	2.0318	No	
3	SASDAC5	SASBDB	56.5	80	190.0	No Yes (1.60, 0.77)	54.3	80.3	1.4817	0.741018	2.1704	No	Noisy high-resolution data required truncation before Guinier Peak Analysis
3	SASDAL5	SASBDB	33.0	45.6	106.0	No	33.0	45.6	1.562542	0.751594	2.4225	No	
3	2TIAKP	BIOISIS	30.3	1.48	100.0	No	30.3	1.48	1.6884	0.764981	2.9826	**Yes**	

3	SASDAF5	SASBDB	41.0	88	144.0	No	41.0	88	1.7961	0.741403	2.3297	No	
3	1SF1KP	BIOISIS	30.2	120.3	105.0	No	30.2	120.3	1.5827	0.737833	2.0182	No	
3	SASDAY4	SASBDB	30.0	1.62	104.0	No	30.0	1.62	1.6256	0.753509	3.1643	No	
3	1TIAKP	BIOISIS	27.2	172	100.0	No	27.2	172	1.2838	0.737583	3.2107	No	
3	SASDAC4	SASBDB	35.0	122	130.0	Yes (1.83, 0.77)	32.5	117	1.5778	0.744143	2.4545	No	
3	SASDA25	SASBDB	20.0	0.194	71.0	Yes (1.48, 0.77)	20.4	0.197	1.5435	0.77381	2.8271	**Yes**	
3	2TM1KP	BIOISIS	29.6	3.52	100.0	No	29.6	3.52	1.6468	0.746663	3.1378	No	
3	1U2FKP	BIOISIS	31.4	1001	115.0	Yes (1.42, 0.14)	31.3	192.6	1.4153	0.743583	3.5279	No	
3	SASDAR4	SASBDB	39.7	206	165.0	No	39.7	206	1.6185	0.746448	3.1685	No	
3	6HYPHP	BIOISIS	58.2	1102.5	280.0	No	58.2	1102.5	1.7616	0.758572	2.9934	No	
3	2U2FKP	BIOISIS	24.6	196.2	85.0	No	24.6	196.2	1.6360	0.745241	2.4572	No	
3	SASDAU3	SASBDB	27.6	34.3	90.0	No	27.6	34.3	1.987162	0.772487	2.5508	**Yes**	Possible aggregation
3	SASDA46	SASBDB	30.0	1800	100.0	No	30.0	1800	2.0888	0.755409	2.8290	**Yes**	
3	SASDAC7	SASBDB	35.5	0.02362	125.0	No	35.5	0.02362	1.7941	0.752962	2.1771	No	
3	SASDAA7	SASBDB	39.8	0.07466	160.0	Yes (1.70, 0.76)	39.6	0.0744	1.6786	0.761283	1.6314	**Yes**	
3	SASDA95	SASBDB	40.0	71.4	145.0	No	40.0	71.4	1.5696	0.746533	1.6264	No	
3	SASDAY6	SASBDB	35.8	112.4	121.4	No	35.8	112.4	1.7378	0.762116	1.9850	**Yes**	
3	SASDAH5	SASBDB	43.0	58	145.0	No	43.0	58	1.7202	0.75699	1.6866	No	
3	SASDAT4	SASBDB	28.0	49.3	97.0	No	28.0	49.3	1.5965	0.756121	1.6818	No	
3	SASDAW5	SASBDB	35.0	78.3	115.0	No	35.0	78.3	1.7316	0.754853	2.0481	No	Noisy high-resolution data required truncation before Guinier Peak Analysis
3	SASDAG7	SASBDB	26.9	8235	94.0	No	26.9	8235	1.5557	0.744839	3.1415	No	
3	SASDAS4	SASBDB	28.5	43.3	107.0	Yes (1.32, 0.70)	30.4	43.17	1.587472	0.744794	2.0373	No	

3	SASDA84	SASBDB	22.5	170	80.0	Yes (1.67, 0.81)	20.5	171	1.6656	0.812158	1.7491	**Yes**	Sample defeated automated heuristic for identifying Guinier peak position
3	SASDAT5	SASBDB	31.0	1158700	120.0	Yes (1.86, 0.77)	29.2	1130000	1.6482	0.74266	2.5741	No	
3	2HYPHP	BIOISIS	17.1	35.27	60.0	Yes (1.96, 0.78)	15.4	33.3	1.5866	0.748622	1.4980	No	
3	5HYPHP	BIOISIS	28.4	0.74	99.0	Yes (2.19, 131)	24.6	113.05	1.6440	0.747264	1.7268	No	
3	1LYSRR	BIOISIS	30.5	183	108.0	No	30.5	183	1.661734	0.746091	1.6735	No	
3	1P4P6R_1	BIOISIS	29.6	379	110.0	No	29.6	379	1.5651	0.742906	1.5252	No	
3	SASDAH4	SASBDB	29.0	0.378	90.0	No	29.0	0.378	1.2824	0.754232	2.3587	No	
3	2PSUKX	BIOISIS	37.7	442.14	105.0	No	37.7	442.14	1.7411	0.75145	1.3032	No	
3	SASDA94	SASBDB	26.5	98.1	85.0	No	26.5	98.1	1.5187	0.740274	1.3136	No	
3	SASDAP5	SASBDB	29.0	11.3	95.0	No	29.0	11.3	1.4412	0.760932	3.8579	**Yes**	
3	SASDAG4	SASBDB	46.0	121	150.0	No	46.0	121	1.599853	0.75468	1.0529	No	
3	1TIAKX	BIOISIS	24.7	331	80.0	No	24.7	331	1.4621	0.742017	1.9811	No	
3	SASDAT6	SASBDB	22.0	590	70.0	No	22.0	590	1.6346	0.743326	1.7352	No	
3	SASDAE5	SASBDB	37.0	86.9	128.0	No	37.0	86.9	1.5121	0.753815	1.8257	No	
3	BoNT6P	BIOISIS	47.3	2513.6	153.0	Yes (1.86, 0.81)	43.6	2510	1.5820	0.74483	1.6448	No	
3	BoNT8P	BIOISIS	43.3	1009.3	150.0	No	43.3	1009.3	1.4613	0.743991	1.6984	No	
3	C3bE2P	BIOISIS	48.2	155	180.0	No	48.2	155	1.553172	0.739958	1.3834	No	
3	C3bEfP	BIOISIS	48.6	160	160.0	Yes (1.58, 0.72)	48.6	155.2	1.576162	0.744359	1.2462	No	
3	DBC30Y	BIOISIS	34.9	1028.1	116.0	No	34.9	1028.1	1.5947	0.744852	1.9962	No	
3	C3BSAP	BIOISIS	46.7	133	176.0	No	46.7	133	1.5997	0.742634	1.2780	No	
3	C3BXXP	BIOISIS	46.8	133	161.0	No	46.8	133	1.6004	0.742792	1.2395	No	
3	SASDAB5	SASBDB	30.0	38.14	105.0	No	30.0	38.14	1.5859	0.709536	1.8236	**Yes**	

3	3LYSRR	BIOISIS	29.7	183	108.0	Yes (1.19, 0.54)	29.0	130.9	1.1384	0.736788	1.7344	No	
3	RBFSHP	BIOISIS	24.0	3226	95.0	Yes (1.63, 0.79)	22.9	3260	1.4876	0.744379	1.7546	No	
3	SASDAH6	SASBDB	31.0	47.4	100.0	No	31.0	47.4	1.5850	0.736363	2.1704	No	
3	SASDAN4	SASBDB	21.0	107.587	70.0	No	21.0	107.587	1.5207	0.749344	2.1737	No	
3	SASDAT3	SASBDB	21.0	98.309	65.0	No	21.0	98.309	1.6058	0.75813	2.1239	No	
4	SASDAS7	SASBDB	85.0	249	300.0	No	85.0	249	1.7884	0.749406	3.7165	No	
4	SASDAF6	SASBDB	42.9	0.172	147.0	No	42.9	0.172	1.8192	0.743617	5.5491	No	
4	SASDAZ4	SASBDB	30.0	0.38	105.0	Yes (1.66, 0.724)	30.6	0.376	1.72	0.745718	1.2908	No	
4	SASDAB8	SASBDB	60.2	1.07	200.0	No	60.2	1.07	1.6751	0.753025	4.1392	No	
4	SASDAM5	SASBDB	42.0	3664	147.0	No	42.0	3664	1.8825	0.752219	3.5554	No	
4	SASDAX5	SASBDB	59.0	435.06	190.0	No	59.0	435.06	1.6055	0.746565	2.3318	No	
4	SASDAG6	SASBDB	29.2	0.093	95.0	No	29.2	0.093	1.5235	0.73786	3.1415	No	
4	SASDA24	SASBDB	78.0	274	270.0	No	78.0	274	1.4546	0.744826	2.8313	No	
4	SASDAQ3	SASBDB	78.0	274	280.0	No	78.0	274	1.4546	0.742858	2.9930	No	
4	SASDAX3	SASBDB	85.0	301	290.0	No	85.0	301	1.8518	0.742074	3.3326	No	
4	SASDAY3	SASBDB	83.0	356	290.0	No	83.0	356	1.8265	0.745091	3.2330	No	
4	SASDAZ3	SASBDB	80.0	280	0.0	No	80.0	280	1.812771	0.740641	2.8414	No	
5	SASDA65	SASBDB	52.0	0.474	167.0	No	52.0	0.474	1.6027	0.741047	2.7473	No	
5	SASDA74	SASBDB	24.0	207	85.0	No	24.0	207	2.962136	0.774485	1.8404	**Yes**	
5	SASDAP4	SASBDB	32.0	2850	110.0	No	32.0	2850	2.0000	0.75656	2.3352	**Yes**	
6	SASDA37	SASBDB	47.2	4140.4	190.0	No	47.2	4140.4	6.3091	0.772973	8.8173	**Yes**	Elongated
6	SASDA47	SASBDB	77.0	7363.77	305.0	No	77.0	7363.77	10.5351	0.815768	11.6919	**Yes**	Elongated
6	SASDA57	SASBDB	97.0	8587.8	385.0	No	97.0	8587.8	11.3802	0.800121	18.0543	**Yes**	Elongated
6	SASDA67	SASBDB	120.0	9924.5	480.0	No	120.0	9924.5	10.4013	0.815834	21.5990	**Yes**	Elongated
6	SASDA77	SASBDB	141.0	10488.6	570.0	No	141.0	10488.6	30.2271	0.783354	30.3913	**Yes**	Elongated

6	SASDA87	SASBDB	159.0	14578	630.0	No	159.0	14578	35.8846	0.789852	29.1923	**Yes**	Elongated
6	SASDAA4	SASBDB	39.0	160	145.0	No	39.0	160	1.773824	0.750228	5.7315	No	
6	SASDA56	SASBDB	40.0	28	145.0	No	40.0	28	1.9554	0.763189	6.5088	**Yes**	Elongated
6	SASDA66	SASBDB	42.0	37.5	160.0	No	42.0	37.5	2.2238	0.765393	6.6023	**Yes**	Elongated
7	SASDA54	SASBDB	28.0	225.0	100.0	No	28.0	225.0	2.0478	0.803131	1.9935	**Yes**	
7	SASDAU5	SASBDB	43.0	2365600.0	160.0	No Yes (2.01, 0.79)	38.2	2230000	1.585305	0.743525	2.8308	No	
7	SASDA88	SASBDB	27.0	0.0	100.0	No	27.0	0.0	2.897361	0.768371	2.1630	**Yes**	
7	SASDA86	SASBDB	40.0	1270.0	140.0	No	40.0	1270.0	1.774991	0.772738	2.4964	**Yes**	
7	1U2FKX	BIOISIS	32.1	349.0	115.0	No	32.1	349.0	1.7881	0.746182	3.0494	No	
7	MnmGEP	BIOISIS	67.4	0.2	236.0	No	67.4	0.2	1.6654	0.744035	2.7329	No	
7	SASDAK5	SASBDB	40.0	10070.0	145.0	No Yes (2.24, 0.78)	35.7	9530.0	1.783373	0.735475	3.8135	No	
7	SASDAE4	SASBDB	55.0	10500.0	200.0	No	55.0	10500.0	2.2760	0.747438	5.4312	**Yes**	
7	SASDA26	SASBDB	32.0	1284.0	110.0	No	32.0	1284.0	1.910251	0.757498	4.0485	No	
7	SASDAB4	SASBDB	36.0	169.0	125.0	No	36.0	169.0	2.0663	0.75174	4.5736	**Yes**	
7	SASDAS6	SASBDB	44.0	23.7	145.0	No	44.0	23.7	2.6066	0.779872	5.9151	**Yes**	
7	SASDA76	SASBDB	51.0	1370.0	170.0	No	51.0	1370.0	2.5866	0.804183	2.7228	**Yes**	