

**Summary of integrative structure determination of Structures of multiple states of the hGBP1 resolved by FRET, SAXS, and EPR (PDB ID: 9A1G, PDB-Dev ID: PDBDEV\_00000088)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	hGBP1 wildtype: Chain A (583 residues)
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- Experimental model, PDB ID: 1DG3</li> <li>- SAS data, SASBDB: SASDDD6</li> <li>- Single molecule FRET data, File: 10.5281/zenodo.6534557</li> <li>- Single molecule FRET data, File: 10.5281/zenodo.6534557</li> <li>- Single molecule FRET data, File: 10.5281/zenodo.6534557</li> <li>- Single molecule FRET data, File: 10.5281/zenodo.6534557</li> <li>- Single molecule FRET data, File: 10.5281/zenodo.6534557</li> <li>- Single molecule FRET data, File: 10.5281/zenodo.6534557</li> <li>- Single molecule FRET data, File: 10.5281/zenodo.6534557</li> <li>- Single molecule FRET data, File: 10.5281/zenodo.6534557</li> <li>- Single molecule FRET data, File: 10.5281/zenodo.6534557</li> <li>- Single molecule FRET data, File: 10.5281/zenodo.6534557</li> <li>- Single molecule FRET data, File: 10.5281/zenodo.6534557</li> <li>- Single molecule FRET data, File: 10.5281/zenodo.6534557</li> <li>- Single molecule FRET data, File: 10.5281/zenodo.6534557</li> <li>- Other, File: 10.5281/zenodo.6534557</li> <li>- Other, File: 10.5281/zenodo.6534557</li> <li>- Other, File: 10.5281/zenodo.6534557</li> <li>- Other, File: 10.5281/zenodo.6534557</li> <li>- Other, File: 10.5281/zenodo.6534557</li> <li>- Other, File: 10.5281/zenodo.6534557</li> <li>- Other, File: 10.5281/zenodo.6534557</li> <li>- Other, File: 10.5281/zenodo.6534557</li> </ul>
<b>2. Representation</b>	
<a href="#">Resolution</a>	Atomic
<a href="#">Number of rigid bodies, flexible units</a>	0, 1
<a href="#">Flexible units</a>	A: 1-583
<a href="#">Structural coverage (rigid bodies)</a>	100%
<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided

<a href="#"><i>Experimental data</i></a>	
<b>4. Validation</b>	
<a href="#"><i>Number of ensembles</i></a>	2
<a href="#"><i>Number of models in ensembles</i></a>	100, 106
<a href="#"><i>Number of deposited models</i></a>	206
<a href="#"><i>Model precision (uncertainty of models)</i></a>	None, Å, None, Å
<a href="#"><i>Data quality</i></a>	SASDDD6: Rg from Gunier is 3.89nm and Rg from p(r) is 4.02nm
	<ul style="list-style-type: none"> <li>- Model-1: Clashscore = 2.87, Number of Ramachandran outliers = 14, Number of sidechain outliers = 103</li> <li>- Model-2: Clashscore = 2.76, Number of Ramachandran outliers = 5, Number of sidechain outliers = 100</li> <li>- Model-3: Clashscore = 3.72, Number of Ramachandran outliers = 10, Number of sidechain outliers = 103</li> <li>- Model-4: Clashscore = 2.98, Number of Ramachandran outliers = 9, Number of sidechain outliers = 102</li> <li>- Model-5: Clashscore = 3.51, Number of Ramachandran outliers = 8, Number of sidechain outliers = 105</li> <li>- Model-6: Clashscore = 1.06, Number of Ramachandran outliers = 9, Number of sidechain outliers = 33</li> <li>- Model-7: Clashscore = 0.64, Number of Ramachandran outliers = 15, Number of sidechain outliers = 27</li> <li>- Model-8: Clashscore = 0.85, Number of Ramachandran outliers = 6, Number of sidechain outliers = 25</li> <li>- Model-9: Clashscore = 3.19, Number of Ramachandran outliers = 10, Number of sidechain outliers = 102</li> <li>- Model-10: Clashscore = 1.17, Number of Ramachandran outliers = 4, Number of sidechain outliers = 29</li> <li>- Model-11: Clashscore = 1.06, Number of Ramachandran outliers = 4, Number of sidechain outliers = 17</li> <li>- Model-12: Clashscore = 1.38, Number of Ramachandran outliers = 9, Number of sidechain outliers = 27</li> <li>- Model-13: Clashscore = 2.98, Number of Ramachandran outliers = 11, Number of sidechain outliers = 105</li> <li>- Model-14: Clashscore = 0.96, Number of Ramachandran outliers = 8, Number of sidechain outliers = 18</li> <li>- Model-15: Clashscore = 1.6, Number of Ramachandran outliers = 6, Number of sidechain outliers = 25</li> </ul>

- Model-16: Clashscore = 0.53, Number of Ramachandran outliers = 6, Number of sidechain outliers = 22
- Model-17: Clashscore = 1.7, Number of Ramachandran outliers = 6, Number of sidechain outliers = 19
- Model-18: Clashscore = 0.53, Number of Ramachandran outliers = 9, Number of sidechain outliers = 21
- Model-19: Clashscore = 3.3, Number of Ramachandran outliers = 17, Number of sidechain outliers = 113
- Model-20: Clashscore = 4.04, Number of Ramachandran outliers = 8, Number of sidechain outliers = 118
- Model-21: Clashscore = 3.72, Number of Ramachandran outliers = 10, Number of sidechain outliers = 109
- Model-22: Clashscore = 3.3, Number of Ramachandran outliers = 7, Number of sidechain outliers = 94
- Model-23: Clashscore = 1.28, Number of Ramachandran outliers = 11, Number of sidechain outliers = 29
- Model-24: Clashscore = 2.87, Number of Ramachandran outliers = 7, Number of sidechain outliers = 105
- Model-25: Clashscore = 1.81, Number of Ramachandran outliers = 7, Number of sidechain outliers = 29
- Model-26: Clashscore = 1.49, Number of Ramachandran outliers = 14, Number of sidechain outliers = 21
- Model-27: Clashscore = 1.28, Number of Ramachandran outliers = 7, Number of sidechain outliers = 37
- Model-28: Clashscore = 1.49, Number of Ramachandran outliers = 5, Number of sidechain outliers = 26
- Model-29: Clashscore = 0.96, Number of Ramachandran outliers = 8, Number of sidechain outliers = 23
- Model-30: Clashscore = 2.02, Number of Ramachandran outliers = 6, Number of sidechain outliers = 103
- Model-31: Clashscore = 1.49, Number of Ramachandran outliers = 9, Number of sidechain outliers = 34
- Model-32: Clashscore = 1.49, Number of Ramachandran outliers = 9, Number of sidechain outliers = 21
- Model-33: Clashscore = 1.06, Number of Ramachandran outliers = 5, Number of sidechain outliers = 31
- Model-34: Clashscore = 1.06, Number of Ramachandran outliers = 7, Number of sidechain outliers = 21
- Model-35: Clashscore = 1.06, Number of Ramachandran outliers = 17, Number of sidechain outliers = 27
- Model-36: Clashscore = 0.74, Number of Ramachandran outliers = 10, Number of sidechain outliers = 24
- Model-37: Clashscore = 1.06, Number of

Ramachandran outliers = 6, Number of sidechain outliers = 21

- Model-38: Clashscore = 1.17, Number of Ramachandran outliers = 5, Number of sidechain outliers = 27
- Model-39: Clashscore = 0.85, Number of Ramachandran outliers = 12, Number of sidechain outliers = 26
- Model-40: Clashscore = 1.28, Number of Ramachandran outliers = 5, Number of sidechain outliers = 32
- Model-41: Clashscore = 2.87, Number of Ramachandran outliers = 9, Number of sidechain outliers = 90
- Model-42: Clashscore = 1.06, Number of Ramachandran outliers = 5, Number of sidechain outliers = 23
- Model-43: Clashscore = 1.38, Number of Ramachandran outliers = 6, Number of sidechain outliers = 39
- Model-44: Clashscore = 2.23, Number of Ramachandran outliers = 6, Number of sidechain outliers = 100
- Model-45: Clashscore = 1.6, Number of Ramachandran outliers = 7, Number of sidechain outliers = 19
- Model-46: Clashscore = 1.06, Number of Ramachandran outliers = 7, Number of sidechain outliers = 40
- Model-47: Clashscore = 1.06, Number of Ramachandran outliers = 12, Number of sidechain outliers = 27
- Model-48: Clashscore = 1.06, Number of Ramachandran outliers = 10, Number of sidechain outliers = 18
- Model-49: Clashscore = 0.64, Number of Ramachandran outliers = 8, Number of sidechain outliers = 19
- Model-50: Clashscore = 3.62, Number of Ramachandran outliers = 6, Number of sidechain outliers = 96
- Model-51: Clashscore = 1.06, Number of Ramachandran outliers = 8, Number of sidechain outliers = 23
- Model-52: Clashscore = 0.74, Number of Ramachandran outliers = 4, Number of sidechain outliers = 31
- Model-53: Clashscore = 2.98, Number of Ramachandran outliers = 10, Number of sidechain outliers = 105
- Model-54: Clashscore = 4.36, Number of Ramachandran outliers = 12, Number of sidechain outliers = 111
- Model-55: Clashscore = 4.15, Number of Ramachandran outliers = 8, Number of sidechain outliers = 86
- Model-56: Clashscore = 3.72, Number of Ramachandran outliers = 8, Number of sidechain outliers = 108
- Model-57: Clashscore = 0.85, Number of Ramachandran outliers = 5, Number of sidechain outliers = 22
- Model-58: Clashscore = 0.64, Number of Ramachandran outliers = 2, Number of sidechain

outliers = 18  
- Model-59: Clashscore = 1.38, Number of Ramachandran outliers = 10, Number of sidechain outliers = 28  
- Model-60: Clashscore = 1.49, Number of Ramachandran outliers = 13, Number of sidechain outliers = 41  
- Model-61: Clashscore = 0.96, Number of Ramachandran outliers = 7, Number of sidechain outliers = 50  
- Model-62: Clashscore = 0.64, Number of Ramachandran outliers = 12, Number of sidechain outliers = 27  
- Model-63: Clashscore = 0.96, Number of Ramachandran outliers = 10, Number of sidechain outliers = 26  
- Model-64: Clashscore = 0.85, Number of Ramachandran outliers = 9, Number of sidechain outliers = 27  
- Model-65: Clashscore = 0.96, Number of Ramachandran outliers = 9, Number of sidechain outliers = 29  
- Model-66: Clashscore = 1.06, Number of Ramachandran outliers = 6, Number of sidechain outliers = 26  
- Model-67: Clashscore = 2.87, Number of Ramachandran outliers = 12, Number of sidechain outliers = 100  
- Model-68: Clashscore = 2.13, Number of Ramachandran outliers = 8, Number of sidechain outliers = 44  
- Model-69: Clashscore = 4.36, Number of Ramachandran outliers = 10, Number of sidechain outliers = 113  
- Model-70: Clashscore = 1.06, Number of Ramachandran outliers = 11, Number of sidechain outliers = 19  
- Model-71: Clashscore = 0.85, Number of Ramachandran outliers = 10, Number of sidechain outliers = 20  
- Model-72: Clashscore = 0.53, Number of Ramachandran outliers = 9, Number of sidechain outliers = 13  
- Model-73: Clashscore = 1.06, Number of Ramachandran outliers = 9, Number of sidechain outliers = 24  
- Model-74: Clashscore = 2.02, Number of Ramachandran outliers = 8, Number of sidechain outliers = 88  
- Model-75: Clashscore = 4.04, Number of Ramachandran outliers = 4, Number of sidechain outliers = 101  
- Model-76: Clashscore = 1.49, Number of Ramachandran outliers = 5, Number of sidechain outliers = 21  
- Model-77: Clashscore = 0.74, Number of Ramachandran outliers = 7, Number of sidechain outliers = 17  
- Model-78: Clashscore = 0.64, Number of Ramachandran outliers = 7, Number of sidechain outliers = 21  
- Model-79: Clashscore = 1.6, Number of Ramachandran outliers = 8, Number of sidechain outliers = 17

- Model-80: Clashscore = 0.85, Number of Ramachandran outliers = 5, Number of sidechain outliers = 18
- Model-81: Clashscore = 0.96, Number of Ramachandran outliers = 9, Number of sidechain outliers = 21
- Model-82: Clashscore = 0.85, Number of Ramachandran outliers = 8, Number of sidechain outliers = 22
- Model-83: Clashscore = 1.17, Number of Ramachandran outliers = 12, Number of sidechain outliers = 18
- Model-84: Clashscore = 4.68, Number of Ramachandran outliers = 13, Number of sidechain outliers = 88
- Model-85: Clashscore = 1.28, Number of Ramachandran outliers = 4, Number of sidechain outliers = 26
- Model-86: Clashscore = 0.96, Number of Ramachandran outliers = 9, Number of sidechain outliers = 22
- Model-87: Clashscore = 2.34, Number of Ramachandran outliers = 11, Number of sidechain outliers = 120
- Model-88: Clashscore = 3.4, Number of Ramachandran outliers = 8, Number of sidechain outliers = 105
- Model-89: Clashscore = 2.98, Number of Ramachandran outliers = 5, Number of sidechain outliers = 100
- Model-90: Clashscore = 1.28, Number of Ramachandran outliers = 8, Number of sidechain outliers = 23
- Model-91: Clashscore = 2.76, Number of Ramachandran outliers = 8, Number of sidechain outliers = 41
- Model-92: Clashscore = 0.85, Number of Ramachandran outliers = 9, Number of sidechain outliers = 35
- Model-93: Clashscore = 1.06, Number of Ramachandran outliers = 16, Number of sidechain outliers = 29
- Model-94: Clashscore = 3.51, Number of Ramachandran outliers = 18, Number of sidechain outliers = 95
- Model-95: Clashscore = 1.49, Number of Ramachandran outliers = 18, Number of sidechain outliers = 16
- Model-96: Clashscore = 3.3, Number of Ramachandran outliers = 8, Number of sidechain outliers = 96
- Model-97: Clashscore = 0.64, Number of Ramachandran outliers = 11, Number of sidechain outliers = 29
- Model-98: Clashscore = 3.72, Number of Ramachandran outliers = 14, Number of sidechain outliers = 95
- Model-99: Clashscore = 1.49, Number of Ramachandran outliers = 11, Number of sidechain outliers = 22
- Model-100: Clashscore = 1.38, Number of Ramachandran outliers = 10, Number of sidechain outliers = 17
- Model-101: Clashscore = 1.38, Number of

[\*Model quality: assessment of atomic segments\*](#)

Ramachandran outliers = 7, Number of sidechain outliers = 20

- Model-102: Clashscore = 0.96, Number of Ramachandran outliers = 9, Number of sidechain outliers = 38
- Model-103: Clashscore = 1.06, Number of Ramachandran outliers = 10, Number of sidechain outliers = 23
- Model-104: Clashscore = 2.13, Number of Ramachandran outliers = 4, Number of sidechain outliers = 42
- Model-105: Clashscore = 0.64, Number of Ramachandran outliers = 13, Number of sidechain outliers = 23
- Model-106: Clashscore = 0.21, Number of Ramachandran outliers = 10, Number of sidechain outliers = 25
- Model-107: Clashscore = 1.6, Number of Ramachandran outliers = 15, Number of sidechain outliers = 20
- Model-108: Clashscore = 1.49, Number of Ramachandran outliers = 10, Number of sidechain outliers = 26
- Model-109: Clashscore = 1.6, Number of Ramachandran outliers = 13, Number of sidechain outliers = 20
- Model-110: Clashscore = 1.17, Number of Ramachandran outliers = 9, Number of sidechain outliers = 23
- Model-111: Clashscore = 1.17, Number of Ramachandran outliers = 10, Number of sidechain outliers = 21
- Model-112: Clashscore = 0.74, Number of Ramachandran outliers = 18, Number of sidechain outliers = 25
- Model-113: Clashscore = 1.7, Number of Ramachandran outliers = 19, Number of sidechain outliers = 31
- Model-114: Clashscore = 1.38, Number of Ramachandran outliers = 13, Number of sidechain outliers = 24
- Model-115: Clashscore = 0.96, Number of Ramachandran outliers = 12, Number of sidechain outliers = 30
- Model-116: Clashscore = 1.17, Number of Ramachandran outliers = 7, Number of sidechain outliers = 34
- Model-117: Clashscore = 1.06, Number of Ramachandran outliers = 8, Number of sidechain outliers = 23
- Model-118: Clashscore = 0.32, Number of Ramachandran outliers = 7, Number of sidechain outliers = 23
- Model-119: Clashscore = 0.74, Number of Ramachandran outliers = 6, Number of sidechain outliers = 13
- Model-120: Clashscore = 0.64, Number of Ramachandran outliers = 4, Number of sidechain outliers = 25
- Model-121: Clashscore = 1.6, Number of Ramachandran outliers = 16, Number of sidechain outliers = 17
- Model-122: Clashscore = 0.74, Number of Ramachandran outliers = 16, Number of sidechain

outliers = 20

- Model-123: Clashscore = 1.17, Number of Ramachandran outliers = 14, Number of sidechain outliers = 22
- Model-124: Clashscore = 1.17, Number of Ramachandran outliers = 12, Number of sidechain outliers = 24
- Model-125: Clashscore = 0.74, Number of Ramachandran outliers = 13, Number of sidechain outliers = 21
- Model-126: Clashscore = 1.49, Number of Ramachandran outliers = 9, Number of sidechain outliers = 22
- Model-127: Clashscore = 0.43, Number of Ramachandran outliers = 9, Number of sidechain outliers = 11
- Model-128: Clashscore = 0.53, Number of Ramachandran outliers = 7, Number of sidechain outliers = 17
- Model-129: Clashscore = 0.96, Number of Ramachandran outliers = 9, Number of sidechain outliers = 17
- Model-130: Clashscore = 1.28, Number of Ramachandran outliers = 14, Number of sidechain outliers = 21
- Model-131: Clashscore = 1.38, Number of Ramachandran outliers = 12, Number of sidechain outliers = 21
- Model-132: Clashscore = 1.38, Number of Ramachandran outliers = 10, Number of sidechain outliers = 26
- Model-133: Clashscore = 0.96, Number of Ramachandran outliers = 6, Number of sidechain outliers = 23
- Model-134: Clashscore = 1.17, Number of Ramachandran outliers = 16, Number of sidechain outliers = 35
- Model-135: Clashscore = 1.06, Number of Ramachandran outliers = 11, Number of sidechain outliers = 22
- Model-136: Clashscore = 0.96, Number of Ramachandran outliers = 8, Number of sidechain outliers = 16
- Model-137: Clashscore = 2.02, Number of Ramachandran outliers = 7, Number of sidechain outliers = 24
- Model-138: Clashscore = 1.17, Number of Ramachandran outliers = 7, Number of sidechain outliers = 21
- Model-139: Clashscore = 1.06, Number of Ramachandran outliers = 7, Number of sidechain outliers = 22
- Model-140: Clashscore = 1.38, Number of Ramachandran outliers = 10, Number of sidechain outliers = 19
- Model-141: Clashscore = 0.64, Number of Ramachandran outliers = 10, Number of sidechain outliers = 33
- Model-142: Clashscore = 3.62, Number of Ramachandran outliers = 7, Number of sidechain outliers = 113
- Model-143: Clashscore = 1.38, Number of Ramachandran outliers = 13, Number of sidechain outliers = 23



- Model-144: Clashscore = 0.85, Number of Ramachandran outliers = 16, Number of sidechain outliers = 23
- Model-145: Clashscore = 1.28, Number of Ramachandran outliers = 10, Number of sidechain outliers = 21
- Model-146: Clashscore = 1.28, Number of Ramachandran outliers = 17, Number of sidechain outliers = 22
- Model-147: Clashscore = 1.6, Number of Ramachandran outliers = 7, Number of sidechain outliers = 29
- Model-148: Clashscore = 1.17, Number of Ramachandran outliers = 9, Number of sidechain outliers = 34
- Model-149: Clashscore = 0.53, Number of Ramachandran outliers = 2, Number of sidechain outliers = 17
- Model-150: Clashscore = 0.64, Number of Ramachandran outliers = 3, Number of sidechain outliers = 21
- Model-151: Clashscore = 1.06, Number of Ramachandran outliers = 8, Number of sidechain outliers = 30
- Model-152: Clashscore = 1.49, Number of Ramachandran outliers = 10, Number of sidechain outliers = 30
- Model-153: Clashscore = 3.83, Number of Ramachandran outliers = 13, Number of sidechain outliers = 97
- Model-154: Clashscore = 0.85, Number of Ramachandran outliers = 11, Number of sidechain outliers = 26
- Model-155: Clashscore = 1.38, Number of Ramachandran outliers = 3, Number of sidechain outliers = 34
- Model-156: Clashscore = 0.64, Number of Ramachandran outliers = 17, Number of sidechain outliers = 19
- Model-157: Clashscore = 1.17, Number of Ramachandran outliers = 15, Number of sidechain outliers = 36
- Model-158: Clashscore = 1.28, Number of Ramachandran outliers = 12, Number of sidechain outliers = 32
- Model-159: Clashscore = 0.64, Number of Ramachandran outliers = 16, Number of sidechain outliers = 33
- Model-160: Clashscore = 1.49, Number of Ramachandran outliers = 8, Number of sidechain outliers = 29
- Model-161: Clashscore = 0.21, Number of Ramachandran outliers = 7, Number of sidechain outliers = 17
- Model-162: Clashscore = 0.96, Number of Ramachandran outliers = 9, Number of sidechain outliers = 35
- Model-163: Clashscore = 0.64, Number of Ramachandran outliers = 7, Number of sidechain outliers = 18
- Model-164: Clashscore = 1.38, Number of Ramachandran outliers = 13, Number of sidechain outliers = 29
- Model-165: Clashscore = 3.51, Number of

Ramachandran outliers = 11, Number of sidechain outliers = 108

- Model-166: Clashscore = 1.38, Number of Ramachandran outliers = 7, Number of sidechain outliers = 21
- Model-167: Clashscore = 3.72, Number of Ramachandran outliers = 10, Number of sidechain outliers = 100
- Model-168: Clashscore = 3.62, Number of Ramachandran outliers = 5, Number of sidechain outliers = 89
- Model-169: Clashscore = 1.6, Number of Ramachandran outliers = 13, Number of sidechain outliers = 23
- Model-170: Clashscore = 0.64, Number of Ramachandran outliers = 12, Number of sidechain outliers = 20
- Model-171: Clashscore = 0.96, Number of Ramachandran outliers = 12, Number of sidechain outliers = 22
- Model-172: Clashscore = 1.17, Number of Ramachandran outliers = 11, Number of sidechain outliers = 17
- Model-173: Clashscore = 0.96, Number of Ramachandran outliers = 9, Number of sidechain outliers = 24
- Model-174: Clashscore = 1.38, Number of Ramachandran outliers = 9, Number of sidechain outliers = 28
- Model-175: Clashscore = 1.06, Number of Ramachandran outliers = 7, Number of sidechain outliers = 31
- Model-176: Clashscore = 2.55, Number of Ramachandran outliers = 10, Number of sidechain outliers = 97
- Model-177: Clashscore = 3.4, Number of Ramachandran outliers = 9, Number of sidechain outliers = 94
- Model-178: Clashscore = 1.06, Number of Ramachandran outliers = 12, Number of sidechain outliers = 20
- Model-179: Clashscore = 1.17, Number of Ramachandran outliers = 12, Number of sidechain outliers = 18
- Model-180: Clashscore = 2.34, Number of Ramachandran outliers = 11, Number of sidechain outliers = 25
- Model-181: Clashscore = 3.51, Number of Ramachandran outliers = 11, Number of sidechain outliers = 113
- Model-182: Clashscore = 3.3, Number of Ramachandran outliers = 12, Number of sidechain outliers = 104
- Model-183: Clashscore = 5.21, Number of Ramachandran outliers = 3, Number of sidechain outliers = 123
- Model-184: Clashscore = 3.3, Number of Ramachandran outliers = 14, Number of sidechain outliers = 92
- Model-185: Clashscore = 2.87, Number of Ramachandran outliers = 10, Number of sidechain outliers = 93
- Model-186: Clashscore = 0.74, Number of Ramachandran outliers = 8, Number of sidechain

	<p>outliers = 31</p> <ul style="list-style-type: none"> <li>- Model-187: Clashscore = 1.81, Number of Ramachandran outliers = 7, Number of sidechain outliers = 92</li> <li>- Model-188: Clashscore = 3.3, Number of Ramachandran outliers = 5, Number of sidechain outliers = 108</li> <li>- Model-189: Clashscore = 0.96, Number of Ramachandran outliers = 12, Number of sidechain outliers = 20</li> <li>- Model-190: Clashscore = 1.06, Number of Ramachandran outliers = 12, Number of sidechain outliers = 34</li> <li>- Model-191: Clashscore = 1.49, Number of Ramachandran outliers = 4, Number of sidechain outliers = 29</li> <li>- Model-192: Clashscore = 1.49, Number of Ramachandran outliers = 7, Number of sidechain outliers = 22</li> <li>- Model-193: Clashscore = 1.91, Number of Ramachandran outliers = 14, Number of sidechain outliers = 37</li> <li>- Model-194: Clashscore = 3.62, Number of Ramachandran outliers = 9, Number of sidechain outliers = 96</li> <li>- Model-195: Clashscore = 3.93, Number of Ramachandran outliers = 10, Number of sidechain outliers = 100</li> <li>- Model-196: Clashscore = 2.55, Number of Ramachandran outliers = 14, Number of sidechain outliers = 80</li> <li>- Model-197: Clashscore = 0.43, Number of Ramachandran outliers = 6, Number of sidechain outliers = 17</li> <li>- Model-198: Clashscore = 1.28, Number of Ramachandran outliers = 13, Number of sidechain outliers = 35</li> <li>- Model-199: Clashscore = 0.74, Number of Ramachandran outliers = 14, Number of sidechain outliers = 21</li> <li>- Model-200: Clashscore = 3.93, Number of Ramachandran outliers = 12, Number of sidechain outliers = 109</li> <li>- Model-201: Clashscore = 0.96, Number of Ramachandran outliers = 7, Number of sidechain outliers = 35</li> <li>- Model-202: Clashscore = 1.17, Number of Ramachandran outliers = 10, Number of sidechain outliers = 25</li> <li>- Model-203: Clashscore = 1.81, Number of Ramachandran outliers = 13, Number of sidechain outliers = 33</li> <li>- Model-204: Clashscore = 1.38, Number of Ramachandran outliers = 10, Number of sidechain outliers = 28</li> <li>- Model-205: Clashscore = 1.28, Number of Ramachandran outliers = 10, Number of sidechain outliers = 36</li> <li>- Model-206: Clashscore = 0.64, Number of Ramachandran outliers = 12, Number of sidechain outliers = 31</li> </ul>
<a href="#"><i>Model quality: assessment of excluded volume</i></a>	Not applicable

<a href="#"><i>Fit to data used for modeling</i></a>	Fit of model to information used to compute it has not been determined
<a href="#"><i>Fit to data used for validation</i></a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
1. <a href="#"><i>Method</i></a>	Rigid body docking
<a href="#"><i>Name</i></a>	None
2. <a href="#"><i>Method</i></a>	Targeted NMSim
<a href="#"><i>Name</i></a>	None
3. <a href="#"><i>Method</i></a>	MD simulation
<a href="#"><i>Name</i></a>	None
<a href="#"><i>Software</i></a>	<ul style="list-style-type: none"> <li>- FPS (version Not available)</li> <li>- <a href="#">NMSim</a> (version Not available)</li> <li>- Amber 14 (version Not available)</li> <li>- DeerAnalysis2006 (version Not available)</li> </ul>