

Integrative Structure Validation Report ?

April 10, 2025 - 12:58 PM PDT

The following software was used in the production of this report:

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

ATSAS Version 3.2.1 (r14885)

PDB ID	8ZZC
PDB-Dev ID	PDBDEV_00000012
Structure Title	Integrative structure and functional anatomy of eight spokes of a nuclear pore complex
Structure Authors	Kim SJ; Fernandez-Martinez J; Nudelman I; Shi Y; Zhang W; Raveh B; Herricks T; Slaughter BD; Hogan JA; Upla P; Chemmama IE; Pellarin R; Echeverria I; Shivaraju M; Chaudhury AS; Wang J; Williams R; Unruh JR; Greenberg CH; Jacobs EY; Yu Z; de la Cruz MJ; Mironska R; Stokes DL; Aitchison JD; Jarrold MF; Gerton JL; Ludtke SJ; Akey CW; Chait BT; Sali A; Rout MP
Deposited on	2018-01-18

This is a PDB-IHM IM Structure Validation Report for a publicly released PDB-IHM entry.

We welcome your comments at helpdesk@pdb-ihm.org

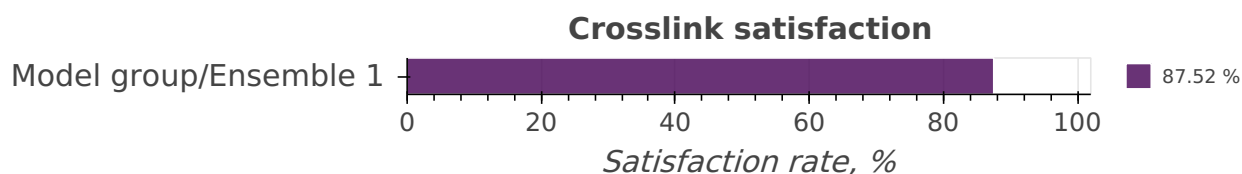
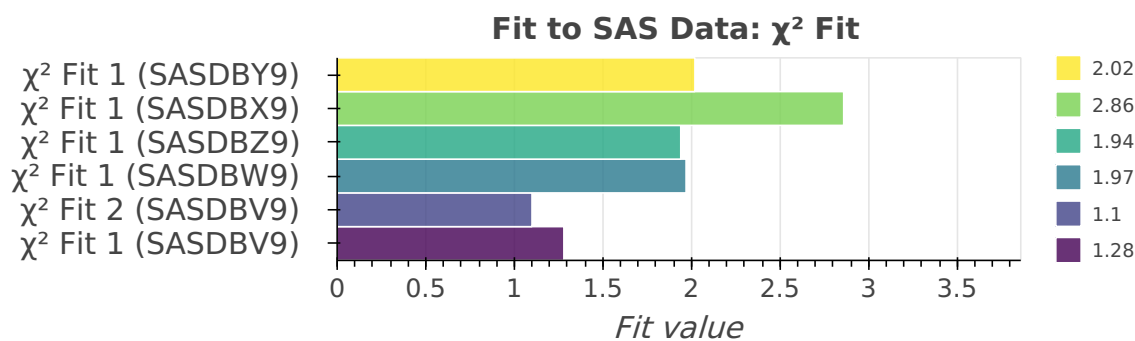
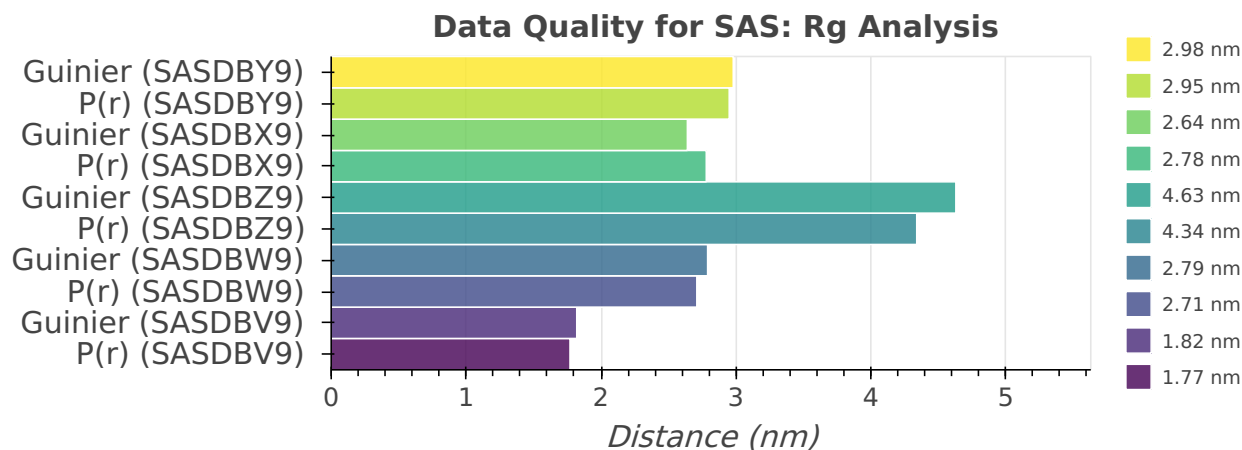
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available [here](#).

Overall quality ?

This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: Excluded Volume Analysis



Ensemble information ?

This entry consists of 2 distinct ensemble(s).

Summary ?

This entry consists of 2 model(s). A total of 65 datasets were used to build this entry.

Representation ?

This entry has 2 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1	1	Nup84	A	726	-	1-6, 7-20, 21-26, 27-80, 81-95, 96-126, 127-135, 136-364, 365-371, 372-483, 484-505, 506-562, 563-574, 575-726	100.00 / 89.39	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
				H					
				BR					
				BY					
				CF					
				CM					
				CT					
				DA					
				DH					
				DO					
				DV					
				EC					
				EJ					
				EQ					
				EX					
				FE					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		2	Nup85	B	744	-	1-46, 47-126, 127-131, 132-230, 231-234, 235-436, 437-450, 451-492, 493-495, 496-544, 545-552, 553-560, 561-566, 567-585, 586-589, 590-597, 598-602, 603-612, 613-615, 616-634, 635-637, 638-655, 656-660, 661-675, 676-684, 685-699, 700-706, 707-719, 720-724, 725-744	100.00 / 82.93	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
				I					
				BS					
				BZ					
				CG					
				CN					
				CU					
				DB					
				DI					
				DP					
				DW					
				ED					
				EK					
				ER					
				EY					
				FF					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		3	Nup120	C	1037	-	1, 2-29, 30-52, 53-305, 306-310, 311-711, 712-714, 715-726, 727-732, 733-746, 747-753, 754-766, 767-769, 770-781, 782-806, 807-818, 819-820, 821-833, 834-837, 838-853, 854-861, 862-879, 880-883, 884-895, 896-900, 901-913, 914-916, 917-931, 932-942, 943-955, 956-959, 960-971, 972-975, 976-987, 988-993, 994-1008, 1009-1024, 1025-1036, 1037	100.00 / 86.40	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
			J						
			BT						
			CA						
			CH						
			CO						
			CV						
			DC						
			DJ						
			DQ						
			DX						
			EE						
			EL						
			ES						
			EZ						
			FG						

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		4	Nup133	D	1157	-	1-55, 56-78, 79-85, 86-125, 126-132, 133-144, 145-161, 162-184, 185-192, 193-200, 201-205, 206-249, 250-257, 258-480, 481-489, 490-763, 764-771, 772-1155, 1156-1157	100.00 / 89.11	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
			K						
			BU						
			CB						
			CI						
			CP						
			CW						
			DD						
			DK						
			DR						
			DY						
			EF						
			EM						
			ET						
			FA						
			FH						

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		5	Nup145c	E	712	-	1-91, 92-99, 100-125, 126-144, 145-550, 551-553, 554-560, 561-565, 566-576, 577-586, 587-602, 603-611, 612-624, 625-630, 631-645, 646-653, 654-673, 674-680, 681-689, 690-702, 703-712	100.00 / 74.44	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
				L					
				BV					
				CC					
				CJ					
				CQ					
				CX					
				DE					
				DL					
				DS					
				DZ					
				EG					
				EN					
				EU					
				FB					
				FI					
		6	Seh1	F	349	-	1-248, 249-287, 288-346, 347-349	100.00 / 87.97	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
				M					
				BW					
				CD					
				CK					
				CR					
				CY					
				DF					
				DM					
				DT					
				EA					
				EH					
				EO					
				EV					
				FC					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				FJ					
		7	Sec13	G	297	-	1-9, 10-158, 159-165, 166-296, 297	100.00 / 94.28	Multiscale: Coarse-grained: 1 - 9 residue(s) per bead
				N					
				BX					
				CE					
				CL					
				CS					
				CZ					
				DG					
				DN					
				DU					
				EB					
				EI					
				EP					
				EW					
				FD					
				FK					
		8	Dyn2	O	92	-	1-6, 7-92	100.00 / 93.48	Multiscale: Coarse-grained: 1 - 6 residue(s) per bead
				P					
				FL					
				FM					
				FT					
				FU					
				GB					
				GC					
				GJ					
				GK					
				GR					
				GS					
				GZ					
				HA					
				HH					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				HI					
		9	Nup82	Q	713	-	1-6, 7-16, 17-22, 23-120, 121-122, 123-452, 453-521, 522-612, 613-624, 625-669, 670-677, 678-713	100.00 / 85.55	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
				R					
				FN					
				FO					
				FV					
				FW					
				GD					
				GE					
				GL					
				GM					
				GT					
				GU					
				HB					
				HC					
				HJ					
				HK					
		10	Nup159	S	1460	-	1082-1116, 1117-1126, 1127-1210, 1211-1239, 1240-1265, 1266-1321, 1322-1331, 1332-1372, 1373-1381, 1382-1412, 1413-1428, 1429-1456, 1457-1460	25.96 / 51.45	Multiscale: Coarse-grained: 1 - 35 residue(s) per bead
				T					
				FP					
				FQ					
				FX					
				FY					
				GF					
				GG					
				GN					
				GO					
				GV					
				GW					
				HD					
				HE					
				HL					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				HM					
		11	Nsp1	U	823	-	601-636, 637-727, 728-741, 742-778, 779-787, 788-823	27.10 / 73.54	Multiscale: Coarse-grained: 1 - 36 residue(s) per bead
				V					
				AF					
				AJ					
				FR					
				FS					
				FZ					
				GA					
				GH					
				GI					
				GP					
				GQ					
				GX					
				GY					
				HF					
				HG					
				HN					
				HO					
				JV					
				JW					
				KD					
				KE					
				KL					
				KM					
				KT					
				KU					
				LB					
				LC					
				LJ					
				LK					
				LR					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				LS					
		12	Nic96	W	839	20-56	1-19, 57-204, 205-360, 361-365, 366-374, 375-404, 405-444, 445-454, 455-515, 516-532, 533-747, 748-752, 753-835, 836-839	100.00 / 71.63	Multiscale: Coarse-grained: 1 - 25 residue(s) per bead
				AA					
				HP					
				HQ					
				HX					
				HY					
				IF					
				IG					
				IN					
				IO					
				IV					
				IW					
				JD					
				JE					
				JL					
				JM					
		11	Nsp1	X	823	637-727, 742-778, 788-823	601-636, 728-741, 779-787	27.10 / 73.54	Multiscale: Coarse-grained: 1 - 36 residue(s) per bead
				AB					
				HR					
				HS					
				HZ					
				IA					
				IH					
				II					
				IP					
				IQ					
				IX					
				IY					
				JF					
				JG					
				JN					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				JO					
		13	Nup49	Y	472	270-359, 369-407, 433-472	201-269, 360-368, 408-432	57.63 / 62.13	Multiscale: Coarse-grained: 1 - 69 residue(s) per bead
				AC					
				HT					
				HU					
				IB					
				IC					
				IJ					
				IK					
				IR					
				IS					
				IZ					
				JA					
				JH					
				JI					
				JP					
				JQ					
		14	Nup57	Z	541	287-423, 433-476, 505-540	201-286, 424-432, 477-504, 541	63.03 / 63.64	Multiscale: Coarse-grained: 1 - 86 residue(s) per bead
				AD					
				HV					
				HW					
				ID					
				IE					
				IL					
				IM					
				IT					
				IU					
				JB					
				JC					
				JJ					
				JK					
				JR					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				JS					
		12	Nic96	AE	839	-	1-19, 20-56, 57-204, 205-360, 361-365, 366-374, 375-404, 405-444, 445-454, 455-515, 516-532, 533-747, 748-752, 753-835, 836-839	100.00 / 71.63	Multiscale: Coarse-grained: 1 - 25 residue(s) per bead
				AI					
				JT					
				JU					
				KB					
				KC					
				KJ					
				KK					
				KR					
				KS					
				KZ					
				LA					
				LH					
				LI					
				LP					
				LQ					
		13	Nup49	AG	472	-	201-269, 270-359, 360-368, 369-407, 408-432, 433-472	57.63 / 62.13	Multiscale: Coarse-grained: 1 - 69 residue(s) per bead
				AK					
				JX					
				JY					
				KF					
				KG					
				KN					
				KO					
				KV					
				KW					
				LD					
				LE					
				LL					
				LM					
				LT					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				LU					
		14	Nup57	AH	541	-	201-286, 287-423, 424-432, 433-476, 477-504, 505-540, 541	63.03 / 63.64	Multiscale: Coarse-grained: 1 - 86 residue(s) per bead
				AL					
				JZ					
				KA					
				KH					
				KI					
				KP					
				KQ					
				KX					
				KY					
				LF					
				LG					
				LN					
				LO					
				LV					
				LW					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		15	Nup157	AM	1391	-	1-87, 88-289, 290-300, 301-309, 310-338, 339-457, 458-480, 481-515, 516-534, 535-679, 680-703, 704-730, 731-743, 744-775, 776-785, 786-830, 831-835, 836-892, 893-899, 900-916, 917-920, 921-933, 934-943, 944-1016, 1017-1038, 1039-1141, 1142-1154, 1155-1390, 1391	100.00 / 80.01	Multiscale: Coarse-grained: 1 - 25 residue(s) per bead
				AQ					
				LX					
				MB					
				MF					
				MJ					
				MN					
				MR					
				MV					
				MZ					
				ND					
				NH					
				NL					
				NP					
				NT					
				NX					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		16	Nup170	AN	1502	-	1-97, 98-299, 300-310, 311-319, 320-352, 353-471, 472-504, 505-537, 538-573, 574-717, 718-764, 765-791, 792-830, 831-862, 863-883, 884-916, 917-918, 919-930, 931-935, 936-992, 993-999, 1000-1016, 1017-1020, 1021-1033, 1034-1043, 1044-1116, 1117-1140, 1141-1191, 1192-1194, 1195-1243, 1244-1256, 1257-1502	100.00 / 74.37	Multiscale: Coarse-grained: 1 - 25 residue(s) per bead
				AR					
				LY					
				MC					
				MG					
				MK					
				MO					
				MS					
				MW					
				NA					
				NE					
				NI					
				NM					
				NQ					
				NU					
				NY					
		17	Nup188	AO	1655	-	1-11, 12-34, 35-39, 40-91, 92-100, 101-123, 124-130, 131-166, 167-173, 174-224, 225-255, 256-282, 283-287, 288-	100.00 / 82.18	Multiscale: Coarse-grained: 1 - 25 residue(s) per bead
				AS					
				LZ					
				MD					
				MH					
				ML					
				MP					
				MT					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				MX			304, 305-317, 318-434, 435-438, 439-479, 480-492, 493-		
				NB			508, 509-514, 515-		
				NF			530, 531-		
				NJ			550, 551-		
				NN			577, 578-		
				NR			583, 584-		
				NV			605, 606-		
				NZ			607, 608-		
							619, 620-		
							631, 632-		
	785, 786-792, 793-889, 890-891, 892-1100, 1101-1118, 1119-1133, 1134-1156, 1157-1241, 1242-1246, 1247-1265, 1266-1275, 1276-1292, 1293-1302, 1303-1322, 1323-1331, 1332-1354, 1355-1382, 1383-1567, 1568-1592, 1593-1628, 1629-1632, 1633-1652, 1653-1655								

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		18	Nup192	AP	1683	-	1-362, 363-416, 417-574, 575-601, 602-798, 799-813, 814-849, 850-856, 857-953, 954-960, 961-1126, 1127-1136, 1137-1226, 1227-1233, 1234-1258, 1259-1271, 1272-1366, 1367-1370, 1371-1418, 1419-1420, 1421-1502, 1503-1510, 1511-1559, 1560-1583, 1584-1590, 1591-1596, 1597-1619, 1620-1622, 1623-1644, 1645-1650, 1651-1683	100.00 / 88.53	Multiscale: Coarse-grained: 1 - 25 residue(s) per bead
				AT					
				MA					
				ME					
				MI					
				MM					
				MQ					
				MU					
				MY					
				NC					
				NG					
				NK					
				NO					
				NS					
				NW					
				OA					
		19	Nup53	AU	475	-	1-247, 248-284, 285-303, 304-360, 361-475	100.00 / 19.79	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
				AZ					
				OB					
				OG					
				OL					
				OQ					
				OV					
				PA					
				PF					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				PK					
				PP					
				PU					
				PZ					
				QE					
				QJ					
				QO					
		20	Nup59	AV	528	-	1-265, 266-302, 303-345, 346-402, 403-528	100.00 / 17.80	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
				BA					
				OC					
				OH					
				OM					
				OR					
				OW					
				PB					
				PG					
				PL					
				PQ					
				PV					
				QA					
				QF					
				QK					
				QP					
		21	Ndc1	AW	655	-	1-655	100.00 / 0.00	Multiscale: Coarse-grained: 55 - 100 residue(s) per bead
				BB					
				OD					
				OI					
				ON					
				OS					
				OX					
				PC					
				PH					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				PM					
				PR					
				PW					
				QB					
				QG					
				QL					
				QQ					
		22	Pom34	AX	299	-	1-299	100.00 / 0.00	Multiscale: Coarse-grained: 49 - 50 residue(s) per bead
				BC					
				OE					
				OJ					
				OO					
				OT					
				OY					
				PD					
				PI					
				PN					
				PS					
				PX					
				QC					
				QH					
				QM					
				QR					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		23	Pom152	AY	1337	-	1-378, 379-472, 473-519, 520-611, 612-615, 616-714, 715-721, 722-818, 819-823, 824-918, 919-930, 931-1026, 1027-1035, 1036-1141, 1142-1149, 1150-1229, 1230-1243, 1244-1337	100.00 / 63.80	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
				BD					
				OF					
				OK					
				OP					
				OU					
				OZ					
				PE					
				PJ					
				PO					
				PT					
				PY					
				QD					
				QI					
				QN					
				QS					
		24	Nup100	BE	959	816-958	551-815, 959	42.65 / 34.96	Multiscale: Coarse-grained: 1 - 25 residue(s) per bead
				BF					
				QT					
				QU					
				QZ					
				RA					
				RF					
				RG					
				RL					
				RM					
				RR					
				RS					
				RX					
				RY					
				SD					
				SE					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		25	Nup116	BG	1113	-	751-965, 966-1111, 1112-1113	32.61 / 40.22	Multiscale: Coarse-grained: 1 - 25 residue(s) per bead
				BH					
				QV					
				QW					
				RB					
				RC					
				RH					
				RI					
				RN					
				RO					
				RT					
				RU					
				RZ					
				SA					
				SF					
				SG					
		27	Gle1	BJ	538	-	1-120	22.30 / 0.00	Multiscale: Coarse-grained: 20 - 50 residue(s) per bead
				QY					
				RE					
				RK					
				RQ					
				RW					
				SC					
				SI					
		28	Nup145	BK	1317	459-605	201-458	30.75 / 36.30	Multiscale: Coarse-grained: 1 - 25 residue(s) per bead
				BL					
				SJ					
				SK					
				SO					
				SP					
				ST					
				SU					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				SY					
				SZ					
				TD					
				TE					
				TI					
				TJ					
				TN					
				TO					
		29	Nup1	BM	1076	-	1-351	32.62 / 0.00	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
				SN					
				SS					
				SX					
				TC					
				TH					
				TM					
				TR					
		30	Nup60	BN	539	-	1-398	73.84 / 0.00	Multiscale: Coarse-grained: 48 - 50 residue(s) per bead
				BO					
				SL					
				SM					
				SQ					
				SR					
				SV					
				SW					
				TA					
				TB					
				TF					
				TG					
				TK					
				TL					
				TP					
				TQ					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		31	Mlp1	BP	1875	-	238-716	25.55 / 0.00	Multiscale: Coarse-grained: 29 - 50 residue(s) per bead
				TS					
				TU					
				TW					
				TY					
				UA					
				UC					
				UE					
		32	Mlp2	BQ	1679	-	215-690	28.35 / 0.00	Multiscale: Coarse-grained: 26 - 50 residue(s) per bead
				TT					
				TV					
				TX					
				TZ					
				UB					
				UD					
				UF					
2	2	10	Nup159	S	1460	-	482-1081	41.10 / 0.00	Coarse-grained: 20 residue(s) per bead
				T					
				FP					
				FQ					
				FX					
				FY					
				GF					
				GG					
				GN					
				GO					
				GV					
				GW					
				HD					
				HE					
				HL					
				HM					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		11	Nsp1	U	823	-	1-600	72.90 / 0.00	Coarse-grained: 20 residue(s) per bead
				V					
				X					
				AB					
				AF					
				AJ					
				FR					
				FS					
				FZ					
				GA					
				GH					
				GI					
				GP					
				GQ					
				GX					
				GY					
				HF					
				HG					
				HN					
				HO					
				HR					
				HS					
				HZ					
				IA					
				IH					
				II					
				IP					
				IQ					
				IX					
				IY					
				JF					
				JG					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				JN					
				JO					
				JV					
				JW					
				KD					
				KE					
				KL					
				KM					
				KT					
				KU					
				LB					
				LC					
				LJ					
				LK					
				LR					
				LS					
		13	Nup49	Y	472	-	1-200	42.37 / 0.00	Coarse-grained: 20 residue(s) per bead
				AC					
				AG					
				AK					
				HT					
				HU					
				IB					
				IC					
				IJ					
				IK					
				IR					
				IS					
				IZ					
				JA					
				JH					
				JI					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				JP					
				JQ					
				JX					
				JY					
				KF					
				KG					
				KN					
				KO					
				KV					
				KW					
				LD					
				LE					
				LL					
				LM					
				LT					
				LU					
		14	Nup57	Z	541	-	1-200	36.97 / 0.00	Coarse-grained: 20 residue(s) per bead
				AD					
				AH					
				AL					
				HV					
				HW					
				ID					
				IE					
				IL					
				IM					
				IT					
				IU					
				JB					
				JC					
				JJ					
				JK					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				JR					
				JS					
				JZ					
				KA					
				KH					
				KI					
				KP					
				KQ					
				KX					
				KY					
				LF					
				LG					
				LN					
				LO					
				LV					
				LW					
		24	Nup100	BE	959	-	11-550	56.31 / 0.00	Coarse-grained: 20 residue(s) per bead
				BF					
				QT					
				QU					
				QZ					
				RA					
				RF					
				RG					
				RL					
				RM					
				RR					
				RS					
				RX					
				RY					
				SD					
				SE					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		25	Nup116	BG	1113	-	11-750	66.49 / 0.00	Coarse-grained: 20 residue(s) per bead
				BH					
				QV					
				QW					
				RB					
				RC					
				RH					
				RI					
				RN					
				RO					
				RT					
				RU					
				RZ					
				SA					
				SF					
				SG					
		28	Nup145	BK	1317	-	1-200	15.19 / 0.00	Coarse-grained: 20 residue(s) per bead
				BL					
				SJ					
				SK					
				SO					
				SP					
				ST					
				SU					
				SY					
				SZ					
				TD					
				TE					
				TI					
				TJ					
				TN					
				TO					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		29	Nup1	BM	1076	-	352-1049	64.87 / 0.00	Multiscale: Coarse-grained: 18 - 20 residue(s) per bead
				SN					
				SS					
				SX					
				TC					
				TH					
				TM					
				TR					
		30	Nup60	BN	539	-	399-498	18.55 / 0.00	Coarse-grained: 20 residue(s) per bead
				BO					
				SL					
				SM					
				SQ					
				SR					
				SV					
				SW					
				TA					
				TB					
				TF					
				TG					
				TK					
				TL					
				TP					
				TQ					

Datasets used for modeling ?

There are 65 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Integrative model	Not available	10.1016/j.cell.2016.10.028
2	Integrative model	Zenodo	10.5281/zenodo.1194547

ID	Dataset type	Database name	Data access code
3	Experimental model	PDB	5CWS
4	Comparative model	Zenodo	10.5281/zenodo.1194547
5	Experimental model	PDB	2QX5
6	Experimental model	Zenodo	10.5281/zenodo.1194547
7	Experimental model	Zenodo	10.5281/zenodo.1194547
8	Comparative model	Zenodo	10.5281/zenodo.1194547
9	Comparative model	Zenodo	10.5281/zenodo.1194547
10	Comparative model	Zenodo	10.5281/zenodo.1194547
11	Comparative model	Zenodo	10.5281/zenodo.1194547
12	Comparative model	Zenodo	10.5281/zenodo.1194547
13	Comparative model	Zenodo	10.5281/zenodo.1194547
14	Integrative model	Not available	10.1016/j.str.2017.01.006
15	Integrative model	Zenodo	10.5281/zenodo.1194547
16	Experimental model	PDB	3NF5
17	Comparative model	Zenodo	10.5281/zenodo.1194547
18	Comparative model	Zenodo	10.5281/zenodo.1194547
19	Experimental model	PDB	3KEP
20	Experimental model	Zenodo	10.5281/zenodo.1194547
21	Mass Spectrometry data	Zenodo	10.5281/zenodo.1149746
22	Crosslinking-MS data	Zenodo	10.5281/zenodo.1194547
23	Crosslinking-MS data	Zenodo	10.5281/zenodo.1194547
24	EM raw micrographs	EMPIAR	EMPIAR-10155
25	3DEM volume	EMDB	EMD-7321
26	3DEM volume	Zenodo	10.5281/zenodo.1194547
27	SAS data	Zenodo	10.5281/zenodo.1194547
28	SAS data	Zenodo	10.5281/zenodo.1194547
29	SAS data	Zenodo	10.5281/zenodo.1194547
30	SAS data	Zenodo	10.5281/zenodo.1194547
31	SAS data	Zenodo	10.5281/zenodo.1194547
32	SAS data	Zenodo	10.5281/zenodo.1194547
33	SAS data	Zenodo	10.5281/zenodo.1194547
34	SAS data	Zenodo	10.5281/zenodo.1194547
35	SAS data	Zenodo	10.5281/zenodo.1194547
36	SAS data	Zenodo	10.5281/zenodo.1194547
37	SAS data	Zenodo	10.5281/zenodo.1194547

ID	Dataset type	Database name	Data access code
38	SAS data	Zenodo	10.5281/zenodo.1194547
39	SAS data	Zenodo	10.5281/zenodo.1194547
40	SAS data	Zenodo	10.5281/zenodo.1194547
41	SAS data	Zenodo	10.5281/zenodo.1194547
42	SAS data	Zenodo	10.5281/zenodo.1194547
43	SAS data	Zenodo	10.5281/zenodo.1194547
44	SAS data	Zenodo	10.5281/zenodo.1194547
45	SAS data	Zenodo	10.5281/zenodo.1194547
46	SAS data	Zenodo	10.5281/zenodo.1194547
47	SAS data	Zenodo	10.5281/zenodo.1194547
48	SAS data	SASBDB	SASDBV9
49	SAS data	SASBDB	SASDBW9
50	SAS data	SASBDB	SASDBZ9
51	SAS data	SASBDB	SASDBX9
52	SAS data	SASBDB	SASDBY9
53	SAS data	Zenodo	10.5281/zenodo.1194547
54	SAS data	Zenodo	10.5281/zenodo.1194547
55	SAS data	Zenodo	10.5281/zenodo.1194547
56	SAS data	Zenodo	10.5281/zenodo.1194547
57	SAS data	Zenodo	10.5281/zenodo.1194547
58	SAS data	Zenodo	10.5281/zenodo.1194547
59	SAS data	Zenodo	10.5281/zenodo.1194547
60	SAS data	Zenodo	10.5281/zenodo.1194547
61	SAS data	Zenodo	10.5281/zenodo.1194547
62	SAS data	Zenodo	10.5281/zenodo.1194547
63	EM raw micrographs	EMPIAR	EMPIAR-10162
64	2DEM class average	Zenodo	10.5281/zenodo.1194547
65	2DEM class average	Zenodo	10.5281/zenodo.1194547

Methodology and software ?

This entry is a result of 2 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Sampling	Replica exchange monte carlo	None	500	False	True
2	1	Sampling	Replica exchange monte carlo	None	3000	False	True
3	1	Sampling	Replica exchange monte carlo	None	1000	False	True
1	2	Sampling	Brownian dynamics	None	1000	False	True

There are 13 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Integrative Modeling Platform (IMP)	develop-0a5706e202	integrative model building	https://integrativemodeling.org
2	IMP PMI module	67456c0	integrative model building	https://integrativemodeling.org
3	HHpred	2.0.16	protein homology detection	https://toolkit.tuebingen.mpg.de/hhpred
4	PSIPRED	4.00	secondary structure prediction	http://bioinf.cs.ucl.ac.uk/psipred/
5	DISOPRED	3	disorder prediction	http://bioinf.cs.ucl.ac.uk/psipred/?disopred=1
6	DomPred	Not available	domain boundary prediction	http://bioinf.cs.ucl.ac.uk/dompred
7	COILS/PCOILS	Not available	coiled-coil prediction	https://toolkit.tuebingen.mpg.de/#/tools/pcoils
8	EMAN2	2.20	image processing	http://blake.bcm.edu/emanwiki/EMAN2
9	RELION	1.40	image processing	https://www2.mrc-lmb.cam.ac.uk/relion/
10	SGD	Not available	database	https://www.yeastgenome.org/
11	HeliQuest	Not available	helix prediction	http://heliquest.ipmc.cnrs.fr/

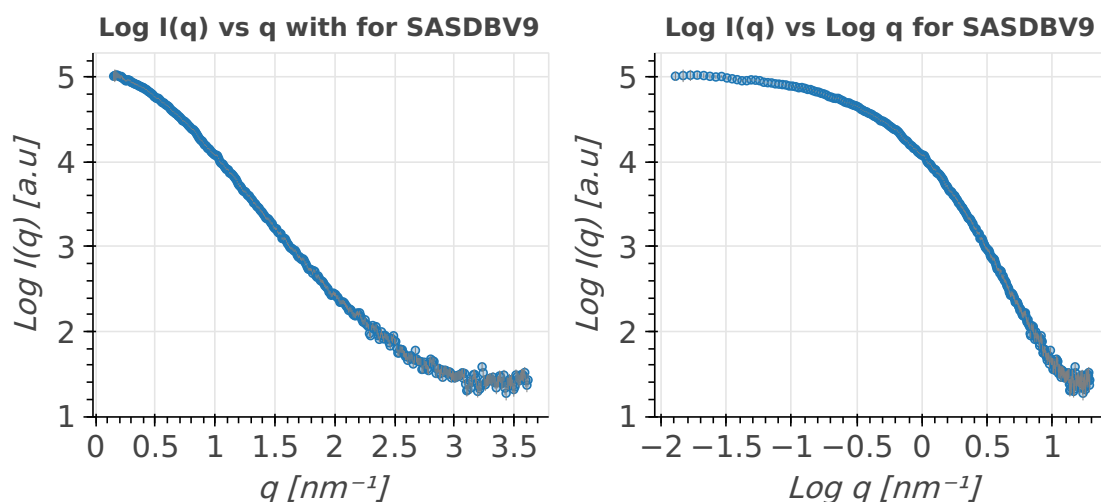
ID	Software name	Software version	Software classification	Software location
12	MODELLER	9.15	comparative modeling	https://salilab.org/modeller/
13	MODELLER	9.13	comparative modeling	https://salilab.org/modeller/

Data quality ?

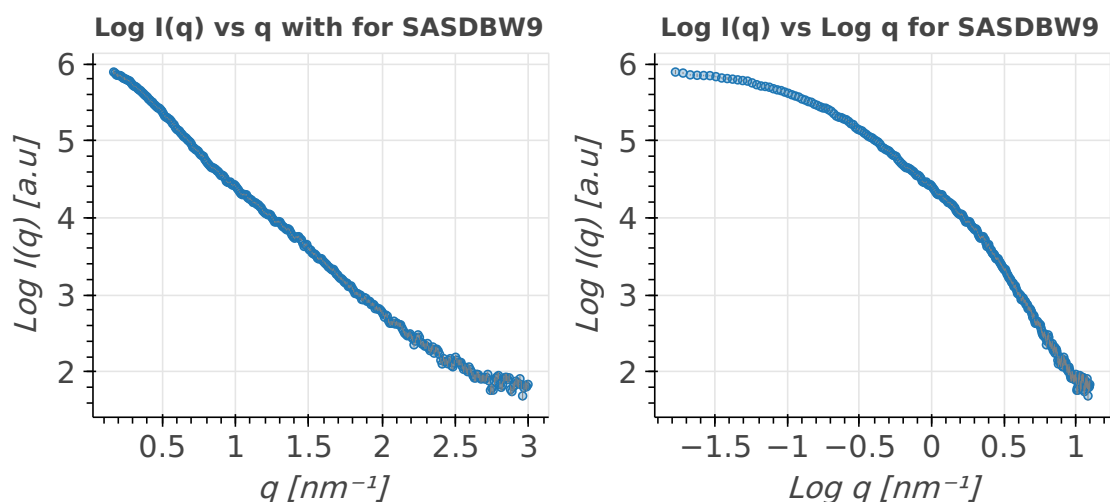
Scattering profile ?

SAS data used in this integrative model was obtained from 5 deposited SASDBD entry (entries).

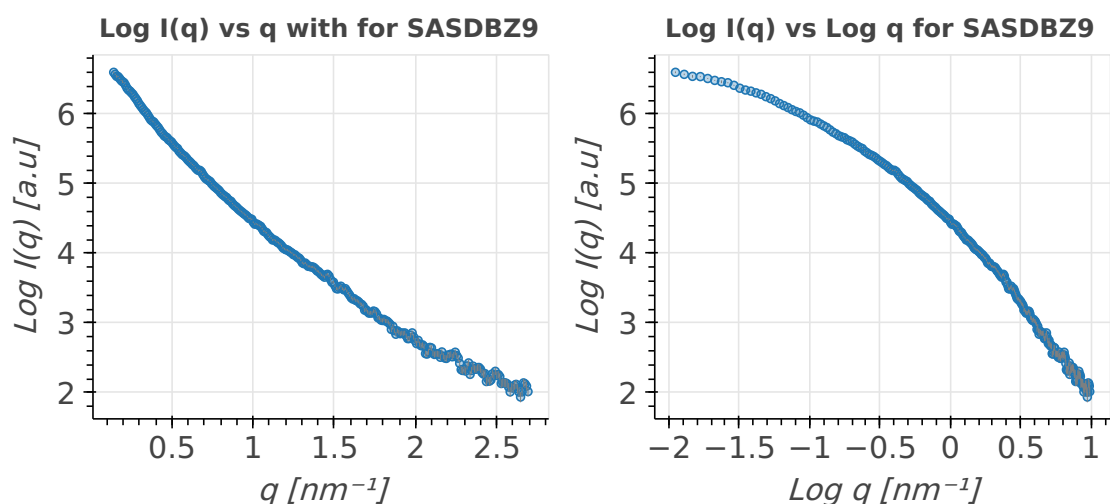
Scattering profile for [SASDBV9](#): data from solutions of biological macromolecules are presented as both log $I(q)$ vs q and log $I(q)$ vs log q based on [SAS validation task force \(SASvtf\) recommendations](#). $I(q)$ is the intensity (in arbitrary units) and q is the modulus of the scattering vector.



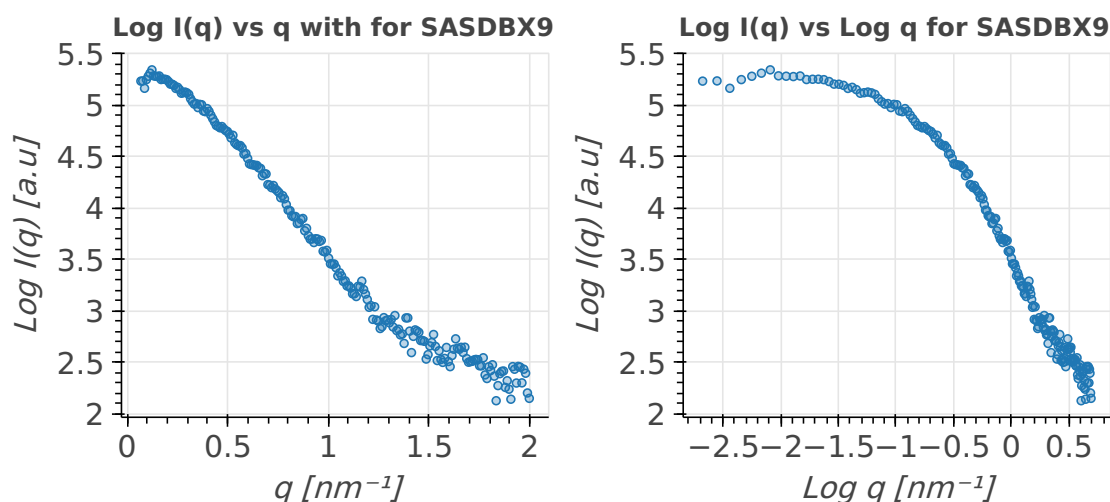
Scattering profile for [SASDBW9](#): data from solutions of biological macromolecules are presented as both log $I(q)$ vs q and log $I(q)$ vs log q based on [SAS validation task force \(SASvtf\) recommendations](#). $I(q)$ is the intensity (in arbitrary units) and q is the modulus of the scattering vector.



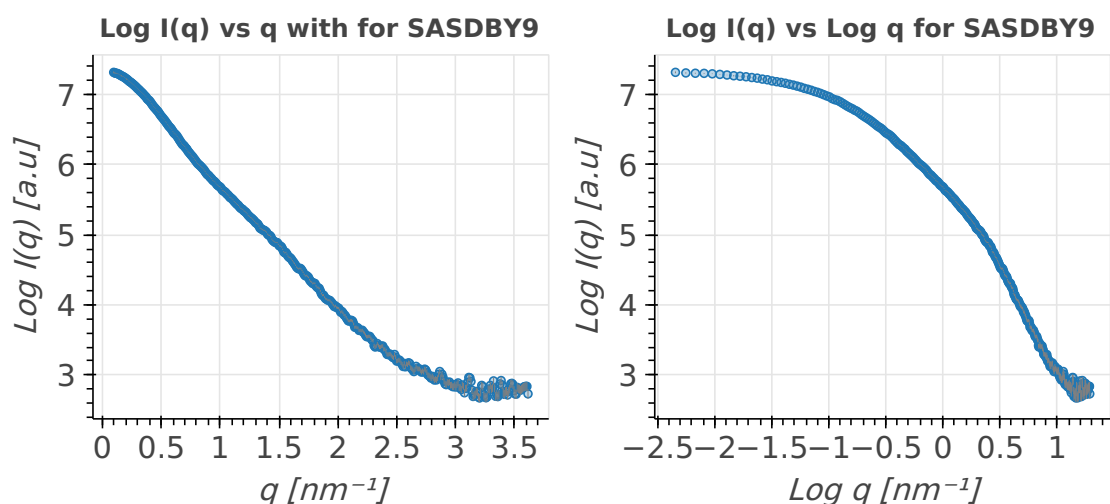
Scattering profile for [SASDBZ9](#): data from solutions of biological macromolecules are presented as both $\log I(q)$ vs q and $\log I(q)$ vs $\log(q)$ based on [SAS validation task force \(SASvtf\) recommendations](#). $I(q)$ is the intensity (in arbitrary units) and q is the modulus of the scattering vector.



Scattering profile for [SASDBX9](#): data from solutions of biological macromolecules are presented as both $\log I(q)$ vs q and $\log I(q)$ vs $\log(q)$ based on [SAS validation task force \(SASvtf\) recommendations](#). $I(q)$ is the intensity (in arbitrary units) and q is the modulus of the scattering vector.



Scattering profile for [SASDBY9](#): data from solutions of biological macromolecules are presented as both $\text{log } I(q)$ vs q and $\text{log } I(q)$ vs $\text{log } (q)$ based on [SAS validation task force \(SASvtf\) recommendations](#). $I(q)$ is the intensity (in arbitrary units) and q is the modulus of the scattering vector.



Key experimental estimates ?

Molecular weight (MW) estimates from experiments and analysis: true molecular weight can be compared to the Porod estimate from scattering profiles.

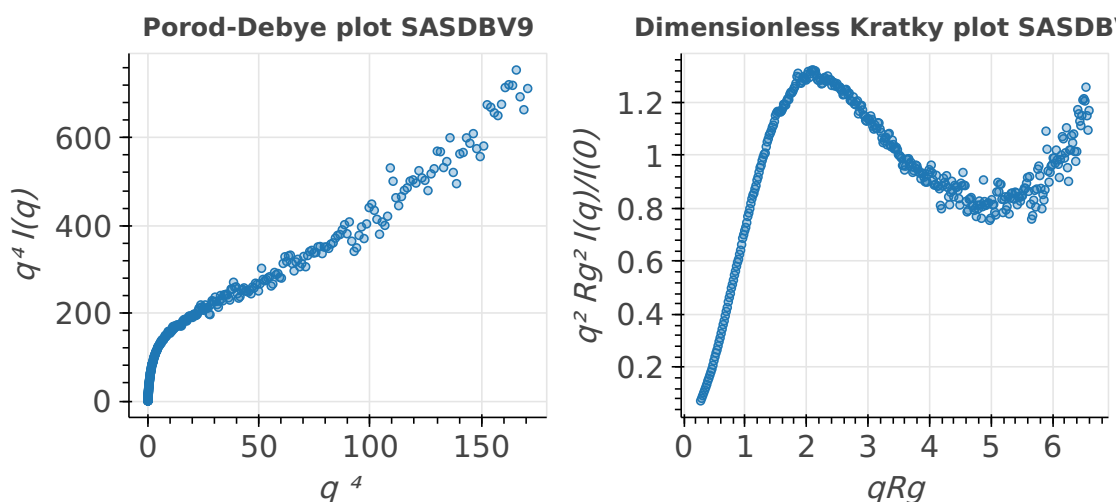
SASDB ID	Chemical composition MW	Standard MW	Porod Volume/MW
SASDBV9	12.6 kDa	12.2 kDa	Not available
SASDBW9	24.1 kDa	25.2 kDa	Not available
SASDBZ9	49.4 kDa	48.3 kDa	Not available
SASDBX9	12.5 kDa	14.7 kDa	Not available
SASDBY9	25.9 kDa	25.2 kDa	Not available

Volume estimates from experiments and analysis: estimated volume can be compared to Porod volume obtained from scattering profiles.

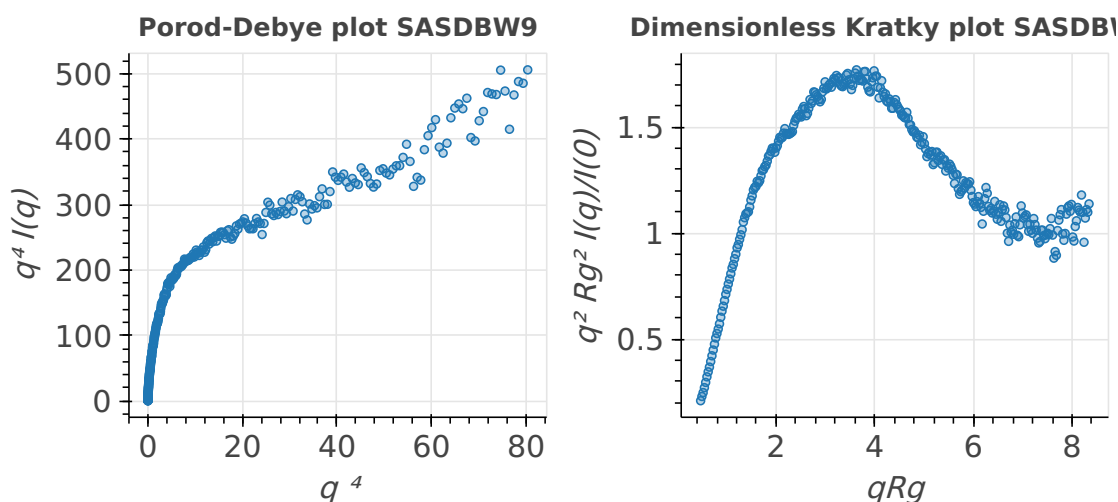
SASDB ID	Estimated Volume	Porod Volume	Specific Volume	Sample Contrast	Sample Concentration
SASDBV9	Not available	17.94 nm ³	Not available	Not available	Not available
SASDBW9	Not available	22.50 nm ³	Not available	Not available	Not available
SASDBZ9	Not available	66.59 nm ³	Not available	Not available	Not available
SASDBX9	Not available	56.68 nm ³	Not available	Not available	Not available
SASDBY9	Not available	27.97 nm ³	Not available	Not available	Not available

Flexibility analysis ?

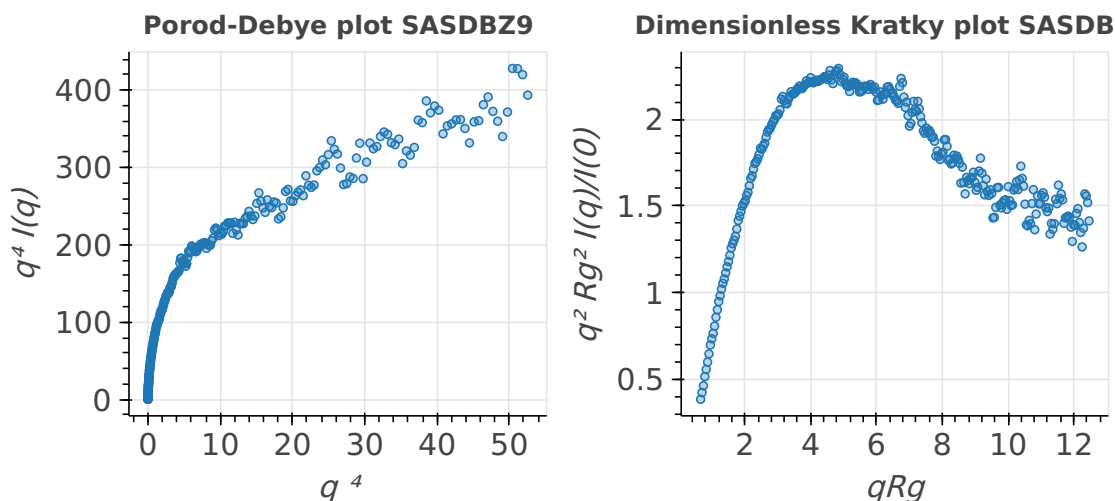
Flexibility analysis for SASDBV9: In a Porod-Debye plot, a clear plateau is observed for globular (partial or fully folded) domains, whereas, fully unfolded domains are devoid of any discernable plateau. For details, refer to Figure 5 in [Rambo and Tainer, 2011](#). In a Kratky plot, a parabolic shape is observed for globular (partial or fully folded) domains and a hyperbolic shape is observed for fully unfolded domains.



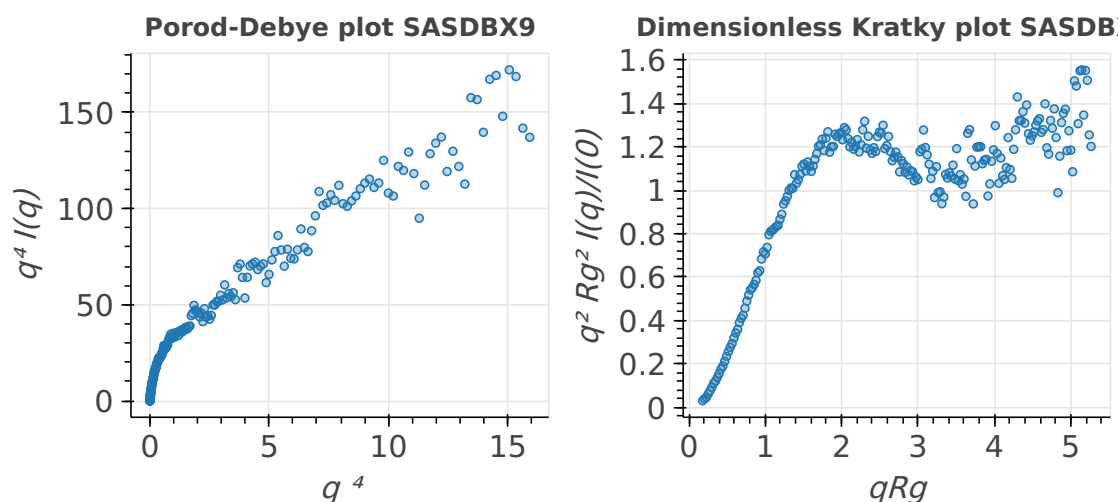
Flexibility analysis for SASDBW9: In a Porod-Debye plot, a clear plateau is observed for globular (partial or fully folded) domains, whereas, fully unfolded domains are devoid of any discernable plateau. For details, refer to Figure 5 in [Rambo and Tainer, 2011](#). In a Kratky plot, a parabolic shape is observed for globular (partial or fully folded) domains and a hyperbolic shape is observed for fully unfolded domains.



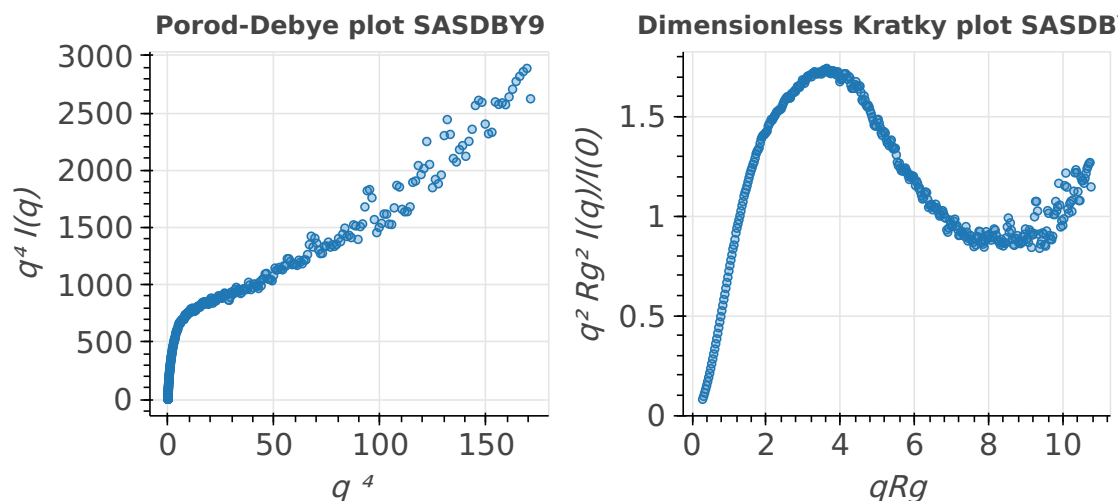
Flexibility analysis for SASDBZ9: In a Porod-Debye plot, a clear plateau is observed for globular (partial or fully folded) domains, whereas, fully unfolded domains are devoid of any discernable plateau. For details, refer to Figure 5 in [Rambo and Tainer, 2011](#). In a Kratky plot, a parabolic shape is observed for globular (partial or fully folded) domains and a hyperbolic shape is observed for fully unfolded domains.



Flexibility analysis for SASDBX9: In a Porod-Debye plot, a clear plateau is observed for globular (partial or fully folded) domains, whereas, fully unfolded domains are devoid of any discernable plateau. For details, refer to Figure 5 in [Rambo and Tainer, 2011](#). In a Kratky plot, a parabolic shape is observed for globular (partial or fully folded) domains and a hyperbolic shape is observed for fully unfolded domains.



Flexibility analysis for SASDBY9: In a Porod-Debye plot, a clear plateau is observed for globular (partial or fully folded) domains, whereas, fully unfolded domains are devoid of any discernable plateau. For details, refer to Figure 5 in [Rambo and Tainer, 2011](#). In a Kratky plot, a parabolic shape is observed for globular (partial or fully folded) domains and a hyperbolic shape is observed for fully unfolded domains.



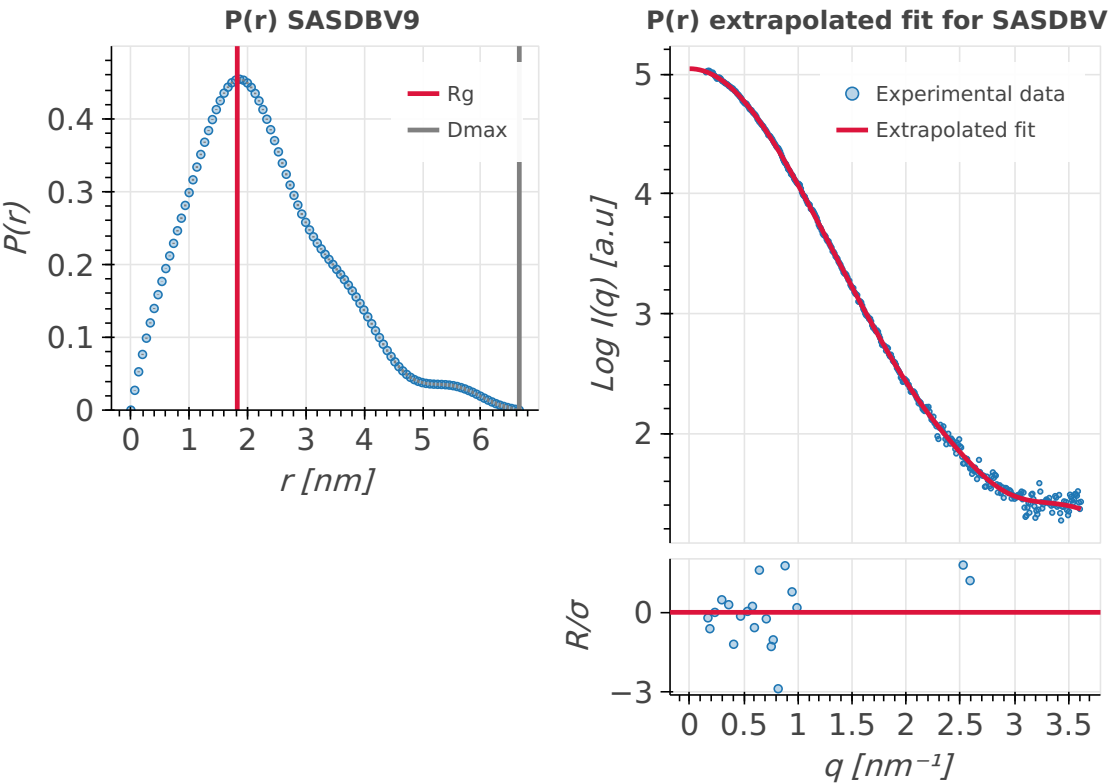
Pair-distance distribution analysis ?

P(r) analysis: P(r) represents the distribution of distances between all pairs of atoms within the particle weighted by the respective electron densities. P(r) is the Fourier transform of I(s) (and vice versa). R_g can be estimated from integrating the P(r) function. Agreement between the P(r) and Guinier-determined R_g (table below) is a good measure of the self-consistency of the SAS profile. R_g is a measure for the overall size of a macromolecule; e.g. a protein with a smaller R_g is more compact than a protein with a larger R_g , provided both have the same molecular weight (MW). The point where P(r) is decaying to zero is called D_{max} and represents the maximum size of the particle.

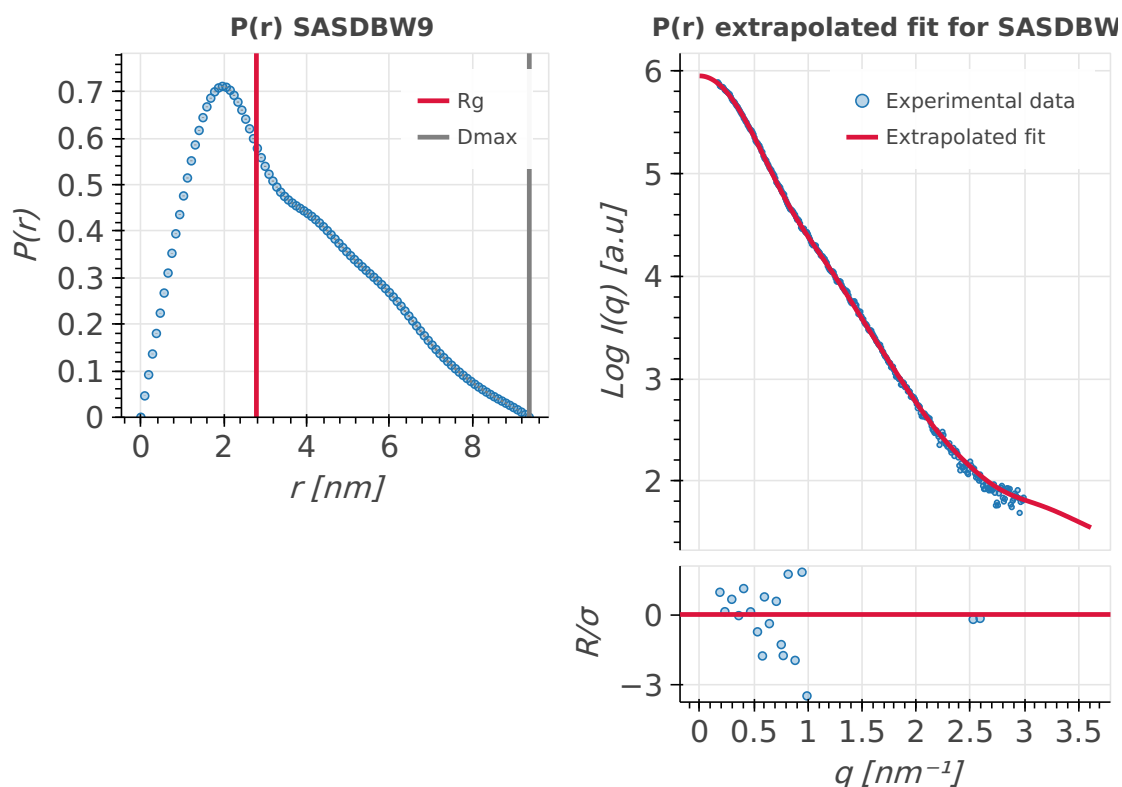
SASDB ID	Software used	D_{max}	D_{max} error	R_g	R_g error
SASDBV9	GNOM 4.5a	6.660 nm	Not available	1.824 nm	0.006 nm
SASDBW9	GNOM 4.5a	9.370 nm	Not available	2.787 nm	0.007 nm
SASDBZ9	GNOM 4.5a	15.430 nm	Not available	4.629 nm	0.011 nm

SASDB ID	Software used	D	D error	R	R error
SASDBX9	GNOM 4.5a	7.930 nm	Not available	2.636 nm	0.008 nm
SASDBY9	GNOM 4.5a	10.450 nm	Not available	2.976 nm	0.005 nm

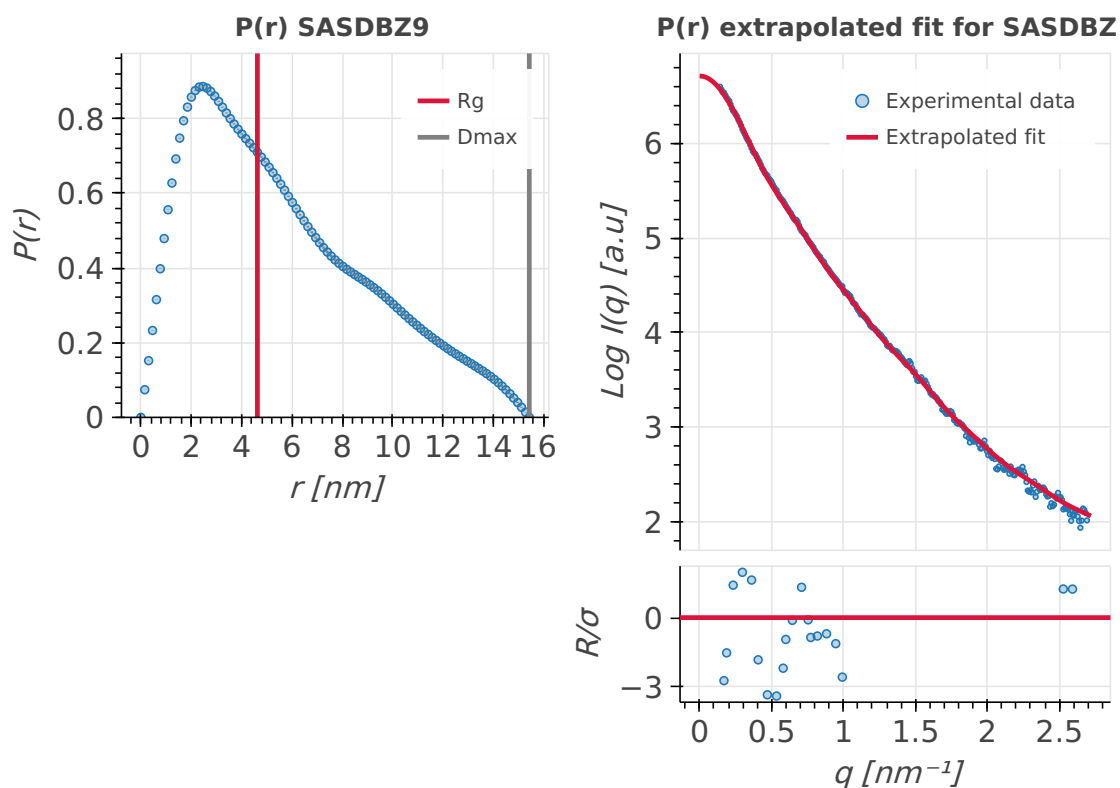
P(r) for SASDBV9: The value of P(r) should be zero beyond $r=D_{\text{max}}$.



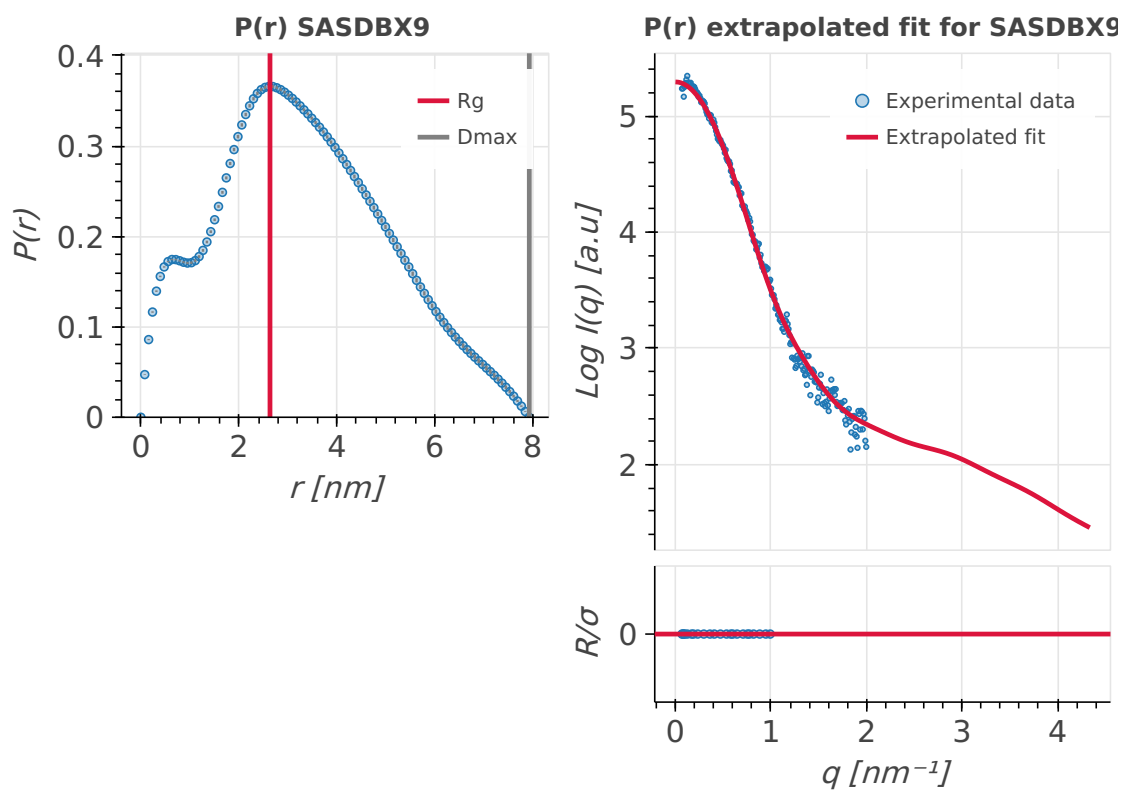
P(r) for SASDBW9: The value of P(r) should be zero beyond $r=D_{\text{max}}$.



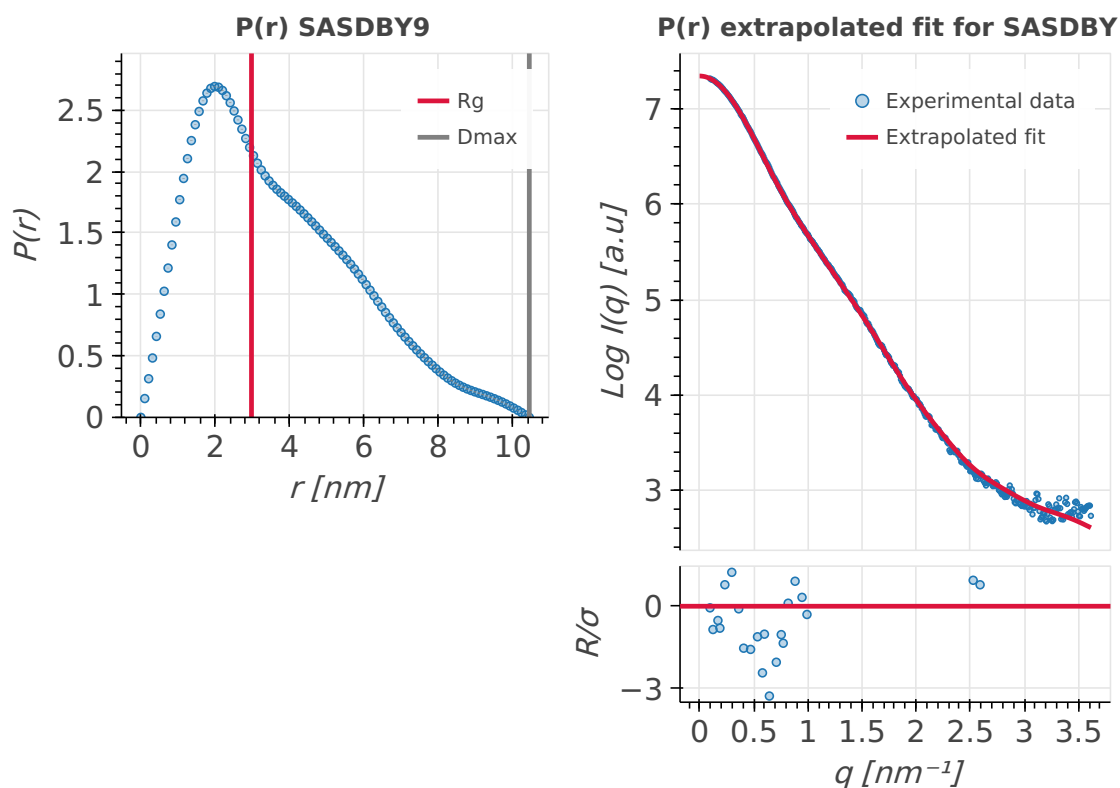
P(r) for SASDBZ9: The value of $P(r)$ should be zero beyond $r=D_{max}$.



P(r) for SASDBX9: The value of $P(r)$ should be zero beyond $r=D_{max}$.



P(r) for SASDBY9: The value of $P(r)$ should be zero beyond $r=D_{max}$.

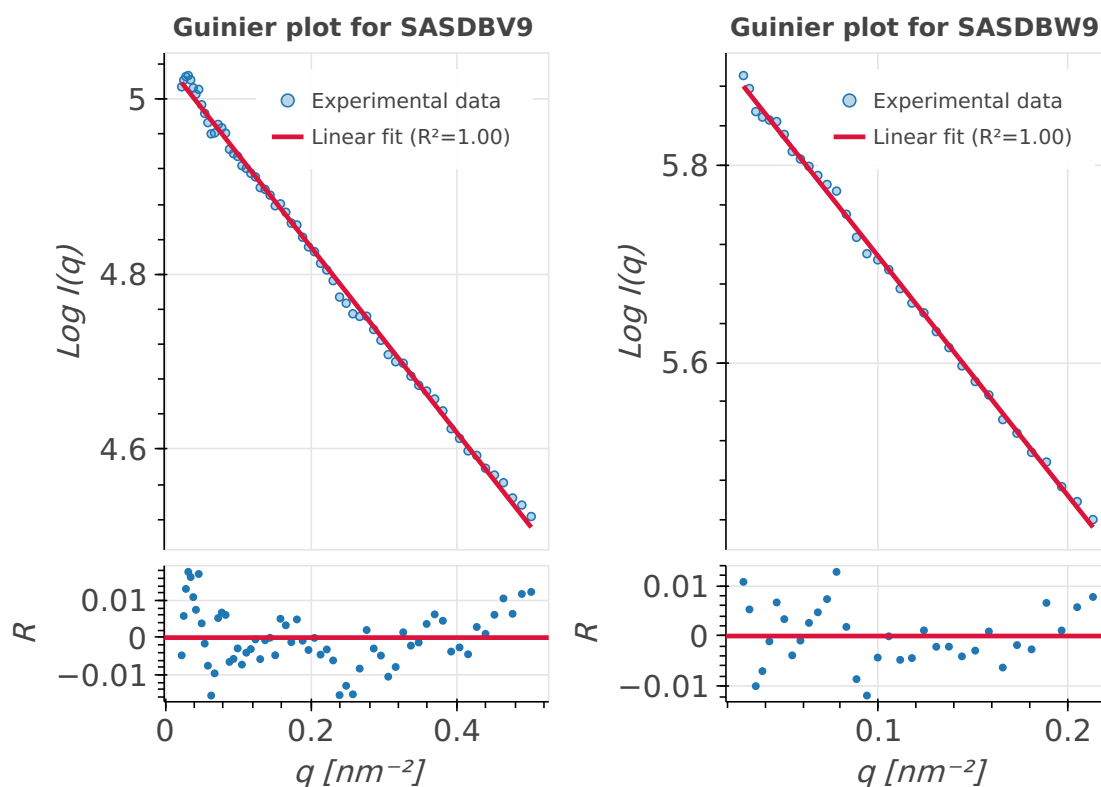


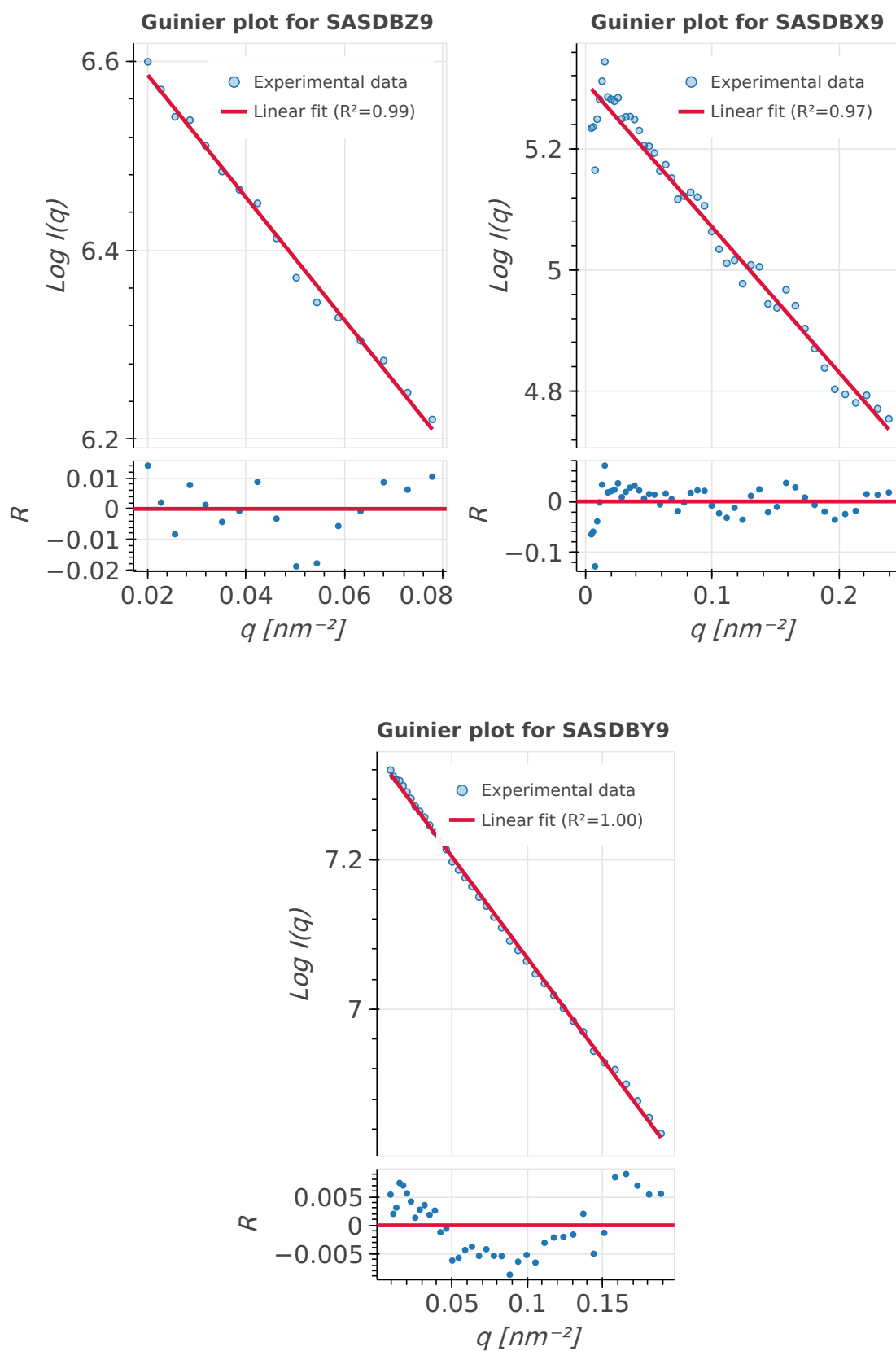
Guinier analysis ?

Guinier analysis: agreement between the $P(r)$ and Guinier-determined R_g (table below) is a good measure of the self-consistency of the SAS profile. Molecular weight estimates can also be compared to Porod and sample molecular weights for consistency.

SASDB ID	R_g	R_g error	MW	MW error
SASDBV9	1.77 nm	0.05 nm	12.2 kDa	Not available
SASDBW9	2.71 nm	0.06 nm	25.2 kDa	Not available
SASDBZ9	4.34 nm	0.17 nm	48.3 kDa	Not available
SASDBX9	2.78 nm	0.18 nm	14.7 kDa	Not available
SASDBY9	2.95 nm	0.11 nm	25.2 kDa	Not available

Guinier analysis: the linearity of the Guinier plot is a sensitive indicator of the quality of the experimental SAS data; a linear Guinier plot is a necessary but not sufficient demonstration that a solution contains monodisperse particles of the same size. Deviations from linearity usually point to strong interference effects, polydispersity of the samples or improper background subtraction. Residual value plot and coefficient of determination (R^2) are measures to assess linear fit to the data. A perfect fit has an R^2 value of 1. Residual values should be equally and randomly spaced around the horizontal axis.





Crosslinking-MS

At the moment, data validation is only available for crosslinking-MS data deposited as a fully *compliant* dataset in the [PRIDE Crosslinking](#) database. Correspondence between crosslinking-MS

and entry entities is established using [pyHMMER](#). Only residue pairs that passed the reported threshold are used for the analysis. The values in the report have to be interpreted in the context of the experiment (i.e. only a minor fraction of in-situ or in-vivo dataset can be used for modeling).

Crosslinking-MS dataset is not available in the [PRIDE Crosslinking](#) database.

2DEM class average

Validation for this section is under development.

Mass Spectrometry

Validation for this section is under development.

EM raw micrographs

Validation for this section is under development.

3DEM volume

Validation for this section is under development.

Model quality ?

For models with atomic structures, MolProbity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Excluded volume satisfaction ?

Excluded volume satisfaction for the models in the entry are listed below. The Analysed column shows the number of particle-particle or particle-atom pairs for which excluded volume was analysed.

Model ID	Analysed	Number of violations	Excluded Volume Satisfaction (%)
1	27420955836	611820	100.00
2	8419356	156	100.00

Fit of model to data used for modeling ?

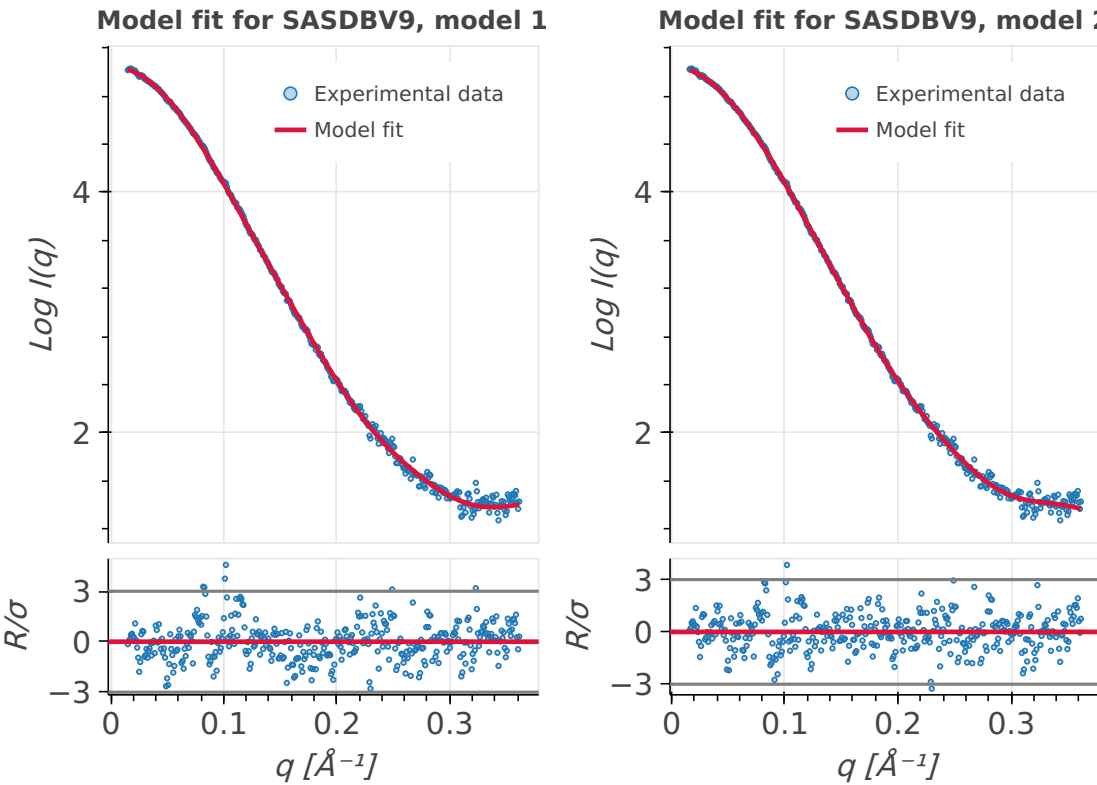
Fit of model(s) to SAS data

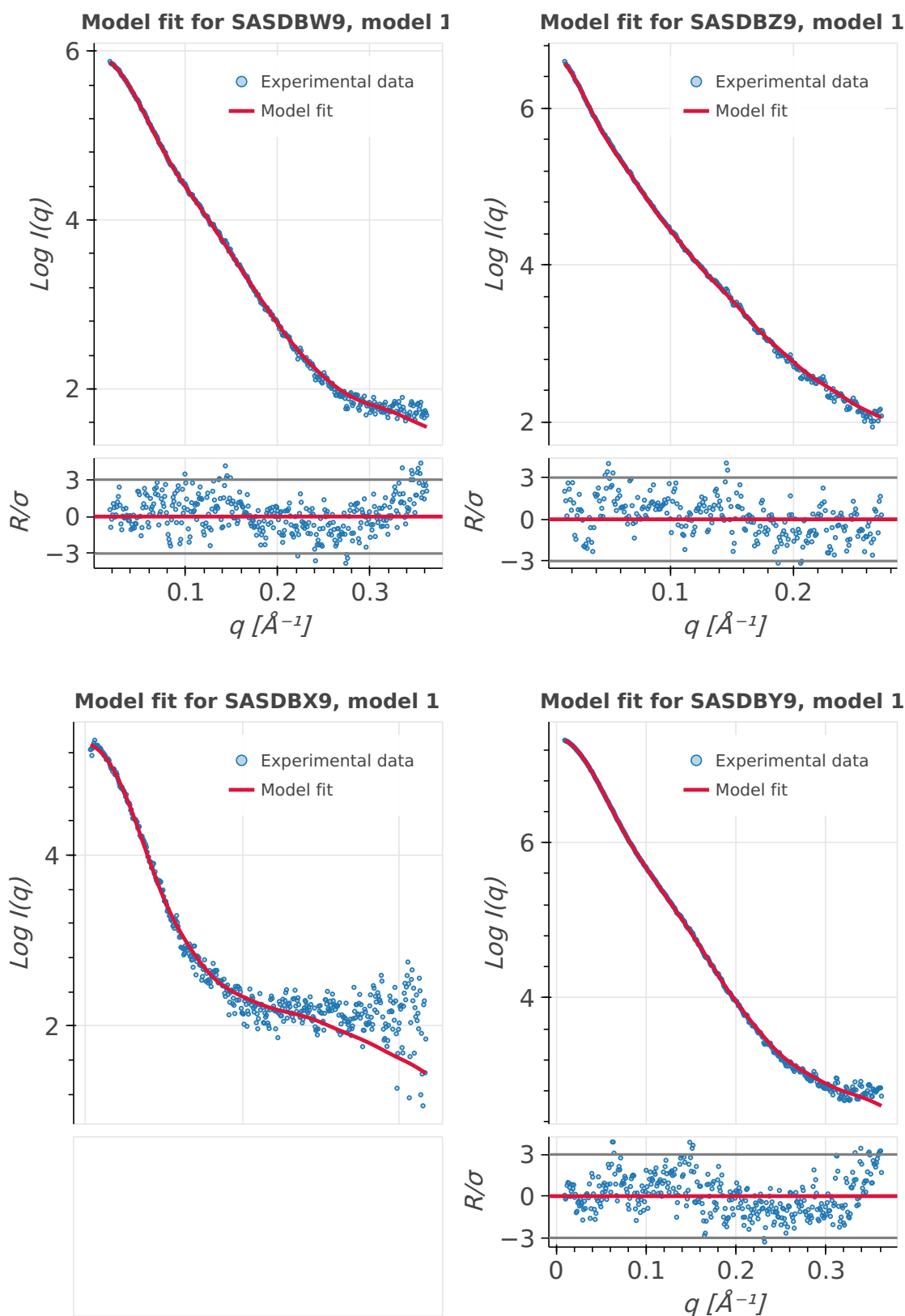
χ^2 goodness of fit and cormap analysis ?

Model and fits displayed below were obtained from SASBDB. χ^2 values are a measure of fit of the model to data. A perfect fit has a χ^2 value of 1.0. ATSAS DATCMP was used for hypothesis testing. All data sets are similar (i.e. the fit and the data collected) is the null hypothesis. p-value is a measure of evidence against the null hypothesis, smaller the value, the stronger the evidence that you should reject the null hypothesis.

SASDB ID	Model	χ^2	p-value
SASDBV9	1	1.28	0.02
SASDBV9	2	1.10	0.01
SASDBW9	1	1.97	0.00
SASDBZ9	1	1.94	0.00
SASDBX9	1	2.86	0.00
SASDBY9	1	2.02	0.00

Model fit(s): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.





Fit of model(s) to crosslinking-MS data

Restraint types

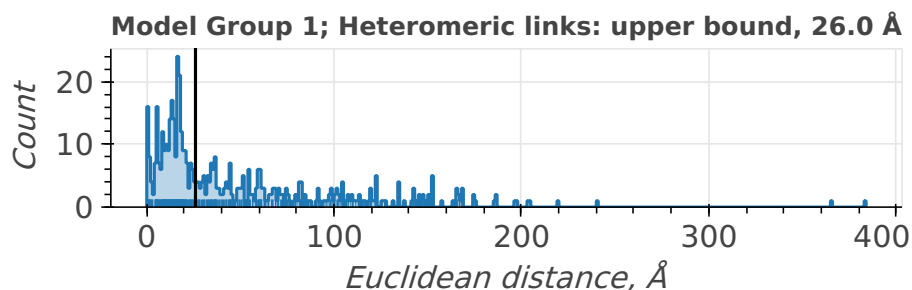
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

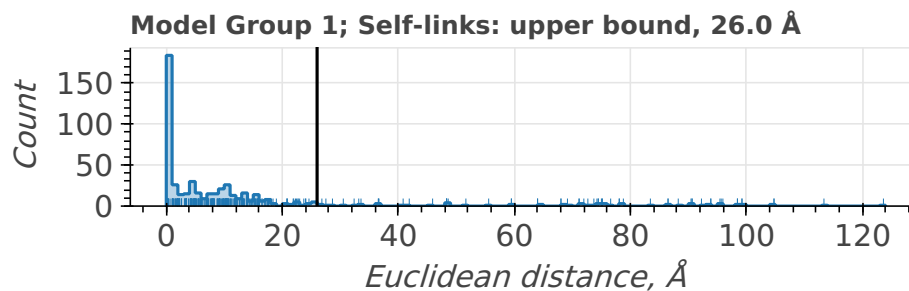
There are 1071 crosslinking restraints combined in 615 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSS	LYS	coarse-grained	LYS	coarse-grained	upper bound	26.0	916
DSS	LYS	CA	LYS	CA	upper bound	26.0	102
DSS	LYS	coarse-grained	THR	coarse-grained	upper bound	26.0	13
DSS	LYS	coarse-grained	MET	coarse-grained	upper bound	26.0	27
DSS	ASN	coarse-grained	LYS	coarse-grained	upper bound	26.0	2
DSS	ARG	coarse-grained	LYS	coarse-grained	upper bound	26.0	2
DSS	GLN	coarse-grained	LYS	coarse-grained	upper bound	26.0	2
DSS	ALA	coarse-grained	LYS	coarse-grained	upper bound	26.0	2
DSS	LYS	coarse-grained	VAL	coarse-grained	upper bound	26.0	3
DSS	GLN	coarse-grained	MET	coarse-grained	upper bound	26.0	1
DSS	LYS	CA	MET	CA	upper bound	26.0	1

Distograms of individual restraints

Restraints with identical thresholds are grouped into one plot. Only the best distance per restraint per model group/ensemble is plotted. Inter- and intramolecular (including self-links) restraints are also grouped into one plot. Distance for a restraint between coarse-grained beads is calculated as a minimal distance between shells; if beads intersect, the distance will be reported as 0.0. A bead with the highest available resolution for a given residue is used for the assessment.





Satisfaction of restraints

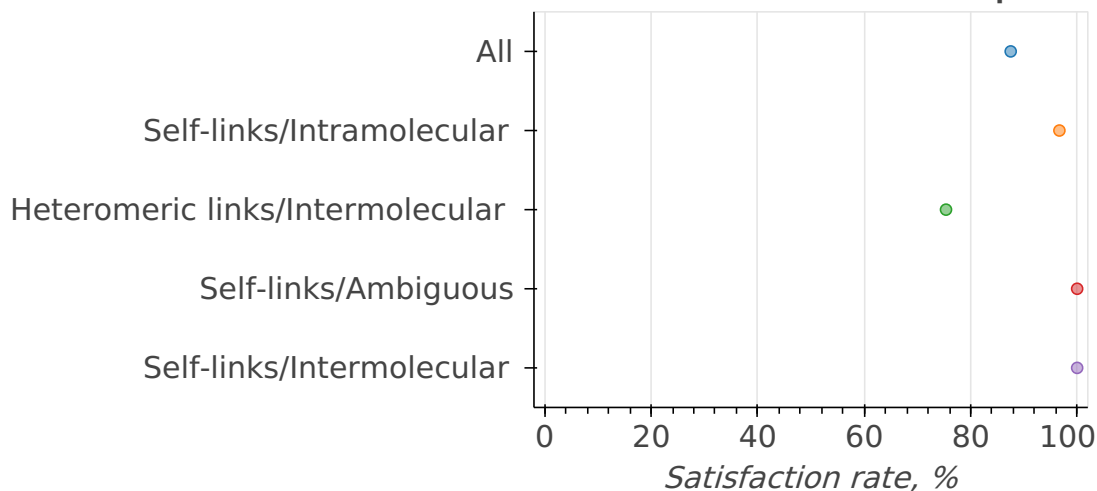
Satisfaction of restraints is calculated on a [restraint group](#) (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered satisfied, if the condition was met in at least one model of the model group/ensemble. The number of measured restraints can be smaller than the total number of restraint groups if crosslinks involve non-modeled residues. Only deposited models are used for validation right now.

State group	State	Model group	# of Deposited models/Total	Restraint group type	Satisfied (%)	Violated (%)	Count (Total=615)
1	1	1	1/5	All	87.52	12.48	609
				Self-links/ Intramolecular	96.67	3.33	300
				Heteromeric links/ Intermolecular	75.37	24.63	268
				Self-links/ Ambiguous	100.00	0.00	37
				Self-links/ Intermolecular	100.00	0.00	4
1	1	2	1/1000	All	Not available	Not available	0

Per-model satisfaction rates in ensembles

Every point represents one model in a model group/ensemble. Where possible, boxplots with quartile marks are also plotted.

Satisfaction rates in Model Group 1



2DEM class average

Validation for this section is under development.

Mass Spectrometry

Validation for this section is under development.

EM raw micrographs

Validation for this section is under development.

3DEM volume

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

The development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures are funded by NSF awards to the [PDB-IHM team](#) (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the [RCSB PDB](#) (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the [Sali lab](#) contributed model validation metrics and software packages.

Dr. Jill Trewhella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods. Team members from the labs of Dr. Juri Rappsilber, Dr. Alexander Leitner, Dr. Andrea Graziadei, and members of [PRIDE](#) database are acknowledged for their advice and support in implementing crosslinking-MS validation methods. We

are grateful to Dr. Shruthi Viswanath for discussions about uncertainty assessment of integrative structural models.

Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.