Summary of integrative structure determination of Structures of the PSG Supramodule of PSD-95 Resolved by Screening of FRET-derived Distance Restraints against Simulated Structures (PDB ID: 9A2F, PDB-Dev ID: PDBDEV_00000164)

1. Model Composition	
Entry composition	Postsynaptic density protein 95 (PSD95) PDZ3-SH3-GuK Module: Chain A (417 residues)
	- Other, File: 10.5281/zenodo.7125978
	- Single molecule FRET data, File:
	10.5281/zenodo.7125978
	- Single molecule FRET data, File: 10.5281/zenodo.7125978
	- Single molecule FRET data, File:
	10.5281/zenodo.7125978
	- Single molecule FRET data, File:
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	- Single molecule FRET data, File:
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	- Single molecule FRET data, File:
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	10.5281/zenodo.7125978
	- Single molecule FRET data, File:
	10.5281/zenodo.7125978 - Single molecule FRET data, File:
	10.5281/zenodo.7125978
Detector would form the U.S.	- Single molecule FRET data, File:
Datasets used for modeling	10.5281/zenodo.7125978
	- Single molecule FRET data, File:
	10.5281/zenodo.7125978
	- Single molecule FRET data, File:
	10.5281/zenodo.7125978 - Single molecule FRET data, File:
	10.5281/zenodo.7125978
	- Single molecule FRET data, File:
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	- Single molecule FRET data, File:
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	- Single molecule FRET data, File:
	10.5281/zenodo.7125978
	- Single molecule FRET data, File:

	10.5281/zenodo.7125978 - Single molecule FRET data, File: 10.5281/zenodo.7125978 - Single molecule FRET data, File: 10.5281/zenodo.7125978 - Single molecule FRET data, File: 10.5281/zenodo.7125978 - Integrative model, File: 10.5281/zenodo.7125978 - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 6QJD - Experimental model, PDB ID: 1KJW
2. Representation	
Resolution	Atomic
Number of <u>rigid bodies</u> , <u>flexible units</u>	0, 1
Flexible units	A: 1-417
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	
4. Validation	
4. Validation Number of ensembles	2
	2 4325, 114
Number of ensembles	
Number of ensembles Number of models in ensembles	4325, 114
Number of ensembles Number of models in ensembles Number of deposited models	4325, 114 200

- outliers = 66
- Model-7: Clashscore = 8.32, Number of Ramachandran outliers = 16, Number of sidechain outliers = 67
- Model-8: Clashscore = 7.41, Number of Ramachandran outliers = 15, Number of sidechain outliers = 59
- Model-9: Clashscore = 6.8, Number of Ramachandran outliers = 18, Number of sidechain outliers = 72
- Model-10: Clashscore = 11.04, Number of Ramachandran outliers = 15, Number of sidechain outliers = 71
- Model-11: Clashscore = 10.58, Number of Ramachandran outliers = 21, Number of sidechain outliers = 67
- Model-12: Clashscore = 9.83, Number of Ramachandran outliers = 15, Number of sidechain outliers = 67
- Model-13: Clashscore = 8.47, Number of Ramachandran outliers = 21, Number of sidechain outliers = 70
- Model-14: Clashscore = 8.47, Number of Ramachandran outliers = 16, Number of sidechain outliers = 65
- Model-15: Clashscore = 10.28, Number of Ramachandran outliers = 13, Number of sidechain outliers = 66
- Model-16: Clashscore = 6.8, Number of Ramachandran outliers = 16, Number of sidechain outliers = 62
- Model-17: Clashscore = 7.56, Number of Ramachandran outliers = 16, Number of sidechain outliers = 66
- Model-18: Clashscore = 7.26, Number of Ramachandran outliers = 16, Number of sidechain outliers = 64
- Model-19: Clashscore = 7.41, Number of Ramachandran outliers = 15, Number of sidechain outliers = 62
- Model-20: Clashscore = 8.62, Number of Ramachandran outliers = 15, Number of sidechain outliers = 67
- Model-21: Clashscore = 9.37, Number of Ramachandran outliers = 15, Number of sidechain outliers = 61
- Model-22: Clashscore = 9.22, Number of Ramachandran outliers = 13, Number of sidechain outliers = 68
- Model-23: Clashscore = 8.47, Number of Ramachandran outliers = 16, Number of sidechain outliers = 68
- Model-24: Clashscore = 8.16, Number of Ramachandran outliers = 20, Number of sidechain outliers = 67
- Model-25: Clashscore = 8.16, Number of Ramachandran outliers = 18, Number of sidechain outliers = 68
- Model-26: Clashscore = 7.86, Number of Ramachandran outliers = 15, Number of sidechain outliers = 67
- Model-27: Clashscore = 9.22, Number of Ramachandran outliers = 21, Number of sidechain outliers = 62

- Model-28: Clashscore = 8.62, Number of Ramachandran outliers = 20, Number of sidechain outliers = 72
- Model-29: Clashscore = 6.65, Number of Ramachandran outliers = 15, Number of sidechain outliers = 58
- Model-30: Clashscore = 7.56, Number of Ramachandran outliers = 15, Number of sidechain outliers = 62
- Model-31: Clashscore = 6.95, Number of Ramachandran outliers = 18, Number of sidechain outliers = 59
- Model-32: Clashscore = 8.92, Number of Ramachandran outliers = 16, Number of sidechain outliers = 68
- Model-33: Clashscore = 6.65, Number of Ramachandran outliers = 19, Number of sidechain outliers = 75
- Model-34: Clashscore = 7.11, Number of Ramachandran outliers = 18, Number of sidechain outliers = 72
- Model-35: Clashscore = 8.16, Number of Ramachandran outliers = 13, Number of sidechain outliers = 69
- Model-36: Clashscore = 10.28, Number of Ramachandran outliers = 18, Number of sidechain outliers = 62
- Model-37: Clashscore = 8.01, Number of Ramachandran outliers = 16, Number of sidechain outliers = 66
- Model-38: Clashscore = 8.01, Number of Ramachandran outliers = 14, Number of sidechain outliers = 66
- Model-39: Clashscore = 7.86, Number of Ramachandran outliers = 17, Number of sidechain outliers = 64
- Model-40: Clashscore = 8.32, Number of Ramachandran outliers = 15, Number of sidechain outliers = 76
- Model-41: Clashscore = 8.01, Number of Ramachandran outliers = 17, Number of sidechain outliers = 66
- Model-42: Clashscore = 8.01, Number of Ramachandran outliers = 15, Number of sidechain outliers = 66
- Model-43: Clashscore = 7.26, Number of Ramachandran outliers = 15, Number of sidechain outliers = 67
- Model-44: Clashscore = 9.68, Number of Ramachandran outliers = 17, Number of sidechain outliers = 75
- Model-45: Clashscore = 5.75, Number of Ramachandran outliers = 20, Number of sidechain outliers = 73
- Model-46: Clashscore = 8.32, Number of Ramachandran outliers = 14, Number of sidechain outliers = 60
- Model-47: Clashscore = 9.68, Number of Ramachandran outliers = 17, Number of sidechain outliers = 66
- Model-48: Clashscore = 8.32, Number of Ramachandran outliers = 17, Number of sidechain outliers = 67
- Model-49: Clashscore = 6.95, Number of

- Ramachandran outliers = 14, Number of sidechain outliers = 66
- Model-50: Clashscore = 8.01, Number of Ramachandran outliers = 15, Number of sidechain outliers = 61
- Model-51: Clashscore = 7.11, Number of Ramachandran outliers = 18, Number of sidechain outliers = 64
- Model-52: Clashscore = 8.47, Number of Ramachandran outliers = 17, Number of sidechain outliers = 71
- Model-53: Clashscore = 7.86, Number of Ramachandran outliers = 14, Number of sidechain outliers = 66
- Model-54: Clashscore = 5.59, Number of Ramachandran outliers = 18, Number of sidechain outliers = 69
- Model-55: Clashscore = 8.62, Number of Ramachandran outliers = 16, Number of sidechain outliers = 74
- Model-56: Clashscore = 10.13, Number of Ramachandran outliers = 13, Number of sidechain outliers = 78
- Model-57: Clashscore = 7.26, Number of Ramachandran outliers = 17, Number of sidechain outliers = 70
- Model-58: Clashscore = 7.41, Number of Ramachandran outliers = 20, Number of sidechain outliers = 59
- Model-59: Clashscore = 8.92, Number of Ramachandran outliers = 15, Number of sidechain outliers = 54
- Model-60: Clashscore = 8.01, Number of Ramachandran outliers = 17, Number of sidechain outliers = 77
- Model-61: Clashscore = 10.13, Number of Ramachandran outliers = 15, Number of sidechain outliers = 64
- Model-62: Clashscore = 10.73, Number of Ramachandran outliers = 17, Number of sidechain outliers = 72
- Model-63: Clashscore = 6.95, Number of Ramachandran outliers = 16, Number of sidechain outliers = 60
- Model-64: Clashscore = 8.47, Number of Ramachandran outliers = 16, Number of sidechain outliers = 75
- Model-65: Clashscore = 7.71, Number of Ramachandran outliers = 14, Number of sidechain outliers = 61
- Model-66: Clashscore = 6.35, Number of Ramachandran outliers = 17, Number of sidechain outliers = 69
- Model-67: Clashscore = 9.37, Number of Ramachandran outliers = 17, Number of sidechain outliers = 62
- Model-68: Clashscore = 6.65, Number of Ramachandran outliers = 16, Number of sidechain outliers = 66
- Model-69: Clashscore = 8.77, Number of Ramachandran outliers = 17, Number of sidechain outliers = 61
- Model-70: Clashscore = 7.71, Number of Ramachandran outliers = 14, Number of sidechain

- outliers = 71
- Model-71: Clashscore = 8.01, Number of Ramachandran outliers = 17, Number of sidechain outliers = 71
- Model-72: Clashscore = 8.62, Number of Ramachandran outliers = 15, Number of sidechain outliers = 62
- Model-73: Clashscore = 8.62, Number of Ramachandran outliers = 18, Number of sidechain outliers = 63
- Model-74: Clashscore = 8.32, Number of Ramachandran outliers = 16, Number of sidechain outliers = 74
- Model-75: Clashscore = 8.77, Number of Ramachandran outliers = 13, Number of sidechain outliers = 78
- Model-76: Clashscore = 8.01, Number of Ramachandran outliers = 17, Number of sidechain outliers = 65
- Model-77: Clashscore = 6.8, Number of Ramachandran outliers = 18, Number of sidechain outliers = 73
- Model-78: Clashscore = 8.47, Number of Ramachandran outliers = 15, Number of sidechain outliers = 68
- Model-79: Clashscore = 8.01, Number of Ramachandran outliers = 14, Number of sidechain outliers = 59
- Model-80: Clashscore = 8.01, Number of Ramachandran outliers = 16, Number of sidechain outliers = 71
- Model-81: Clashscore = 6.5, Number of Ramachandran outliers = 13, Number of sidechain outliers = 67
- Model-82: Clashscore = 7.86, Number of Ramachandran outliers = 14, Number of sidechain outliers = 66
- Model-83: Clashscore = 6.8, Number of Ramachandran outliers = 19, Number of sidechain outliers = 61
- Model-84: Clashscore = 9.98, Number of Ramachandran outliers = 15, Number of sidechain outliers = 66
- Model-85: Clashscore = 8.01, Number of Ramachandran outliers = 15, Number of sidechain outliers = 69
- Model-86: Clashscore = 9.98, Number of Ramachandran outliers = 14, Number of sidechain outliers = 70
- Model-87: Clashscore = 5.44, Number of Ramachandran outliers = 19, Number of sidechain outliers = 72
- Model-88: Clashscore = 8.01, Number of Ramachandran outliers = 18, Number of sidechain outliers = 77
- Model-89: Clashscore = 6.5, Number of Ramachandran outliers = 16, Number of sidechain outliers = 70
- Model-90: Clashscore = 8.32, Number of Ramachandran outliers = 23, Number of sidechain outliers = 56
- Model-91: Clashscore = 9.68, Number of Ramachandran outliers = 15, Number of sidechain outliers = 77

Model quality: assessment of atomic segments

- Model-92: Clashscore = 7.11, Number of Ramachandran outliers = 14, Number of sidechain outliers = 62
- Model-93: Clashscore = 8.77, Number of Ramachandran outliers = 16, Number of sidechain outliers = 62
- Model-94: Clashscore = 7.26, Number of Ramachandran outliers = 16, Number of sidechain outliers = 63
- Model-95: Clashscore = 9.83, Number of Ramachandran outliers = 17, Number of sidechain outliers = 72
- Model-96: Clashscore = 9.22, Number of Ramachandran outliers = 15, Number of sidechain outliers = 70
- Model-97: Clashscore = 8.92, Number of Ramachandran outliers = 17, Number of sidechain outliers = 62
- Model-98: Clashscore = 8.62, Number of Ramachandran outliers = 17, Number of sidechain outliers = 64
- Model-99: Clashscore = 8.16, Number of Ramachandran outliers = 17, Number of sidechain outliers = 67
- Model-100: Clashscore = 11.19, Number of Ramachandran outliers = 17, Number of sidechain outliers = 62
- Model-101: Clashscore = 6.95, Number of Ramachandran outliers = 19, Number of sidechain outliers = 61
- Model-102: Clashscore = 4.23, Number of Ramachandran outliers = 16, Number of sidechain outliers = 59
- Model-103: Clashscore = 7.41, Number of Ramachandran outliers = 19, Number of sidechain outliers = 65
- Model-104: Clashscore = 5.9, Number of Ramachandran outliers = 16, Number of sidechain outliers = 76
- Model-105: Clashscore = 7.71, Number of Ramachandran outliers = 16, Number of sidechain outliers = 59
- Model-106: Clashscore = 9.07, Number of Ramachandran outliers = 17, Number of sidechain outliers = 77
- Model-107: Clashscore = 6.05, Number of Ramachandran outliers = 14, Number of sidechain outliers = 70
- Model-108: Clashscore = 7.86, Number of Ramachandran outliers = 15, Number of sidechain outliers = 67
- Model-109: Clashscore = 7.11, Number of Ramachandran outliers = 18, Number of sidechain outliers = 73
- Model-110: Clashscore = 6.8, Number of Ramachandran outliers = 15, Number of sidechain outliers = 63
- Model-111: Clashscore = 7.26, Number of Ramachandran outliers = 17, Number of sidechain outliers = 77
- Model-112: Clashscore = 8.47, Number of Ramachandran outliers = 17, Number of sidechain outliers = 73
- Model-113: Clashscore = 7.86, Number of

- Ramachandran outliers = 18, Number of sidechain outliers = 65
- Model-114: Clashscore = 8.16, Number of Ramachandran outliers = 15, Number of sidechain outliers = 62
- Model-115: Clashscore = 7.56, Number of Ramachandran outliers = 15, Number of sidechain outliers = 72
- Model-116: Clashscore = 7.56, Number of Ramachandran outliers = 18, Number of sidechain outliers = 69
- Model-117: Clashscore = 9.98, Number of Ramachandran outliers = 21, Number of sidechain outliers = 62
- Model-118: Clashscore = 8.01, Number of Ramachandran outliers = 17, Number of sidechain outliers = 64
- Model-119: Clashscore = 8.62, Number of Ramachandran outliers = 15, Number of sidechain outliers = 62
- Model-120: Clashscore = 8.92, Number of Ramachandran outliers = 14, Number of sidechain outliers = 67
- Model-121: Clashscore = 7.41, Number of Ramachandran outliers = 12, Number of sidechain outliers = 54
- Model-122: Clashscore = 6.95, Number of Ramachandran outliers = 17, Number of sidechain outliers = 65
- Model-123: Clashscore = 7.26, Number of Ramachandran outliers = 18, Number of sidechain outliers = 65
- Model-124: Clashscore = 6.65, Number of Ramachandran outliers = 16, Number of sidechain outliers = 62
- Model-125: Clashscore = 7.56, Number of Ramachandran outliers = 14, Number of sidechain outliers = 68
- Model-126: Clashscore = 7.26, Number of Ramachandran outliers = 16, Number of sidechain outliers = 67
- Model-127: Clashscore = 7.86, Number of Ramachandran outliers = 17, Number of sidechain outliers = 61
- Model-128: Clashscore = 7.11, Number of Ramachandran outliers = 14, Number of sidechain outliers = 67
- Model-129: Clashscore = 6.95, Number of Ramachandran outliers = 18, Number of sidechain outliers = 75
- Model-130: Clashscore = 7.56, Number of Ramachandran outliers = 15, Number of sidechain outliers = 70
- Model-131: Clashscore = 7.71, Number of Ramachandran outliers = 20, Number of sidechain outliers = 80
- Model-132: Clashscore = 9.07, Number of Ramachandran outliers = 17, Number of sidechain outliers = 76
- Model-133: Clashscore = 7.86, Number of Ramachandran outliers = 16, Number of sidechain outliers = 64
- Model-134: Clashscore = 7.56, Number of Ramachandran outliers = 16, Number of sidechain

- outliers = 63
- Model-135: Clashscore = 7.26, Number of Ramachandran outliers = 14, Number of sidechain outliers = 59
- Model-136: Clashscore = 6.8, Number of Ramachandran outliers = 13, Number of sidechain outliers = 65
- Model-137: Clashscore = 9.37, Number of Ramachandran outliers = 18, Number of sidechain outliers = 70
- Model-138: Clashscore = 8.62, Number of Ramachandran outliers = 16, Number of sidechain outliers = 68
- Model-139: Clashscore = 6.8, Number of Ramachandran outliers = 17, Number of sidechain outliers = 62
- Model-140: Clashscore = 7.26, Number of Ramachandran outliers = 17, Number of sidechain outliers = 66
- Model-141: Clashscore = 7.26, Number of Ramachandran outliers = 17, Number of sidechain outliers = 64
- Model-142: Clashscore = 8.16, Number of Ramachandran outliers = 21, Number of sidechain outliers = 69
- Model-143: Clashscore = 8.92, Number of Ramachandran outliers = 18, Number of sidechain outliers = 62
- Model-144: Clashscore = 7.41, Number of Ramachandran outliers = 16, Number of sidechain outliers = 62
- Model-145: Clashscore = 5.59, Number of Ramachandran outliers = 18, Number of sidechain outliers = 67
- Model-146: Clashscore = 8.01, Number of Ramachandran outliers = 15, Number of sidechain outliers = 69
- Model-147: Clashscore = 9.07, Number of Ramachandran outliers = 18, Number of sidechain outliers = 54
- Model-148: Clashscore = 8.77, Number of Ramachandran outliers = 20, Number of sidechain outliers = 84
- Model-149: Clashscore = 7.41, Number of Ramachandran outliers = 20, Number of sidechain outliers = 65
- Model-150: Clashscore = 8.77, Number of Ramachandran outliers = 17, Number of sidechain outliers = 65
- Model-151: Clashscore = 8.62, Number of Ramachandran outliers = 17, Number of sidechain outliers = 54
- Model-152: Clashscore = 5.9, Number of Ramachandran outliers = 15, Number of sidechain outliers = 71
- Model-153: Clashscore = 8.01, Number of Ramachandran outliers = 20, Number of sidechain outliers = 65
- Model-154: Clashscore = 6.65, Number of Ramachandran outliers = 20, Number of sidechain outliers = 72
- Model-155: Clashscore = 8.47, Number of Ramachandran outliers = 14, Number of sidechain outliers = 68

- Model-156: Clashscore = 10.58, Number of Ramachandran outliers = 15, Number of sidechain outliers = 70
- Model-157: Clashscore = 8.32, Number of Ramachandran outliers = 15, Number of sidechain outliers = 67
- Model-158: Clashscore = 8.62, Number of Ramachandran outliers = 18, Number of sidechain outliers = 62
- Model-159: Clashscore = 8.62, Number of Ramachandran outliers = 16, Number of sidechain outliers = 58
- Model-160: Clashscore = 6.8, Number of Ramachandran outliers = 18, Number of sidechain outliers = 70
- Model-161: Clashscore = 7.71, Number of Ramachandran outliers = 15, Number of sidechain outliers = 71
- Model-162: Clashscore = 7.11, Number of Ramachandran outliers = 15, Number of sidechain outliers = 58
- Model-163: Clashscore = 6.5, Number of Ramachandran outliers = 15, Number of sidechain outliers = 62
- Model-164: Clashscore = 6.95, Number of Ramachandran outliers = 17, Number of sidechain outliers = 65
- Model-165: Clashscore = 6.35, Number of Ramachandran outliers = 18, Number of sidechain outliers = 63
- Model-166: Clashscore = 8.77, Number of Ramachandran outliers = 18, Number of sidechain outliers = 69
- Model-167: Clashscore = 8.01, Number of Ramachandran outliers = 19, Number of sidechain outliers = 71
- Model-168: Clashscore = 5.9, Number of Ramachandran outliers = 15, Number of sidechain outliers = 74
- Model-169: Clashscore = 8.47, Number of Ramachandran outliers = 18, Number of sidechain outliers = 59
- Model-170: Clashscore = 7.56, Number of Ramachandran outliers = 13, Number of sidechain outliers = 70
- Model-171: Clashscore = 8.62, Number of Ramachandran outliers = 16, Number of sidechain outliers = 67
- Model-172: Clashscore = 8.01, Number of Ramachandran outliers = 21, Number of sidechain outliers = 65
- Model-173: Clashscore = 8.16, Number of Ramachandran outliers = 15, Number of sidechain outliers = 75
- Model-174: Clashscore = 8.92, Number of Ramachandran outliers = 13, Number of sidechain outliers = 75
- Model-175: Clashscore = 8.32, Number of Ramachandran outliers = 14, Number of sidechain outliers = 84
- Model-176: Clashscore = 6.95, Number of Ramachandran outliers = 16, Number of sidechain outliers = 80
- Model-177: Clashscore = 8.62, Number of

- Ramachandran outliers = 16, Number of sidechain outliers = 77
- Model-178: Clashscore = 9.53, Number of Ramachandran outliers = 19, Number of sidechain outliers = 70
- Model-179: Clashscore = 7.71, Number of Ramachandran outliers = 16, Number of sidechain outliers = 56
- Model-180: Clashscore = 9.68, Number of Ramachandran outliers = 17, Number of sidechain outliers = 59
- Model-181: Clashscore = 8.32, Number of Ramachandran outliers = 15, Number of sidechain outliers = 62
- Model-182: Clashscore = 8.62, Number of Ramachandran outliers = 13, Number of sidechain outliers = 75
- Model-183: Clashscore = 8.77, Number of Ramachandran outliers = 17, Number of sidechain outliers = 64
- Model-184: Clashscore = 7.26, Number of Ramachandran outliers = 20, Number of sidechain outliers = 56
- Model-185: Clashscore = 8.92, Number of Ramachandran outliers = 18, Number of sidechain outliers = 69
- Model-186: Clashscore = 7.11, Number of Ramachandran outliers = 15, Number of sidechain outliers = 60
- Model-187: Clashscore = 9.37, Number of Ramachandran outliers = 15, Number of sidechain outliers = 51
- Model-188: Clashscore = 8.32, Number of Ramachandran outliers = 19, Number of sidechain outliers = 79
- Model-189: Clashscore = 7.26, Number of Ramachandran outliers = 13, Number of sidechain outliers = 54
- Model-190: Clashscore = 7.11, Number of Ramachandran outliers = 19, Number of sidechain outliers = 66
- Model-191: Clashscore = 8.47, Number of Ramachandran outliers = 17, Number of sidechain outliers = 59
- Model-192: Clashscore = 9.22, Number of Ramachandran outliers = 17, Number of sidechain outliers = 73
- Model-193: Clashscore = 8.01, Number of Ramachandran outliers = 16, Number of sidechain outliers = 69
- Model-194: Clashscore = 6.8, Number of Ramachandran outliers = 18, Number of sidechain outliers = 67
- Model-195: Clashscore = 7.41, Number of Ramachandran outliers = 18, Number of sidechain outliers = 54
- Model-196: Clashscore = 6.95, Number of Ramachandran outliers = 19, Number of sidechain outliers = 63
- Model-197: Clashscore = 8.92, Number of Ramachandran outliers = 16, Number of sidechain outliers = 74
- Model-198: Clashscore = 7.26, Number of Ramachandran outliers = 15, Number of sidechain

	outliers = 64 - Model-199: Clashscore = 8.01, Number of Ramachandran outliers = 17, Number of sidechain outliers = 71 - Model-200: Clashscore = 7.26, Number of Ramachandran outliers = 18, Number of sidechain outliers = 64
Model quality: assessment of excluded volume	Not applicable
Fit to data used for modeling	Fit of model to information used to compute it has not been determined
Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <u>Method</u>	Unbiased DMD Simulations
<u>Name</u>	DMD simulations
Number of computed models	20871
2. <u>Method</u>	FRET-guided screening of structures from molecular dynamics simulations
<u>Name</u>	None
Number of computed models	4439