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Supporting information for article:

Crystallization and preliminary X-ray crystallographic analysis of the sclerostin-neutralizing Fab AbD09097

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Table S1 Molecular replacement solutions for the Fab AbD09097 obtained with the software Phaser and using the coordinates of the Fab AbD1556 (PDB entry 3NH7) as search template.

Run A[a]	RFZ[e]	TFZ[f]	LLG[g]
variable domain, heavy chain[e]	11.1	9.2	170
variable domain, light chain	5.7	15.6	258
constant domain, heavy chain	4.9	17.2	130
constant domain, light chain	8.5	27.3	377
Run B[b]			
variable domains of heavy & light chain	7.9	7.3	68
constant domains of heavy & light chain	3.7	10.6	74
Run C[c]			
heavy chain	8.6	5.8	-53
light chain	3.6	4.4	-166
Run D[d]			
complete Fab	3.3	2.9	-7

All MR runs using Phaser were done using a resolution limit of 20 - 1.85Å. Similarity of template was set to 0.6, one Fab was assumed in the asymmetric unit, packing tolerance was set to a maximum of 10 clashes.

a) variable and constant domain: the search template Fab AbD1556 (PDB 3NH7) was separated into the four search templates containing the variable and constant domains of the heavy and light chain separately (VH: aa 1 - 120; VL: aa 2 - 111; CH: aa 121 - 220; CL: aa 112 - 211)

b) two search templates were used, of which one comprised residues 1-120 and 2-111 of the variable domains of the heavy and light chain and the other consisted of residues 2-111 and 112-211 of the constant domains of the heavy and light chain of the Fab AbD1556 (PDB 3NH7).

c) two search templates consisting of the heavy chain (aa 1-220) or the light chain (aa 2-211) of the Fab AbD1556 (PDB 3NH7)

d) the full Fab AbD1556 structure was used as search template (PDB 3NH7)

[b] RFZ: rotation function Z-score

[c] TFZ: translation function Z-score

[d] LLG: least-likelihood gain. For judgment of a correct MR solution, TFZ should be higher than five and for consecutive searches of substructures LLG should be positive and increase with the addition of correctly placed search templates.