

Integrative Structure Validation Report

July 22, 2024 - 03:38 PM PDT

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

Python-IHM Version 1.3

ATSAS Version 3.2.1 (r14885)

Integrative Modeling Validation Version 1.2

| | |
|-------------------|--|
| PDB ID | 8ZZB |
| PDB-Dev ID | PDBDEV_00000011 |
| Structure Title | Integrative structure and functional anatomy of three 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 |

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

We welcome your comments at pdb-dev@mail.wwpdb.org

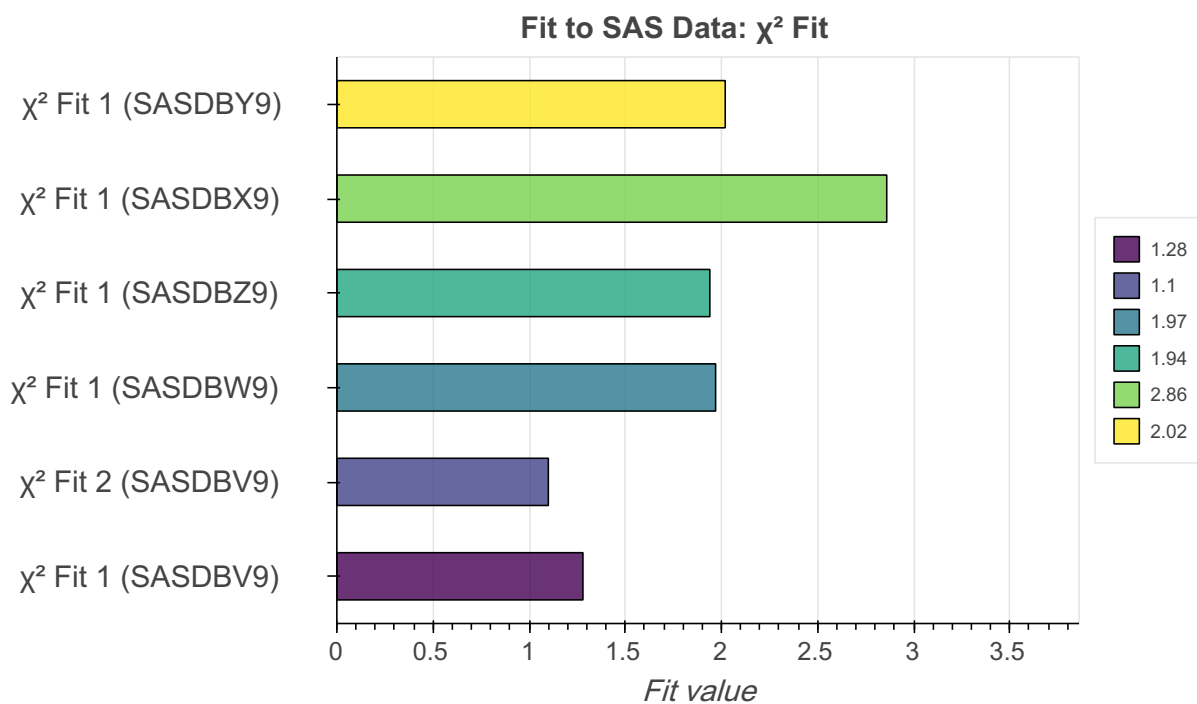
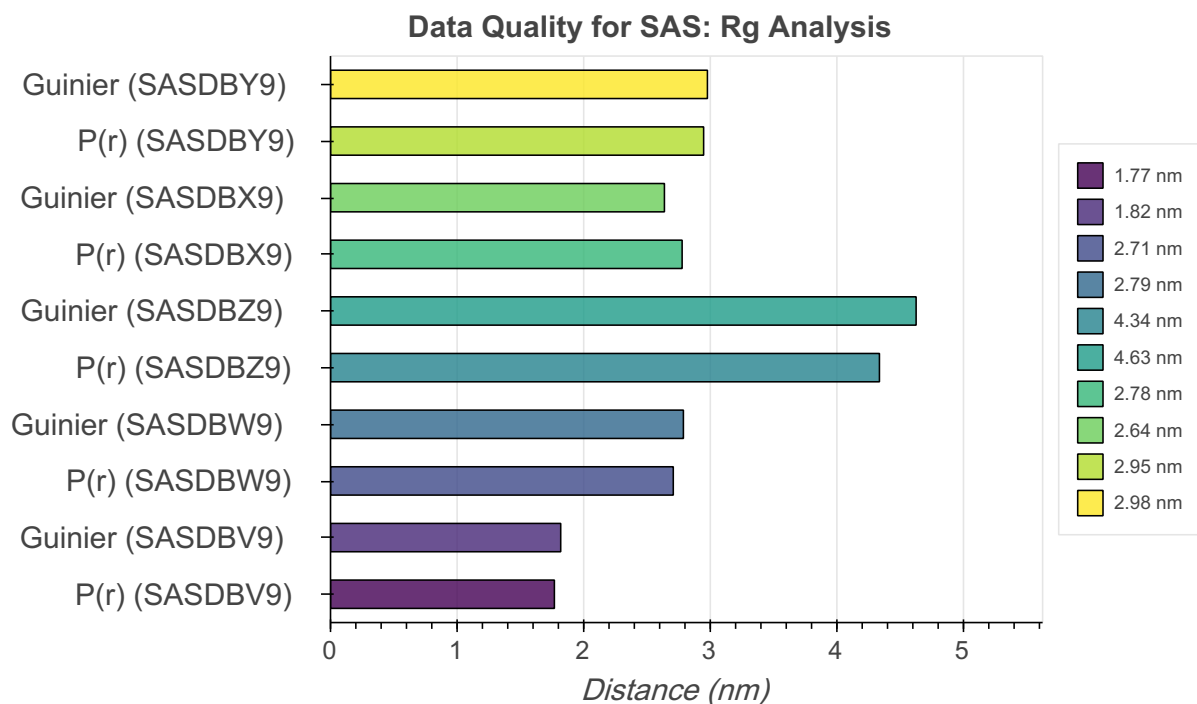
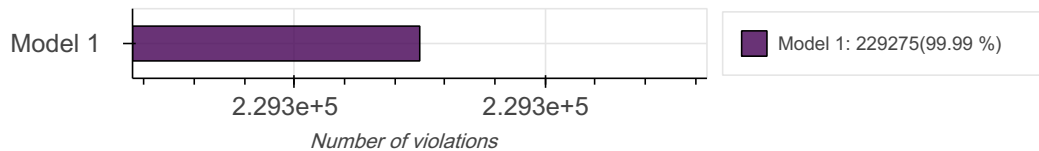
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

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 assessment for SAS datasets and fit to model assessments for SAS 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 1 distinct ensemble(s).

Summary ?

This entry consists of 1 unique models, with 207 subunits in each model. A total of 65 datasets or restraints were used to build this entry. Each model is represented by 24 rigid bodies and 2496 flexible or non-rigid units.

Entry composition ?

There is 1 unique type of models in this entry. This model is titled Scaffold cluster 1/None.

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 1 | 1 | 1 | Nup84 | A | A | 726 |
| 1 | 2 | 1 | Nup84 | H | H | 726 |
| 1 | 3 | 1 | Nup84 | O | O | 726 |
| 1 | 4 | 1 | Nup84 | V | V | 726 |
| 1 | 5 | 1 | Nup84 | AC | AC | 726 |
| 1 | 6 | 1 | Nup84 | AJ | AJ | 726 |
| 1 | 7 | 2 | Nup85 | B | B | 744 |
| 1 | 8 | 2 | Nup85 | I | I | 744 |
| 1 | 9 | 2 | Nup85 | P | P | 744 |
| 1 | 10 | 2 | Nup85 | W | W | 744 |
| 1 | 11 | 2 | Nup85 | AD | AD | 744 |
| 1 | 12 | 2 | Nup85 | AK | AK | 744 |
| 1 | 13 | 3 | Nup120 | C | C | 1037 |
| 1 | 14 | 3 | Nup120 | J | J | 1037 |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 1 | 15 | 3 | Nup120 | Q | Q | 1037 |
| 1 | 16 | 3 | Nup120 | X | X | 1037 |
| 1 | 17 | 3 | Nup120 | AE | AE | 1037 |
| 1 | 18 | 3 | Nup120 | AL | AL | 1037 |
| 1 | 19 | 4 | Nup133 | D | D | 1157 |
| 1 | 20 | 4 | Nup133 | K | K | 1157 |
| 1 | 21 | 4 | Nup133 | R | R | 1157 |
| 1 | 22 | 4 | Nup133 | Y | Y | 1157 |
| 1 | 23 | 4 | Nup133 | AF | AF | 1157 |
| 1 | 24 | 4 | Nup133 | AM | AM | 1157 |
| 1 | 25 | 5 | Nup145c | E | E | 712 |
| 1 | 26 | 5 | Nup145c | L | L | 712 |
| 1 | 27 | 5 | Nup145c | S | S | 712 |
| 1 | 28 | 5 | Nup145c | Z | Z | 712 |
| 1 | 29 | 5 | Nup145c | AG | AG | 712 |
| 1 | 30 | 5 | Nup145c | AN | AN | 712 |
| 1 | 31 | 6 | Seh1 | F | F | 349 |
| 1 | 32 | 6 | Seh1 | M | M | 349 |
| 1 | 33 | 6 | Seh1 | T | T | 349 |
| 1 | 34 | 6 | Seh1 | AA | AA | 349 |
| 1 | 35 | 6 | Seh1 | AH | AH | 349 |
| 1 | 36 | 6 | Seh1 | AO | AO | 349 |
| 1 | 37 | 7 | Sec13 | G | G | 297 |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 1 | 38 | 7 | Sec13 | N | N | 297 |
| 1 | 39 | 7 | Sec13 | U | U | 297 |
| 1 | 40 | 7 | Sec13 | AB | AB | 297 |
| 1 | 41 | 7 | Sec13 | AI | AI | 297 |
| 1 | 42 | 7 | Sec13 | AP | AP | 297 |
| 1 | 43 | 8 | Dyn2 | AQ | AQ | 92 |
| 1 | 44 | 8 | Dyn2 | AR | AR | 92 |
| 1 | 45 | 8 | Dyn2 | AY | AY | 92 |
| 1 | 46 | 8 | Dyn2 | AZ | AZ | 92 |
| 1 | 47 | 8 | Dyn2 | BG | BG | 92 |
| 1 | 48 | 8 | Dyn2 | BH | BH | 92 |
| 1 | 49 | 9 | Nup82 | AS | AS | 713 |
| 1 | 50 | 9 | Nup82 | AT | AT | 713 |
| 1 | 51 | 9 | Nup82 | BA | BA | 713 |
| 1 | 52 | 9 | Nup82 | BB | BB | 713 |
| 1 | 53 | 9 | Nup82 | BI | BI | 713 |
| 1 | 54 | 9 | Nup82 | BJ | BJ | 713 |
| 1 | 55 | 10 | Nup159 | AU | AU | 1460 |
| 1 | 56 | 10 | Nup159 | AV | AV | 1460 |
| 1 | 57 | 10 | Nup159 | BC | BC | 1460 |
| 1 | 58 | 10 | Nup159 | BD | BD | 1460 |
| 1 | 59 | 10 | Nup159 | BK | BK | 1460 |
| 1 | 60 | 10 | Nup159 | BL | BL | 1460 |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 1 | 61 | 11 | Nsp1 | AW | AW | 823 |
| 1 | 62 | 11 | Nsp1 | AX | AX | 823 |
| 1 | 63 | 11 | Nsp1 | BE | BE | 823 |
| 1 | 64 | 11 | Nsp1 | BF | BF | 823 |
| 1 | 65 | 11 | Nsp1 | BM | BM | 823 |
| 1 | 66 | 11 | Nsp1 | BN | BN | 823 |
| 1 | 67 | 11 | Nsp1 | BP | BP | 823 |
| 1 | 68 | 11 | Nsp1 | BT | BT | 823 |
| 1 | 69 | 11 | Nsp1 | BX | BX | 823 |
| 1 | 70 | 11 | Nsp1 | CB | CB | 823 |
| 1 | 71 | 11 | Nsp1 | CF | CF | 823 |
| 1 | 72 | 11 | Nsp1 | CJ | CJ | 823 |
| 1 | 73 | 11 | Nsp1 | CN | CN | 823 |
| 1 | 74 | 11 | Nsp1 | CR | CR | 823 |
| 1 | 75 | 11 | Nsp1 | CV | CV | 823 |
| 1 | 76 | 11 | Nsp1 | CZ | CZ | 823 |
| 1 | 77 | 11 | Nsp1 | DD | DD | 823 |
| 1 | 78 | 11 | Nsp1 | DH | DH | 823 |
| 1 | 79 | 12 | Nic96 | BO | BO | 839 |
| 1 | 80 | 12 | Nic96 | BS | BS | 839 |
| 1 | 81 | 12 | Nic96 | BW | BW | 839 |
| 1 | 82 | 12 | Nic96 | CA | CA | 839 |
| 1 | 83 | 12 | Nic96 | CE | CE | 839 |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 1 | 84 | 12 | Nic96 | CI | CI | 839 |
| 1 | 85 | 12 | Nic96 | CM | CM | 839 |
| 1 | 86 | 12 | Nic96 | CQ | CQ | 839 |
| 1 | 87 | 12 | Nic96 | CU | CU | 839 |
| 1 | 88 | 12 | Nic96 | CY | CY | 839 |
| 1 | 89 | 12 | Nic96 | DC | DC | 839 |
| 1 | 90 | 12 | Nic96 | DG | DG | 839 |
| 1 | 91 | 13 | Nup49 | BQ | BQ | 472 |
| 1 | 92 | 13 | Nup49 | BU | BU | 472 |
| 1 | 93 | 13 | Nup49 | BY | BY | 472 |
| 1 | 94 | 13 | Nup49 | CC | CC | 472 |
| 1 | 95 | 13 | Nup49 | CG | CG | 472 |
| 1 | 96 | 13 | Nup49 | CK | CK | 472 |
| 1 | 97 | 13 | Nup49 | CO | CO | 472 |
| 1 | 98 | 13 | Nup49 | CS | CS | 472 |
| 1 | 99 | 13 | Nup49 | CW | CW | 472 |
| 1 | 100 | 13 | Nup49 | DA | DA | 472 |
| 1 | 101 | 13 | Nup49 | DE | DE | 472 |
| 1 | 102 | 13 | Nup49 | DI | DI | 472 |
| 1 | 103 | 14 | Nup57 | BR | BR | 541 |
| 1 | 104 | 14 | Nup57 | BV | BV | 541 |
| 1 | 105 | 14 | Nup57 | BZ | BZ | 541 |
| 1 | 106 | 14 | Nup57 | CD | CD | 541 |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 1 | 107 | 14 | Nup57 | CH | CH | 541 |
| 1 | 108 | 14 | Nup57 | CL | CL | 541 |
| 1 | 109 | 14 | Nup57 | CP | CP | 541 |
| 1 | 110 | 14 | Nup57 | CT | CT | 541 |
| 1 | 111 | 14 | Nup57 | CX | CX | 541 |
| 1 | 112 | 14 | Nup57 | DB | DB | 541 |
| 1 | 113 | 14 | Nup57 | DF | DF | 541 |
| 1 | 114 | 14 | Nup57 | DJ | DJ | 541 |
| 1 | 115 | 15 | Nup157 | DK | DK | 1391 |
| 1 | 116 | 15 | Nup157 | DO | DO | 1391 |
| 1 | 117 | 15 | Nup157 | DS | DS | 1391 |
| 1 | 118 | 15 | Nup157 | DW | DW | 1391 |
| 1 | 119 | 15 | Nup157 | EA | EA | 1391 |
| 1 | 120 | 15 | Nup157 | EE | EE | 1391 |
| 1 | 121 | 16 | Nup170 | DL | DL | 1502 |
| 1 | 122 | 16 | Nup170 | DP | DP | 1502 |
| 1 | 123 | 16 | Nup170 | DT | DT | 1502 |
| 1 | 124 | 16 | Nup170 | DX | DX | 1502 |
| 1 | 125 | 16 | Nup170 | EB | EB | 1502 |
| 1 | 126 | 16 | Nup170 | EF | EF | 1502 |
| 1 | 127 | 17 | Nup188 | DM | DM | 1655 |
| 1 | 128 | 17 | Nup188 | DQ | DQ | 1655 |
| 1 | 129 | 17 | Nup188 | DU | DU | 1655 |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 1 | 130 | 17 | Nup188 | DY | DY | 1655 |
| 1 | 131 | 17 | Nup188 | EC | EC | 1655 |
| 1 | 132 | 17 | Nup188 | EG | EG | 1655 |
| 1 | 133 | 18 | Nup192 | DN | DN | 1683 |
| 1 | 134 | 18 | Nup192 | DR | DR | 1683 |
| 1 | 135 | 18 | Nup192 | DV | DV | 1683 |
| 1 | 136 | 18 | Nup192 | DZ | DZ | 1683 |
| 1 | 137 | 18 | Nup192 | ED | ED | 1683 |
| 1 | 138 | 18 | Nup192 | EH | EH | 1683 |
| 1 | 139 | 19 | Nup53 | EI | EI | 475 |
| 1 | 140 | 19 | Nup53 | EN | EN | 475 |
| 1 | 141 | 19 | Nup53 | ES | ES | 475 |
| 1 | 142 | 19 | Nup53 | EX | EX | 475 |
| 1 | 143 | 19 | Nup53 | FC | FC | 475 |
| 1 | 144 | 19 | Nup53 | FH | FH | 475 |
| 1 | 145 | 20 | Nup59 | EJ | EJ | 528 |
| 1 | 146 | 20 | Nup59 | EO | EO | 528 |
| 1 | 147 | 20 | Nup59 | ET | ET | 528 |
| 1 | 148 | 20 | Nup59 | EY | EY | 528 |
| 1 | 149 | 20 | Nup59 | FD | FD | 528 |
| 1 | 150 | 20 | Nup59 | FI | FI | 528 |
| 1 | 151 | 21 | Ndc1 | EK | EK | 655 |
| 1 | 152 | 21 | Ndc1 | EP | EP | 655 |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 1 | 153 | 21 | Ndc1 | EU | EU | 655 |
| 1 | 154 | 21 | Ndc1 | EZ | EZ | 655 |
| 1 | 155 | 21 | Ndc1 | FE | FE | 655 |
| 1 | 156 | 21 | Ndc1 | FJ | FJ | 655 |
| 1 | 157 | 22 | Pom34 | EL | EL | 299 |
| 1 | 158 | 22 | Pom34 | EQ | EQ | 299 |
| 1 | 159 | 22 | Pom34 | EV | EV | 299 |
| 1 | 160 | 22 | Pom34 | FA | FA | 299 |
| 1 | 161 | 22 | Pom34 | FF | FF | 299 |
| 1 | 162 | 22 | Pom34 | FK | FK | 299 |
| 1 | 163 | 23 | Pom152 | EM | EM | 1337 |
| 1 | 164 | 23 | Pom152 | ER | ER | 1337 |
| 1 | 165 | 23 | Pom152 | EW | EW | 1337 |
| 1 | 166 | 23 | Pom152 | FB | FB | 1337 |
| 1 | 167 | 23 | Pom152 | FG | FG | 1337 |
| 1 | 168 | 23 | Pom152 | FL | FL | 1337 |
| 1 | 169 | 24 | Nup100 | FM | FM | 959 |
| 1 | 170 | 24 | Nup100 | FN | FN | 959 |
| 1 | 171 | 24 | Nup100 | FS | FS | 959 |
| 1 | 172 | 24 | Nup100 | FT | FT | 959 |
| 1 | 173 | 24 | Nup100 | FY | FY | 959 |
| 1 | 174 | 24 | Nup100 | FZ | FZ | 959 |
| 1 | 175 | 25 | Nup116 | FO | FO | 1113 |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 1 | 176 | 25 | Nup116 | FP | FP | 1113 |
| 1 | 177 | 25 | Nup116 | FU | FU | 1113 |
| 1 | 178 | 25 | Nup116 | FV | FV | 1113 |
| 1 | 179 | 25 | Nup116 | GA | GA | 1113 |
| 1 | 180 | 25 | Nup116 | GB | GB | 1113 |
| 1 | 181 | 26 | Nup42 | FQ | FQ | 430 |
| 1 | 182 | 26 | Nup42 | FW | FW | 430 |
| 1 | 183 | 26 | Nup42 | GC | GC | 430 |
| 1 | 184 | 27 | Gle1 | FR | FR | 538 |
| 1 | 185 | 27 | Gle1 | FX | FX | 538 |
| 1 | 186 | 27 | Gle1 | GD | GD | 538 |
| 1 | 187 | 28 | Nup145 | GE | GE | 1317 |
| 1 | 188 | 28 | Nup145 | GF | GF | 1317 |
| 1 | 189 | 28 | Nup145 | GJ | GJ | 1317 |
| 1 | 190 | 28 | Nup145 | GK | GK | 1317 |
| 1 | 191 | 28 | Nup145 | GO | GO | 1317 |
| 1 | 192 | 28 | Nup145 | GP | GP | 1317 |
| 1 | 193 | 29 | Nup1 | GG | GG | 1076 |
| 1 | 194 | 29 | Nup1 | GL | GL | 1076 |
| 1 | 195 | 29 | Nup1 | GQ | GQ | 1076 |
| 1 | 196 | 30 | Nup60 | GH | GH | 539 |
| 1 | 197 | 30 | Nup60 | GI | GI | 539 |
| 1 | 198 | 30 | Nup60 | GM | GM | 539 |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 1 | 199 | 30 | Nup60 | GN | GN | 539 |
| 1 | 200 | 30 | Nup60 | GR | GR | 539 |
| 1 | 201 | 30 | Nup60 | GS | GS | 539 |
| 1 | 202 | 31 | Mlp1 | GT | GT | 1875 |
| 1 | 203 | 31 | Mlp1 | GV | GV | 1875 |
| 1 | 204 | 31 | Mlp1 | GX | GX | 1875 |
| 1 | 205 | 32 | Mlp2 | GU | GU | 1679 |
| 1 | 206 | 32 | Mlp2 | GW | GW | 1679 |
| 1 | 207 | 32 | Mlp2 | GY | GY | 1679 |

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 | File | 10.1016/j.cell.2016.10.028 |
| 2 | Integrative model | File | 10.5281/zenodo.1194547 |
| 3 | Experimental model | PDB | 5CWS |
| 4 | Comparative model | File | 10.5281/zenodo.1194547 |
| 5 | Experimental model | PDB | 2QX5 |
| 6 | Experimental model | File | 10.5281/zenodo.1194547 |
| 7 | Experimental model | File | 10.5281/zenodo.1194547 |
| 8 | Comparative model | File | 10.5281/zenodo.1194547 |
| 9 | Comparative model | File | 10.5281/zenodo.1194547 |
| 10 | Comparative model | File | 10.5281/zenodo.1194547 |

| ID | Dataset type | Database name | Data access code |
|-----------|------------------------|----------------------|---------------------------|
| 11 | Comparative model | File | 10.5281/zenodo.1194547 |
| 12 | Comparative model | File | 10.5281/zenodo.1194547 |
| 13 | Comparative model | File | 10.5281/zenodo.1194547 |
| 14 | Integrative model | File | 10.1016/j.str.2017.01.006 |
| 15 | Integrative model | File | 10.5281/zenodo.1194547 |
| 16 | Experimental model | PDB | 3NF5 |
| 17 | Comparative model | File | 10.5281/zenodo.1194547 |
| 18 | Comparative model | File | 10.5281/zenodo.1194547 |
| 19 | Experimental model | PDB | 3KEP |
| 20 | Experimental model | File | 10.5281/zenodo.1194547 |
| 21 | Mass Spectrometry data | File | 10.5281/zenodo.1149746 |
| 22 | Crosslinking-MS data | File | 10.5281/zenodo.1194547 |
| 23 | Crosslinking-MS data | File | 10.5281/zenodo.1194547 |
| 24 | EM raw micrographs | EMPIAR | EMPIAR-10155 |
| 25 | 3DEM volume | EMDB | EMD-7321 |
| 26 | 3DEM volume | File | 10.5281/zenodo.1194547 |
| 27 | SAS data | File | 10.5281/zenodo.1194547 |
| 28 | SAS data | File | 10.5281/zenodo.1194547 |
| 29 | SAS data | File | 10.5281/zenodo.1194547 |
| 30 | SAS data | File | 10.5281/zenodo.1194547 |
| 31 | SAS data | File | 10.5281/zenodo.1194547 |
| 32 | SAS data | File | 10.5281/zenodo.1194547 |
| 33 | SAS data | File | 10.5281/zenodo.1194547 |

| ID | Dataset type | Database name | Data access code |
|----|--------------|---------------|------------------------|
| 34 | SAS data | File | 10.5281/zenodo.1194547 |
| 35 | SAS data | File | 10.5281/zenodo.1194547 |
| 36 | SAS data | File | 10.5281/zenodo.1194547 |
| 37 | SAS data | File | 10.5281/zenodo.1194547 |
| 38 | SAS data | File | 10.5281/zenodo.1194547 |
| 39 | SAS data | File | 10.5281/zenodo.1194547 |
| 40 | SAS data | File | 10.5281/zenodo.1194547 |
| 41 | SAS data | File | 10.5281/zenodo.1194547 |
| 42 | SAS data | File | 10.5281/zenodo.1194547 |
| 43 | SAS data | File | 10.5281/zenodo.1194547 |
| 44 | SAS data | File | 10.5281/zenodo.1194547 |
| 45 | SAS data | File | 10.5281/zenodo.1194547 |
| 46 | SAS data | File | 10.5281/zenodo.1194547 |
| 47 | SAS data | File | 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 | File | 10.5281/zenodo.1194547 |
| 54 | SAS data | File | 10.5281/zenodo.1194547 |
| 55 | SAS data | File | 10.5281/zenodo.1194547 |
| 56 | SAS data | File | 10.5281/zenodo.1194547 |

| ID | Dataset type | Database name | Data access code |
|----|--------------------|---------------|------------------------|
| 57 | SAS data | File | 10.5281/zenodo.1194547 |
| 58 | SAS data | File | 10.5281/zenodo.1194547 |
| 59 | SAS data | File | 10.5281/zenodo.1194547 |
| 60 | SAS data | File | 10.5281/zenodo.1194547 |
| 61 | SAS data | File | 10.5281/zenodo.1194547 |
| 62 | SAS data | File | 10.5281/zenodo.1194547 |
| 63 | EM raw micrographs | EMPIAR | EMPIAR-10162 |
| 64 | 2DEM class average | File | 10.5281/zenodo.1194547 |
| 65 | 2DEM class average | File | 10.5281/zenodo.1194547 |

Representation

This entry has only one representation and includes 24 rigid bodies and 2496 flexible units

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--------------|--|
| A | - | 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 |
| B | - | 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 |
| C | - | 1-1, 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, 1037-1037 |
| D | - | 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 |
| E | - | 1-91, 92-99, 100-125, 126-144, 145-148, 149-550, 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 |

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--------------|--|
| F | - | 1-248, 249-287, 288-346, 347-349 |
| G | - | 1-9, 10-158, 159-165, 166-296, 297-297 |
| H | - | 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 |
| I | - | 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 |
| J | - | 1-1, 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, 1037-1037 |
| K | - | 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 |
| L | - | 1-91, 92-99, 100-125, 126-144, 145-148, 149-550, 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 |
| M | - | 1-248, 249-287, 288-346, 347-349 |
| N | - | 1-9, 10-158, 159-165, 166-296, 297-297 |
| O | - | 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 |
| P | - | 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 |
| Q | - | 1-1, 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, 1037-1037 |
| R | - | 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 |

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--------------|--|
| S | - | 1-91, 92-99, 100-125, 126-144, 145-148, 149-550, 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 |
| T | - | 1-248, 249-287, 288-346, 347-349 |
| U | - | 1-9, 10-158, 159-165, 166-296, 297-297 |
| V | - | 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 |
| W | - | 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 |
| X | - | 1-1, 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, 1037-1037 |
| Y | - | 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 |
| Z | - | 1-91, 92-99, 100-125, 126-144, 145-148, 149-550, 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 |
| AA | - | 1-248, 249-287, 288-346, 347-349 |
| AB | - | 1-9, 10-158, 159-165, 166-296, 297-297 |
| AC | - | 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 |
| AD | - | 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 |
| AE | - | 1-1, 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, 1037-1037 |

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--------------|--|
| AF | - | 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 |
| AG | - | 1-91, 92-99, 100-125, 126-144, 145-148, 149-550, 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 |
| AH | - | 1-248, 249-287, 288-346, 347-349 |
| AI | - | 1-9, 10-158, 159-165, 166-296, 297-297 |
| AJ | - | 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 |
| AK | - | 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 |
| AL | - | 1-1, 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, 1037-1037 |
| AM | - | 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 |
| AN | - | 1-91, 92-99, 100-125, 126-144, 145-148, 149-550, 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 |
| AO | - | 1-248, 249-287, 288-346, 347-349 |
| AP | - | 1-9, 10-158, 159-165, 166-296, 297-297 |
| AQ | - | 1-6, 7-92 |
| AR | - | 1-6, 7-92 |
| AS | - | 1-6, 7-16, 17-22, 23-120, 121-122, 123-452, 453-521, 522-612, 613-624, 625-669, 670-677, 678-713 |
| AT | - | 1-6, 7-16, 17-22, 23-120, 121-122, 123-452, 453-521, 522-612, 613-624, 625-669, 670-677, 678-713 |

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--------------|---|
| AU | - | 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 |
| AV | - | 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 |
| AW | - | 601-636, 637-727, 728-741, 742-778, 779-787, 788-823 |
| AX | - | 601-636, 637-727, 728-741, 742-778, 779-787, 788-823 |
| AY | - | 1-6, 7-92 |
| AZ | - | 1-6, 7-92 |
| BA | - | 1-6, 7-16, 17-22, 23-120, 121-122, 123-452, 453-521, 522-612, 613-624, 625-669, 670-677, 678-713 |
| BB | - | 1-6, 7-16, 17-22, 23-120, 121-122, 123-452, 453-521, 522-612, 613-624, 625-669, 670-677, 678-713 |
| BC | - | 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 |
| BD | - | 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 |
| BE | - | 601-636, 637-727, 728-741, 742-778, 779-787, 788-823 |
| BF | - | 601-636, 637-727, 728-741, 742-778, 779-787, 788-823 |
| BG | - | 1-6, 7-92 |
| BH | - | 1-6, 7-92 |
| BI | - | 1-6, 7-16, 17-22, 23-120, 121-122, 123-452, 453-521, 522-612, 613-624, 625-669, 670-677, 678-713 |
| BJ | - | 1-6, 7-16, 17-22, 23-120, 121-122, 123-452, 453-521, 522-612, 613-624, 625-669, 670-677, 678-713 |
| BK | - | 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 |
| BL | - | 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 |

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|---------------------------------|--|
| BM | - | 601-636, 637-727, 728-741, 742-778, 779-787, 788-823 |
| BN | - | 601-636, 637-727, 728-741, 742-778, 779-787, 788-823 |
| BO | 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 |
| BP | 637-727, 742-778, 788-823 | 601-636, 728-741, 779-787 |
| BQ | 270-359, 369-407, 433-472 | 201-269, 360-368, 408-432 |
| BR | 287-423, 433-476, 505-540 | 201-286, 424-432, 477-504, 541-541 |
| BS | 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 |
| BT | 637-727, 742-778, 788-823 | 601-636, 728-741, 779-787 |
| BU | 270-359, 369-407, 433-472 | 201-269, 360-368, 408-432 |

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|---------------------------|---|
| BV | 287-423, 433-476, 505-540 | 201-286, 424-432, 477-504, 541-541 |
| BW | - | 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 |
| BX | - | 601-636, 637-727, 728-741, 742-778, 779-787, 788-823 |
| BY | - | 201-269, 270-359, 360-368, 369-407, 408-432, 433-472 |
| BZ | - | 201-286, 287-423, 424-432, 433-476, 477-504, 505-540, 541-541 |
| CA | - | 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 |
| CB | - | 601-636, 637-727, 728-741, 742-778, 779-787, 788-823 |
| CC | - | 201-269, 270-359, 360-368, 369-407, 408-432, 433-472 |
| CD | - | 201-286, 287-423, 424-432, 433-476, 477-504, 505-540, 541-541 |
| CE | - | 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 |
| CF | - | 601-636, 637-727, 728-741, 742-778, 779-787, 788-823 |
| CG | - | 201-269, 270-359, 360-368, 369-407, 408-432, 433-472 |
| CH | - | 201-286, 287-423, 424-432, 433-476, 477-504, 505-540, 541-541 |
| CI | - | 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 |
| CJ | - | 601-636, 637-727, 728-741, 742-778, 779-787, 788-823 |
| CK | - | 201-269, 270-359, 360-368, 369-407, 408-432, 433-472 |
| CL | - | 201-286, 287-423, 424-432, 433-476, 477-504, 505-540, 541-541 |

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--------------|---|
| CM | - | 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 |
| CN | - | 601-636, 637-727, 728-741, 742-778, 779-787, 788-823 |
| CO | - | 201-269, 270-359, 360-368, 369-407, 408-432, 433-472 |
| CP | - | 201-286, 287-423, 424-432, 433-476, 477-504, 505-540, 541-541 |
| CQ | - | 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 |
| CR | - | 601-636, 637-727, 728-741, 742-778, 779-787, 788-823 |
| CS | - | 201-269, 270-359, 360-368, 369-407, 408-432, 433-472 |
| CT | - | 201-286, 287-423, 424-432, 433-476, 477-504, 505-540, 541-541 |
| CU | - | 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 |
| CV | - | 601-636, 637-727, 728-741, 742-778, 779-787, 788-823 |
| CW | - | 201-269, 270-359, 360-368, 369-407, 408-432, 433-472 |
| CX | - | 201-286, 287-423, 424-432, 433-476, 477-504, 505-540, 541-541 |
| CY | - | 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 |
| CZ | - | 601-636, 637-727, 728-741, 742-778, 779-787, 788-823 |
| DA | - | 201-269, 270-359, 360-368, 369-407, 408-432, 433-472 |
| DB | - | 201-286, 287-423, 424-432, 433-476, 477-504, 505-540, 541-541 |
| DC | - | 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 |
| DD | - | 601-636, 637-727, 728-741, 742-778, 779-787, 788-823 |
| DE | - | 201-269, 270-359, 360-368, 369-407, 408-432, 433-472 |
| DF | - | 201-286, 287-423, 424-432, 433-476, 477-504, 505-540, 541-541 |

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--------------|--|
| DG | - | 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 |
| DH | - | 601-636, 637-727, 728-741, 742-778, 779-787, 788-823 |
| DI | - | 201-269, 270-359, 360-368, 369-407, 408-432, 433-472 |
| DJ | - | 201-286, 287-423, 424-432, 433-476, 477-504, 505-540, 541-541 |
| DK | - | 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, 1391-1391 |
| DL | - | 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 |
| DM | - | 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, 288-304, 305-317, 318-434, 435-438, 439-479, 480-492, 493-508, 509-514, 515-530, 531-550, 551-577, 578-583, 584-605, 606-607, 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 |
| DN | - | 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 |
| DO | - | 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, 1391-1391 |
| DP | - | 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 |

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--------------|--|
| DQ | - | 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, 288-304, 305-317, 318-434, 435-438, 439-479, 480-492, 493-508, 509-514, 515-530, 531-550, 551-577, 578-583, 584-605, 606-607, 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 |
| DR | - | 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 |
| DS | - | 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, 1391-1391 |
| DT | - | 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 |
| DU | - | 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, 288-304, 305-317, 318-434, 435-438, 439-479, 480-492, 493-508, 509-514, 515-530, 531-550, 551-577, 578-583, 584-605, 606-607, 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 |
| DV | - | 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 |
| DW | - | 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, 1391-1391 |
| DX | - | 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 |

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--------------|--|
| DY | - | 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, 288-304, 305-317, 318-434, 435-438, 439-479, 480-492, 493-508, 509-514, 515-530, 531-550, 551-577, 578-583, 584-605, 606-607, 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 |
| DZ | - | 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 |
| EA | - | 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, 1391-1391 |
| EB | - | 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 |
| EC | - | 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, 288-304, 305-317, 318-434, 435-438, 439-479, 480-492, 493-508, 509-514, 515-530, 531-550, 551-577, 578-583, 584-605, 606-607, 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 |
| ED | - | 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 |
| EE | - | 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, 1391-1391 |
| EF | - | 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 |

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--------------|--|
| EG | - | 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, 288-304, 305-317, 318-434, 435-438, 439-479, 480-492, 493-508, 509-514, 515-530, 531-550, 551-577, 578-583, 584-605, 606-607, 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 |
| EH | - | 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 |
| EI | - | 1-247, 248-284, 285-303, 304-360, 361-475 |
| EJ | - | 1-265, 266-302, 303-345, 346-402, 403-528 |
| EK | - | 1-655 |
| EL | - | 1-299 |
| EM | - | 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 |
| EN | - | 1-247, 248-284, 285-303, 304-360, 361-475 |
| EO | - | 1-265, 266-302, 303-345, 346-402, 403-528 |
| EP | - | 1-655 |
| EQ | - | 1-299 |
| ER | - | 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 |
| ES | - | 1-247, 248-284, 285-303, 304-360, 361-475 |
| ET | - | 1-265, 266-302, 303-345, 346-402, 403-528 |
| EU | - | 1-655 |
| EV | - | 1-299 |
| EW | - | 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 |

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--------------|---|
| EX | - | 1-247, 248-284, 285-303, 304-360, 361-475 |
| EY | - | 1-265, 266-302, 303-345, 346-402, 403-528 |
| EZ | - | 1-655 |
| FA | - | 1-299 |
| FB | - | 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 |
| FC | - | 1-247, 248-284, 285-303, 304-360, 361-475 |
| FD | - | 1-265, 266-302, 303-345, 346-402, 403-528 |
| FE | - | 1-655 |
| FF | - | 1-299 |
| FG | - | 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 |
| FH | - | 1-247, 248-284, 285-303, 304-360, 361-475 |
| FI | - | 1-265, 266-302, 303-345, 346-402, 403-528 |
| FJ | - | 1-655 |
| FK | - | 1-299 |
| FL | - | 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 |
| FM | 816-958 | 551-815, 959-959 |
| FN | 816-958 | 551-815, 959-959 |
| FO | - | 751-965, 966-1111, 1112-1113 |
| FP | - | 751-965, 966-1111, 1112-1113 |
| FQ | - | - |

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--------------|------------------------------|
| FR | - | 1-120 |
| FS | - | 551-815, 816-958, 959-959 |
| FT | - | 551-815, 816-958, 959-959 |
| FU | - | 751-965, 966-1111, 1112-1113 |
| FV | - | 751-965, 966-1111, 1112-1113 |
| FW | - | - |
| FX | - | 1-120 |
| FY | - | 551-815, 816-958, 959-959 |
| FZ | - | 551-815, 816-958, 959-959 |
| GA | - | 751-965, 966-1111, 1112-1113 |
| GB | - | 751-965, 966-1111, 1112-1113 |
| GC | - | - |
| GD | - | 1-120 |
| GE | 459-605 | 201-458 |
| GF | 459-605 | 201-458 |
| GG | - | 1-351 |
| GH | - | 1-398 |
| GI | - | 1-398 |
| GJ | - | 201-458, 459-605 |
| GK | - | 201-458, 459-605 |
| GL | - | 1-351 |
| GM | - | 1-398 |

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--------------|--------------------|
| GN | - | 1-398 |
| GO | - | 201-458, 459-605 |
| GP | - | 201-458, 459-605 |
| GQ | - | 1-351 |
| GR | - | 1-398 |
| GS | - | 1-398 |
| GT | - | 238-716 |
| GU | - | 215-690 |
| GV | - | 238-716 |
| GW | - | 215-690 |
| GX | - | 238-716 |
| GY | - | 215-690 |

Methodology and software

This entry is a result of 1 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 | Replica exchange monte carlo | Sampling | None | 500 | False | True |
| 2 | 1 | Replica exchange monte carlo | Sampling | None | 3000 | False | True |
| 3 | 1 | Replica exchange monte carlo | Sampling | 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 | 4.0 | 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 | 2.2 | image processing | http://blake.bcm.edu/emanwiki/EMAN2 |
| 9 | RELION | 1.4 | 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/ |
| 12 | MODELLER | 9.15 | comparative modeling | https://salilab.org/modeller/ |
| 13 | MODELLER | 9.13 | comparative modeling | https://salilab.org/modeller/ |

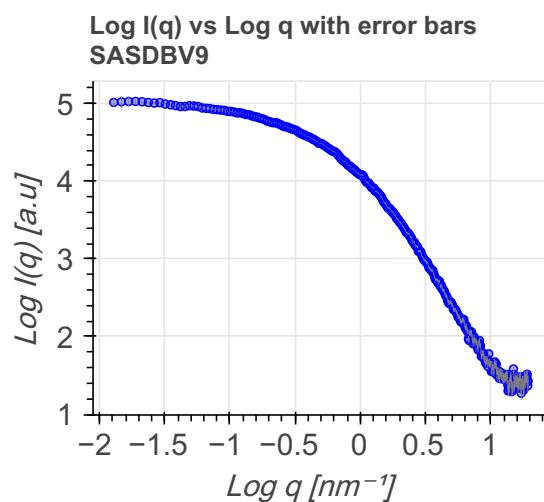
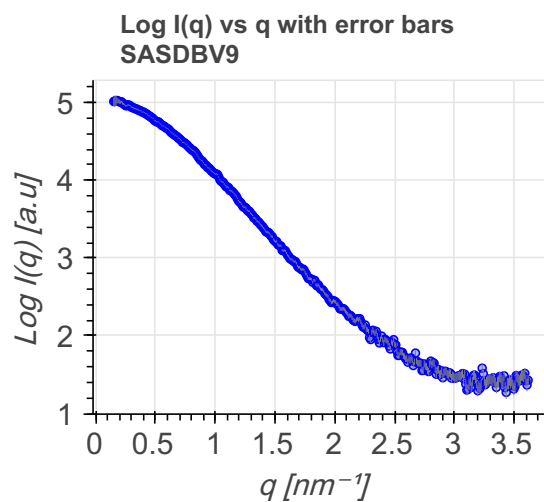
Data quality ?

Scattering profile ?

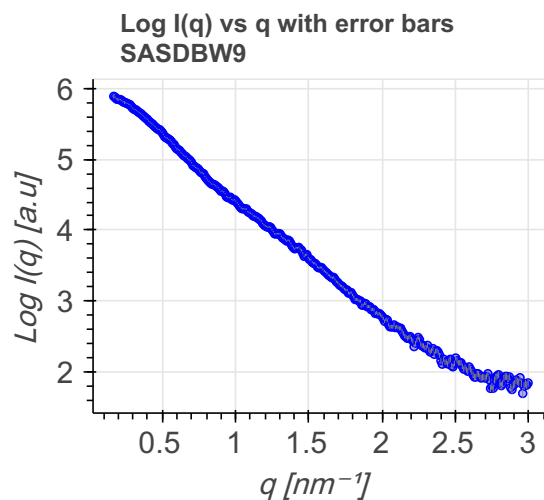
SAS data used in this integrative model was obtained from 5 deposited SASBDB entry (entries).

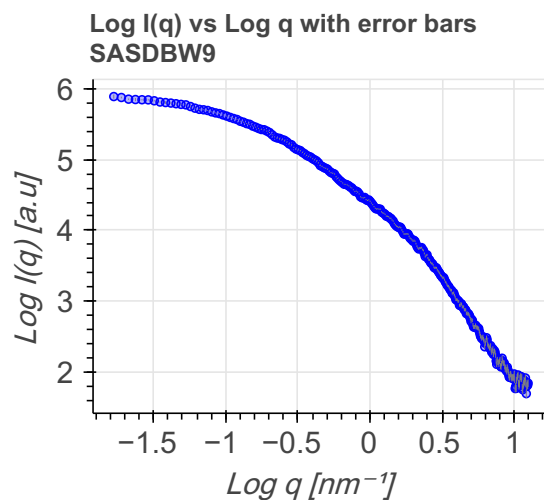
Scattering profile for SASDBV9: data from solutions of biological macromolecules are presented as both log I(q) vs q and

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.

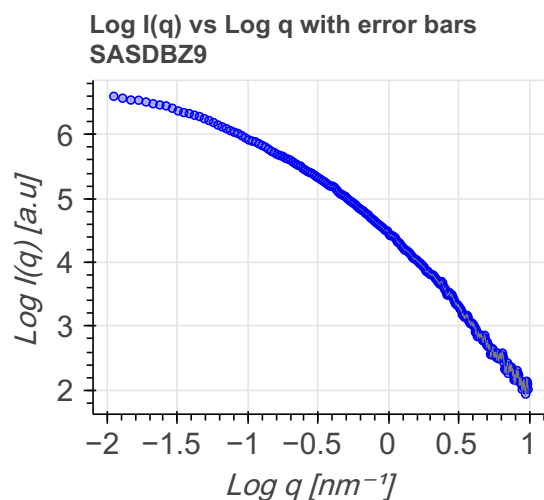
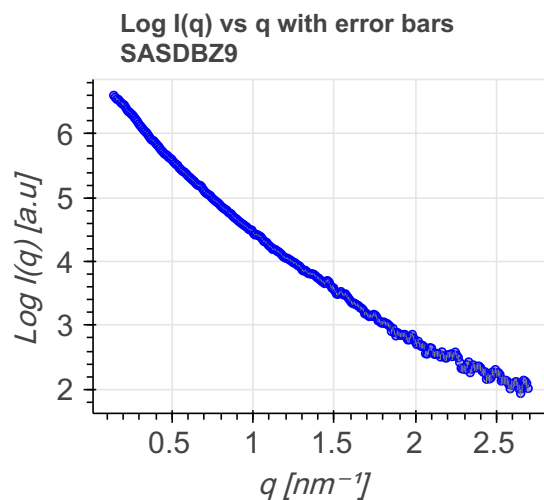


Scattering profile for SASDBW9: data from solutions of biological macromolecules are presented as both log I(q) vs q and log I(q) vs log (q) based on SAS validation task force (SASvtf) recommendations. I(q) is the intensity (in arbitrary units) and q is the modulus of the scattering vector.

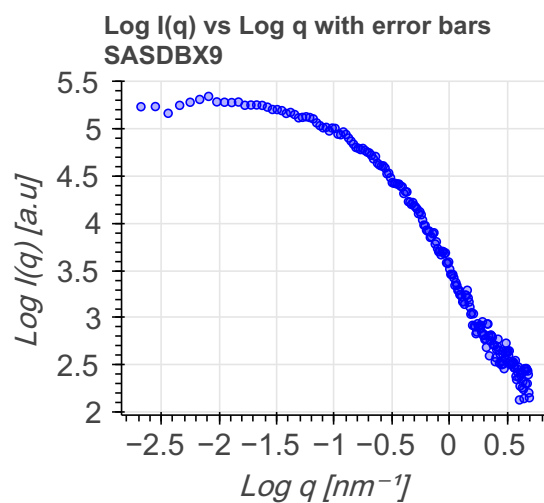
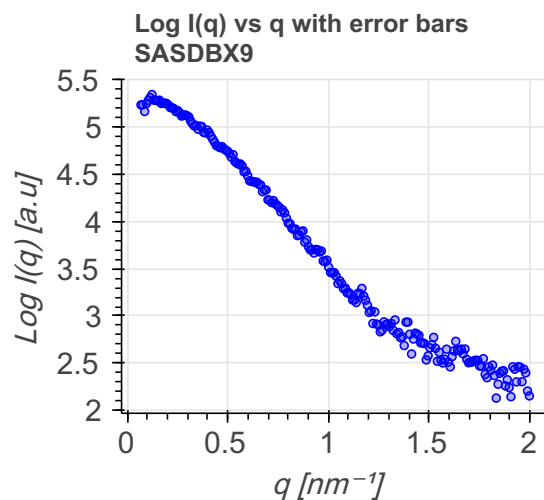




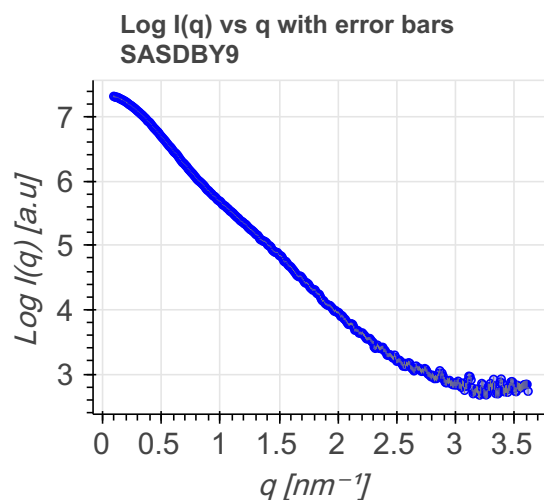
Scattering profile for [SASDBZ9](#): data from solutions of biological macromolecules are presented as both $\log I(q)$ vs q and $\log I(q)$ vs $\log(q)$ based on [SAS validation task force \(SASvtf\) recommendations](#). $I(q)$ is the intensity (in arbitrary units) and q is the modulus of the scattering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

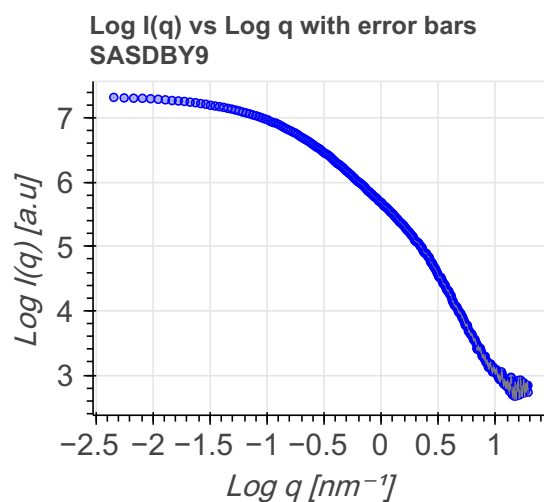


Scattering profile for [SASDBX9](#): data from solutions of biological macromolecules are presented as both $\log I(q)$ vs q and $\log I(q)$ vs $\log(q)$ based on [SAS validation task force \(SASvtf\) recommendations](#). $I(q)$ is the intensity (in arbitrary units) and q is the modulus of the scattering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



Scattering profile for [SASDBY9](#): data from solutions of biological macromolecules are presented as both $\log I(q)$ 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.





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 | N/A |
| SASDBW9 | 24.1 kDa | 25.2 kDa | N/A |
| SASDBZ9 | 49.4 kDa | 48.3 kDa | N/A |
| SASDBX9 | 12.5 kDa | 14.7 kDa | N/A |
| SASDBY9 | 25.9 kDa | 25.2 kDa | N/A |

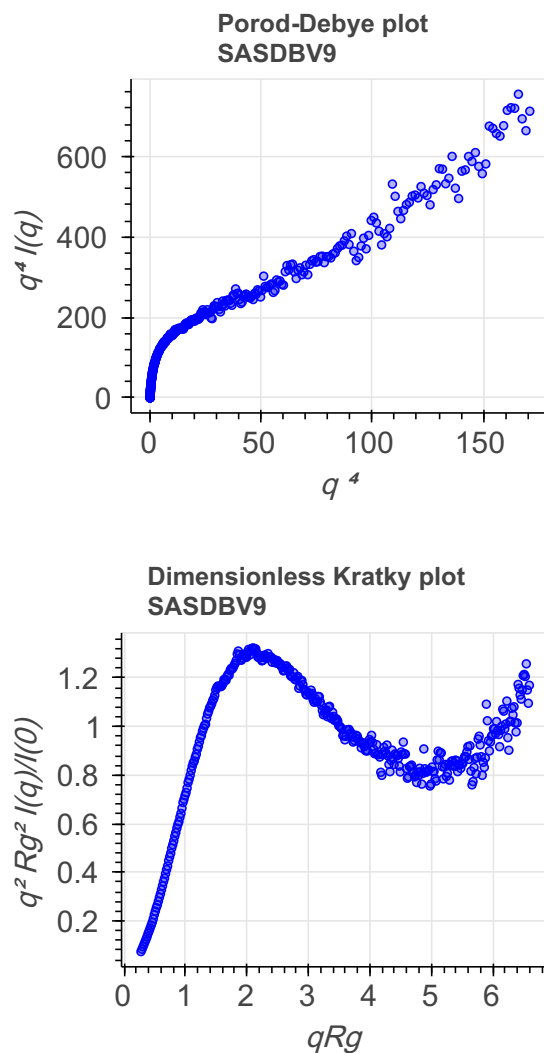
Volume estimates from experiments and analysis: estimated volume can be compared to Porod volume obtained from scattering profiles.

| SASDB ID | Estimated Volume | Porod Volume | Specific Volume | Sample Contrast | Sample Concentration |
|----------|------------------|-----------------------|-----------------|-----------------|----------------------|
| SASDBV9 | N/A | 17.94 nm ³ | N/A | N/A | N/A |
| SASDBW9 | N/A | 22.50 nm ³ | N/A | N/A | N/A |
| SASDBZ9 | N/A | 66.59 nm ³ | N/A | N/A | N/A |
| SASDBX9 | N/A | 56.68 nm ³ | N/A | N/A | N/A |
| SASDBY9 | N/A | 27.97 nm ³ | N/A | N/A | N/A |

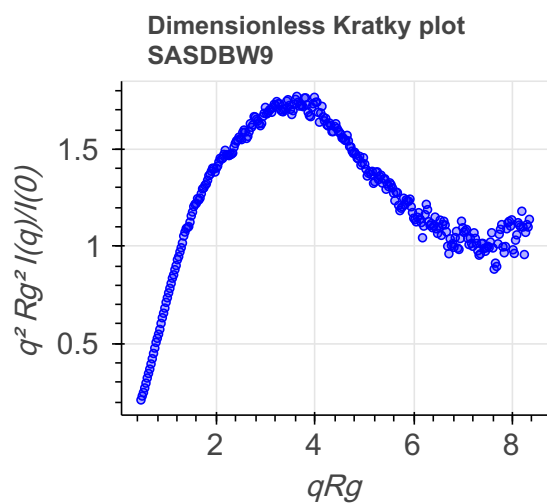
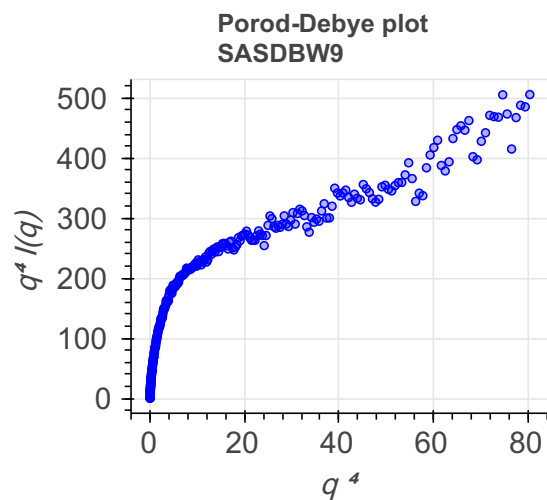
Flexibility analysis ?

Flexibility analysis for SASDBV9: In a Porod-Debye plot, a clear plateau is observed for globular (partial or fully folded)

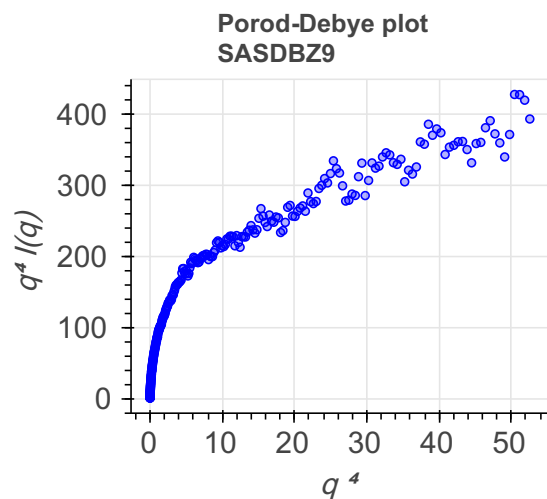
domains, whereas, fully unfolded domains are devoid of any discernable plateau. For details, refer to Figure 5 in [Rambo and Tainer, 2011](#) . In a Kratky plot, a parabolic shape is observed for globular (partial or fully folded) domains and a hyperbolic shape is observed for fully unfolded domains.

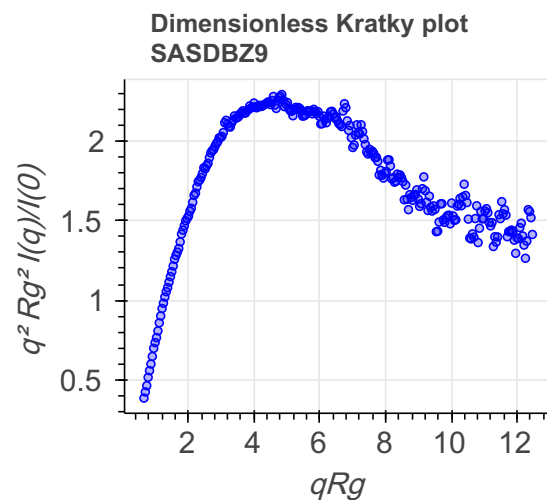


Flexibility analysis for SASDBV9: In a Porod-Debye plot, a clear plateau is observed for globular (partial or fully folded) domains, whereas, fully unfolded domains are devoid of any discernable plateau. For details, refer to Figure 5 in [Rambo and Tainer, 2011](#) . In a Kratky plot, a parabolic shape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

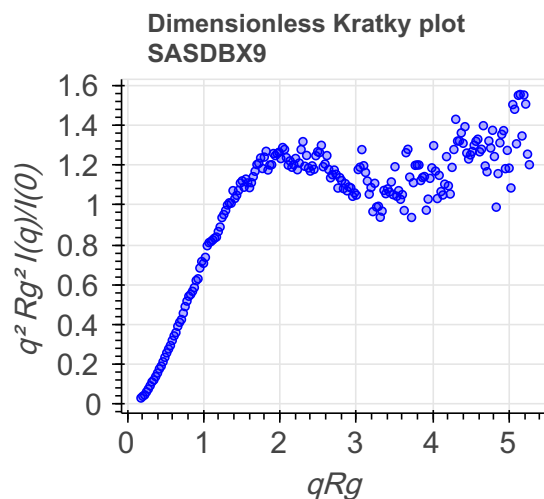
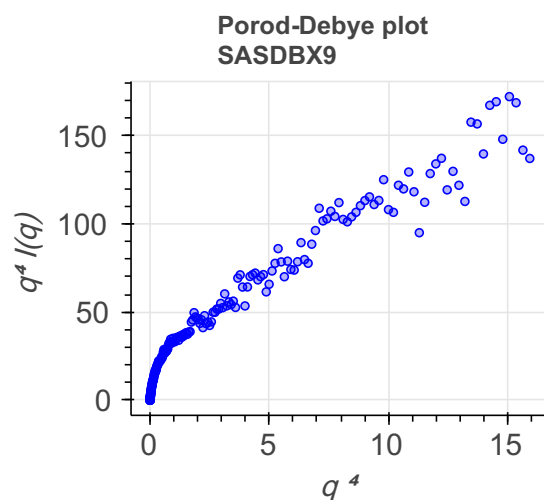


Flexibility analysis for SASDBZ9: In a Porod-Debye plot, a clear plateau is observed for globular (partial or fully folded) domains, whereas, fully unfolded domains are devoid of any discernable plateau. For details, refer to Figure 5 in [Rambo and Tainer, 2011](#). In a Kratky plot, a parabolic shape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



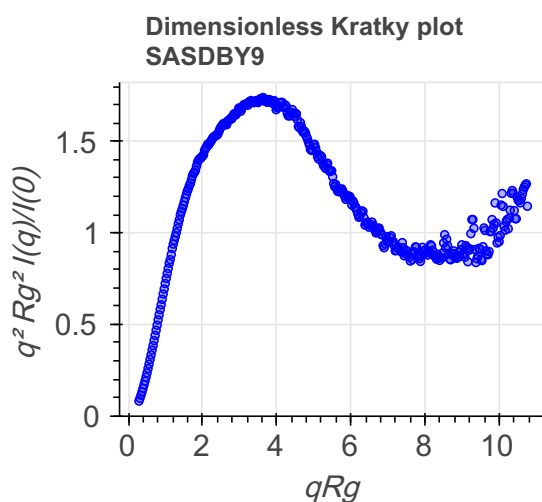
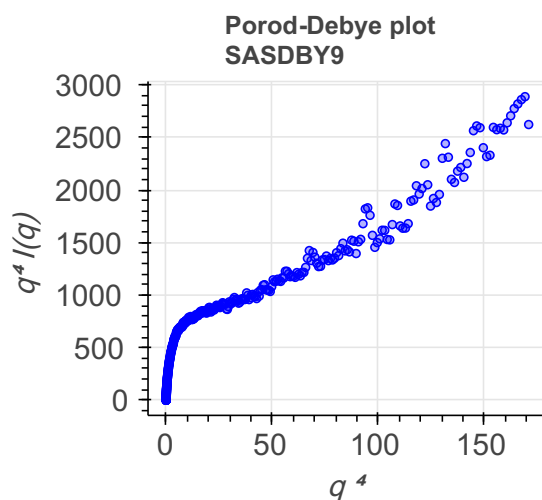


Flexibility analysis for SASDBX9: In a Porod-Debye plot, a clear plateau is observed for globular (partial or fully folded) domains, whereas, fully unfolded domains are devoid of any discernable plateau. For details, refer to Figure 5 in [Rambo and Tainer, 2011](#). In a Kratky plot, a parabolic shape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



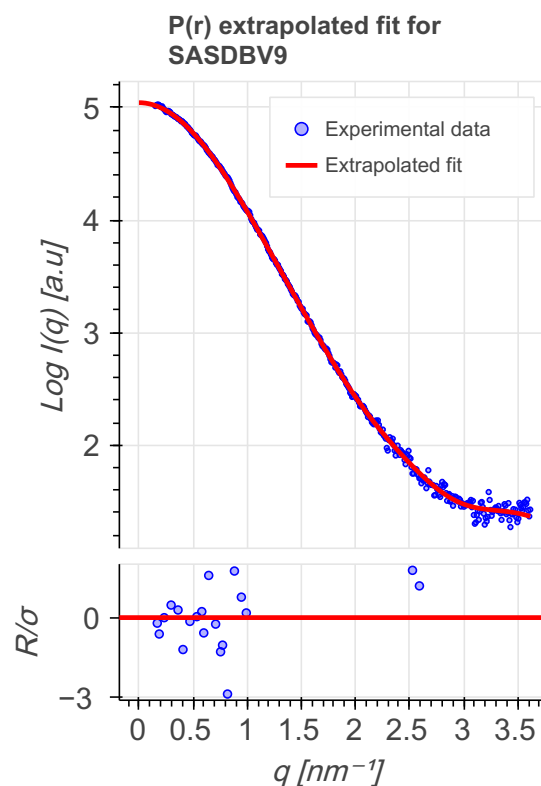
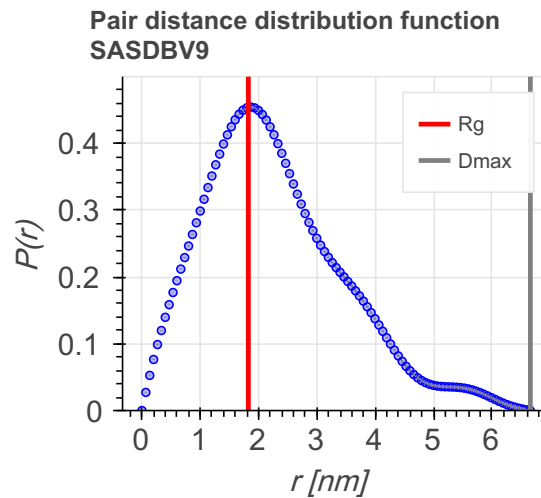
Pair-distance distribution analysis

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.

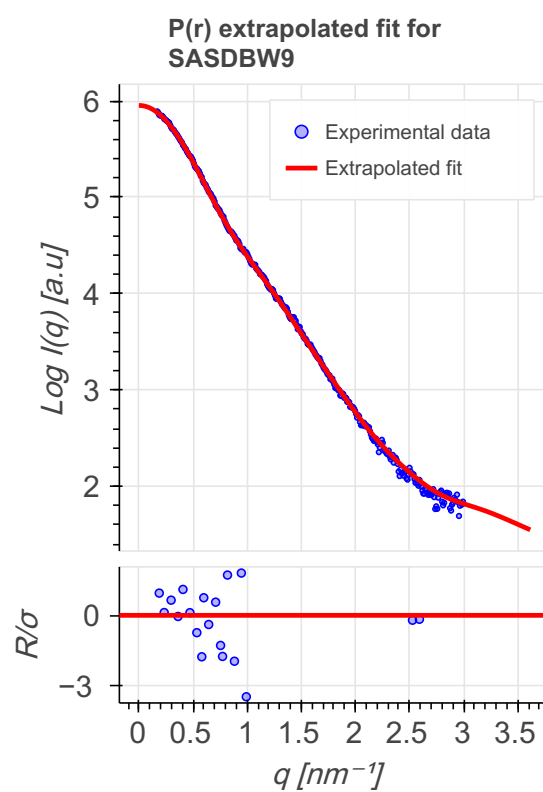
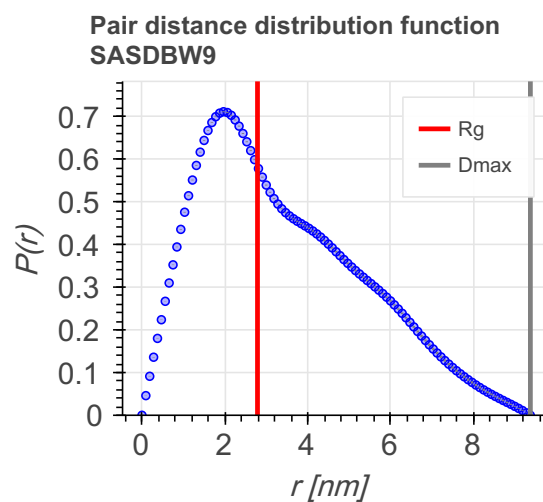
| SASDB ID | Software used | Dmax | Dmax error | Rg | Rg error |
|----------|---------------|-----------|------------|----------|----------|
| SASDBV9 | GNOM 4.5a | 6.660 nm | N/A | 1.824 nm | 0.006 nm |
| SASDBW9 | GNOM 4.5a | 9.370 nm | N/A | 2.787 nm | 0.007 nm |
| SASDBZ9 | GNOM 4.5a | 15.430 nm | N/A | 4.629 nm | 0.011 nm |
| SASDBX9 | GNOM 4.5a | 7.930 nm | N/A | 2.636 nm | 0.008 nm |

| SASDB ID | Software used | Dmax | Dmax error | Rg | Rg error |
|----------|---------------|-----------|------------|----------|----------|
| SASDBV9 | GNOM 4.5a | 10.450 nm | N/A | 2.976 nm | 0.005 nm |

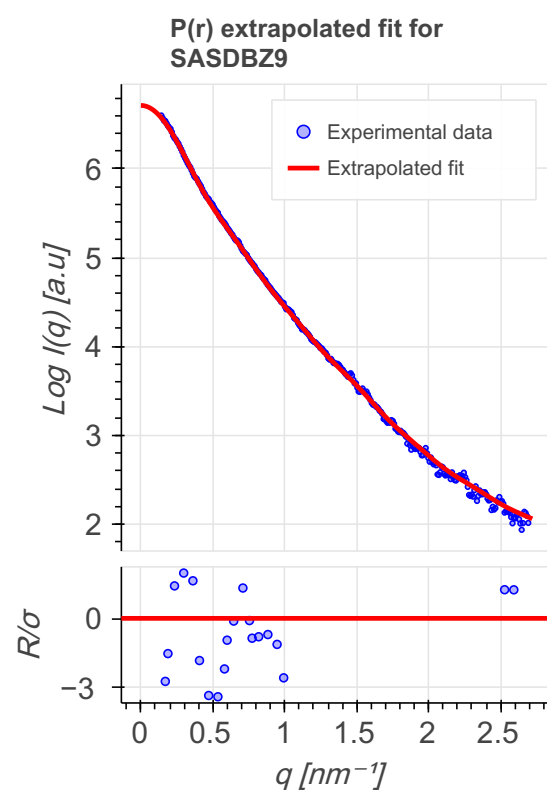
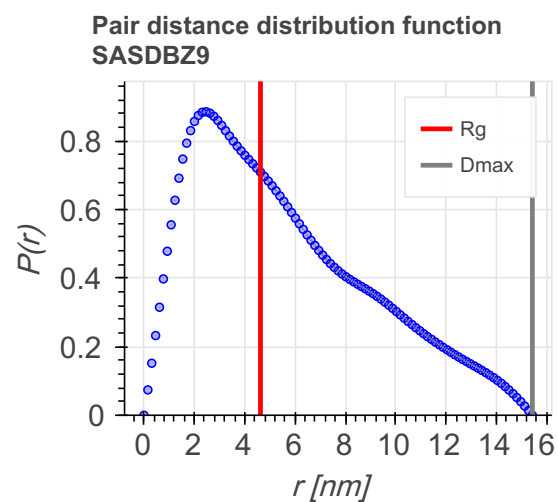
P(r) for SASDBV9: The value of P(r) should be zero beyond $r=D_{\max}$.



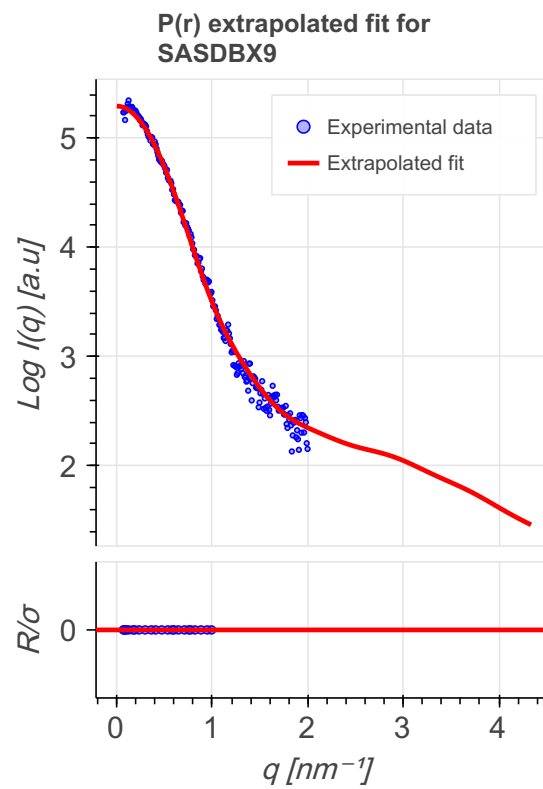
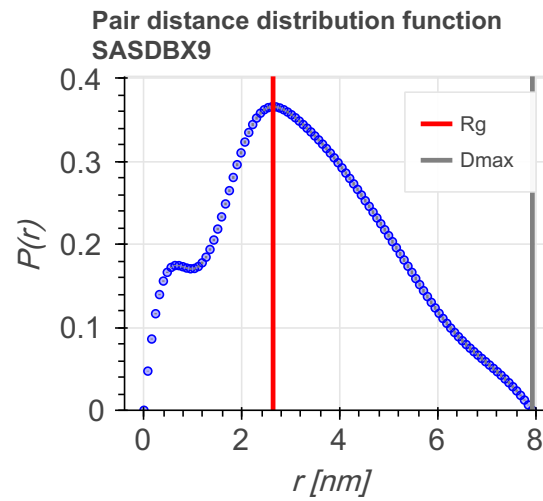
P(r) for SASDBW9: The value of P(r) should be zero beyond $r=D_{\max}$.



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

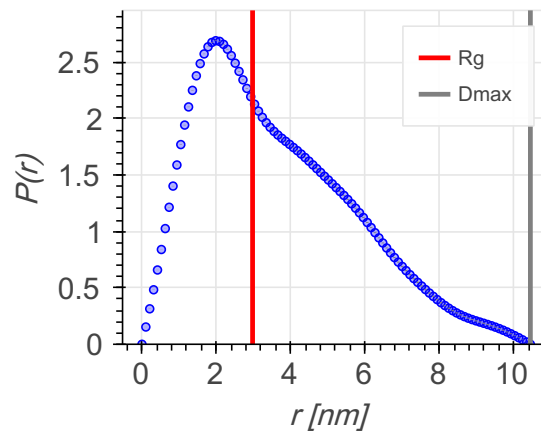


P(r) for SASDBZ9: The value of $P(r)$ should be zero beyond $r=D_{max}$.

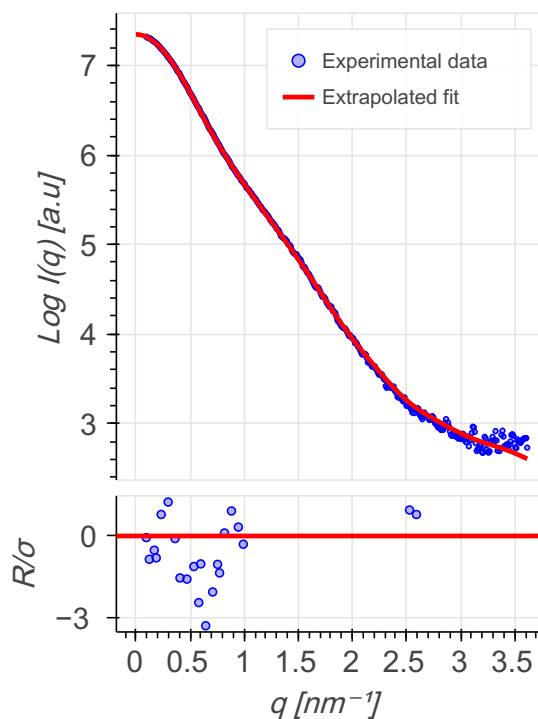


$P(r)$ for SASDBY9: The value of $P(r)$ should be zero beyond $r=D_{max}$.

Pair distance distribution function
SASDBY9



P(r) extrapolated fit for
SASDBY9



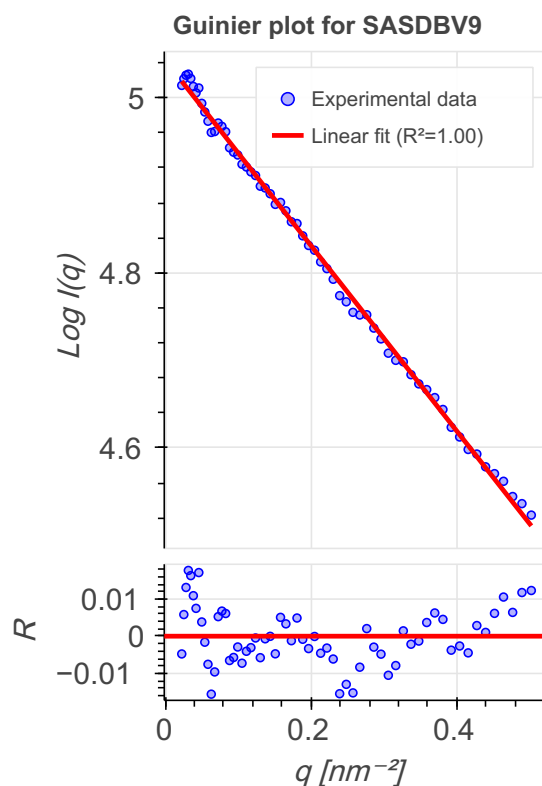
Guinier analysis ?

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.

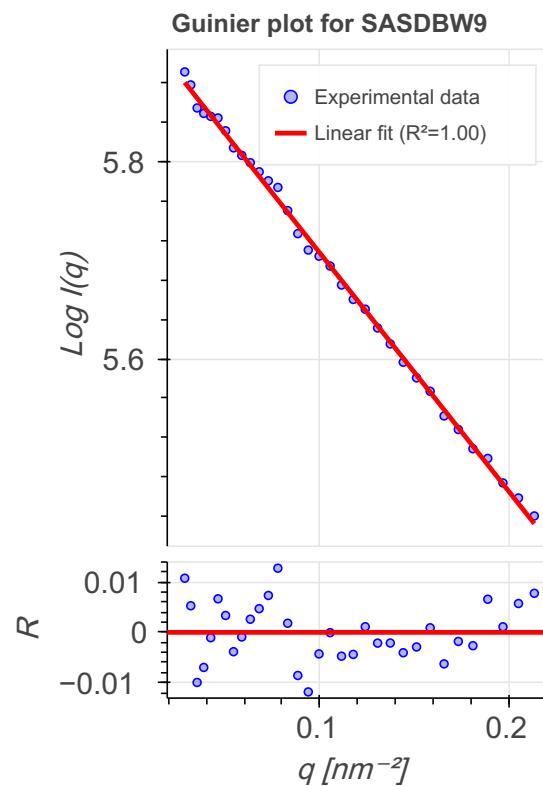
| SASDB ID | R_g | R_g error | MW | MW error |
|----------|---------|-------------|----------|----------|
| SASDBV9 | 1.77 nm | 0.05 nm | 12.2 kDa | N/A |
| SASDBW9 | 2.71 nm | 0.06 nm | 25.2 kDa | N/A |

| SASDB ID | Rg | Rg error | MW | MW error |
|----------|---------|----------|----------|----------|
| SASDBZ9 | 4.34 nm | 0.17 nm | 48.3 kDa | N/A |
| SASDBX9 | 2.78 nm | 0.18 nm | 14.7 kDa | N/A |
| SASDBY9 | 2.95 nm | 0.11 nm | 25.2 kDa | N/A |

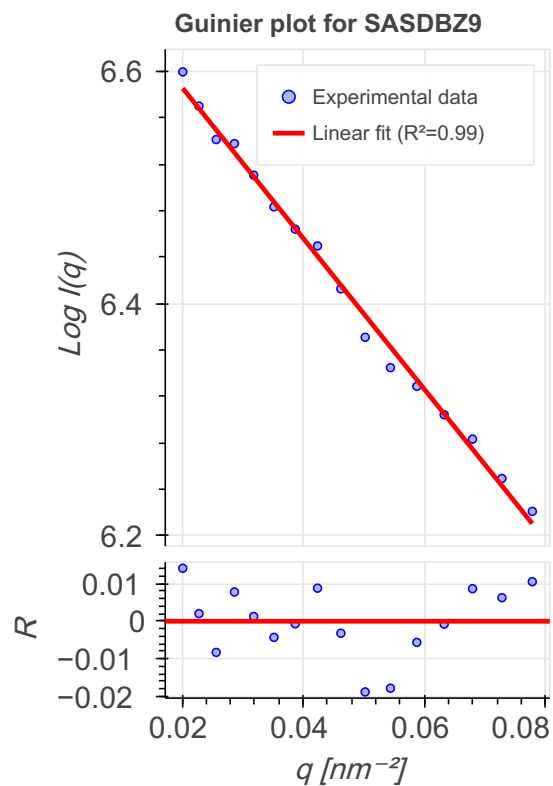
Guinier analysis for SASDBV9: the linearity of the Guinier plot is a sensitive indicator of the quality of the experimental SAS data; a linear Guinier plot is a necessary but not sufficient demonstration that a solution contains monodisperse particles of the same size. Deviations from linearity usually 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.



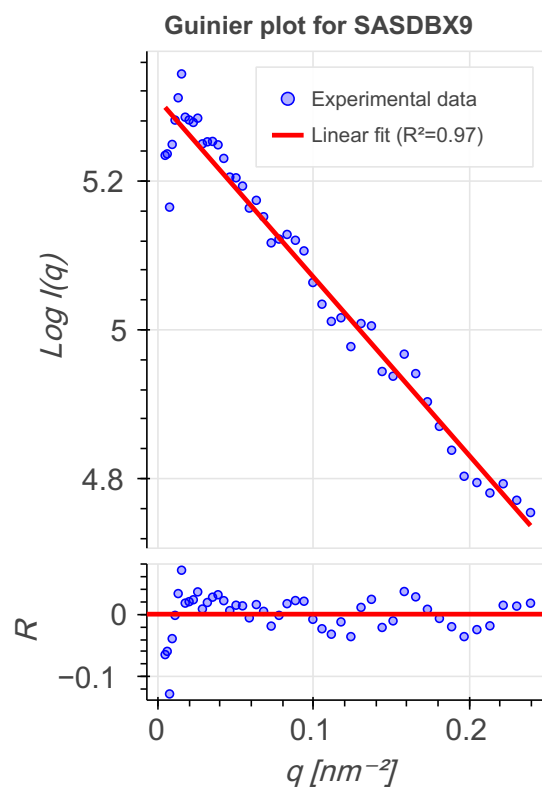
Guinier analysis for SASDBW9: the linearity of the Guinier plot is a sensitive indicator of the quality of the experimental SAS data; a linear Guinier plot is a necessary but not sufficient demonstration that a solution contains monodisperse particles of the same size. Deviations from linearity usually 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.



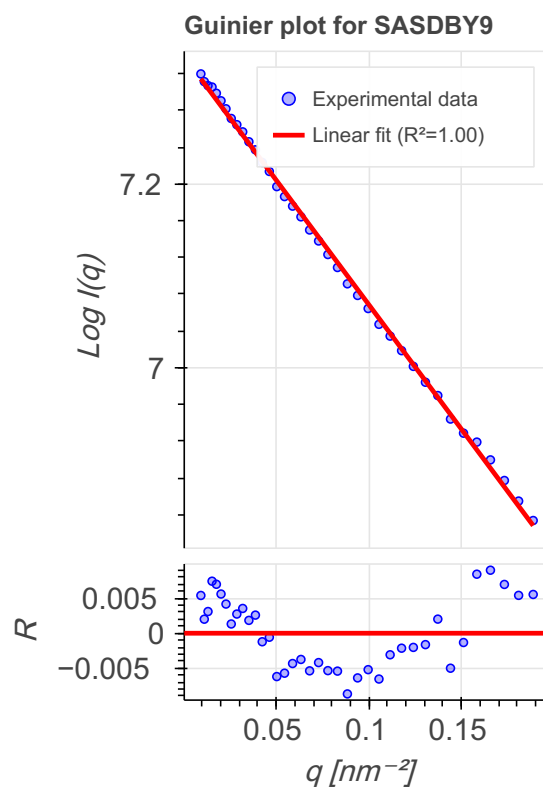
Guinier analysis for SASDBZ9: the linearity of the Guinier plot is a sensitive indicator of the quality of the experimental SAS data; a linear Guinier plot is a necessary but not sufficient demonstration that a solution contains monodisperse particles of the same size. Deviations from linearity usually 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.



Guinier analysis for SASDBX9: 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.



Guinier analysis for SASDBY9: 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.



2DEM class average

Validation for this section is under development.

3DEM volume

Validation for this section is under development.

EM raw micrographs

Validation for this section is under development.

Crosslinking-MS

Validation for this section is under development.

Mass Spectrometry

Validation for this section is under development.

Model quality ?

For models with atomic structures, molprobability 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.

| Models | Excluded Volume Satisfaction (%) | Number of violations |
|--------|----------------------------------|----------------------|
| | | |

| Models | Excluded Volume Satisfaction (%) | Number of violations |
|--------|----------------------------------|----------------------|
| 1 | 99.99 | 229275.0 |

Fit of model to data used for modeling ?

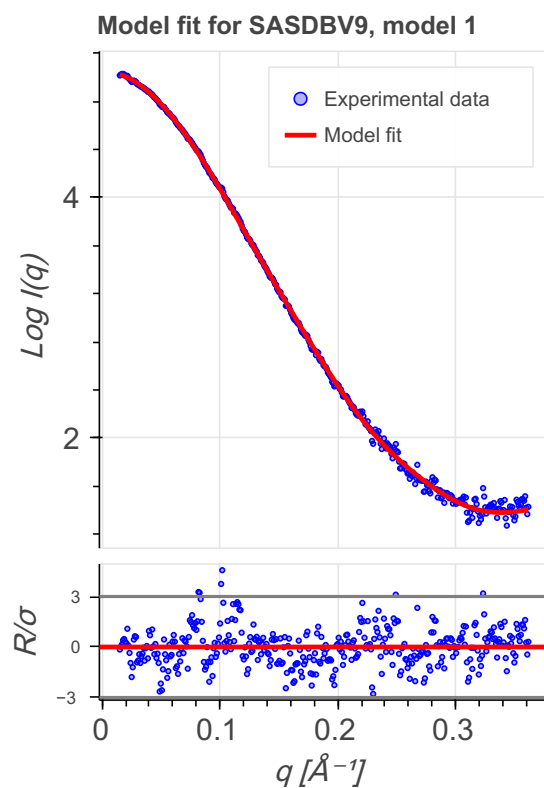
Fit of model(s) to SAS data

χ^2 goodness of fit and cormap analysis ?

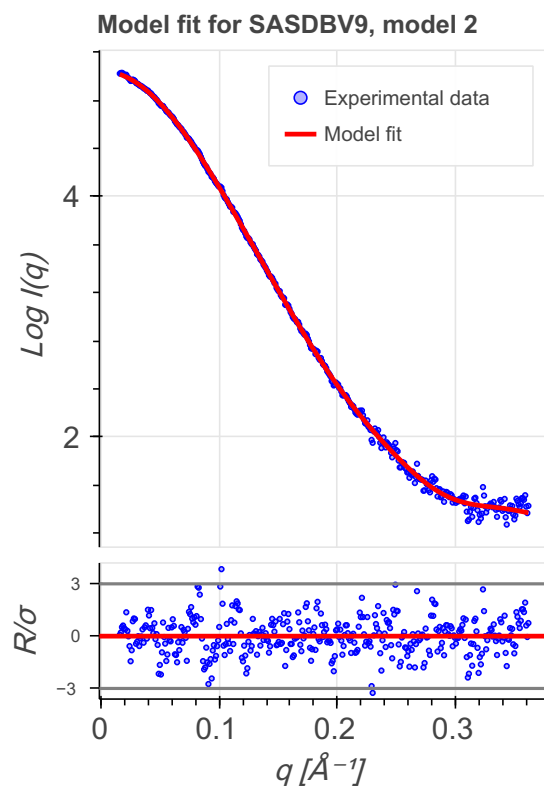
Model and fits displayed below were obtained from SASBDB. χ^2 values are a measure of fit of the model to data. A perfect fit has a χ^2 value of 1.0. ATSAS datcmp was used for hypothesis testing. All data sets are similar (i.e. the fit and the data collected) is the null hypothesis. *p*-value is a measure 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 | 2.22E-02 |
| SASDBV9 | 2 | 1.10 | 5.56E-03 |
| SASDBW9 | 1 | 1.97 | 1.10E-05 |
| SASDBZ9 | 1 | 1.94 | 0.00E+00 |
| SASDBX9 | 1 | 2.86 | 0.00E+00 |
| SASDBY9 | 1 | 2.02 | 3.00E-06 |

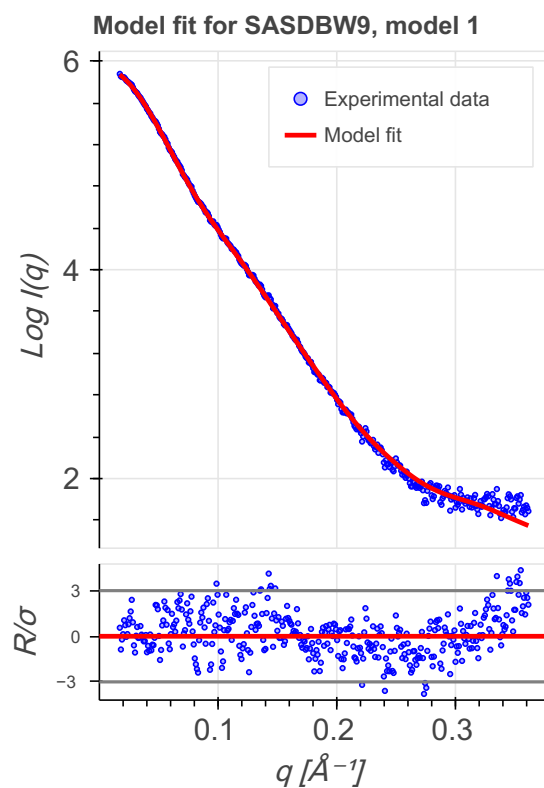
Model fit for SASDBV9 (fit/model number 1): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.



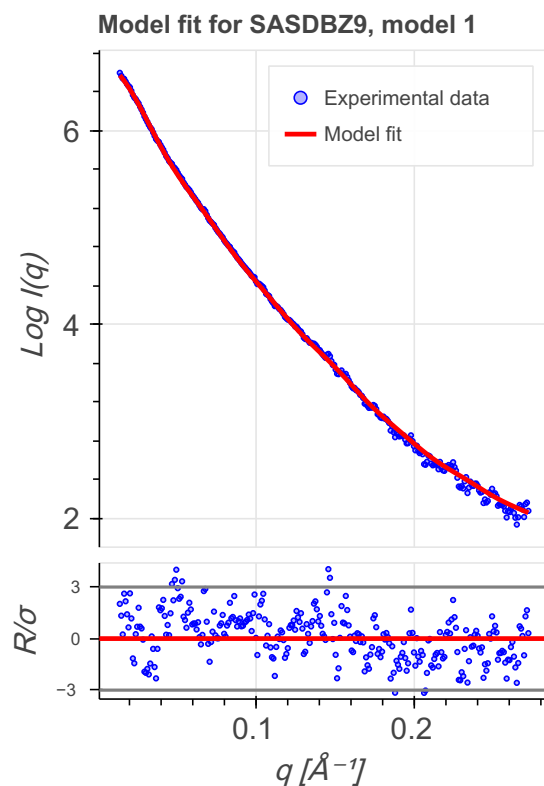
Model fit for SASDBV9 (fit/model number 2): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.



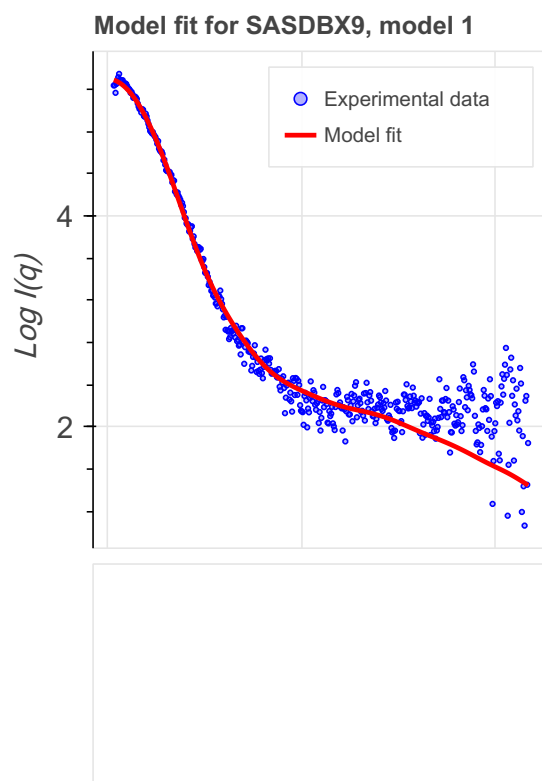
Model fit for SASDBV9 (fit/model number 1): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.



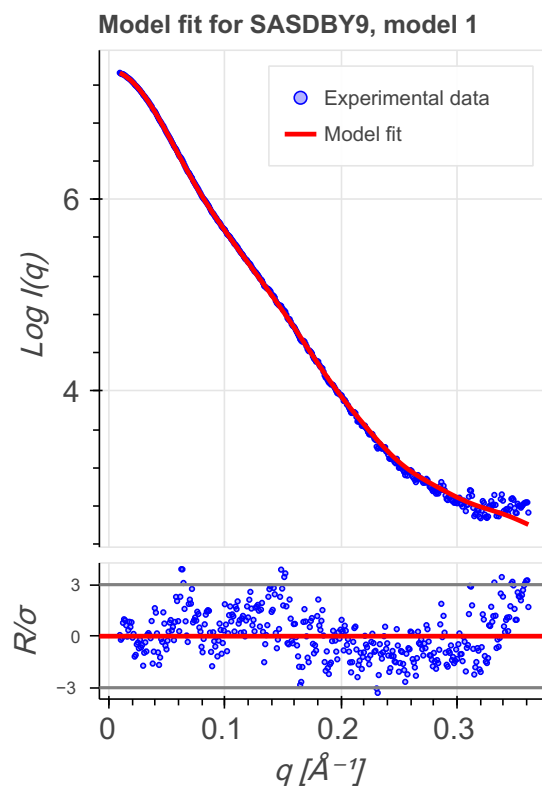
Model fit for SASDBZ9 (fit/model number 1): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.



Model fit for SASDBX9 (fit/model number 1): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.



Model fit for SASDBY9 (fit/model number 1): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.



2DEM class average

Validation for this section is under development.

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EM raw micrographs

Validation for this section is under development.

Crosslinking-MS

Validation for this section is under development.

Mass Spectrometry

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgements

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Implementation of validation methods for SAS data and SAS-based models are funded by [RCSB PDB](#) (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from [RCSB PDB](#), Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods.

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