Summary of integrative structure determination of Structures of multiple states of the T4 lysozyme resolved by FRET (PDB ID: 9A08, PDB-Dev ID: PDBDEV_00000044)

1. Model Composition	
Entry composition	T4L: Chain A (164 residues)
Datasets used for modeling	- Single molecule FRET data, File: 10.5281/zenodo.3376527 - Single molecule FRET data, File: 10.5281/zenodo.3376527

	- Single molecule FRET data, File: 10.5281/zenodo.3376527
	- Single molecule FRET data, File: 10.5281/zenodo.3376527
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	- Single molecule FRET data, File: 10.5281/zenodo.3376527
	- Single molecule FRET data, File: 10.5281/zenodo.3376527
	- Single molecule FRET data, File: 10.5281/zenodo.3376527
	- Experimental model, PDB ID: 172L
	- Experimental model, PDB ID: 148L

2. Representation	
Resolution	Atomic
Number of *rigid bodies*, *flexible units*	2, 0
Rigid bodies	- A: 1-1621-162 - B: - - C: - - D: - - E: - - F: - - G: - - H: -
Structural coverage (rigid bodies)	100%

3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	

4. Validation	
Number of ensembles	2
Number of models in ensembles	119, 164
Number of deposited models	283
Model precision (uncertainty of models)	None, Å, None, Å
Data quality	Data quality has not been assessed
	- Model-1: Clashscore = 44.11, Number of Ramachandran outliers = 4, Number of sidechain outliers = 32 - Model-2: Clashscore = 39.89, Number of Ramachandran outliers = 5, Number of sidechain outliers = 21

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- Model-3: Clashscore = 47.18, Number of Ramachandran outliers = 2, Number of sidechain outliers = 29
- Model-4: Clashscore = 53.32, Number of Ramachandran outliers = 5, Number of sidechain outliers = 31
- Model-5: Clashscore = 45.65, Number of Ramachandran outliers = 4, Number of sidechain outliers = 26
- Model-6: Clashscore = 43.73, Number of Ramachandran outliers = 3, Number of sidechain outliers = 26
- Model-7: Clashscore = 64.44, Number of Ramachandran outliers = 3, Number of sidechain outliers = 36
- Model-8: Clashscore = 53.7, Number of Ramachandran outliers = 2, Number of sidechain outliers = 32
- Model-9: Clashscore = 36.07, Number of Ramachandran outliers = 3, Number of sidechain outliers = 20
- Model-10: Clashscore = 46.03, Number of Ramachandran outliers = 7, Number of sidechain outliers = 27
- Model-11: Clashscore = 41.81, Number of Ramachandran outliers = 3, Number of sidechain outliers = 29
- Model-12: Clashscore = 46.41, Number of Ramachandran outliers = 3, Number of sidechain outliers = 28
- Model-13: Clashscore = 53.7, Number of Ramachandran outliers = 4, Number of sidechain outliers = 22
- Model-14: Clashscore = 41.81, Number of Ramachandran outliers = 4, Number of sidechain outliers = 17
- Model-15: Clashscore = 39.89, Number of Ramachandran outliers = 5, Number of sidechain outliers = 25
- Model-16: Clashscore = 47.18, Number of Ramachandran outliers = 2, Number of sidechain outliers = 26
- Model-17: Clashscore = 34.91, Number of Ramachandran outliers = 1, Number of sidechain outliers = 27
- Model-18: Clashscore = 42.58, Number of Ramachandran outliers = 5, Number of sidechain outliers = 25
- Model-19: Clashscore = 37.59, Number of Ramachandran outliers = 2, Number of sidechain outliers = 26
- Model-20: Clashscore = 44.11, Number of Ramachandran outliers = 1, Number of sidechain outliers = 31
- Model-21: Clashscore = 40.28, Number of Ramachandran outliers = 5, Number of sidechain outliers = 25
- Model-22: Clashscore = 42.58, Number of Ramachandran outliers = 1, Number of sidechain outliers = 17
- Model-23: Clashscore = 36.06, Number of Ramachandran outliers = 1, Number of sidechain outliers = 17
- Model-24: Clashscore = 46.41, Number of

Ramachandran outliers = 1, Number of sidechain outliers = 22
- Model-25: Clashscore = 37.21, Number of Ramachandran outliers = 1, Number of sidechain outliers = 29
- Model-26: Clashscore = 47.56, Number of Ramachandran outliers = 3, Number of sidechain outliers = 26
- Model-27: Clashscore = 32.22, Number of Ramachandran outliers = 2, Number of sidechain outliers = 24
- Model-28: Clashscore = 46.41, Number of Ramachandran outliers = 4, Number of sidechain outliers = 17
- Model-29: Clashscore = 33.37, Number of Ramachandran outliers = 0, Number of sidechain outliers = 23
- Model-30: Clashscore = 41.43, Number of Ramachandran outliers = 0, Number of sidechain outliers = 21
- Model-31: Clashscore = 39.13, Number of Ramachandran outliers = 2, Number of sidechain outliers = 30
- Model-32: Clashscore = 39.51, Number of Ramachandran outliers = 4, Number of sidechain outliers = 23
- Model-33: Clashscore = 44.5, Number of Ramachandran outliers = 4, Number of sidechain outliers = 16
- Model-34: Clashscore = 40.28, Number of Ramachandran outliers = 2, Number of sidechain outliers = 29
- Model-35: Clashscore = 38.74, Number of Ramachandran outliers = 3, Number of sidechain outliers = 18
- Model-36: Clashscore = 47.18, Number of Ramachandran outliers = 1, Number of sidechain outliers = 22
- Model-37: Clashscore = 43.34, Number of Ramachandran outliers = 1, Number of sidechain outliers = 22
- Model-38: Clashscore = 46.41, Number of Ramachandran outliers = 1, Number of sidechain outliers = 27
- Model-39: Clashscore = 28.0, Number of Ramachandran outliers = 1, Number of sidechain outliers = 22
- Model-40: Clashscore = 38.74, Number of Ramachandran outliers = 2, Number of sidechain outliers = 23
- Model-41: Clashscore = 40.66, Number of Ramachandran outliers = 0, Number of sidechain outliers = 22
- Model-42: Clashscore = 43.73, Number of Ramachandran outliers = 1, Number of sidechain outliers = 25
- Model-43: Clashscore = 52.55, Number of Ramachandran outliers = 2, Number of sidechain outliers = 29
- Model-44: Clashscore = 43.34, Number of Ramachandran outliers = 4, Number of sidechain outliers = 25
- Model-45: Clashscore = 38.36, Number of Ramachandran outliers = 2, Number of sidechain

outliers = 27
- Model-46: Clashscore = 41.04, Number of Ramachandran outliers = 3, Number of sidechain outliers = 24
- Model-47: Clashscore = 45.26, Number of Ramachandran outliers = 1, Number of sidechain outliers = 18
- Model-48: Clashscore = 47.56, Number of Ramachandran outliers = 2, Number of sidechain outliers = 21
- Model-49: Clashscore = 40.28, Number of Ramachandran outliers = 3, Number of sidechain outliers = 20
- Model-50: Clashscore = 44.5, Number of Ramachandran outliers = 3, Number of sidechain outliers = 25
- Model-51: Clashscore = 46.41, Number of Ramachandran outliers = 2, Number of sidechain outliers = 38
- Model-52: Clashscore = 35.29, Number of Ramachandran outliers = 2, Number of sidechain outliers = 25
- Model-53: Clashscore = 42.96, Number of Ramachandran outliers = 2, Number of sidechain outliers = 28
- Model-54: Clashscore = 41.81, Number of Ramachandran outliers = 3, Number of sidechain outliers = 20
- Model-55: Clashscore = 42.58, Number of Ramachandran outliers = 0, Number of sidechain outliers = 28
- Model-56: Clashscore = 50.63, Number of Ramachandran outliers = 0, Number of sidechain outliers = 29
- Model-57: Clashscore = 34.91, Number of Ramachandran outliers = 6, Number of sidechain outliers = 23
- Model-58: Clashscore = 36.82, Number of Ramachandran outliers = 3, Number of sidechain outliers = 17
- Model-59: Clashscore = 41.81, Number of Ramachandran outliers = 2, Number of sidechain outliers = 16
- Model-60: Clashscore = 41.81, Number of Ramachandran outliers = 1, Number of sidechain outliers = 17
- Model-61: Clashscore = 37.97, Number of Ramachandran outliers = 2, Number of sidechain outliers = 20
- Model-62: Clashscore = 46.8, Number of Ramachandran outliers = 2, Number of sidechain outliers = 31
- Model-63: Clashscore = 39.51, Number of Ramachandran outliers = 1, Number of sidechain outliers = 24
- Model-64: Clashscore = 50.63, Number of Ramachandran outliers = 1, Number of sidechain outliers = 24
- Model-65: Clashscore = 33.37, Number of Ramachandran outliers = 2, Number of sidechain outliers = 27
- Model-66: Clashscore = 36.06, Number of Ramachandran outliers = 2, Number of sidechain outliers = 16

- Model-67: Clashscore = 41.81, Number of Ramachandran outliers = 1, Number of sidechain outliers = 27
- Model-68: Clashscore = 42.58, Number of Ramachandran outliers = 1, Number of sidechain outliers = 30
- Model-69: Clashscore = 41.43, Number of Ramachandran outliers = 0, Number of sidechain outliers = 31
- Model-70: Clashscore = 46.41, Number of Ramachandran outliers = 2, Number of sidechain outliers = 22
- Model-71: Clashscore = 49.87, Number of Ramachandran outliers = 3, Number of sidechain outliers = 18
- Model-72: Clashscore = 52.17, Number of Ramachandran outliers = 4, Number of sidechain outliers = 34
- Model-73: Clashscore = 33.37, Number of Ramachandran outliers = 5, Number of sidechain outliers = 25
- Model-74: Clashscore = 29.54, Number of Ramachandran outliers = 2, Number of sidechain outliers = 18
- Model-75: Clashscore = 43.34, Number of Ramachandran outliers = 0, Number of sidechain outliers = 18
- Model-76: Clashscore = 51.4, Number of Ramachandran outliers = 0, Number of sidechain outliers = 29
- Model-77: Clashscore = 41.04, Number of Ramachandran outliers = 2, Number of sidechain outliers = 27
- Model-78: Clashscore = 37.59, Number of Ramachandran outliers = 2, Number of sidechain outliers = 29
- Model-79: Clashscore = 39.89, Number of Ramachandran outliers = 4, Number of sidechain outliers = 30
- Model-80: Clashscore = 36.06, Number of Ramachandran outliers = 0, Number of sidechain outliers = 29
- Model-81: Clashscore = 37.21, Number of Ramachandran outliers = 2, Number of sidechain outliers = 30
- Model-82: Clashscore = 47.56, Number of Ramachandran outliers = 1, Number of sidechain outliers = 28
- Model-83: Clashscore = 38.74, Number of Ramachandran outliers = 0, Number of sidechain outliers = 22
- Model-84: Clashscore = 48.71, Number of Ramachandran outliers = 0, Number of sidechain outliers = 23
- Model-85: Clashscore = 38.36, Number of Ramachandran outliers = 3, Number of sidechain outliers = 22
- Model-86: Clashscore = 30.3, Number of Ramachandran outliers = 2, Number of sidechain outliers = 13
- Model-87: Clashscore = 35.67, Number of Ramachandran outliers = 1, Number of sidechain outliers = 20
- Model-88: Clashscore = 34.91, Number of

Ramachandran outliers = 0, Number of sidechain outliers = 19
- Model-89: Clashscore = 41.81, Number of Ramachandran outliers = 1, Number of sidechain outliers = 26
- Model-90: Clashscore = 36.82, Number of Ramachandran outliers = 5, Number of sidechain outliers = 27
- Model-91: Clashscore = 41.81, Number of Ramachandran outliers = 4, Number of sidechain outliers = 21
- Model-92: Clashscore = 44.11, Number of Ramachandran outliers = 2, Number of sidechain outliers = 30
- Model-93: Clashscore = 39.13, Number of Ramachandran outliers = 2, Number of sidechain outliers = 20
- Model-94: Clashscore = 41.04, Number of Ramachandran outliers = 1, Number of sidechain outliers = 23
- Model-95: Clashscore = 46.8, Number of Ramachandran outliers = 5, Number of sidechain outliers = 33
- Model-96: Clashscore = 35.67, Number of Ramachandran outliers = 1, Number of sidechain outliers = 22
- Model-97: Clashscore = 43.34, Number of Ramachandran outliers = 3, Number of sidechain outliers = 17
- Model-98: Clashscore = 32.6, Number of Ramachandran outliers = 1, Number of sidechain outliers = 20
- Model-99: Clashscore = 44.88, Number of Ramachandran outliers = 0, Number of sidechain outliers = 23
- Model-100: Clashscore = 45.65, Number of Ramachandran outliers = 5, Number of sidechain outliers = 25
- Model-101: Clashscore = 37.21, Number of Ramachandran outliers = 5, Number of sidechain outliers = 28
- Model-102: Clashscore = 44.88, Number of Ramachandran outliers = 3, Number of sidechain outliers = 32
- Model-103: Clashscore = 46.03, Number of Ramachandran outliers = 3, Number of sidechain outliers = 28
- Model-104: Clashscore = 34.14, Number of Ramachandran outliers = 1, Number of sidechain outliers = 22
- Model-105: Clashscore = 40.66, Number of Ramachandran outliers = 2, Number of sidechain outliers = 25
- Model-106: Clashscore = 42.19, Number of Ramachandran outliers = 0, Number of sidechain outliers = 24
- Model-107: Clashscore = 44.88, Number of Ramachandran outliers = 1, Number of sidechain outliers = 26
- Model-108: Clashscore = 42.58, Number of Ramachandran outliers = 2, Number of sidechain outliers = 18
- Model-109: Clashscore = 38.36, Number of Ramachandran outliers = 0, Number of sidechain

outliers = 17
- Model-110: Clashscore = 42.19, Number of Ramachandran outliers = 4, Number of sidechain outliers = 22
- Model-111: Clashscore = 47.95, Number of Ramachandran outliers = 0, Number of sidechain outliers = 28
- Model-112: Clashscore = 32.99, Number of Ramachandran outliers = 3, Number of sidechain outliers = 20
- Model-113: Clashscore = 39.51, Number of Ramachandran outliers = 1, Number of sidechain outliers = 13
- Model-114: Clashscore = 40.28, Number of Ramachandran outliers = 3, Number of sidechain outliers = 25
- Model-115: Clashscore = 41.81, Number of Ramachandran outliers = 3, Number of sidechain outliers = 22
- Model-116: Clashscore = 36.44, Number of Ramachandran outliers = 0, Number of sidechain outliers = 22
- Model-117: Clashscore = 43.73, Number of Ramachandran outliers = 3, Number of sidechain outliers = 27
- Model-118: Clashscore = 42.96, Number of Ramachandran outliers = 1, Number of sidechain outliers = 29
- Model-119: Clashscore = 47.95, Number of Ramachandran outliers = 0, Number of sidechain outliers = 33
- Model-120: Clashscore = 35.44, Number of Ramachandran outliers = 1, Number of sidechain outliers = 24
- Model-121: Clashscore = 38.91, Number of Ramachandran outliers = 1, Number of sidechain outliers = 24
- Model-122: Clashscore = 43.14, Number of Ramachandran outliers = 2, Number of sidechain outliers = 23
- Model-123: Clashscore = 39.68, Number of Ramachandran outliers = 5, Number of sidechain outliers = 30
- Model-124: Clashscore = 29.66, Number of Ramachandran outliers = 2, Number of sidechain outliers = 28
- Model-125: Clashscore = 35.44, Number of Ramachandran outliers = 0, Number of sidechain outliers = 17
- Model-126: Clashscore = 42.76, Number of Ramachandran outliers = 0, Number of sidechain outliers = 27
- Model-127: Clashscore = 35.82, Number of Ramachandran outliers = 0, Number of sidechain outliers = 24
- Model-128: Clashscore = 35.82, Number of Ramachandran outliers = 2, Number of sidechain outliers = 22
- Model-129: Clashscore = 36.21, Number of Ramachandran outliers = 2, Number of sidechain outliers = 23
- Model-130: Clashscore = 35.44, Number of Ramachandran outliers = 1, Number of sidechain outliers = 23

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| Model quality: assessment of atomic segments | - Model-131: Clashscore = 38.91, Number of Ramachandran outliers = 1, Number of sidechain outliers = 18
- Model-132: Clashscore = 40.45, Number of Ramachandran outliers = 1, Number of sidechain outliers = 27
- Model-133: Clashscore = 31.59, Number of Ramachandran outliers = 0, Number of sidechain outliers = 29
- Model-134: Clashscore = 42.76, Number of Ramachandran outliers = 2, Number of sidechain outliers = 23
- Model-135: Clashscore = 25.81, Number of Ramachandran outliers = 4, Number of sidechain outliers = 16
- Model-136: Clashscore = 30.82, Number of Ramachandran outliers = 2, Number of sidechain outliers = 18
- Model-137: Clashscore = 32.74, Number of Ramachandran outliers = 3, Number of sidechain outliers = 22
- Model-138: Clashscore = 40.06, Number of Ramachandran outliers = 2, Number of sidechain outliers = 25
- Model-139: Clashscore = 36.59, Number of Ramachandran outliers = 3, Number of sidechain outliers = 26
- Model-140: Clashscore = 35.44, Number of Ramachandran outliers = 1, Number of sidechain outliers = 20
- Model-141: Clashscore = 39.68, Number of Ramachandran outliers = 2, Number of sidechain outliers = 27
- Model-142: Clashscore = 33.13, Number of Ramachandran outliers = 3, Number of sidechain outliers = 22
- Model-143: Clashscore = 33.13, Number of Ramachandran outliers = 0, Number of sidechain outliers = 25
- Model-144: Clashscore = 28.12, Number of Ramachandran outliers = 1, Number of sidechain outliers = 25
- Model-145: Clashscore = 33.9, Number of Ramachandran outliers = 2, Number of sidechain outliers = 24
- Model-146: Clashscore = 41.6, Number of Ramachandran outliers = 4, Number of sidechain outliers = 32
- Model-147: Clashscore = 30.82, Number of Ramachandran outliers = 1, Number of sidechain outliers = 23
- Model-148: Clashscore = 35.05, Number of Ramachandran outliers = 0, Number of sidechain outliers = 23
- Model-149: Clashscore = 32.74, Number of Ramachandran outliers = 2, Number of sidechain outliers = 25
- Model-150: Clashscore = 37.37, Number of Ramachandran outliers = 0, Number of sidechain outliers = 27
- Model-151: Clashscore = 29.66, Number of Ramachandran outliers = 3, Number of sidechain outliers = 19
- Model-152: Clashscore = 40.06, Number of |

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Ramachandran outliers = 1, Number of sidechain outliers = 26
- Model-153: Clashscore = 30.05, Number of Ramachandran outliers = 1, Number of sidechain outliers = 19
- Model-154: Clashscore = 33.51, Number of Ramachandran outliers = 1, Number of sidechain outliers = 18
- Model-155: Clashscore = 33.9, Number of Ramachandran outliers = 3, Number of sidechain outliers = 26
- Model-156: Clashscore = 33.51, Number of Ramachandran outliers = 3, Number of sidechain outliers = 21
- Model-157: Clashscore = 37.37, Number of Ramachandran outliers = 6, Number of sidechain outliers = 25
- Model-158: Clashscore = 25.81, Number of Ramachandran outliers = 2, Number of sidechain outliers = 22
- Model-159: Clashscore = 26.19, Number of Ramachandran outliers = 1, Number of sidechain outliers = 21
- Model-160: Clashscore = 33.9, Number of Ramachandran outliers = 3, Number of sidechain outliers = 24
- Model-161: Clashscore = 41.22, Number of Ramachandran outliers = 0, Number of sidechain outliers = 27
- Model-162: Clashscore = 43.14, Number of Ramachandran outliers = 1, Number of sidechain outliers = 24
- Model-163: Clashscore = 45.84, Number of Ramachandran outliers = 2, Number of sidechain outliers = 27
- Model-164: Clashscore = 40.06, Number of Ramachandran outliers = 1, Number of sidechain outliers = 29
- Model-165: Clashscore = 37.37, Number of Ramachandran outliers = 2, Number of sidechain outliers = 28
- Model-166: Clashscore = 27.35, Number of Ramachandran outliers = 0, Number of sidechain outliers = 28
- Model-167: Clashscore = 30.43, Number of Ramachandran outliers = 1, Number of sidechain outliers = 21
- Model-168: Clashscore = 35.82, Number of Ramachandran outliers = 7, Number of sidechain outliers = 26
- Model-169: Clashscore = 36.59, Number of Ramachandran outliers = 6, Number of sidechain outliers = 23
- Model-170: Clashscore = 26.96, Number of Ramachandran outliers = 2, Number of sidechain outliers = 22
- Model-171: Clashscore = 37.37, Number of Ramachandran outliers = 3, Number of sidechain outliers = 23
- Model-172: Clashscore = 33.51, Number of Ramachandran outliers = 2, Number of sidechain outliers = 27
- Model-173: Clashscore = 28.51, Number of Ramachandran outliers = 1, Number of sidechain

outliers = 23
- Model-174: Clashscore = 34.67, Number of Ramachandran outliers = 2, Number of sidechain outliers = 21
- Model-175: Clashscore = 36.98, Number of Ramachandran outliers = 1, Number of sidechain outliers = 24
- Model-176: Clashscore = 36.21, Number of Ramachandran outliers = 2, Number of sidechain outliers = 24
- Model-177: Clashscore = 36.21, Number of Ramachandran outliers = 0, Number of sidechain outliers = 18
- Model-178: Clashscore = 33.51, Number of Ramachandran outliers = 0, Number of sidechain outliers = 24
- Model-179: Clashscore = 36.21, Number of Ramachandran outliers = 2, Number of sidechain outliers = 17
- Model-180: Clashscore = 39.29, Number of Ramachandran outliers = 2, Number of sidechain outliers = 19
- Model-181: Clashscore = 39.68, Number of Ramachandran outliers = 0, Number of sidechain outliers = 21
- Model-182: Clashscore = 41.22, Number of Ramachandran outliers = 1, Number of sidechain outliers = 23
- Model-183: Clashscore = 42.37, Number of Ramachandran outliers = 0, Number of sidechain outliers = 28
- Model-184: Clashscore = 44.3, Number of Ramachandran outliers = 1, Number of sidechain outliers = 26
- Model-185: Clashscore = 31.97, Number of Ramachandran outliers = 1, Number of sidechain outliers = 16
- Model-186: Clashscore = 40.45, Number of Ramachandran outliers = 1, Number of sidechain outliers = 17
- Model-187: Clashscore = 33.9, Number of Ramachandran outliers = 3, Number of sidechain outliers = 18
- Model-188: Clashscore = 31.97, Number of Ramachandran outliers = 1, Number of sidechain outliers = 26
- Model-189: Clashscore = 29.28, Number of Ramachandran outliers = 2, Number of sidechain outliers = 26
- Model-190: Clashscore = 39.29, Number of Ramachandran outliers = 2, Number of sidechain outliers = 29
- Model-191: Clashscore = 35.82, Number of Ramachandran outliers = 2, Number of sidechain outliers = 22
- Model-192: Clashscore = 16.18, Number of Ramachandran outliers = 5, Number of sidechain outliers = 14
- Model-193: Clashscore = 30.05, Number of Ramachandran outliers = 2, Number of sidechain outliers = 25
- Model-194: Clashscore = 32.74, Number of Ramachandran outliers = 0, Number of sidechain outliers = 22

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- Model-195: Clashscore = 34.67, Number of Ramachandran outliers = 2, Number of sidechain outliers = 22
- Model-196: Clashscore = 32.36, Number of Ramachandran outliers = 2, Number of sidechain outliers = 21
- Model-197: Clashscore = 31.59, Number of Ramachandran outliers = 1, Number of sidechain outliers = 24
- Model-198: Clashscore = 36.59, Number of Ramachandran outliers = 1, Number of sidechain outliers = 31
- Model-199: Clashscore = 38.52, Number of Ramachandran outliers = 1, Number of sidechain outliers = 32
- Model-200: Clashscore = 38.14, Number of Ramachandran outliers = 4, Number of sidechain outliers = 29
- Model-201: Clashscore = 39.29, Number of Ramachandran outliers = 5, Number of sidechain outliers = 24
- Model-202: Clashscore = 26.96, Number of Ramachandran outliers = 0, Number of sidechain outliers = 21
- Model-203: Clashscore = 38.91, Number of Ramachandran outliers = 4, Number of sidechain outliers = 26
- Model-204: Clashscore = 30.05, Number of Ramachandran outliers = 3, Number of sidechain outliers = 24
- Model-205: Clashscore = 25.42, Number of Ramachandran outliers = 1, Number of sidechain outliers = 20
- Model-206: Clashscore = 34.28, Number of Ramachandran outliers = 2, Number of sidechain outliers = 23
- Model-207: Clashscore = 26.96, Number of Ramachandran outliers = 7, Number of sidechain outliers = 25
- Model-208: Clashscore = 33.51, Number of Ramachandran outliers = 4, Number of sidechain outliers = 26
- Model-209: Clashscore = 34.28, Number of Ramachandran outliers = 2, Number of sidechain outliers = 27
- Model-210: Clashscore = 38.14, Number of Ramachandran outliers = 2, Number of sidechain outliers = 23
- Model-211: Clashscore = 31.59, Number of Ramachandran outliers = 3, Number of sidechain outliers = 17
- Model-212: Clashscore = 32.36, Number of Ramachandran outliers = 2, Number of sidechain outliers = 24
- Model-213: Clashscore = 38.91, Number of Ramachandran outliers = 3, Number of sidechain outliers = 18
- Model-214: Clashscore = 39.29, Number of Ramachandran outliers = 3, Number of sidechain outliers = 22
- Model-215: Clashscore = 33.9, Number of Ramachandran outliers = 3, Number of sidechain outliers = 24
- Model-216: Clashscore = 33.13, Number of

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Ramachandran outliers = 3, Number of sidechain outliers = 22
- Model-217: Clashscore = 33.51, Number of Ramachandran outliers = 5, Number of sidechain outliers = 29
- Model-218: Clashscore = 30.43, Number of Ramachandran outliers = 10, Number of sidechain outliers = 29
- Model-219: Clashscore = 38.52, Number of Ramachandran outliers = 3, Number of sidechain outliers = 20
- Model-220: Clashscore = 45.84, Number of Ramachandran outliers = 3, Number of sidechain outliers = 28
- Model-221: Clashscore = 36.98, Number of Ramachandran outliers = 4, Number of sidechain outliers = 25
- Model-222: Clashscore = 31.97, Number of Ramachandran outliers = 7, Number of sidechain outliers = 23
- Model-223: Clashscore = 30.05, Number of Ramachandran outliers = 2, Number of sidechain outliers = 21
- Model-224: Clashscore = 24.65, Number of Ramachandran outliers = 1, Number of sidechain outliers = 18
- Model-225: Clashscore = 39.68, Number of Ramachandran outliers = 2, Number of sidechain outliers = 29
- Model-226: Clashscore = 36.59, Number of Ramachandran outliers = 6, Number of sidechain outliers = 33
- Model-227: Clashscore = 25.42, Number of Ramachandran outliers = 12, Number of sidechain outliers = 21
- Model-228: Clashscore = 37.37, Number of Ramachandran outliers = 3, Number of sidechain outliers = 21
- Model-229: Clashscore = 38.14, Number of Ramachandran outliers = 4, Number of sidechain outliers = 31
- Model-230: Clashscore = 28.12, Number of Ramachandran outliers = 8, Number of sidechain outliers = 16
- Model-231: Clashscore = 34.67, Number of Ramachandran outliers = 4, Number of sidechain outliers = 21
- Model-232: Clashscore = 38.91, Number of Ramachandran outliers = 4, Number of sidechain outliers = 22
- Model-233: Clashscore = 30.82, Number of Ramachandran outliers = 2, Number of sidechain outliers = 27
- Model-234: Clashscore = 35.05, Number of Ramachandran outliers = 2, Number of sidechain outliers = 29
- Model-235: Clashscore = 31.97, Number of Ramachandran outliers = 3, Number of sidechain outliers = 21
- Model-236: Clashscore = 38.52, Number of Ramachandran outliers = 4, Number of sidechain outliers = 29
- Model-237: Clashscore = 34.28, Number of Ramachandran outliers = 3, Number of sidechain

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outliers = 23
- Model-238: Clashscore = 31.2, Number of Ramachandran outliers = 4, Number of sidechain outliers = 25
- Model-239: Clashscore = 33.13, Number of Ramachandran outliers = 4, Number of sidechain outliers = 24
- Model-240: Clashscore = 38.91, Number of Ramachandran outliers = 1, Number of sidechain outliers = 23
- Model-241: Clashscore = 33.13, Number of Ramachandran outliers = 2, Number of sidechain outliers = 17
- Model-242: Clashscore = 41.6, Number of Ramachandran outliers = 4, Number of sidechain outliers = 28
- Model-243: Clashscore = 29.66, Number of Ramachandran outliers = 3, Number of sidechain outliers = 21
- Model-244: Clashscore = 34.28, Number of Ramachandran outliers = 5, Number of sidechain outliers = 28
- Model-245: Clashscore = 33.9, Number of Ramachandran outliers = 3, Number of sidechain outliers = 25
- Model-246: Clashscore = 30.82, Number of Ramachandran outliers = 2, Number of sidechain outliers = 25
- Model-247: Clashscore = 30.05, Number of Ramachandran outliers = 4, Number of sidechain outliers = 30
- Model-248: Clashscore = 26.96, Number of Ramachandran outliers = 4, Number of sidechain outliers = 25
- Model-249: Clashscore = 39.29, Number of Ramachandran outliers = 2, Number of sidechain outliers = 27
- Model-250: Clashscore = 48.15, Number of Ramachandran outliers = 3, Number of sidechain outliers = 27
- Model-251: Clashscore = 31.2, Number of Ramachandran outliers = 7, Number of sidechain outliers = 18
- Model-252: Clashscore = 39.29, Number of Ramachandran outliers = 3, Number of sidechain outliers = 27
- Model-253: Clashscore = 32.36, Number of Ramachandran outliers = 2, Number of sidechain outliers = 25
- Model-254: Clashscore = 37.75, Number of Ramachandran outliers = 3, Number of sidechain outliers = 24
- Model-255: Clashscore = 28.12, Number of Ramachandran outliers = 4, Number of sidechain outliers = 20
- Model-256: Clashscore = 34.28, Number of Ramachandran outliers = 1, Number of sidechain outliers = 24
- Model-257: Clashscore = 36.98, Number of Ramachandran outliers = 1, Number of sidechain outliers = 30
- Model-258: Clashscore = 29.66, Number of Ramachandran outliers = 3, Number of sidechain outliers = 28

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- Model-259: Clashscore = 36.98, Number of Ramachandran outliers = 3, Number of sidechain outliers = 24
- Model-260: Clashscore = 32.74, Number of Ramachandran outliers = 2, Number of sidechain outliers = 22
- Model-261: Clashscore = 32.36, Number of Ramachandran outliers = 2, Number of sidechain outliers = 16
- Model-262: Clashscore = 29.66, Number of Ramachandran outliers = 7, Number of sidechain outliers = 23
- Model-263: Clashscore = 34.28, Number of Ramachandran outliers = 6, Number of sidechain outliers = 23
- Model-264: Clashscore = 30.82, Number of Ramachandran outliers = 3, Number of sidechain outliers = 16
- Model-265: Clashscore = 33.9, Number of Ramachandran outliers = 1, Number of sidechain outliers = 21
- Model-266: Clashscore = 44.3, Number of Ramachandran outliers = 4, Number of sidechain outliers = 18
- Model-267: Clashscore = 39.68, Number of Ramachandran outliers = 4, Number of sidechain outliers = 24
- Model-268: Clashscore = 37.37, Number of Ramachandran outliers = 4, Number of sidechain outliers = 18
- Model-269: Clashscore = 35.44, Number of Ramachandran outliers = 1, Number of sidechain outliers = 19
- Model-270: Clashscore = 38.91, Number of Ramachandran outliers = 4, Number of sidechain outliers = 32
- Model-271: Clashscore = 35.05, Number of Ramachandran outliers = 3, Number of sidechain outliers = 27
- Model-272: Clashscore = 42.37, Number of Ramachandran outliers = 4, Number of sidechain outliers = 22
- Model-273: Clashscore = 32.74, Number of Ramachandran outliers = 2, Number of sidechain outliers = 23
- Model-274: Clashscore = 29.28, Number of Ramachandran outliers = 0, Number of sidechain outliers = 20
- Model-275: Clashscore = 38.14, Number of Ramachandran outliers = 2, Number of sidechain outliers = 28
- Model-276: Clashscore = 34.28, Number of Ramachandran outliers = 3, Number of sidechain outliers = 20
- Model-277: Clashscore = 42.76, Number of Ramachandran outliers = 4, Number of sidechain outliers = 26
- Model-278: Clashscore = 32.74, Number of Ramachandran outliers = 1, Number of sidechain outliers = 16
- Model-279: Clashscore = 41.22, Number of Ramachandran outliers = 5, Number of sidechain outliers = 26
- Model-280: Clashscore = 40.45, Number of

IM Summary Table

	Ramachandran outliers = 3, Number of sidechain outliers = 26 - Model-281: Clashscore = 36.98, Number of Ramachandran outliers = 3, Number of sidechain outliers = 27 - Model-282: Clashscore = 32.74, Number of Ramachandran outliers = 2, Number of sidechain outliers = 17 - Model-283: Clashscore = 38.91, Number of Ramachandran outliers = 3, Number of sidechain outliers = 21
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. *Method*	free NMSim
Name	None
2. *Method*	FRET-guided NMSim
Name	None
3. *Method*	FRET screening
Name	None
Software	- Olga (version Not available) - NMSim (version Not available)