Supporting Information

Accelerated Molecular Dynamics for Peptide Folding: Benchmarking Different Combinations of Amber Force Fields and Explicit Solvent Models

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Table S1. Total Potential Energy (EPTOT) Average and dihedral angle (DHIED) average values obtained by cMD

ff99SB TIP3P	**Average EPTOT***	**Average DHIED***
H1 EXTENDED	-24216.6	171.0
H1 MISFOLDED	-27050.1	172.3
H2 EXTENDED	-10078.0	58.3
H2 MISFOLDED	-10244.8	60.0
B1 EXTENDED	-30044.5	165.0
B1 MISFOLDED	-23632.6	168.4
B2 EXTENDED	-22522.8	135.8
B2 MISFOLDED	-22541.2	139.2
B3 EXTENDED	-34514.5	159.1
B3 MISFOLDED	-22223.9	162.8
ID1 EXTENDED	-15929.4	150.4
ID1 MISFOLDED	-20480.7	148.2
ID2 EXTENDED	-24007.8	137.4
ID2 MISFOLDED	-18957.1	140.8
ID3 EXTENDED	-21743.6	139.0
ID3 MISFOLDED	-17957.3	149.8
ff99SB OPC	**Average EPTOT***	**Average DHIED***
H1 EXTENDED	-39642.5	171.0
H1 MISFOLDED	-35971.0	171.1
H2 EXTENDED	-14029.0	58.1
H2 MISFOLDED	-13261.7	60.1
B1 EXTENDED	-37900.0	162.0
B1 MISFOLDED	-30039.4	162.8
B2 EXTENDED	-25786.0	134.5
B2 MISFOLDED	-28368.7	136.4
B3 EXTENDED	-39629.6	160.8
B3 MISFOLDED	-28127.9	163.6
ID1 EXTENDED	-20304.9	146.8
ID1 MISFOLDED	-26763.9	152.7
ID2 EXTENDED	-30045.8	135.1
ID2 MISFOLDED	-21756.8	142.4
ID3 EXTENDED	-29418.7	136.8
ID3 MISFOLDED	-24346.0	142.1
ff14SB TIP3P	**Average EPTOT***	**Average DHIED***
H1 EXTENDED	-40384.0	191.6
H1 MISFOLDED	-27024.7	191.5
H2 EXTENDED	-10100.9	55.8
H2 MISFOLDED	-10244.7	58.2
B1 EXTENDED	-25237.0	210.9
B1 MISFOLDED	-23582.6	215.6
B2 EXTENDED	-20087.7	163.6

B2 MISFOLDED	-22518.1	163.5
B3 EXTENDED	-25025.7	199.6
B3 MISFOLDED	-22192.7	202.4
ID1 EXTENDED	-24497.5	169.2
ID1 MISFOLDED	-20454.6	174.7
ID2 EXTENDED	-25311.8	161.4
ID2 MISFOLDED	-18934.8	166.9
ID3 EXTENDED	-24036.5	169.4
ID3 MISFOLDED	-17935.0	173.9
ff14SB OPC	**Average EPTOT***	**Average DHIED***
H1 EXTENDED	-41568.5	191.2
H1 MISFOLDED	-35941.6	198.5
H2 EXTENDED	-13718.6	53.5
H2 MISFOLDED	-13261.2	58.8
B1 EXTENDED	-41820.8	192.9
B1 MISFOLDED	-29989.0	216.8
B2 EXTENDED	-28981.6	162.4
B2 MISFOLDED	-28345.7	164.1
B3 EXTENDED	-41820.8	192.9
B3 MISFOLDED	-28091.5	203.0
ID1 EXTENDED	-28280.6	170.2
ID1 MISFOLDED	-26743.3	172.6
ID2 EXTENDED	-31638.8	160.8
ID2 MISFOLDED	-21731.1	167.0
ID3 EXTENDED	-3331.1	159.4
ID3 MISFOLDED	-24324.5	172.2
ff19SB TIP3P	**Average EPTOT***	**Average DHIED***
H1 EXTENDED	-21846.2	93.3
H1 MISFOLDED	-27115.7	95.0
H2 EXTENDED	-95440.8	43.0
H2 MISFOLDED	-10259.3	45.5
B1 EXTENDED	-33799.7	96.9
B1 MISFOLDED	-23683.7	97.1
B2 EXTENDED	-19732.3	79.5
B2 MISFOLDED	-22595.7	79.4
B3 EXTENDED	-23016.5	88.2
B3 MISFOLDED	-22285.6	90.8
ID1 EXTENDED	-17731.1	74.5
ID1 MISFOLDED	-20548.9	74.1
ID2 EXTENDED	-26174.8	77.2
ID2 MISFOLDED	-19015.7	77.6
ID3 EXTENDED	-19476.7	70.7
ID3 MISFOLDED	-18060.0	72.7
ff19SB OPC	**Average EPTOT***	**Average DHIED***
H1 EXTENDED	-38906.2	94.8
H1 MISFOLDED	-36042.9	97.6

H2 EXTENDED	-11618.7	43.5
H2 MISFOLDED	-13272.9	47.0
B1 EXTENDED	-38353.5	92.1
B1 MISFOLDED	-30120.1	97.4
B2 EXTENDED	-20528.5	81.2
B2 MISFOLDED	-28711.7	81.5
B3 EXTENDED	-29998.9	90.9
B3 MISFOLDED	-28189.3	90.2
ID1 EXTENDED	-19186.2	75.2
ID1 MISFOLDED	-26824.6	74.0
ID2 EXTENDED	-41710.2	78.8
ID2 MISFOLDED	-21815.0	78.6
ID3 EXTENDED	-25853.0	72.0
ID3 MISFOLDED	-24403.9	72.7
ff15ipq-m TIP3P	**Average EPTOT***	**Average DHIED***
H2 EXTENDED	-15450.5	-47.5
ff15ipq-m OPC	**Average EPTOT***	**Average DHIED***
H2 EXTENDED	-9985.6	-43.8
ff15ipq-m SPC/E	**Average EPTOT***	**Average DHIED***
H2 EXTENDED	-17038.3	-45.7

* values are reported in kcal/mol

Table S2. parameters used in aMDs simulations

ff99SB TIP3P	**ethreshd ***	**alphad***	**ethreshp***	**alphap***
H1 EXTENDED	239.0	13.6	-22981.4	1235.2
H1 MISFOLDED	240.3	13.6	-25672.3	1377.8
H2 EXTENDED	86.3	5.6	-9561.2	516.8
H2 MISFOLDED	87.9	5.6	-9719.4	525.4
B1 EXTENDED	237.0	14.4	-28535.2	1509.3
B1 MISFOLDED	240.4	14.4	-22445.9	1186.7
B2 EXTENDED	191.8	11.2	-21372.3	1150.6
B2 MISFOLDED	195.2	11.2	-21389.7	1151.5
B3 EXTENDED	227.1	13.6	-32759.6	1754.9
B3 MISFOLDED	230.8	13.6	-21087.3	1136.6
ID1 EXTENDED	214.4	12.8	-15107.2	822.2
ID1 MISFOLDED	212.2	12.8	-19429.5	1051.2
ID2 EXTENDED	193.4	11.2	-22797.8	1210.1
ID2 MISFOLDED	196.8	11.2	-18000.9	956.2
ID3 EXTENDED	199.0	12.0	-20646.8	1096.8
ID3 MISFOLDED	209.8	12.0	-17054.1	903.2
ff99SB OPC	**ethreshd ***	**alphad***	**ethreshp***	**alphap***
H1 EXTENDED	239.0	13.6	-37555.3	2087.2
H1 MISFOLDED	239.0	13.6	-34075.8	1895.2
H2 EXTENDED	86.1	5.6	-13286.6	742.4
H2 MISFOLDED	88.1	5.6	-12559.0	702.7

B1 EXTENDED	234.0	14.4	-35925.0	1975.0
B1 MISFOLDED	234.8	14.4	-28475.2	1564.2
B2 EXTENDED	190.5	11.2	-24422.0	1364.0
B2 MISFOLDED	192.4	11.2	-26869.7	1499.0
B3 EXTENDED	228.8	13.6	-37541.8	2087.8
B3 MISFOLDED	231.6	13.6	-26641.0	1486.9
ID1 EXTENDED	210.8	12.8	-19224.4	1080.5
ID1 MISFOLDED	216.7	12.8	-25345.5	1418.4
ID2 EXTENDED	191.1	11.2	-28475.0	1570.7
ID2 MISFOLDED	198.4	11.2	-20618.7	1138.1
ID3 EXTENDED	196.8	12.0	-27879.5	1539.2
ID3 MISFOLDED	202.1	12.0	-23074.7	1271.4
ff14SB TIP3P	**ethreshd ***	**alphad***	**ethreshp***	**alphap***
H1 EXTENDED	259.6	13.6	-38334.2	2049.8
H1 MISFOLDED	259.5	13.6	-25646.9	1377.8
H2 EXTENDED	83.8	5.6	-9583.2	517.8
H2 MISFOLDED	86.2	5.6	-9719.3	525.4
B1 EXTENDED	282.9	14.4	-23967.3	1269.7
B1 MISFOLDED	287.6	14.4	-22395.9	1186.7
B2 EXTENDED	219.6	11.2	-19058.6	1029.1
B2 MISFOLDED	219.6	11.2	-21366.6	1151.5
B3 EXTENDED	267.6	13.6	-23746.5	1279.2
B3 MISFOLDED	270.4	13.6	-21056.1	1136.6
ID1 EXTENDED	233.2	12.8	-23242.8	1254.7
ID1 MISFOLDED	238.7	12.8	-19403.4	1051.2
ID2 EXTENDED	217.4	11.2	-24034.5	1277.3
ID2 MISFOLDED	222.9	11.2	-17978.6	956.2
ID3 EXTENDED	229.5	12.0	-22823.1	1213.4
ID3 MISFOLDED	233.9	12.0	-17031.8	903.2
ff14SB OPC	**ethreshd ***	**alphad***	**ethreshp***	**alphap***
H1 EXTENDED	259.2	13.6	-39379.5	2189.0
H1 MISFOLDED	266.5	13.6	-34046.4	1895.2
H2 EXTENDED	84.7	5.6	-11814.3	661.1
H2 MISFOLDED	86.8	5.6	-12558.5	702.7
B1 EXTENDED	284.2	14.4	-38756.7	2133.8
B1 MISFOLDED	288.8	14.4	-28424.8	1564.2
B2 EXTENDED	218.4	11.2	-27449.3	1532.3
B2 MISFOLDED	220.1	11.2	-26846.7	1499.0
B3 EXTENDED	260.9	13.6	-39616.5	2204.3
B3 MISFOLDED	271.0	13.6	-26604.6	1486.9
ID1 EXTENDED	234.2	12.8	-26782.2	1498.4
ID1 MISFOLDED	236.6	12.8	-25324.9	1418.4
ID2 EXTENDED	216.8	11.2	-29983.0	1655.8
ID2 MISFOLDED	223.0	11.2	-20593.0	1138.1
ID3 EXTENDED	219.4	12.0	-28743.3	1587.8
ID3 MISFOLDED	232.2	12.0	-23053.2	1271.4

ff19SB TIP3P	ethreshd *	alphad*	ethreshp*	alphap*
H1 EXTENDED	161.3	13.6	-20733.9	1112.3
H1 MISFOLDED	163.0	13.6	-25737.9	1377.8
H2 EXTENDED	71.0	5.6	-9055.1	489.0
H2 MISFOLDED	73.5	5.6	-9733.9	525.4
B1 EXTENDED	168.9	14.4	-32104.1	1695.5
B1 MISFOLDED	169.1	14.4	-22497.0	1186.7
B2 EXTENDED	135.5	11.2	-18724.8	1007.5
B2 MISFOLDED	135.4	11.2	-21444.2	1151.5
B3 EXTENDED	156.2	13.6	-21842.9	1173.6
B3 MISFOLDED	158.7	13.6	-21149.0	1136.6
ID1 EXTENDED	138.5	12.8	-16821.5	909.6
ID1 MISFOLDED	138.1	12.8	-19497.7	1051.2
ID2 EXTENDED	133.2	11.2	-24858.1	1316.6
ID2 MISFOLDED	133.6	11.2	-18059.5	956.2
ID3 EXTENDED	130.8	12.0	-18497.0	979.7
ID3 MISFOLDED	132.7	12.0	-17154.8	905.1
ff19SB OPC	**ethreshd ***	**alphad***	**ethreshp***	**alphap***
H1 EXTENDED	162.8	13.6	-36861.2	2045.0
H1 MISFOLDED	165.6	13.6	-34147.7	1895.2
H2 EXTENDED	71.5	5.6	-11003.0	615.7
H2 MISFOLDED	75.0	5.6	-12570.2	702.7
B1 EXTENDED	164.1	14.4	-36357.3	1996.2
B1 MISFOLDED	169.4	14.4	-28555.9	1564.2
B2 EXTENDED	137.2	11.2	-19441.6	1086.9
B2 MISFOLDED	137.5	11.2	-27197.3	1514.4
B3 EXTENDED	158.9	13.6	-28417.3	1581.6
B3 MISFOLDED	158.2	13.6	-26702.4	1486.9
ID1 EXTENDED	139.2	12.8	-18167.1	1019.0
ID1 MISFOLDED	138.0	12.8	-25406.8	1417.8
ID2 EXTENDED	134.8	11.2	-39532.1	2178.1
ID2 MISFOLDED	134.6	11.2	-20676.9	1138.1
ID3 EXTENDED	131.9	12.0	-24503.2	1349.8
ID3 MISFOLDED	132.7	12.0	-23133.2	1270.7
ff15ipq-m TIP3P	**ethreshd ***	**alphad***	**ethreshp***	**alphap***
H2 EXTENDED	-19.5	5.6	-14669.2	781.3
ff15ipq-m OPC	**ethreshd ***	**alphad***	**ethreshp***	**alphap***
H2 EXTENDED	-15.8	5.6	-9204.3	781.3
ff15ipq-m SPC/E	**ethreshd ***	**alphad***	**ethreshp***	**alphap***
H2 EXTENDED	-17.7	5.6	-16257.0	781.3

* values are reported in kcal/mol

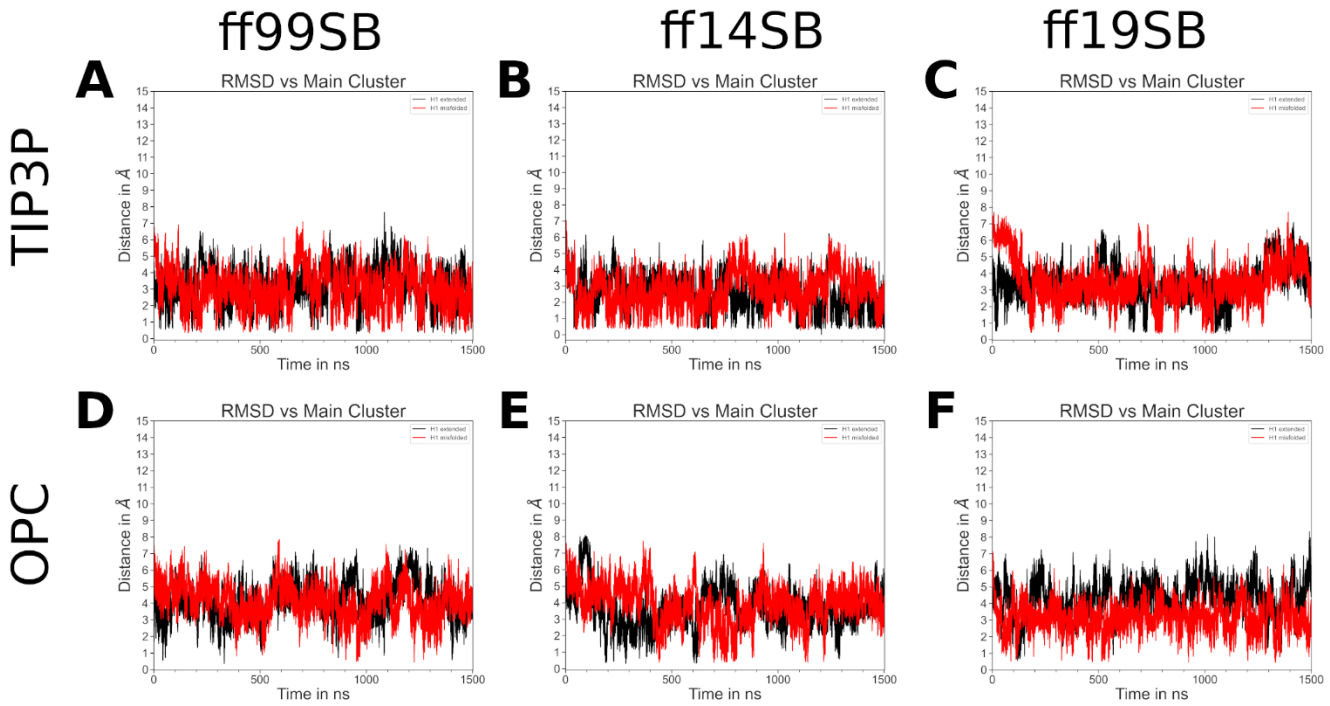

Figure S1. RMSD of H1 for extended (black) and misfolded (red) aMDs. The main cluster obtained from the last 500 ns of ff14SB/TIP3P simulation starting from extended conformation was used as the reference.

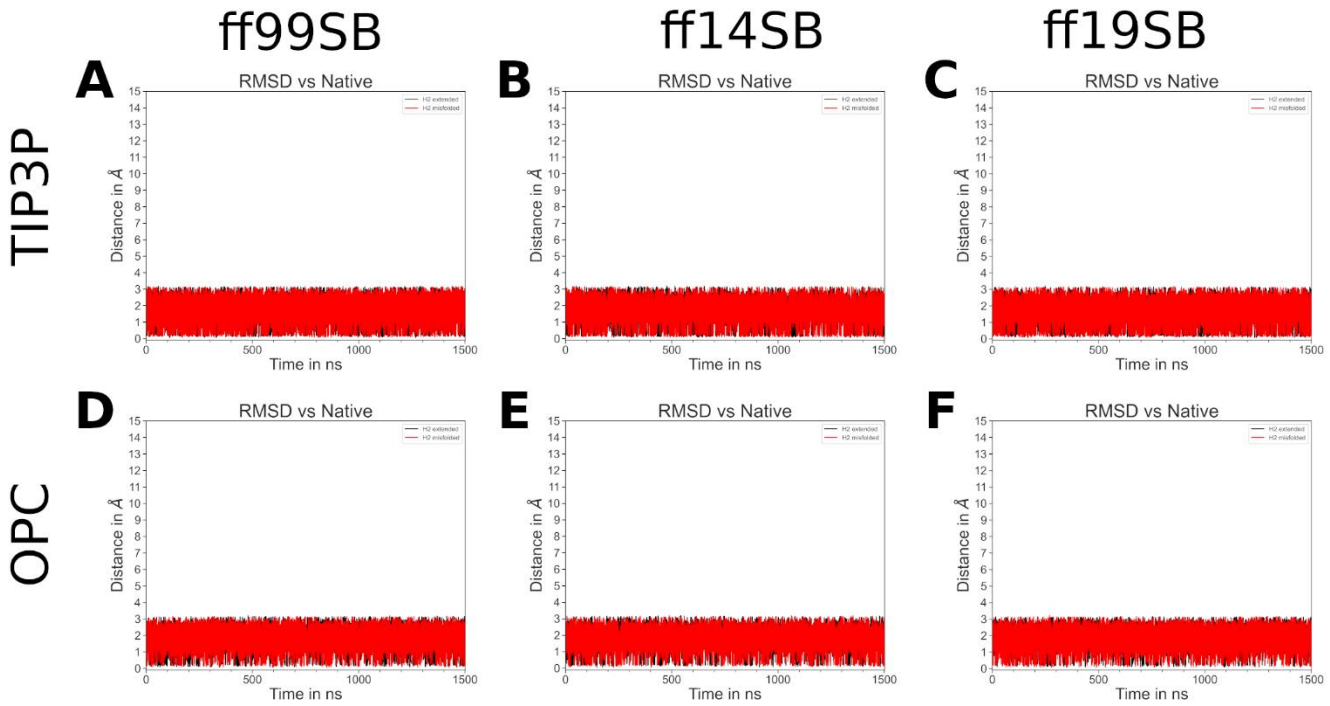

Figure S2. RMSD of H2 for extended (black) and misfolded (red) aMDs. The native structure was used as the reference.

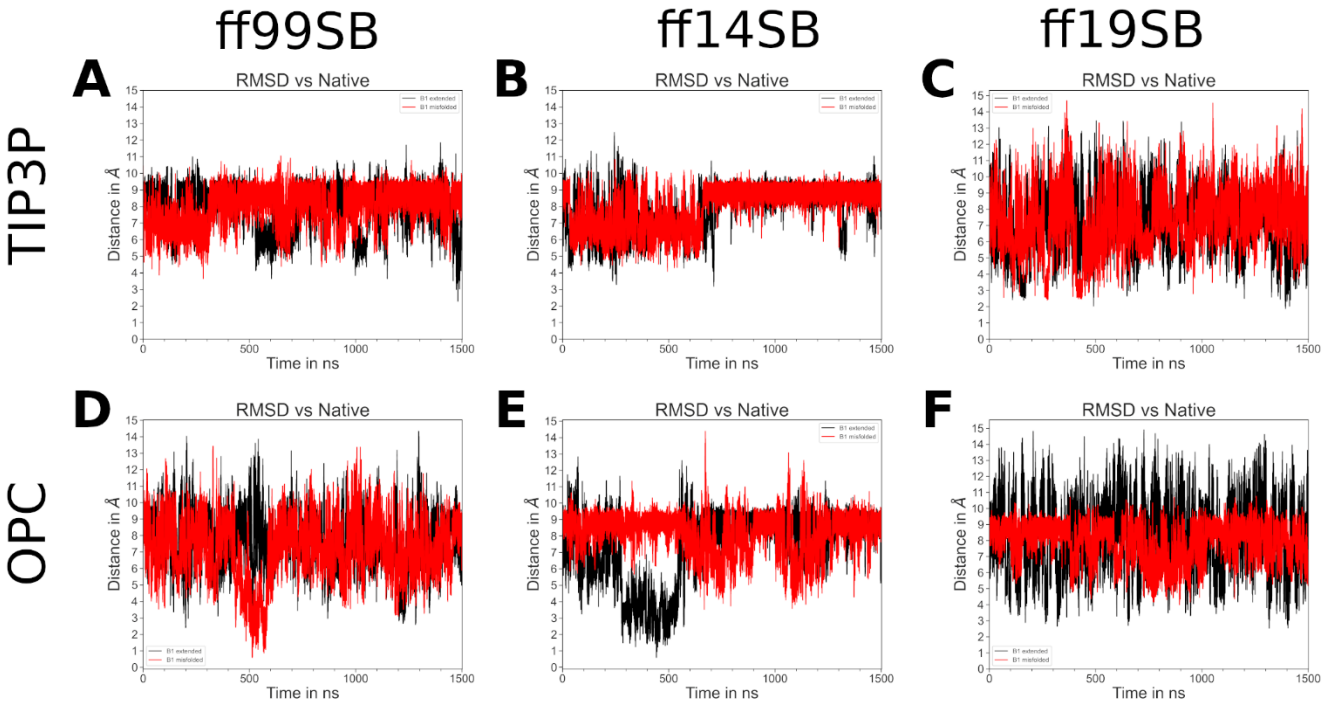

Figure S3. RMSD of B1 for extended (black) and misfolded (red) aMDs. The native structure was used as the reference.

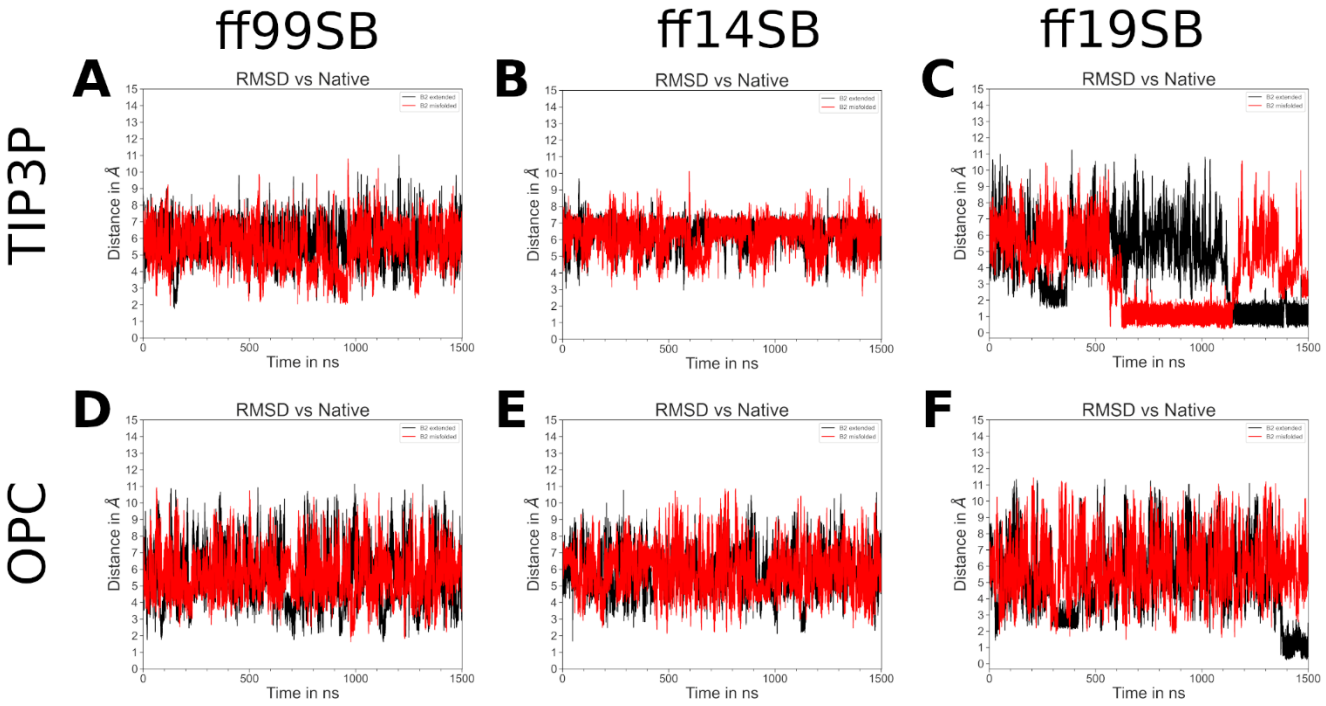

Figure S4. RMSD of B2 for extended (black) and misfolded (red) aMDs. The native structure was used as the reference.

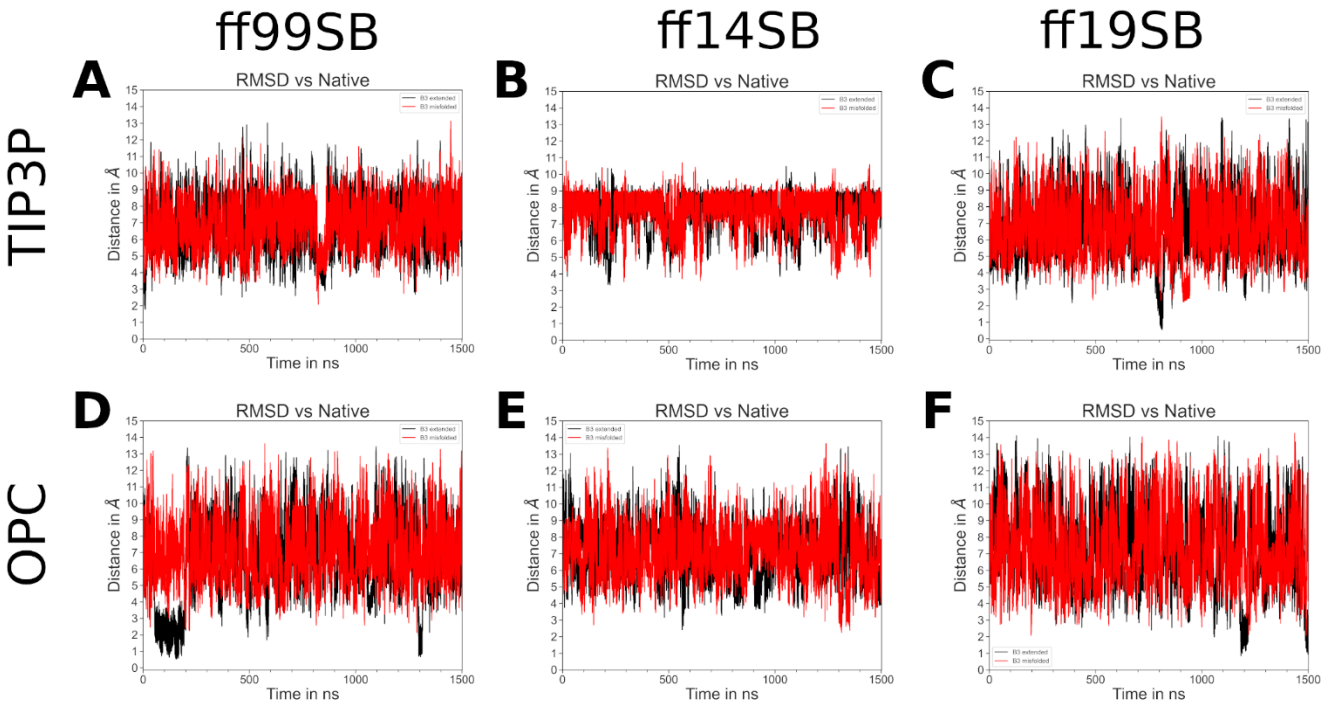

Figure S5. RMSD of B3 for extended (black) and misfolded (red) aMDs. The native structure was used as the reference.

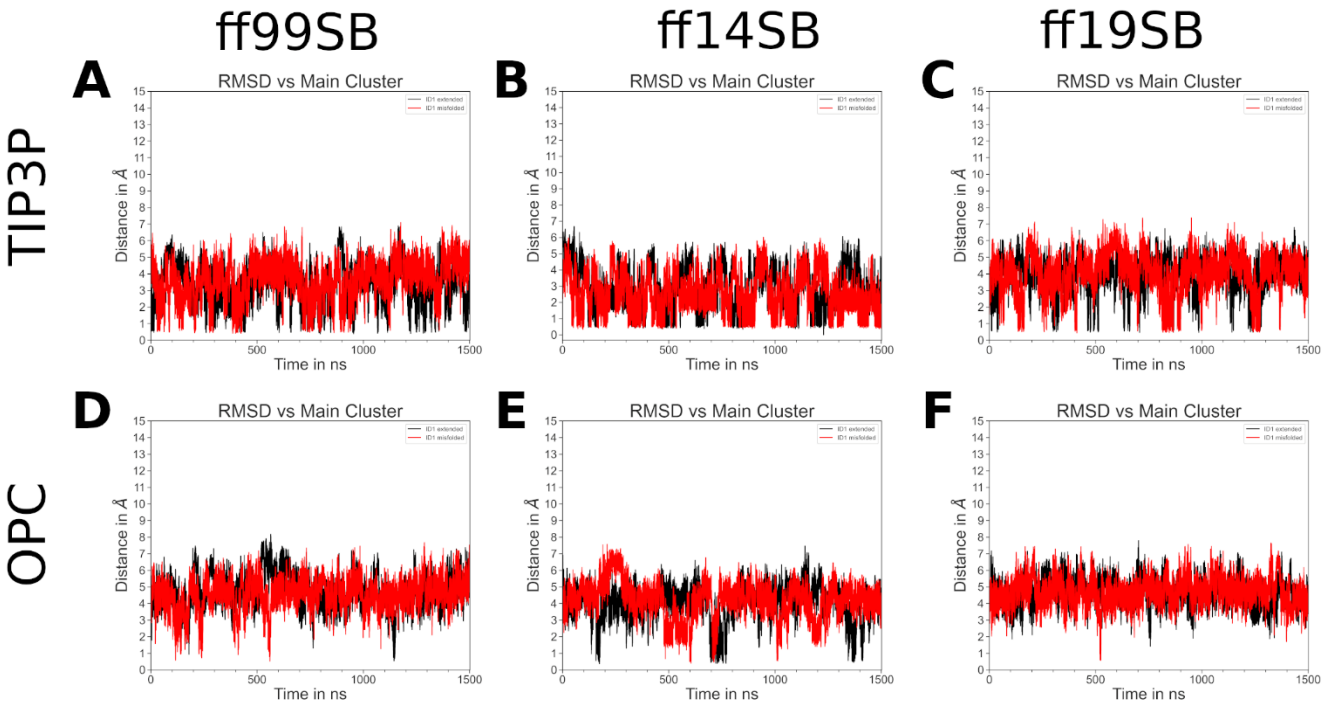

Figure S6. RMSD of ID1 for extended (black) and misfolded (red) aMDs. The main cluster obtained from the last 500 ns of the extended ff14SB/TIP3P simulation was used as the reference.

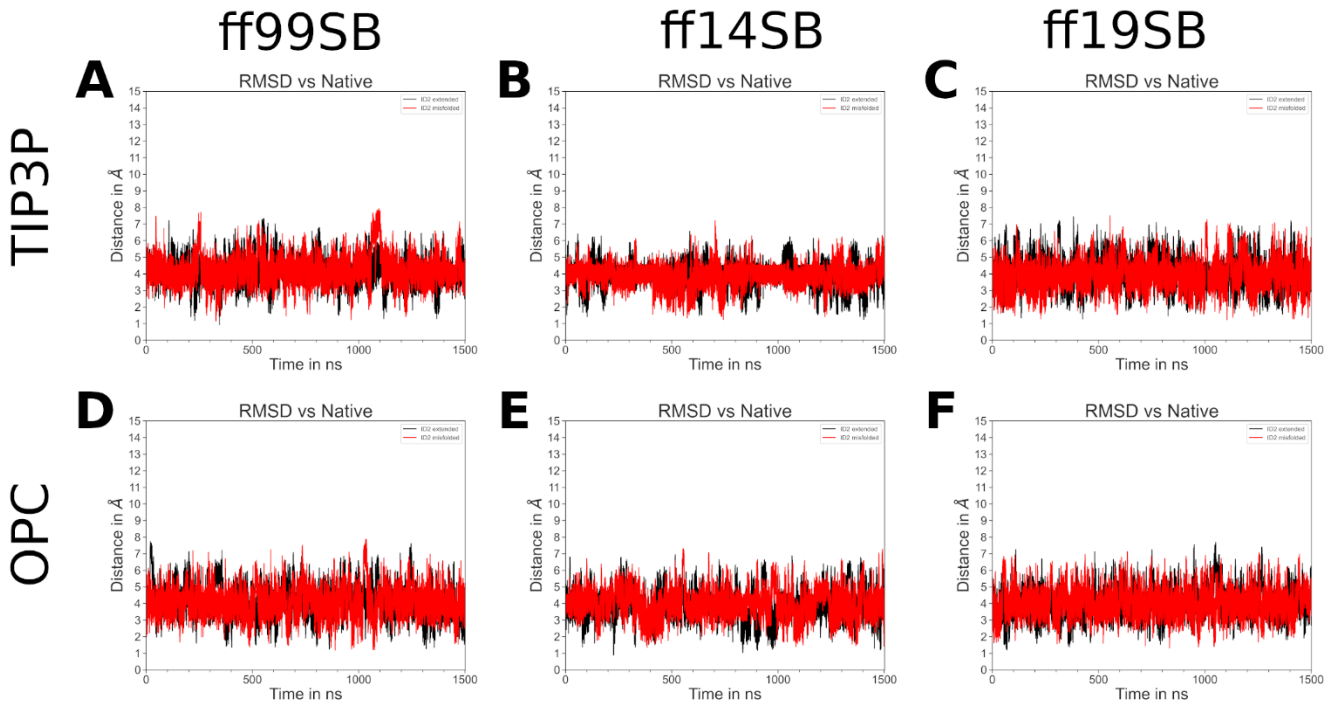

Figure S7. RMSD of ID2 for extended (black) and misfolded (red) aMD. The native structure was used as the reference.

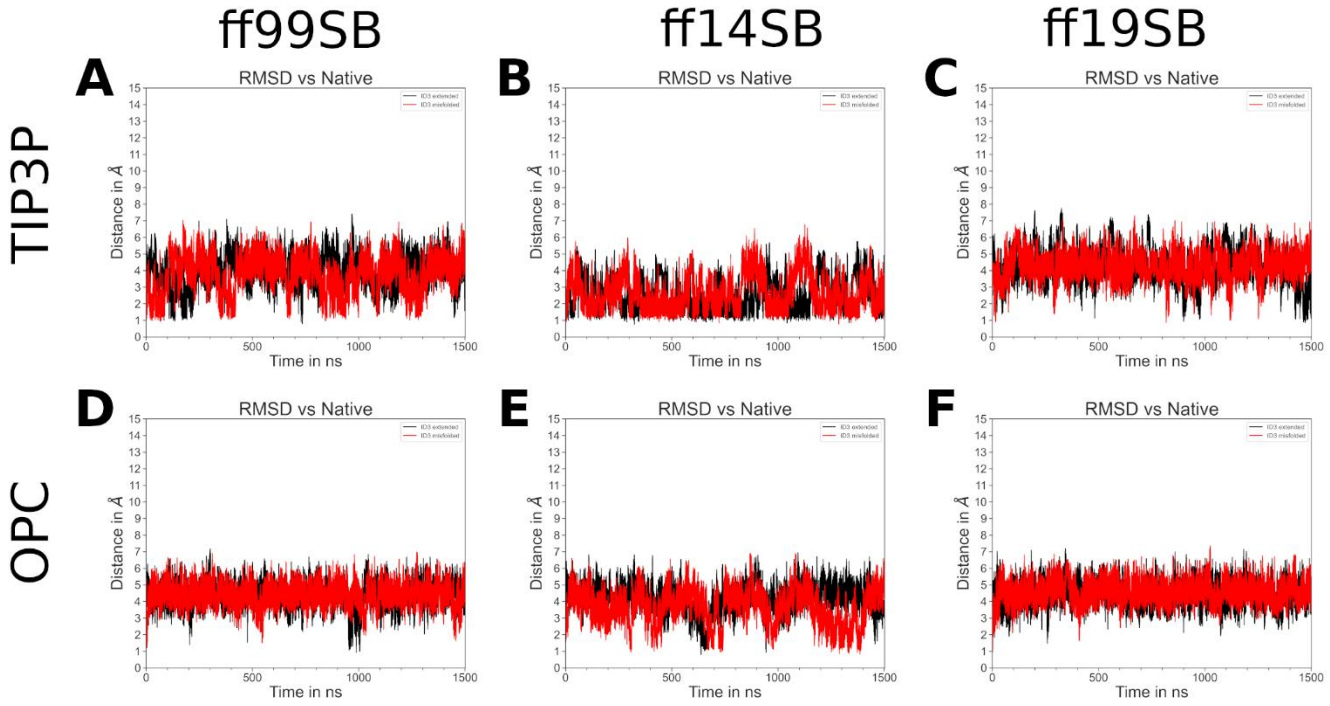

Figure S8. RMSD of ID3 for extended (black) and misfolded (red) aMDs. The native structure was used as the reference.

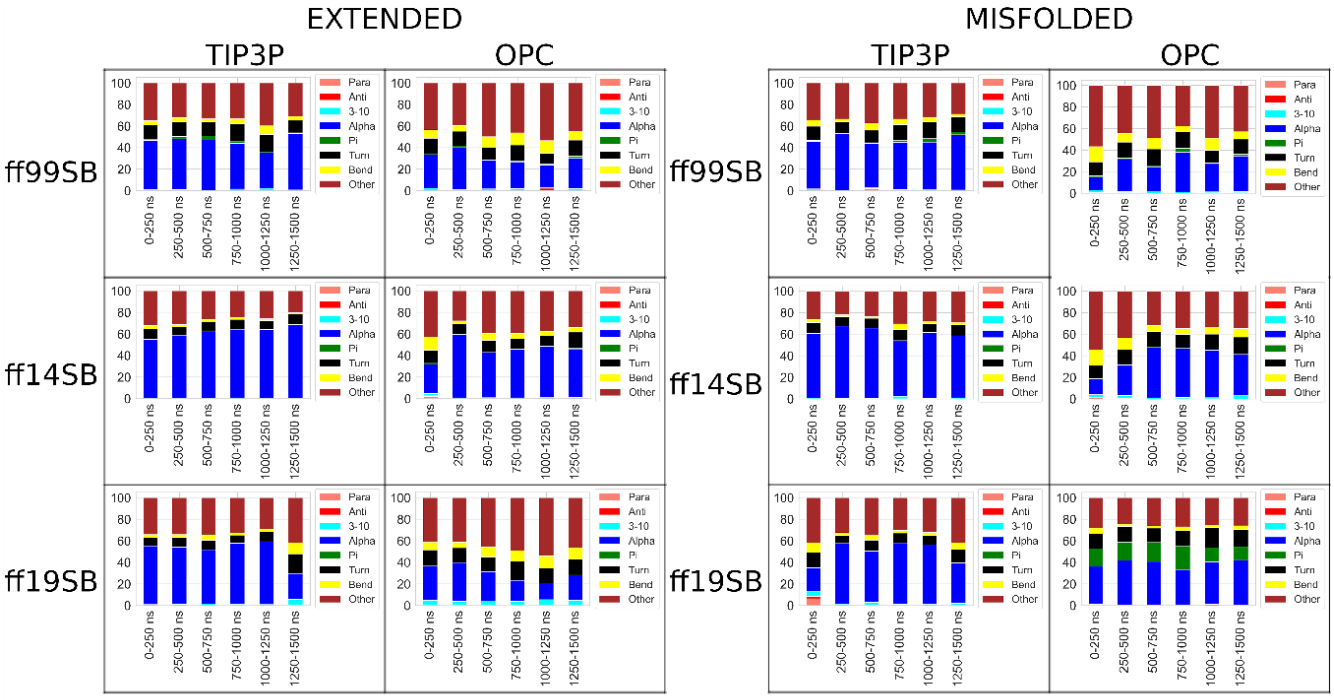

Figure S9. H1 DSSP for extended (left) and misfolded (right) aMDs, calculated at 250 ns intervals.

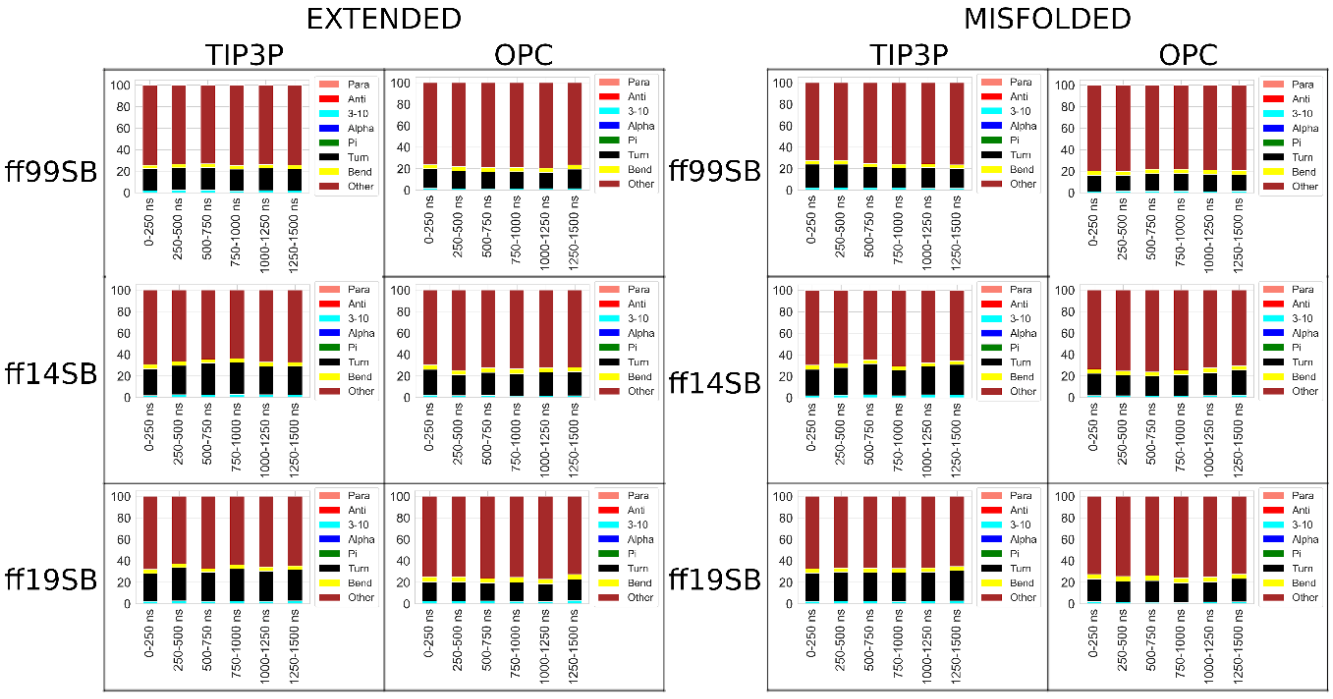

Figure S10. H2 DSSP for extended (left) and misfolded (right) aMDs, calculated at 250 ns intervals.

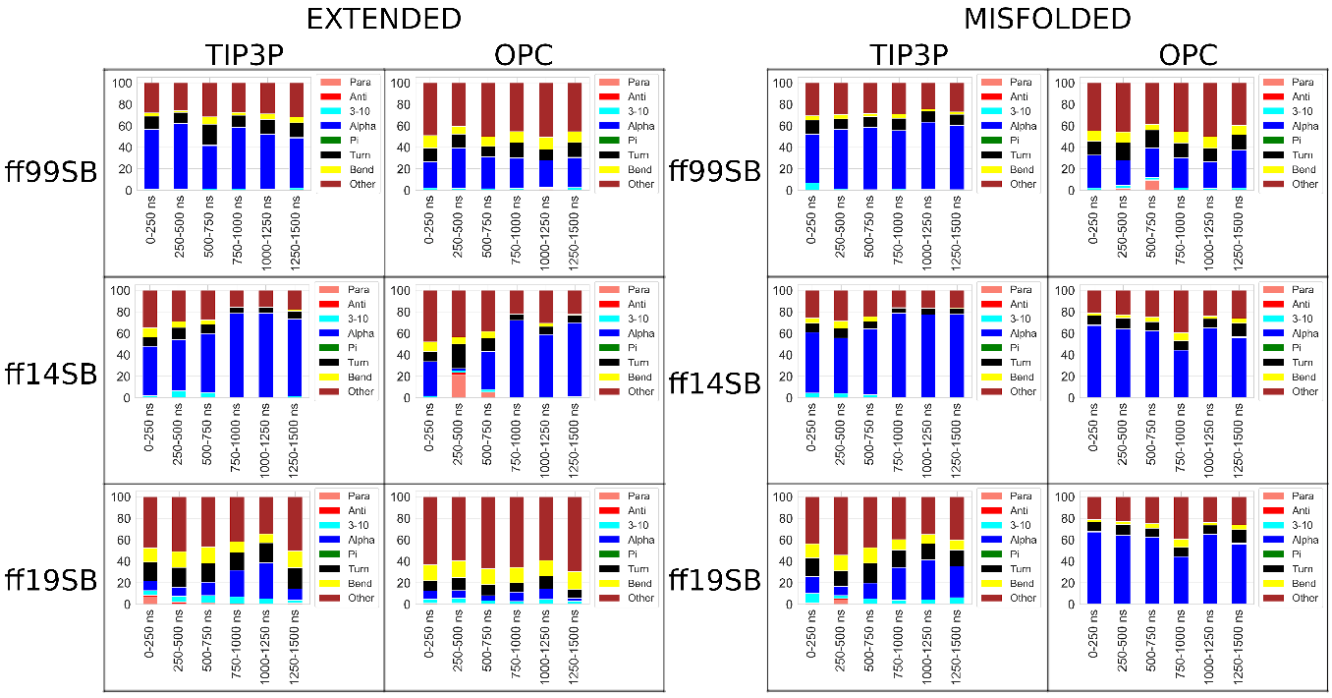

Figure S11. B1 DSSP for extended (left) and misfolded (right) aMDs, calculated at 250 ns intervals.

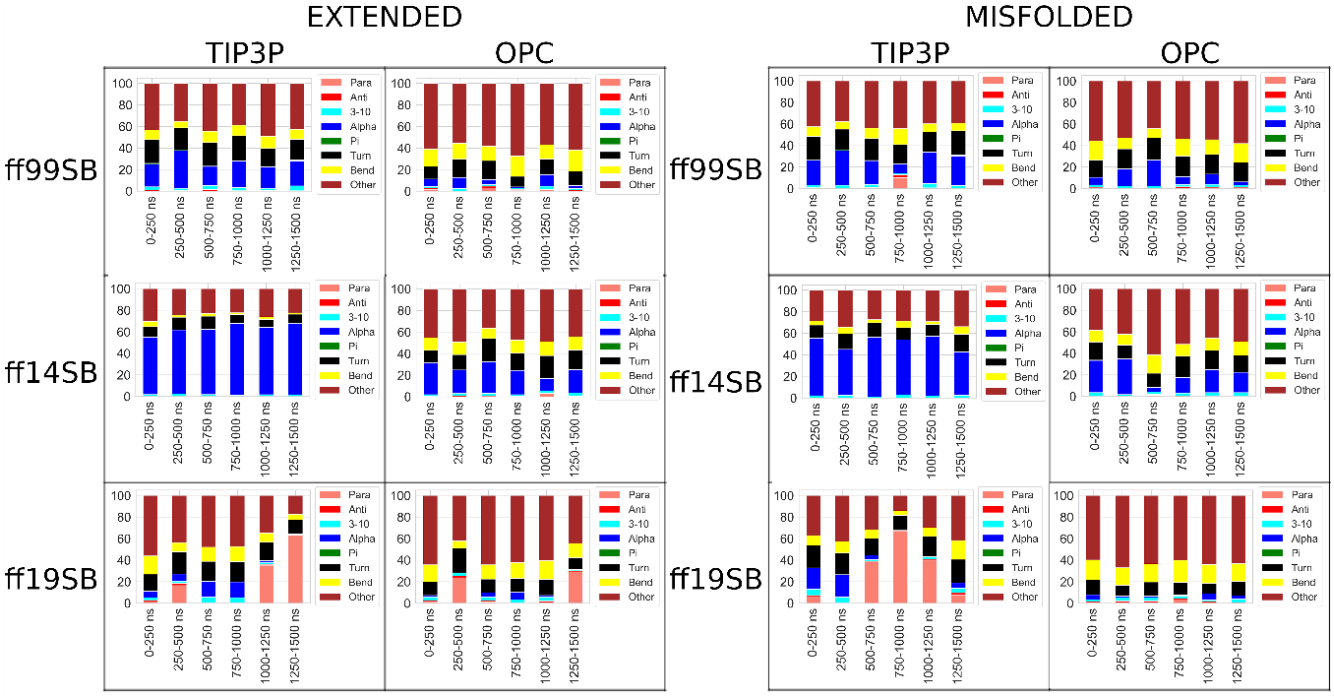

Figure S12. B2 DSSP for extended (left) and misfolded (right) aMDs, calculated at 250 ns intervals.

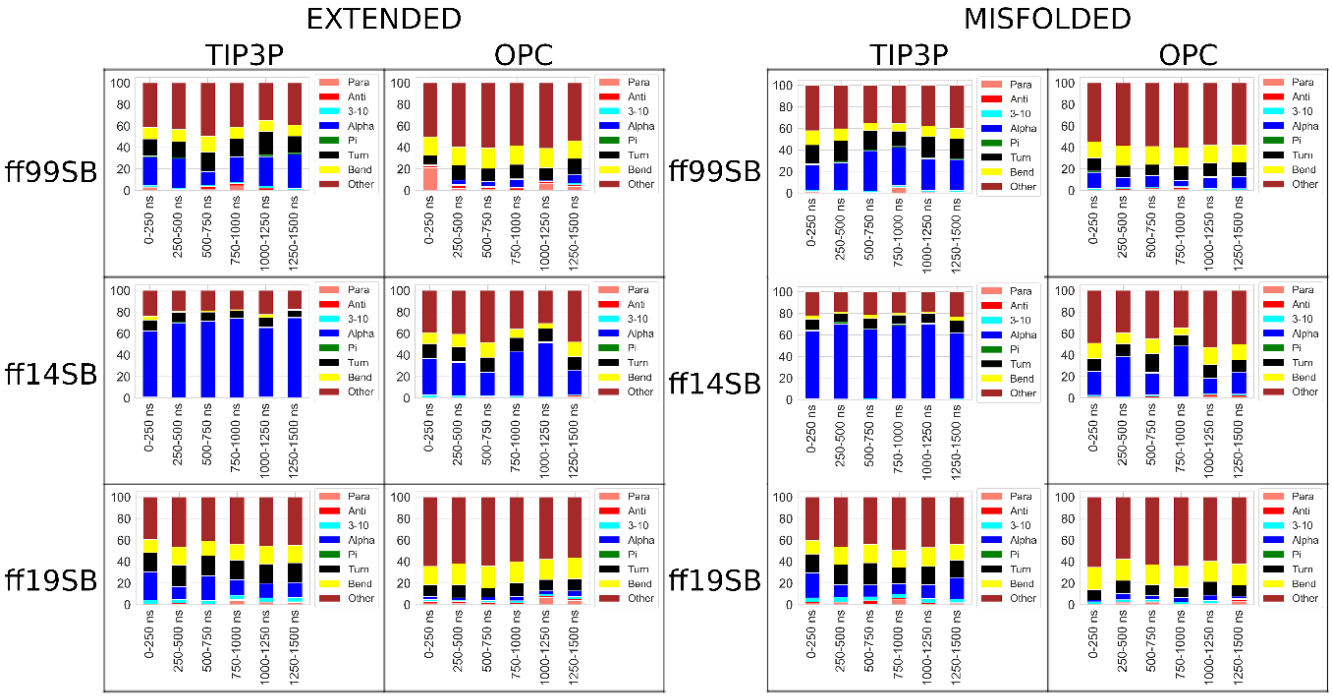

Figure S13. B3 DSSP for extended (left) and misfolded (right) aMDs, calculated at 250 ns intervals.

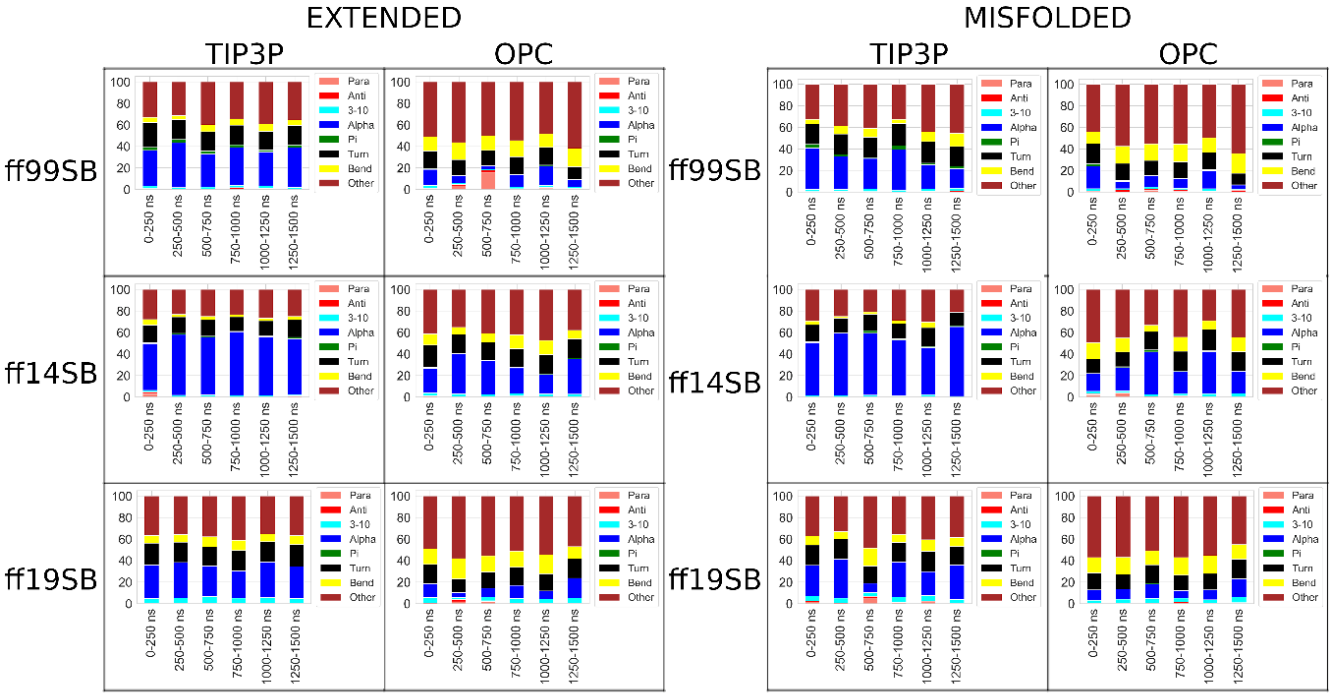

Figure S14. ID1 DSSP for extended (left) and misfolded (right) aMDs, calculated at 250 ns intervals.

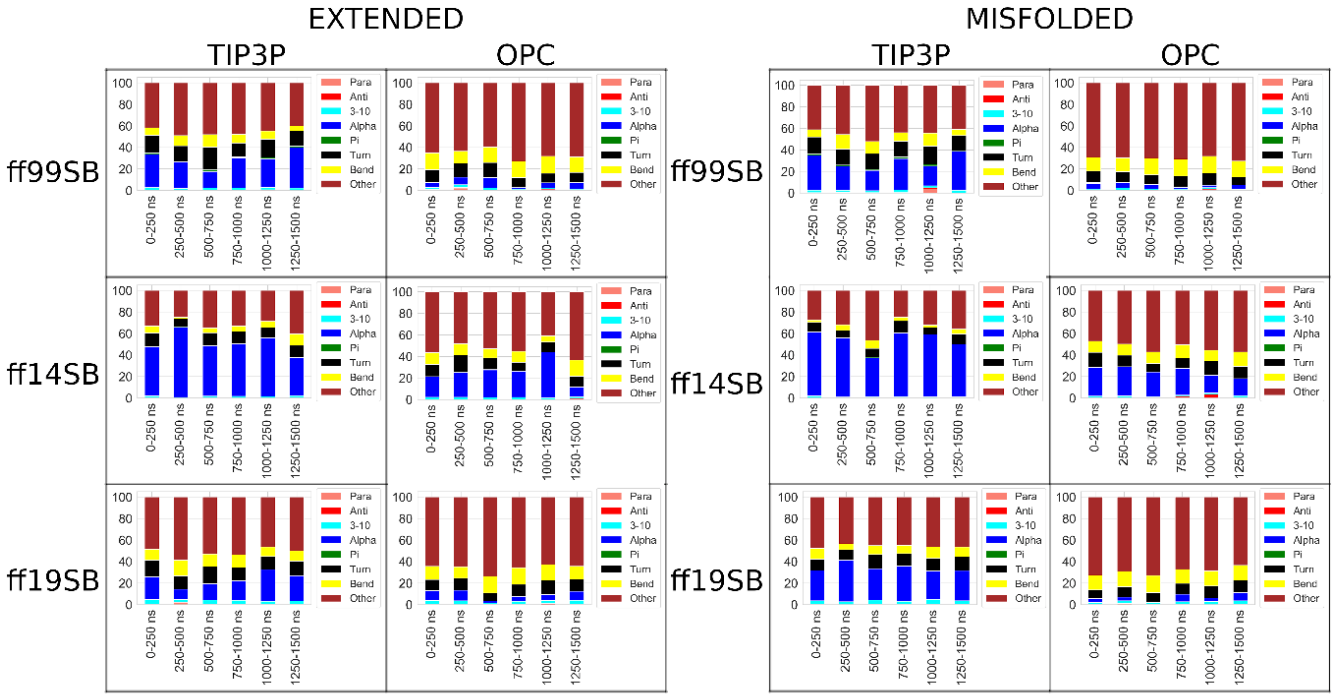

Figure S15. ID2 DSSP for extended (left) and misfolded (right) aMDs, calculated at 250 ns intervals.

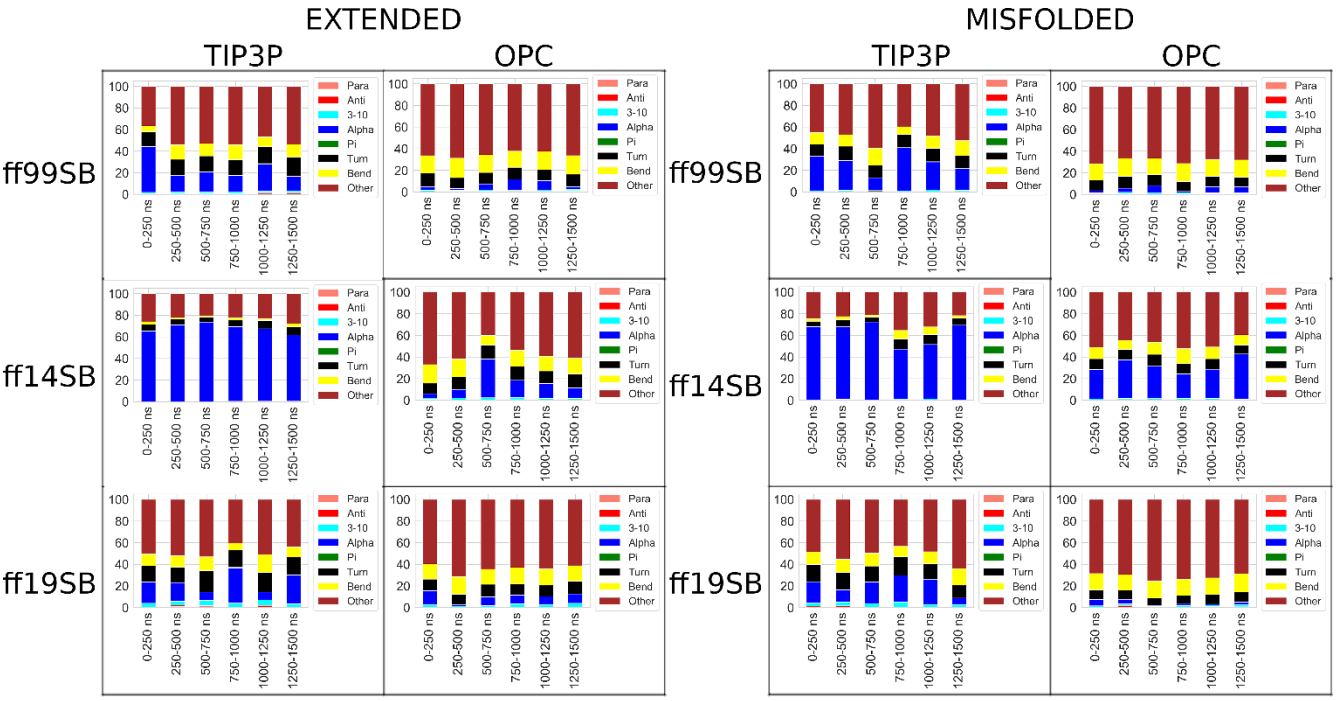

Figure S16. ID3 DSSP for extended (left) and misfolded (right) aMDs, calculated at 250 ns intervals.

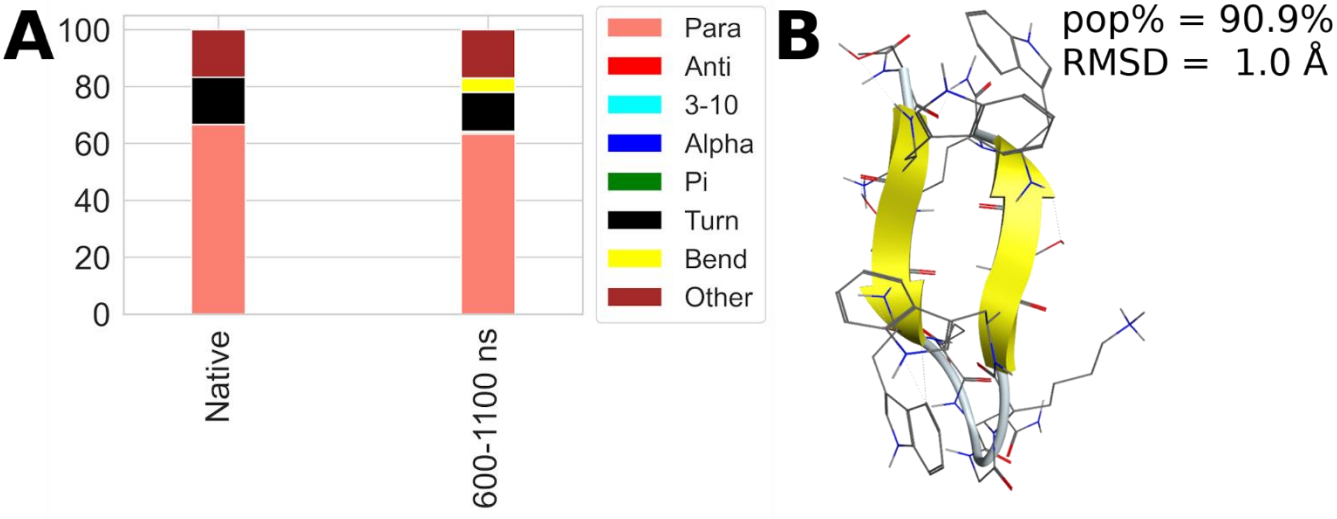

Figure S17. DSSP and main cluster of ff19SB/TIP3P B2 simulation starting from misfolded conformation. The 600 – 1100 ns time interval was considered for the analysis. Population (pop%) and RMSD compared to native structure are also shown.

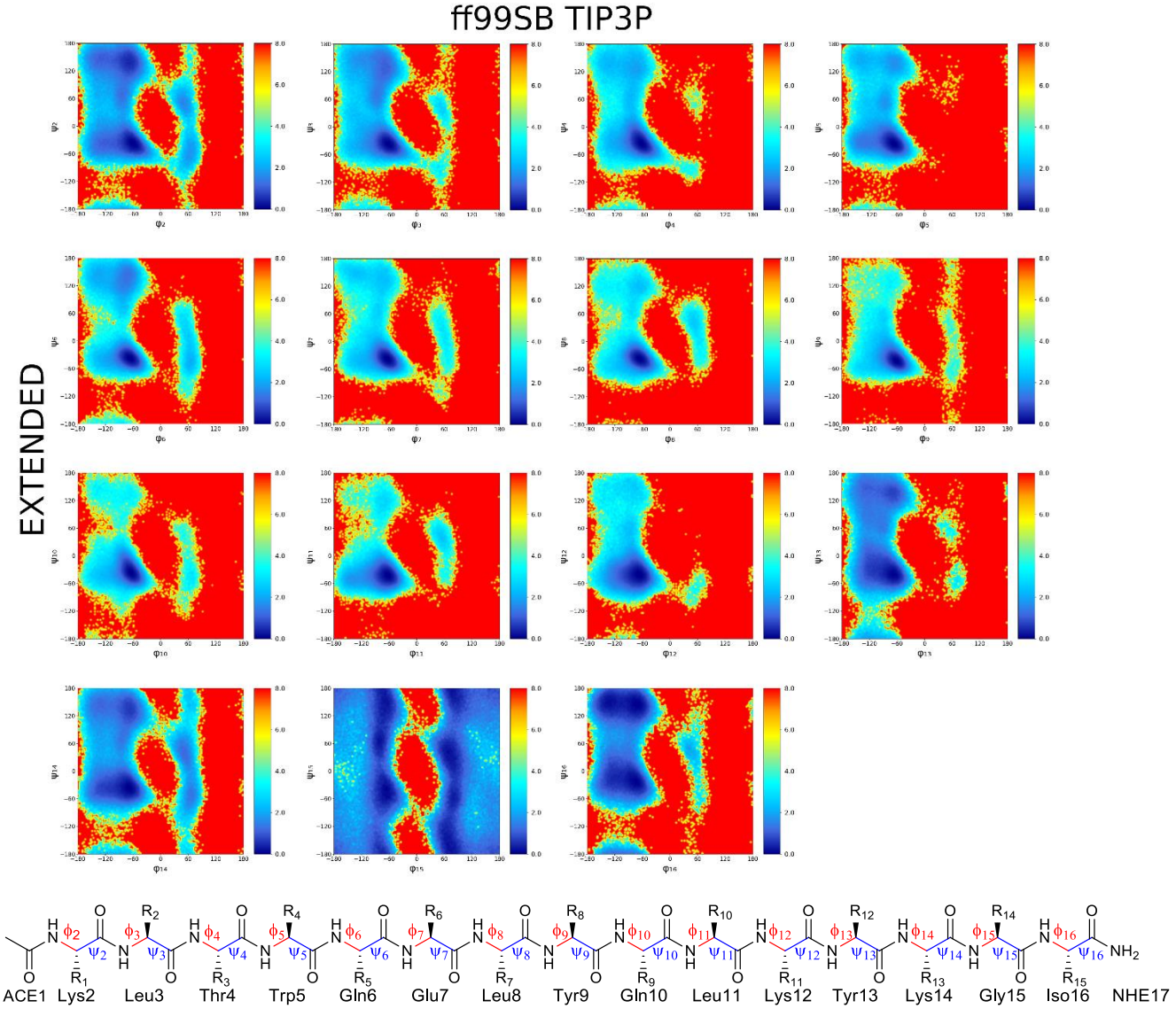

Figure S18. PMFs obtained from φ and ψ dihedral distributions of H1 residues for the ff99SB/TIP3P combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. H1 sequence and representation of φ and ψ angles numbering are also shown.

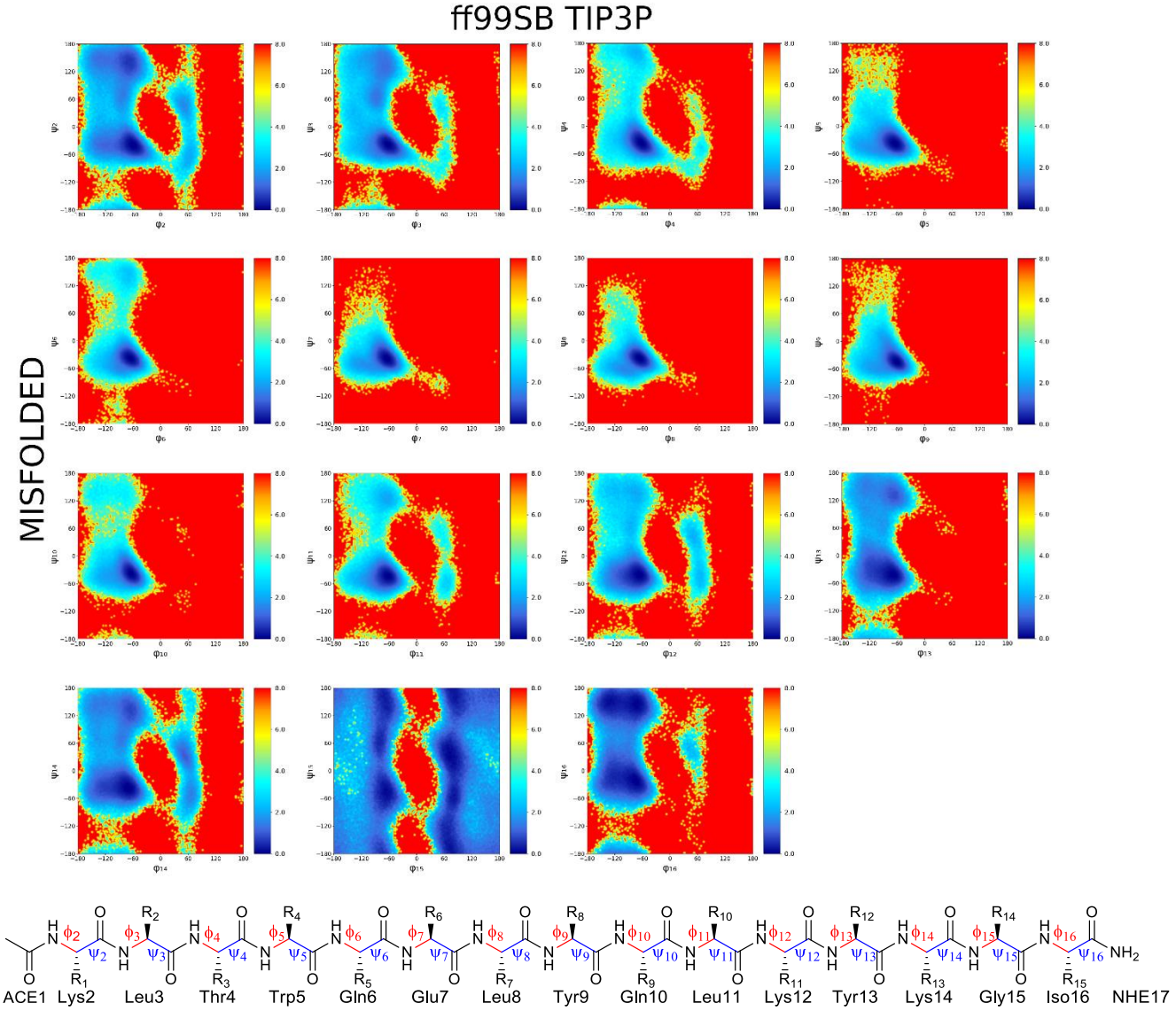

Figure S19. PMFs obtained from φ and ψ dihedral distributions of H1 residues for the ff99SB/TIP3P combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. H1 sequence and representation of φ and ψ angles numbering are also shown.

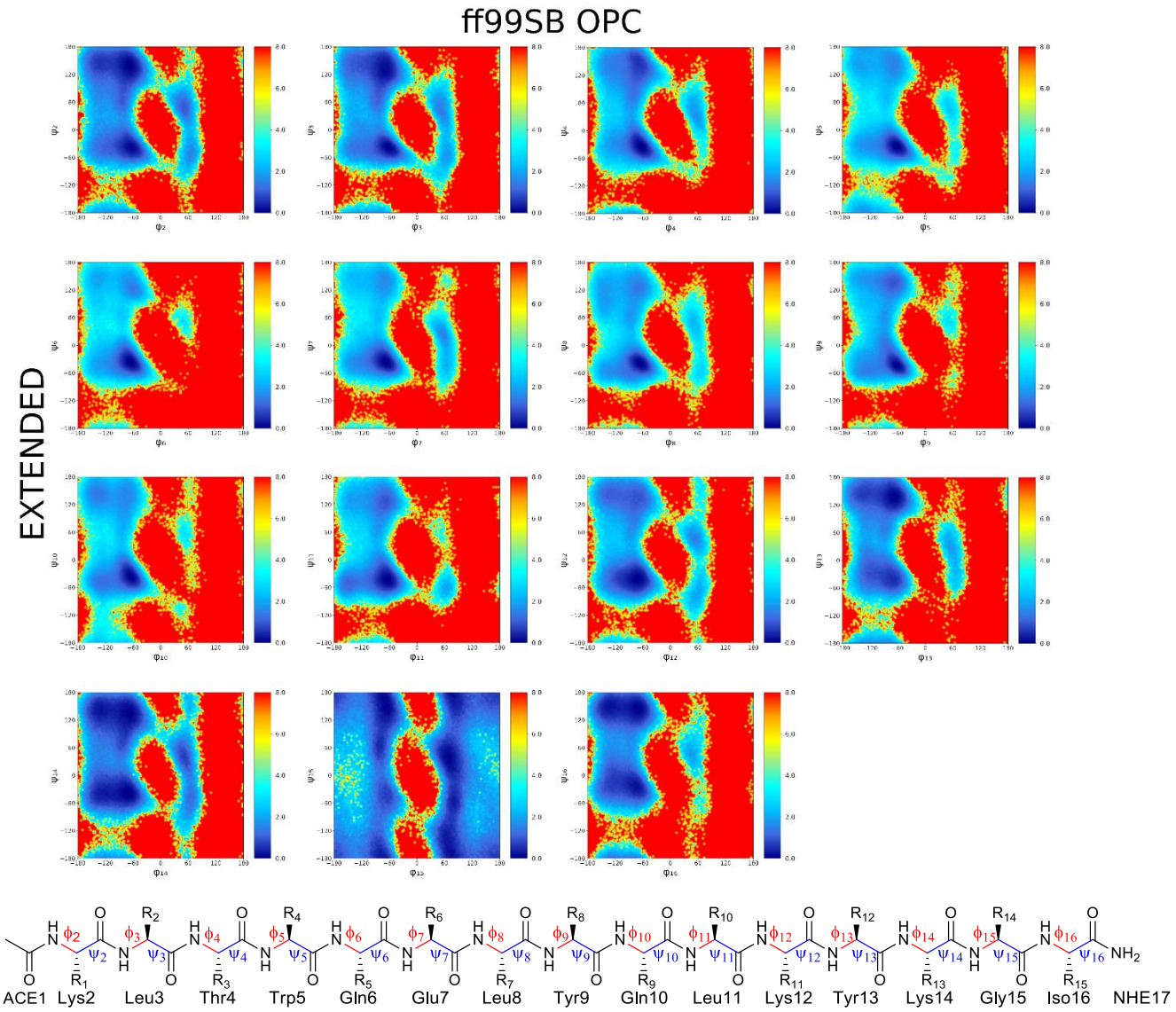

Figure S20. PMFs obtained from φ and ψ dihedral distributions of H1 residues for the ff99SB/OPC combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. H1 sequence and representation of φ and ψ angles numbering are also shown.

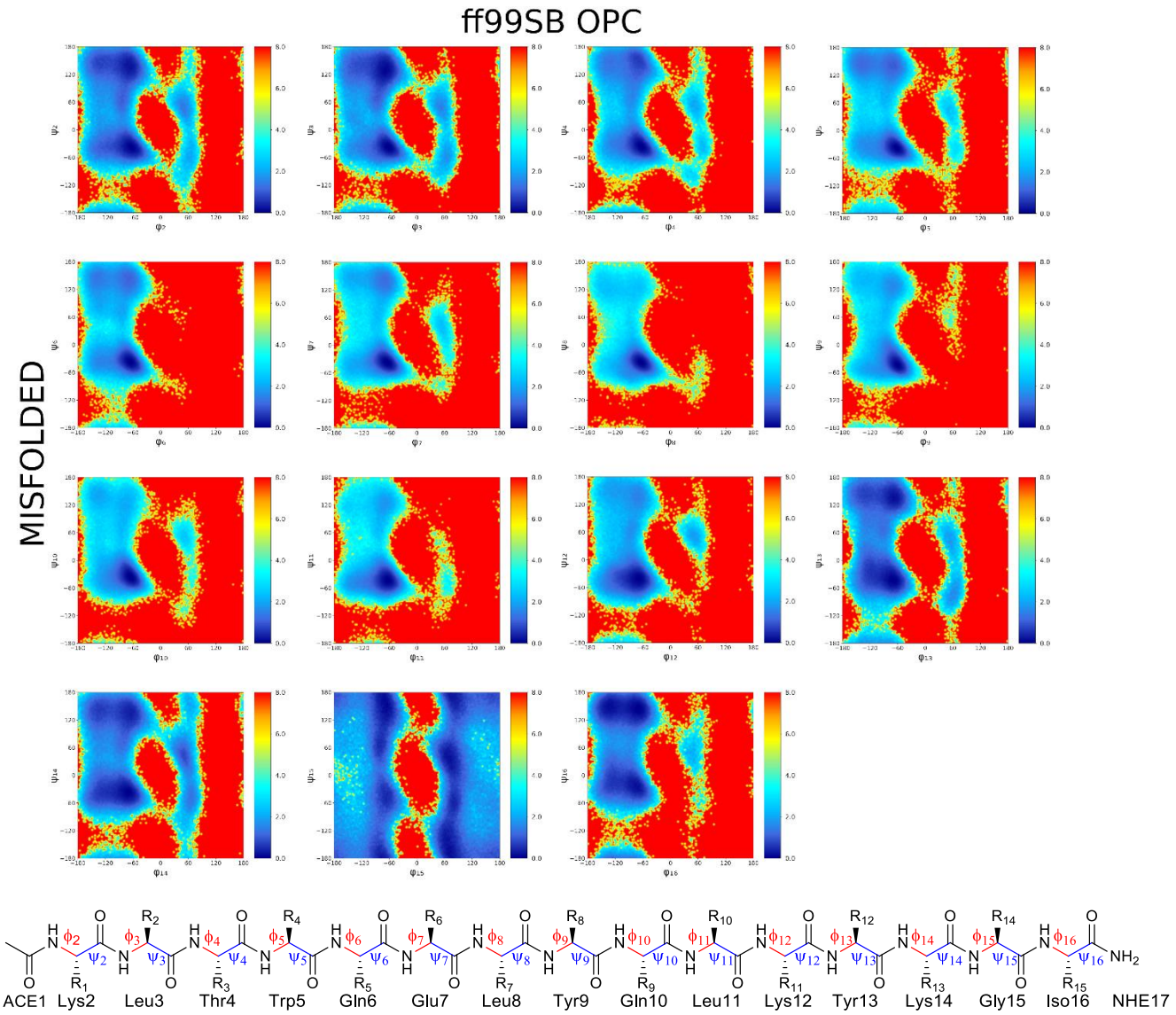

Figure S21. PMFs obtained from φ and ψ dihedral distributions of H1 residues for the ff99SB/OPC combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. H1 sequence and representation of φ and ψ angles numbering are also shown.

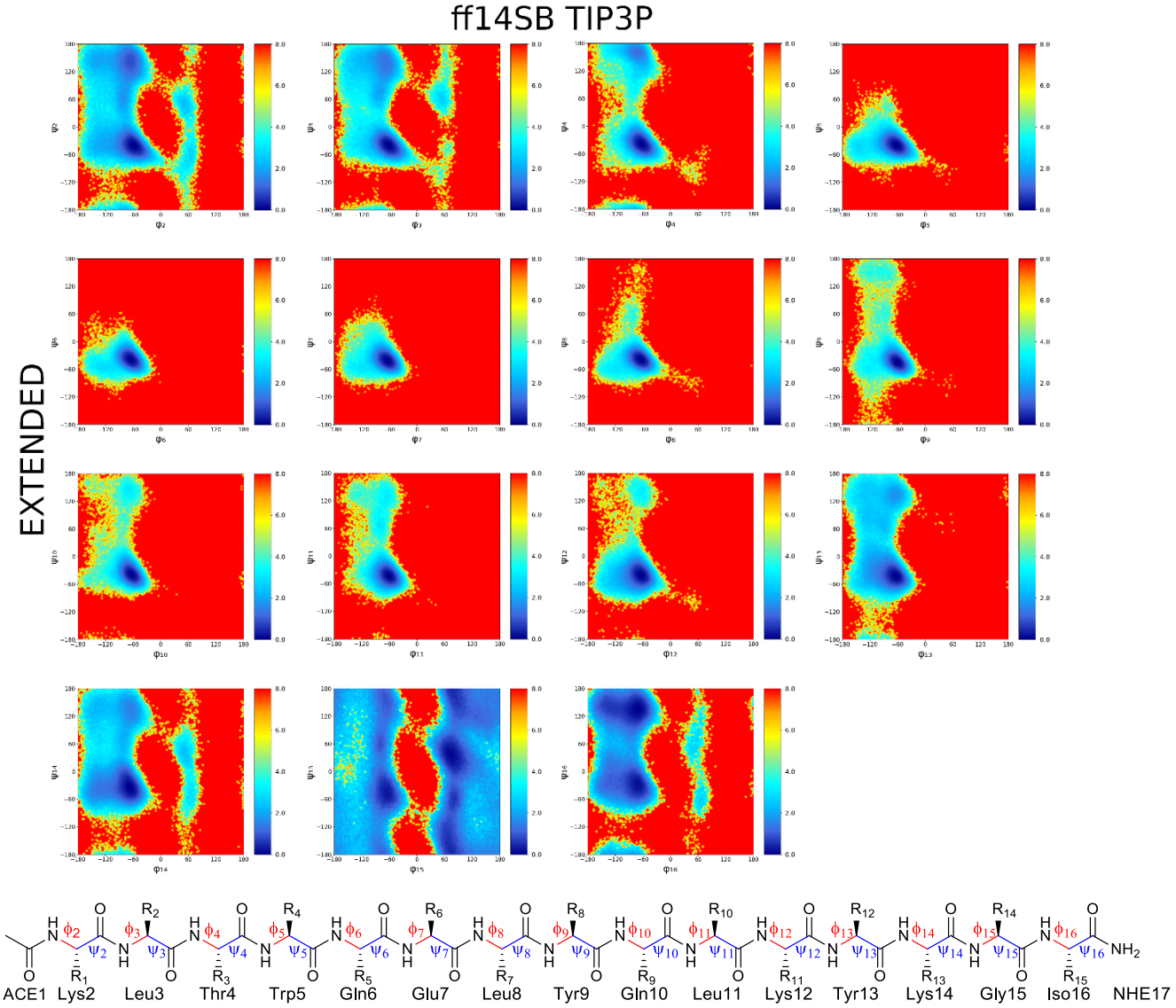

Figure S22. PMFs obtained from φ and ψ dihedral distributions of H1 residues for the ff14SB/TIP3P combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. H1 sequence and representation of φ and ψ angles numbering are also shown.

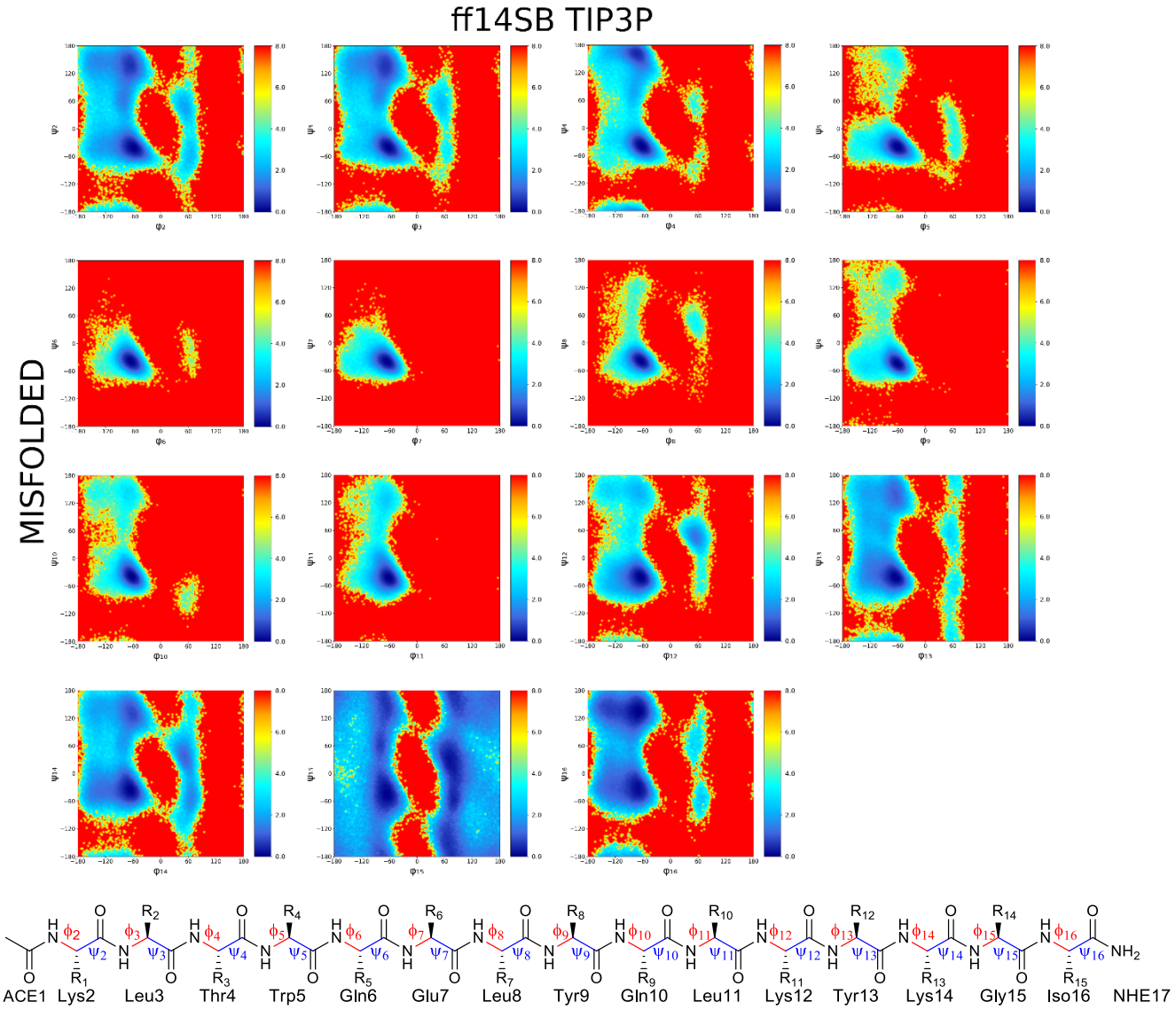

Figure S23. PMFs obtained from φ and ψ dihedral distributions of H1 residues for the ff14SB/TIP3P combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. H1 sequence and representation of φ and ψ angles numbering are also shown.

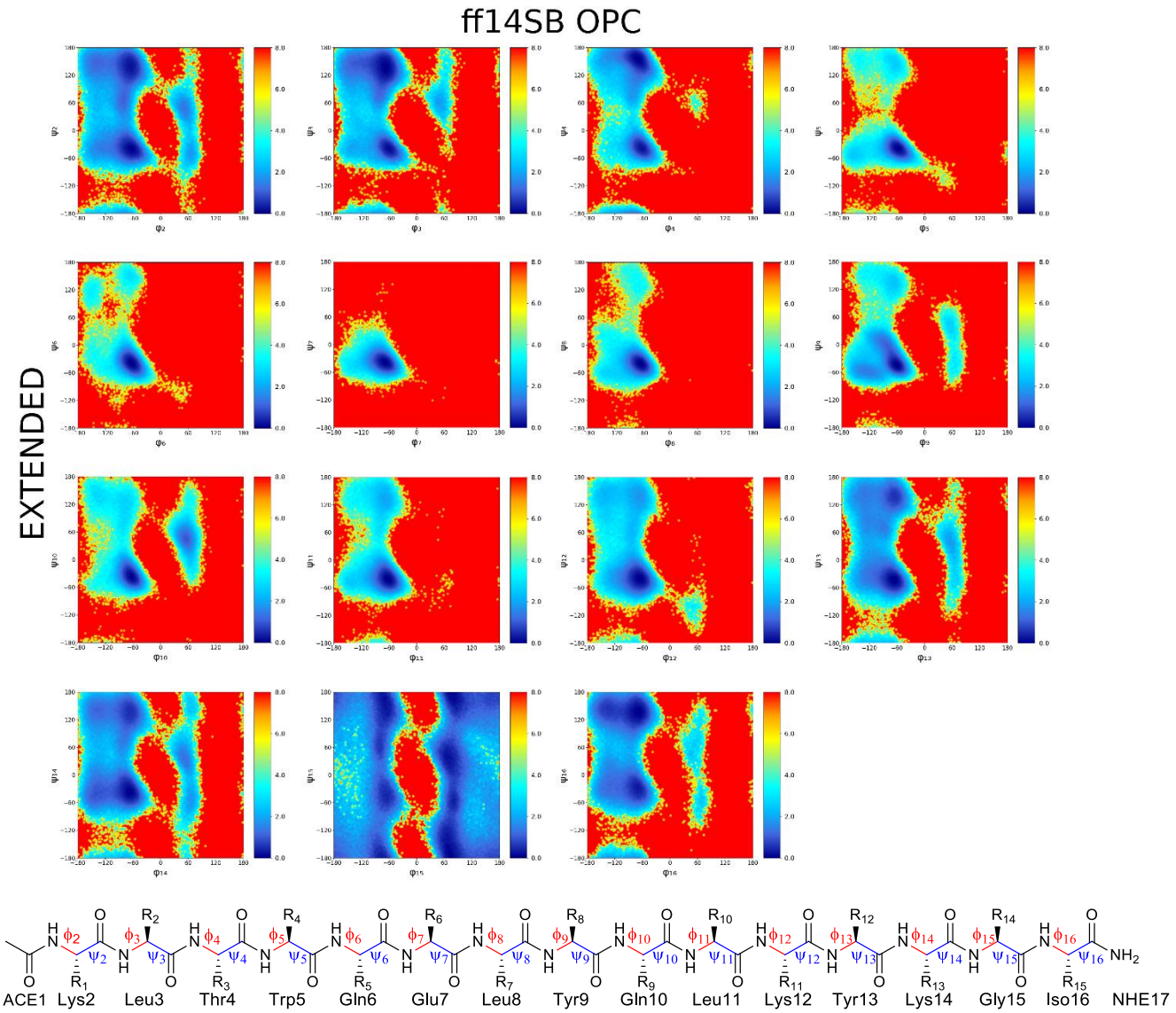

Figure S24. PMFs obtained from φ and ψ dihedral distributions of H1 residues for the ff14SB/OPC combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. H1 sequence and representation of φ and ψ angles numbering are also shown.

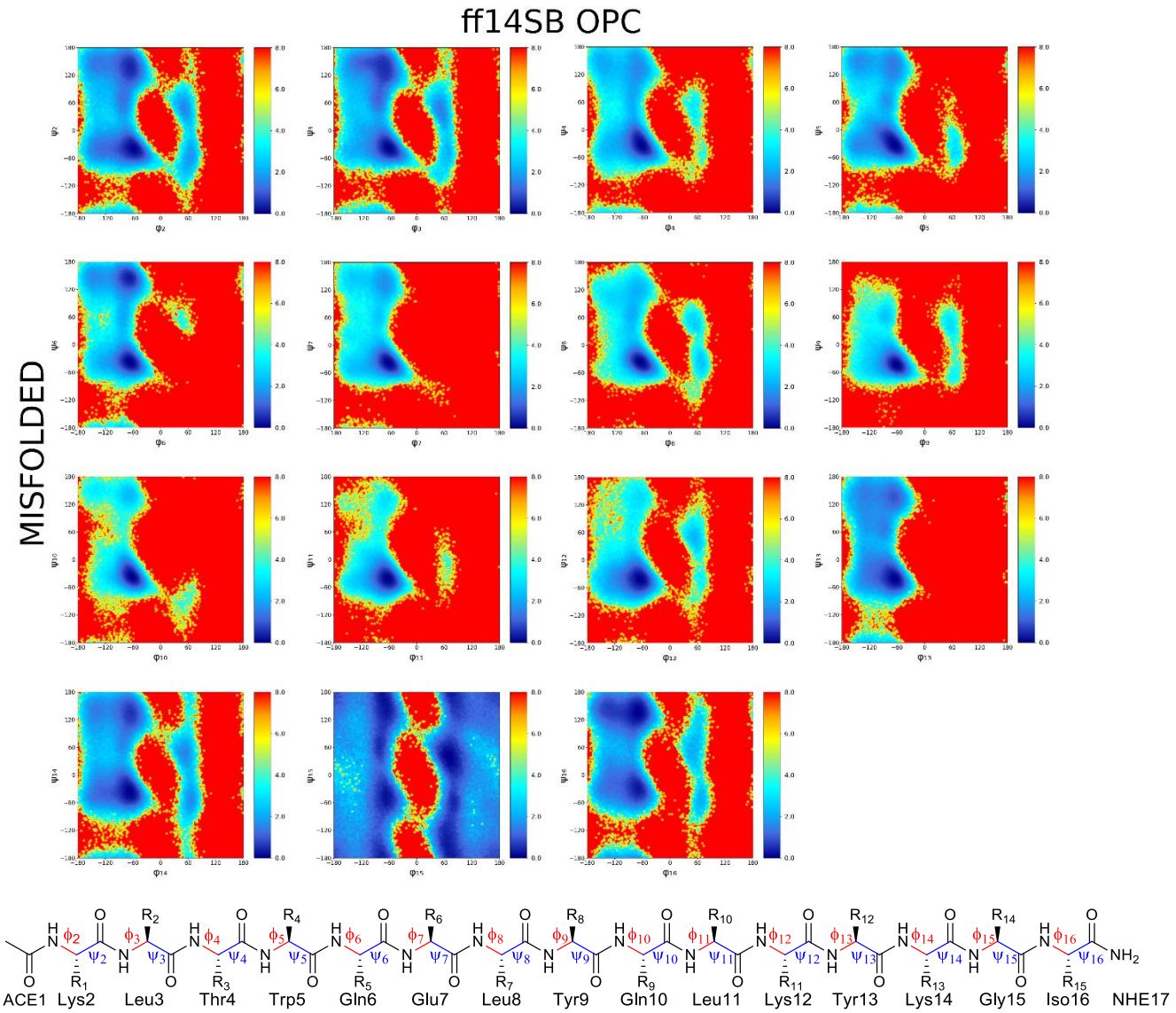

Figure S25. PMFs obtained from φ and ψ dihedral distributions of H1 residues for the ff14SB/OPC combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. H1 sequence and representation of φ and ψ angles numbering are also shown.

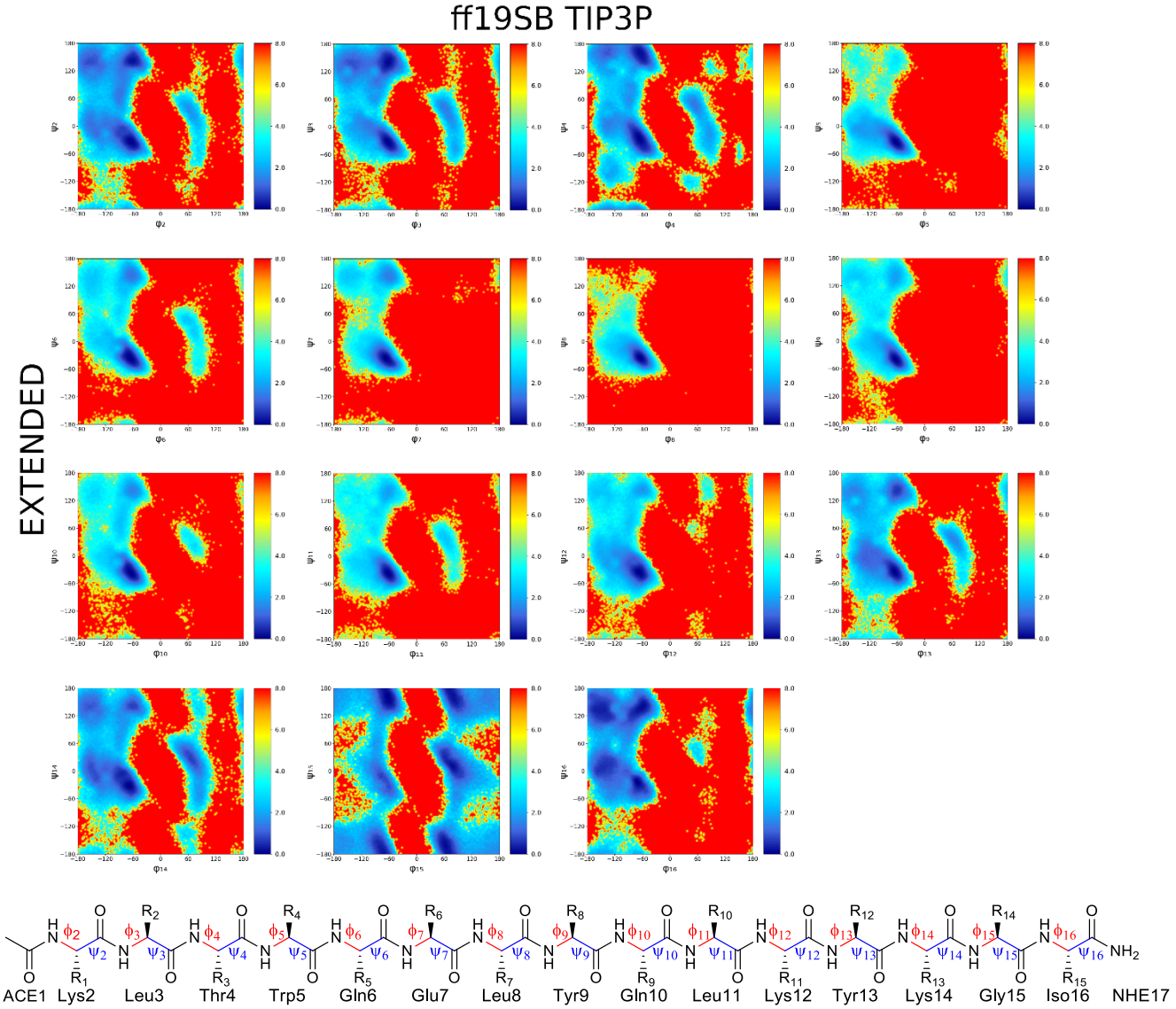

Figure S26. PMFs obtained from φ and ψ dihedral distributions of H1 residues for the ff19SB/TIP3P combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. H1 sequence and representation of φ and ψ angles numbering are also shown.

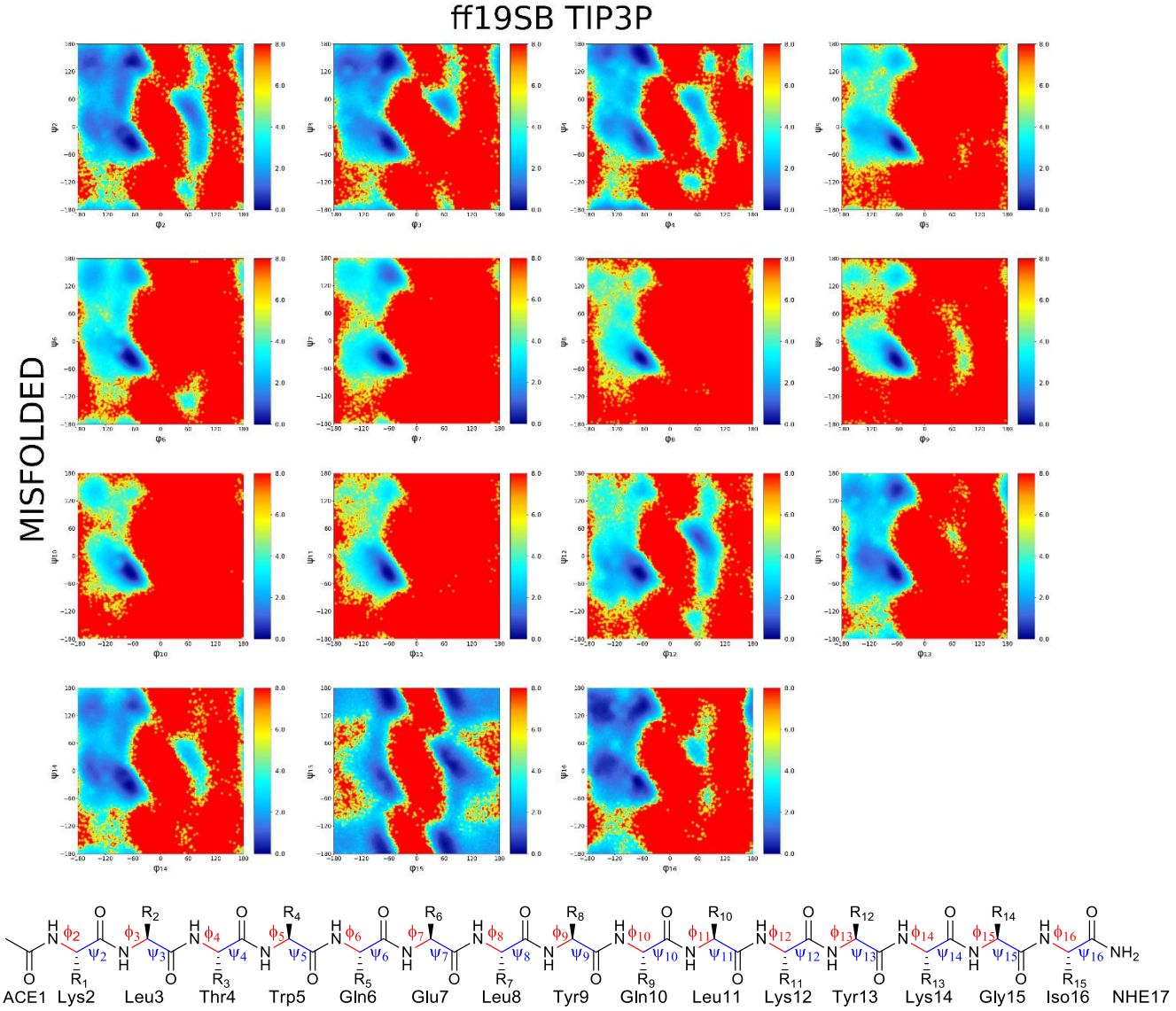

Figure S27. PMFs obtained from φ and ψ dihedral distributions of H1 residues for the ff19SB/TIP3P combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. H1 sequence and representation of φ and ψ angles numbering are also shown.

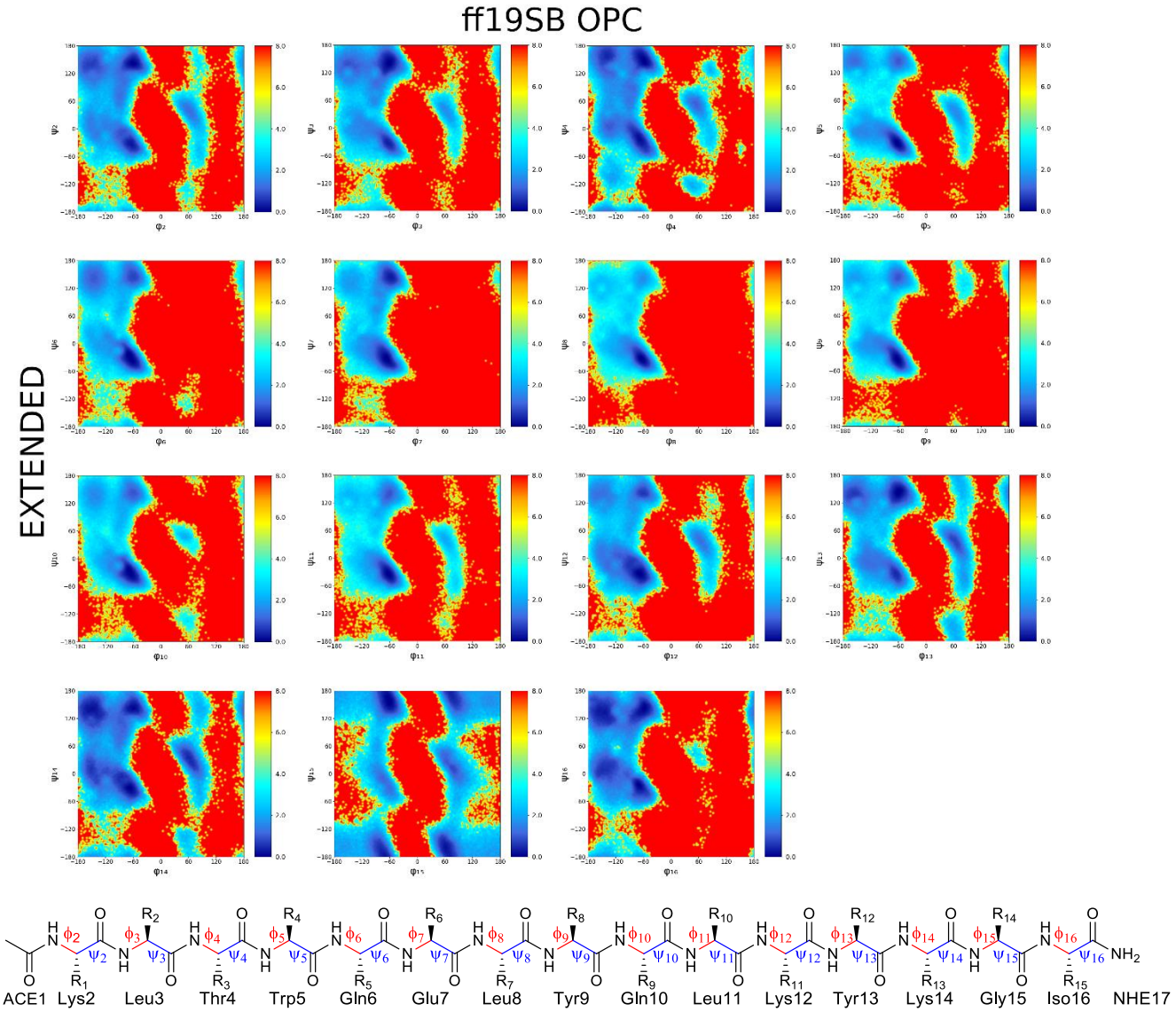

Figure S28. PMFs obtained from φ and ψ dihedral distributions of H1 residues for the ff19SB/OPC combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. H1 sequence and representation of φ and ψ angles numbering are also shown.

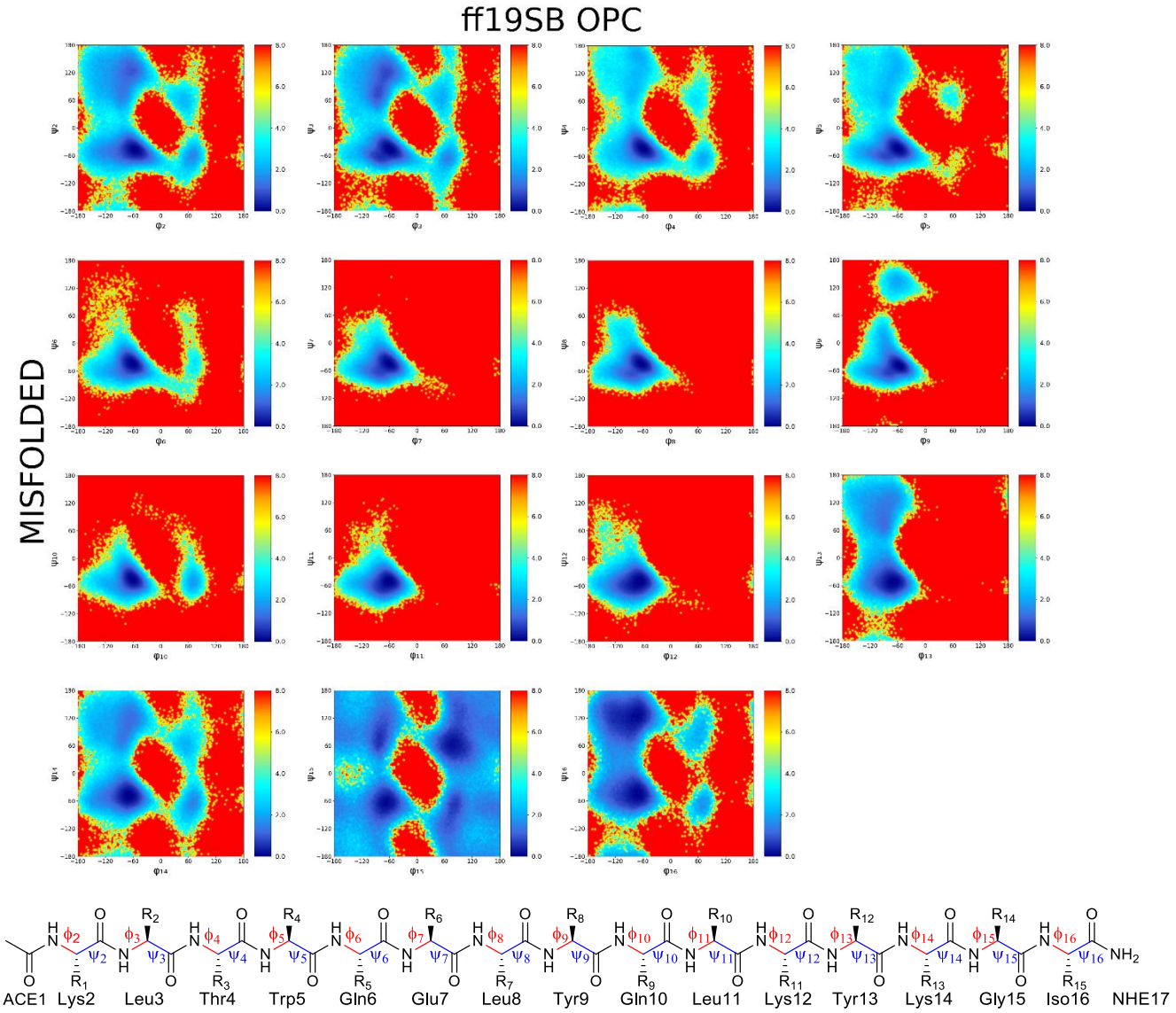

Figure S29. PMFs obtained from φ and ψ dihedral distributions of H1 residues for the ff19SB/OPC combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. H1 sequence and representation of φ and ψ angles numbering are also shown.

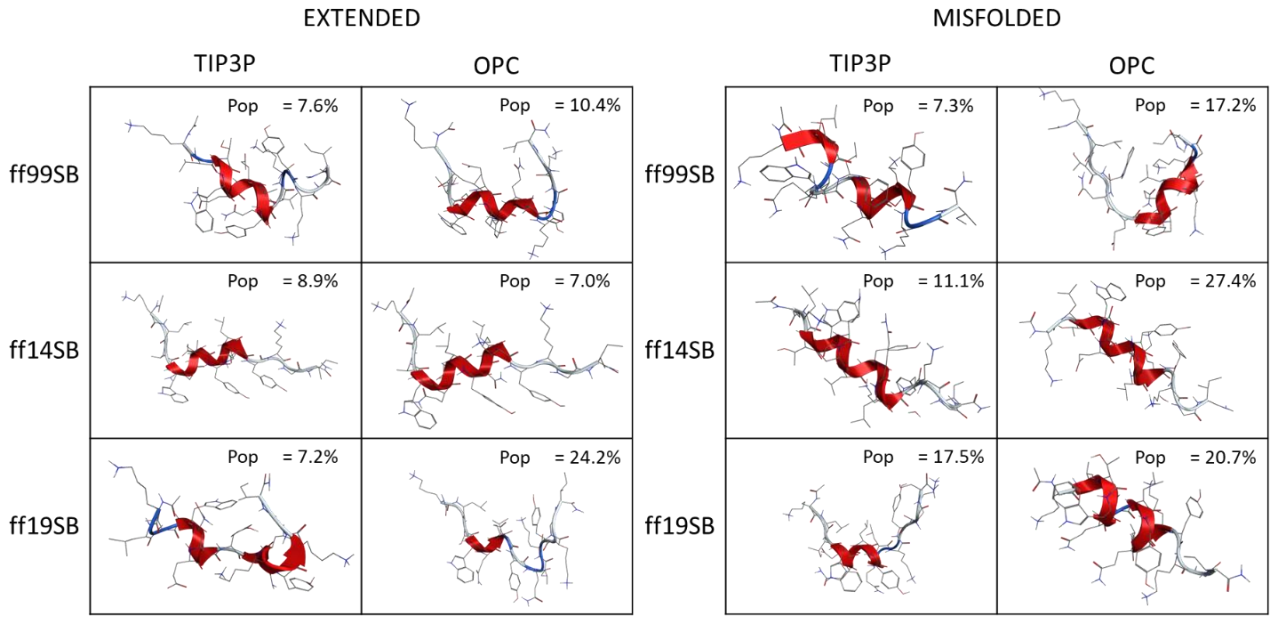

Figure S30. Representative conformation and population (pop%) of the second clusters from H1 trajectories.

Table S3. H-bond analyses from H1 trajectories. Only H-bonds involving the backbone are included in the table (donor N-H, acceptor C=O).

ff99SB OPC

EXTENDED			MISFOLDED		
acceptor	donor	occ%	acceptor	donor	occ%
TRP5	TYR9	23.59	LEU8	LYS12	25.94
THR4	LEU8	17.75	GLU7	LEU11	23.66
LEU8	LYS12	16.61	TYR9	TYR13	21.97
TYR9	TYR13	15.98	TRP5	TYR9	19.9
GLN6	GLN10	15.12	GLN6	GLN10	18.21
GLU7	LEU11	13.93	THR4	LEU8	12.88
LEU3	GLU7	11.74	GLN10	LYS14	12.72
THR4	GLU7	7.01	LEU3	GLU7	8.93
GLN10	LYS14	6.55	TYR9	LYS14	7.53
LYS2	GLN6	6.45	GLU7	GLN10	7.44
LEU3	GLN6	5.73	LYS2	GLN6	7.37
			GLN10	GLY15	6.51

ff99SB TIP3P

EXTENDED			MISFOLDED		
acceptor	donor	occ%	acceptor	donor	occ%
TYR9	TYR13	35.57	TRP5	TYR9	35.42
LEU8	LYS12	33.16	LEU8	LYS12	35.15
GLU7	LEU11	28.72	LEU3	GLU7	31.74
GLN6	GLN10	27.68	TYR9	TYR13	31.54
TRP5	TYR9	23.62	GLU7	LEU11	29.96
LEU3	GLU7	21.77	GLN6	GLN10	28.9
GLN10	LYS14	17.63	THR4	LEU8	23.33
LYS2	GLN6	16.01	GLN10	LYS14	19.72
THR4	LEU8	15.36	LYS2	GLN6	18.57
LEU3	GLN6	9.2	TYR9	LYS14	13.64
TYR9	LYS14	7.89	GLN10	GLY15	10.84
LEU11	GLY15	7.52	ACE1	TRP5	10.64
GLN10	GLY15	7.52	LEU3	GLN6	10.44
ACE1	TRP5	6.78	LEU11	GLY15	8.18
LYS2	TRP5	6.53	GLN6	LEU11	6.47
			LYS2	TRP5	5.57
			TRP5	GLN10	5.28
			LEU8	TYR13	5.13

ff14SB OPC

ff14SB TIP3P

EXTENDED		
acceptor	donor	occ%
TRP5	TYR9	46.2
THR4	LEU8	37.06
TYR9	TYR13	30.25
GLN10	LYS14	21.33
LEU8	LYS12	20.8
GLU7	LEU11	19.11
GLN6	GLN10	19.06
GLN6	LEU11	12.41
THR4	GLU7	11.72
LEU3	GLU7	8.91
LYS2	GLN6	7.74
LEU11	GLY15	7.65
GLN10	GLY15	6.36

MISFOLDED		
acceptor	donor	occ%
TYR9	TYR13	37.81
LEU8	LYS12	29.34
GLU7	LEU11	26.09
GLN6	GLN10	23.74
GLN10	LYS14	20.66
TRP5	TYR9	12.72
LEU3	GLN6	10.95
LEU3	GLU7	10.51
THR4	LEU8	10.07
LEU11	GLY15	9.34
GLN6	TYR9	8.11
LYS2	GLN6	7.7
TYR9	LYS14	5.53
TYR9	LYS12	5.5
GLN10	GLY15	5.37
ACE1	TRP5	5.33

EXTENDED		
acceptor	donor	occ%
TRP5	TYR9	46.13
TYR9	TYR13	45.18
GLU7	LEU11	39.23
LEU8	LYS12	38.88
GLN10	LYS14	35.65
GLN6	GLN10	35.29
THR4	LEU8	31.24
LEU3	GLU7	31.11
LYS2	GLN6	25.18
LEU11	GLY15	18.67
ACE1	TRP5	15.82
GLN10	GLY15	7.97
LEU11	ILE16	7.1

MISFOLDED		
acceptor	donor	occ%
TRP5	TYR9	49.83
TYR9	TYR13	40.46
GLU7	LEU11	39.56
LEU8	LYS12	37.93
THR4	LEU8	34.15
GLN6	GLN10	33.25
GLN10	LYS14	26.96
LEU3	GLU7	19.75
LYS2	GLN6	15.38
LEU11	GLY15	10.46
ACE1	TRP5	10.39
GLN10	GLY15	7.91
THR4	GLU7	7.42
TYR9	LYS14	6

ff19SB OPC		
EXTENDED		
acceptor	donor	occ%
LEU8	LYS12	14.25
TYR9	TYR13	14.02
GLU7	LEU11	13.2
TRP5	TYR9	12.92
GLU7	GLN10	11.43
THR4	LEU8	9.88
TYR9	LYS12	8.26
GLN6	GLN10	8.07
THR4	GLU7	7.32
GLN10	LYS14	7.11
GLN10	TYR13	5.5

MISFOLDED		
acceptor	donor	occ%
LEU8	LYS12	34.48
TRP5	TYR9	32.19
TYR9	LYS14	26.75
LEU3	GLU7	25.95
TYR9	TYR13	25.33
GLU7	LEU11	24.86
GLN6	GLN10	23.14
THR4	LEU8	22.81
TRP5	GLN10	17.07
LEU8	TYR13	16.75
LYS2	GLN6	15.89
GLN10	GLY15	15.7
ACE1	TRP5	14.54
GLN10	LYS14	13.21
GLU7	LYS12	11.39
GLN6	LEU11	11.02
LEU3	LEU8	10.15
ACE1	GLN6	8
LEU11	ILE16	7.72
THR4	TYR9	7.66
LEU11	GLY15	7.02
GLN10	ILE16	5.63
LEU3	GLN6	5.45

ff19SB TIP3P		
EXTENDED		
acceptor	donor	occ%
TRP5	TYR9	31.45
GLU7	LEU11	29.39
TYR9	TYR13	26.5
LEU8	LYS12	24.05
THR4	LEU8	21.95
GLN6	GLN10	21.9
GLN10	LYS14	20.12
LEU11	GLY15	9.3
THR4	GLU7	7.78
LEU3	GLU7	7.56
LYS2	GLN6	6.9
LEU3	GLN6	6.75
GLN10	TYR13	5.99
GLU7	GLN10	5.82
TYR9	LYS12	5.74

MISFOLDED		
acceptor	donor	occ%
GLU7	LEU11	39.46
TRP5	TYR9	37.55
LEU8	LYS12	30.56
TYR9	TYR13	27.23
THR4	LEU8	27
GLN10	LYS14	21.8
GLN6	GLN10	20.3
GLU7	GLN10	9.53
LEU11	GLY15	9.03
THR4	GLU7	8.81
TYR9	LYS12	6.21
LYS2	GLN6	5.35

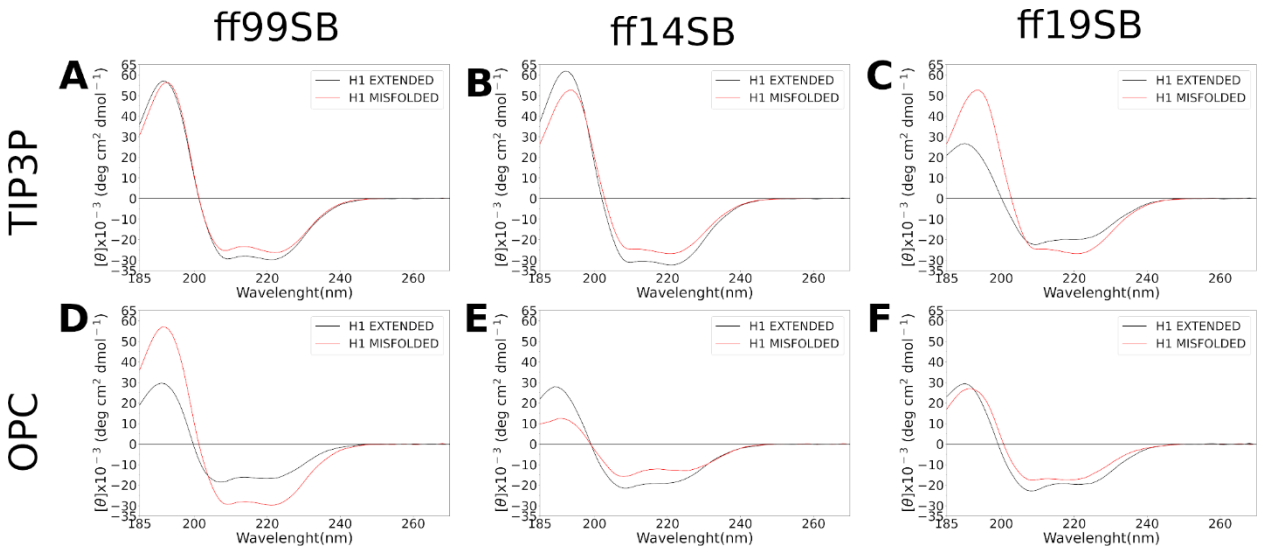

Figure 31. SESCA CD spectra of H1 calculated using the main cluster obtained from the last 500 ns of aMD trajectory, for each combination. Results from extended and misfolded simulations are reported in black and red lines, respectively.

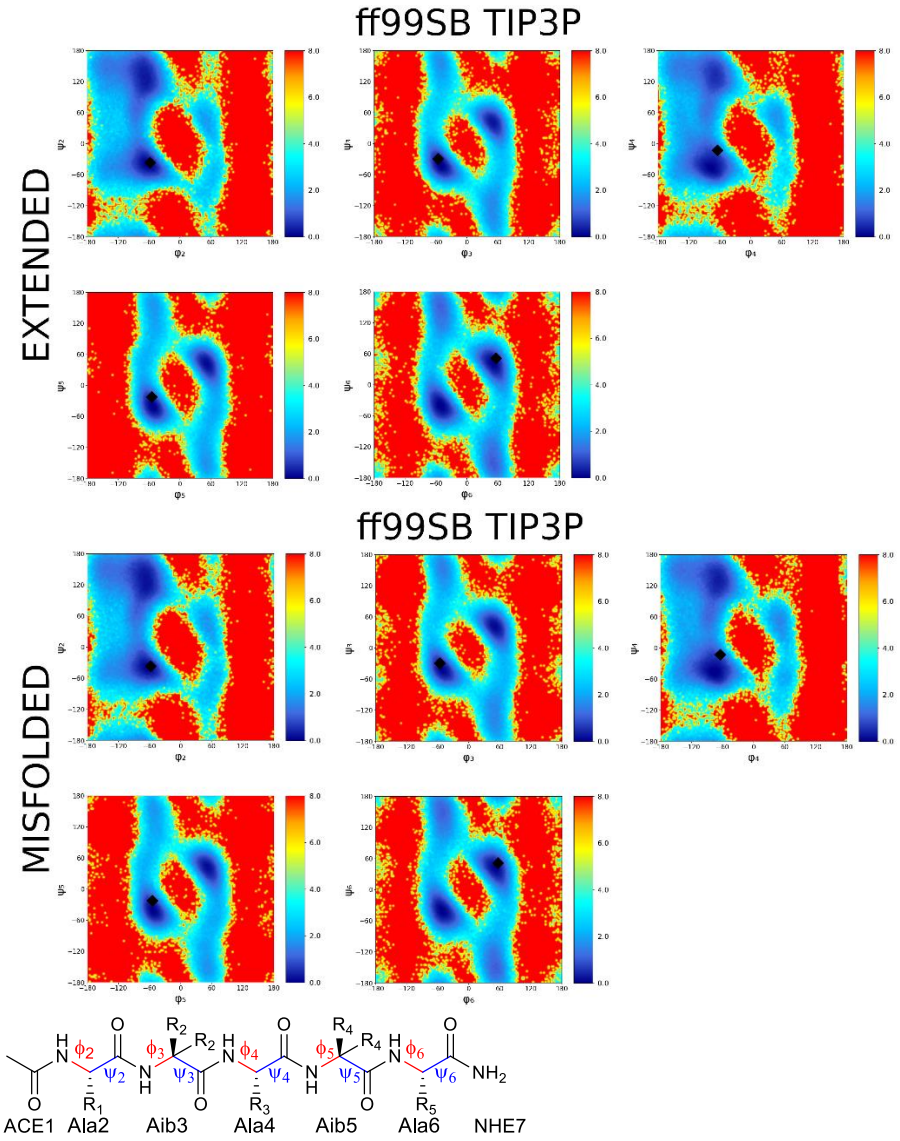

Figure S32. PMFs obtained from φ and ψ dihedral distributions of H2 residues for the ff99SB/TIP3P combination from extended (top panels) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. H2 sequence and representation of φ and ψ angles numbering are also shown.

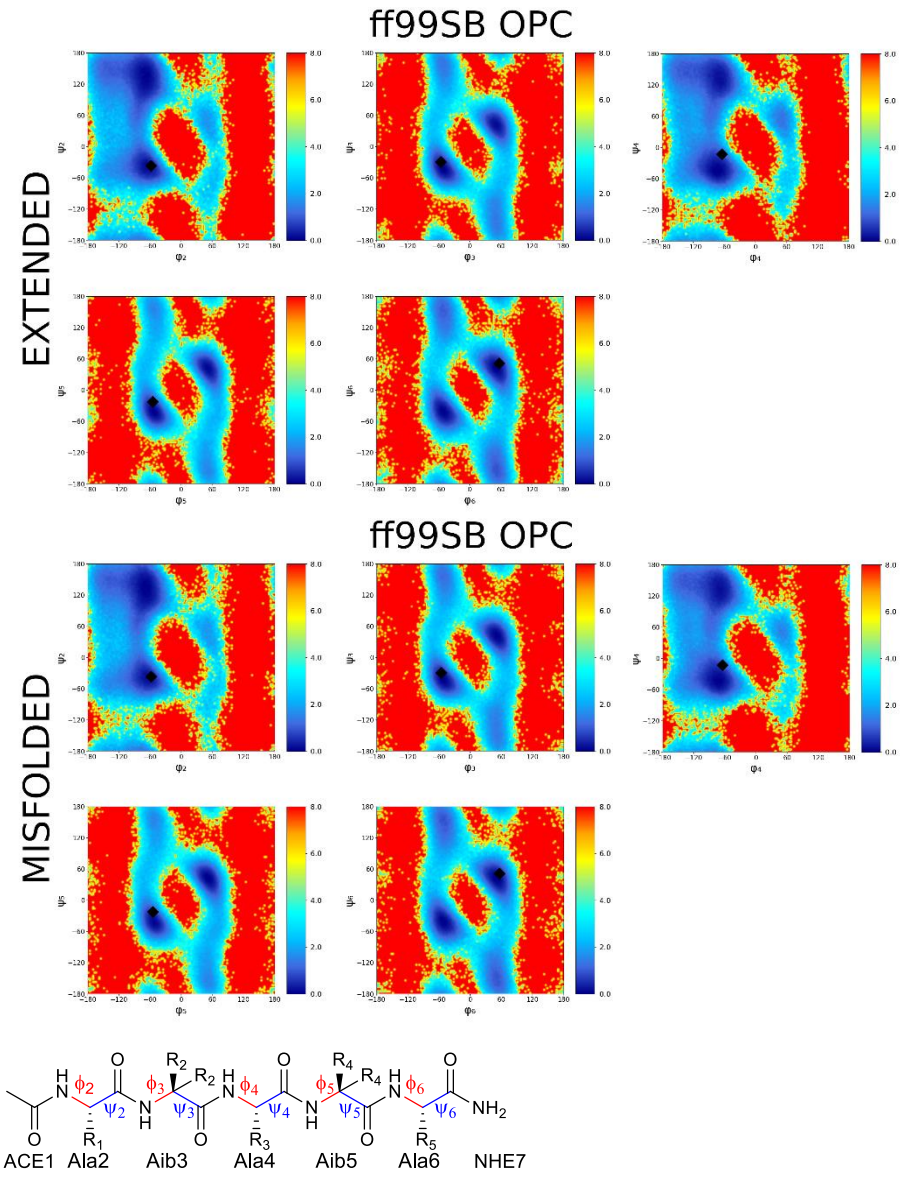

Figure S33. PMFs obtained from φ and ψ dihedral distributions of H2 residues for the ff99SB/OPC combination from extended (top panels) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. H2 sequence and representation of φ and ψ angles numbering are also shown.

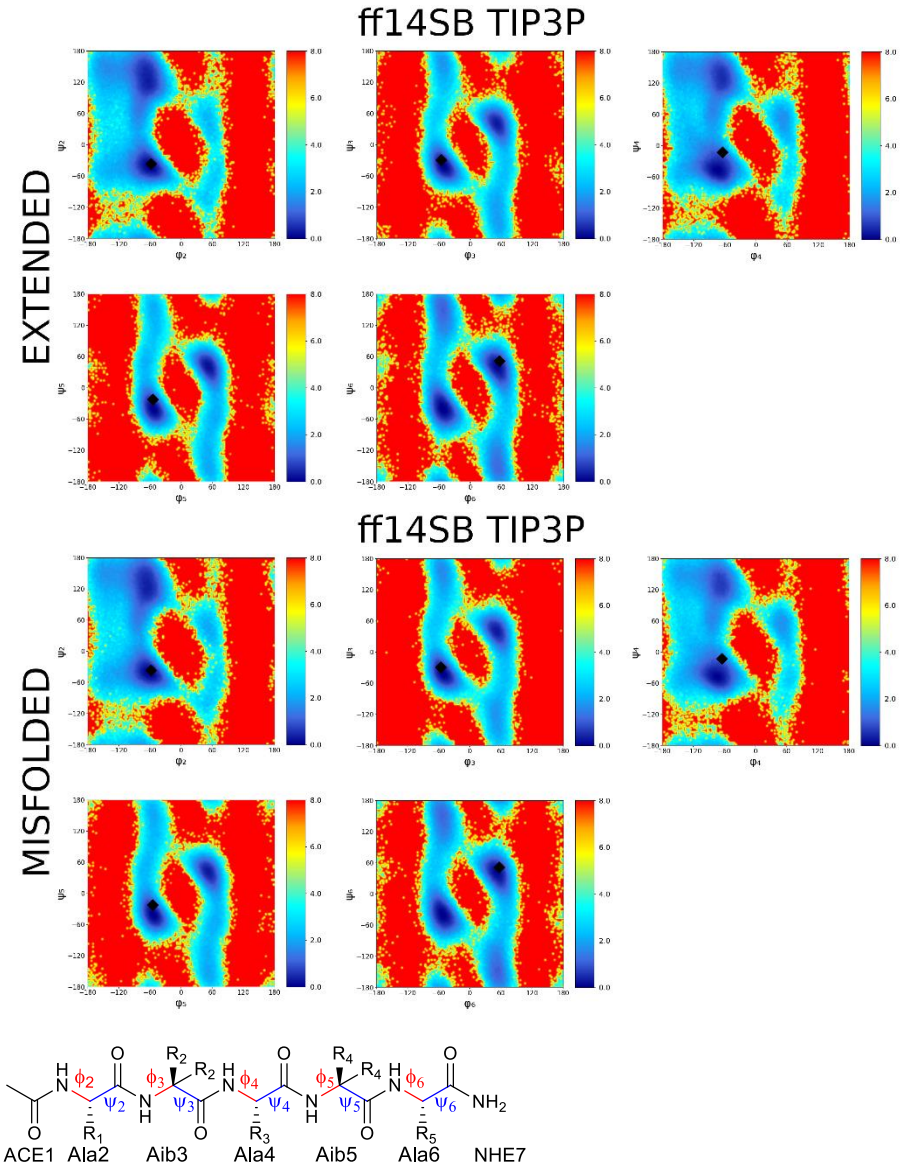

Figure S34. PMFs obtained from φ and ψ dihedral distributions of H2 residues for the ff14SB/TIP3P combination from extended (top panels) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. H2 sequence and representation of φ and ψ angles numbering are also shown.

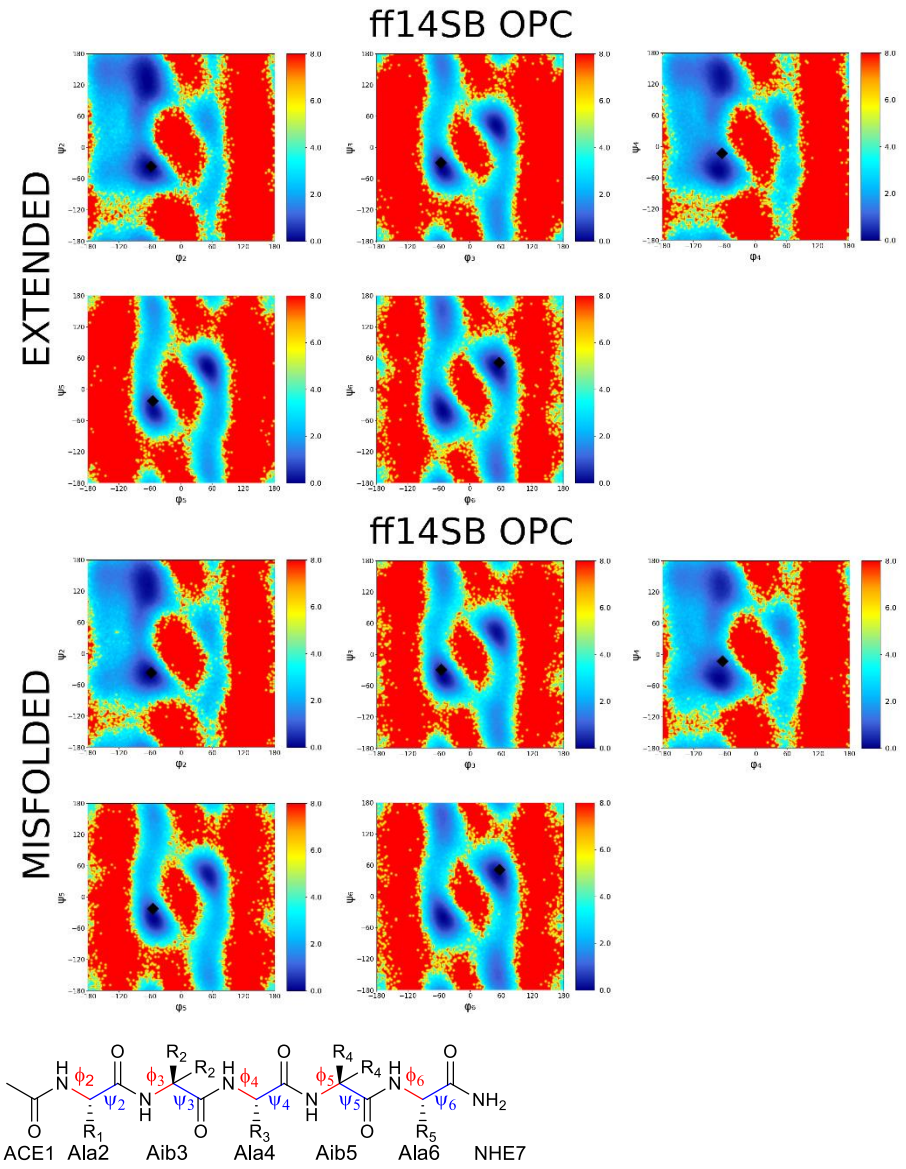

Figure S35. PMFs obtained from φ and ψ dihedral distributions of H2 residues for the ff14SB/OPC combination from extended (top panels) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. H2 sequence and representation of φ and ψ angles numbering are also shown.

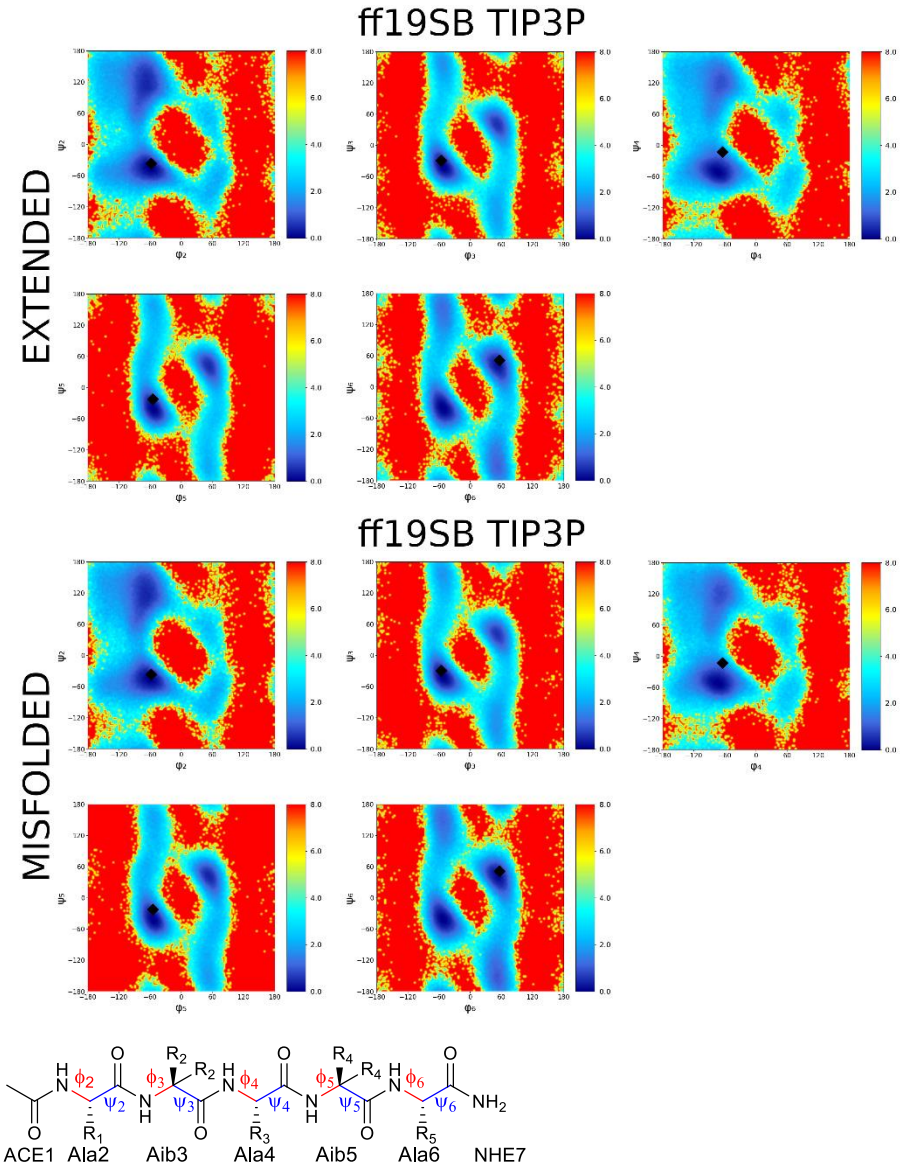

Figure S36. PMFs obtained from φ and ψ dihedral distributions of H2 residues for the ff19SB/TIP3P combination from extended (top panels) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. H2 sequence and representation of φ and ψ angles numbering are also shown.

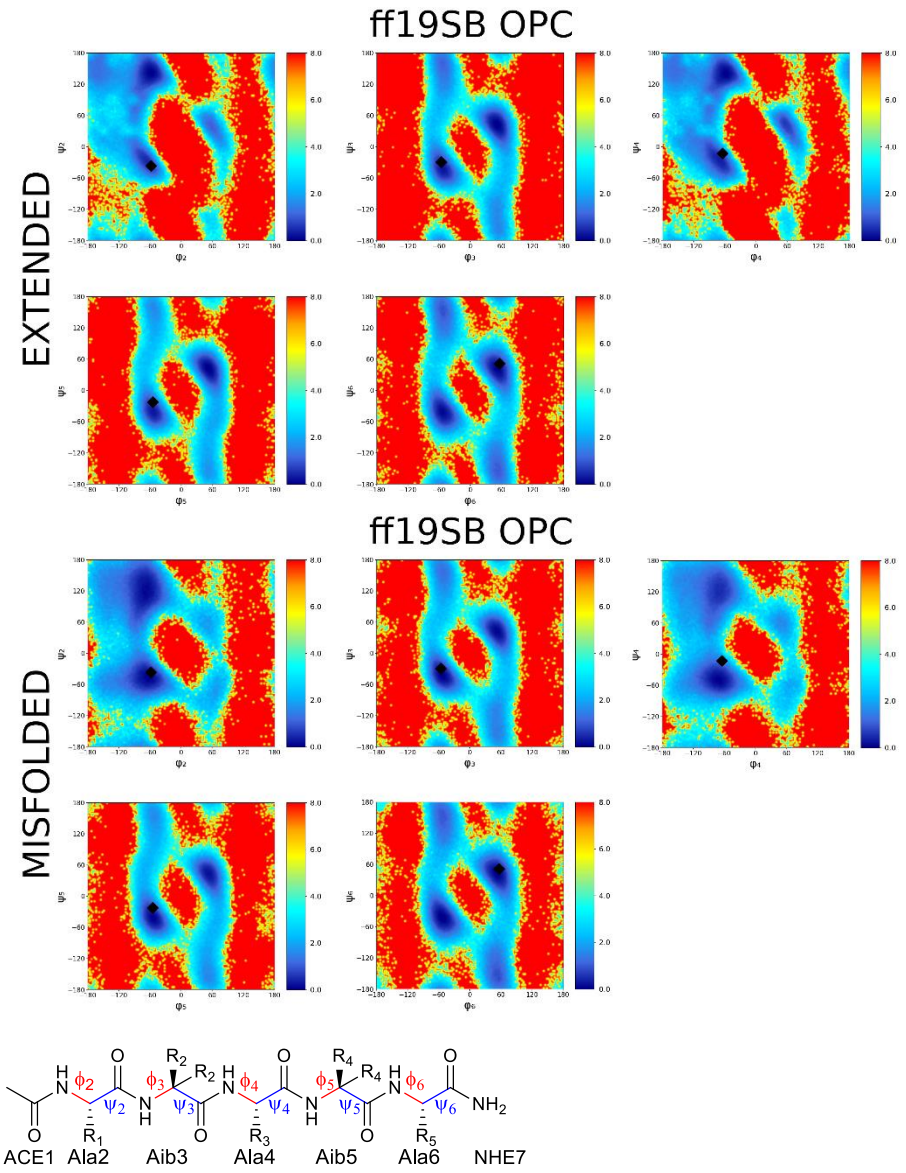

Figure S37. PMFs obtained from φ and ψ dihedral distributions of H2 residues for the ff19SB/OPC combination from extended (top panels) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. H2 sequence and representation of φ and ψ angles numbering are also shown.

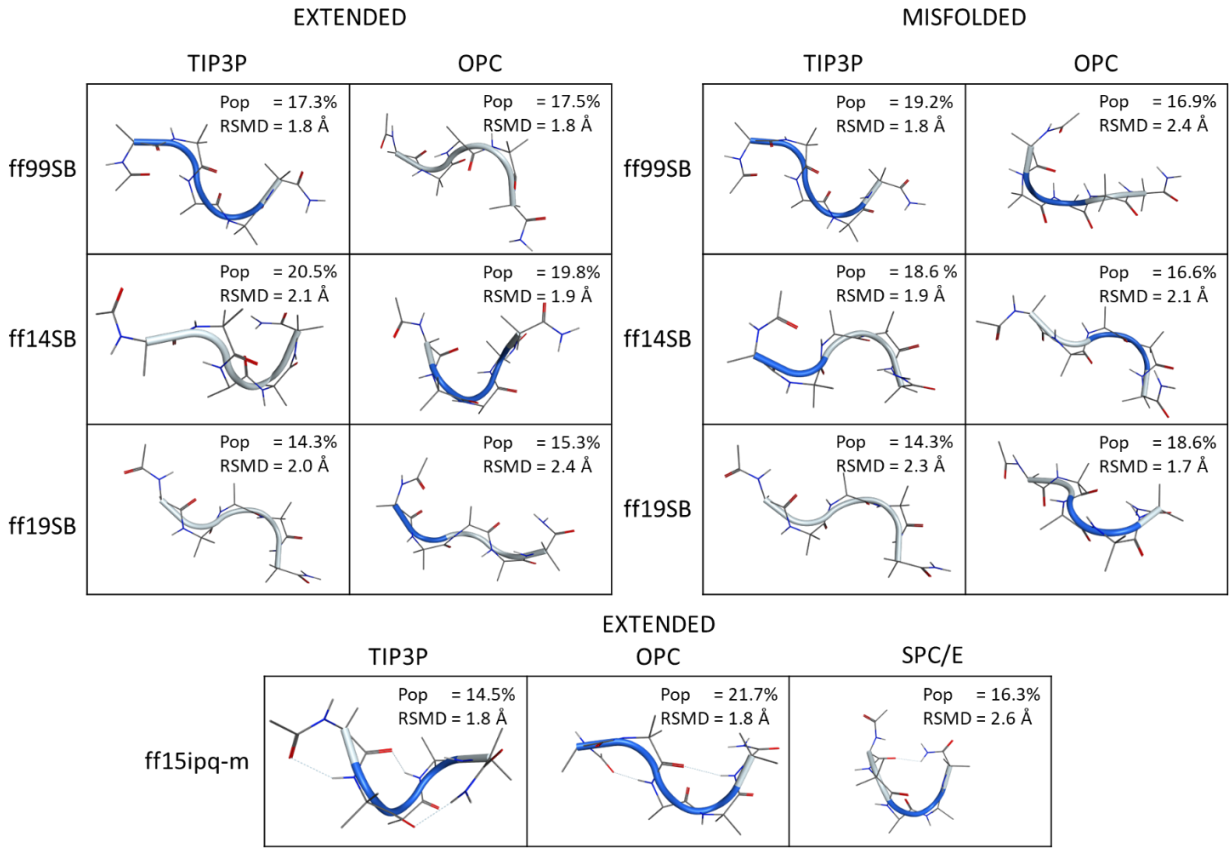

Figure S38. Representative conformation of the second clusters from H2 trajectories. Population (pop%) and RMSD vs native structure are also shown in the figure.

Table S4. H-bond analyses from H2 trajectories. Only H-bonds involving the backbone are included in the table (donor N-H, acceptor C=O). Native H-bonds are highlighted in bold.

NATIVE		
acceptor	donor	Distance
AIB3	**AIB6**	2.91
AIB3	**AIB5**	2.94
ALA2	**AIB5**	2.97
ALA2	**ALA4**	3.02
ALA4	**AIB6**	3.04
ACE1	**ALA4**	3.13
ACE1	**AIB3**	3.22
AIB5	**NHE7**	3.34
ACE1	**AIB5**	4.43

ff99SB OPC					
EXTENDED			MISFOLDED		
acceptor	donor	occ%	acceptor	donor	occ%
ALA2	AIB6	5.34	**ACE1**	**ALA4**	5.22

ff99SB TIP3P					
EXTENDED			MISFOLDED		
acceptor	donor	occ%	acceptor	donor	occ%
ACE1	**ALA4**	8.63	**ACE1**	**ALA4**	7.75
ALA2	AIB6	8.01	ALA2	AIB6	6.82

ff14SB OPC									ff14SB TIP3P								
EXTENDED				MISFOLDED					EXTENDED				MISFOLDED				
acceptor	donor	occ%		acceptor	donor	occ%			acceptor	donor	occ%		acceptor	donor	occ%		
ACE1	**ALA4**	5.90		ALA2	AIB6	6.90			ALA2	AIB6	8.68		ALA2	AIB6	9.88		
ALA2	AIB6	5.86		**ACE1**	**ALA4**	5.82			**ACE1**	**ALA4**	8.58		**ACE1**	**ALA4**	8.25		
									ACE1	**AIB5**	6.74		**ACE1**	**AIB5**	6.63		
ACE1	**AIB5**	5.30		**ALA4**	**AIB6**	5.02											

ff19SB OPC						ff19SB TIP3P					
EXTENDED				MISFOLDED		EXTENDED			MISFOLDED		
acceptor	donor	occ%	acceptor	donor	occ%	acceptor	donor	occ%	acceptor	donor	occ%
			ALA2	AIB6	6.06	ALA2	AIB6	11.35	ALA2	AIB6	10.86
			ACE1	**ALA4**	5.30	**ACE1**	**ALA4**	8.56	**ACE1**	**ALA4**	8.16
						ACE1	**AIB5**	7.12	**ACE1**	**AIB5**	6.66
									ALA4	**AIB6**	5.54

ff15ipq-m OPC		
acceptor	donor	occ%
ALA4	NHE7	12.43
ACE1	**ALA4**	8.05
AIB3	**AIB5**	7.62
ACE1	**AIB3**	7.38

ff15ipq-m TIP3P		
acceptor	donor	occ%
ALA4	NHE7	10.13
ACE1	**ALA4**	6.00
ACE1	**AIB3**	5.11

ff15ipq-m SPC/E		
acceptor	donor	occ%
ALA4	NHE7	8.50
ACE1	**ALA4**	6.30

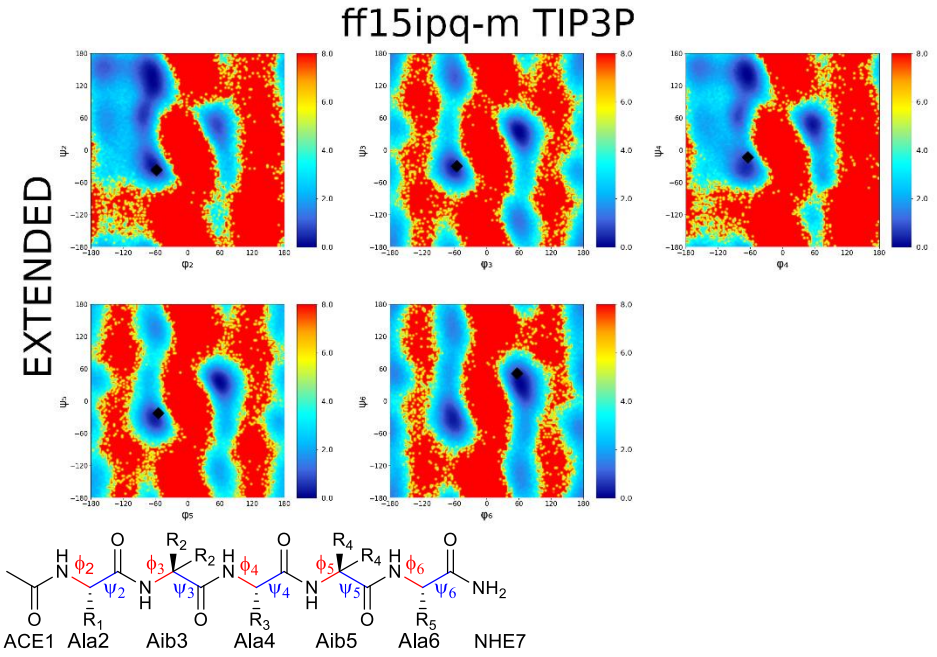

Figure S39. PMFs obtained from φ and ψ dihedral distributions of H2 residues for the ff115ipq-m/TIP3P combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. H2 sequence and representation of φ and ψ angles numbering are also shown.

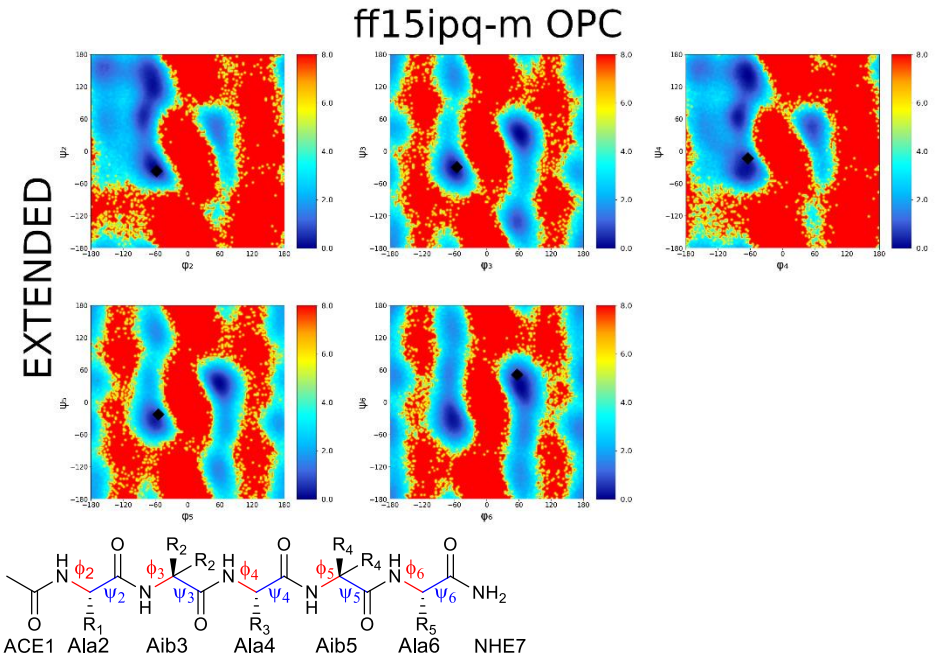

Figure S40. PMFs obtained from φ and ψ dihedral distributions of H2 residues for the ff115ipq-m/OPC combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. H2 sequence and representation of φ and ψ angles numbering are also shown.

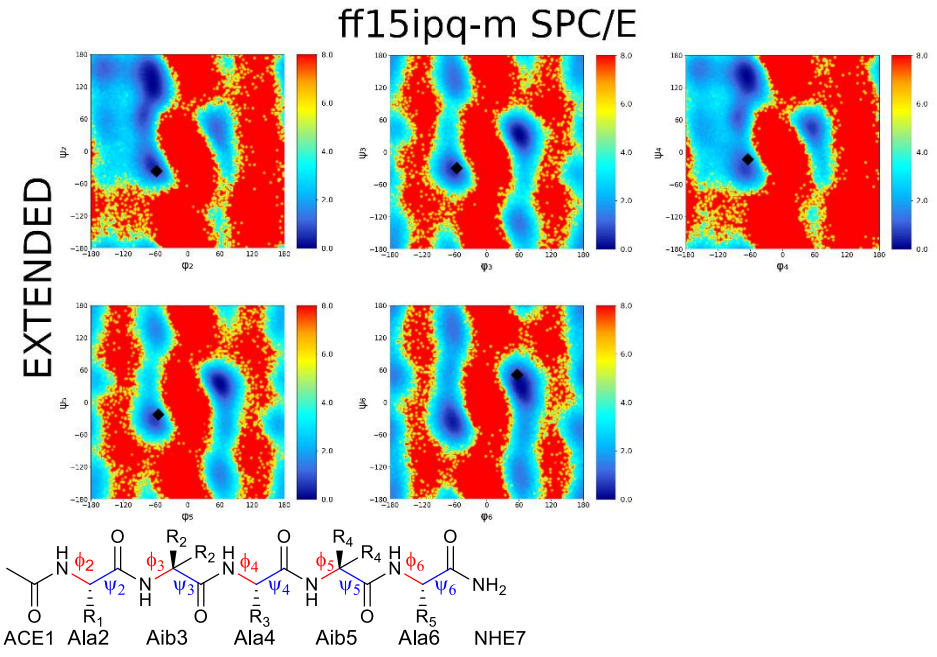

Figure S41. PMFs obtained from φ and ψ dihedral distributions of H2 residues for the ff115ipq-m/SPC/E combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. H2 sequence and representation of φ and ψ angles numbering are also shown.

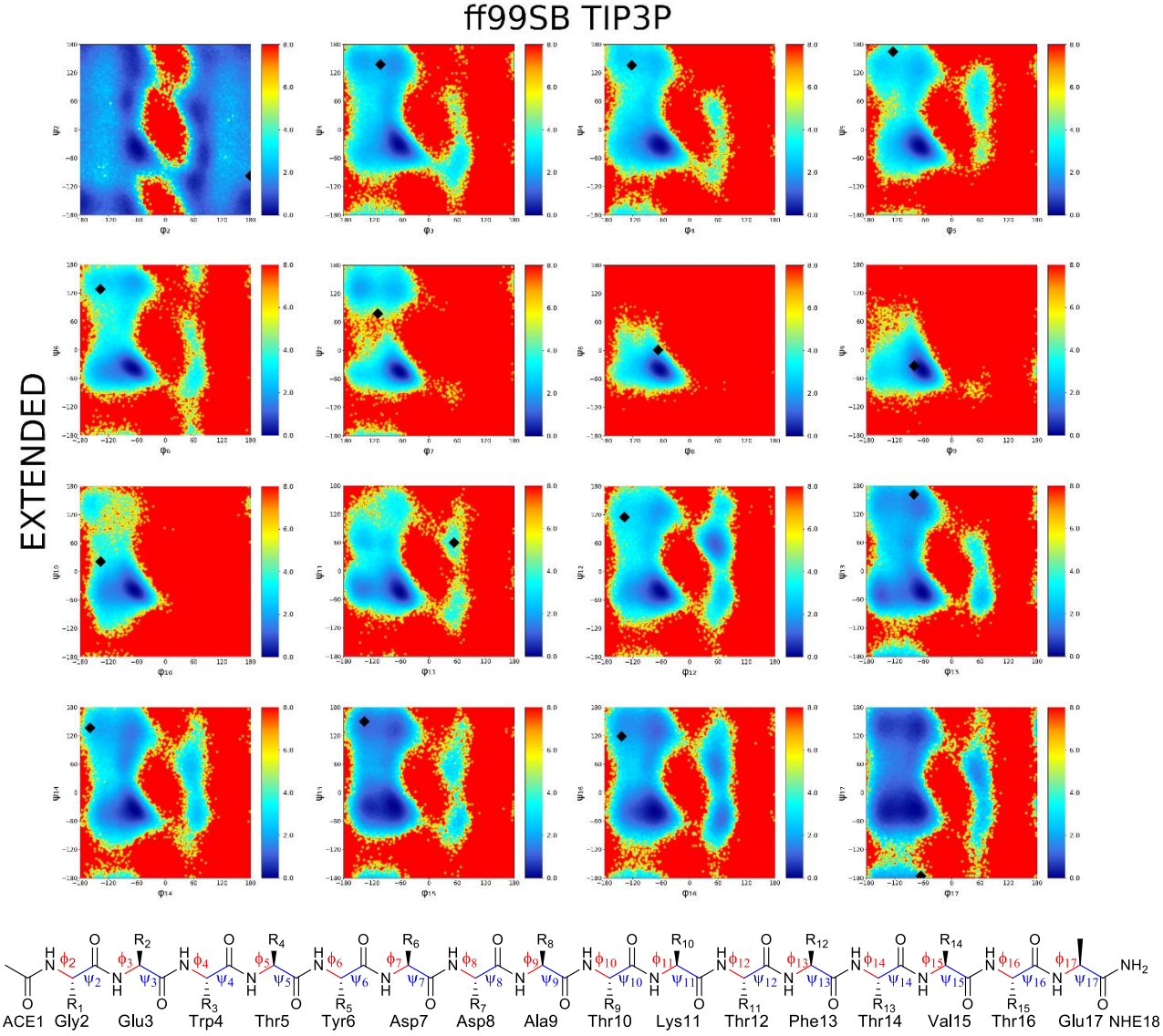

Figure S42. PMFs obtained from φ and ψ dihedral distributions of B1 residues for the ff99SB/TIP3P combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B1 sequence and representation of φ and ψ angles numbering are also shown.

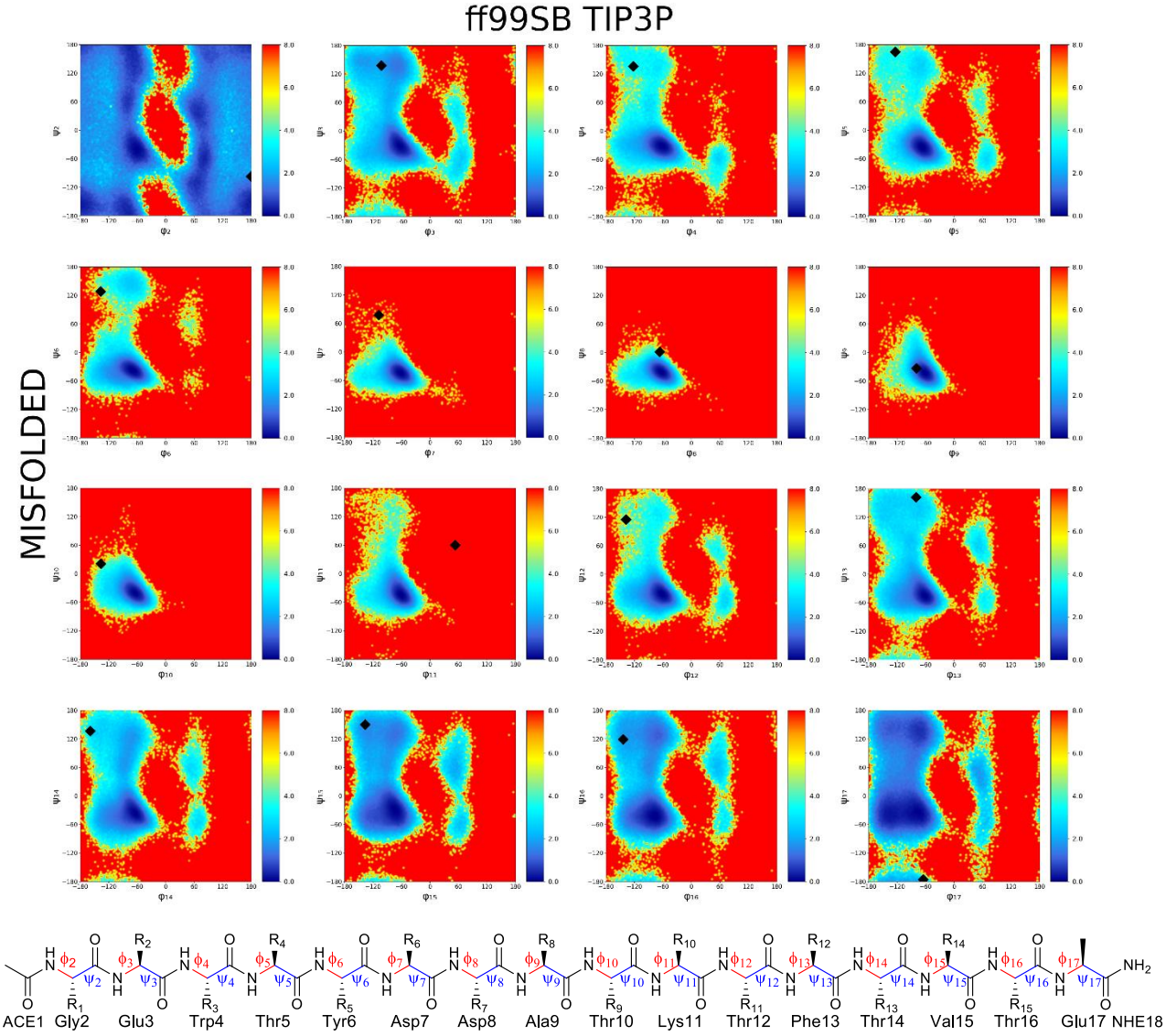

Figure S43. PMFs obtained from φ and ψ dihedral distributions of B1 residues for the ff99SB/TIP3P combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B1 sequence and representation of φ and ψ angles numbering are also shown.

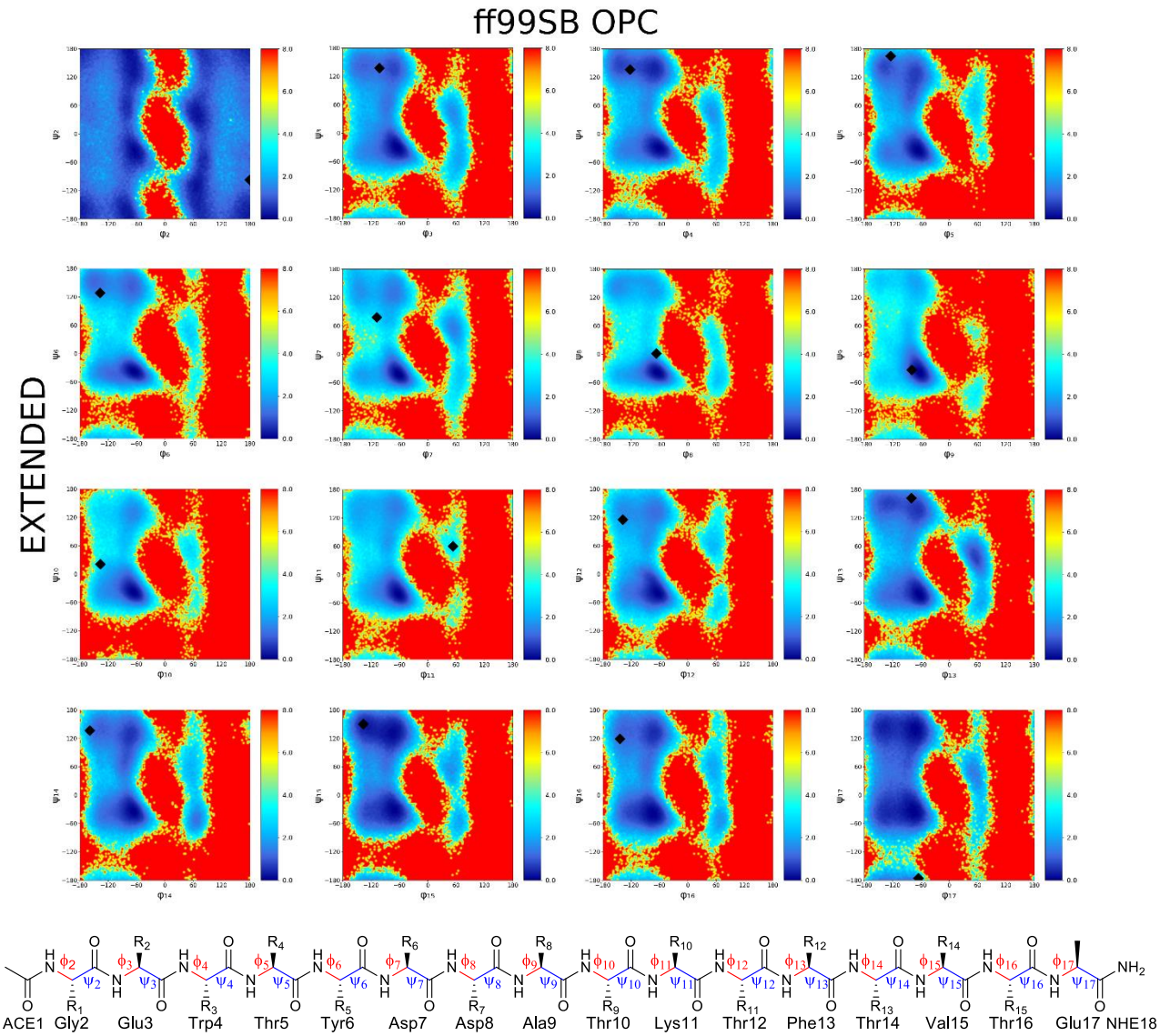

Figure S44. PMFs obtained from φ and ψ dihedral distributions of B1 residues for the ff99SB/OPC combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B1 sequence and representation of φ and ψ angles numbering are also shown.

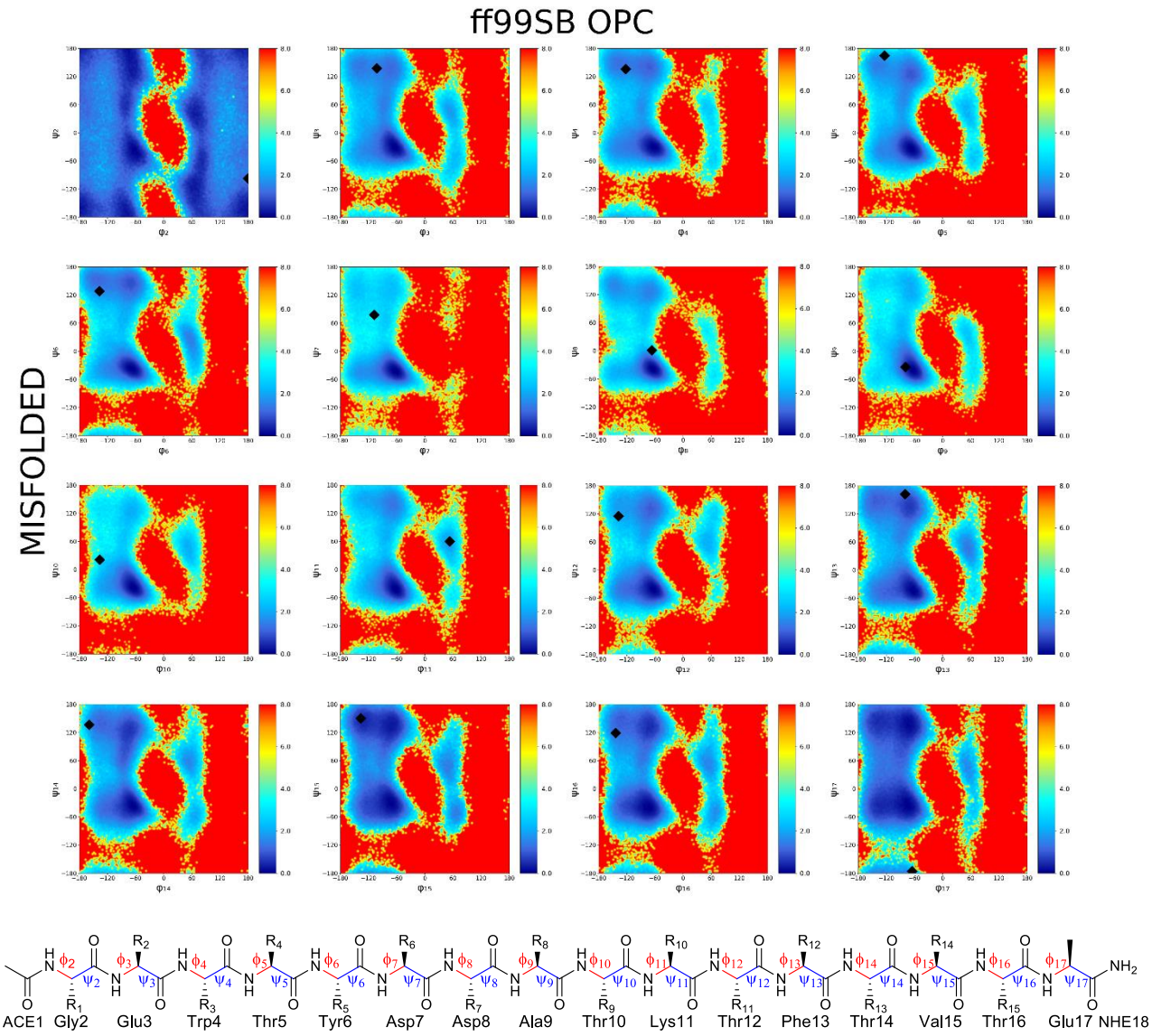

Figure S45. PMFs obtained from φ and ψ dihedral distributions of B1 residues for the ff99SB/OPC combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B1 sequence and representation of φ and ψ angles numbering are also shown.

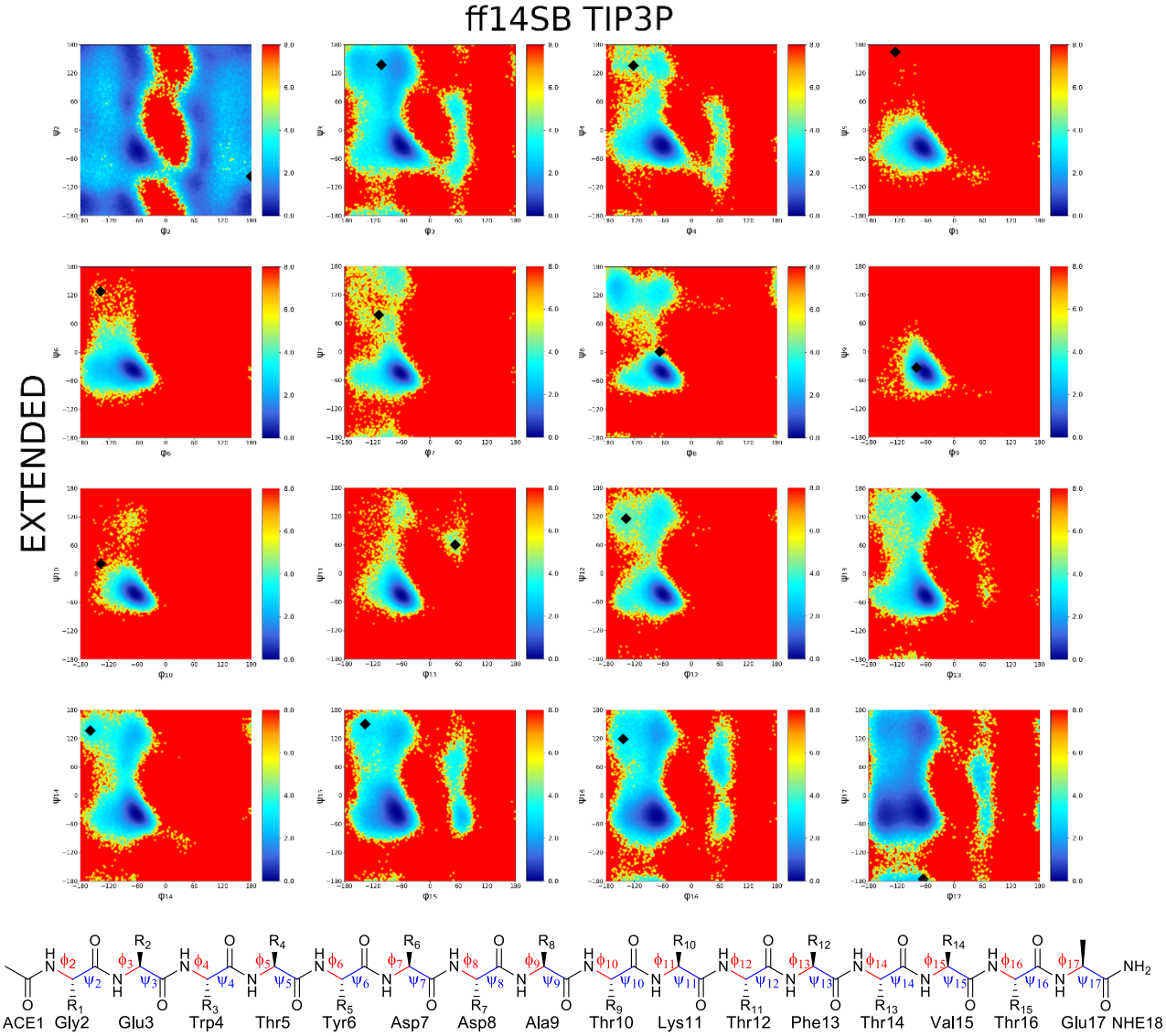

Figure S46. PMFs obtained from φ and ψ dihedral distributions of B1 residues for the ff14SB/TIP3P combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B1 sequence and representation of φ and ψ angles numbering are also shown.

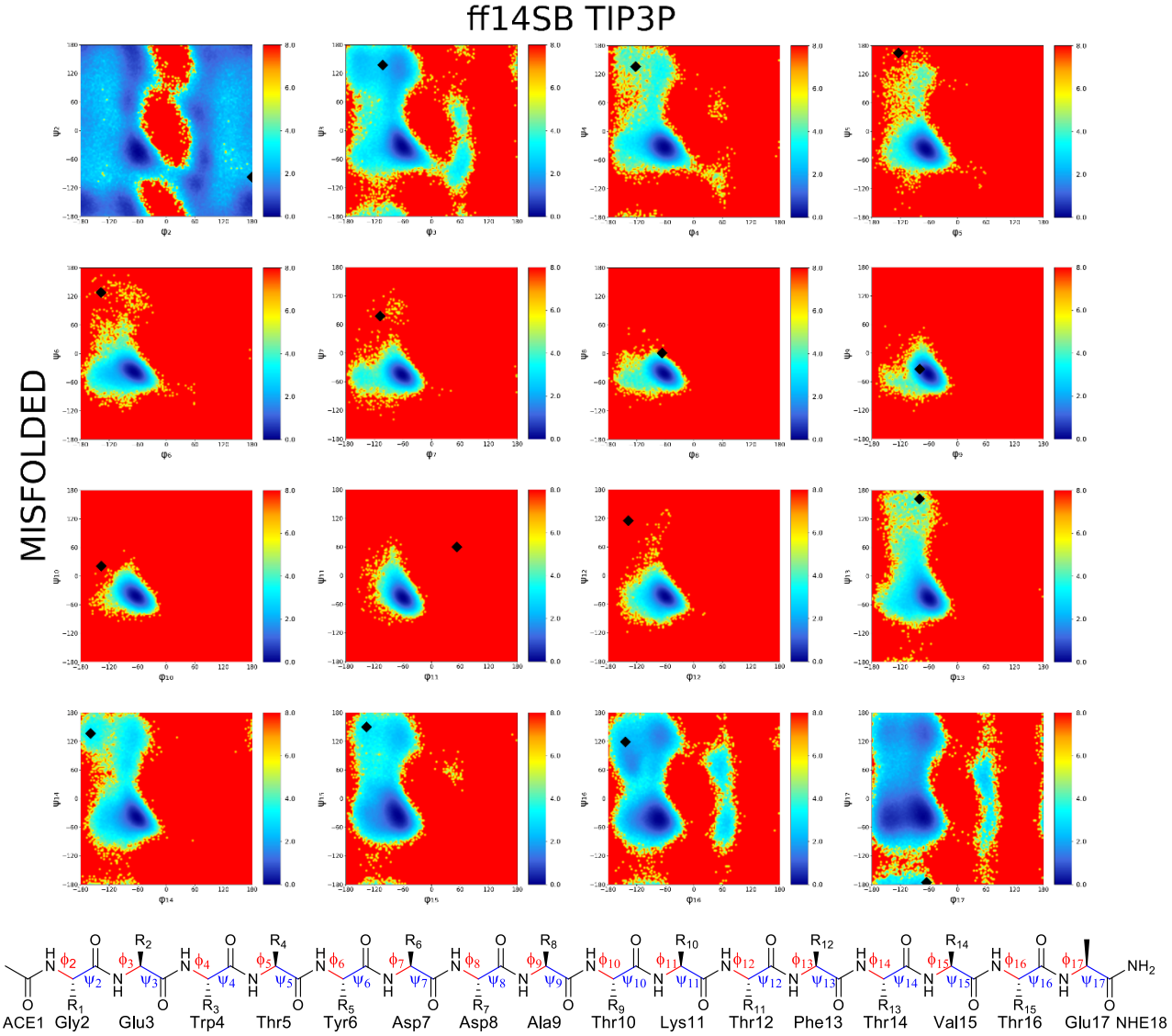

Figure S47. PMFs obtained from φ and ψ dihedral distributions of B1 residues for the ff14SB/TIP3P combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B1 sequence and representation of φ and ψ angles numbering are also shown.

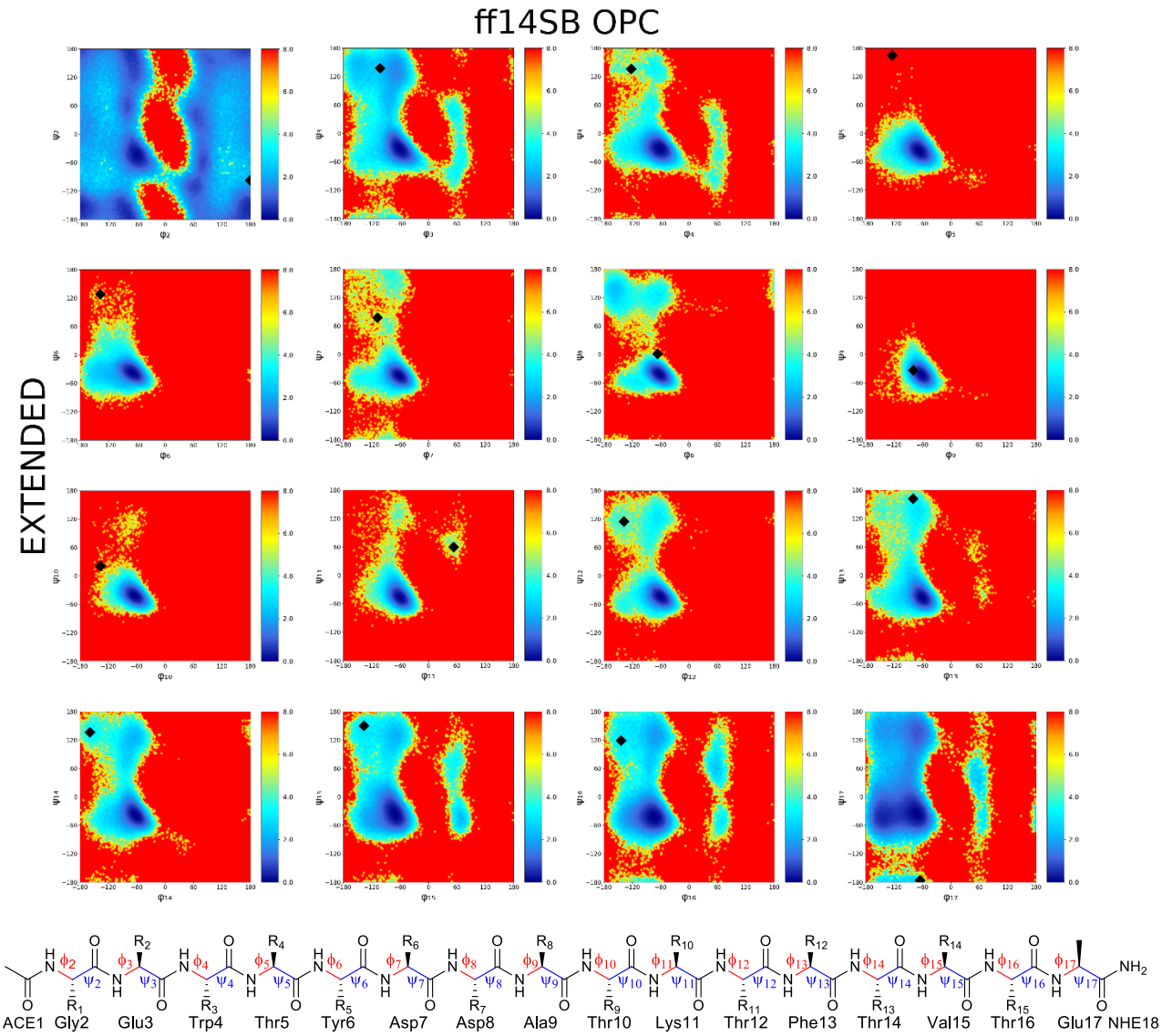

Figure S48. PMFs obtained from φ and ψ dihedral distributions of B1 residues for the ff14SB/OPC combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B1 sequence and representation of φ and ψ angles numbering are also shown.

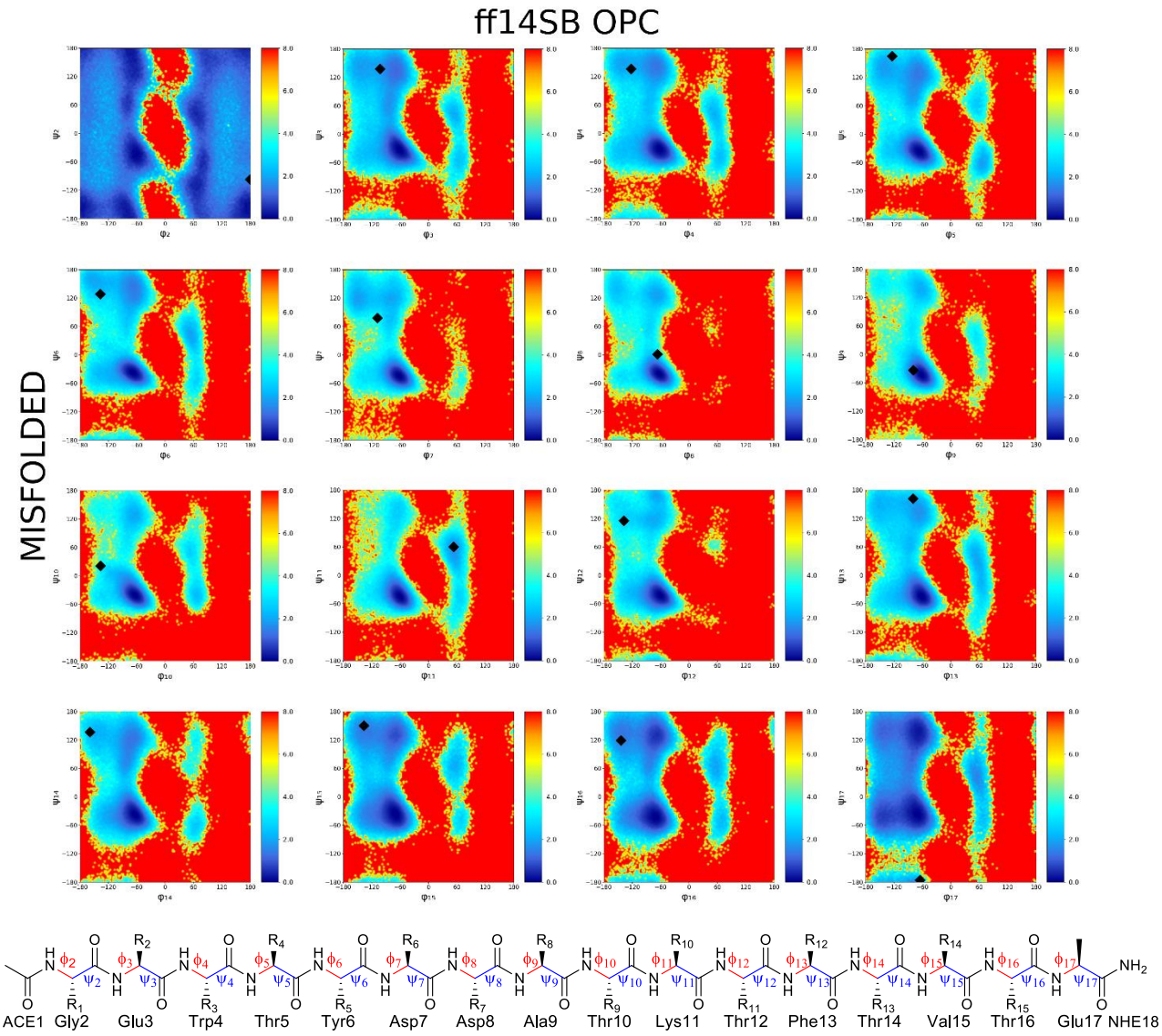

Figure S49. PMFs obtained from φ and ψ dihedral distributions of B1 residues for the ff14SB/OPC combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B1 sequence and representation of φ and ψ angles numbering are also shown.

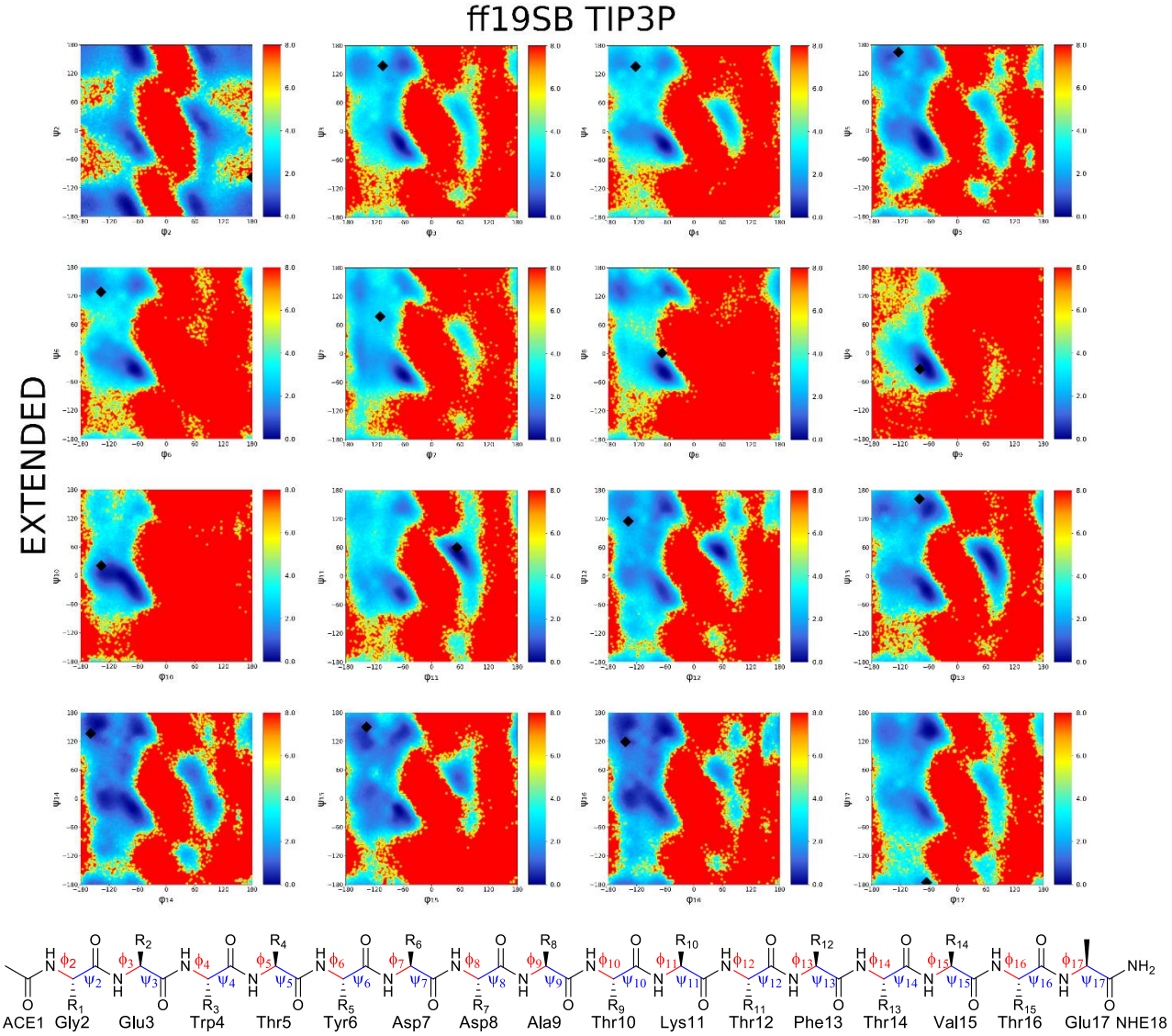

Figure S50. PMFs obtained from φ and ψ dihedral distributions of B1 residues for the ff19SB/TIP3P combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B1 sequence and representation of φ and ψ angles numbering are also shown.

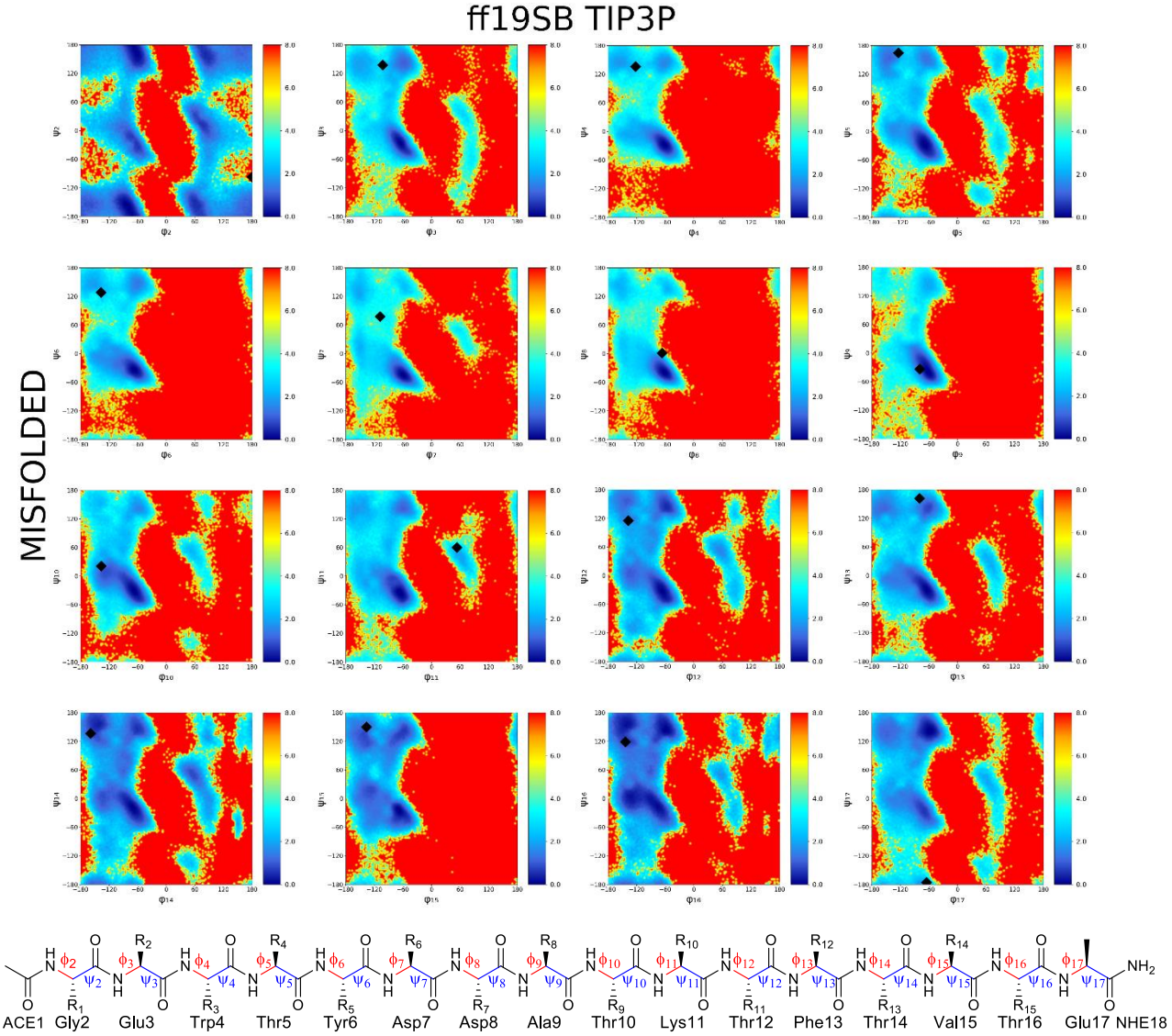

Figure S51. PMFs obtained from φ and ψ dihedral distributions of B1 residues for the ff19SB/TIP3P combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B1 sequence and representation of φ and ψ angles numbering are also shown.

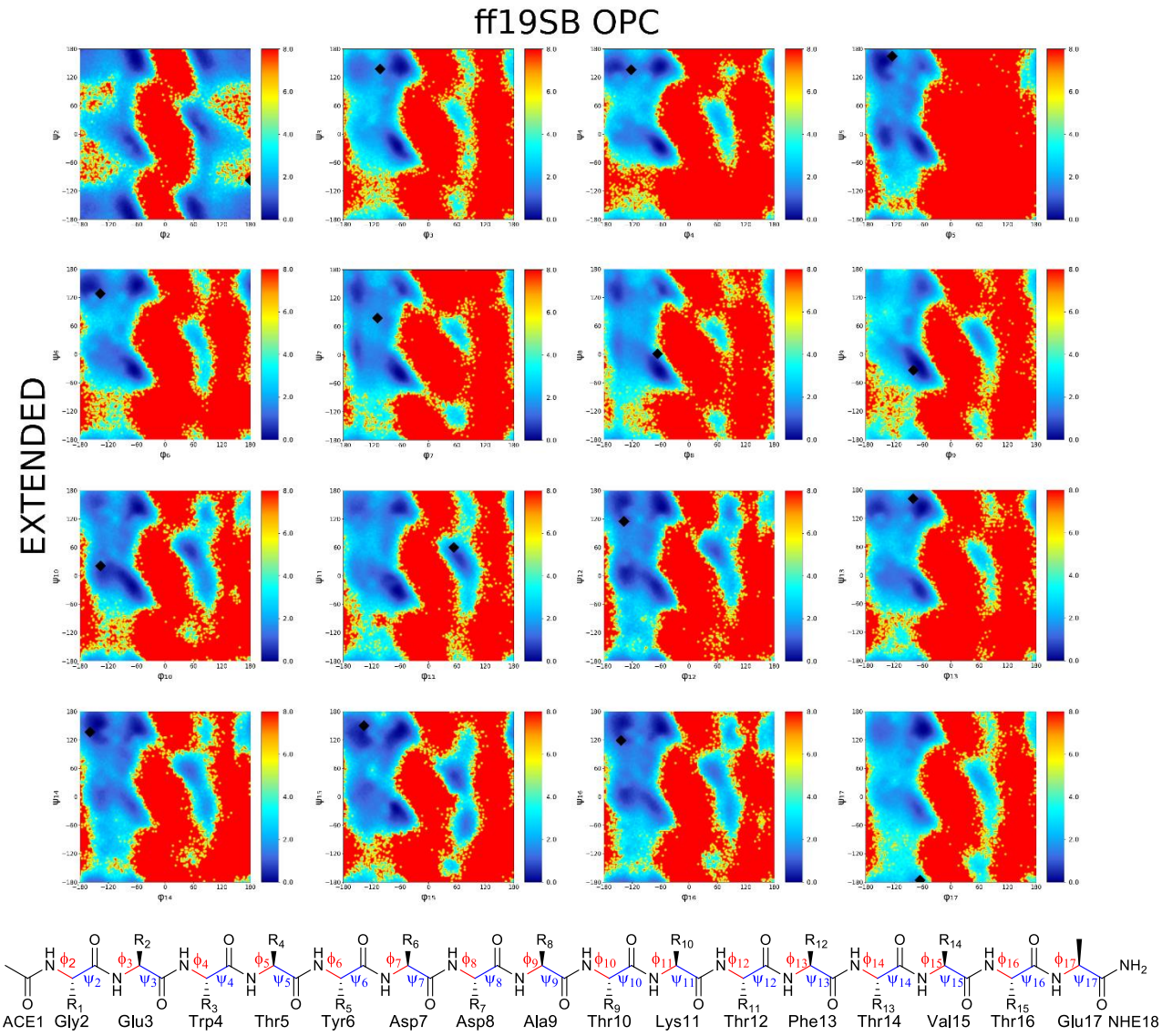

Figure S52. PMFs obtained from φ and ψ dihedral distributions of B1 residues for the ff19SB/OPC combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B1 sequence and representation of φ and ψ angles numbering are also shown.

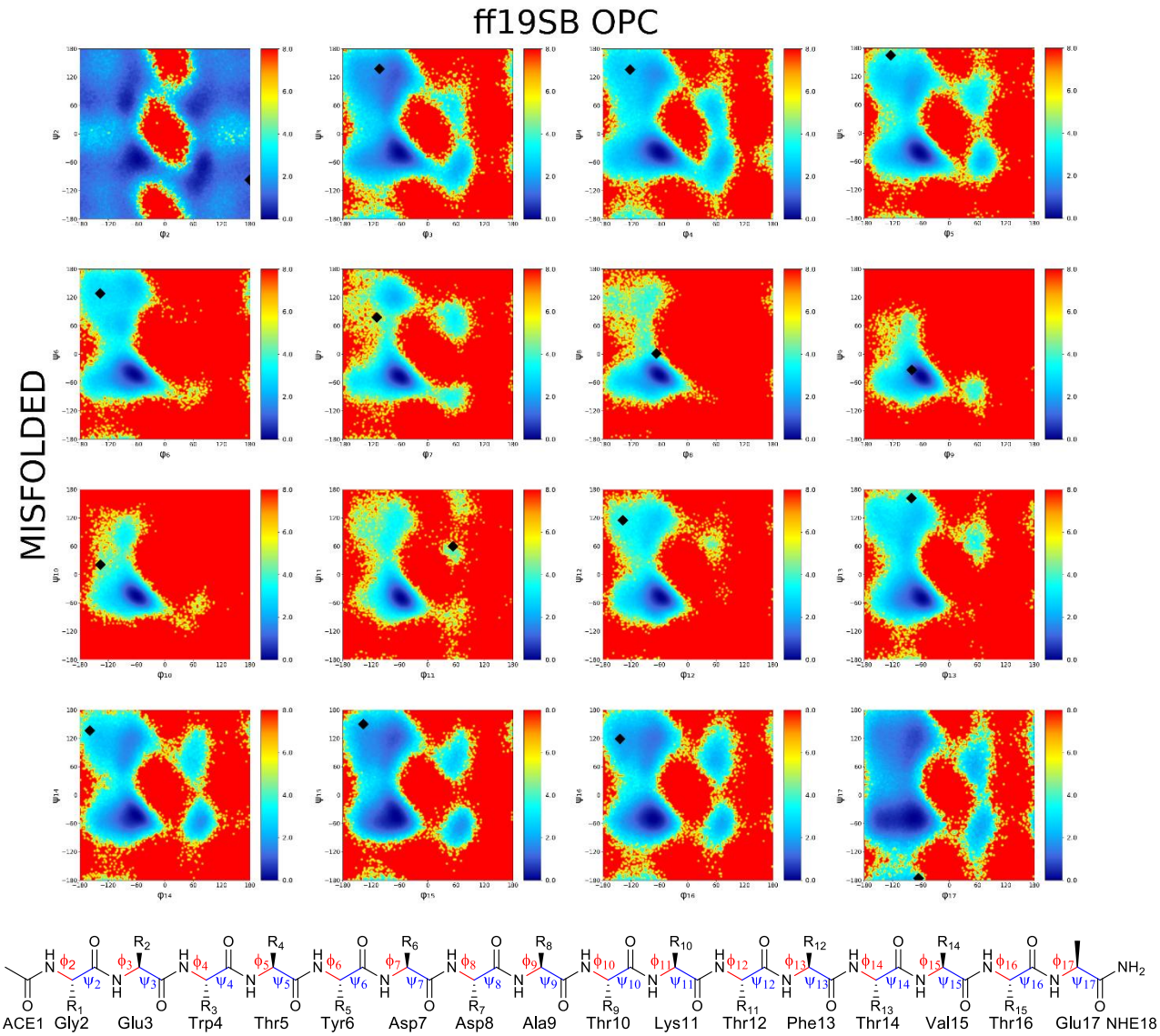

Figure S53. PMFs obtained from φ and ψ dihedral distributions of B1 residues for the ff19SB/OPC combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B1 sequence and representation of φ and ψ angles numbering are also shown.

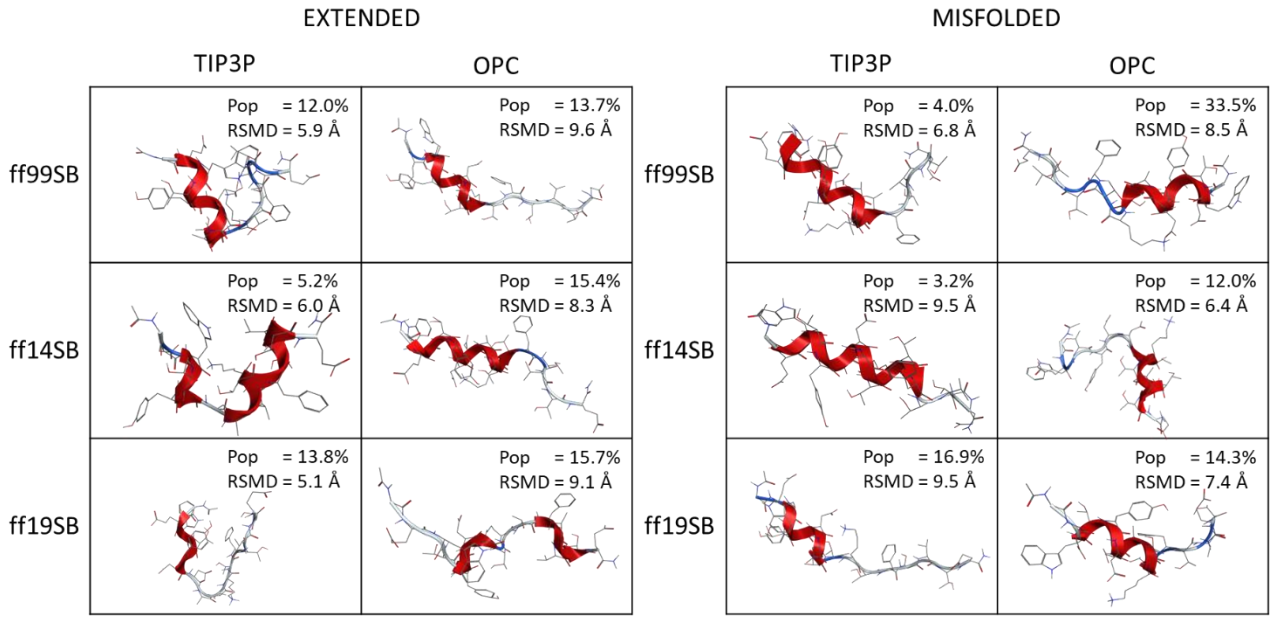

Figure S54. Representative conformation and population (pop%) of the second clusters from B1 trajectories. RMSD vs native structure are also shown.

Table S5. H-bond analyses from B1 trajectories. Only H-bonds involving the backbone are included in the table (donor N-H, acceptor C=O). Native H-bonds are highlighted in bold.

NATIVE		
acceptor	donor	Distance
ASP7	**ALA9**	**2.78**
ASP7	**LYS11**	**2.98**
GLU3	**THR16**	**3.06**
THR12	**ASP7**	**3.08**
ASP7	**THR10**	**3.18**
ASP7	**THR12**	**3.22**
THR5	**THR14**	**3.33**
THR16	**GLU3**	**3.37**
THR10	**THR12**	**3.38**
TYR6	**ASP8**	**3.59**
ASP8	**THR10**	**3.68**
THR12	**THR14**	**3.95**
GLY2	**TRP4**	**4.04**
ASP8	**LYS11**	**4.29**
ALA9	**LYS11**	**4.32**
GLU3	**THR5**	**4.35**
LYS11	**PHE13**	**4.46**

ff99SB OPC						ff99SB TIP3P					
EXTENDED			MISFOLDED			EXTENDED			MISFOLDED		
acceptor	donor	occ%	acceptor	donor	occ%	acceptor	donor	occ%	acceptor	donor	occ%
ASP8	THR12	23.70	ALA9	PHE13	24.34	**ASP7**	**LYS11**	43.99	**ASP7**	**LYS11**	48.48

TYR6	THR10	21.02
ASP7	**LYS11**	20.94
ALA9	PHE13	18.57
THR5	ALA9	13.73
THR10	THR14	10.03
GLU3	ASP7	9.80
TRP4	ASP8	8.05
PHE13	GLU17	6.38
LYS11	VAL15	6.28
ALA9	THR14	5.52
GLU3	TYR6	5.51
ASP8	**LYS11**	5.31
GLY2	THR5	5.04

TYR6	THR10	22.35
ASP8	THR12	21.02
ASP7	**LYS11**	19.94
TRP4	ASP8	13.16
THR5	ALA9	12.28
THR10	THR14	12.16
GLU3	ASP7	10.75
LYS11	VAL15	9.02
PHE13	GLU17	8.40
GLY2	THR5	7.70
GLY2	TYR6	5.49
ALA9	THR12	5.23

TYR6	THR10	34.59
ASP8	THR12	33.73
ALA9	PHE13	32.19
GLU3	ASP7	27.93
TRP4	ASP8	25.80
THR5	ALA9	24.74
THR10	THR14	18.67
PHE13	GLU17	17.70
LYS11	VAL15	15.99
GLY2	TYR6	14.25
GLY2	THR5	12.01
ASP7	**THR12**	8.92
GLU3	TYR6	8.41
THR12	THR16	6.61

ALA9	PHE13	46.09
ASP8	THR12	45.21
TYR6	THR10	45.01
GLU3	ASP7	31.71
TRP4	ASP8	31.07
THR5	ALA9	30.43
THR10	THR14	29.85
LYS11	VAL15	24.85
PHE13	GLU17	24.25
GLY2	THR5	12.05
GLY2	TYR6	11.81
GLU3	TYR6	10.96
THR12	THR16	10.90
THR12	GLU17	5.61
PHE13	THR16	5.08

ff14SB OPC

EXTENDED

acceptor	donor	occ%
ASP7	**LYS11**	50.91
ALA9	PHE13	48.16
TYR6	THR10	46.74
ASP8	THR12	46.41
THR5	ALA9	33.42
THR10	THR14	33.24
TRP4	ASP8	28.98
GLU3	ASP7	26.93
LYS11	VAL15	24.34
PHE13	GLU17	23.66
GLY2	THR5	20.68
THR12	THR16	14.24
GLY2	TYR6	11.73
GLU3	TYR6	7.91

MISFOLDED

acceptor	donor	occ%
ALA9	PHE13	36.34
ASP7	**LYS11**	35.76
ASP8	THR12	33.62
TYR6	THR10	32.01
THR10	THR14	25.41
THR5	ALA9	21.26
LYS11	VAL15	20.82
PHE13	GLU17	18.83
TRP4	ASP8	18.30
GLU3	ASP7	17.30
THR12	THR16	11.90
GLY2	THR5	10.97
GLY2	TYR6	9.29
GLU3	TYR6	5.30

ff14SB TIP3P

EXTENDED

acceptor	donor	occ%
ASP7	**LYS11**	54.92
ALA9	PHE13	54.72
ASP8	THR12	54.03
TYR6	THR10	46.93
PHE13	GLU17	43.61
THR10	THR14	41.88
LYS11	VAL15	36.09
THR5	ALA9	34.81
TRP4	ASP8	34.22
GLU3	ASP7	32.97
THR12	THR16	22.82
GLY2	THR5	17.65
GLY2	TYR6	14.09
GLU3	TYR6	9.99
PHE13	THR16	5.75

MISFOLDED

acceptor	donor	occ%
ASP7	**LYS11**	58.56
ALA9	PHE13	57.31
ASP8	THR12	55.66
TYR6	THR10	51.25
THR10	THR14	41.59
PHE13	GLU17	39.88
THR5	ALA9	38.29
LYS11	VAL15	37.43
TRP4	ASP8	35.49
GLU3	ASP7	34.04
THR12	THR16	22.97
GLY2	TYR6	16.03
GLY2	THR5	16.00
GLU3	TYR6	8.67
ACE1	THR5	5.71
PHE13	THR16	5.66

ff19SB OPC

EXTENDED

acceptor	donor	occ%
GLY2	THR5	6.51
ASP7	**THR10**	5.01

MISFOLDED

acceptor	donor	occ%
ALA9	PHE13	47.92
ASP7	**LYS11**	46.64
ASP8	THR12	45.65
TYR6	THR10	41.59
THR10	THR14	35.62
LYS11	VAL15	28.43
THR5	ALA9	27.90
TRP4	ASP8	26.64
GLU3	ASP7	23.23

ff19SB TIP3P

EXTENDED

acceptor	donor	occ%
GLY2	THR5	15.31
TYR6	THR10	15.07
THR5	ALA9	14.54
ASP7	**LYS11**	14.16
ASP7	**THR12**	12.26
ASP8	LYS11	12.23
GLU3	ASP7	11.55
ASP8	**THR12**	11.12
THR10	THR14	10.58

MISFOLDED

acceptor	donor	occ%
ASP7	**LYS11**	25.16
TYR6	THR10	24.81
GLY2	THR5	19.04
THR5	ALA9	18.78
ASP8	THR12	18.51
GLU3	ASP7	16.70
ALA9	PHE13	15.98
TRP4	ASP8	15.57
GLU3	TYR6	10.86

PHE13	GLU17	21.77
THR12	THR16	13.94
GLY2	TYR6	11.76
THR12	GLU17	10.28
GLU3	TYR6	7.11
GLY2	THR5	6.56
THR10	VAL15	5.76
TYR6	LYS11	5.57

TRP4	ASP8	9.63
GLU3	TYR6	7.71
ALA9	PHE13	5.96

ASP7	**THR10**	7.58
THR10	THR14	6.48

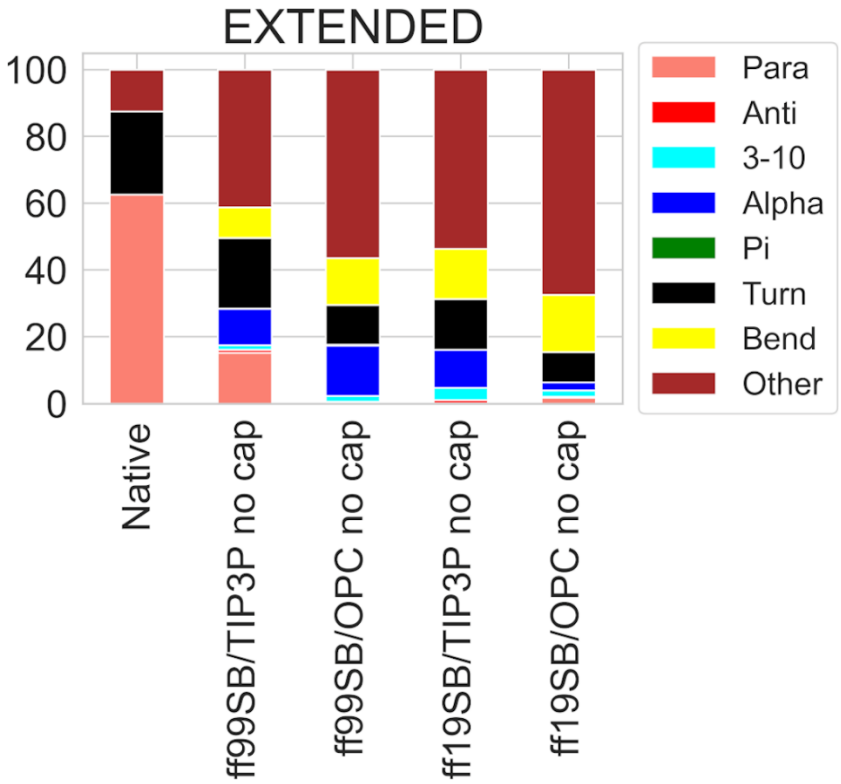

Figure S55. DSSP analysis of B1 uncapped trajectories from extended conformation. Data are reported as percentage of the distributions of all the residues considering the last 500 ns frames.

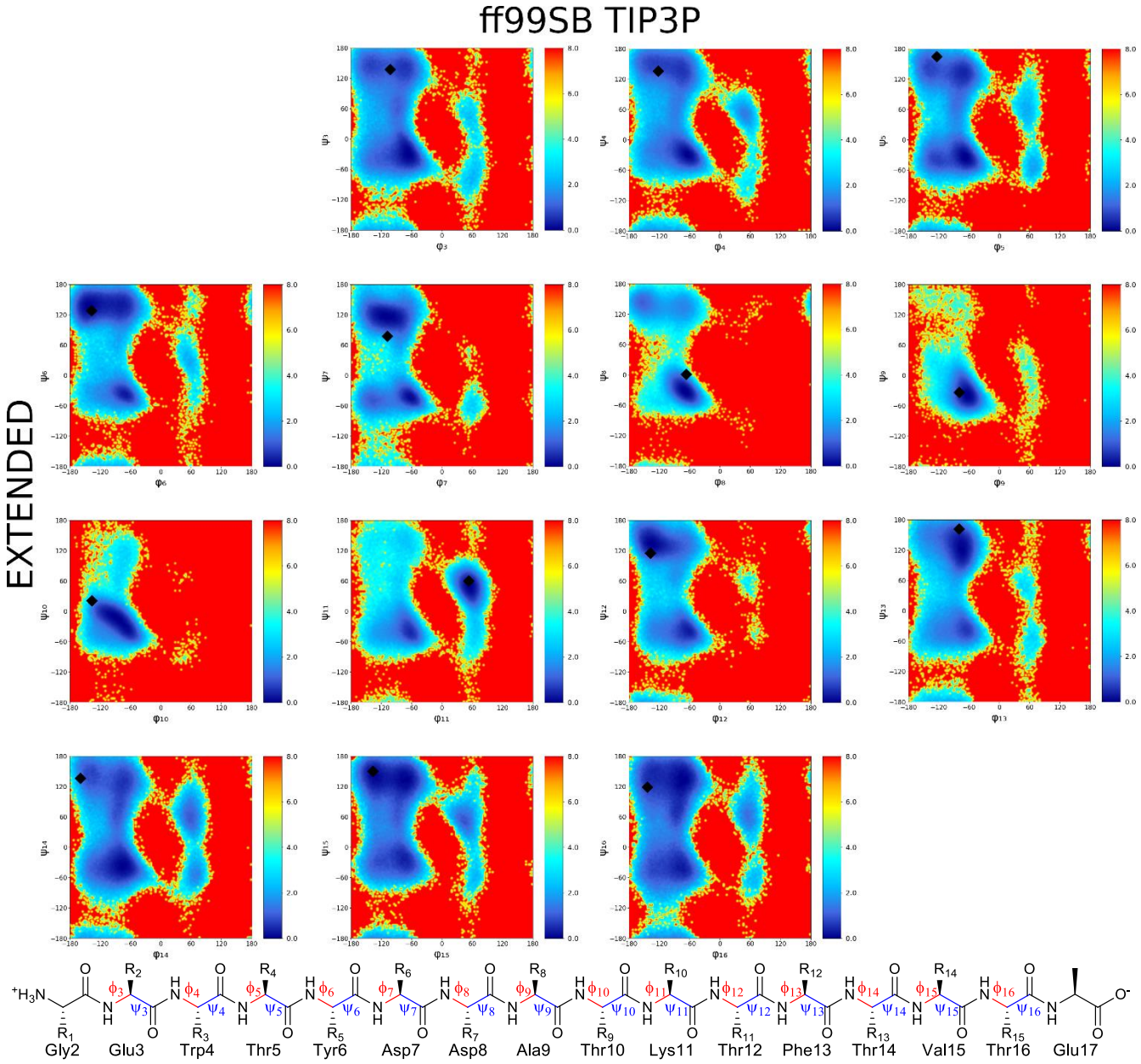

Figure S56. PMFs obtained from φ and ψ dihedral distributions of B1 uncapped residues for the ff99SB/TIP3P combination from extended (top panel) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B1 uncapped sequence and representation of φ and ψ angles numbering are also shown.

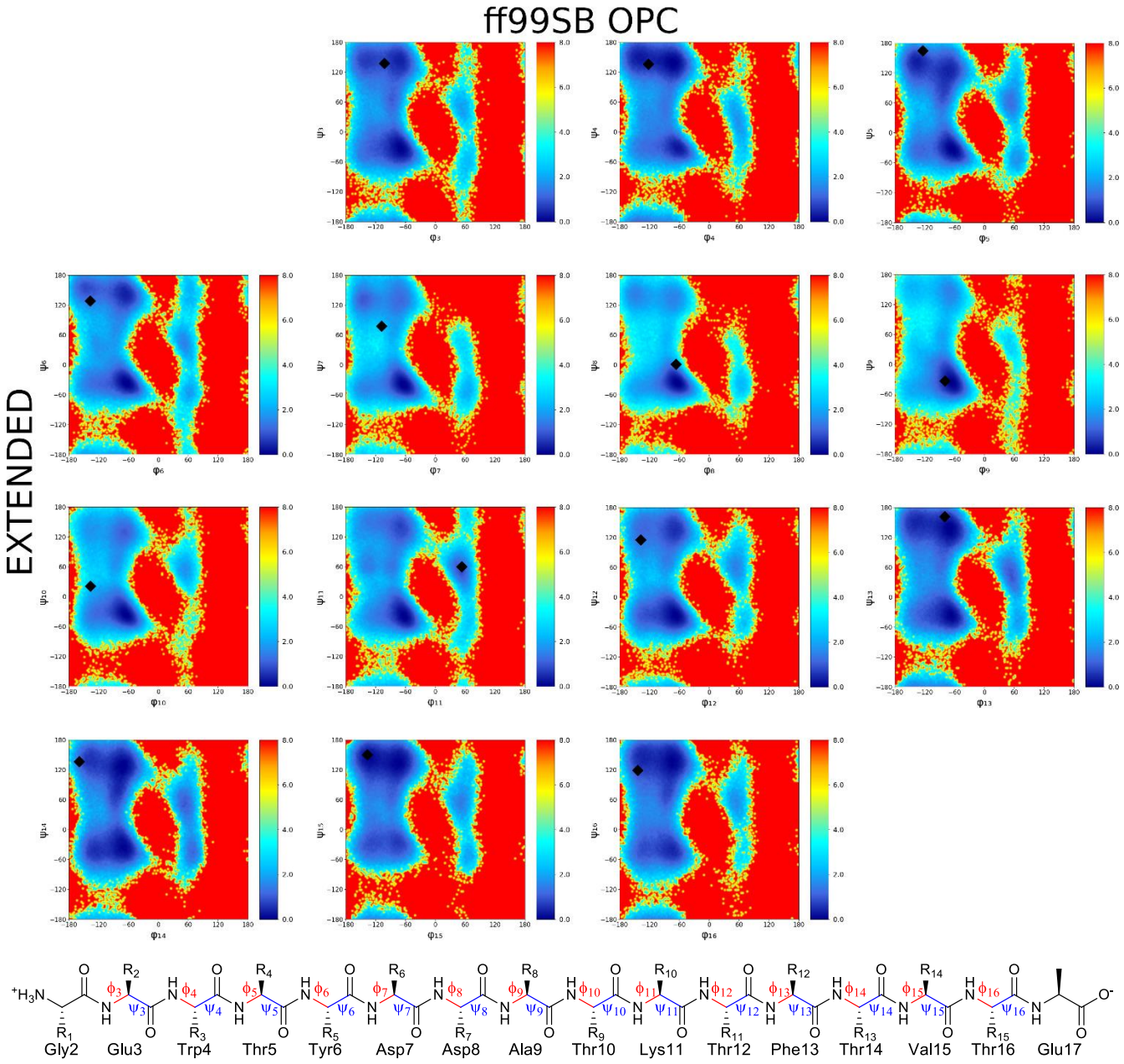

Figure S57. PMFs obtained from φ and ψ dihedral distributions of B1 uncapped residues for the ff99SB/OPC combination from extended (top panel) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B1 uncapped sequence and representation of φ and ψ angles numbering are also shown.

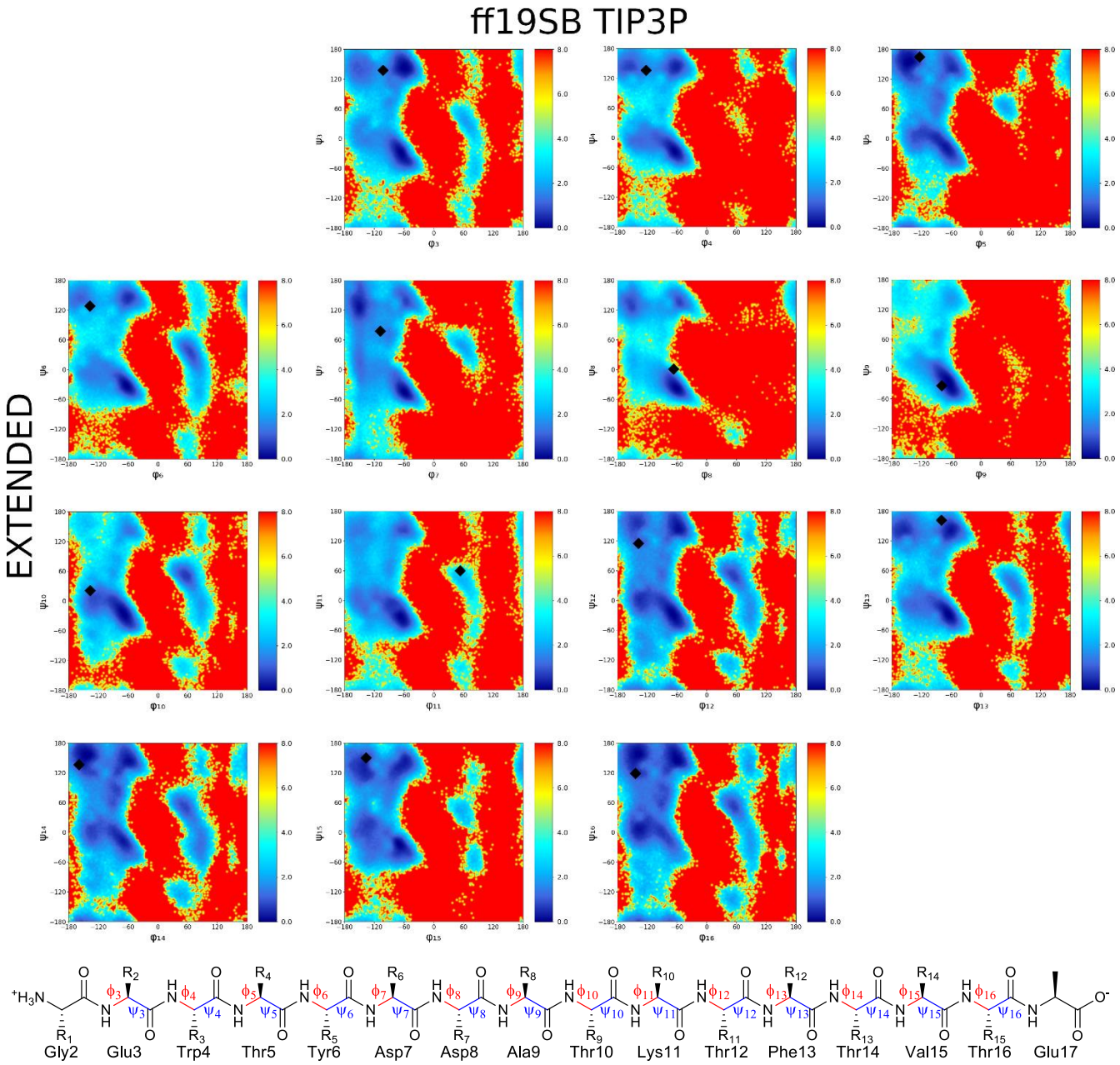

Figure S58. PMFs obtained from φ and ψ dihedral distributions of B1 uncapped residues for the ff99SB/TIP3P combination from extended (top panel) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B1 uncapped sequence and representation of φ and ψ angles numbering are also shown.

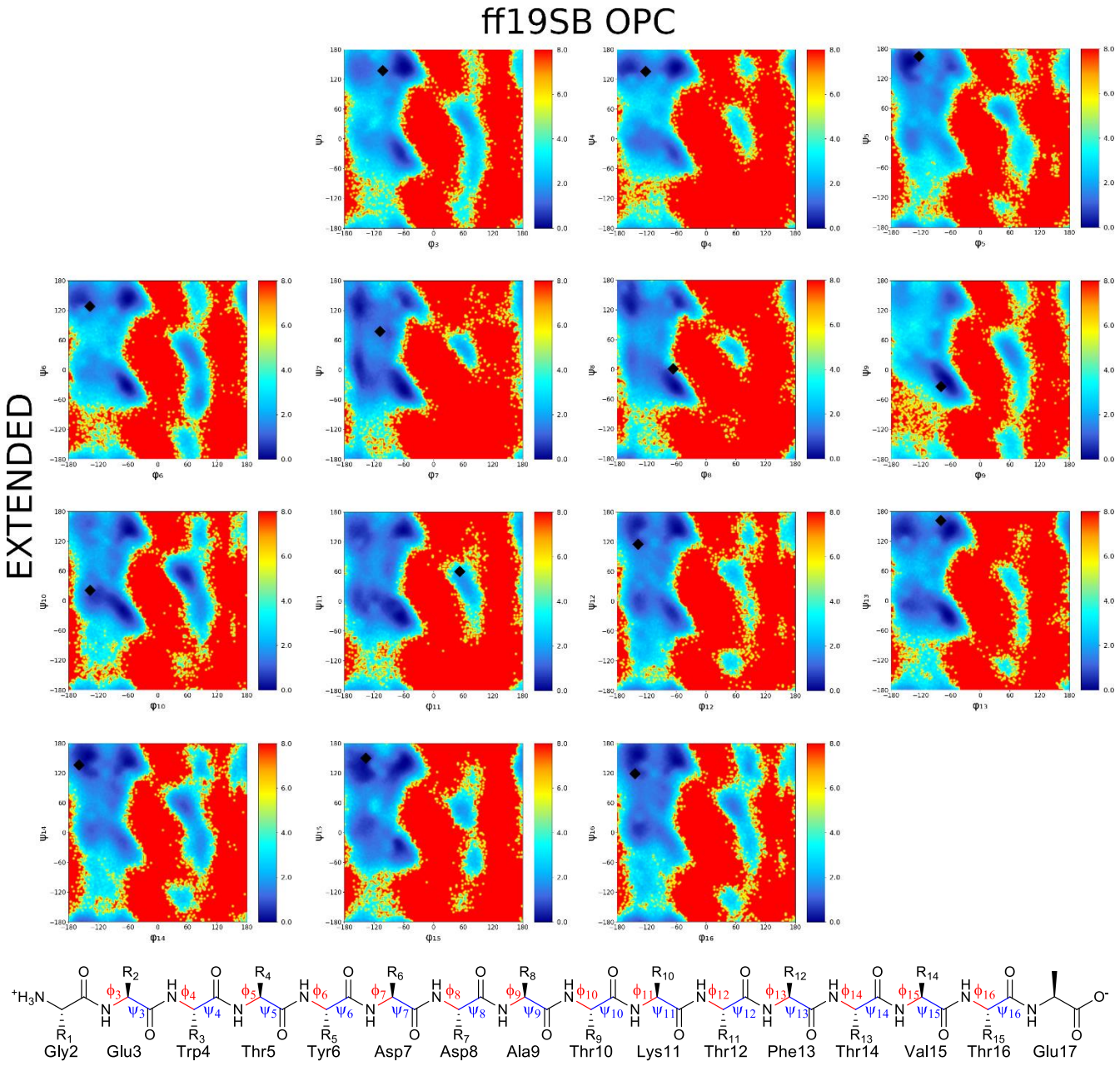

Figure S59. PMFs obtained from φ and ψ dihedral distributions of B1 uncapped residues for the ff19SB/OPC combination from extended (top panel) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B1 uncapped sequence and representation of φ and ψ angles numbering are also shown.

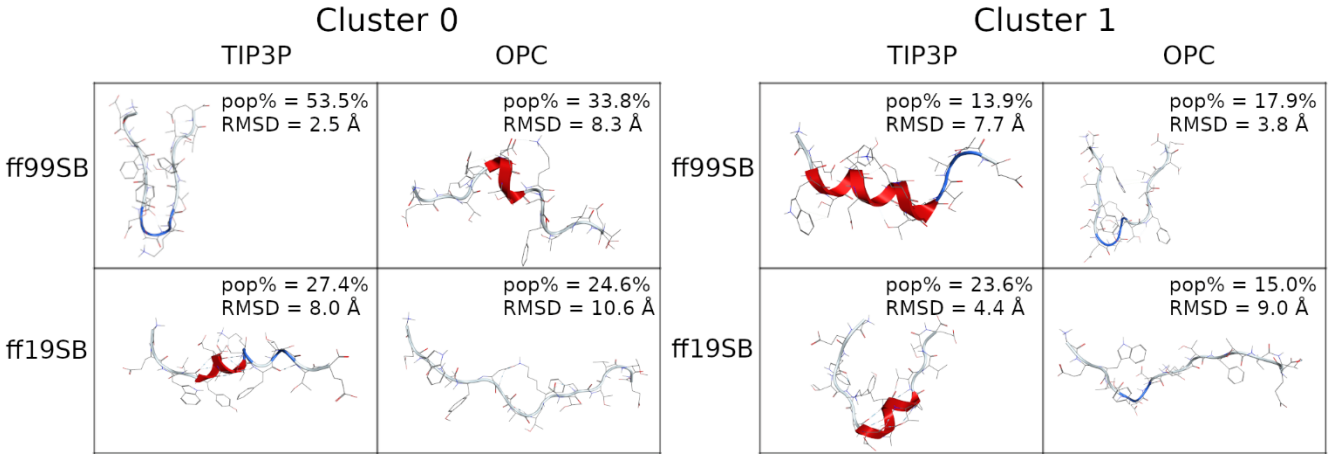

Figure S60. Representative conformation of the main and second clusters from B1 uncapped trajectories. Population (pop%) and RMSD vs native structure are also shown in the figure.

Table S6. H-bond analyses from B1 uncapped trajectories. Only H-bonds involving the backbone are included in the table (donor N-H, acceptor C=O). Native H-bonds are highlighted in bold.

ff99SB OPC		
EXTENDED		
acceptor	donor	occ%
ASP7	**LYS11**	15.63
TYR6	THR10	13.4
ASP8	THR12	11.24
ALA9	PHE13	11.05
THR5	ALA9	7.97
THR10	THR14	5.29
TRP4	ASP8	5

ff99SB TIP3P		
EXTENDED		
acceptor	donor	occ%
THR12	**ASP7**	33.31
THR5	**THR14**	25.12
ASP7	**THR12**	17.09
ASP7	**LYS11**	15.83
ASP8	THR12	12.2
ALA9	PHE13	10.78
ASP8	**LYS11**	8.42
TYR6	THR10	6.36
THR14	THR5	5.64
THR10	THR14	5.33
TRP4	ASP8	5

ff19SB OPC		
EXTENDED		
acceptor	donor	occ%
ASP8	**LYS11**	5

ff19SB TIP3P		
EXTENDED		
acceptor	donor	occ%
ASP7	**LYS11**	13.68
ASP8	THR12	12.69
ALA9	PHE13	8.22
ASP8	**LYS11**	7.85
TYR6	THR10	7.18
ASP7	**THR10**	6.5
THR5	ALA9	5.45

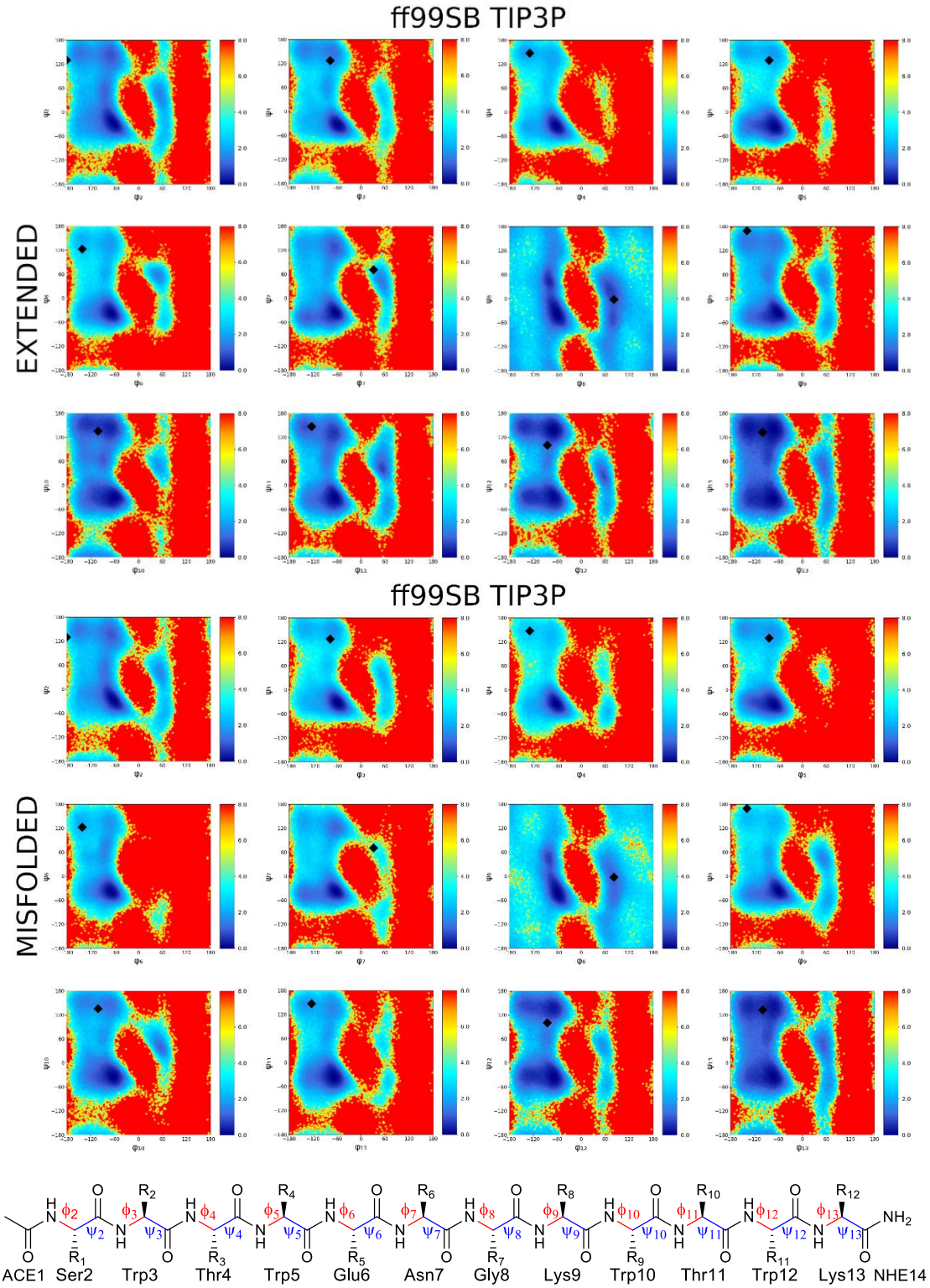

Figure S61. PMFs obtained from φ and ψ dihedral distributions of B2 residues for the ff99SB/TIP3P combination from extended (top panel) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B2 sequence and representation of φ and ψ angles numbering are also shown.

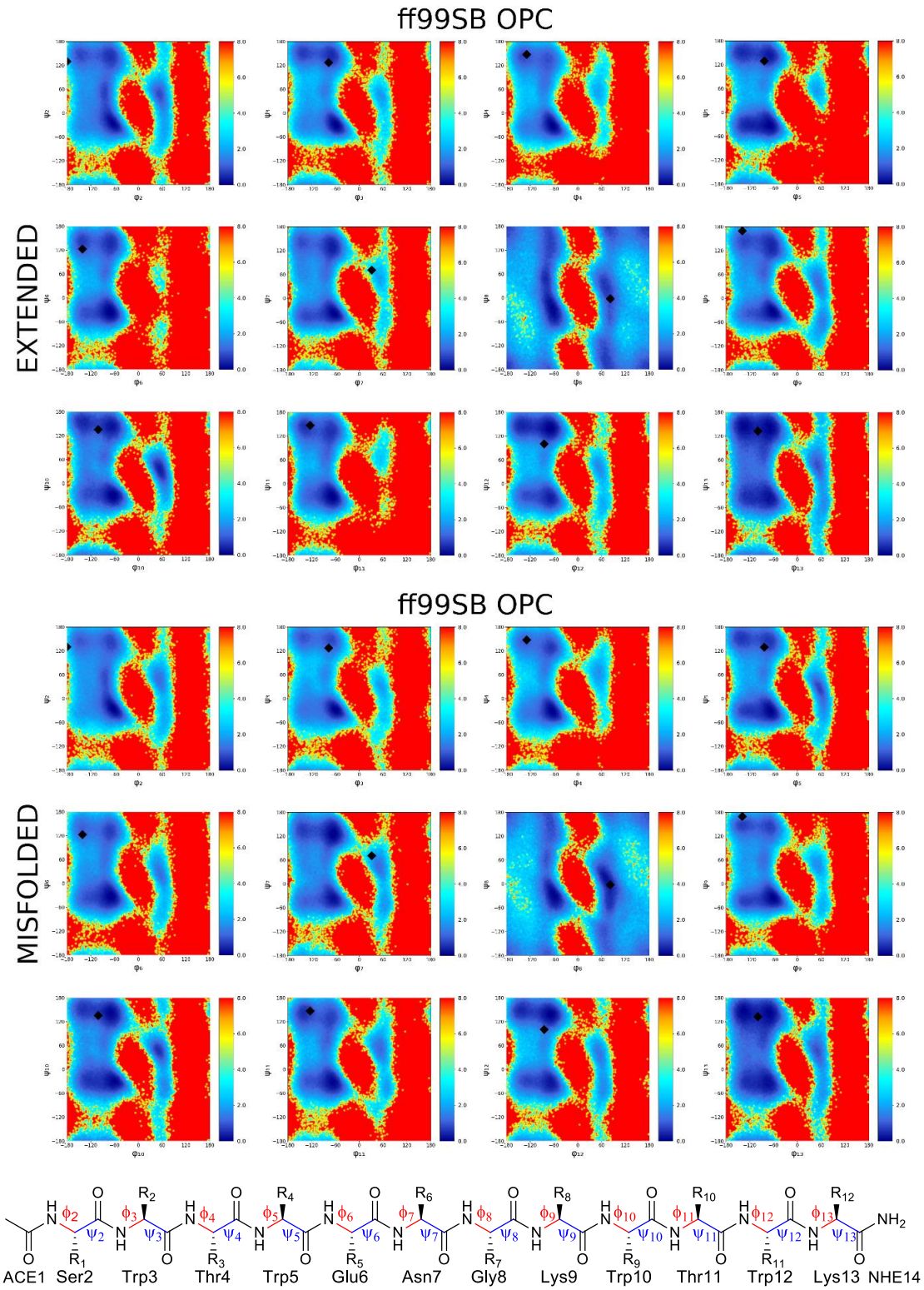

Figure S62. PMFs obtained from φ and ψ dihedral distributions of B2 residues for the ff99SB/OPC combination from extended (top panel) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B2 sequence and representation of φ and ψ angles numbering are also shown.

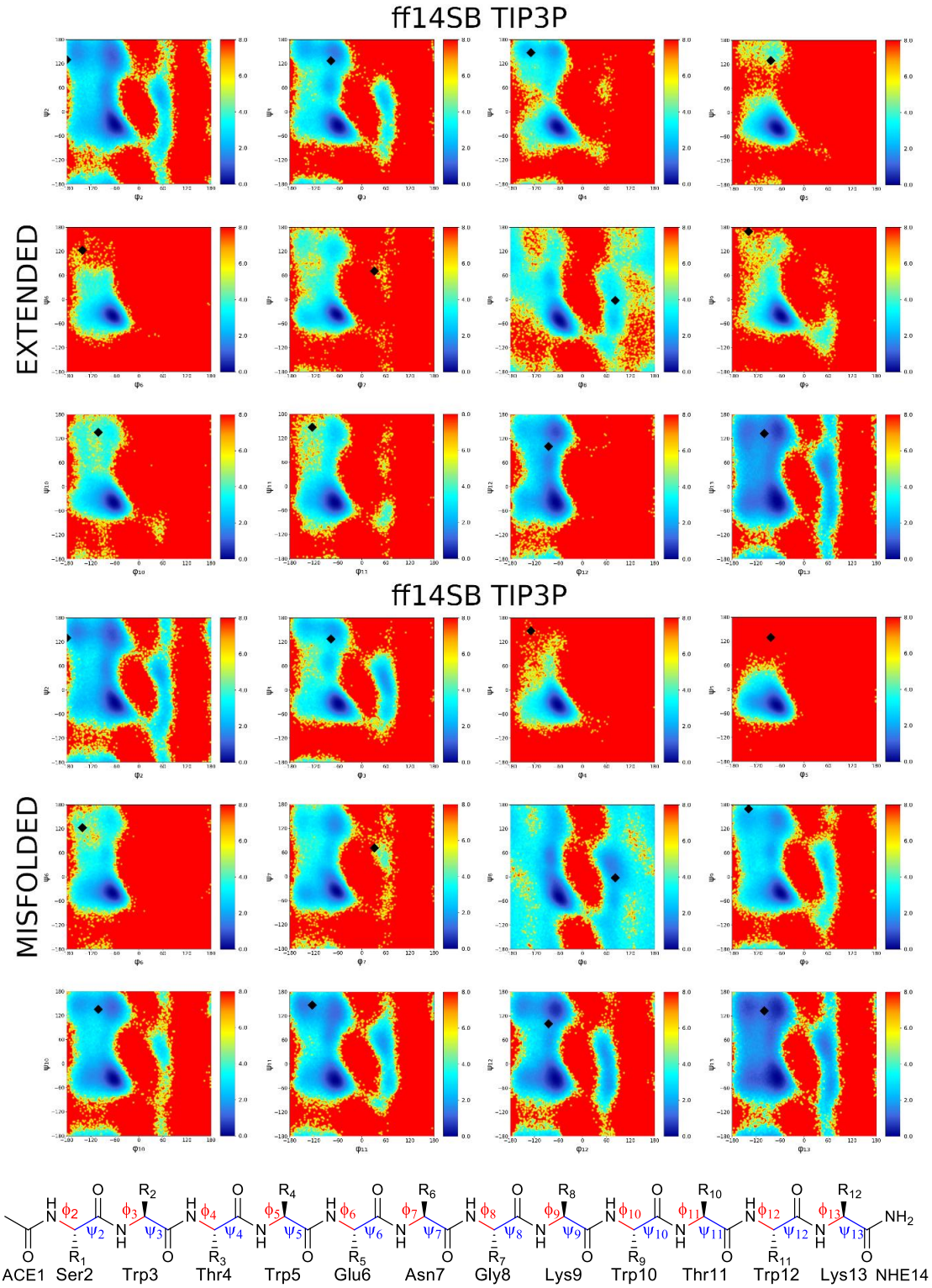

Figure S63. PMFs obtained from φ and ψ dihedral distributions of B2 residues for the ff14SB/TIP3P combination from extended (top panel) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B2 sequence and representation of φ and ψ angles numbering are also shown.

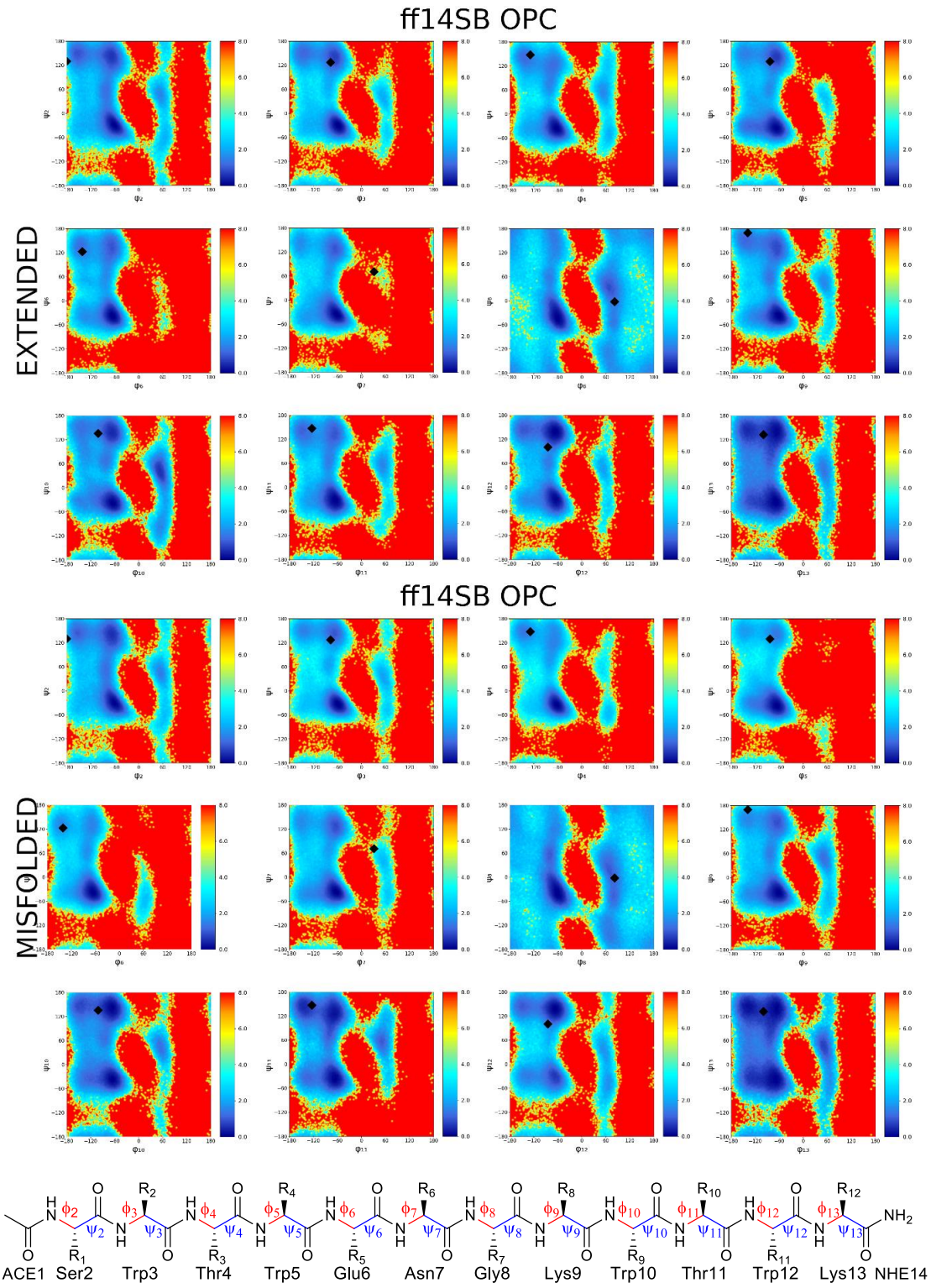

Figure S64. PMFs obtained from φ and ψ dihedral distributions of B2 residues for the ff14SB/OPC combination from extended (top panel) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B2 sequence and representation of φ and ψ angles numbering are also shown.

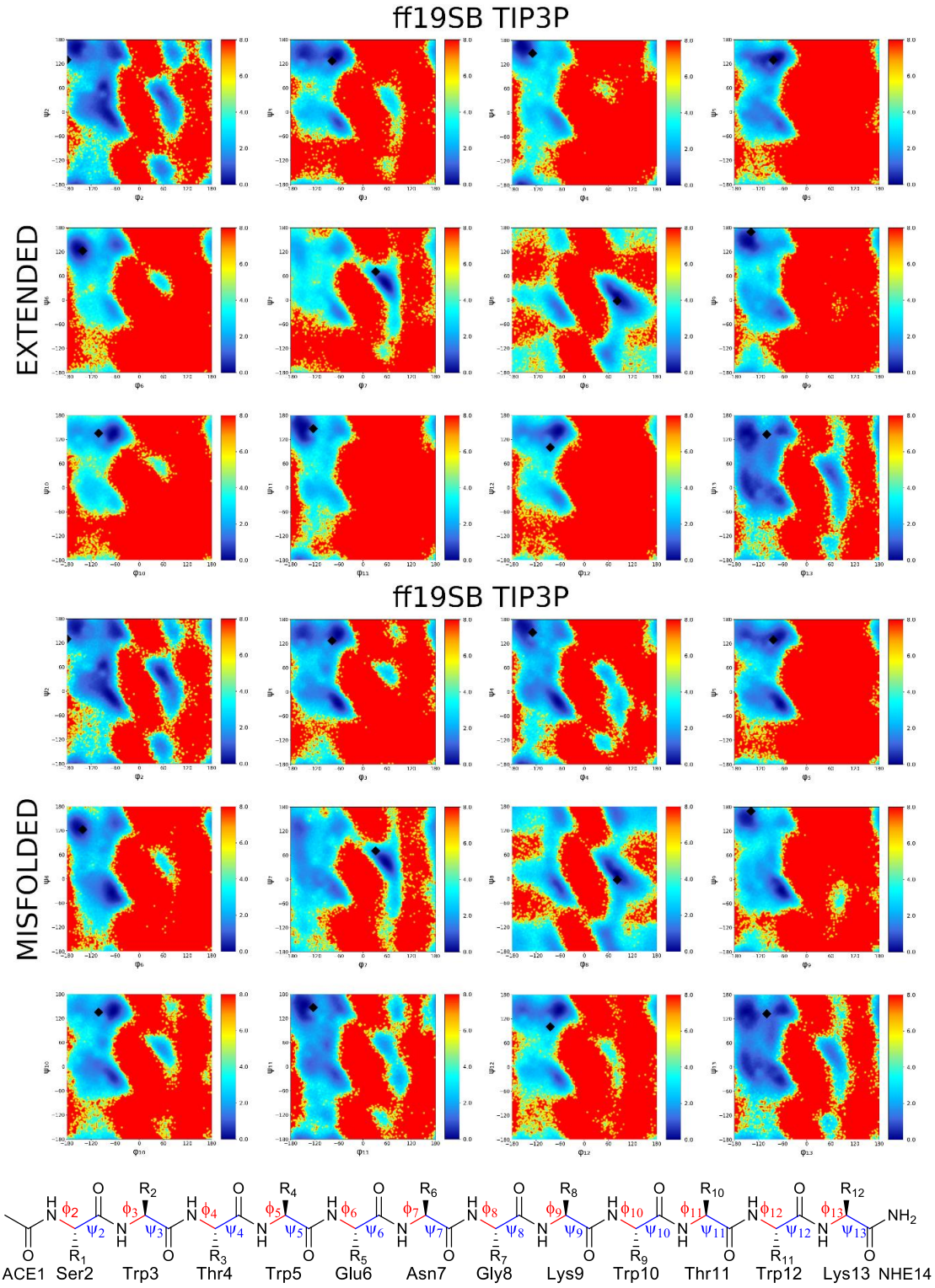

Figure S65. PMFs obtained from φ and ψ dihedral distributions of B2 residues for the ff19SB/TIP3P combination from extended (top panel) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds.

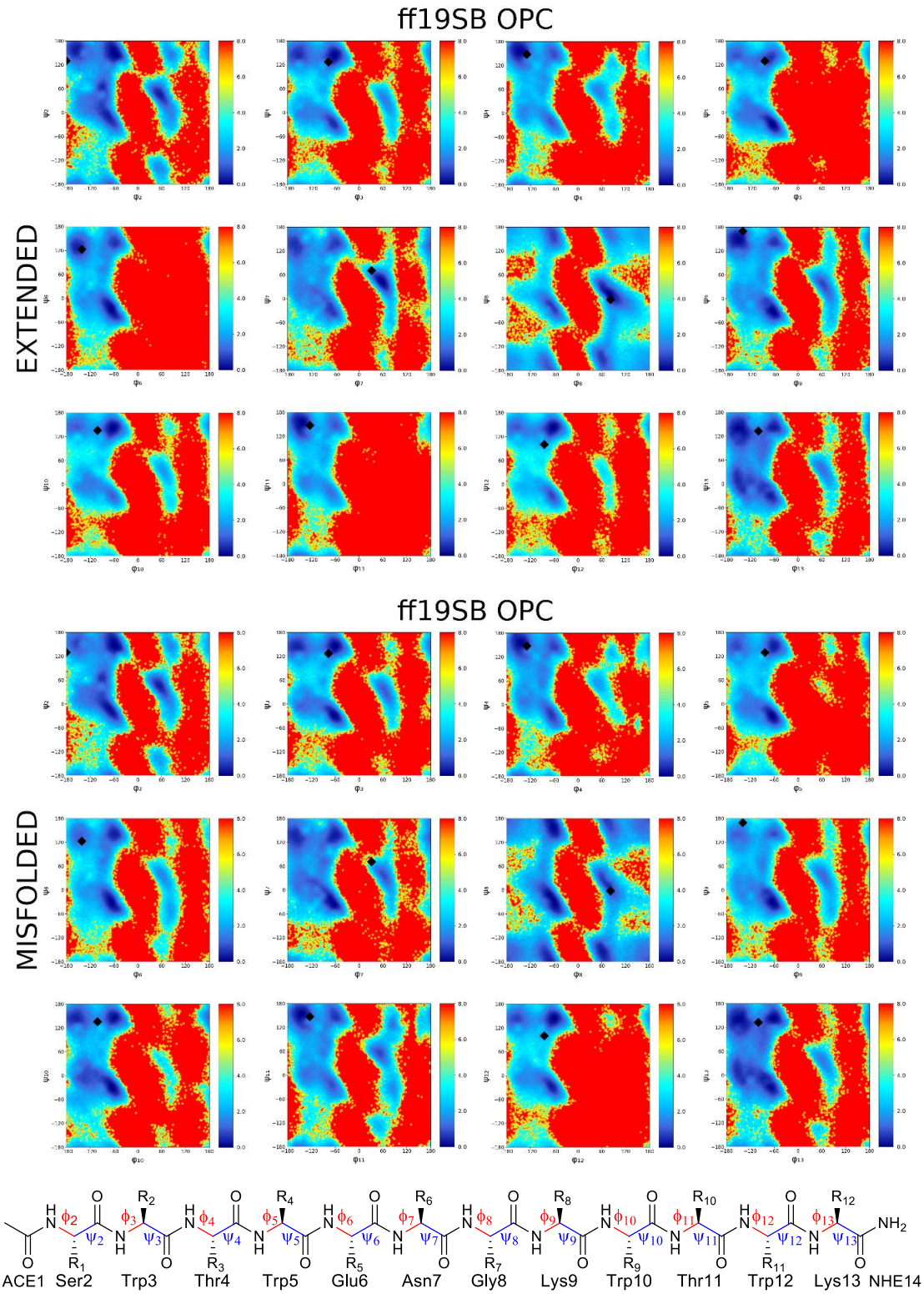

Figure S66. PMFs obtained from φ and ψ dihedral distributions of B2 residues for the ff19SB/OPC combination from extended (top panel) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B2 sequence and representation of φ and ψ angles numbering are also shown.

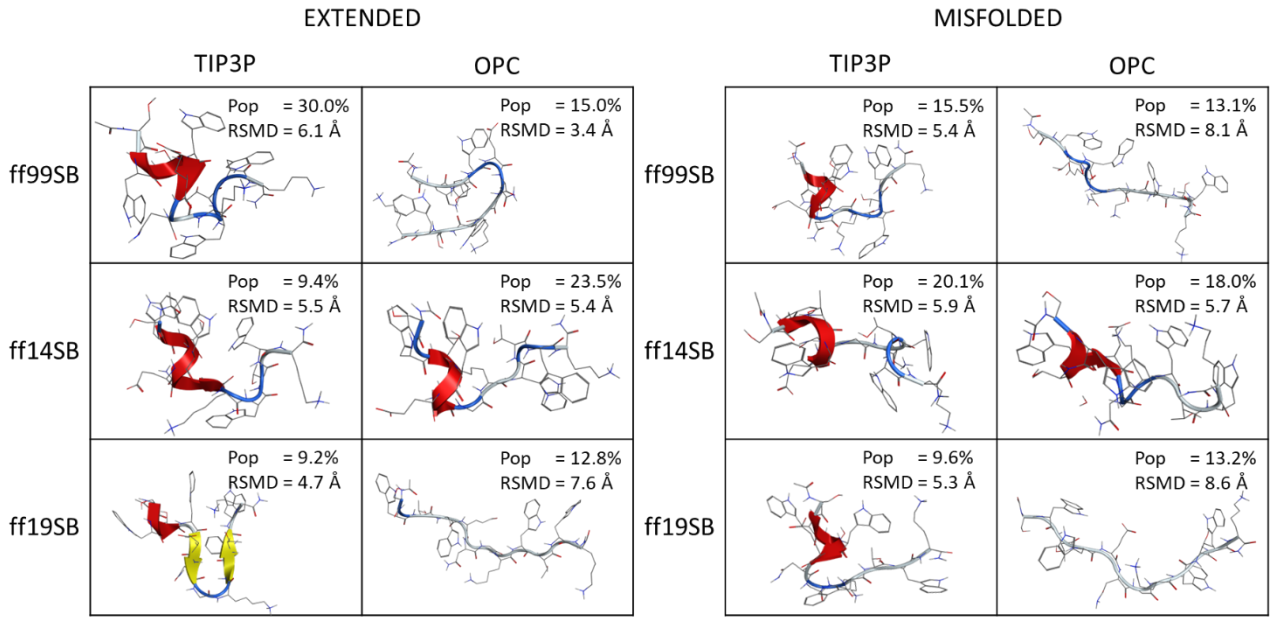

Figure S67. Representative conformation of the second cluster from B2 trajectories. Population (pop%) and RMSD vs native structure are also shown in the figure.

Table S7. H-bond analyses from B2 trajectories. Only H-bonds involving the backbone are included in the table (donor N-H, acceptor C=O). Native H-bonds are highlighted in bold.

NATIVE		
donor	acceptor	Distance
SER2	**LYS13**	**2.74**
LYS9	**GLU6**	**2.84**
THR4	**THR11**	**2.9**
GLU6	**LYS9**	**2.92**
LYS13	**SER2**	**2.96**
THR11	**THR4**	**2.99**
GLU6	**GLY8**	**3.31**
THR11	**LYS13**	**3.37**
ASN7	**LYS9**	**3.47**
SER2	**THR4**	**3.62**
THR4	**GLU6**	**3.78**
TRP12	**NME**	**4.15**
LYS9	**THR11**	**4.21**
THR11	**TRP3**	**4.47**
SER2	**TRP12**	**4.47**
LYS9	**TRP5**	**4.49**

ff99SB OPC						ff99SB TIP3P					
EXTENDED			MISFOLDED			EXTENDED			MISFOLDED		
donor	acceptor	occ%	donor	acceptor	occ%	donor	acceptor	occ%	donor	acceptor	occ%
SER2	GLU6	10.61	TRP3	ASN7	9.59	TRP3	ASN7	28.69	TRP3	ASN7	30.04

TRP3	ASN7	8.46
SER2	TRP5	6.53
LYS9	LYS13	5.14

SER2	GLU6	9.54
GLU6	TRP10	6.92
ACE1	THR4	6.15
SER2	TRP5	5.83
GLU6	**LYS9**	5.25
ACE1	TRP3	5.04
ASN7	**LYS9**	5.02

SER2	GLU6	19.53
THR4	GLY8	11.81
TRP5	LYS9	10.37
GLU6	TRP10	10.22
SER2	TRP5	10.03
TRP3	GLY8	9.55
ASN7	**LYS9**	9.43
LYS9	LYS13	7.70
ACE1	THR4	7.06
ASN7	THR11	5.76
TRP3	GLU6	5.65

SER2	GLU6	24.18
GLU6	TRP10	15.15
GLY8	TRP12	14.70
LYS9	LYS13	13.42
ASN7	THR11	12.85
THR4	GLY8	12.51
SER2	TRP5	12.14
TRP3	GLY8	10.66
TRP5	LYS9	10.02
ACE1	THR4	9.21
ASN7	**LYS9**	8.61
GLY8	THR11	6.92
GLU6	**LYS9**	6.57
ACE1	TRP5	6.26
GLY8	LYS13	5.13

ff14SB OPC

EXTENDED

donor	acceptor	occ%
GLU6	TRP10	12.89
SER2	GLU6	12.83
TRP3	ASN7	10.45
ASN7	THR11	10.33
THR4	GLY8	7.23
GLY8	TRP12	7.20
SER2	TRP5	6.86
ACE1	THR4	6.65
GLU6	**LYS9**	5.15

MISFOLDED

donor	acceptor	occ%
TRP3	ASN7	18.92
SER2	GLU6	15.66
THR4	GLY8	10.85
GLU6	TRP10	9.50
SER2	TRP5	8.25
ASN7	THR11	7.26
ACE1	THR4	6.42
TRP5	LYS9	5.89
ASN7	**LYS9**	5.33

ff14SB TIP3P

EXTENDED

donor	acceptor	occ%
TRP3	ASN7	44.90
GLY8	TRP12	42.56
TRP5	LYS9	39.18
ASN7	THR11	36.49
THR4	GLY8	33.59
GLU6	TRP10	32.53
LYS9	LYS13	23.56
SER2	GLU6	20.88
ACE1	THR4	10.49
GLY8	THR11	8.97
ACE1	TRP5	6.69
SER2	TRP5	6.29

MISFOLDED

donor	acceptor	occ%
TRP3	ASN7	46.71
SER2	GLU6	25.95
THR4	GLY8	22.48
TRP5	LYS9	22.47
GLY8	TRP12	22.33
ASN7	THR11	21.49
GLU6	TRP10	18.96
LYS9	LYS13	15.37
SER2	TRP5	9.74
ACE1	THR4	9.21
ACE1	TRP5	7.78
TRP3	GLU6	6.71
GLY8	THR11	5.46

ff19SB OPC

EXTENDED

donor	acceptor	occ%
THR4	**THR11**	16.90
THR11	**THR4**	15.63
SER2	**LYS13**	12.73
LYS9	**GLU6**	12.19

MISFOLDED

donor	acceptor	occ%
TRP3	ASN7	22.38
SER2	GLU6	21.11
GLU6	TRP10	17.28
GLY8	TRP12	15.13
ASN7	THR11	13.77
TRP5	LYS9	12.00
THR4	GLY8	11.87
LYS9	LYS13	8.02
ACE1	TRP5	7.77
TRP3	GLY8	6.10
ACE1	THR4	5.97
SER2	TRP5	5.96

ff19SB TIP3P

EXTENDED

donor	acceptor	occ%
THR4	**THR11**	53.39
THR11	**THR4**	45.56
SER2	**LYS13**	45.01
LYS9	**GLU6**	40.83
GLU6	**LYS9**	17.20
LYS13	**SER2**	7.96
ACE1	TRP3	5.30

MISFOLDED

donor	acceptor	occ%
THR4	**THR11**	24.54
LYS9	**GLU6**	20.21
THR11	**THR4**	17.66
SER2	**LYS13**	16.02
GLY8	THR11	8.47
GLU6	**LYS9**	6.31
TRP3	GLU6	5.88
TRP3	ASN7	5.41
THR4	LYS13	5.03

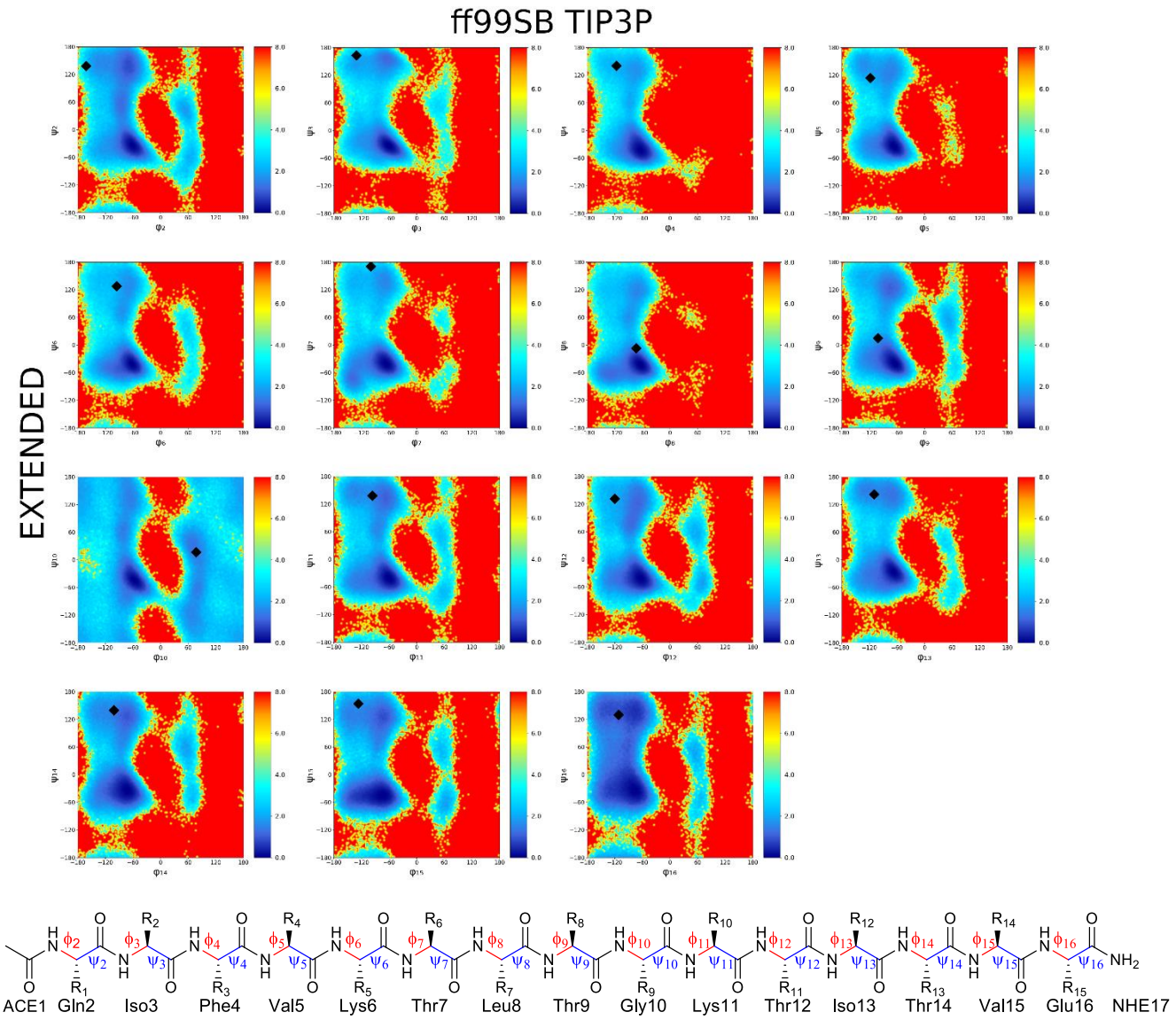

Figure S68. PMFs obtained from φ and ψ dihedral distributions of B3 residues for the ff99SB/TIP3P combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B3 sequence and representation of φ and ψ angles numbering are also shown.

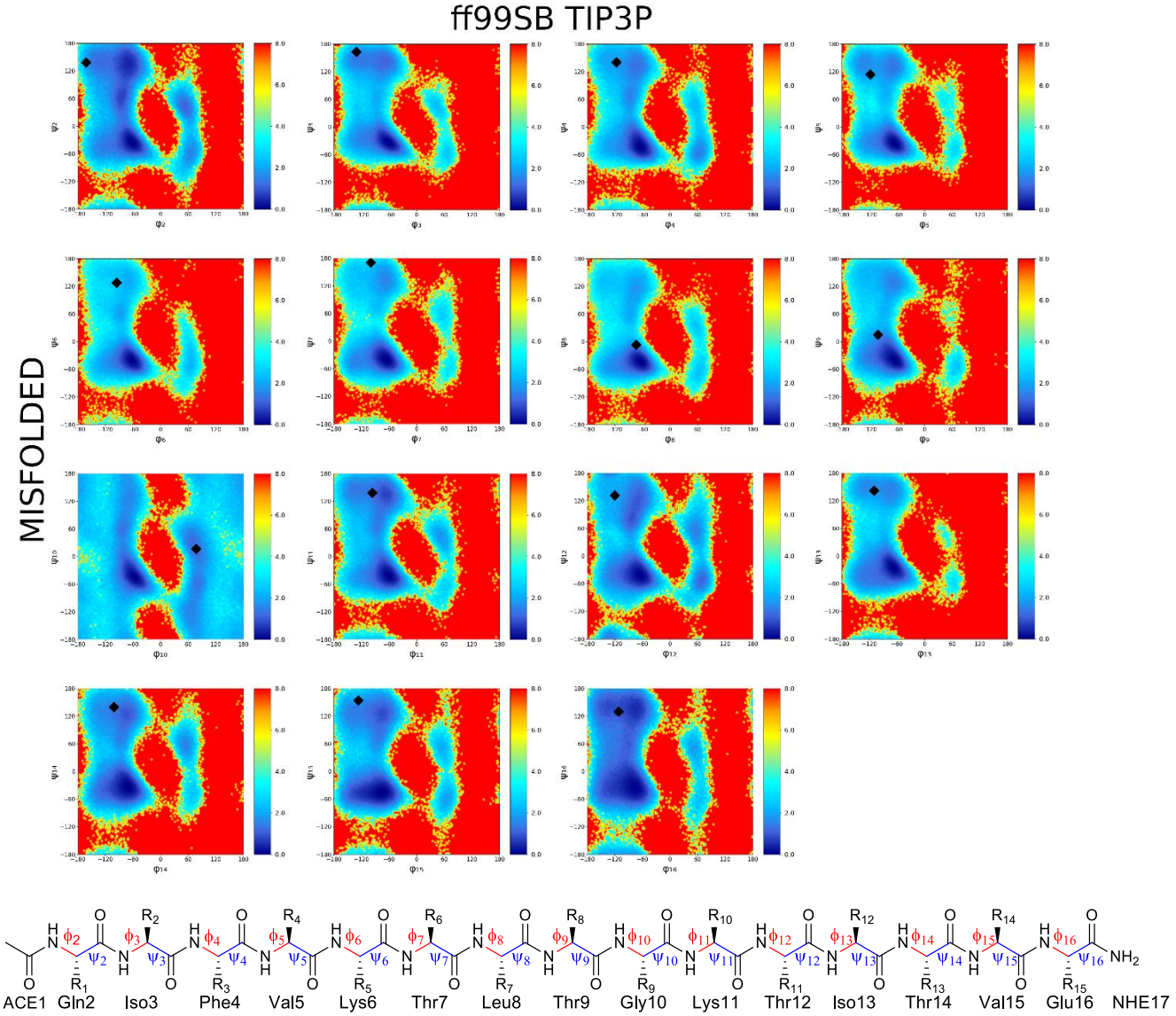

Figure S69. PMFs obtained from φ and ψ dihedral distributions of B3 residues for the ff99SB/TIP3P combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B3 sequence and representation of φ and ψ angles numbering are also shown.

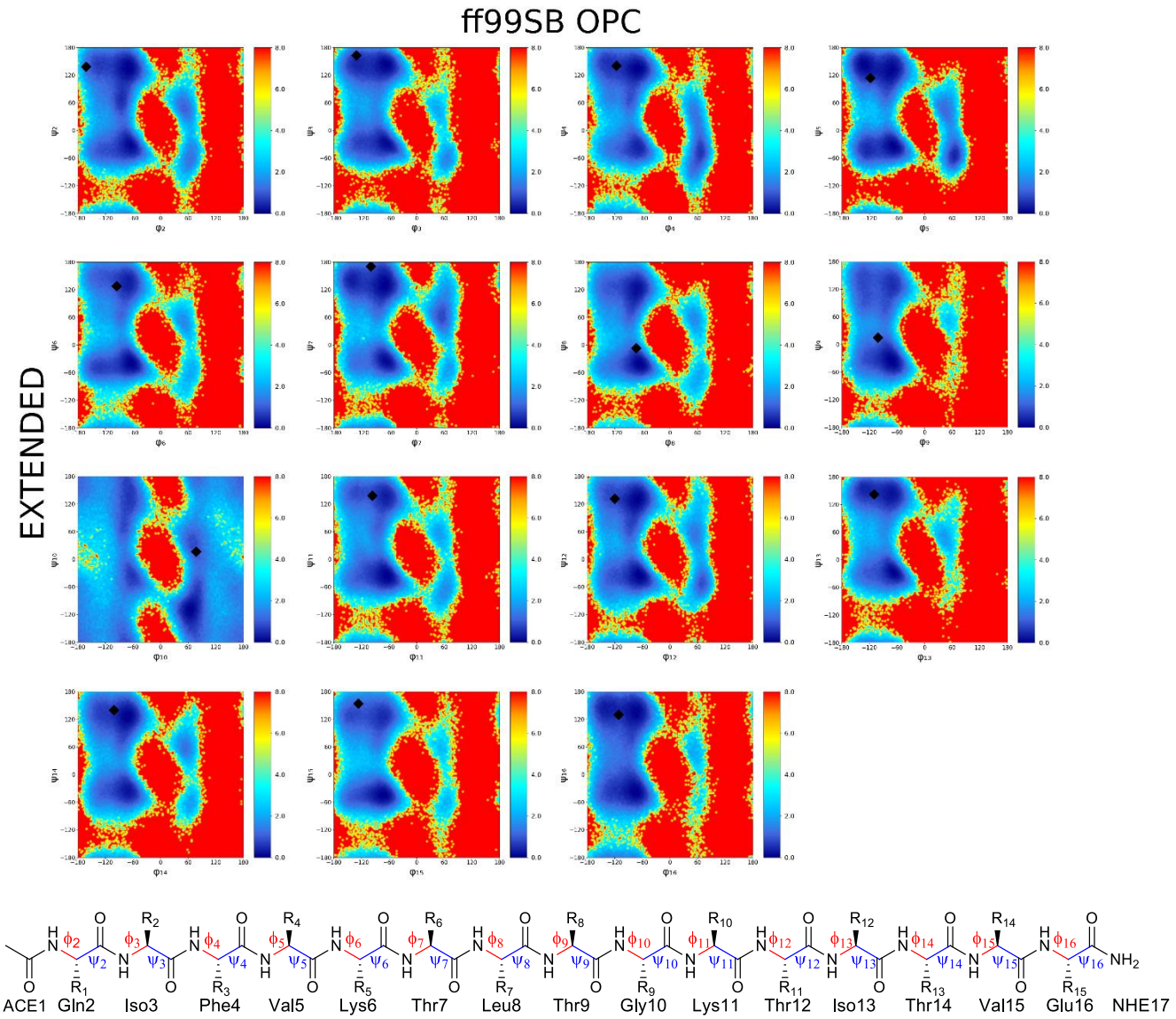

Figure S70. PMFs obtained from φ and ψ dihedral distributions of B3 residues for the ff99SB/OPC combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B3 sequence and representation of φ and ψ angles numbering are also shown.

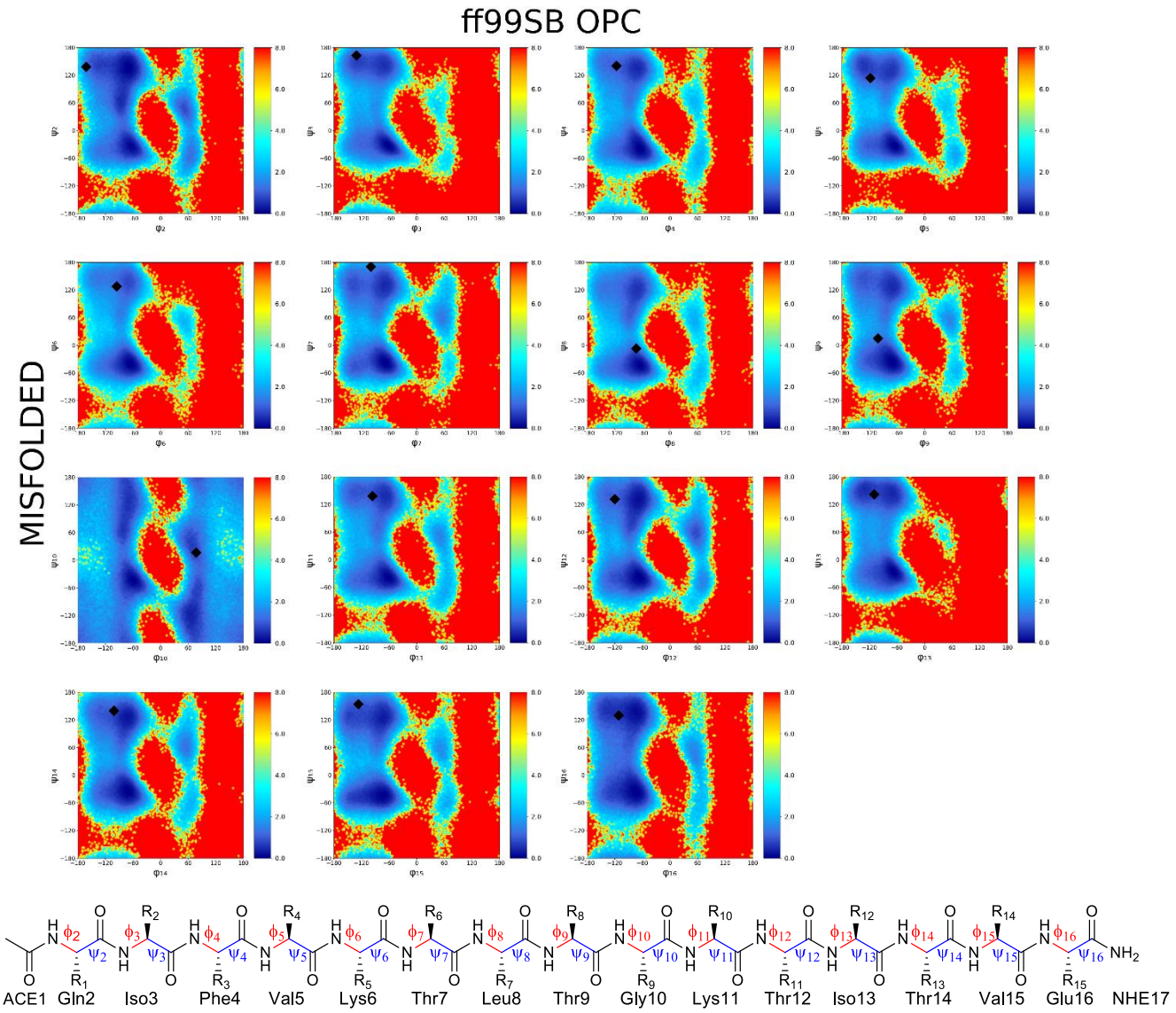

Figure S71. PMFs obtained from φ and ψ dihedral distributions of B3 residues for the ff99SB/OPC combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B3 sequence and representation of φ and ψ angles numbering are also shown.

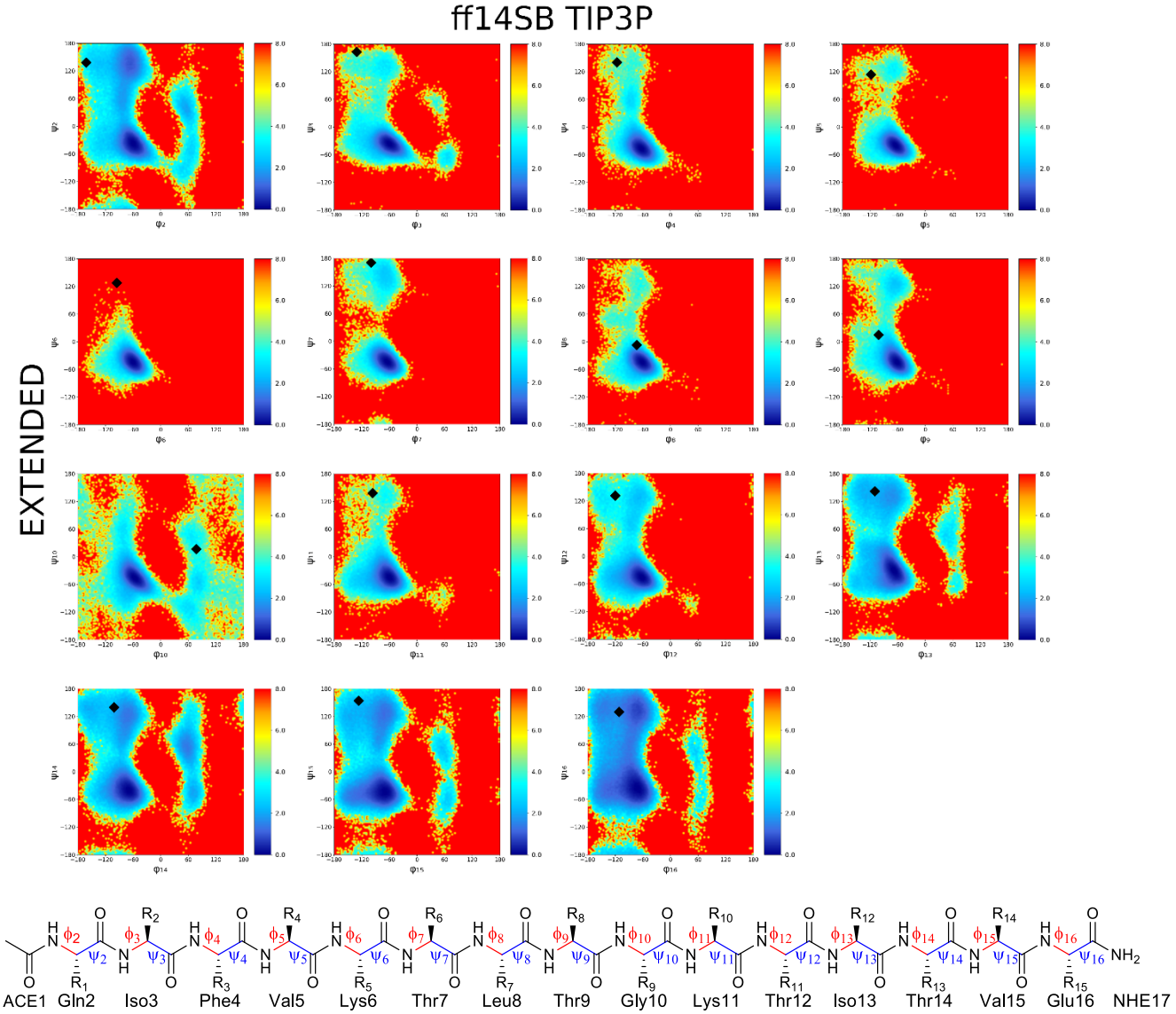

Figure S72. PMFs obtained from φ and ψ dihedral distributions of B3 residues for the ff14SB/TIP3P combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B3 sequence and representation of φ and ψ angles numbering are also shown.

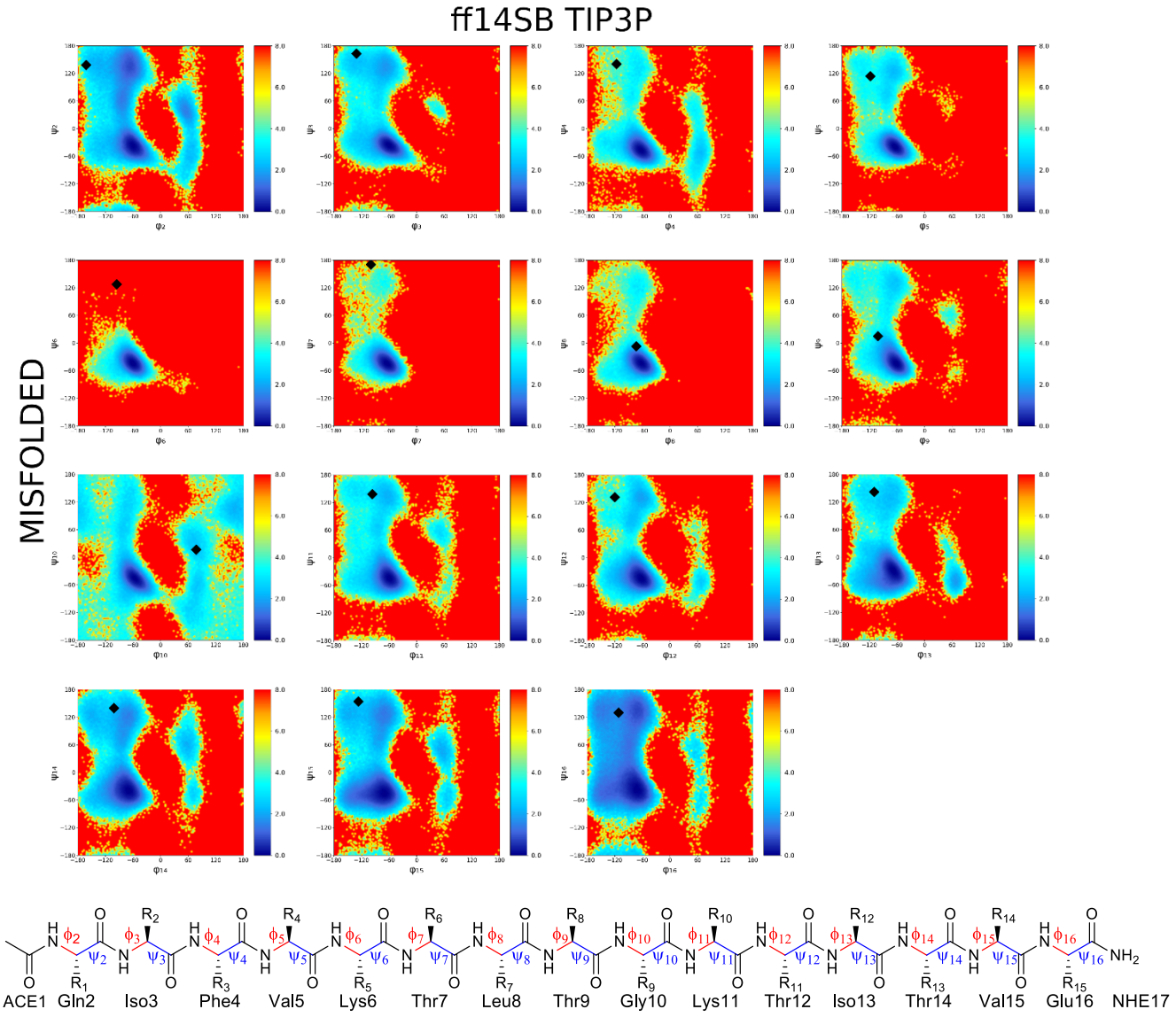

Figure S73. PMFs obtained from φ and ψ dihedral distributions of B3 residues for the ff14SB/TIP3P combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B3 sequence and representation of φ and ψ angles numbering are also shown.

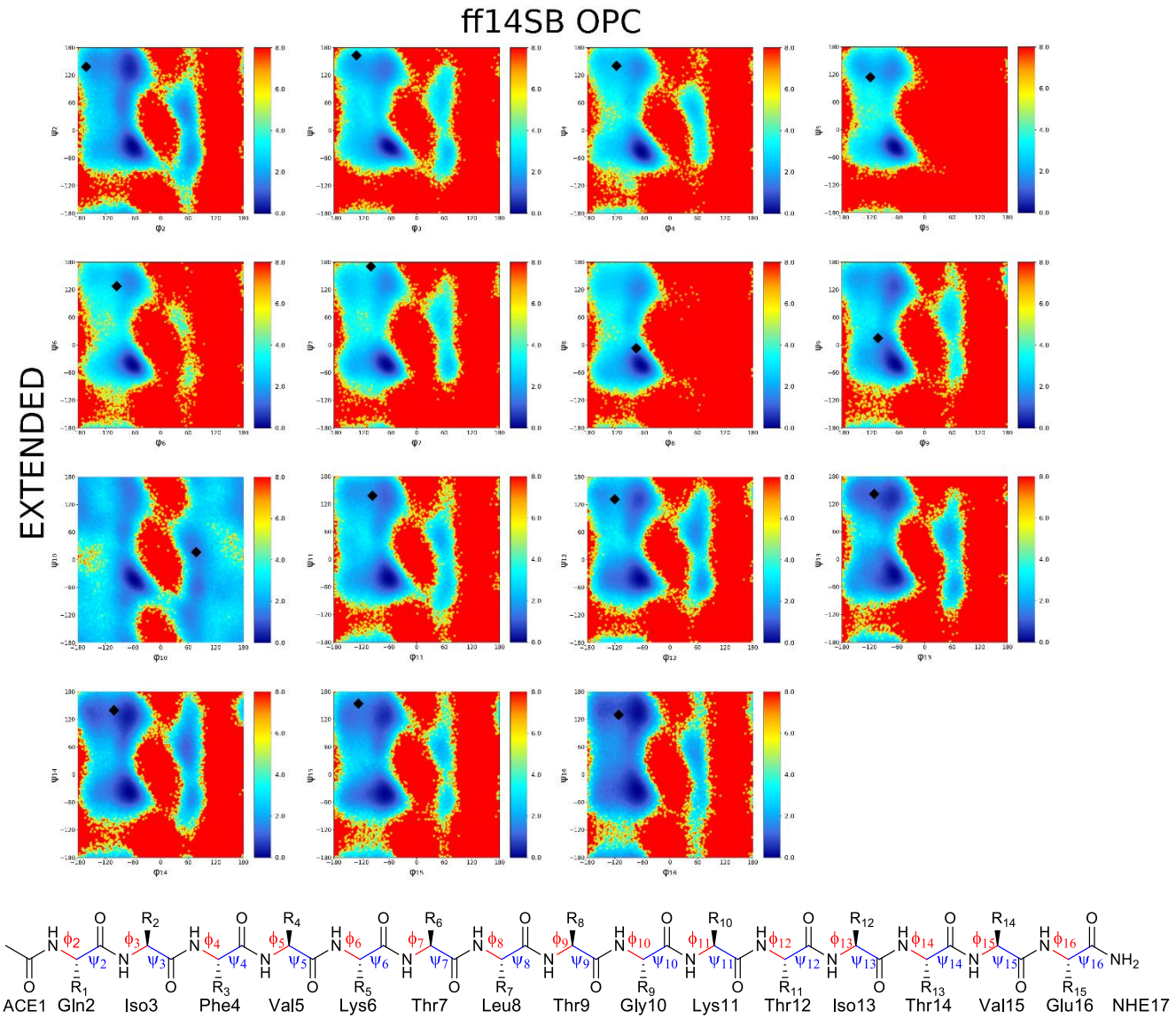

Figure S74. PMFs obtained from φ and ψ dihedral distributions of B3 residues for the ff14SB/OPC combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B3 sequence and representation of φ and ψ angles numbering are also shown.

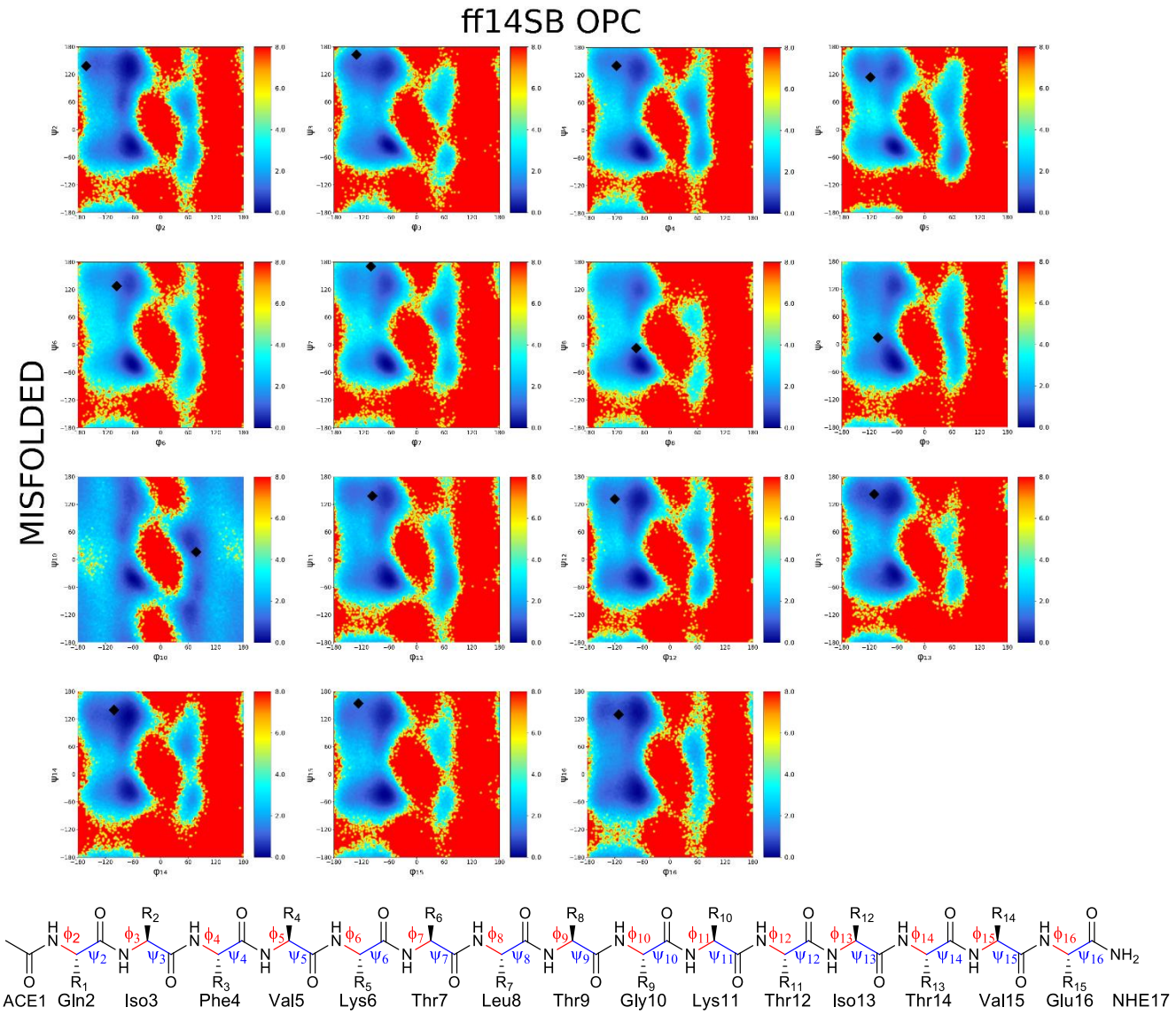

Figure S75. PMFs obtained from φ and ψ dihedral distributions of B3 residues for the ff14SB/OPC combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B3 sequence and representation of φ and ψ angles numbering are also shown.

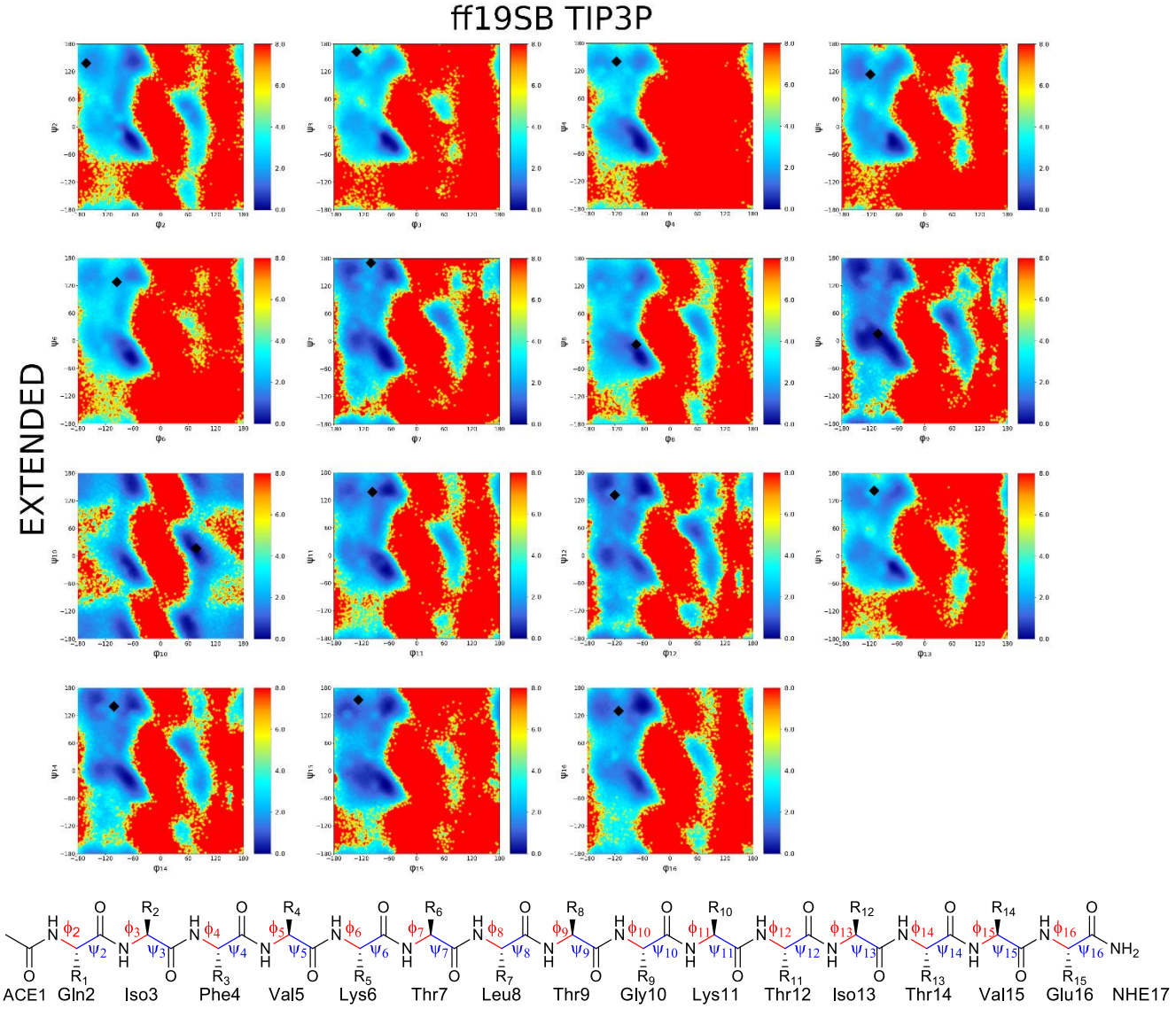

Figure S76. PMFs obtained from φ and ψ dihedral distributions of B3 residues for the ff19SB/TIP3P combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B3 sequence and representation of φ and ψ angles numbering are also shown.

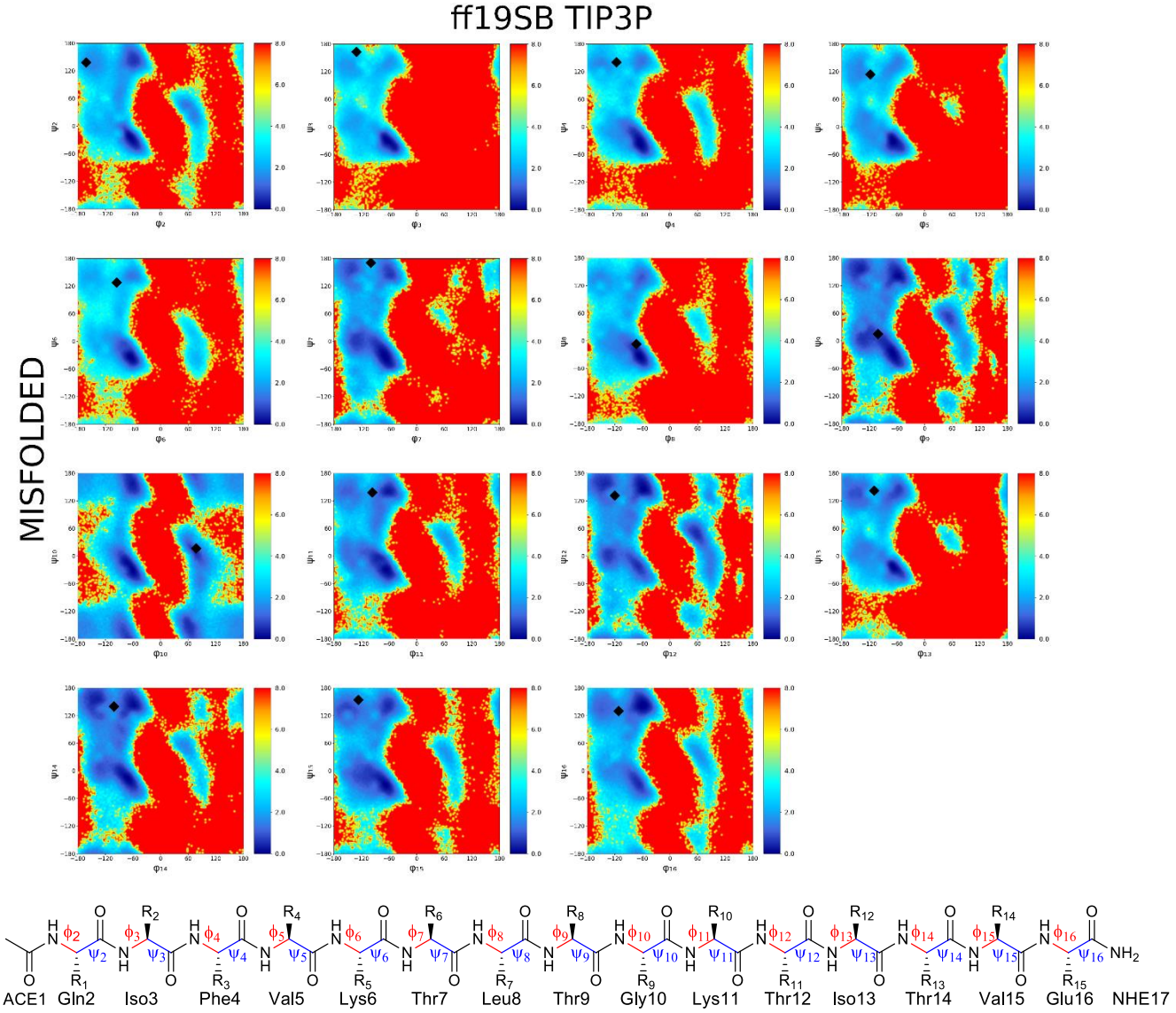

Figure S77. PMFs obtained from φ and ψ dihedral distributions of B3 residues for the ff19SB/TIP3P combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B3 sequence and representation of φ and ψ angles numbering are also shown.

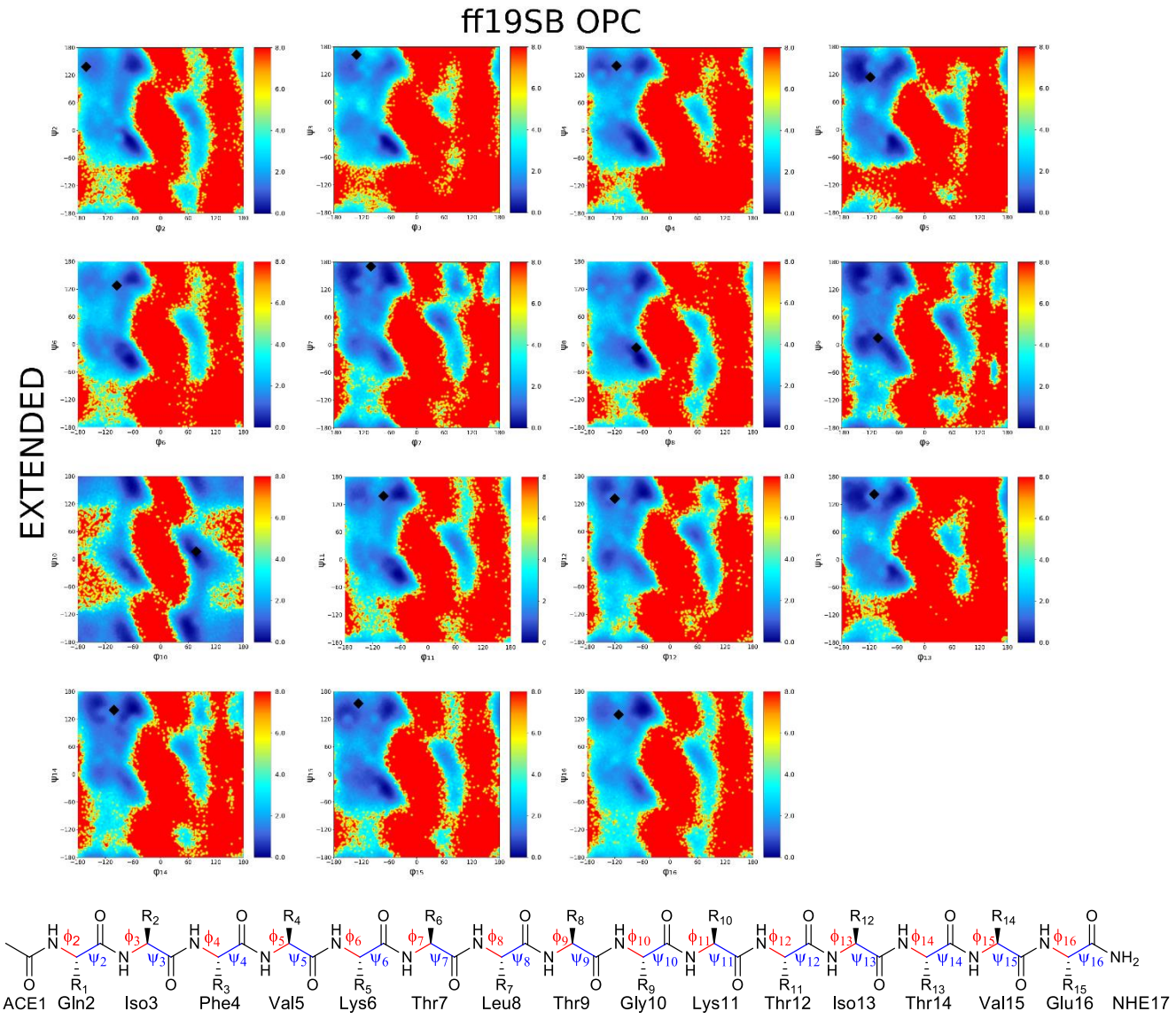

Figure S78. PMFs obtained from φ and ψ dihedral distributions of B3 residues for the ff19SB/OPC combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B3 sequence and representation of φ and ψ angles numbering are also shown.

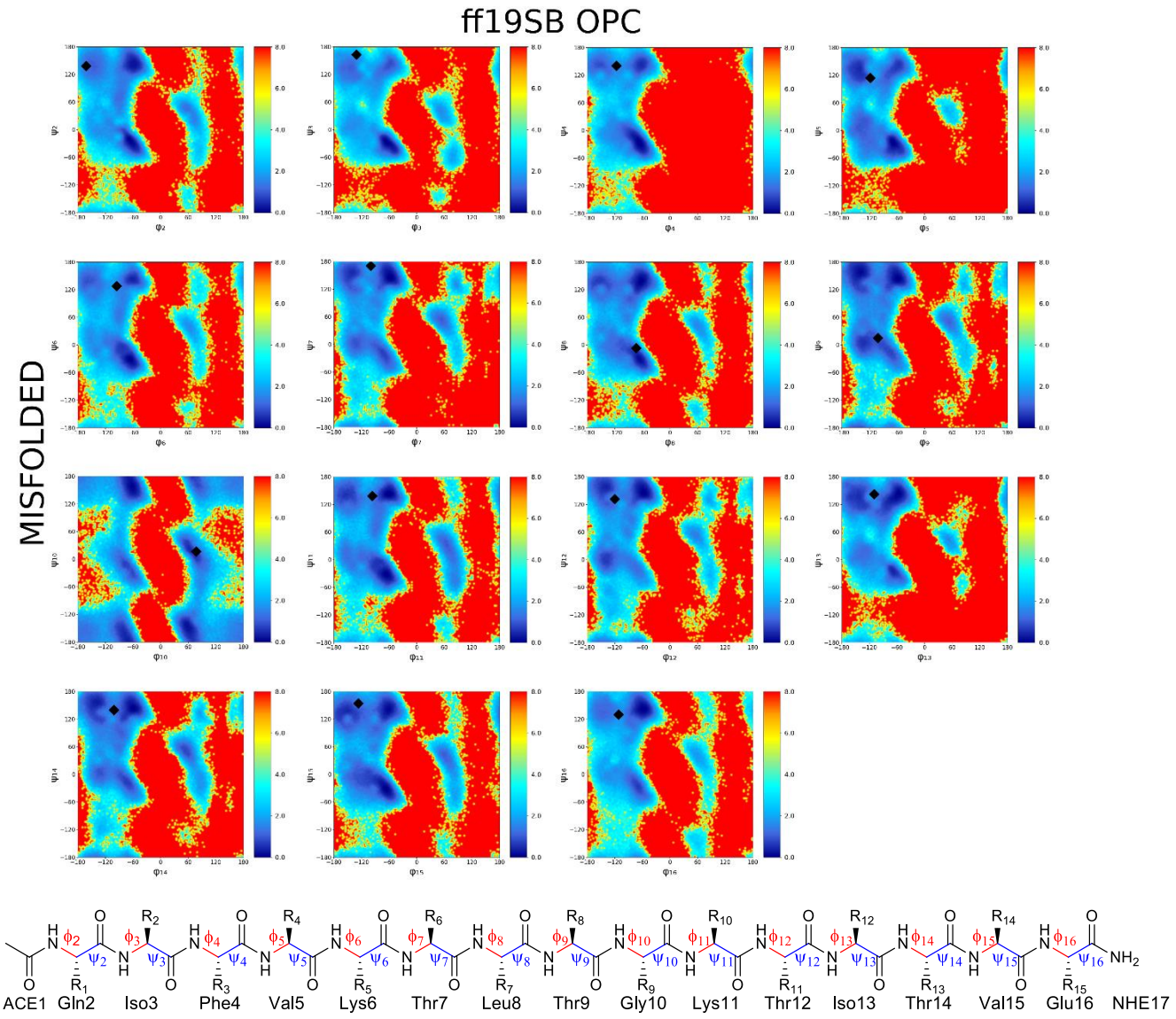

Figure S79. PMFs obtained from φ and ψ dihedral distributions of B3 residues for the ff19SB/OPC combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. B3 sequence and representation of φ and ψ angles numbering are also shown.

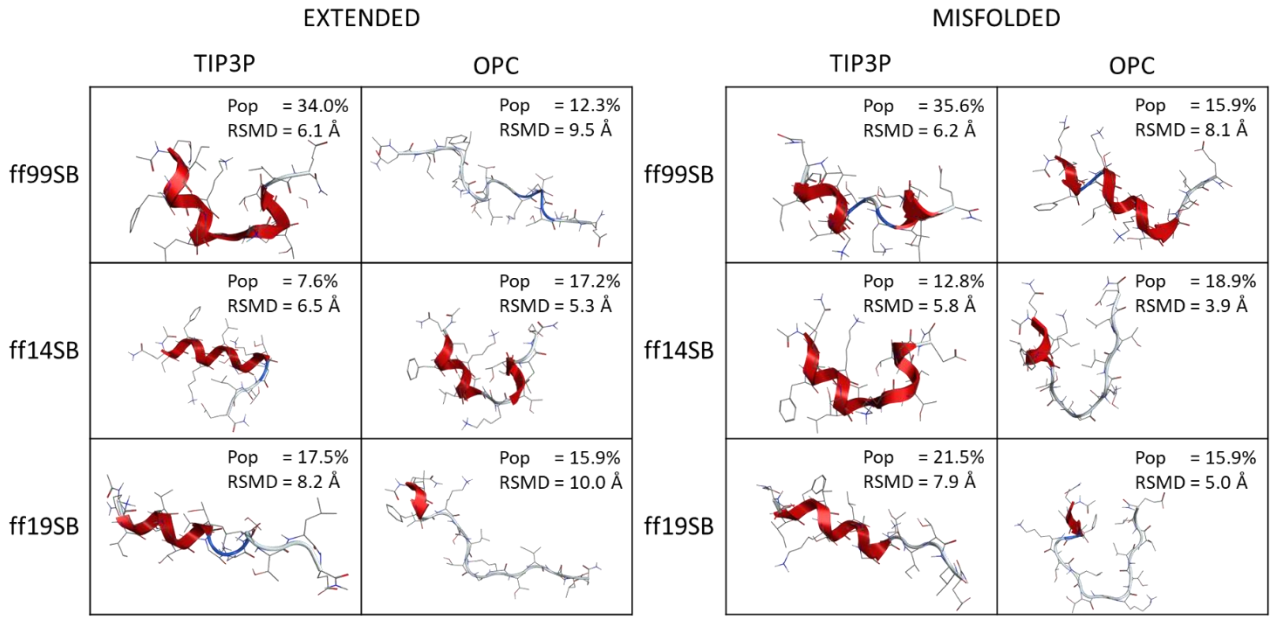

Figure S80. Representative conformation and population (pop%) of the second cluster from B3 trajectories. RMSD vs native structure are also shown.

Table S8. H-bond analyses from B3 trajectories. Only H-bonds involving the backbone are included in the table (donor N-H, acceptor C=O). Native H-bonds are highlighted in bold.

NATIVE		
acceptor	donor	Distance
VAL5	ILE13	2.72
ILE13	VAL5	2.79
LYS11	THR7	2.91
ILE3	LEU15	3.05
LEU15	ILE3	3.05
THR7	THR9	3.15
THR7	GLY10	3.37
THR9	LYS11	3.42
LEU8	GLY10	3.6
VAL5	THR7	3.9
GLY10	THR12	4.02
ILE13	LEU15	4.02
PHE4	LYS6	4.12
LEU15	NME	4.15
THR12	THR14	4.17
LYS11	ILE13	4.29
THR7	LYS11	4.3
LYS6	LEU8	4.43
ILE3	VAL5	4.45
LEU15	GLN2	4.47
ff99SB OPC		ff99SB TIP3P

EXTENDED		
acceptor	donor	occ%
ILE3	**VAL5**	7.07
GLN2	LYS6	6.25
PHE4	**LYS6**	5.83

MISFOLDED		
acceptor	donor	occ%
PHE4	LEU8	8.69
GLN2	LYS6	8.12
ILE3	THR7	8.02
VAL5	THR9	6.34
THR12	GLU16	5.88
ACE1	ILE3	5.16

EXTENDED		
acceptor	donor	occ%
GLN2	LYS6	22.07
ILE3	THR7	21.90
PHE4	LEU8	21.28
VAL5	THR9	17.91
THR12	GLU16	17.33
LYS6	GLY10	16.09
THR7	**LYS11**	13.77
THR9	ILE13	12.93
LYS11	LEU15	11.46
LEU8	THR12	10.18
GLY10	THR14	9.42
ILE3	LYS6	8.74
ACE1	PHE4	8.45
THR12	LEU15	7.05
ACE1	VAL5	6.97
GLN2	VAL5	6.50
LYS11	GLU16	5.73

MISFOLDED		
acceptor	donor	occ%
PHE4	LEU8	24.76
VAL5	THR9	22.40
GLN2	LYS6	19.08
LYS6	GLY10	18.29
ILE3	THR7	16.13
THR12	GLU16	15.92
THR7	**LYS11**	13.36
THR9	ILE13	11.74
LEU8	THR12	10.74
GLY10	THR14	8.63
LYS11	LEU15	8.39
THR12	LEU15	8.14
GLN2	VAL5	5.89
ACE1	ILE3	5.62
ILE3	LYS6	5.48
ACE1	PHE4	5.41
ILE3	**VAL5**	5.25
LYS11	**ILE13**	5.16

ff14SB OPC

EXTENDED		
acceptor	donor	occ%
PHE4	LEU8	34.19
VAL5	THR9	29.81
ILE3	THR7	27.15
GLN2	LYS6	23.29
LYS6	GLY10	17.73
THR7	**LYS11**	12.25
THR9	ILE13	11.88
LEU8	THR12	11.78
GLY10	THR14	8.72
THR12	GLU16	6.68
ACE1	VAL5	5.89
LYS11	LEU15	5.84
GLN2	VAL5	5.31

MISFOLDED		
acceptor	donor	occ%
VAL5	THR9	14.89
PHE4	LEU8	13.29
ILE3	THR7	9.79
GLN2	LYS6	8.99
LYS6	GLY10	8.41
PHE4	**LYS6**	6.13
LEU8	THR12	6.02
THR9	ILE13	5.94
THR7	**LYS11**	5.93
THR12	GLU16	5.52
GLY10	THR14	5.38

ff14SB TIP3P

EXTENDED		
acceptor	donor	occ%
PHE4	LEU8	53.03
VAL5	THR9	51.95
THR7	**LYS11**	44.33
GLN2	LYS6	43.51
THR9	ILE13	40.66
ILE3	THR7	40.28
LYS6	GLY10	37.95
LEU8	THR12	35.48
LYS11	LEU15	23.08
THR12	GLU16	20.48
GLY10	THR14	19.79
ACE1	VAL5	12.19
ACE1	PHE4	8.72
LYS11	GLU16	6.66
GLN2	VAL5	6.50

MISFOLDED		
acceptor	donor	occ%
PHE4	LEU8	50.57
VAL5	THR9	50.13
LYS6	GLY10	38.09
GLN2	LYS6	36.04
THR7	**LYS11**	35.90
ILE3	THR7	35.51
THR9	ILE13	34.71
LEU8	THR12	28.11
LYS11	LEU15	22.87
THR12	GLU16	21.59
GLY10	THR14	20.92
ACE1	VAL5	9.90
LYS11	GLU16	8.93
ACE1	PHE4	7.17
GLN2	VAL5	5.47
THR12	LEU15	5.05

ff19SB OPC

EXTENDED		
acceptor	donor	occ%
GLN2	LYS6	6.24
ACE1	PHE4	5.61
GLN2	VAL5	5.40
ILE13	**VAL5**	5.24

MISFOLDED		
acceptor	donor	occ%
GLN2	LYS6	7.48
GLN2	VAL5	7.16

ff19SB TIP3P

EXTENDED		
acceptor	donor	occ%
GLN2	LYS6	17.75
PHE4	LEU8	13.10
ILE3	THR7	12.21
GLN2	VAL5	10.37

MISFOLDED		
acceptor	donor	occ%
GLN2	LYS6	17.52
PHE4	LEU8	15.49
ILE3	THR7	14.31
VAL5	THR9	11.04

VAL5	**ILE13**	5.10

VAL5	THR9	9.34
ACE1	PHE4	8.68
THR12	LEU15	8.61
THR12	GLU16	6.44

GLN2	VAL5	10.72
ACE1	PHE4	8.58
THR12	LEU15	6.64
PHE4	THR7	5.78
LYS6	GLY10	5.31
THR12	GLU16	5.10

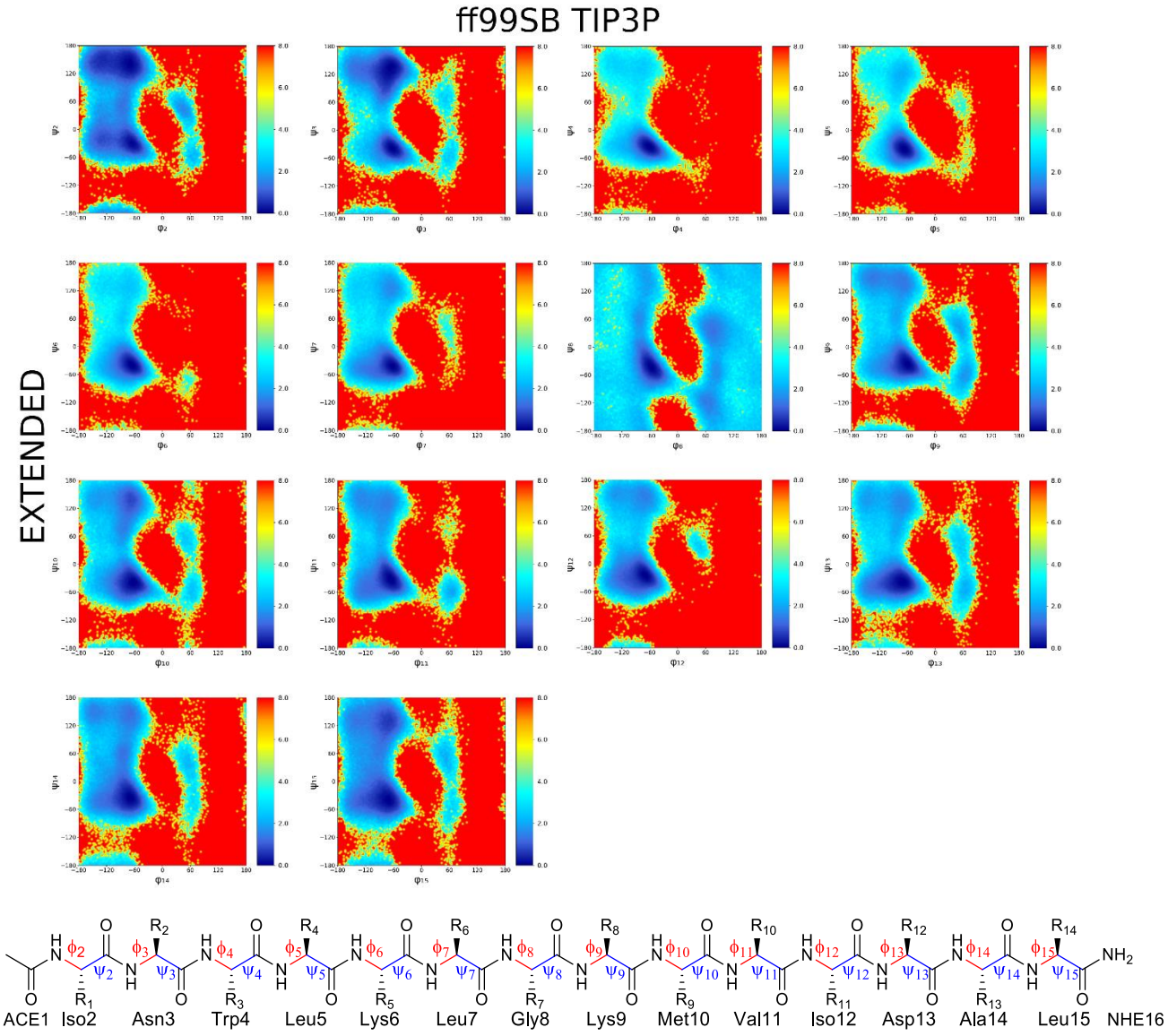

Figure S81. PMFs obtained from φ and ψ dihedral distributions of ID1 residues for the ff99SB/TIP3P combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID1 sequence and representation of φ and ψ angles numbering are also shown.

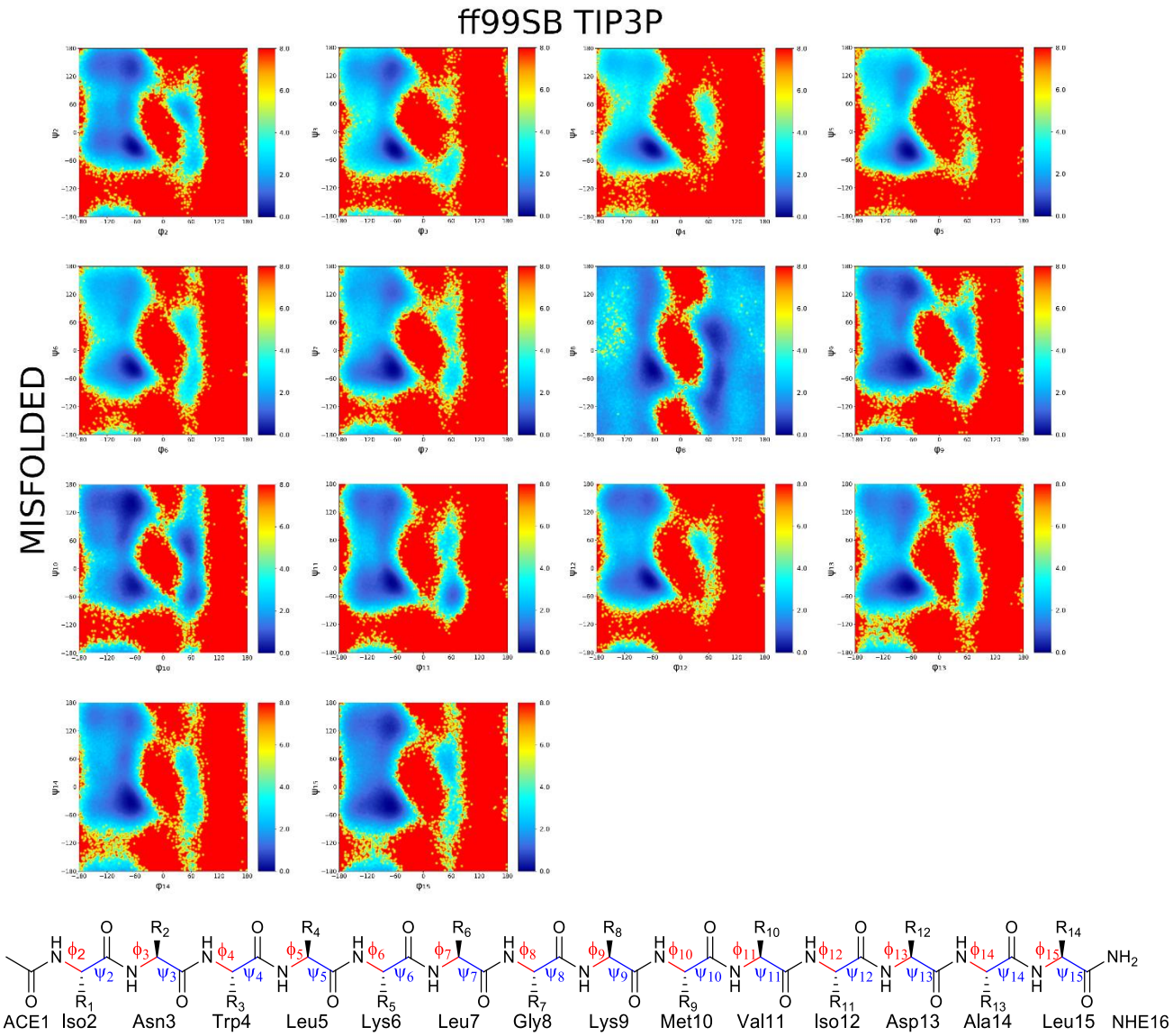

Figure S82. PMFs obtained from φ and ψ dihedral distributions of ID1 residues for the ff99SB/TIP3P combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID1 sequence and representation of φ and ψ angles numbering are also shown.

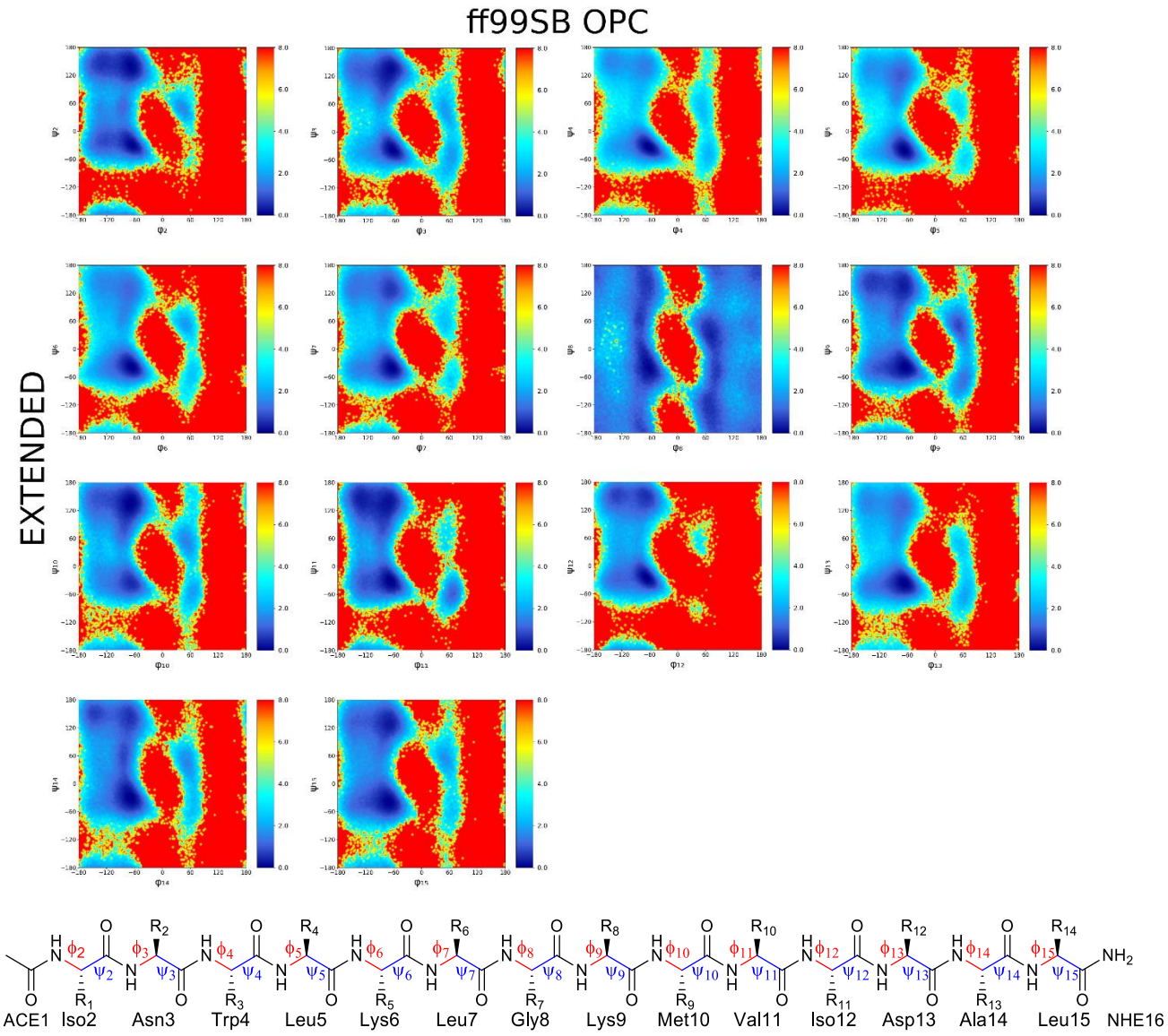

Figure S83. PMFs obtained from φ and ψ dihedral distributions of ID1 residues for the ff99SB/OPC combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID1 sequence and representation of φ and ψ angles numbering are also shown.

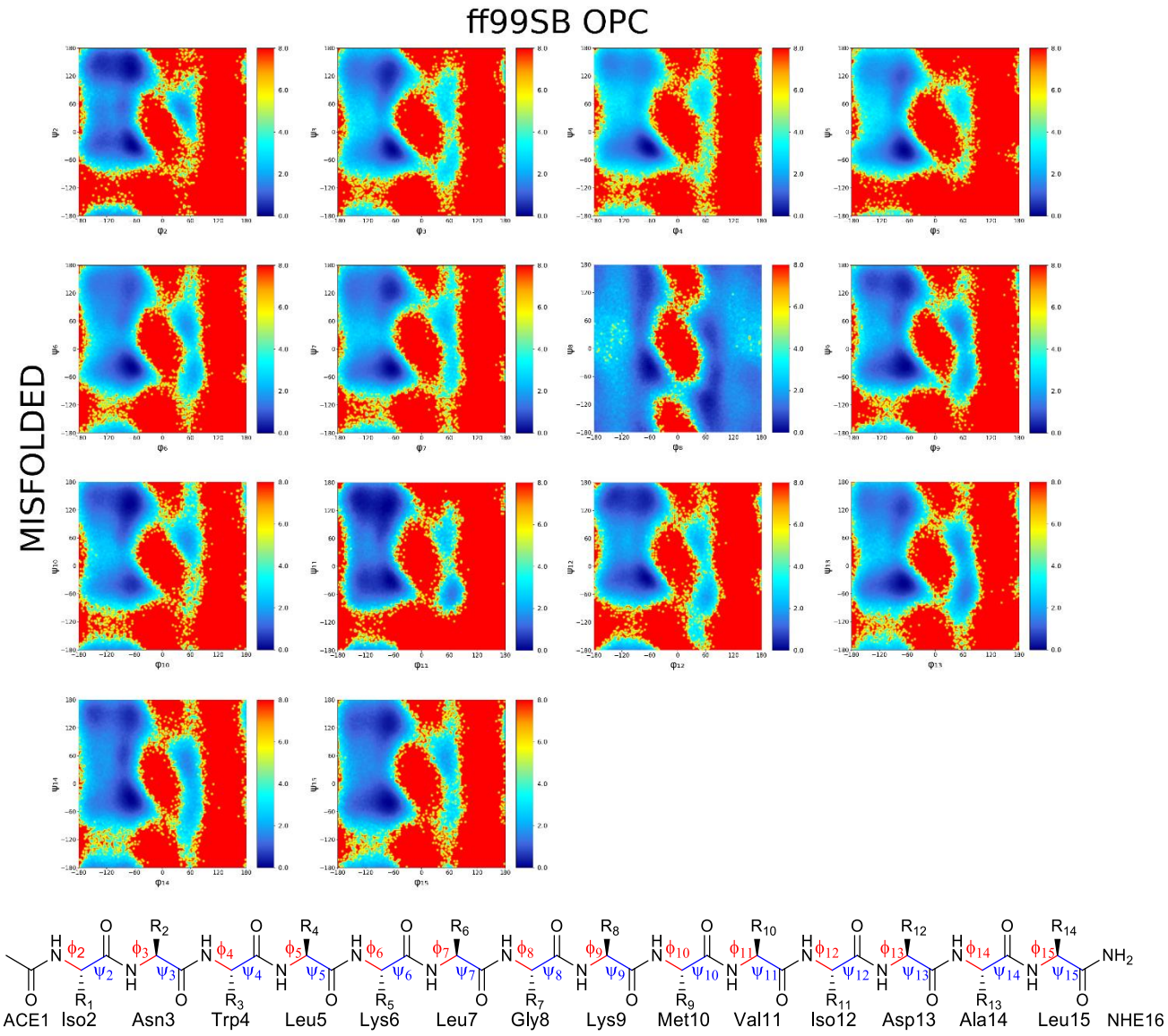

Figure S84. PMFs obtained from φ and ψ dihedral distributions of ID1 residues for the ff99SB/OPC combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID1 sequence and representation of φ and ψ angles numbering are also shown.

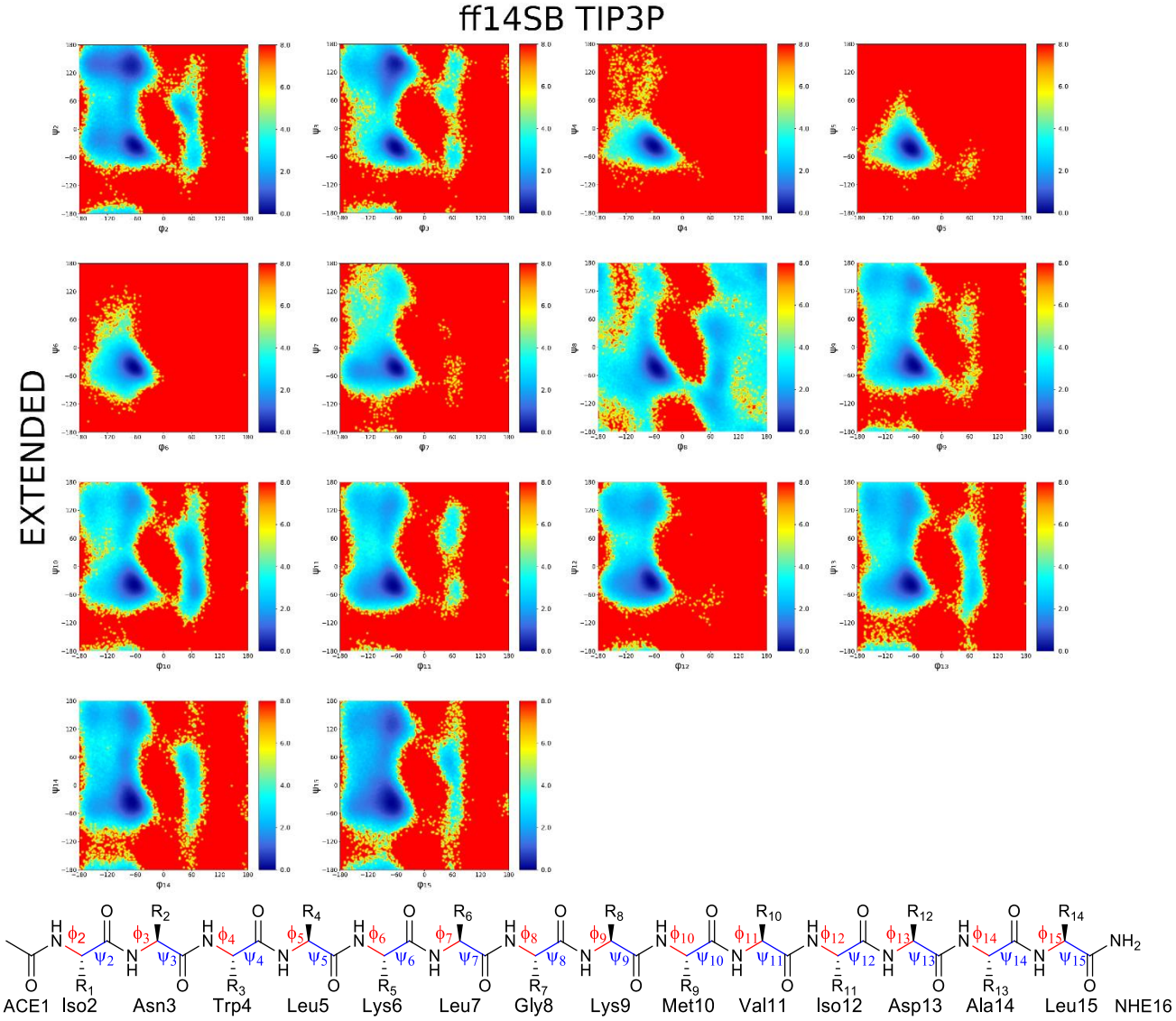

Figure S85. PMFs obtained from φ and ψ dihedral distributions of ID1 residues for the ff14SB/TIP3P combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID1 sequence and representation of φ and ψ angles numbering are also shown.

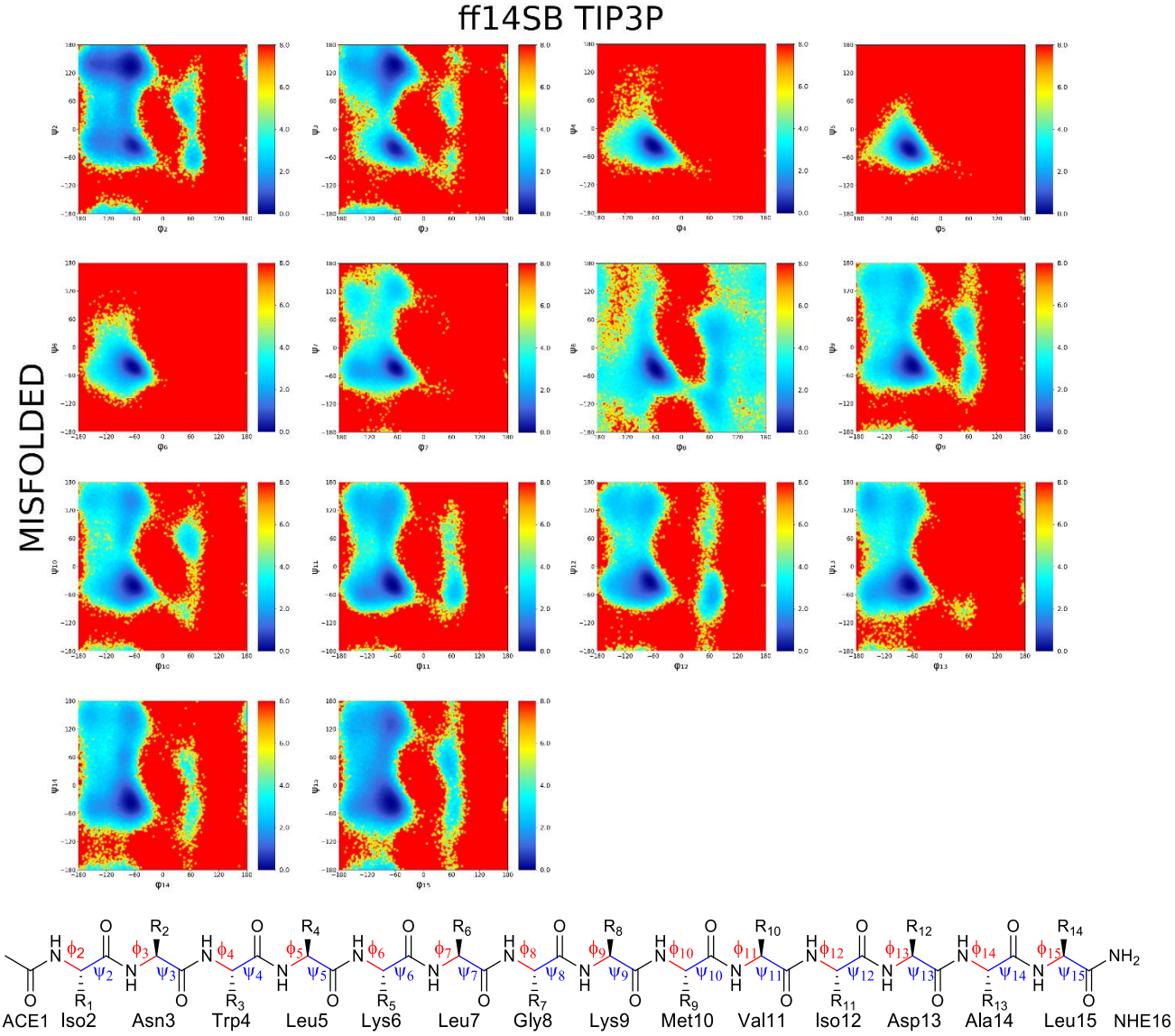

Figure S86. PMFs obtained from φ and ψ dihedral distributions of ID1 residues for the ff14SB/TIP3P combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID1 sequence and representation of φ and ψ angles numbering are also shown.

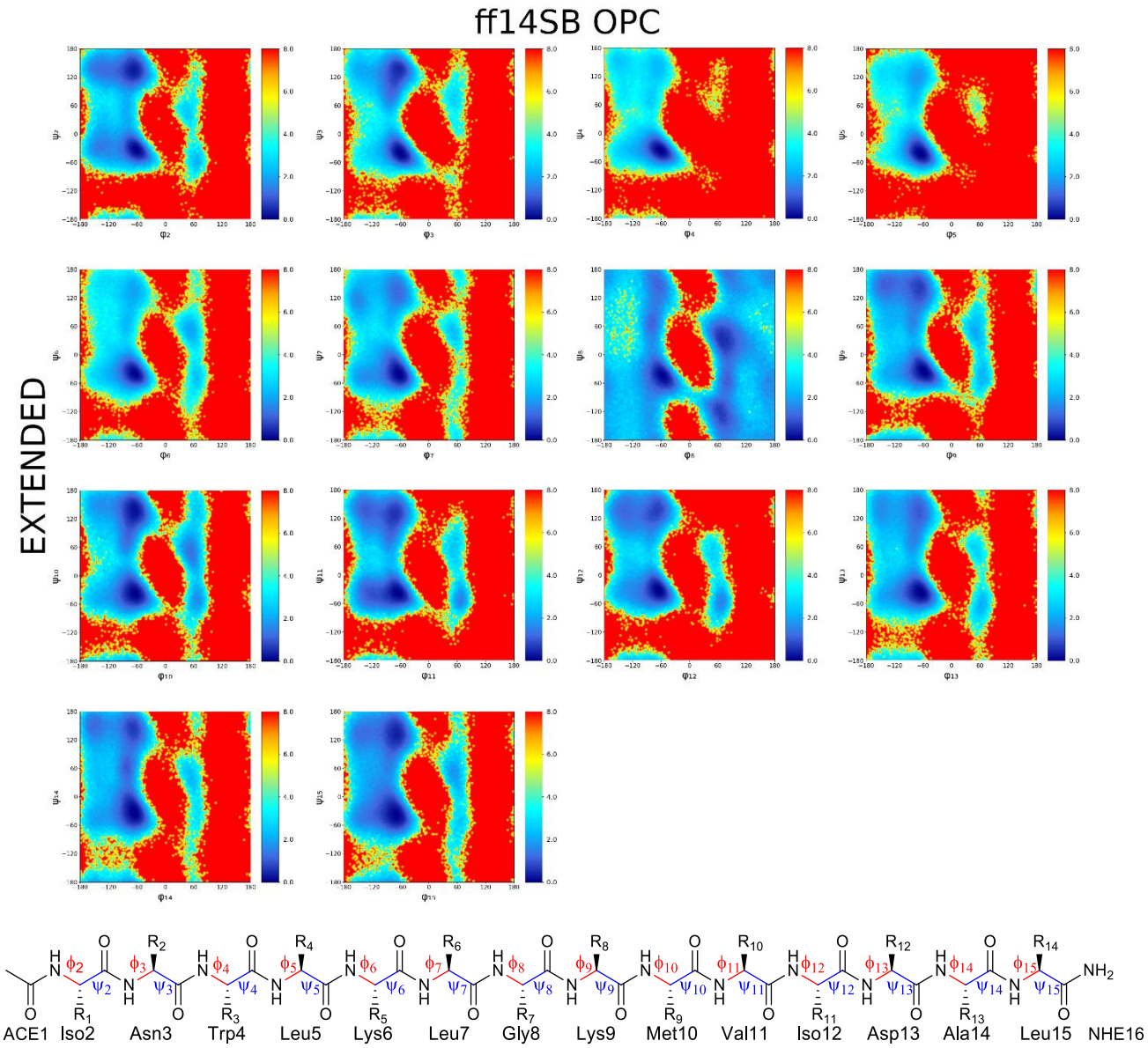

Figure S87. PMFs obtained from φ and ψ dihedral distributions of ID1 residues for the ff14SB/OPC combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID1 sequence and representation of φ and ψ angles numbering are also shown.

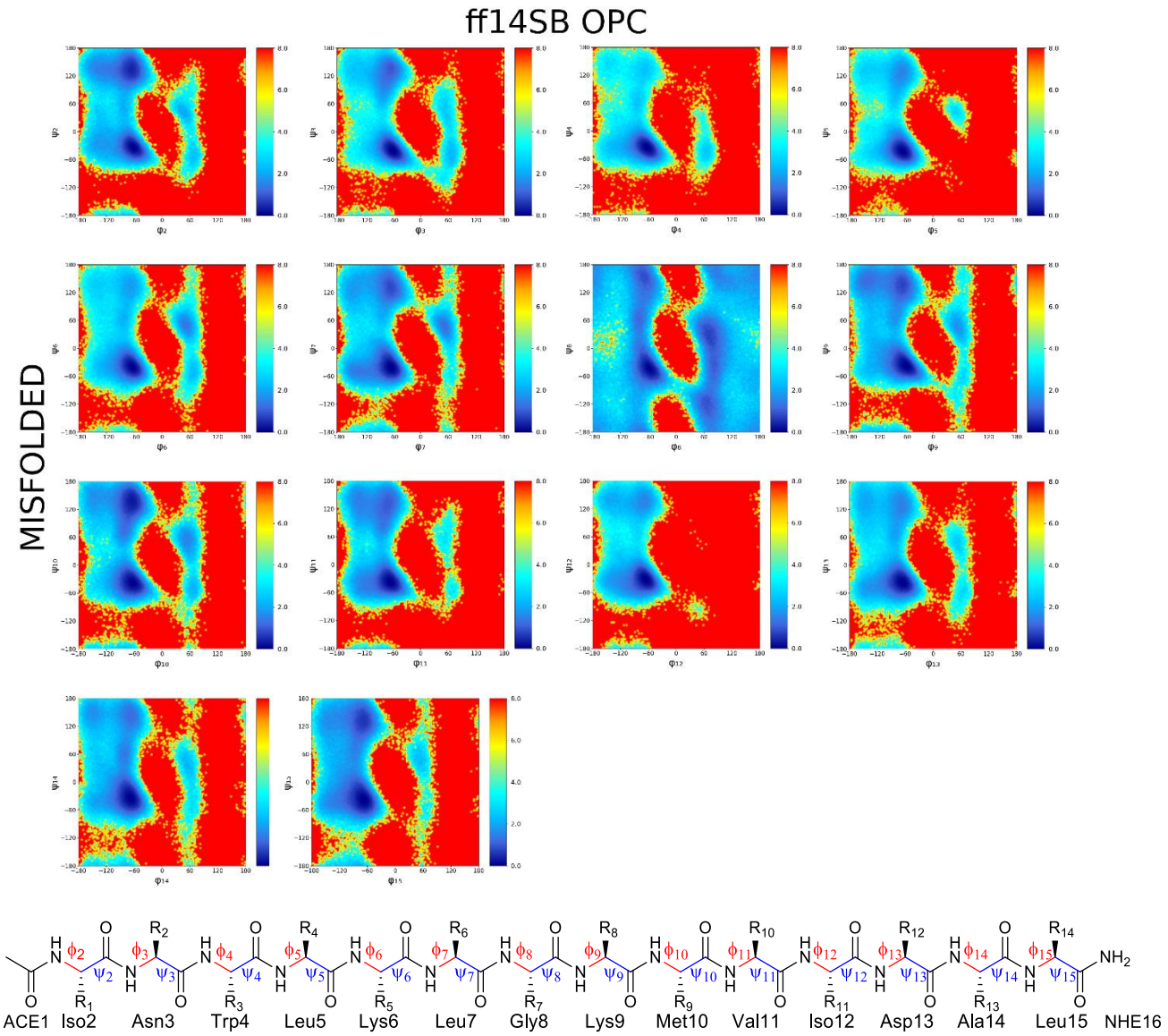

Figure S88. PMFs obtained from φ and ψ dihedral distributions of ID1 residues for the ff14SB/OPC combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID1 sequence and representation of φ and ψ angles numbering are also shown.

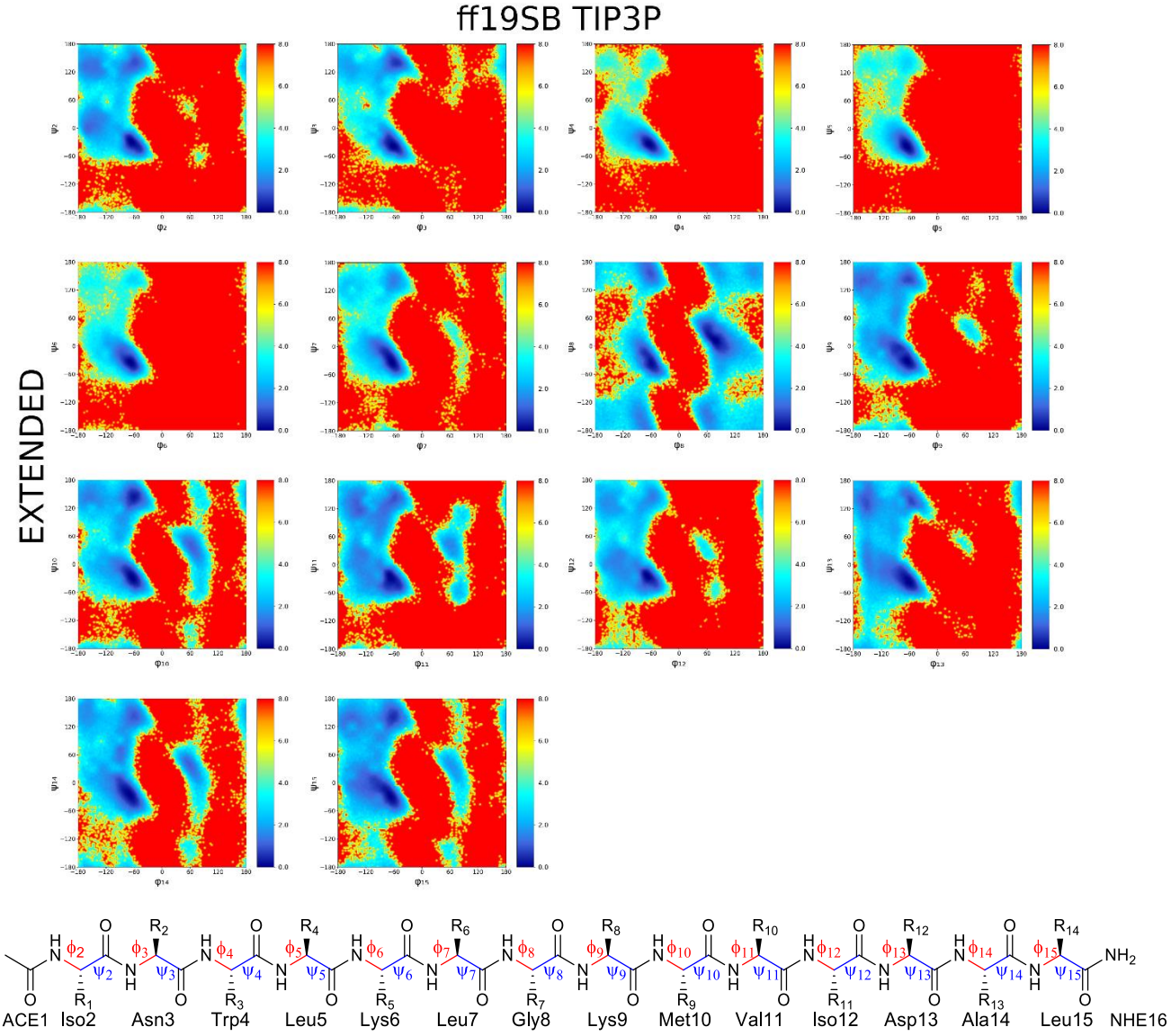

Figure S89. PMFs obtained from φ and ψ dihedral distributions of ID1 residues for the ff19SB/TIP3P combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID1 sequence and representation of φ and ψ angles numbering are also shown.

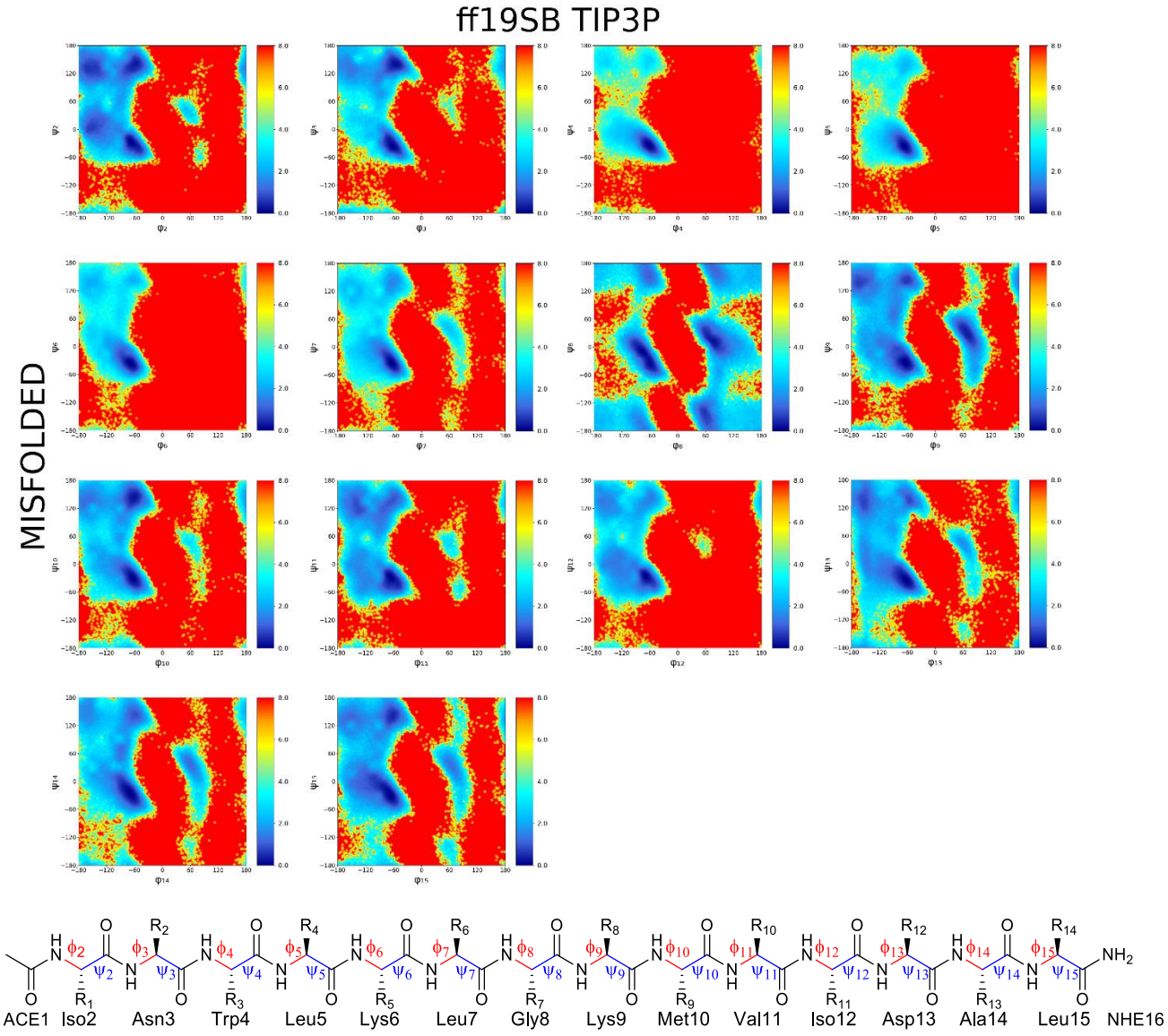

Figure S90. PMFs obtained from φ and ψ dihedral distributions of ID1 residues for the ff19SB/TIP3P combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID1 sequence and representation of φ and ψ angles numbering are also shown.

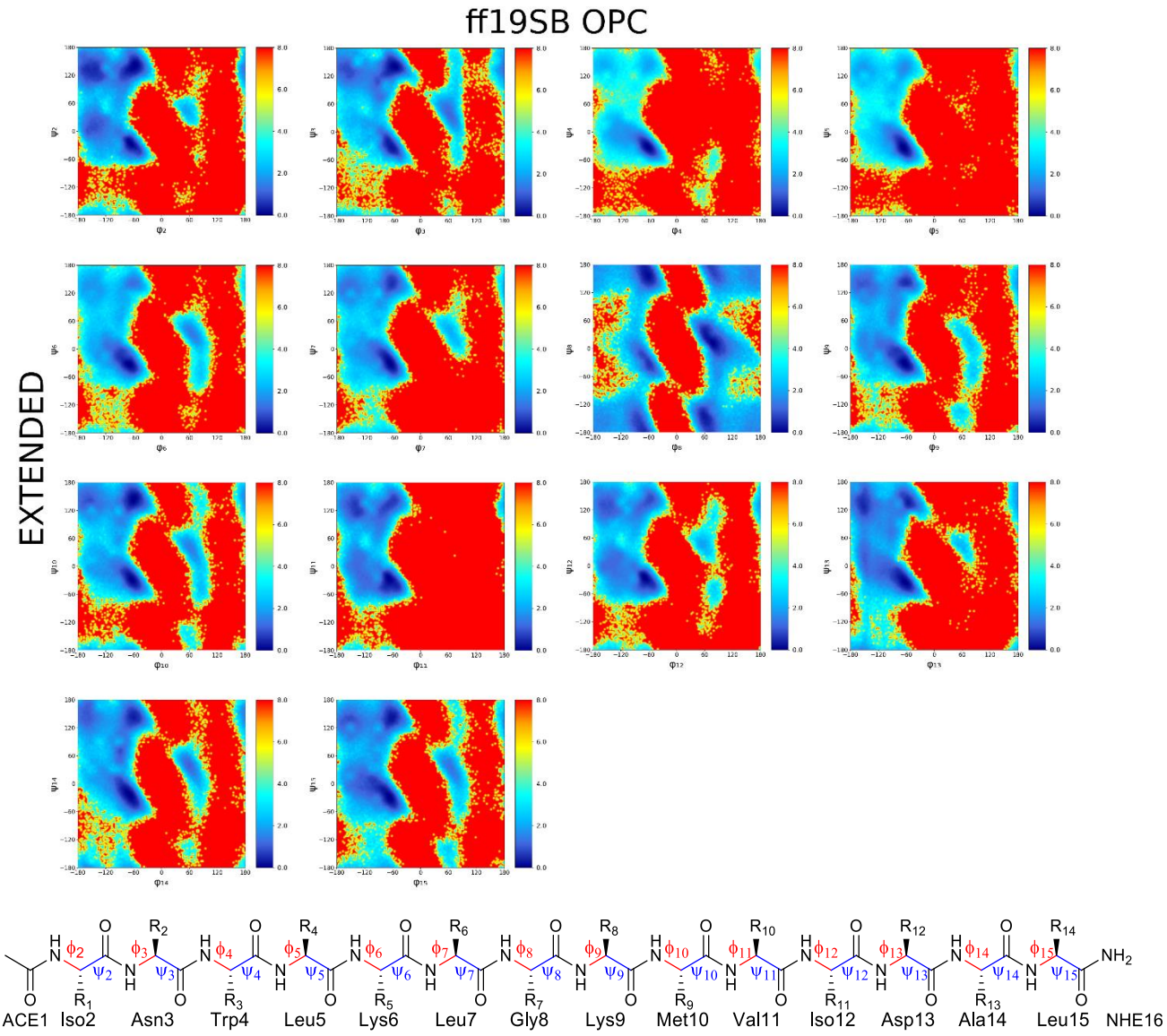

Figure S91. PMFs obtained from φ and ψ dihedral distributions of ID1 residues for the ff19SB/OPC combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID1 sequence and representation of φ and ψ angles numbering are also shown.

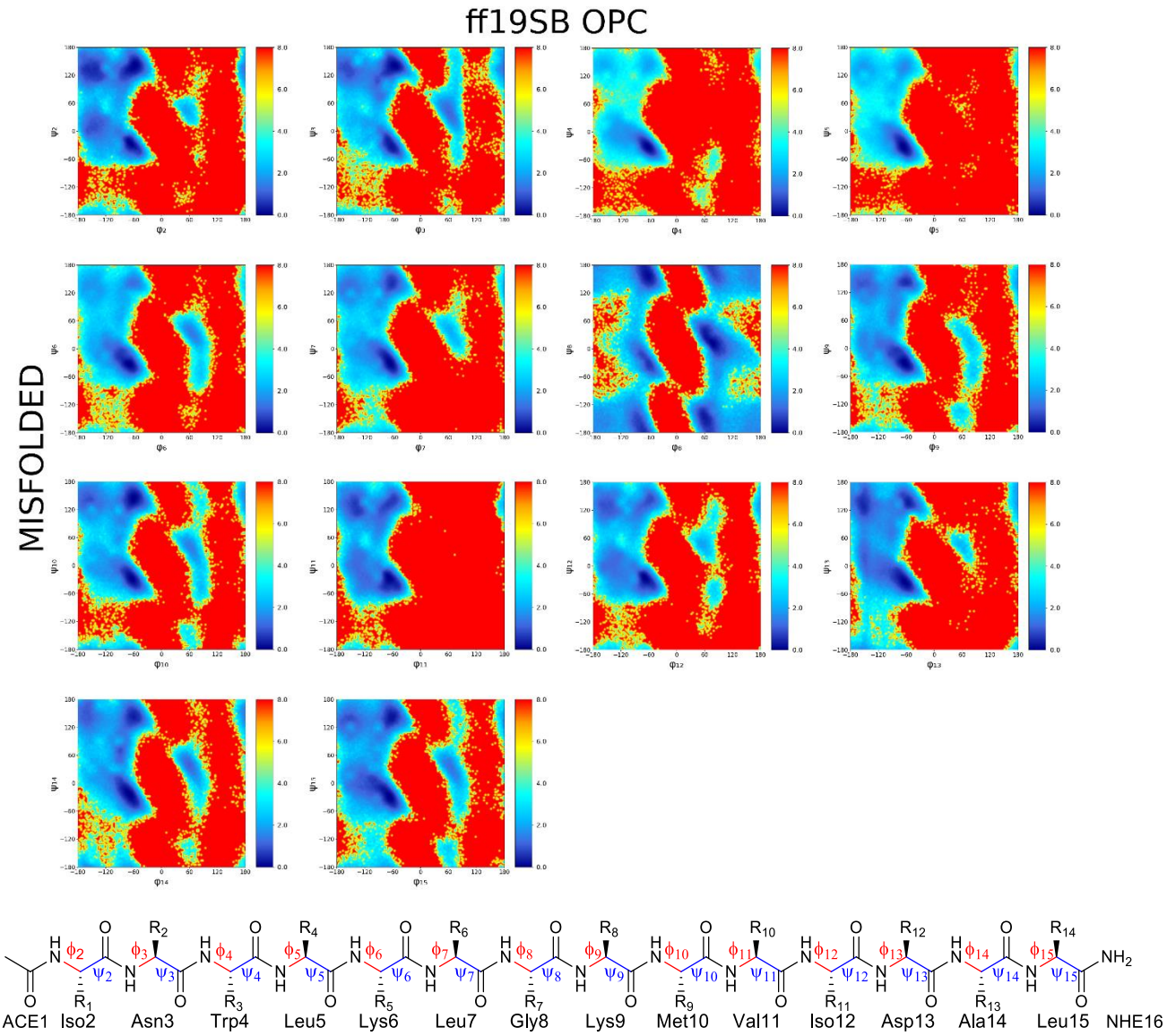

Figure S92. PMFs obtained from φ and ψ dihedral distributions of ID1 residues for the ff19SB/OPC combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID1 sequence and representation of φ and ψ angles numbering are also shown.

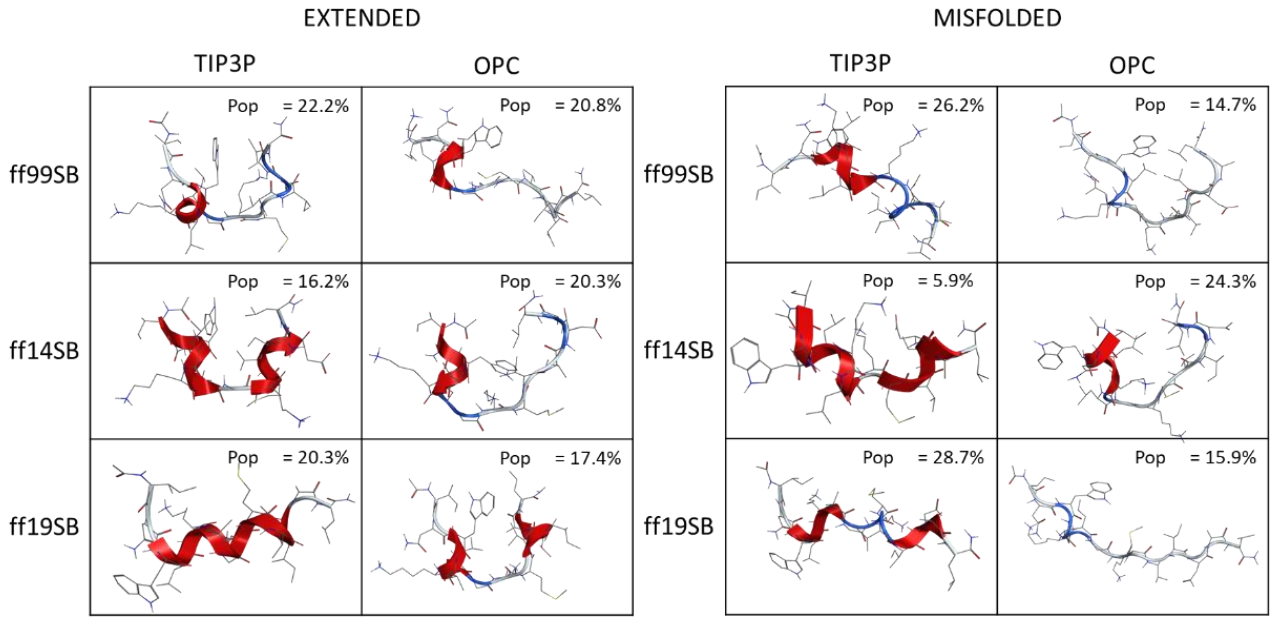

Figure S93. Representative conformation and population (pop%) of the second clusters from ID1 trajectories.

Table S9. H-bond analyses from ID1 trajectories. Only H-bonds involving the backbone are included in the table (donor N-H, acceptor C=O). Native H-bonds are highlighted in bold.

ff99SB OPC					
EXTENDED			MISFOLDED		
acceptor	donor	occ%	acceptor	donor	occ%
ASN3	LEU7	19.47	ASN3	LEU7	15.24
TRP4	GLY8	13.95	TRP4	GLY8	10.11
VAL11	LEU15	6.93	ILE2	LYS6	7.64
ILE2	LYS6	6.57			

ff99SB TIP3P					
EXTENDED			MISFOLDED		
acceptor	donor	occ%	acceptor	donor	occ%
ASN3	LEU7	34.89	ASN3	LEU7	28.27
TRP4	GLY8	28.97	TRP4	GLY8	17.39
MET10	ALA14	15.99	ILE2	LYS6	17.07
LEU7	VAL11	14.86	TRP4	LYS9	12.50
VAL11	LEU15	14.50	VAL11	LEU15	11.37
LYS9	ASP13	12.16	ACE1	LEU5	10.64
LEU5	LYS9	12.14	MET10	ALA14	8.04
TRP4	LYS9	11.69	ILE2	LEU5	7.02
LYS6	MET10	10.72	GLY8	ILE12	6.15
GLY8	ILE12	9.99	LEU7	LYS9	5.98
ILE2	LYS6	9.10	ASN3	GLY8	5.86
MET10	ASP13	7.25	LYS9	VAL11	5.53
ASN3	GLY8	6.49	MET10	ASP13	5.38
MET10	LEU15	6.36	MET10	ILE12	5.19
ASN3	LYS6	5.88	VAL11	ALA14	5.19
LEU7	MET10	5.81			

ff14SB OPC					
EXTENDED			MISFOLDED		
acceptor	donor	occ%	acceptor	donor	occ%

ff14SB TIP3P					
EXTENDED			MISFOLDED		
acceptor	donor	occ%	acceptor	donor	occ%

ASN3	LEU7	29.46
TRP4	GLY8	19.73
ILE2	LYS6	13.91
TRP4	LYS9	10.69
GLY8	ILE12	10.11
VAL11	LEU15	8.97
ACE1	LEU5	8.90
MET10	ALA14	7.05
GLY8	VAL11	6.12
ASN3	LYS6	5.58
LEU7	VAL11	5.52
LYS9	ASP13	5.47

ASN3	LEU7	27.03
ILE2	LYS6	20.96
TRP4	GLY8	16.92
VAL11	LEU15	14.70
MET10	ALA14	11.98
ACE1	LEU5	11.43
LYS9	ASP13	9.76
GLY8	ILE12	8.38
TRP4	LYS9	8.25
ILE2	LEU5	6.61
LEU7	VAL11	5.78
VAL11	ALA14	5.75
LEU5	LYS9	5.56
GLY8	VAL11	5.11
MET10	ASP13	5.04

ASN3	LEU7	44.94
TRP4	GLY8	34.08
LEU7	VAL11	21.72
GLY8	ILE12	20.38
LEU5	LYS9	20.37
VAL11	LEU15	19.04
ILE2	LYS6	18.77
LYS6	MET10	18.20
LYS9	ASP13	18.05
MET10	ALA14	15.95
TRP4	LYS9	12.66
ACE1	LEU5	10.67
GLY8	VAL11	7.00
LEU7	MET10	6.15
GLY8	ASP13	5.71

TRP5	TYR9	49.83
TYR9	TYR13	40.46
GLU7	LEU11	39.56
LEU8	LYS12	37.93
THR4	LEU8	34.15
GLN6	GLN10	33.25
GLN10	LYS14	26.96
LEU3	GLU7	19.75
LYS2	GLN6	15.38
LEU11	GLY15	10.46
ACE1	TRP5	10.39
GLN10	GLY15	7.91
THR4	GLU7	7.42
TYR9	LYS14	6.00

ff19SB OPC

EXTENDED

acceptor	donor	occ%
ASN3	LEU7	18.17
ASN3	LYS6	11.41
TRP4	GLY8	10.93
TRP4	LYS9	6.03
GLY8	VAL11	5.81
LYS9	ASP13	5.09

MISFOLDED

acceptor	donor	occ%
LEU8	LYS12	34.48
TRP5	TYR9	32.19
TYR9	LYS14	26.75
LEU3	GLU7	25.95
TYR9	TYR13	25.33
GLU7	LEU11	24.86
GLN6	GLN10	23.14
THR4	LEU8	22.81
TRP5	GLN10	17.07
LEU8	TYR13	16.75
LYS2	GLN6	15.89
GLN10	GLY15	15.70
ACE1	TRP5	14.54
GLN10	LYS14	13.21
GLU7	LYS12	11.39
GLN6	LEU11	11.02
LEU3	LEU8	10.15
ACE1	GLN6	8.00
LEU11	ILE16	7.72
THR4	TYR9	7.66
LEU11	GLY15	7.02
GLN10	ILE16	5.63
LEU3	GLN6	5.45

ff19SB TIP3P

EXTENDED

acceptor	donor	occ%
ASN3	LEU7	35.90
TRP4	GLY8	20.21
ILE2	LYS6	19.84
TRP4	LYS9	14.58
ACE1	LEU5	12.13
LEU5	GLY8	9.42
VAL11	LEU15	9.06
ASN3	LYS6	8.35
LYS9	ASP13	7.68
MET10	ALA14	7.08
LEU5	LYS9	6.80
VAL11	ALA14	6.30
ACE1	TRP4	6.20
GLY8	VAL11	6.13
MET10	ASP13	6.07
LYS6	MET10	5.88
ILE2	LEU5	5.67
GLY8	ILE12	5.06

MISFOLDED

acceptor	donor	occ%
GLU7	LEU11	39.46
TRP5	TYR9	37.55
LEU8	LYS12	30.56
TYR9	TYR13	27.23
THR4	LEU8	27.00
GLN10	LYS14	21.80
GLN6	GLN10	20.30
GLU7	GLN10	9.53
LEU11	GLY15	9.03
THR4	GLU7	8.81
TYR9	LYS12	6.21
LYS2	GLN6	5.35

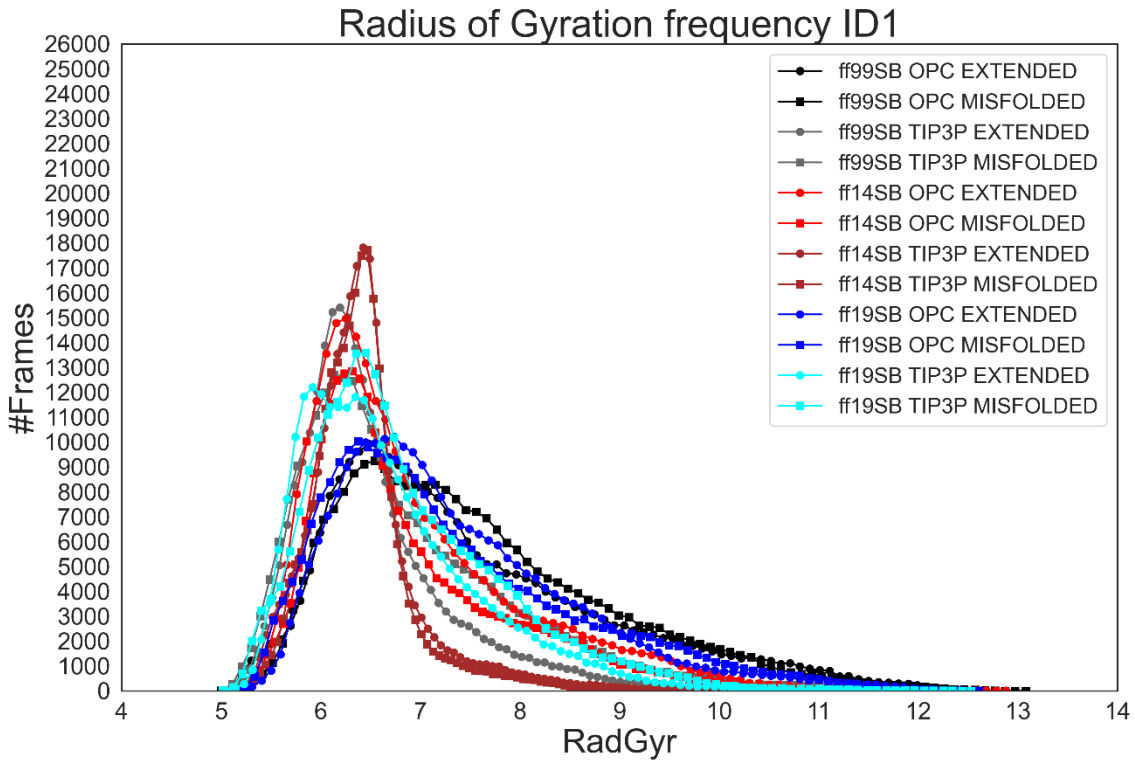

Figure S94. Radius of gyration frequencies calculated on the last 500ns of ID1 trajectories.

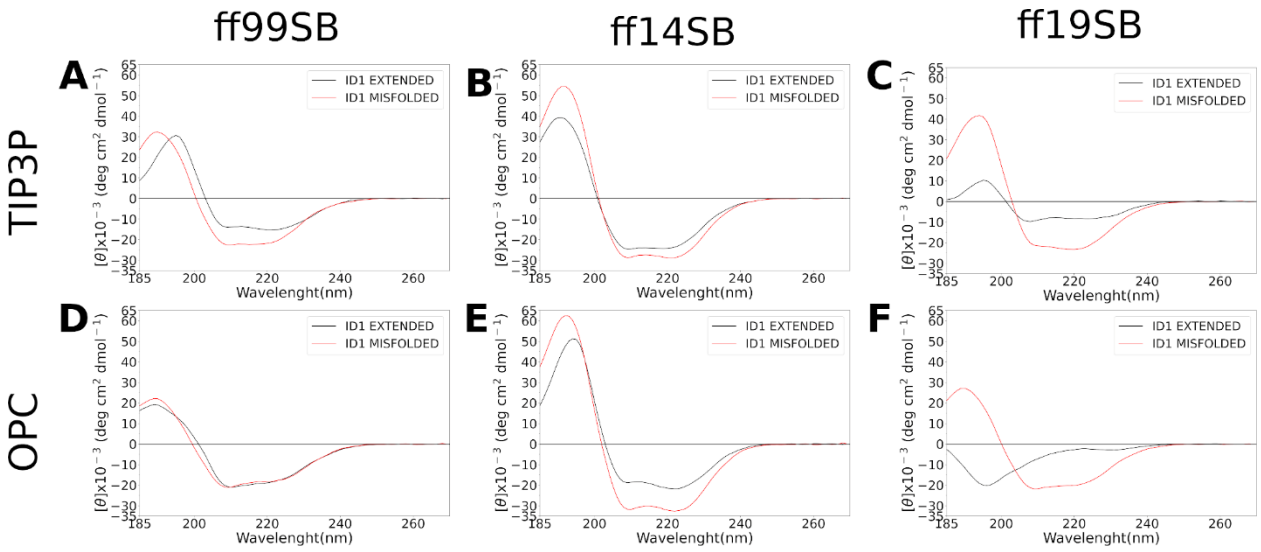

Figure S95. SESCA CD spectra of ID1 calculated on the main cluster obtained from the last 500 ns of aMD trajectory. Results from extended and misfolded simulations are reported in black and red lines, respectively.

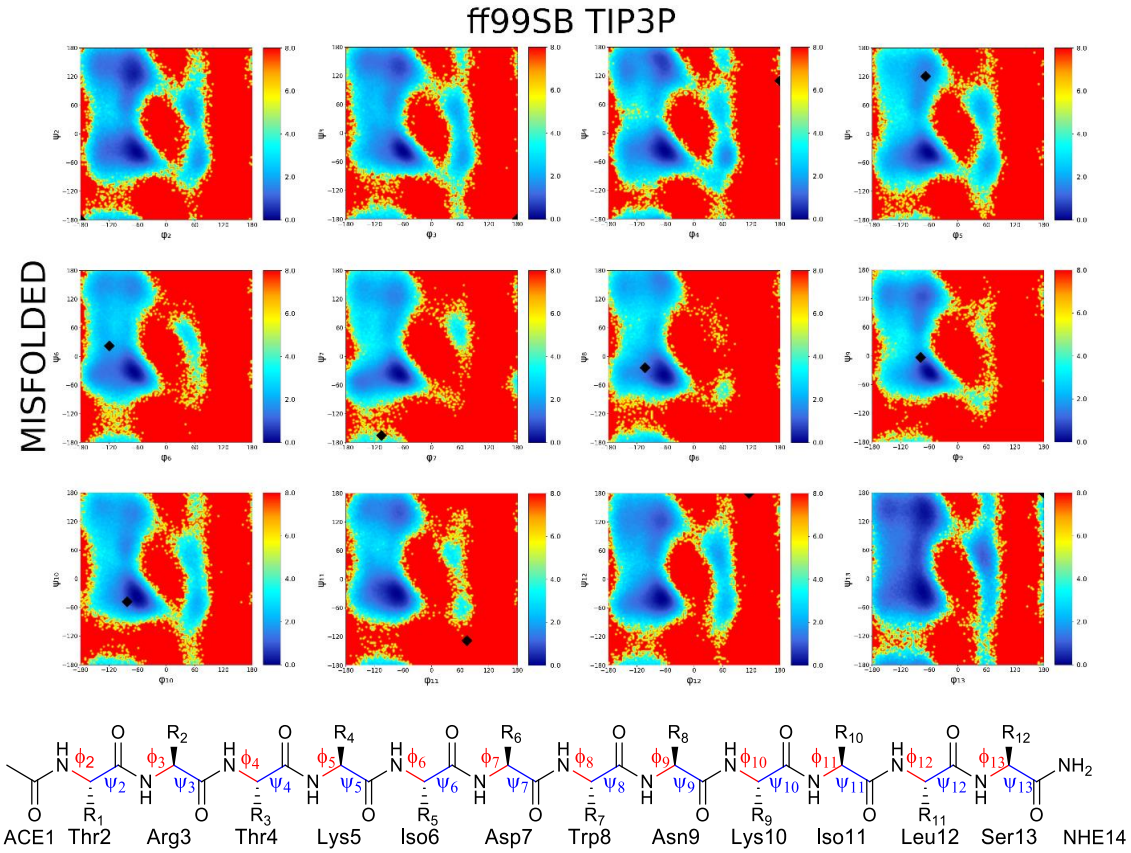

Figure S96. PMFs obtained from φ and ψ dihedral distributions of ID2 residues for the ff99SB/TIP3P combination from extended (top panels) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID2 sequence and representation of φ and ψ angles numbering are also shown.

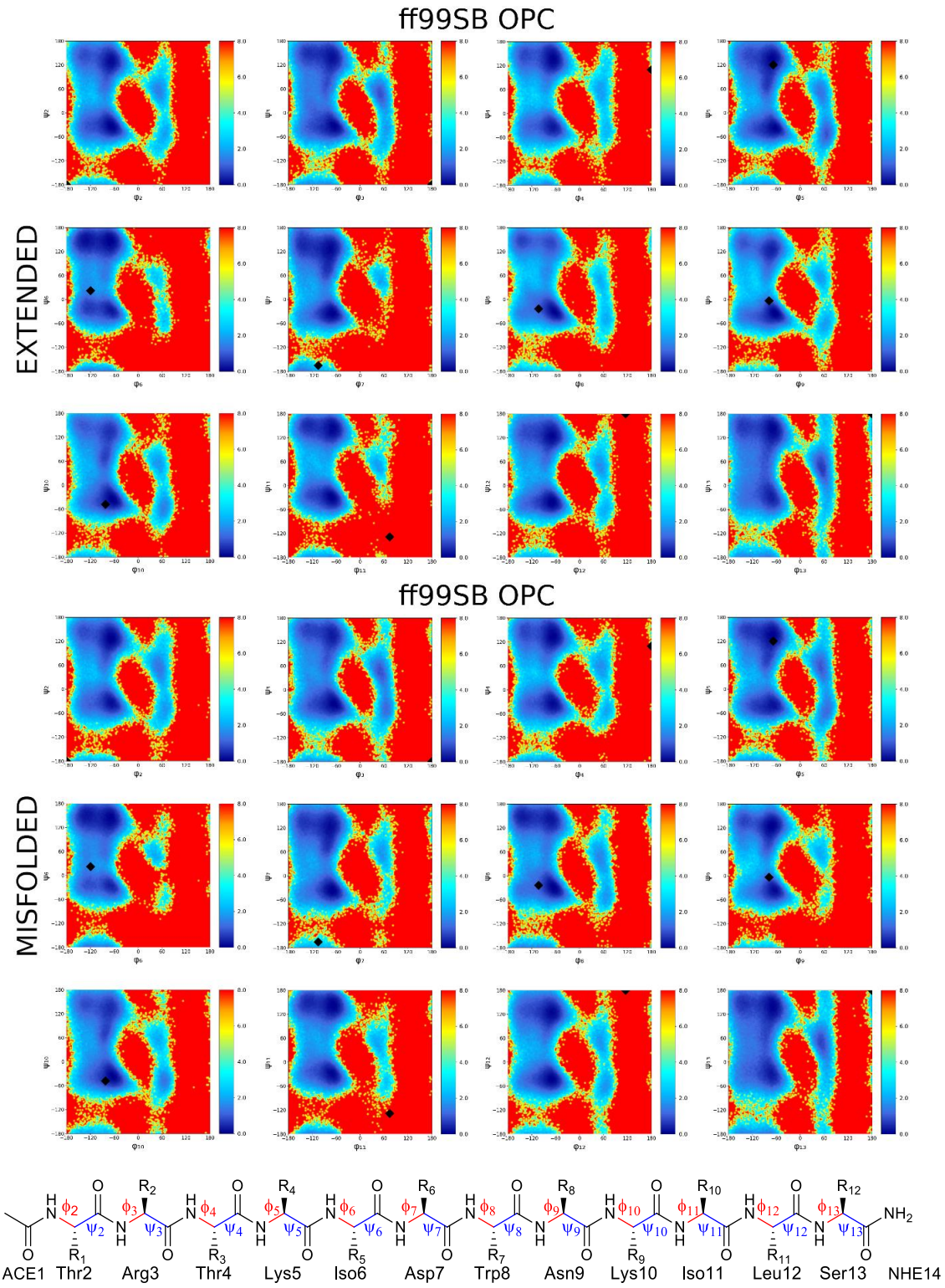

Figure S97. PMFs obtained from φ and ψ dihedral distributions of ID2 residues for the ff99SB/OPC combination from extended (top panels) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID2 sequence and representation of φ and ψ angles numbering are also shown.

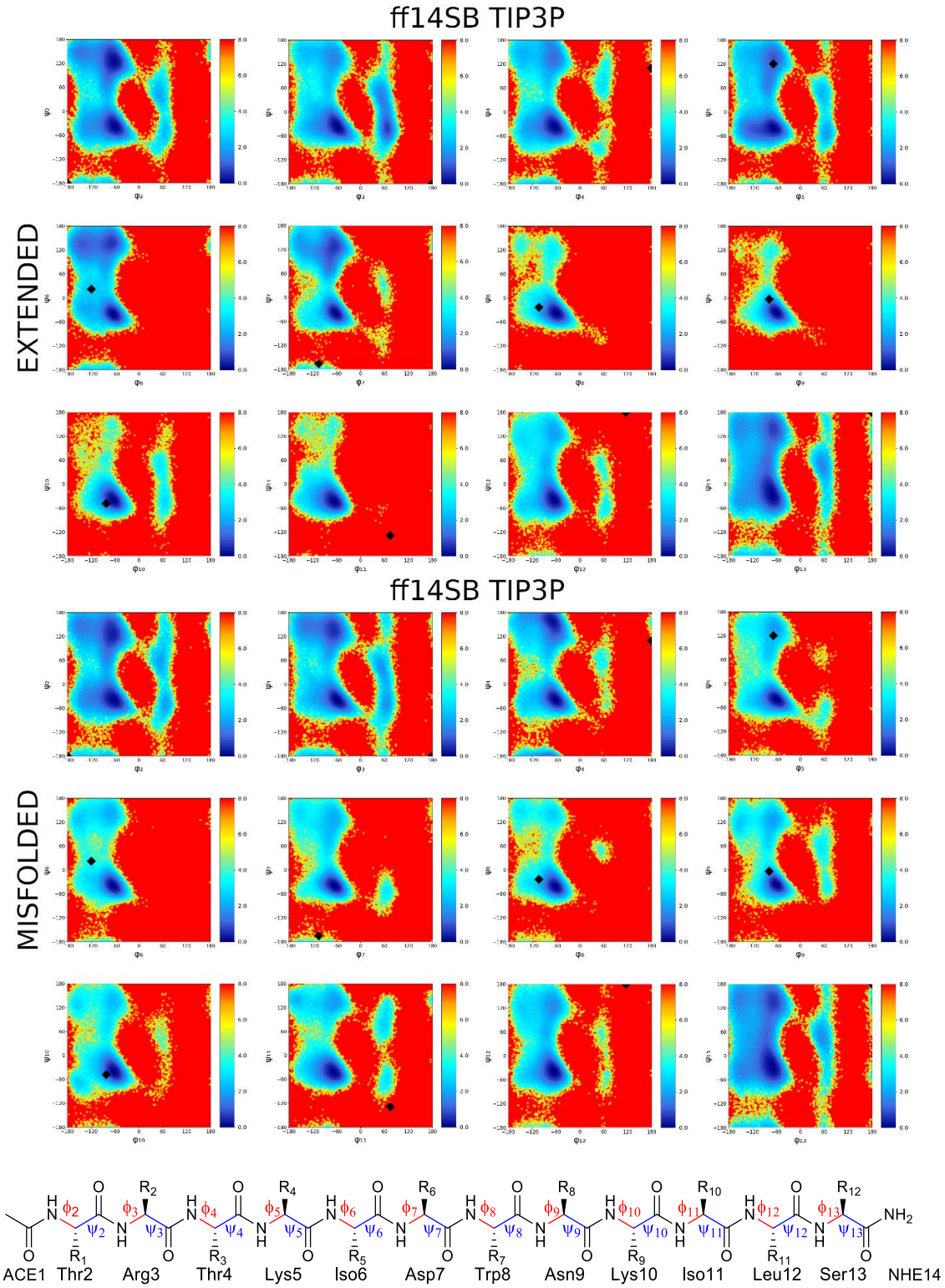

Figure S98. PMFs obtained from φ and ψ dihedral distributions of ID2 residues for the ff14SB/TIP3P combination from extended (top panels) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID2 sequence and representation of φ and ψ angles numbering are also shown.

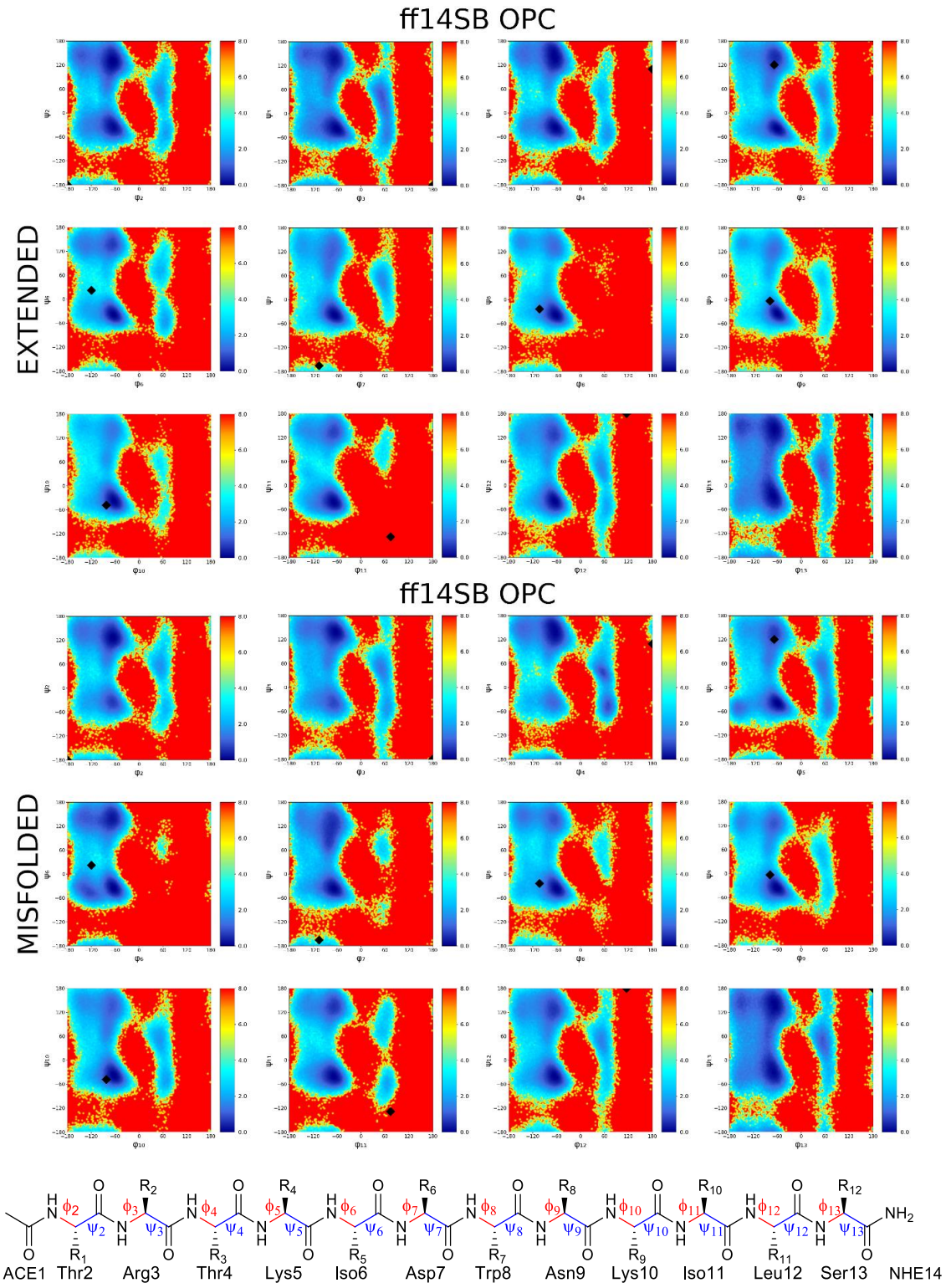

Figure S99. PMFs obtained from φ and ψ dihedral distributions of ID2 residues for the ff14SB/OPC combination from extended (top panels) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID2 sequence and representation of φ and ψ angles numbering are also shown.

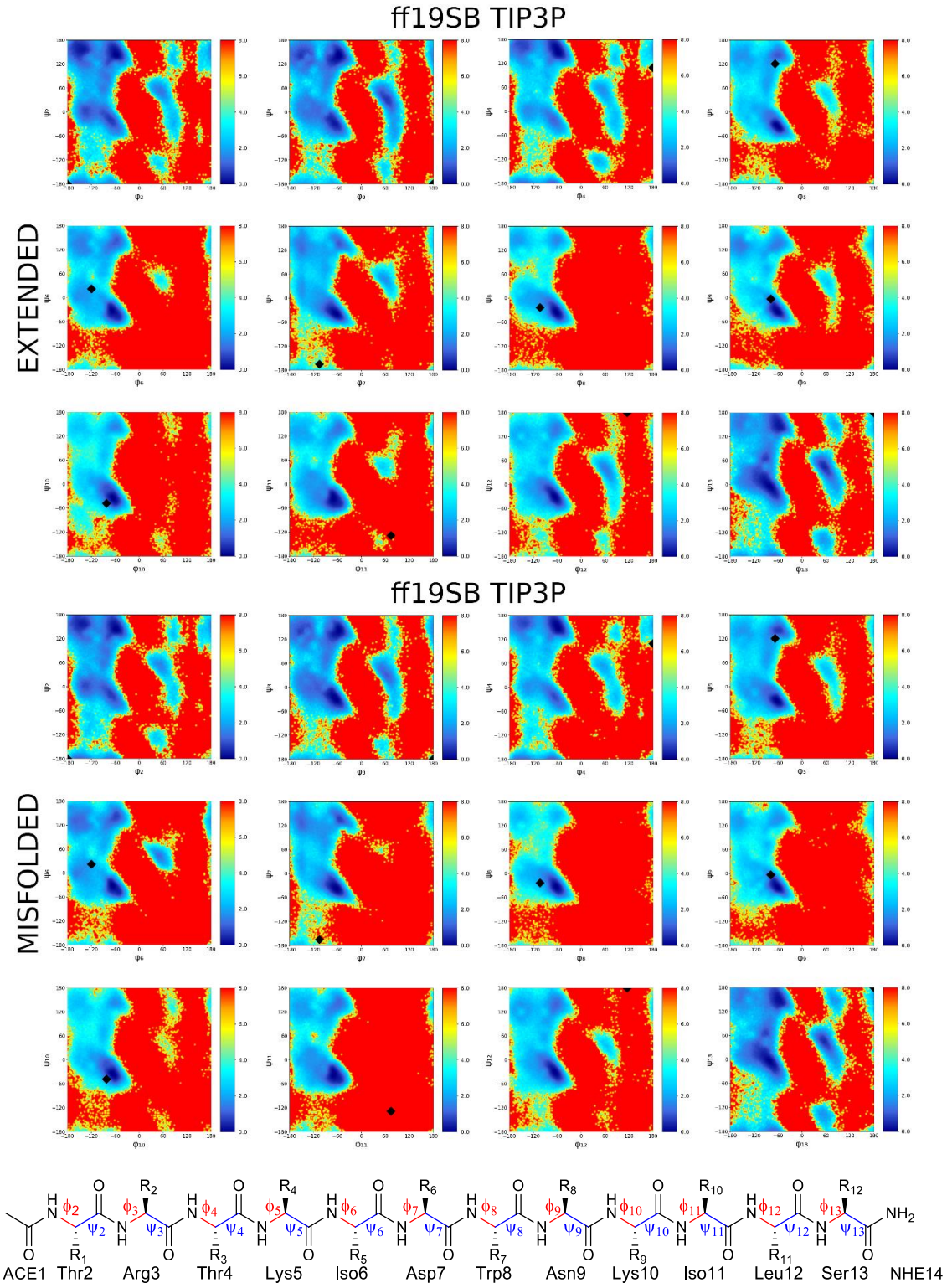

Figure S100. PMFs obtained from φ and ψ dihedral distributions of ID2 residues for the ff19SB/TIP3P combination from extended (top panels) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID2 sequence and representation of φ and ψ angles numbering are also shown.

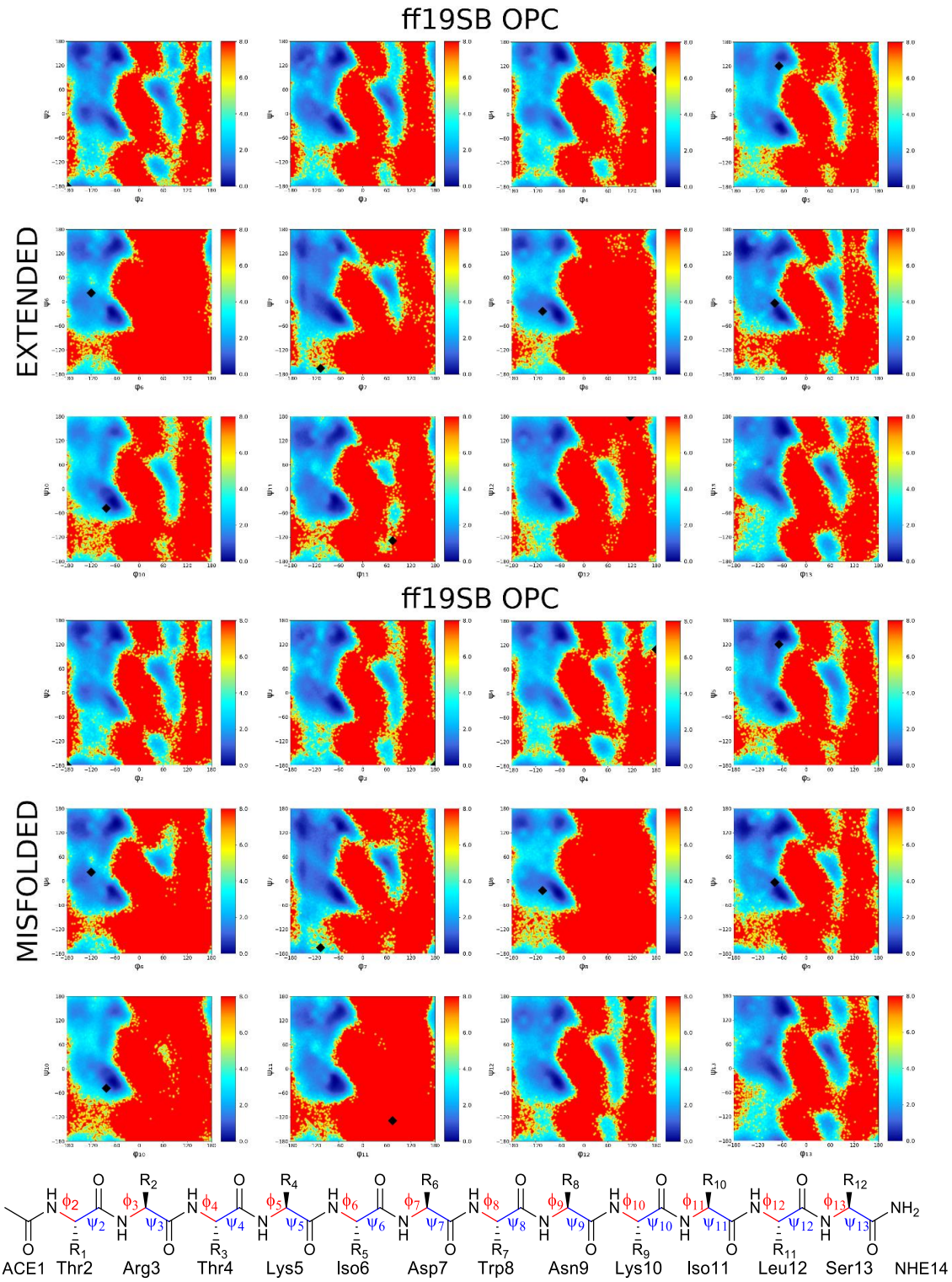

Figure S101. PMFs obtained from φ and ψ dihedral distributions of ID2 residues for the ff19SB/OPC combination from extended (top panels) and misfolded (bottom panels) conformations. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID2 sequence and representation of φ and ψ angles numbering are also shown.

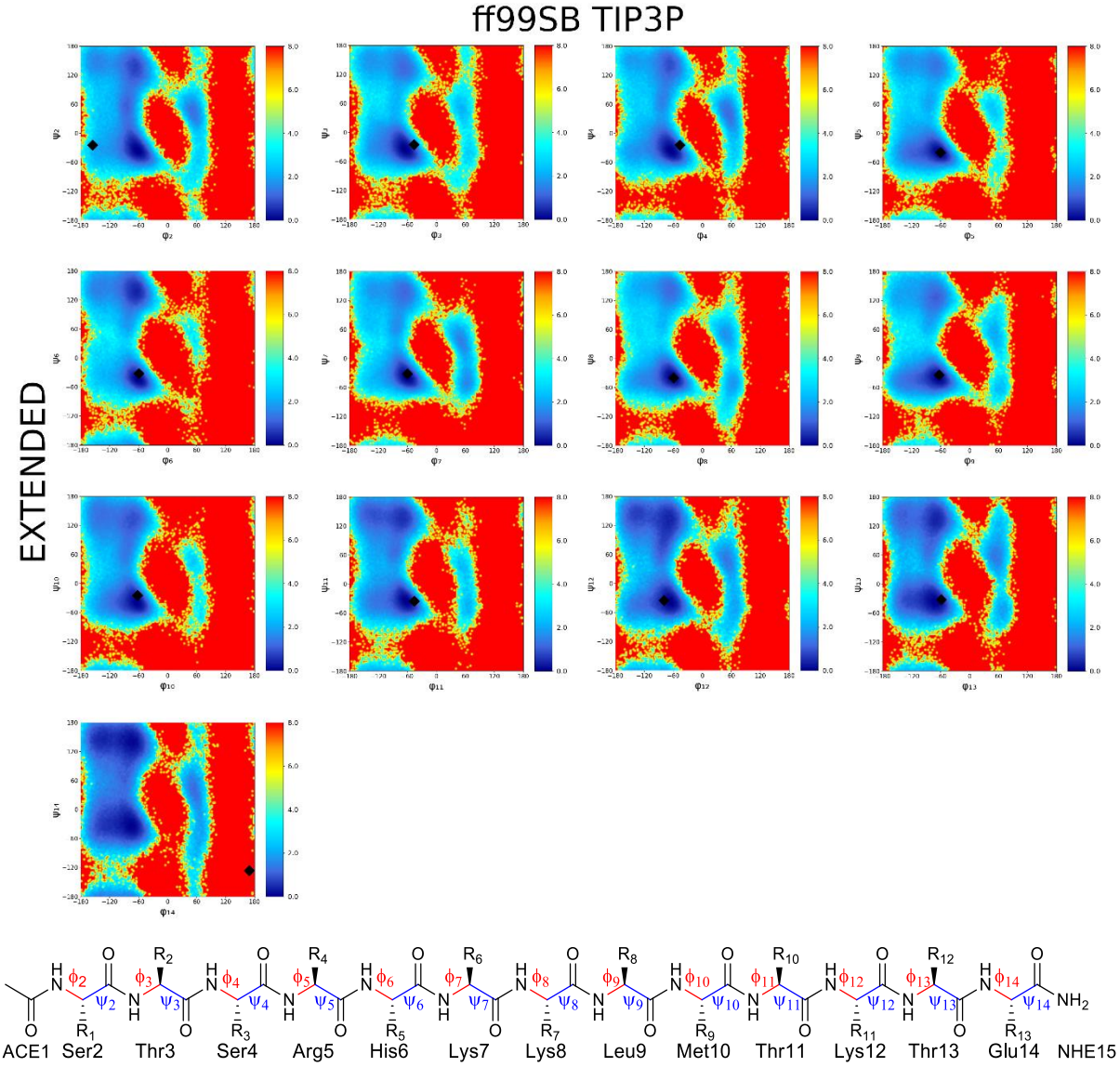

Figure S102. PMFs obtained from φ and ψ dihedral distributions of ID3 residues for ff99SB/TIP3P combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID3 sequence and representation of φ and ψ angles numbering are also shown.

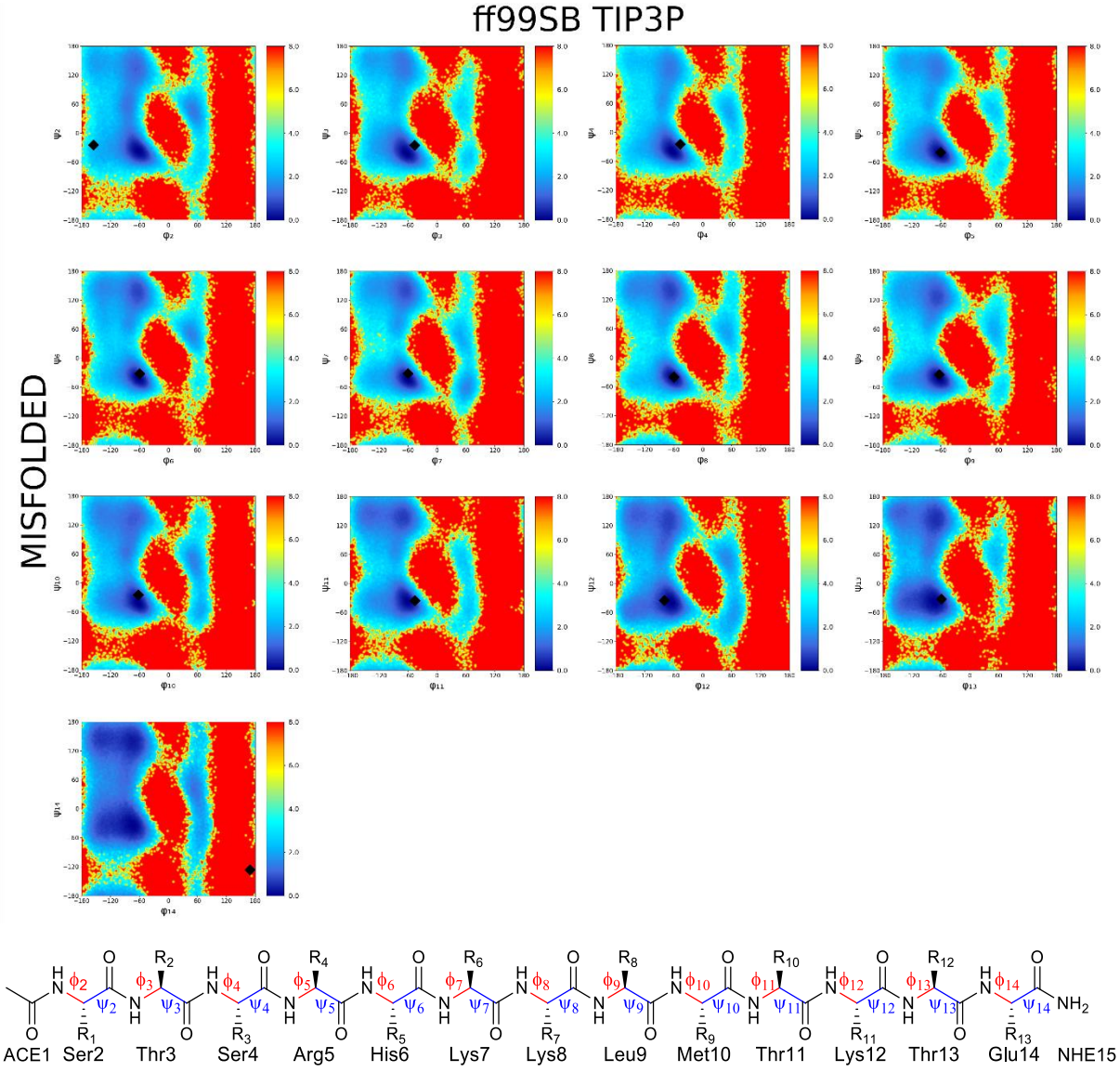

Figure S103. PMFs obtained from φ and ψ dihedral distributions of ID3 residues for the ff99SB/TIP3P combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID3 sequence and representation of φ and ψ angles numbering are also shown.

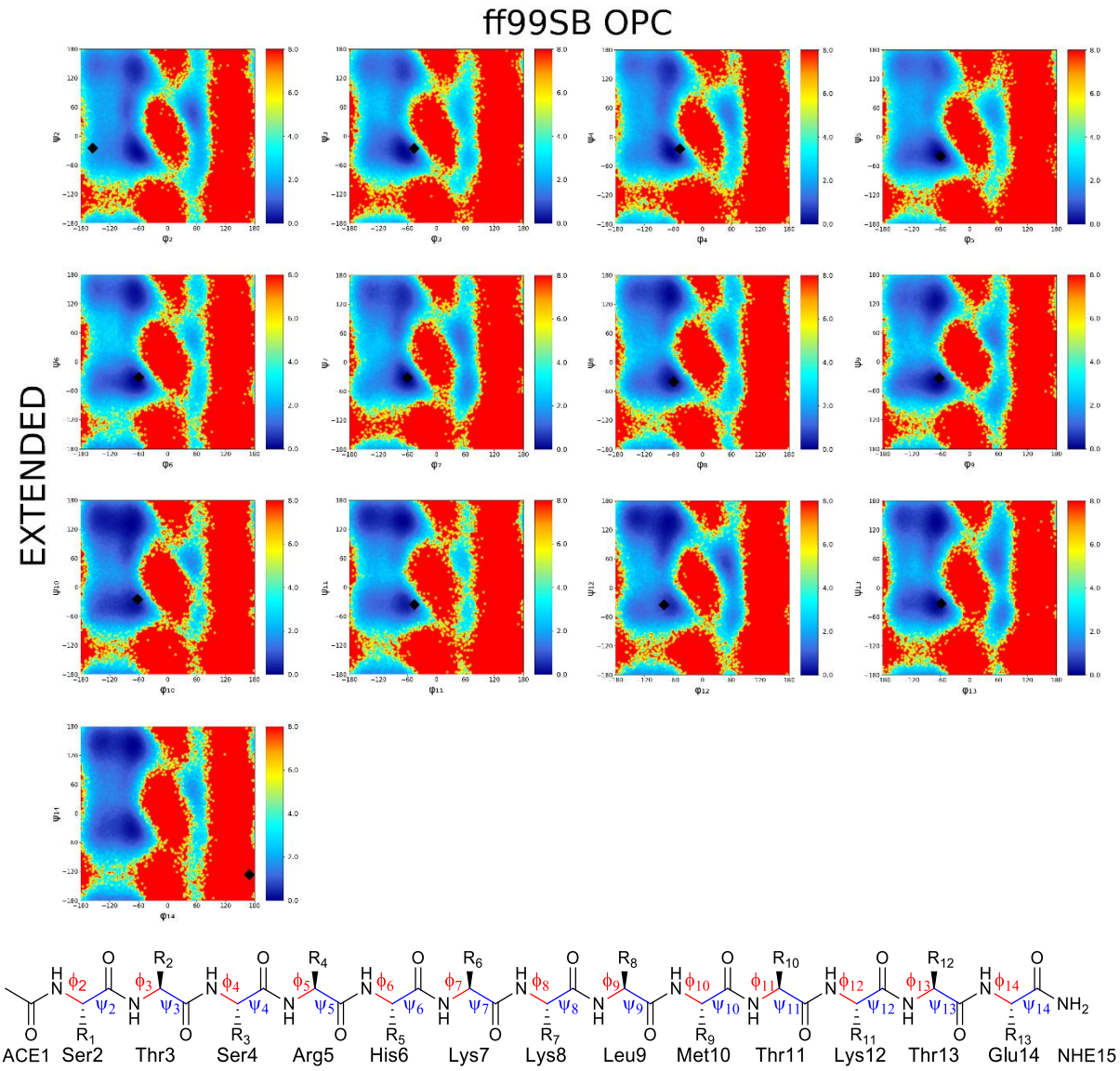

Figure S104. PMFs obtained from φ and ψ dihedral distributions of ID3 residues for the ff99SB/OPC combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID3 sequence and representation of φ and ψ angles numbering are also shown.

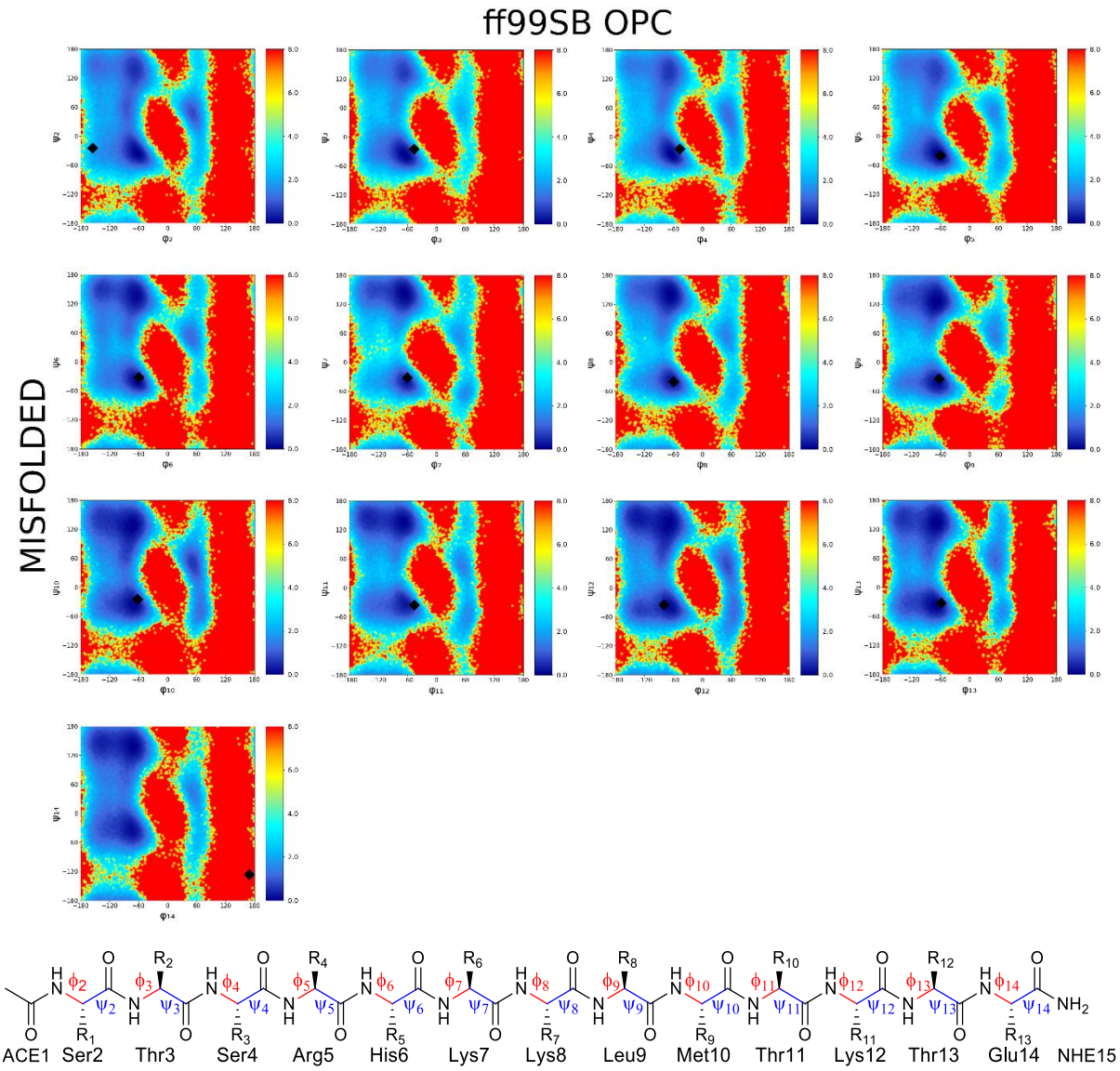

Figure S105. PMFs obtained from φ and ψ dihedral distributions of ID3 residues for the ff99SB/OPC combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID3 sequence and representation of φ and ψ angles numbering are also shown.

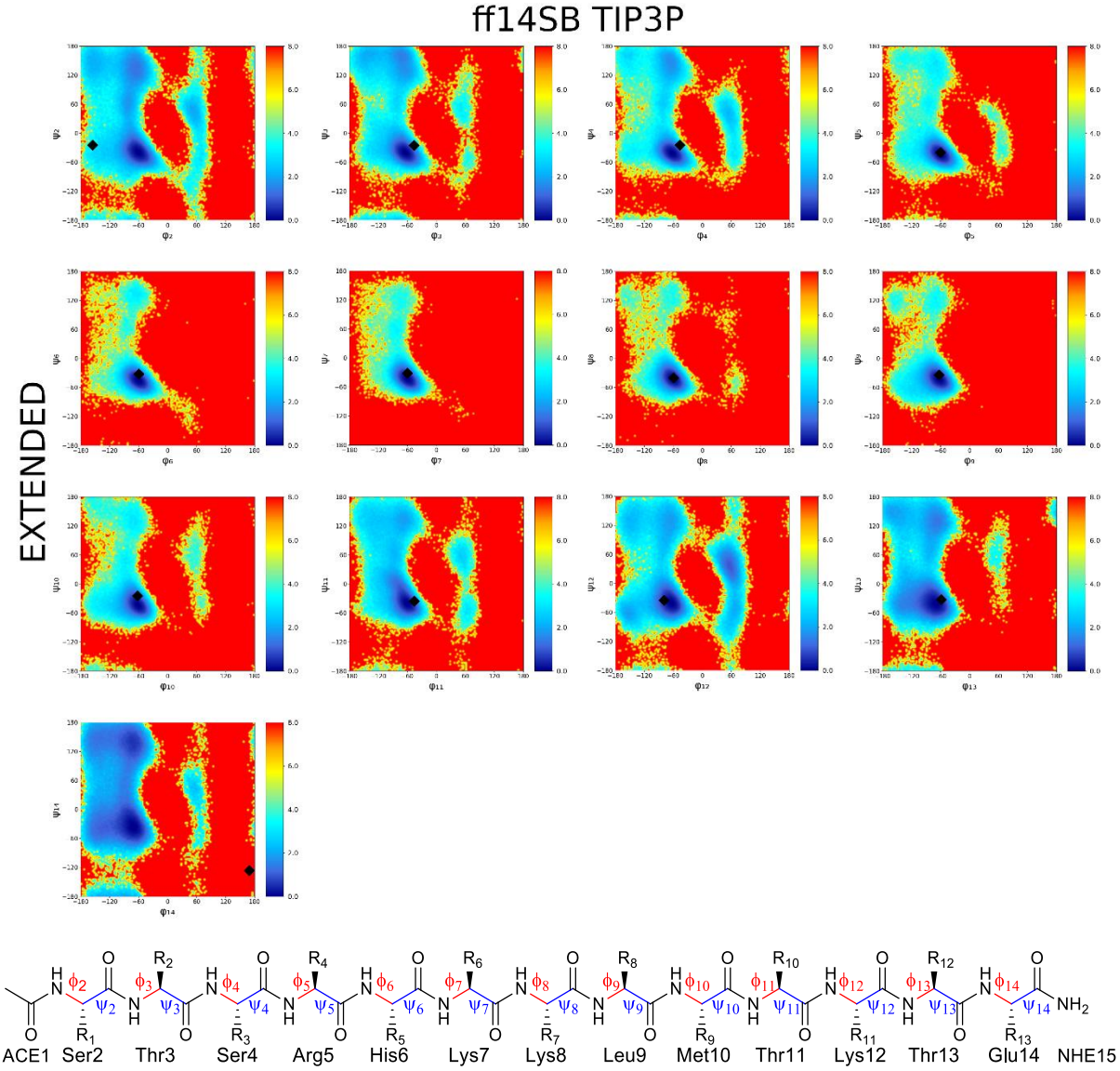

Figure S106. PMFs obtained from φ and ψ dihedral distributions of ID3 residues for the ff14SB/TIP3P combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID3 sequence and representation of φ and ψ angles numbering are also shown.

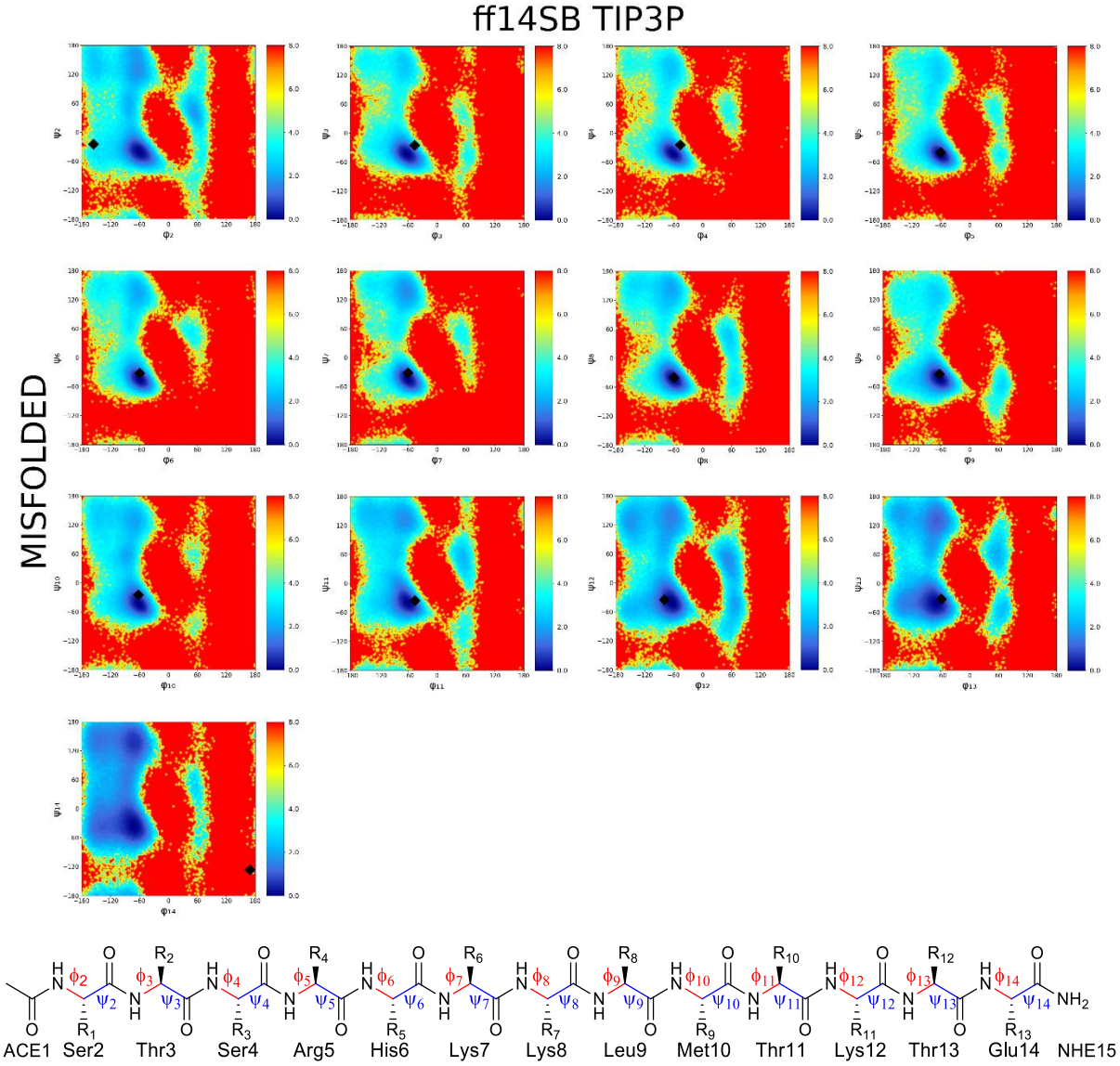

Figure S107. PMFs obtained from φ and ψ dihedral distributions of ID3 residues for the ff14SB/TIP3P combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID3 sequence and representation of φ and ψ angles numbering are also shown.

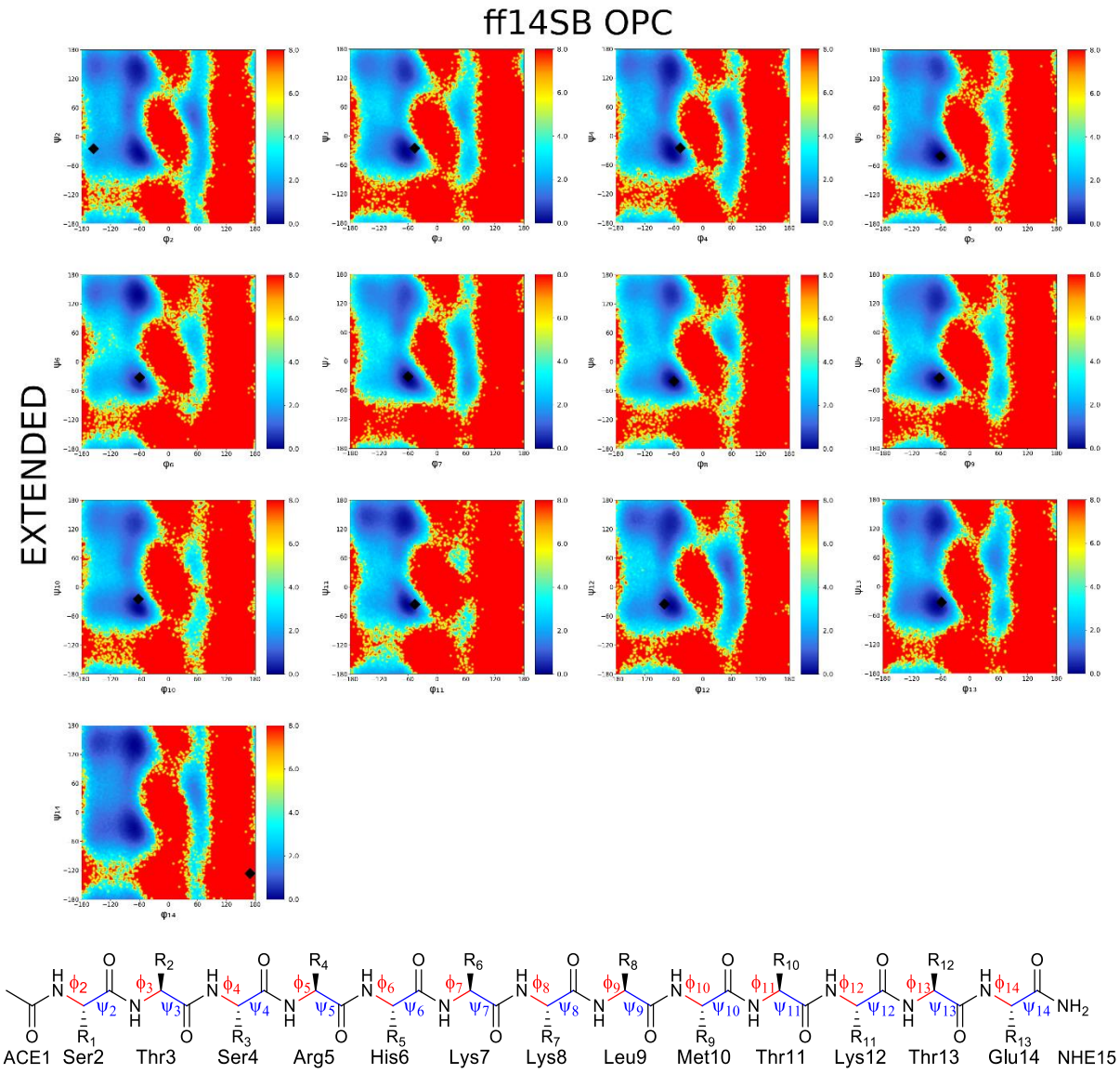

Figure S108. PMFs obtained from φ and ψ dihedral distributions of ID3 residues for the ff14SB/OPC combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID3 sequence and representation of φ and ψ angles numbering are also shown.

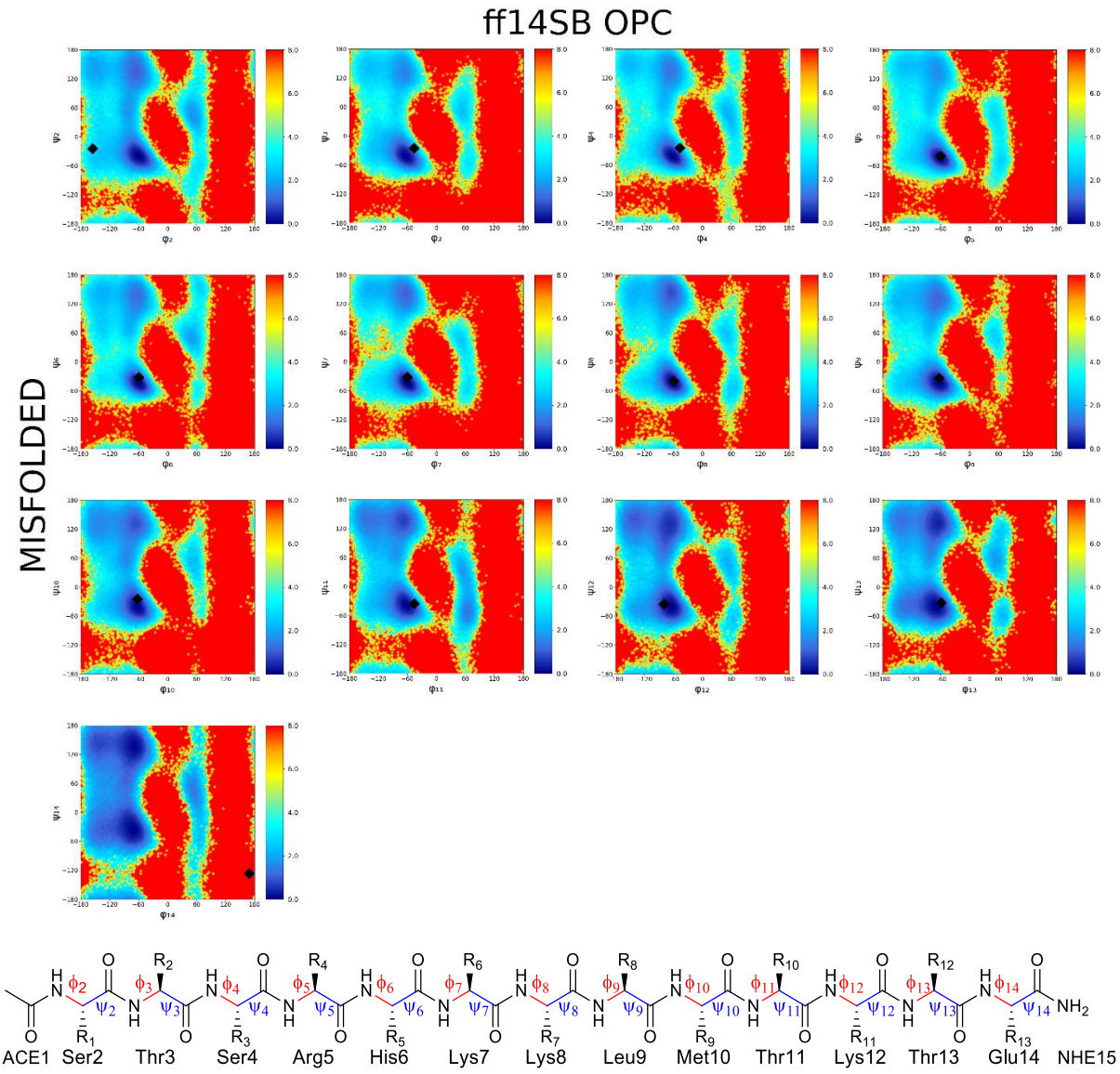

Figure S109. PMFs obtained from φ and ψ dihedral distributions of ID3 residues for the ff14SB/OPC combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID3 sequence and representation of φ and ψ angles numbering are also shown.

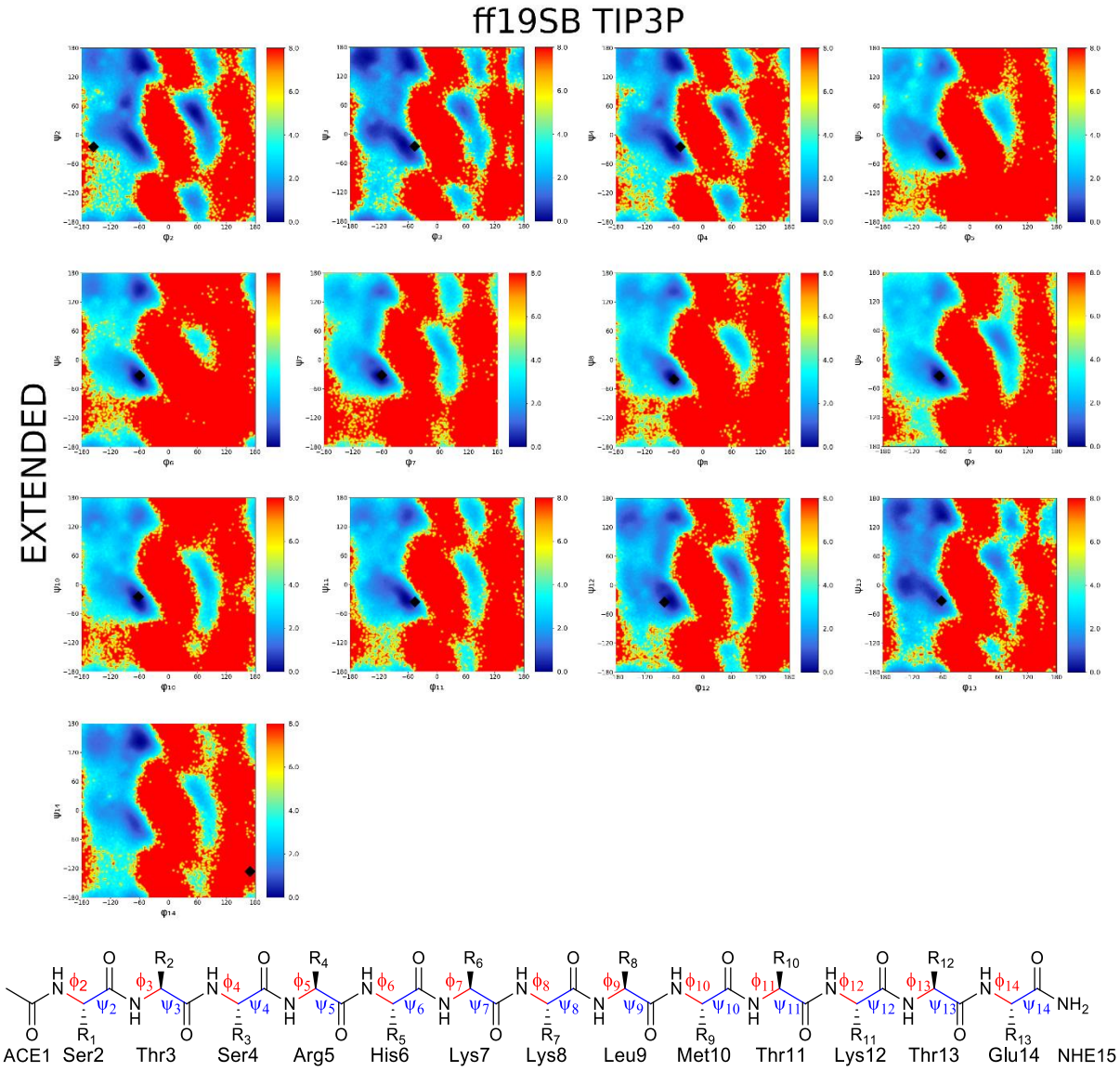

Figure S110. PMFs obtained from φ and ψ dihedral distributions of ID3 residues for the ff19SB/TIP3P combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID3 sequence and representation of φ and ψ angles numbering are also shown.

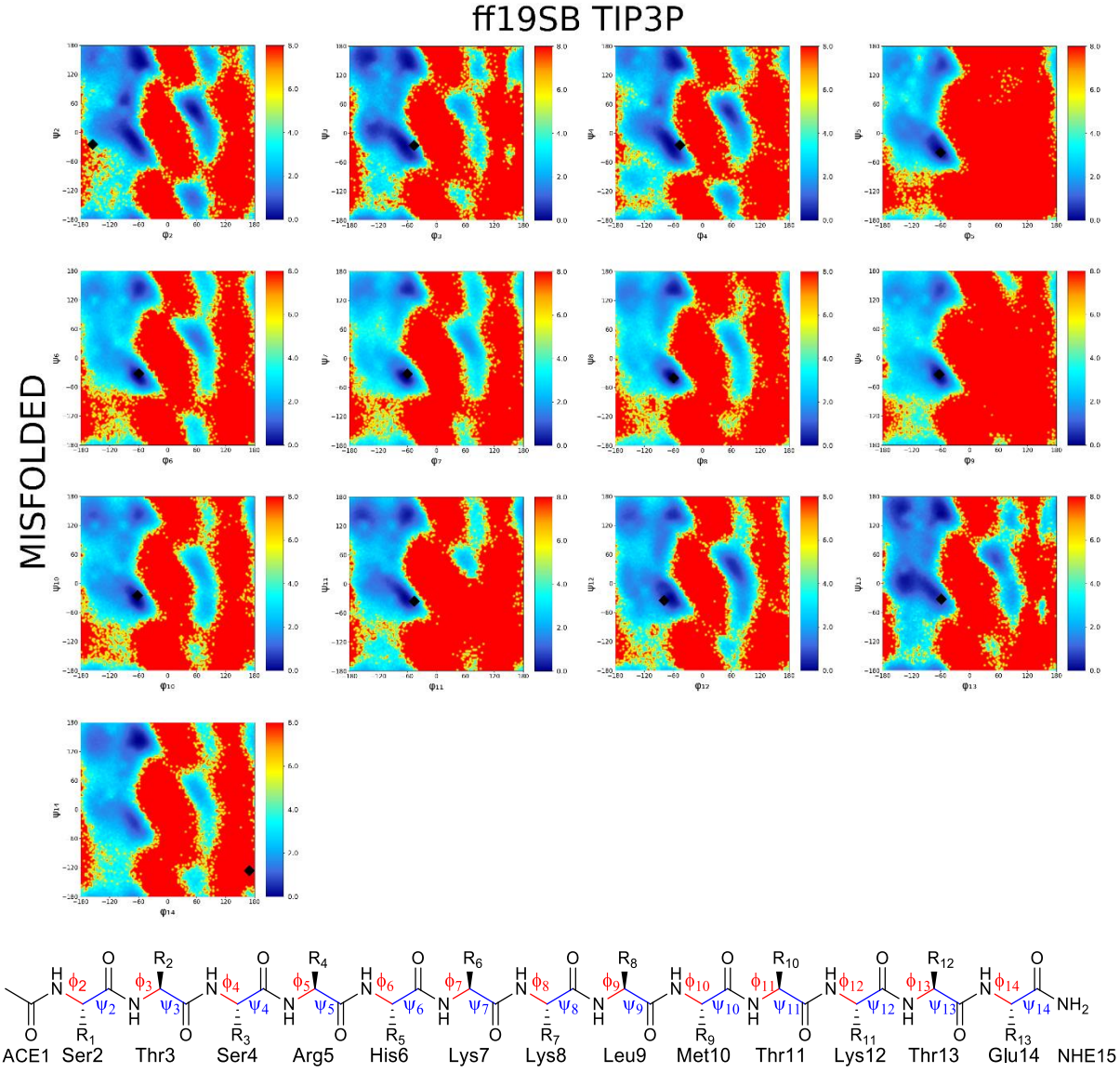

Figure S111. PMFs obtained from φ and ψ dihedral distributions of ID3 residues for the ff19SB/TIP3P combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID3 sequence and representation of φ and ψ angles numbering are also shown.

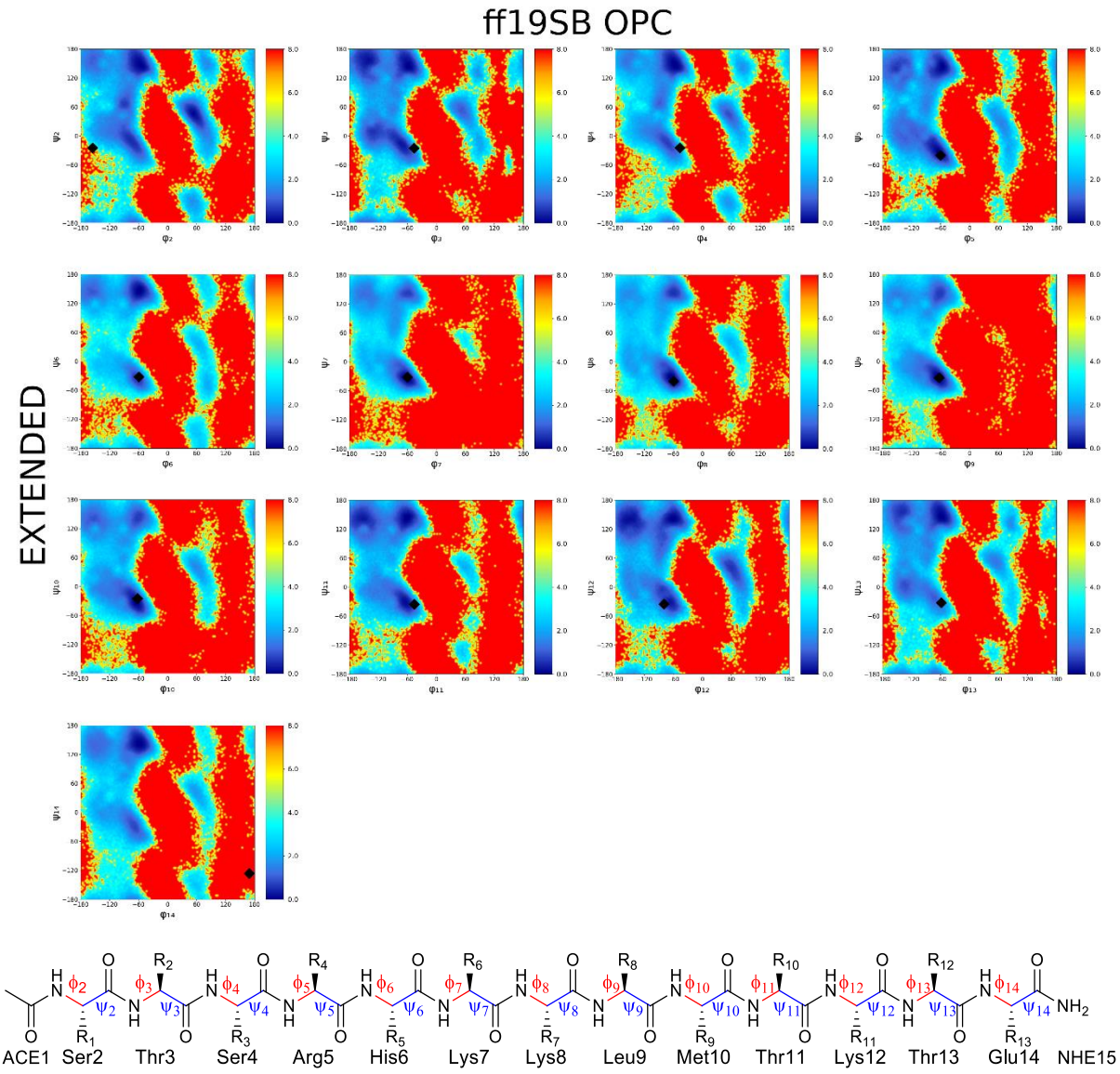

Figure S112. PMFs obtained from φ and ψ dihedral distributions of ID3 residues for the ff19SB/OPC combination from an extended conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID3 sequence and representation of φ and ψ angles numbering are also shown.

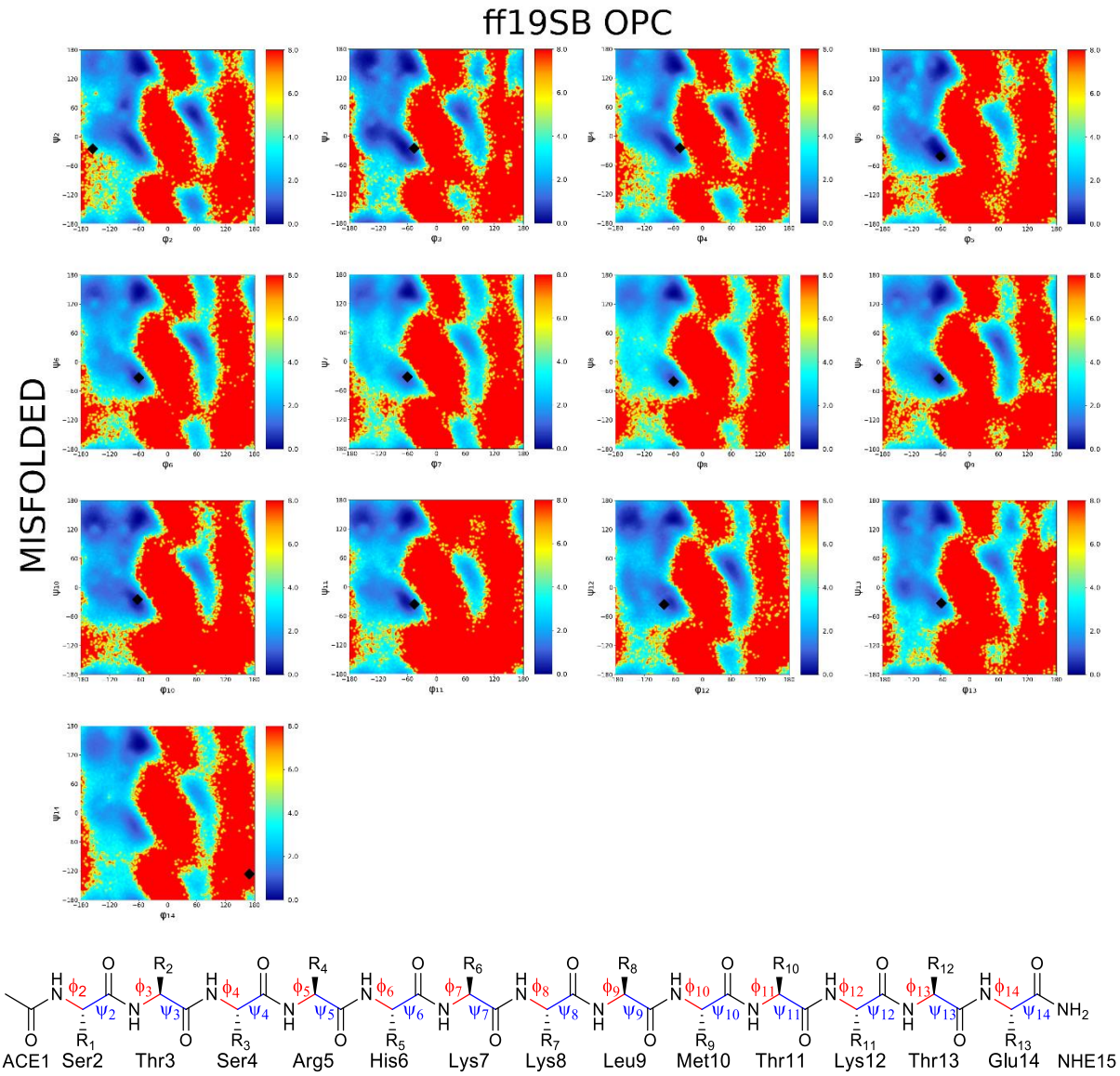

Figure S113. PMFs obtained from φ and ψ dihedral distributions of ID3 residues for the ff19SB/OPC combination from a misfolded conformation. PMFs are shown as heat maps (0.0 – 8.0 kcal/mol range) from dark blue to red. The native conformation's φ and ψ angles are reported as black diamonds. ID3 sequence and representation of φ and ψ angles numbering are also shown.

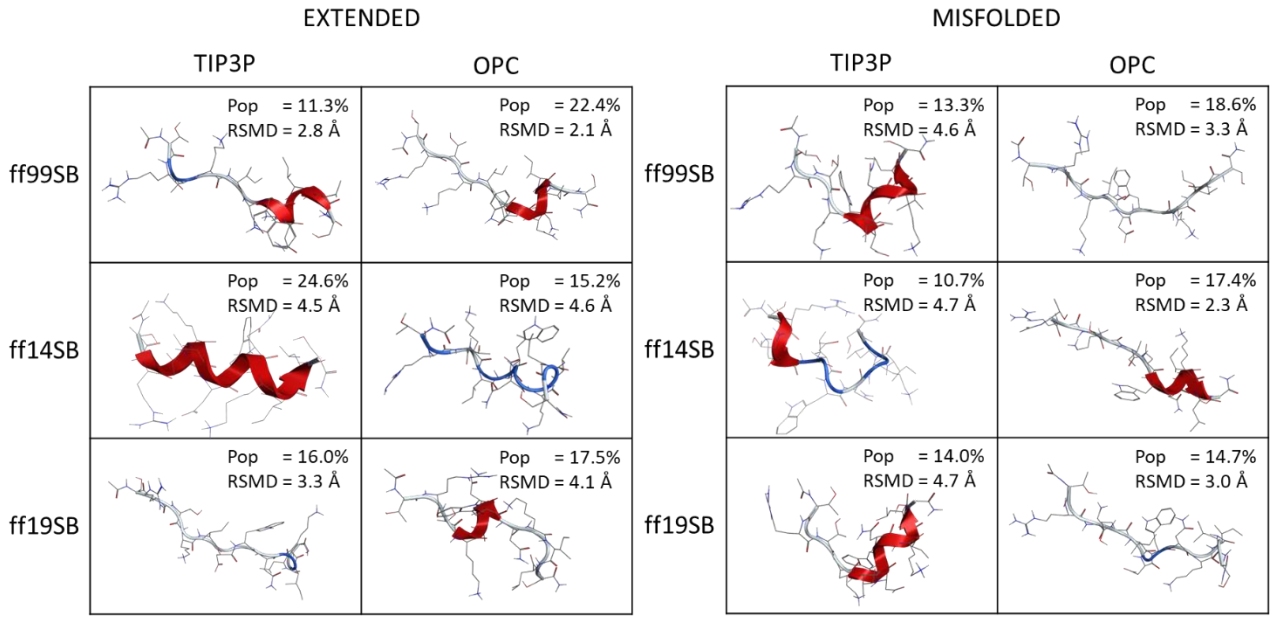

Figure S114. Representative conformation and population (pop%) of the second clusters from ID2 trajectories. RMSDs vs native structure are also shown.

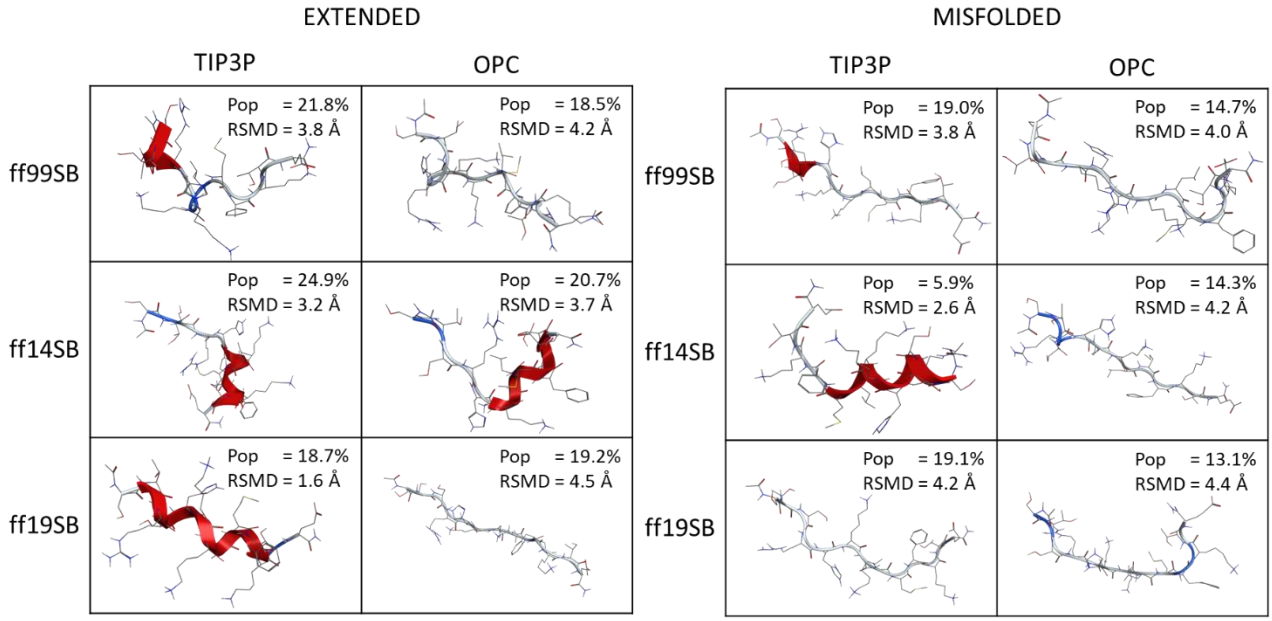

Figure S115. Representative conformation and population (pop%) of the second clusters from ID3 trajectories. RMSDs vs native structure are also shown.

Table S10. H-bond analyses from ID2 trajectories. Only H-bonds involving the backbone are included in the table (donor N-H, acceptor C=O). Native H-bonds are highlighted in bold.

NATIVE		
acceptor	donor	Distance
TRP8	**LEU12**	**2.52**
THR4	**ILE6**	**3.16**
TRP8	**LYS10**	**3.21**
ASP7	**ASN9**	**3.51**
ASP7	**LYS10**	**3.54**
LYS5	**ASP7**	**3.68**
ASN9	**LEU12**	**3.92**
ASN9	**ILE11**	**4.13**

ff99SB OPC

EXTENDED			MISFOLDED		
acceptor	donor	occ%	acceptor	donor	occ%
TRP8	**LEU12**	23.83	ASN9	SER13	18.21
ASN9	SER13	21.21	LYS5	ASN9	17.94
LYS5	ASN9	20.76	TRP8	LEU12	17.24
THR4	TRP8	17.57	THR4	TRP8	14.43
ILE6	LYS10	13.69	THR2	ILE6	12.52
THR2	ILE6	12.48	ILE6	LYS10	12.19
ARG3	ASP7	11.66	ARG3	ASP7	11.98
TRP8	ILE11	9.84	ACE1	LYS5	8.34
THR4	ASP7	7.66	THR2	LYS5	7.32
THR2	LYS5	7.37	TRP8	ILE11	7.25
ASP7	ILE11	7.35	THR4	ASP7	6.16
ACE1	LYS5	6.38	ASP7	ILE11	5.49
ASP7	LYS10	6.07	ARG3	TRP8	5.33

ff99SB TIP3P

EXTENDED			MISFOLDED		
acceptor	donor	occ%	acceptor	donor	occ%
TRP8	**LEU12**	6.58	**ASN9**	**ILE11**	5.02
THR4	**ILE6**	5.49			
ASN9	SER13	5.42			
ASN9	**ILE11**	5.04			

ff14SB OPC

EXTENDED			MISFOLDED		
acceptor	donor	occ%	acceptor	donor	occ%
TRP8	**LEU12**	21.07	**TRP8**	**LEU12**	14.48
ASN9	SER13	16.54	ASN9	SER13	13.31
LYS5	ASN9	15.67	LYS5	ASN9	7.78
THR4	TRP8	11.90	THR4	TRP8	7.24
ILE6	LYS10	9.60	THR2	ILE6	6.60
TRP8	ILE11	9.34	ASP7	ILE11	6.57
ASP7	ILE11	7.37	TRP8	ILE11	6.11
ASP7	**LYS10**	5.09	**ASP7**	**LYS10**	6.09
			ARG3	LYS5	5.35
			THR4	**ILE6**	5.08
			THR2	ASP7	5.07

ff14SB TIP3P

EXTENDED			MISFOLDED		
acceptor	donor	occ%	acceptor	donor	occ%
TRP8	**LEU12**	43.80	LYS5	ASN9	34.73
ASN9	SER13	32.73	**TRP8**	**LEU12**	34.35
ASP7	ILE11	17.49	ASN9	SER13	32.10
ACE1	LYS5	16.26	THR4	TRP8	31.02
LYS5	ASN9	14.05	ILE6	LYS10	26.98
ASP7	**LYS10**	13.33	ASP7	ILE11	16.05
ILE6	LYS10	13.16	ARG3	ASP7	14.02
THR2	ILE6	12.04	THR2	ILE6	10.92
ARG3	ASP7	10.51	TRP8	ILE11	7.68
THR2	THR4	10.23	THR4	ASP7	6.43
THR4	TRP8	9.43	ACE1	LYS5	6.14
THR2	LYS5	9.35	THR2	LYS5	5.27
TRP8	ILE11	9.11			
ACE1	ILE6	7.38			
ILE6	ARG3	6.30			

ff19SB OPC					
EXTENDED			MISFOLDED		
acceptor	donor	occ%	acceptor	donor	occ%
LYS5	ASN9	8.84	ASN9	SER13	6.87
THR4	ASP7	6.32	**TRP8**	**LEU12**	5.89
THR4	TRP8	6.11			
ASN9	SER13	5.41			

ff19SB TIP3P					
EXTENDED			MISFOLDED		
acceptor	donor	occ%	acceptor	donor	occ%
TRP8	**LEU12**	20.56	**TRP8**	**LEU12**	24.94
ASN9	SER13	17.23	ASN9	SER13	16.97
THR4	TRP8	15.66	LYS5	ASN9	13.61
LYS5	ASN9	15.54	**ASP7**	**LYS10**	10.49
ILE6	LYS10	9.85	ASP7	ILE11	10.13
ASP7	ILE11	8.63	THR4	TRP8	9.96
THR4	ASP7	7.66	ILE6	LYS10	9.49
ASP7	**LYS10**	7.05	TRP8	ILE11	7.73
TRP8	ILE11	6.77	ILE6	ASN9	6.92

Table S11. H-bond analyses from ID3 trajectories. Only H-bonds involving the backbone are included in the table (donor N-H, acceptor C=O). Native H-bonds are highlighted in bold.

NATIVE		
acceptor	donor	Distance
THR3	**ARG5**	**2.56**
MET10	**THR13**	**2.59**
SER2	**SER4**	**2.59**
THR3	**HIE6**	**2.61**
SER2	**ARG5**	**2.7**
MET10	**LYS12**	**2.78**
ARG5	**LYS8**	**2.83**
HIE6	**LEU9**	**2.88**
MET10	**GLU14**	**2.92**
SER4	**LYS7**	**2.93**
LYS7	**MET10**	**2.95**
LYS12	**GLU14**	**3.01**
ARG5	**LYS7**	**3.07**
LYS8	**PHE11**	**3.08**
LEU9	**PHE11**	**3.08**
HIE6	**LYS8**	**3.09**
LYS7	**LEU9**	**3.19**
SER4	**HIE6**	**3.25**
LYS8	**MET10**	**3.26**
LEU9	**LYS12**	**3.3**
HIE6	**MET10**	**3.34**
PHE11	**GLU14**	**3.48**
LYS7	**PHE11**	**3.49**
SER4	**LYS8**	**3.56**
PHE11	**THR13**	**3.67**
ARG5	**LEU9**	**3.68**
THR3	**LYS7**	**3.78**
LEU9	**THR13**	**3.99**
GLU14	**LYS12**	**4.16**
ff99SB OPC		ff99SB TIP3P

EXTENDED		
acceptor	donor	occ%
1792	**LYS7**	7.65
SER2	HIE6	6.12
HIE6	**MET10**	5.10
SER4	**LYS8**	5.01

MISFOLDED		
acceptor	donor	occ%
SER2	HIP6	8.15
THR3	**LYS7**	7.12
ACE1	ARG5	5.41

EXTENDED		
acceptor	donor	occ%
HIE6	**MET10**	17.34
SER2	HIE6	15.73
ARG5	**LEU9**	14.42
LYS7	**PHE11**	14.16
SER4	**LYS8**	12.11
ACE1	ARG5	10.18
THR3	**LYS7**	9.37
MET10	**GLU14**	8.13
LYS8	LYS12	7.92
SER2	**ARG5**	7.02
LEU9	**THR13**	6.04
HIE6	**LEU9**	5.01

MISFOLDED		
acceptor	donor	occ%
THR3	**LYS7**	18.82
SER2	HIP6	18.13
SER4	**LYS8**	15.22
HIP6	MET10	15.17
ACE1	ARG5	14.59
LYS7	**PHE11**	13.56
MET10	**GLU14**	11.67
LYS8	LYS12	11.44
ARG5	**LEU9**	11.24
LEU9	**THR13**	7.87

ff14SB OPC

EXTENDED		
acceptor	donor	occ%
HIE6	**MET10**	13.64
LYS7	**PHE11**	10.50
MET10	**GLU14**	9.14
SER2	HIE6	6.32
LEU9	**THR13**	5.44
HIE6	**LEU9**	5.04

MISFOLDED		
acceptor	donor	occ%
THR3	**LYS7**	27.30
SER2	HIP6	25.49
SER4	**LYS8**	24.71
HIP6	MET10	23.50
ARG5	**LEU9**	19.84
ACE1	ARG5	17.80
LYS7	**PHE11**	16.73
LEU9	**THR13**	10.52
LYS8	LYS12	10.38
MET10	**GLU14**	10.33

ff14SB TIP3P

EXTENDED		
acceptor	donor	occ%
HIE6	**MET10**	50.07
LYS7	**PHE11**	42.78
SER4	**LYS8**	41.18
ARG5	**LEU9**	39.36
THR3	**LYS7**	37.22
MET10	**GLU14**	26.65
LYS8	LYS12	26.30
SER2	HIE6	25.43
LEU9	**THR13**	23.56
ACE1	ARG5	22.46
LYS8	THR13	5.00

MISFOLDED		
acceptor	donor	occ%
THR3	**LYS7**	48.00
SER2	HIP6	43.97
SER4	**LYS8**	40.34
HIP6	MET10	37.80
ARG5	**LEU9**	35.00
LYS7	**PHE11**	32.72
ACE1	ARG5	30.94
MET10	**GLU14**	26.32
LYS8	LYS12	25.39
LEU9	**THR13**	21.77

ff19SB OPC

EXTENDED		
acceptor	donor	occ%
HIE6	**MET10**	9.60
LYS7	**PHE11**	9.57
HIE6	**LEU9**	8.39
LYS7	**MET10**	5.89

MISFOLDED		
acceptor	donor	occ%

ff19SB TIP3P

EXTENDED		
acceptor	donor	occ%
HIE6	**MET10**	13.28
SER4	**LYS8**	11.79
LYS7	**PHE11**	11.03
ARG5	**LEU9**	9.60
LYS8	LYS12	8.91
LEU9	**LYS12**	6.82
LYS8	**PHE11**	6.66
HIE6	**LEU9**	6.13
THR3	**LYS7**	6.09
LEU9	**THR13**	5.63
MET10	**GLU14**	5.49
SER4	**LYS7**	5.17

MISFOLDED		
acceptor	donor	occ%
HIP6	MET10	11.72
ARG5	**LEU9**	11.58
LYS7	**PHE11**	10.63
SER4	**LYS8**	10.11
THR3	**LYS7**	5.80

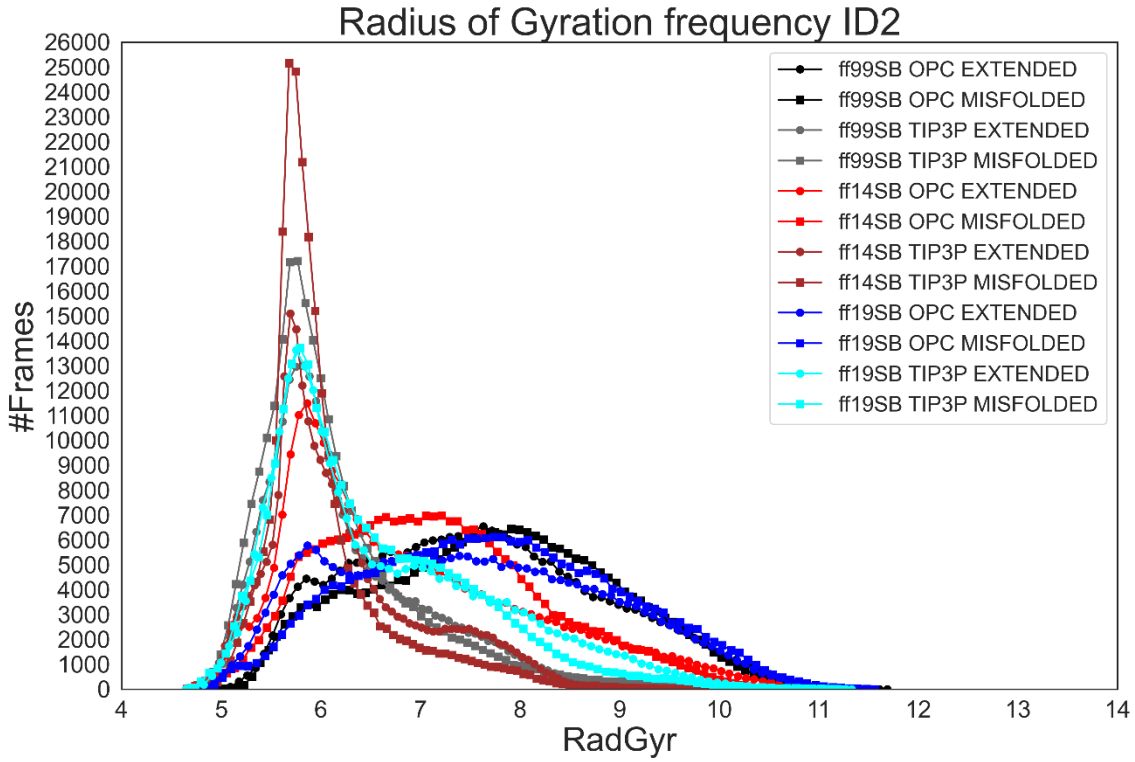

Figure S116. Radius of gyration frequencies calculated on the last 500 ns of ID2 trajectories.

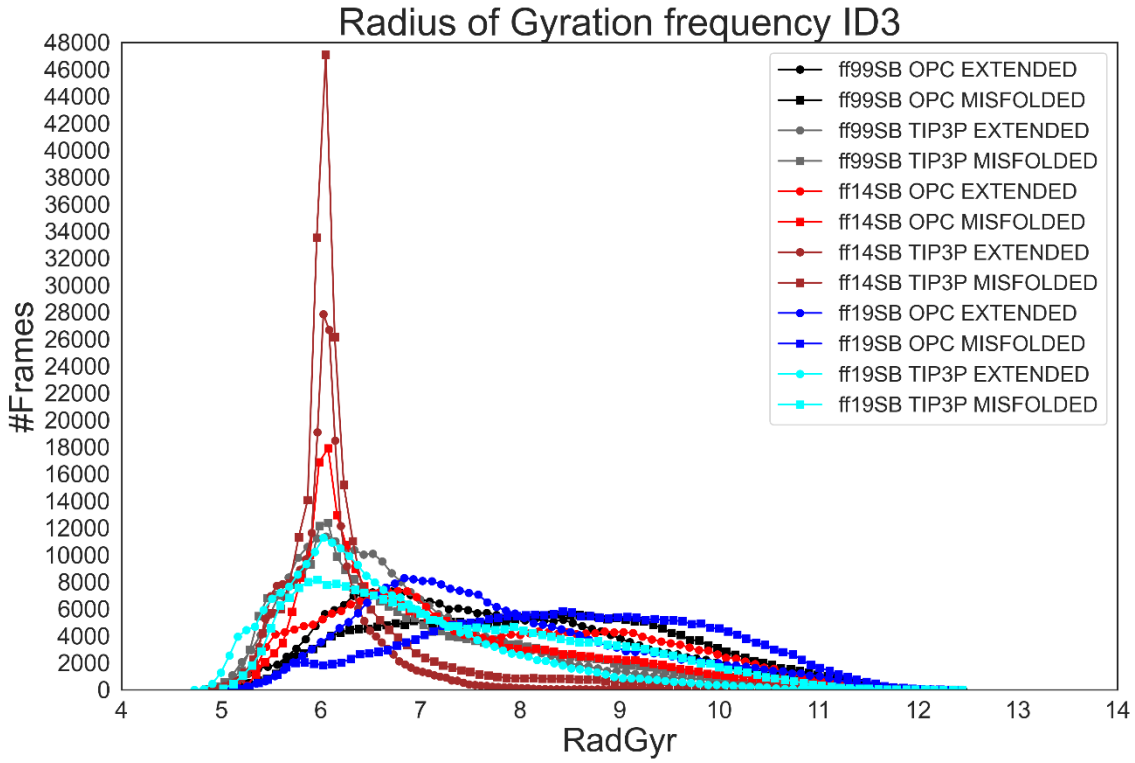

Figure S117. Radius of gyration frequencies calculated on the last 500 ns of ID3 trajectories.

PDB coordinate of the starting structures.

H1 extended

```
ATOM   1  CH3 ACE  1   33.886  24.866  20.687  1.00  0.00   C
ATOM   2  C   ACE  1   34.349  25.487  22.029  1.00  0.00   C
ATOM   3  O   ACE  1   35.523  25.237  22.383  1.00  0.00   O
ATOM   4  N   LYS  2   33.495  26.383  22.610  1.00  0.00   N
ATOM   5  CA  LYS  2   33.521  27.193  23.881  1.00  0.00   C
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ATOM   7  CG  LYS  2   33.715  29.463  22.665  1.00  0.00   C
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ATOM   9  CE  LYS  2   34.253  31.767  23.672  1.00  0.00   C
ATOM  10  NZ  LYS  2   34.819  33.142  23.409  1.00  0.00   N1+
ATOM  11  C   LYS  2   32.059  27.345  24.436  1.00  0.00   C
ATOM  12  O   LYS  2   31.046  27.373  23.727  1.00  0.00   O
ATOM  13  N   LEU  3   31.923  27.417  25.779  1.00  0.00   N
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ATOM  15  CB  LEU  3   30.847  25.882  27.303  1.00  0.00   C
ATOM  16  CG  LEU  3   29.715  25.411  28.161  1.00  0.00   C
ATOM  17  CD1 LEU  3   28.525  24.979  27.268  1.00  0.00   C
ATOM  18  CD2 LEU  3   30.147  24.264  28.963  1.00  0.00   C
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ATOM  20  O   LEU  3   30.770  28.660  28.174  1.00  0.00   O
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ATOM  22  CA  THR  4   28.124  29.588  27.862  1.00  0.00   C
ATOM  23  CB  THR  4   27.292  30.615  27.131  1.00  0.00   C
ATOM  24  CG2 THR  4   28.245  31.849  26.715  1.00  0.00   C
ATOM  25  OG1 THR  4   26.516  30.116  26.042  1.00  0.00   O
ATOM  26  C   THR  4   27.170  28.751  28.688  1.00  0.00   C
ATOM  27  O   THR  4   26.631  27.757  28.164  1.00  0.00   O
ATOM  28  N   TRP  5   26.992  29.046  30.013  1.00  0.00   N
ATOM  29  CA  TRP  5   26.156  28.193  30.953  1.00  0.00   C
ATOM  30  CB  TRP  5   26.186  28.781  32.341  1.00  0.00   C
ATOM  31  CG  TRP  5   25.582  30.165  32.384  1.00  0.00   C
ATOM  32  CD1 TRP  5   26.288  31.318  32.276  1.00  0.00   C
ATOM  33  NE1 TRP  5   25.329  32.344  32.241  1.00  0.00   N
ATOM  34  CE2 TRP  5   24.063  31.879  32.527  1.00  0.00   C
ATOM  35  CZ2 TRP  5   22.846  32.559  32.674  1.00  0.00   C
ATOM  36  CH2 TRP  5   21.722  31.764  32.868  1.00  0.00   C
ATOM  37  CZ3 TRP  5   21.804  30.382  33.043  1.00  0.00   C
ATOM  38  CE3 TRP  5   23.013  29.735  32.875  1.00  0.00   C
ATOM  39  CD2 TRP  5   24.210  30.482  32.643  1.00  0.00   C
ATOM  40  C   TRP  5   24.728  27.828  30.447  1.00  0.00   C
ATOM  41  O   TRP  5   24.091  26.781  30.816  1.00  0.00   O
ATOM  42  N   GLN  6   24.172  28.762  29.668  1.00  0.00   N
ATOM  43  CA  GLN  6   22.885  28.523  28.973  1.00  0.00   C
ATOM  44  CB  GLN  6   22.498  29.852  28.287  1.00  0.00   C
ATOM  45  CG  GLN  6   22.587  31.121  29.099  1.00  0.00   C
ATOM  46  CD  GLN  6   22.412  32.291  28.172  1.00  0.00   C
ATOM  47  OE1 GLN  6   23.316  32.556  27.384  1.00  0.00   O
ATOM  48  NE2 GLN  6   21.203  32.738  28.006  1.00  0.00   N
ATOM  49  C   GLN  6   22.814  27.395  27.871  1.00  0.00   C
ATOM  50  O   GLN  6   21.666  27.039  27.608  1.00  0.00   O
ATOM  51  N   GLU  7   23.965  26.797  27.497  1.00  0.00   N
ATOM  52  CA  GLU  7   23.863  25.708  26.404  1.00  0.00   C
ATOM  53  CB  GLU  7   25.123  25.744  25.455  1.00  0.00   C
ATOM  54  CG  GLU  7   25.083  27.024  24.556  1.00  0.00   C
ATOM  55  CD  GLU  7   26.410  27.203  23.864  1.00  0.00   C
ATOM  56  OE1 GLU  7   27.263  27.882  24.478  1.00  0.00   O
ATOM  57  OE2 GLU  7   26.527  26.829  22.708  1.00  0.00   O1-
ATOM  58  C   GLU  7   23.726  24.335  27.089  1.00  0.00   C
ATOM  59  O   GLU  7   23.169  23.430  26.517  1.00  0.00   O
ATOM  60  N   LEU  8   24.224  24.139  28.346  1.00  0.00   N
ATOM  61  CA  LEU  8   23.976  22.903  29.089  1.00  0.00   C
ATOM  62  CB  LEU  8   24.497  23.062  30.515  1.00  0.00   C
ATOM  63  CG  LEU  8   26.076  23.131  30.667  1.00  0.00   C
ATOM  64  CD1 LEU  8   26.270  22.916  32.210  1.00  0.00   C
ATOM  65  CD2 LEU  8   26.762  21.929  30.005  1.00  0.00   C
ATOM  66  C   LEU  8   22.526  22.391  29.168  1.00  0.00   C
ATOM  67  O   LEU  8   22.319  21.195  29.108  1.00  0.00   O
ATOM  68  N   TYR  9   21.535  23.194  29.197  1.00  0.00   N
ATOM  69  CA  TYR  9   20.129  22.872  29.380  1.00  0.00   C
ATOM  70  CB  TYR  9   19.533  23.856  30.394  1.00  0.00   C
ATOM  71  CG  TYR  9   20.105  23.674  31.790  1.00  0.00   C
ATOM  72  CD1 TYR  9   19.691  22.512  32.511  1.00  0.00   C
ATOM  73  CE1 TYR  9   20.159  22.268  33.858  1.00  0.00   C
ATOM  74  CZ  TYR  9   21.124  23.171  34.354  1.00  0.00   C
ATOM  75  OH  TYR  9   21.570  23.102  35.677  1.00  0.00   O
ATOM  76  CE2 TYR  9   21.672  24.205  33.572  1.00  0.00   C
ATOM  77  CD2 TYR  9   21.107  24.533  32.340  1.00  0.00   C
ATOM  78  C   TYR  9   19.399  22.689  28.048  1.00  0.00   C
ATOM  79  O   TYR  9   18.208  22.392  28.037  1.00  0.00   O
ATOM  80  N   GLN  10   20.046  22.820  26.873  1.00  0.00   N
ATOM  81  CA  GLN  10   19.725  22.145  25.615  1.00  0.00   C
ATOM  82  CB  GLN  10   19.687  23.127  24.450  1.00  0.00   C
ATOM  83  CG  GLN  10   18.307  23.884  24.531  1.00  0.00   C
ATOM  84  CD  GLN  10   18.061  24.905  23.403  1.00  0.00   C
ATOM  85  OE1 GLN  10   18.436  24.799  22.242  1.00  0.00   O
ATOM  86  NE2 GLN  10   17.273  25.924  23.717  1.00  0.00   N
ATOM  87  C   GLN  10   20.656  20.884  25.312  1.00  0.00   C
ATOM  88  O   GLN  10   20.165  19.845  24.826  1.00  0.00   O
ATOM  89  N   LEU  11   21.923  20.962  25.703  1.00  0.00   N
ATOM  90  CA  LEU  11   22.962  19.918  25.650  1.00  0.00   C
ATOM  91  CB  LEU  11   24.332  20.488  26.010  1.00  0.00   C
ATOM  92  CG  LEU  11   25.533  19.676  25.462  1.00  0.00   C
ATOM  93  CD1 LEU  11   25.720  19.993  23.943  1.00  0.00   C
ATOM  94  CD2 LEU  11   26.969  19.826  26.081  1.00  0.00   C
ATOM  95  C   LEU  11   22.673  18.635  26.492  1.00  0.00   C
ATOM  96  O   LEU  11   22.929  17.594  26.006  1.00  0.00   O
ATOM  97  N   LYS  12   22.036  18.756  27.632  1.00  0.00   N
ATOM  98  CA  LYS  12   21.665  17.559  28.524  1.00  0.00   C
ATOM  99  CB  LYS  12   21.353  18.149  29.969  1.00  0.00   C
ATOM 100  CG  LYS  12   21.380  17.101  31.048  1.00  0.00   C
ATOM 101  CD  LYS  12   21.158  17.717  32.393  1.00  0.00   C
ATOM 102  CE  LYS  12   21.488  16.864  33.631  1.00  0.00   C
ATOM 103  NZ  LYS  12   20.608  15.707  33.921  1.00  0.00   N1+
ATOM 104  C   LYS  12   20.617  16.610  27.890  1.00  0.00   C
ATOM 105  O   LYS  12   20.562  15.449  28.258  1.00  0.00   O
ATOM 106  N   TYR  13   19.785  17.090  26.935  1.00  0.00   N
ATOM 107  CA  TYR  13   18.585  16.440  26.332  1.00  0.00   C
ATOM 108  CB  TYR  13   17.327  17.308  26.571  1.00  0.00   C
ATOM 109  CG  TYR  13   16.976  17.423  28.029  1.00  0.00   C
ATOM 110  CD1 TYR  13   16.988  18.661  28.705  1.00  0.00   C
ATOM 111  CE1 TYR  13   16.699  18.801  30.061  1.00  0.00   C
ATOM 112  CZ  TYR  13   16.417  17.628  30.792  1.00  0.00   C
ATOM 113  OH  TYR  13   16.188  17.721  32.137  1.00  0.00   O
ATOM 114  CE2 TYR  13   16.410  16.340  30.155  1.00  0.00   C
ATOM 115  CD2 TYR  13   16.697  16.268  28.734  1.00  0.00   C
ATOM 116  C   TYR  13   18.859  16.159  24.831  1.00  0.00   C
ATOM 117  O   TYR  13   18.509  15.087  24.317  1.00  0.00   O
ATOM 118  N   LYS  14   19.424  17.062  24.051  1.00  0.00   N
ATOM 119  CA  LYS  14   19.886  16.800  22.689  1.00  0.00   C
ATOM 120  CB  LYS  14   20.306  18.148  22.094  1.00  0.00   C
ATOM 121  CG  LYS  14   20.753  18.075  20.557  1.00  0.00   C
ATOM 122  CD  LYS  14   21.616  19.231  20.084  1.00  0.00   C
ATOM 123  CE  LYS  14   20.796  20.538  20.141  1.00  0.00   C
ATOM 124  NZ  LYS  14   21.556  21.656  19.644  1.00  0.00   N1+
ATOM 125  C   LYS  14   20.837  15.685  22.495  1.00  0.00   C
ATOM 126  O   LYS  14   20.658  14.937  21.495  1.00  0.00   O
ATOM 127  N   GLY  15   21.813  15.564  23.421  1.00  0.00   N
ATOM 128  CA  GLY  15   23.008  14.810  23.424  1.00  0.00   C
ATOM 129  C   GLY  15   24.087  15.227  22.415  1.00  0.00   C
ATOM 130  O   GLY  15   23.803  15.951  21.463  1.00  0.00   O
ATOM 131  N   ILE  16   25.315  14.697  22.628  1.00  0.00   N
ATOM 132  CA  ILE  16   26.475  15.229  21.913  1.00  0.00   C
ATOM 133  CB  ILE  16   27.655  14.961  22.930  1.00  0.00   C
ATOM 134  CG2 ILE  16   27.542  15.868  24.167  1.00  0.00   C
ATOM 135  CG1 ILE  16   28.106  13.472  23.104  1.00  0.00   C
ATOM 136  CD1 ILE  16   29.241  13.161  24.170  1.00  0.00   C
ATOM 137  C   ILE  16   26.685  14.560  20.547  1.00  0.00   C
ATOM 138  O   ILE  16   26.046  13.594  20.109  1.00  0.00   O
ATOM 139  N   NHE  17   27.545  15.187  19.756  1.00  0.00   N
TER  140   NHE  17
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H1 misfolded

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ATOM   1 CH3 ACE  1   16.354  36.122  18.628  1.00  0.00   C
ATOM   2 C   ACE  1   16.263  34.604  18.876  1.00  0.00   C
ATOM   3 O   ACE  1   15.147  34.127  19.105  1.00  0.00   O
ATOM   4 N   LYS  2   17.384  33.844  18.658  1.00  0.00   N
ATOM   5 CA  LYS  2   17.445  32.376  18.946  1.00  0.00   C
ATOM   6 CB  LYS  2   17.580  31.658  17.542  1.00  0.00   C
ATOM   7 CG  LYS  2   17.449  30.116  17.547  1.00  0.00   C
ATOM   8 CD  LYS  2   17.430  29.435  16.187  1.00  0.00   C
ATOM   9 CE  LYS  2   18.808  29.378  15.551  1.00  0.00   C
ATOM  10 NZ  LYS  2   19.789  28.389  16.064  1.00  0.00   N1+
ATOM  11 C   LYS  2   18.653  32.048  19.804  1.00  0.00   C
ATOM  12 O   LYS  2   19.602  32.839  19.852  1.00  0.00   O
ATOM  13 N   LEU  3   18.656  30.926  20.485  1.00  0.00   N
ATOM  14 CA  LEU  3   19.738  30.456  21.339  1.00  0.00   C
ATOM  15 CB  LEU  3   19.199  29.293  22.198  1.00  0.00   C
ATOM  16 CG  LEU  3   20.199  28.788  23.213  1.00  0.00   C
ATOM  17 CD1 LEU  3   20.671  29.787  24.256  1.00  0.00   C
ATOM  18 CD2 LEU  3   19.597  27.635  23.974  1.00  0.00   C
ATOM  19 C   LEU  3   20.969  29.933  20.524  1.00  0.00   C
ATOM  20 O   LEU  3   20.817  29.097  19.630  1.00  0.00   O
ATOM  21 N   THR  4   22.165  30.418  20.816  1.00  0.00   N
ATOM  22 CA  THR  4   23.411  29.913  20.259  1.00  0.00   C
ATOM  23 CB  THR  4   24.020  30.965  19.267  1.00  0.00   C
ATOM  24 CG2 THR  4   23.177  31.206  18.019  1.00  0.00   C
ATOM  25 OG1 THR  4   24.339  32.238  19.851  1.00  0.00   O
ATOM  26 C   THR  4   24.423  29.597  21.337  1.00  0.00   C
ATOM  27 O   THR  4   24.617  30.282  22.322  1.00  0.00   O
ATOM  28 N   TRP  5   25.125  28.410  21.206  1.00  0.00   N
ATOM  29 CA  TRP  5   26.331  28.005  21.913  1.00  0.00   C
ATOM  30 CB  TRP  5   26.751  26.684  21.191  1.00  0.00   C
ATOM  31 CG  TRP  5   27.720  25.815  21.941  1.00  0.00   C
ATOM  32 CD1 TRP  5   27.434  24.660  22.583  1.00  0.00   C
ATOM  33 NE1 TRP  5   28.644  24.052  22.902  1.00  0.00   N
ATOM  34 CE2 TRP  5   29.690  24.831  22.556  1.00  0.00   C
ATOM  35 CZ2 TRP  5   31.104  24.602  22.607  1.00  0.00   C
ATOM  36 CH2 TRP  5   32.026  25.566  22.177  1.00  0.00   C
ATOM  37 CZ3 TRP  5   31.458  26.573  21.401  1.00  0.00   C
ATOM  38 CE3 TRP  5   30.038  26.820  21.340  1.00  0.00   C
ATOM  39 CD2 TRP  5   29.130  25.972  21.935  1.00  0.00   C
ATOM  40 C   TRP  5   27.411  29.119  21.982  1.00  0.00   C
ATOM  41 O   TRP  5   27.613  29.785  20.985  1.00  0.00   O
ATOM  42 N   GLN  6   28.125  29.253  23.112  1.00  0.00   N
ATOM  43 CA  GLN  6   29.264  30.128  23.304  1.00  0.00   C
ATOM  44 CB  GLN  6   28.911  31.119  24.400  1.00  0.00   C
ATOM  45 CG  GLN  6   29.950  32.195  24.595  1.00  0.00   C
ATOM  46 CD  GLN  6   29.691  33.005  25.773  1.00  0.00   C
ATOM  47 OE1 GLN  6   28.703  33.743  25.843  1.00  0.00   O
ATOM  48 NE2 GLN  6   30.555  32.922  26.764  1.00  0.00   N
ATOM  49 C   GLN  6   30.613  29.338  23.521  1.00  0.00   C
ATOM  50 O   GLN  6   31.478  29.475  22.658  1.00  0.00   O
ATOM  51 N   GLU  7   30.757  28.662  24.625  1.00  0.00   N
ATOM  52 CA  GLU  7   31.953  27.969  25.143  1.00  0.00   C
ATOM  53 CB  GLU  7   32.888  28.982  25.857  1.00  0.00   C
ATOM  54 CG  GLU  7   32.170  29.773  26.962  1.00  0.00   C
ATOM  55 CD  GLU  7   33.142  30.587  27.760  1.00  0.00   C
ATOM  56 OE1 GLU  7   33.329  30.175  28.912  1.00  0.00   O
ATOM  57 OE2 GLU  7   33.675  31.717  27.415  1.00  0.00   O1-
ATOM  58 C   GLU  7   31.759  26.791  26.071  1.00  0.00   C
ATOM  59 O   GLU  7   30.680  26.654  26.730  1.00  0.00   O
ATOM  60 N   LEU  8   32.760  25.962  26.276  1.00  0.00   N
ATOM  61 CA  LEU  8   32.834  24.854  27.255  1.00  0.00   C
ATOM  62 CB  LEU  8   33.878  23.833  26.748  1.00  0.00   C
ATOM  63 CG  LEU  8   33.968  22.503  27.516  1.00  0.00   C
ATOM  64 CD1 LEU  8   32.698  21.763  27.089  1.00  0.00   C
ATOM  65 CD2 LEU  8   35.241  21.739  27.005  1.00  0.00   C
ATOM  66 C   LEU  8   33.128  25.391  28.682  1.00  0.00   C
ATOM  67 O   LEU  8   34.027  26.204  28.867  1.00  0.00   O
ATOM  68 N   TYR  9   32.337  24.905  29.664  1.00  0.00   N
ATOM  69 CA  TYR  9   32.409  25.298  31.083  1.00  0.00   C
ATOM  70 CB  TYR  9   31.238  26.248  31.411  1.00  0.00   C
ATOM  71 CG  TYR  9   31.119  26.892  32.747  1.00  0.00   C
ATOM  72 CD1 TYR  9   29.916  26.753  33.379  1.00  0.00   C
ATOM  73 CE1 TYR  9   29.654  27.315  34.658  1.00  0.00   C
ATOM  74 CZ  TYR  9   30.677  27.931  35.368  1.00  0.00   C
ATOM  75 OH  TYR  9   30.354  28.439  36.610  1.00  0.00   O
ATOM  76 CE2 TYR  9   31.996  28.002  34.755  1.00  0.00   C
ATOM  77 CD2 TYR  9   32.199  27.525  33.439  1.00  0.00   C
ATOM  78 C   TYR  9   32.306  24.033  32.000  1.00  0.00   C
ATOM  79 O   TYR  9   32.253  22.911  31.478  1.00  0.00   O
ATOM  80 N   GLN  10  32.485  24.175  33.348  1.00  0.00   N
ATOM  81 CA  GLN  10  32.258  23.036  34.253  1.00  0.00   C
ATOM  82 CB  GLN  10  32.435  23.560  35.763  1.00  0.00   C
ATOM  83 CG  GLN  10  33.890  23.714  36.151  1.00  0.00   C
ATOM  84 CD  GLN  10  34.333  24.030  37.528  1.00  0.00   C
ATOM  85 OE1 GLN  10  34.381  25.161  37.990  1.00  0.00   O
ATOM  86 NE2 GLN  10  34.681  23.002  38.314  1.00  0.00   N
ATOM  87 C   GLN  10  30.837  22.455  33.989  1.00  0.00   C
ATOM  88 O   GLN  10  30.649  21.279  33.725  1.00  0.00   O
ATOM  89 N   LEU  11  29.829  23.359  34.103  1.00  0.00   N
ATOM  90 CA  LEU  11  28.428  22.992  33.843  1.00  0.00   C
ATOM  91 CB  LEU  11  27.492  23.898  34.670  1.00  0.00   C
ATOM  92 CG  LEU  11  25.985  23.718  34.684  1.00  0.00   C
ATOM  93 CD1 LEU  11  25.568  22.310  34.970  1.00  0.00   C
ATOM  94 CD2 LEU  11  25.306  24.595  35.690  1.00  0.00   C
ATOM  95 C   LEU  11  28.164  23.054  32.294  1.00  0.00   C
ATOM  96 O   LEU  11  27.909  24.141  31.797  1.00  0.00   O
ATOM  97 N   LYS  12  28.264  21.849  31.652  1.00  0.00   N
ATOM  98 CA  LYS  12  28.120  21.651  30.182  1.00  0.00   C
ATOM  99 CB  LYS  12  26.654  21.295  29.829  1.00  0.00   C
ATOM 100 CG  LYS  12  26.165  19.896  30.240  1.00  0.00   C
ATOM 101 CD  LYS  12  24.707  19.636  29.852  1.00  0.00   C
ATOM 102 CE  LYS  12  24.010  18.371  30.344  1.00  0.00   C
ATOM 103 NZ  LYS  12  22.795  18.040  29.592  1.00  0.00   N1+
ATOM 104 C   LYS  12  28.711  22.848  29.383  1.00  0.00   C
ATOM 105 O   LYS  12  29.926  22.936  29.224  1.00  0.00   O
ATOM 106 N   TYR  13  27.891  23.805  28.925  1.00  0.00   N
ATOM 107 CA  TYR  13  28.384  24.923  28.093  1.00  0.00   C
ATOM 108 CB  TYR  13  28.671  24.456  26.691  1.00  0.00   C
ATOM 109 CG  TYR  13  27.807  23.477  25.978  1.00  0.00   C
ATOM 110 CD1 TYR  13  28.184  22.091  25.961  1.00  0.00   C
ATOM 111 CE1 TYR  13  27.233  21.176  25.501  1.00  0.00   C
ATOM 112 CZ  TYR  13  25.968  21.526  25.043  1.00  0.00   C
ATOM 113 OH  TYR  13  25.162  20.527  24.522  1.00  0.00   O
ATOM 114 CE2 TYR  13  25.585  22.903  25.018  1.00  0.00   C
ATOM 115 CD2 TYR  13  26.529  23.857  25.484  1.00  0.00   C
ATOM 116 C   TYR  13  27.393  26.121  28.215  1.00  0.00   C
ATOM 117 O   TYR  13  26.214  26.002  28.553  1.00  0.00   O
ATOM 118 N   LYS  14  27.904  27.356  28.071  1.00  0.00   N
ATOM 119 CA  LYS  14  26.982  28.537  28.065  1.00  0.00   C
ATOM 120 CB  LYS  14  27.938  29.703  28.410  1.00  0.00   C
ATOM 121 CG  LYS  14  28.747  29.455  29.640  1.00  0.00   C
ATOM 122 CD  LYS  14  29.582  30.620  30.027  1.00  0.00   C
ATOM 123 CE  LYS  14  30.438  30.213  31.262  1.00  0.00   C
ATOM 124 NZ  LYS  14  31.220  31.359  31.752  1.00  0.00   N1+
ATOM 125 C   LYS  14  26.453  28.790  26.707  1.00  0.00   C
ATOM 126 O   LYS  14  27.148  28.429  25.769  1.00  0.00   O
ATOM 127 N   GLY  15  25.394  29.560  26.658  1.00  0.00   N
ATOM 128 CA  GLY  15  24.767  30.035  25.457  1.00  0.00   C
ATOM 129 C   GLY  15  24.173  31.476  25.662  1.00  0.00   C
ATOM 130 O   GLY  15  23.902  31.906  26.797  1.00  0.00   O
ATOM 131 N   ILE  16  24.074  32.207  24.582  1.00  0.00   N
ATOM 132 CA  ILE  16  23.423  33.582  24.512  1.00  0.00   C
ATOM 133 CB  ILE  16  24.437  34.691  24.501  1.00  0.00   C
ATOM 134 CG2 ILE  16  25.291  34.921  25.774  1.00  0.00   C
ATOM 135 CG1 ILE  16  25.175  34.743  23.107  1.00  0.00   C
ATOM 136 CD1 ILE  16  26.340  33.834  22.974  1.00  0.00   C
ATOM 137 C   ILE  16  22.341  33.521  23.427  1.00  0.00   C
ATOM 138 O   ILE  16  22.400  32.859  22.373  1.00  0.00   O
ATOM 139 N   NHE  17  21.219  34.128  23.683  1.00  0.00   N
TER  140     NHE  17
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H2 extended

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ATOM   1  CH3 ACE  1   18.616  22.973  24.268  1.00  0.00   C
ATOM   2  C   ACE  1   17.319  22.718  23.497  1.00  0.00   C
ATOM   3  O   ACE  1   16.325  22.950  24.135  1.00  0.00   O
ATOM   4  N   ALA  2   17.399  22.348  22.178  1.00  0.00   N
ATOM   5  CA  ALA  2   16.245  21.977  21.352  1.00  0.00   C
ATOM   6  CB  ALA  2   16.376  22.769  20.037  1.00  0.00   C
ATOM   7  C   ALA  2   15.956  20.463  21.131  1.00  0.00   C
ATOM   8  O   ALA  2   15.127  20.176  20.242  1.00  0.00   O
ATOM   9  N   AIB  3   16.717  19.554  21.753  1.00  0.00   N
ATOM  10  CA  AIB  3   16.899  18.097  21.482  1.00  0.00   C
ATOM  11  CB1 AIB  3   15.605  17.462  21.843  1.00  0.00   C
ATOM  12  CB2 AIB  3   18.007  17.657  22.449  1.00  0.00   C
ATOM  13  C   AIB  3   17.317  17.864  19.972  1.00  0.00   C
ATOM  14  O   AIB  3   16.905  16.856  19.354  1.00  0.00   O
ATOM  15  N   ALA  4   18.206  18.694  19.391  1.00  0.00   N
ATOM  16  CA  ALA  4   18.691  18.534  18.024  1.00  0.00   C
ATOM  17  CB  ALA  4   19.360  19.880  17.652  1.00  0.00   C
ATOM  18  C   ALA  4   19.708  17.388  17.776  1.00  0.00   C
ATOM  19  O   ALA  4   20.542  16.977  18.623  1.00  0.00   O
ATOM  20  N   AIB  5   19.591  16.819  16.543  1.00  0.00   N
ATOM  21  CA  AIB  5   20.489  15.789  16.006  1.00  0.00   C
ATOM  22  CB1 AIB  5   19.981  15.663  14.550  1.00  0.00   C
ATOM  23  CB2 AIB  5   20.289  14.477  16.723  1.00  0.00   C
ATOM  24  C   AIB  5   22.000  16.237  15.973  1.00  0.00   C
ATOM  25  O   AIB  5   22.919  15.409  16.045  1.00  0.00   O
ATOM  26  N   AIB  6   22.241  17.605  16.061  1.00  0.00   N
ATOM  27  CA  AIB  6   23.433  18.358  15.575  1.00  0.00   C
ATOM  28  CB1 AIB  6   23.313  19.835  15.991  1.00  0.00   C
ATOM  29  CB2 AIB  6   23.394  18.398  14.087  1.00  0.00   C
ATOM  30  C   AIB  6   24.801  17.776  16.113  1.00  0.00   C
ATOM  31  O   AIB  6   25.888  17.815  15.456  1.00  0.00   O
ATOM  32  N   NHE  7   24.805  17.527  17.371  1.00  0.00   N
TER   33      NHE  7
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H2 misfolded

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ATOM   1  CH3 ACE  1   15.700  20.901  23.583  1.00  0.00   C
ATOM   2  C   ACE  1   15.782  20.376  22.147  1.00  0.00   C
ATOM   3  O   ACE  1   14.816  19.818  21.631  1.00  0.00   O
ATOM   4  N   ALA  2   16.941  20.556  21.510  1.00  0.00   N
ATOM   5  CA  ALA  2   17.145  20.104  20.149  1.00  0.00   C
ATOM   6  CB  ALA  2   16.156  20.768  19.196  1.00  0.00   C
ATOM   7  C   ALA  2   18.549  20.437  19.667  1.00  0.00   C
ATOM   8  O   ALA  2   19.343  21.015  20.405  1.00  0.00   O
ATOM   9  N   AIB  3   18.856  20.067  18.421  1.00  0.00   N
ATOM  10  CA  AIB  3   20.177  20.329  17.837  1.00  0.00   C
ATOM  11  CB1 AIB  3   21.195  19.529  18.664  1.00  0.00   C
ATOM  12  CB2 AIB  3   20.522  21.820  17.879  1.00  0.00   C
ATOM  13  C   AIB  3   20.284  19.808  16.392  1.00  0.00   C
ATOM  14  O   AIB  3   19.346  19.263  15.879  1.00  0.00   O
ATOM  15  N   ALA  4   21.451  20.000  15.773  1.00  0.00   N
ATOM  16  CA  ALA  4   21.679  19.556  14.412  1.00  0.00   C
ATOM  17  CB  ALA  4   23.091  19.900  13.952  1.00  0.00   C
ATOM  18  C   ALA  4   21.504  18.050  14.289  1.00  0.00   C
ATOM  19  O   ALA  4   21.114  17.551  13.237  1.00  0.00   O
ATOM  20  N   AIB  5   21.794  17.325  15.372  1.00  0.00   N
ATOM  21  CA  AIB  5   21.667  15.863  15.383  1.00  0.00   C
ATOM  22  CB1 AIB  5   22.653  15.337  16.437  1.00  0.00   C
ATOM  23  CB2 AIB  5   21.995  15.261  14.012  1.00  0.00   C
ATOM  24  C   AIB  5   20.265  15.408  15.830  1.00  0.00   C
ATOM  25  O   AIB  5   20.004  14.237  15.890  1.00  0.00   O
ATOM  26  N   AIB  6   19.392  16.371  16.135  1.00  0.00   N
ATOM  27  CA  AIB  6   18.027  16.068  16.575  1.00  0.00   C
ATOM  28  CB1 AIB  6   18.143  15.314  17.908  1.00  0.00   C
ATOM  29  CB2 AIB  6   17.285  15.206  15.548  1.00  0.00   C
ATOM  30  C   AIB  6   17.215  17.345  16.866  1.00  0.00   C
ATOM  31  O   AIB  6   17.723  18.425  16.723  1.00  0.00   O
ATOM  32  N   NHE  7   15.956  17.174  17.274  1.00  0.00   N
TER   33      NHE  7
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B1 extended

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ATOM   1 CH3 ACE  1   19.051  33.832  35.759  1.00  0.00   C
ATOM   2 C   ACE  1   18.351  33.143  34.583  1.00  0.00   C
ATOM   3 O   ACE  1   17.199  33.400  34.331  1.00  0.00   O
ATOM   4 N   GLY  2   19.106  32.321  33.780  1.00  0.00   N
ATOM   5 CA  GLY  2   18.554  31.853  32.435  1.00  0.00   C
ATOM   6 C   GLY  2   19.280  30.641  31.839  1.00  0.00   C
ATOM   7 O   GLY  2   20.329  30.069  32.455  1.00  0.00   O
ATOM   8 N   GLU  3   18.690  30.057  30.782  1.00  0.00   N
ATOM   9 CA  GLU  3   19.126  28.740  30.137  1.00  0.00   C
ATOM  10 CB  GLU  3   18.047  28.303  29.011  1.00  0.00   C
ATOM  11 CG  GLU  3   18.009  26.878  28.481  1.00  0.00   C
ATOM  12 CD  GLU  3   17.686  25.810  29.566  1.00  0.00   C
ATOM  13 OE1 GLU  3   16.590  25.685  30.118  1.00  0.00   O
ATOM  14 OE2 GLU  3   18.584  25.028  29.955  1.00  0.00   O1-
ATOM  15 C   GLU  3   20.497  28.844  29.597  1.00  0.00   C
ATOM  16 O   GLU  3   21.281  27.899  29.667  1.00  0.00   O
ATOM  17 N   TRP  4   20.946  30.045  29.171  1.00  0.00   N
ATOM  18 CA  TRP  4   22.256  30.415  28.703  1.00  0.00   C
ATOM  19 CB  TRP  4   22.213  31.929  28.355  1.00  0.00   C
ATOM  20 CG  TRP  4   22.087  33.014  29.361  1.00  0.00   C
ATOM  21 CD1 TRP  4   20.943  33.623  29.746  1.00  0.00   C
ATOM  22 NE1 TRP  4   21.214  34.587  30.722  1.00  0.00   N
ATOM  23 CE2 TRP  4   22.585  34.527  31.053  1.00  0.00   C
ATOM  24 CZ2 TRP  4   23.323  35.266  31.971  1.00  0.00   C
ATOM  25 CH2 TRP  4   24.682  34.964  32.135  1.00  0.00   C
ATOM  26 CZ3 TRP  4   25.247  34.001  31.319  1.00  0.00   C
ATOM  27 CE3 TRP  4   24.509  33.342  30.352  1.00  0.00   C
ATOM  28 CD2 TRP  4   23.163  33.567  30.154  1.00  0.00   C
ATOM  29 C   TRP  4   23.425  30.165  29.661  1.00  0.00   C
ATOM  30 O   TRP  4   24.549  30.036  29.213  1.00  0.00   O
ATOM  31 N   THR  5   23.125  30.021  30.981  1.00  0.00   N
ATOM  32 CA  THR  5   24.124  29.538  31.953  1.00  0.00   C
ATOM  33 CB  THR  5   23.654  29.541  33.388  1.00  0.00   C
ATOM  34 CG2 THR  5   23.335  30.915  33.938  1.00  0.00   C
ATOM  35 OG1 THR  5   22.552  28.629  33.555  1.00  0.00   O
ATOM  36 C   THR  5   24.614  28.160  31.639  1.00  0.00   C
ATOM  37 O   THR  5   25.730  27.827  31.944  1.00  0.00   O
ATOM  38 N   TYR  6   23.740  27.260  31.121  1.00  0.00   N
ATOM  39 CA  TYR  6   23.954  25.794  30.892  1.00  0.00   C
ATOM  40 CB  TYR  6   22.707  25.285  31.624  1.00  0.00   C
ATOM  41 CG  TYR  6   22.579  23.755  31.605  1.00  0.00   C
ATOM  42 CD1 TYR  6   23.684  23.029  32.097  1.00  0.00   C
ATOM  43 CE1 TYR  6   23.689  21.585  32.093  1.00  0.00   C
ATOM  44 CZ  TYR  6   22.523  20.909  31.654  1.00  0.00   C
ATOM  45 OH  TYR  6   22.468  19.548  31.777  1.00  0.00   O
ATOM  46 CE2 TYR  6   21.481  21.605  30.960  1.00  0.00   C
ATOM  47 CD2 TYR  6   21.520  23.022  30.975  1.00  0.00   C
ATOM  48 C   TYR  6   24.133  25.466  29.432  1.00  0.00   C
ATOM  49 O   TYR  6   24.879  24.521  29.187  1.00  0.00   O
ATOM  50 N   ASP  7   23.417  26.167  28.598  1.00  0.00   N
ATOM  51 CA  ASP  7   23.338  25.843  27.163  1.00  0.00   C
ATOM  52 CB  ASP  7   21.940  25.171  26.854  1.00  0.00   C
ATOM  53 CG  ASP  7   21.548  25.223  25.399  1.00  0.00   C
ATOM  54 OD1 ASP  7   22.373  25.078  24.471  1.00  0.00   O
ATOM  55 OD2 ASP  7   20.374  25.349  25.132  1.00  0.00   O1-
ATOM  56 C   ASP  7   23.529  27.094  26.312  1.00  0.00   C
ATOM  57 O   ASP  7   22.675  28.010  26.238  1.00  0.00   O
ATOM  58 N   ASP  8   24.683  27.127  25.632  1.00  0.00   N
ATOM  59 CA  ASP  8   25.117  28.249  24.756  1.00  0.00   C
ATOM  60 CB  ASP  8   25.875  29.350  25.614  1.00  0.00   C
ATOM  61 CG  ASP  8   26.075  30.700  24.967  1.00  0.00   C
ATOM  62 OD1 ASP  8   27.201  31.229  24.868  1.00  0.00   O
ATOM  63 OD2 ASP  8   25.100  31.257  24.394  1.00  0.00   O1-
ATOM  64 C   ASP  8   26.002  27.814  23.563  1.00  0.00   C
ATOM  65 O   ASP  8   26.288  26.603  23.390  1.00  0.00   O
ATOM  66 N   ALA  9   25.997  28.614  22.567  1.00  0.00   N
ATOM  67 CA  ALA  9   26.384  28.249  21.202  1.00  0.00   C
ATOM  68 CB  ALA  9   26.161  29.489  20.276  1.00  0.00   C
ATOM  69 C   ALA  9   27.813  27.627  21.049  1.00  0.00   C
ATOM  70 O   ALA  9   28.015  27.005  20.004  1.00  0.00   O
ATOM  71 N   THR  10   28.785  27.822  21.929  1.00  0.00   N
ATOM  72 CA  THR  10   30.201  27.331  21.932  1.00  0.00   C
ATOM  73 CB  THR  10   31.107  28.545  22.201  1.00  0.00   C
ATOM  74 CG2 THR  10   31.067  29.466  20.995  1.00  0.00   C
ATOM  75 OG1 THR  10   30.744  29.178  23.434  1.00  0.00   O
ATOM  76 C   THR  10   30.575  26.197  22.908  1.00  0.00   C
ATOM  77 O   THR  10   31.581  25.536  22.765  1.00  0.00   O
ATOM  78 N   LYS  11   29.803  26.124  23.991  1.00  0.00   N
ATOM  79 CA  LYS  11   29.803  25.082  25.051  1.00  0.00   C
ATOM  80 CB  LYS  11   29.587  25.679  26.406  1.00  0.00   C
ATOM  81 CG  LYS  11   28.132  26.163  26.713  1.00  0.00   C
ATOM  82 CD  LYS  11   28.163  27.048  28.012  1.00  0.00   C
ATOM  83 CE  LYS  11   27.899  26.242  29.290  1.00  0.00   C
ATOM  84 NZ  LYS  11   28.258  27.060  30.484  1.00  0.00   N1+
ATOM  85 C   LYS  11   28.894  23.843  24.695  1.00  0.00   C
ATOM  86 O   LYS  11   29.318  22.686  24.988  1.00  0.00   O
ATOM  87 N   THR  12   27.840  24.038  23.860  1.00  0.00   N
ATOM  88 CA  THR  12   26.937  22.902  23.511  1.00  0.00   C
ATOM  89 CB  THR  12   25.375  23.288  23.476  1.00  0.00   C
ATOM  90 CG2 THR  12   24.509  22.023  23.483  1.00  0.00   C
ATOM  91 OG1 THR  12   24.997  24.039  24.634  1.00  0.00   O
ATOM  92 C   THR  12   27.465  22.206  22.275  1.00  0.00   C
ATOM  93 O   THR  12   27.541  20.981  22.228  1.00  0.00   O
ATOM  94 N   PHE  13   27.825  23.003  21.238  1.00  0.00   N
ATOM  95 CA  PHE  13   28.243  22.461  19.934  1.00  0.00   C
ATOM  96 CB  PHE  13   27.479  23.052  18.752  1.00  0.00   C
ATOM  97 CG  PHE  13   25.943  23.070  18.974  1.00  0.00   C
ATOM  98 CD1 PHE  13   25.173  21.903  18.967  1.00  0.00   C
ATOM  99 CE1 PHE  13   23.816  21.888  19.347  1.00  0.00   C
ATOM 100 CZ  PHE  13   23.258  23.056  19.807  1.00  0.00   C
ATOM 101 CE2 PHE  13   24.030  24.246  19.861  1.00  0.00   C
ATOM 102 CD2 PHE  13   25.341  24.274  19.386  1.00  0.00   C
ATOM 103 C   PHE  13   29.733  22.448  19.943  1.00  0.00   C
ATOM 104 O   PHE  13   30.287  22.931  18.965  1.00  0.00   O
ATOM 105 N   THR  14   30.352  21.774  20.881  1.00  0.00   N
ATOM 106 CA  THR  14   31.807  21.539  20.841  1.00  0.00   C
ATOM 107 CB  THR  14   32.149  20.641  22.042  1.00  0.00   C
ATOM 108 CG2 THR  14   32.091  21.198  23.433  1.00  0.00   C
ATOM 109 OG1 THR  14   31.245  19.592  22.058  1.00  0.00   O
ATOM 110 C   THR  14   32.357  20.989  19.526  1.00  0.00   C
ATOM 111 O   THR  14   33.535  21.376  19.167  1.00  0.00   O
ATOM 112 N   VAL  15   31.533  20.290  18.722  1.00  0.00   N
ATOM 113 CA  VAL  15   31.728  19.848  17.317  1.00  0.00   C
ATOM 114 CB  VAL  15   30.522  19.069  16.832  1.00  0.00   C
ATOM 115 CG1 VAL  15   30.436  17.686  17.471  1.00  0.00   C
ATOM 116 CG2 VAL  15   29.121  19.824  16.926  1.00  0.00   C
ATOM 117 C   VAL  15   32.033  20.920  16.276  1.00  0.00   C
ATOM 118 O   VAL  15   32.582  20.641  15.194  1.00  0.00   O
ATOM 119 N   THR  16   31.735  22.215  16.615  1.00  0.00   N
ATOM 120 CA  THR  16   32.098  23.411  15.890  1.00  0.00   C
ATOM 121 CB  THR  16   31.202  24.626  16.233  1.00  0.00   C
ATOM 122 CG2 THR  16   29.748  24.342  15.915  1.00  0.00   C
ATOM 123 OG1 THR  16   31.298  24.973  17.570  1.00  0.00   O
ATOM 124 C   THR  16   33.628  23.793  15.976  1.00  0.00   C
ATOM 125 O   THR  16   34.049  24.807  15.396  1.00  0.00   O
ATOM 126 N   GLU  17   34.410  22.994  16.738  1.00  0.00   N
ATOM 127 CA  GLU  17   35.850  23.317  17.023  1.00  0.00   C
ATOM 128 CB  GLU  17   35.850  23.966  18.427  1.00  0.00   C
ATOM 129 CG  GLU  17   37.295  24.559  18.699  1.00  0.00   C
ATOM 130 CD  GLU  17   37.548  24.750  20.196  1.00  0.00   C
ATOM 131 OE1 GLU  17   36.652  25.322  20.914  1.00  0.00   O
ATOM 132 OE2 GLU  17   38.718  24.458  20.533  1.00  0.00   O1-
ATOM 133 C   GLU  17   36.611  21.936  16.972  1.00  0.00   C
ATOM 134 O   GLU  17   37.625  21.663  17.595  1.00  0.00   O
ATOM 135 N   NHE  18   36.172  21.042  16.100  1.00  0.00   N
TER  136  NHE  18
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B1 misfolded

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ATOM   1 CH3 ACE  1   30.243  19.667  35.960  1.00  0.00   C
ATOM   2 C   ACE  1   30.138  21.124  35.507  1.00  0.00   C
ATOM   3 O   ACE  1   30.051  22.030  36.334  1.00  0.00   O
ATOM   4 N   GLY  2   30.148  21.343  34.212  1.00  0.00   N
ATOM   5 CA  GLY  2   30.055  22.684  33.670  1.00  0.00   C
ATOM   6 C   GLY  2   30.090  22.645  32.149  1.00  0.00   C
ATOM   7 O   GLY  2   29.300  23.317  31.490  1.00  0.00   O
ATOM   8 N   GLU  3   31.010  21.854  31.592  1.00  0.00   N
ATOM   9 CA  GLU  3   31.144  21.730  30.155  1.00  0.00   C
ATOM  10 CB  GLU  3   32.268  20.765  29.789  1.00  0.00   C
ATOM  11 CG  GLU  3   32.375  20.664  28.287  1.00  0.00   C
ATOM  12 CD  GLU  3   33.500  19.699  27.921  1.00  0.00   C
ATOM  13 OE1 GLU  3   33.195  18.483  27.789  1.00  0.00   O
ATOM  14 OE2 GLU  3   34.653  20.186  27.778  1.00  0.00   O1-
ATOM  15 C   GLU  3   29.859  21.207  29.528  1.00  0.00   C
ATOM  16 O   GLU  3   29.406  21.726  28.510  1.00  0.00   O
ATOM  17 N   TRP  4   29.273  20.175  30.139  1.00  0.00   N
ATOM  18 CA  TRP  4   28.047  19.586  29.640  1.00  0.00   C
ATOM  19 CB  TRP  4   27.596  18.428  30.523  1.00  0.00   C
ATOM  20 CG  TRP  4   26.321  17.748  30.082  1.00  0.00   C
ATOM  21 CD1 TRP  4   25.713  16.712  30.676  1.00  0.00   C
ATOM  22 NE1 TRP  4   24.545  16.414  29.904  1.00  0.00   N
ATOM  23 CE2 TRP  4   24.477  17.249  28.896  1.00  0.00   C
ATOM  24 CZ2 TRP  4   23.500  17.313  27.895  1.00  0.00   C
ATOM  25 CH2 TRP  4   23.673  18.305  26.938  1.00  0.00   C
ATOM  26 CZ3 TRP  4   24.728  19.144  26.989  1.00  0.00   C
ATOM  27 CE3 TRP  4   25.701  19.061  28.007  1.00  0.00   C
ATOM  28 CD2 TRP  4   25.526  18.062  28.972  1.00  0.00   C
ATOM  29 C   TRP  4   26.921  20.611  29.606  1.00  0.00   C
ATOM  30 O   TRP  4   26.188  20.699  28.624  1.00  0.00   O
ATOM  31 N   THR  5   26.787  21.386  30.684  1.00  0.00   N
ATOM  32 CA  THR  5   25.755  22.399  30.774  1.00  0.00   C
ATOM  33 CB  THR  5   25.826  23.138  32.107  1.00  0.00   C
ATOM  34 CG2 THR  5   25.636  22.147  33.249  1.00  0.00   C
ATOM  35 OG1 THR  5   27.101  23.773  32.232  1.00  0.00   O
ATOM  36 C   THR  5   25.899  23.429  29.663  1.00  0.00   C
ATOM  37 O   THR  5   24.916  23.805  29.028  1.00  0.00   O
ATOM  38 N   TYR  6   27.131  23.887  29.429  1.00  0.00   N
ATOM  39 CA  TYR  6   27.400  24.869  28.397  1.00  0.00   C
ATOM  40 CB  TYR  6   28.884  25.215  28.343  1.00  0.00   C
ATOM  41 CG  TYR  6   29.122  26.239  27.259  1.00  0.00   C
ATOM  42 CD1 TYR  6   30.417  26.715  27.017  1.00  0.00   C
ATOM  43 CE1 TYR  6   30.637  27.665  26.012  1.00  0.00   C
ATOM  44 CZ  TYR  6   29.564  28.138  25.249  1.00  0.00   C
ATOM  45 OH  TYR  6   29.779  29.059  24.272  1.00  0.00   O
ATOM  46 CE2 TYR  6   28.270  27.661  25.490  1.00  0.00   C
ATOM  47 CD2 TYR  6   28.049  26.712  26.494  1.00  0.00   C
ATOM  48 C   TYR  6   26.993  24.350  27.026  1.00  0.00   C
ATOM  49 O   TYR  6   26.367  25.066  26.248  1.00  0.00   O
ATOM  50 N   ASP  7   27.350  23.097  26.731  1.00  0.00   N
ATOM  51 CA  ASP  7   27.021  22.487  25.458  1.00  0.00   C
ATOM  52 CB  ASP  7   27.546  21.058  25.383  1.00  0.00   C
ATOM  53 CG  ASP  7   27.180  20.452  24.030  1.00  0.00   C
ATOM  54 OD1 ASP  7   28.007  20.599  23.091  1.00  0.00   O
ATOM  55 OD2 ASP  7   26.078  19.847  23.949  1.00  0.00   O1-
ATOM  56 C   ASP  7   25.515  22.442  25.245  1.00  0.00   C
ATOM  57 O   ASP  7   25.028  22.766  24.164  1.00  0.00   O
ATOM  58 N   ASP  8   24.777  22.038  26.281  1.00  0.00   N
ATOM  59 CA  ASP  8   23.332  21.951  26.204  1.00  0.00   C
ATOM  60 CB  ASP  8   22.740  21.464  27.522  1.00  0.00   C
ATOM  61 CG  ASP  8   21.220  21.387  27.400  1.00  0.00   C
ATOM  62 OD1 ASP  8   20.729  20.298  26.999  1.00  0.00   O
ATOM  63 OD2 ASP  8   20.564  22.417  27.710  1.00  0.00   O1-
ATOM  64 C   ASP  8   22.717  23.309  25.892  1.00  0.00   C
ATOM  65 O   ASP  8   21.831  23.412  25.049  1.00  0.00   O
ATOM  66 N   ALA  9   23.193  24.351  26.577  1.00  0.00   N
ATOM  67 CA  ALA  9   22.691  25.695  26.371  1.00  0.00   C
ATOM  68 CB  ALA  9   23.404  26.692  27.279  1.00  0.00   C
ATOM  69 C   ALA  9   22.900  26.144  24.933  1.00  0.00   C
ATOM  70 O   ALA  9   21.997  26.709  24.318  1.00  0.00   O
ATOM  71 N   THR  10   24.096  25.891  24.395  1.00  0.00   N
ATOM  72 CA  THR  10   24.418  26.269  23.034  1.00  0.00   C
ATOM  73 CB  THR  10   25.843  25.864  22.674  1.00  0.00   C
ATOM  74 CG2 THR  10   26.821  26.557  23.617  1.00  0.00   C
ATOM  75 OG1 THR  10   25.982  24.446  22.801  1.00  0.00   O
ATOM  76 C   THR  10   23.479  25.596  22.042  1.00  0.00   C
ATOM  77 O   THR  10   22.982  26.239  21.119  1.00  0.00   O
ATOM  78 N   LYS  11   23.238  24.298  22.233  1.00  0.00   N
ATOM  79 CA  LYS  11   22.362  23.544  21.358  1.00  0.00   C
ATOM  80 CB  LYS  11   22.263  22.089  21.802  1.00  0.00   C
ATOM  81 CG  LYS  11   21.336  21.331  20.858  1.00  0.00   C
ATOM  82 CD  LYS  11   21.236  19.876  21.302  1.00  0.00   C
ATOM  83 CE  LYS  11   20.308  19.119  20.357  1.00  0.00   C
ATOM  84 NZ  LYS  11   20.212  17.716  20.785  1.00  0.00   N1+
ATOM  85 C   LYS  11   20.956  24.126  21.355  1.00  0.00   C
ATOM  86 O   LYS  11   20.349  24.284  20.299  1.00  0.00   O
ATOM  87 N   THR  12   20.440  24.447  22.543  1.00  0.00   N
ATOM  88 CA  THR  12   19.112  25.010  22.674  1.00  0.00   C
ATOM  89 CB  THR  12   18.771  25.281  24.136  1.00  0.00   C
ATOM  90 CG2 THR  12   18.828  23.975  24.922  1.00  0.00   C
ATOM  91 OG1 THR  12   19.715  26.206  24.681  1.00  0.00   O
ATOM  92 C   THR  12   18.997  26.325  21.918  1.00  0.00   C
ATOM  93 O   THR  12   18.018  26.555  21.211  1.00  0.00   O
ATOM  94 N   PHE  13   20.002  27.191  22.068  1.00  0.00   N
ATOM  95 CA  PHE  13   20.011  28.478  21.401  1.00  0.00   C
ATOM  96 CB  PHE  13   21.271  29.265  21.745  1.00  0.00   C
ATOM  97 CG  PHE  13   21.371  30.624  21.095  1.00  0.00   C
ATOM  98 CD1 PHE  13   22.485  31.436  21.338  1.00  0.00   C
ATOM  99 CE1 PHE  13   22.577  32.696  20.735  1.00  0.00   C
ATOM 100 CZ  PHE  13   21.556  33.144  19.889  1.00  0.00   C
ATOM 101 CE2 PHE  13   20.442  32.332  19.645  1.00  0.00   C
ATOM 102 CD2 PHE  13   20.349  31.073  20.248  1.00  0.00   C
ATOM 103 C   PHE  13   19.964  28.311  19.889  1.00  0.00   C
ATOM 104 O   PHE  13   19.210  29.003  19.208  1.00  0.00   O
ATOM 105 N   THR  14   20.775  27.388  19.364  1.00  0.00   N
ATOM 106 CA  THR  14   20.823  27.134  17.938  1.00  0.00   C
ATOM 107 CB  THR  14   21.828  26.036  17.611  1.00  0.00   C
ATOM 108 CG2 THR  14   23.216  26.460  18.078  1.00  0.00   C
ATOM 109 OG1 THR  14   21.448  24.829  18.277  1.00  0.00   O
ATOM 110 C   THR  14   19.464  26.694  17.413  1.00  0.00   C
ATOM 111 O   THR  14   19.011  27.171  16.375  1.00  0.00   O
ATOM 112 N   VAL  15   18.812  25.779  18.136  1.00  0.00   N
ATOM 113 CA  VAL  15   17.510  25.279  17.742  1.00  0.00   C
ATOM 114 CB  VAL  15   16.995  24.248  18.740  1.00  0.00   C
ATOM 115 CG1 VAL  15   16.874  24.889  20.117  1.00  0.00   C
ATOM 116 CG2 VAL  15   15.626  23.746  18.292  1.00  0.00   C
ATOM 117 C   VAL  15   16.490  26.405  17.667  1.00  0.00   C
ATOM 118 O   VAL  15   15.719  26.486  16.713  1.00  0.00   O
ATOM 119 N   THR  16   16.486  27.277  18.679  1.00  0.00   N
ATOM 120 CA  THR  16   15.562  28.392  18.725  1.00  0.00   C
ATOM 121 CB  THR  16   15.772  29.227  19.984  1.00  0.00   C
ATOM 122 CG2 THR  16   15.545  28.356  21.215  1.00  0.00   C
ATOM 123 OG1 THR  16   17.107  29.737  20.001  1.00  0.00   O
ATOM 124 C   THR  16   15.749  29.308  17.523  1.00  0.00   C
ATOM 125 O   THR  16   14.775  29.727  16.901  1.00  0.00   O
ATOM 126 N   GLU  17   17.006  29.618  17.199  1.00  0.00   N
ATOM 127 CA  GLU  17   17.316  30.481  16.076  1.00  0.00   C
ATOM 128 CB  GLU  17   18.822  30.670  15.929  1.00  0.00   C
ATOM 129 CG  GLU  17   19.103  31.573  14.752  1.00  0.00   C
ATOM 130 CD  GLU  17   20.611  31.762  14.604  1.00  0.00   C
ATOM 131 OE1 GLU  17   21.226  30.940  13.874  1.00  0.00   O
ATOM 132 OE2 GLU  17   21.134  32.728  15.222  1.00  0.00   O1-
ATOM 133 C   GLU  17   16.792  29.895  14.774  1.00  0.00   C
ATOM 134 O   GLU  17   16.192  28.822  14.769  1.00  0.00   O
ATOM 135 N   NHE  18   17.015  30.596  13.663  1.00  0.00   N
TER  136  NHE  18
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B2 extended

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ATOM   1 CH3 ACE  1   28.608  21.610  32.298  1.00  0.00   C
ATOM   2 C   ACE  1   29.240  22.384  31.135  1.00  0.00   C
ATOM   3 O   ACE  1   29.406  23.622  31.282  1.00  0.00   O
ATOM   4 N   SER  2   29.453  21.666  30.018  1.00  0.00   N
ATOM   5 CA  SER  2   29.732  22.254  28.643  1.00  0.00   C
ATOM   6 CB  SER  2   30.900  21.463  28.035  1.00  0.00   C
ATOM   7 OG  SER  2   31.572  22.388  27.260  1.00  0.00   O
ATOM   8 C   SER  2   28.518  22.440  27.776  1.00  0.00   C
ATOM   9 O   SER  2   27.356  22.034  28.140  1.00  0.00   O
ATOM  10 N   TRP  3   28.656  23.153  26.639  1.00  0.00   N
ATOM  11 CA  TRP  3   27.523  23.593  25.762  1.00  0.00   C
ATOM  12 CB  TRP  3   28.053  24.667  24.898  1.00  0.00   C
ATOM  13 CG  TRP  3   28.394  25.978  25.633  1.00  0.00   C
ATOM  14 CD1 TRP  3   29.605  26.355  26.004  1.00  0.00   C
ATOM  15 NE1 TRP  3   29.532  27.360  26.916  1.00  0.00   N
ATOM  16 CE2 TRP  3   28.214  27.723  27.232  1.00  0.00   C
ATOM  17 CZ2 TRP  3   27.706  28.702  28.108  1.00  0.00   C
ATOM  18 CH2 TRP  3   26.333  28.774  28.260  1.00  0.00   C
ATOM  19 CZ3 TRP  3   25.473  27.875  27.575  1.00  0.00   C
ATOM  20 CE3 TRP  3   26.047  26.953  26.616  1.00  0.00   C
ATOM  21 CD2 TRP  3   27.409  26.803  26.474  1.00  0.00   C
ATOM  22 C   TRP  3   26.834  22.512  25.015  1.00  0.00   C
ATOM  23 O   TRP  3   25.887  22.712  24.321  1.00  0.00   O
ATOM  24 N   THR  4   27.301  21.234  25.063  1.00  0.00   N
ATOM  25 CA  THR  4   26.759  19.943  24.464  1.00  0.00   C
ATOM  26 CB  THR  4   27.796  18.821  24.565  1.00  0.00   C
ATOM  27 CG2 THR  4   28.595  18.590  23.290  1.00  0.00   C
ATOM  28 OG1 THR  4   28.736  19.049  25.651  1.00  0.00   O
ATOM  29 C   THR  4   25.417  19.451  25.088  1.00  0.00   C
ATOM  30 O   THR  4   24.654  18.647  24.455  1.00  0.00   O
ATOM  31 N   TRP  5   25.180  19.807  26.373  1.00  0.00   N
ATOM  32 CA  TRP  5   24.208  19.233  27.306  1.00  0.00   C
ATOM  33 CB  TRP  5   24.827  18.854  28.665  1.00  0.00   C
ATOM  34 CG  TRP  5   25.740  17.653  28.616  1.00  0.00   C
ATOM  35 CD1 TRP  5   25.680  16.566  27.801  1.00  0.00   C
ATOM  36 NE1 TRP  5   26.569  15.594  28.175  1.00  0.00   N
ATOM  37 CE2 TRP  5   27.394  16.018  29.116  1.00  0.00   C
ATOM  38 CZ2 TRP  5   28.547  15.541  29.735  1.00  0.00   C
ATOM  39 CH2 TRP  5   29.130  16.261  30.755  1.00  0.00   C
ATOM  40 CZ3 TRP  5   28.683  17.516  31.128  1.00  0.00   C
ATOM  41 CE3 TRP  5   27.550  18.077  30.488  1.00  0.00   C
ATOM  42 CD2 TRP  5   26.889  17.316  29.491  1.00  0.00   C
ATOM  43 C   TRP  5   23.020  20.236  27.453  1.00  0.00   C
ATOM  44 O   TRP  5   22.073  19.879  28.201  1.00  0.00   O
ATOM  45 N   GLU  6   23.054  21.383  26.761  1.00  0.00   N
ATOM  46 CA  GLU  6   21.873  22.292  26.659  1.00  0.00   C
ATOM  47 CB  GLU  6   22.303  23.725  27.059  1.00  0.00   C
ATOM  48 CG  GLU  6   22.721  23.701  28.568  1.00  0.00   C
ATOM  49 CD  GLU  6   23.050  25.140  29.036  1.00  0.00   C
ATOM  50 OE1 GLU  6   24.097  25.257  29.745  1.00  0.00   O
ATOM  51 OE2 GLU  6   22.365  26.164  28.672  1.00  0.00  O1-
ATOM  52 C   GLU  6   21.058  22.265  25.318  1.00  0.00   C
ATOM  53 O   GLU  6   20.534  23.255  24.830  1.00  0.00   O
ATOM  54 N   ASN  7   21.236  21.184  24.564  1.00  0.00   N
ATOM  55 CA  ASN  7   20.725  20.855  23.295  1.00  0.00   C
ATOM  56 CB  ASN  7   21.297  19.414  22.986  1.00  0.00   C
ATOM  57 CG  ASN  7   21.523  19.146  21.490  1.00  0.00   C
ATOM  58 OD1 ASN  7   22.446  19.591  20.888  1.00  0.00   O
ATOM  59 ND2 ASN  7   20.669  18.441  20.874  1.00  0.00   N
ATOM  60 C   ASN  7   19.195  20.867  23.124  1.00  0.00   C
ATOM  61 O   ASN  7   18.395  20.668  24.035  1.00  0.00   O
ATOM  62 N   GLY  8   18.829  21.100  21.877  1.00  0.00   N
ATOM  63 CA  GLY  8   17.458  21.148  21.365  1.00  0.00   C
ATOM  64 C   GLY  8   16.554  22.344  21.709  1.00  0.00   C
ATOM  65 O   GLY  8   15.437  22.495  21.231  1.00  0.00   O
ATOM  66 N   LYS  9   17.025  23.197  22.626  1.00  0.00   N
ATOM  67 CA  LYS  9   16.309  24.393  23.063  1.00  0.00   C
ATOM  68 CB  LYS  9   16.810  24.874  24.500  1.00  0.00   C
ATOM  69 CG  LYS  9   16.675  23.793  25.562  1.00  0.00   C
ATOM  70 CD  LYS  9   15.270  23.199  25.749  1.00  0.00   C
ATOM  71 CE  LYS  9   15.353  22.212  26.938  1.00  0.00   C
ATOM  72 NZ  LYS  9   13.964  21.717  27.189  1.00  0.00  N1+
ATOM  73 C   LYS  9   16.151  25.582  22.086  1.00  0.00   C
ATOM  74 O   LYS  9   15.306  26.417  22.176  1.00  0.00   O
ATOM  75 N   TRP  10   16.999  25.527  21.092  1.00  0.00   N
ATOM  76 CA  TRP  10   17.321  26.553  20.122  1.00  0.00   C
ATOM  77 CB  TRP  10   18.784  27.127  20.394  1.00  0.00   C
ATOM  78 CG  TRP  10   18.952  27.885  21.681  1.00  0.00   C
ATOM  79 CD1 TRP  10   19.549  27.338  22.762  1.00  0.00   C
ATOM  80 NE1 TRP  10   19.468  28.206  23.878  1.00  0.00   N
ATOM  81 CE2 TRP  10   18.893  29.356  23.506  1.00  0.00   C
ATOM  82 CZ2 TRP  10   18.580  30.519  24.245  1.00  0.00   C
ATOM  83 CH2 TRP  10   17.937  31.642  23.600  1.00  0.00   C
ATOM  84 CZ3 TRP  10   17.394  31.392  22.316  1.00  0.00   C
ATOM  85 CE3 TRP  10   17.729  30.261  21.607  1.00  0.00   C
ATOM  86 CD2 TRP  10   18.506  29.187  22.133  1.00  0.00   C
ATOM  87 C   TRP  10   17.406  25.945  18.686  1.00  0.00   C
ATOM  88 O   TRP  10   17.922  24.824  18.582  1.00  0.00   O
ATOM  89 N   THR  11   16.954  26.624  17.669  1.00  0.00   N
ATOM  90 CA  THR  11   16.900  26.161  16.209  1.00  0.00   C
ATOM  91 CB  THR  11   15.763  26.801  15.378  1.00  0.00   C
ATOM  92 CG2 THR  11   14.352  26.291  15.692  1.00  0.00   C
ATOM  93 OG1 THR  11   15.703  28.147  15.797  1.00  0.00   O
ATOM  94 C   THR  11   18.307  26.334  15.478  1.00  0.00   C
ATOM  95 O   THR  11   18.325  25.896  14.323  1.00  0.00   O
ATOM  96 N   TRP  12   19.286  26.964  16.034  1.00  0.00   N
ATOM  97 CA  TRP  12   20.536  27.319  15.320  1.00  0.00   C
ATOM  98 CB  TRP  12   20.923  28.819  15.465  1.00  0.00   C
ATOM  99 CG  TRP  12   20.760  29.409  16.863  1.00  0.00   C
ATOM 100 CD1 TRP  12   21.404  28.970  17.955  1.00  0.00   C
ATOM 101 NE1 TRP  12   21.120  29.749  19.009  1.00  0.00   N
ATOM 102 CE2 TRP  12   20.232  30.740  18.711  1.00  0.00   C
ATOM 103 CZ2 TRP  12   19.571  31.695  19.462  1.00  0.00   C
ATOM 104 CH2 TRP  12   18.588  32.588  18.900  1.00  0.00   C
ATOM 105 CZ3 TRP  12   18.254  32.309  17.592  1.00  0.00   C
ATOM 106 CE3 TRP  12   18.820  31.276  16.840  1.00  0.00   C
ATOM 107 CD2 TRP  12   19.938  30.546  17.322  1.00  0.00   C
ATOM 108 C   TRP  12   21.600  26.375  15.769  1.00  0.00   C
ATOM 109 O   TRP  12   21.669  25.883  16.860  1.00  0.00   O
ATOM 110 N   LYS  13   22.504  26.092  14.806  1.00  0.00   N
ATOM 111 CA  LYS  13   23.678  25.181  14.892  1.00  0.00   C
ATOM 112 CB  LYS  13   23.589  23.825  14.290  1.00  0.00   C
ATOM 113 CG  LYS  13   22.606  22.954  15.034  1.00  0.00   C
ATOM 114 CD  LYS  13   22.711  21.451  14.811  1.00  0.00   C
ATOM 115 CE  LYS  13   22.001  21.163  13.431  1.00  0.00   C
ATOM 116 NZ  LYS  13   22.004  19.726  13.112  1.00  0.00  N1+
ATOM 117 C   LYS  13   25.040  25.831  14.504  1.00  0.00   C
ATOM 118 O   LYS  13   25.172  26.598  13.530  1.00  0.00   O
ATOM 119 N   NHE  14   26.102  25.549  15.260  1.00  0.00   N
TER  120   NHE  14
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B2 misfolded

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ATOM   1  CH3 ACE  1   27.375  19.046  34.055  1.00  0.00   C
ATOM   2  C   ACE  1   27.392  20.412  33.367  1.00  0.00   C
ATOM   3  O   ACE  1   27.360  21.446  34.032  1.00  0.00   O
ATOM   4  N   SER  2   27.440  20.412  32.055  1.00  0.00   N
ATOM   5  CA  SER  2   27.461  21.648  31.298  1.00  0.00   C
ATOM   6  CB  SER  2   28.676  22.496  31.664  1.00  0.00   C
ATOM   7  OG  SER  2   28.660  23.704  30.899  1.00  0.00   O
ATOM   8  C   SER  2   27.518  21.375  29.802  1.00  0.00   C
ATOM   9  O   SER  2   26.793  21.994  29.027  1.00  0.00   O
ATOM  10  N   TRP  3   28.383  20.442  29.398  1.00  0.00   N
ATOM  11  CA  TRP  3   28.532  20.090  28.000  1.00  0.00   C
ATOM  12  CB  TRP  3   29.585  19.001  27.817  1.00  0.00   C
ATOM  13  CG  TRP  3   29.810  18.567  26.389  1.00  0.00   C
ATOM  14  CD1 TRP  3   30.671  17.635  25.957  1.00  0.00   C
ATOM  15  NE1 TRP  3   30.535  17.567  24.535  1.00  0.00   N
ATOM  16  CE2 TRP  3   29.627  18.429  24.152  1.00  0.00   C
ATOM  17  CZ2 TRP  3   29.180  18.692  22.851  1.00  0.00   C
ATOM  18  CH2 TRP  3   28.197  19.667  22.729  1.00  0.00   C
ATOM  19  CZ3 TRP  3   27.716  20.310  23.815  1.00  0.00   C
ATOM  20  CE3 TRP  3   28.181  20.028  25.116  1.00  0.00   C
ATOM  21  CD2 TRP  3   29.171  19.046  25.239  1.00  0.00   C
ATOM  22  C   TRP  3   27.222  19.573  27.423  1.00  0.00   C
ATOM  23  O   TRP  3   26.827  19.962  26.326  1.00  0.00   O
ATOM  24  N   THR  4   26.548  18.693  28.167  1.00  0.00   N
ATOM  25  CA  THR  4   25.289  18.126  27.727  1.00  0.00   C
ATOM  26  CB  THR  4   24.734  17.153  28.762  1.00  0.00   C
ATOM  27  CG2 THR  4   25.730  16.019  28.978  1.00  0.00   C
ATOM  28  OG1 THR  4   24.521  17.841  29.998  1.00  0.00   O
ATOM  29  C   THR  4   24.246  19.214  27.507  1.00  0.00   C
ATOM  30  O   THR  4   23.539  19.204  26.503  1.00  0.00   O
ATOM  31  N   TRP  5   24.154  20.153  28.451  1.00  0.00   N
ATOM  32  CA  TRP  5   23.202  21.241  28.357  1.00  0.00   C
ATOM  33  CB  TRP  5   23.306  22.168  29.564  1.00  0.00   C
ATOM  34  CG  TRP  5   22.350  23.337  29.556  1.00  0.00   C
ATOM  35  CD1 TRP  5   22.236  24.292  30.489  1.00  0.00   C
ATOM  36  NE1 TRP  5   21.204  25.180  30.054  1.00  0.00   N
ATOM  37  CE2 TRP  5   20.731  24.757  28.907  1.00  0.00   C
ATOM  38  CZ2 TRP  5   19.715  25.326  28.130  1.00  0.00   C
ATOM  39  CH2 TRP  5   19.410  24.664  26.946  1.00  0.00   C
ATOM  40  CZ3 TRP  5   20.068  23.541  26.589  1.00  0.00   C
ATOM  41  CE3 TRP  5   21.089  22.986  27.386  1.00  0.00   C
ATOM  42  CD2 TRP  5   21.397  23.653  28.579  1.00  0.00   C
ATOM  43  C   TRP  5   23.443  22.075  27.107  1.00  0.00   C
ATOM  44  O   TRP  5   22.503  22.420  26.395  1.00  0.00   O
ATOM  45  N   GLU  6   24.711  22.399  26.841  1.00  0.00   N
ATOM  46  CA  GLU  6   25.072  23.190  25.681  1.00  0.00   C
ATOM  47  CB  GLU  6   26.578  23.413  25.617  1.00  0.00   C
ATOM  48  CG  GLU  6   26.913  24.239  24.398  1.00  0.00   C
ATOM  49  CD  GLU  6   28.423  24.462  24.333  1.00  0.00   C
ATOM  50  OE1 GLU  6   29.105  23.610  23.705  1.00  0.00   O
ATOM  51  OE2 GLU  6   28.879  25.484  24.912  1.00  0.00   O1-
ATOM  52  C   GLU  6   24.649  22.498  24.394  1.00  0.00   C
ATOM  53  O   GLU  6   24.093  23.131  23.498  1.00  0.00   O
ATOM  54  N   ASN  7   24.913  21.192  24.302  1.00  0.00   N
ATOM  55  CA  ASN  7   24.560  20.420  23.127  1.00  0.00   C
ATOM  56  CB  ASN  7   24.975  18.962  23.284  1.00  0.00   C
ATOM  57  CG  ASN  7   24.604  18.151  22.050  1.00  0.00   C
ATOM  58  OD1 ASN  7   24.044  18.687  21.097  1.00  0.00   O
ATOM  59  ND2 ASN  7   24.919  16.853  22.071  1.00  0.00   N
ATOM  60  C   ASN  7   23.059  20.454  22.880  1.00  0.00   C
ATOM  61  O   ASN  7   22.617  20.644  21.750  1.00  0.00   O
ATOM  62  N   GLY  8   22.274  20.269  23.944  1.00  0.00   N
ATOM  63  CA  GLY  8   20.828  20.278  23.841  1.00  0.00   C
ATOM  64  C   GLY  8   20.344  21.619  23.308  1.00  0.00   C
ATOM  65  O   GLY  8   19.485  21.668  22.430  1.00  0.00   O
ATOM  66  N   LYS  9   20.896  22.710  23.844  1.00  0.00   N
ATOM  67  CA  LYS  9   20.520  24.044  23.423  1.00  0.00   C
ATOM  68  CB  LYS  9   21.302  25.103  24.192  1.00  0.00   C
ATOM  69  CG  LYS  9   20.877  26.491  23.721  1.00  0.00   C
ATOM  70  CD  LYS  9   21.659  27.550  24.492  1.00  0.00   C
ATOM  71  CE  LYS  9   21.235  28.937  24.020  1.00  0.00   C
ATOM  72  NZ  LYS  9   21.988  29.958  24.762  1.00  0.00   N1+
ATOM  73  C   LYS  9   20.796  24.249  21.940  1.00  0.00   C
ATOM  74  O   LYS  9   19.959  24.788  21.218  1.00  0.00   O
ATOM  75  N   TRP  10   21.974  23.817  21.486  1.00  0.00   N
ATOM  76  CA  TRP  10   22.355  23.954  20.094  1.00  0.00   C
ATOM  77  CB  TRP  10   23.746  23.379  19.847  1.00  0.00   C
ATOM  78  CG  TRP  10   24.232  23.476  18.420  1.00  0.00   C
ATOM  79  CD1 TRP  10   25.408  23.051  17.938  1.00  0.00   C
ATOM  80  NE1 TRP  10   25.422  23.355  16.541  1.00  0.00   N
ATOM  81  CE2 TRP  10   24.293  23.937  16.220  1.00  0.00   C
ATOM  82  CZ2 TRP  10   23.889  24.399  14.962  1.00  0.00   C
ATOM  83  CH2 TRP  10   22.628  24.984  14.903  1.00  0.00   C
ATOM  84  CZ3 TRP  10   21.858  25.086  16.007  1.00  0.00   C
ATOM  85  CE3 TRP  10   22.286  24.613  17.264  1.00  0.00   C
ATOM  86  CD2 TRP  10   23.555  24.026  17.324  1.00  0.00   C
ATOM  87  C   TRP  10   21.380  23.220  19.184  1.00  0.00   C
ATOM  88  O   TRP  10   20.960  23.754  18.160  1.00  0.00   O
ATOM  89  N   THR  11   21.020  21.990  19.561  1.00  0.00   N
ATOM  90  CA  THR  11   20.099  21.190  18.781  1.00  0.00   C
ATOM  91  CB  THR  11   19.862  19.832  19.435  1.00  0.00   C
ATOM  92  CG2 THR  11   21.185  19.084  19.546  1.00  0.00   C
ATOM  93  OG1 THR  11   19.310  20.022  20.740  1.00  0.00   O
ATOM  94  C   THR  11   18.750  21.882  18.644  1.00  0.00   C
ATOM  95  O   THR  11   18.180  21.928  17.557  1.00  0.00   O
ATOM  96  N   TRP  12   18.241  22.423  19.754  1.00  0.00   N
ATOM  97  CA  TRP  12   16.965  23.109  19.755  1.00  0.00   C
ATOM  98  CB  TRP  12   16.623  23.629  21.147  1.00  0.00   C
ATOM  99  CG  TRP  12   15.306  24.361  21.248  1.00  0.00   C
ATOM 100  CD1 TRP  12   14.773  24.912  22.348  1.00  0.00   C
ATOM 101  NE1 TRP  12   13.524  25.492  21.961  1.00  0.00   N
ATOM 102  CE2 TRP  12   13.336  25.285  20.681  1.00  0.00   C
ATOM 103  CZ2 TRP  12   12.248  25.681  19.894  1.00  0.00   C
ATOM 104  CH2 TRP  12   12.306  25.328  18.551  1.00  0.00   C
ATOM 105  CZ3 TRP  12   13.360  24.642  18.058  1.00  0.00   C
ATOM 106  CE3 TRP  12   14.444  24.253  18.870  1.00  0.00   C
ATOM 107  CD2 TRP  12   14.386  24.610  20.222  1.00  0.00   C
ATOM 108  C   TRP  12   16.983  24.300  18.806  1.00  0.00   C
ATOM 109  O   TRP  12   16.042  24.501  18.041  1.00  0.00   O
ATOM 110  N   LYS  13   18.058  25.089  18.858  1.00  0.00   N
ATOM 111  CA  LYS  13   18.195  26.254  18.006  1.00  0.00   C
ATOM 112  CB  LYS  13   19.512  26.975  18.268  1.00  0.00   C
ATOM 113  CG  LYS  13   19.617  28.191  17.354  1.00  0.00   C
ATOM 114  CD  LYS  13   20.935  28.911  17.617  1.00  0.00   C
ATOM 115  CE  LYS  13   21.040  30.127  16.703  1.00  0.00   C
ATOM 116  NZ  LYS  13   22.310  30.823  16.956  1.00  0.00   N1+
ATOM 117  C   LYS  13   18.163  25.863  16.535  1.00  0.00   C
ATOM 118  O   LYS  13   18.035  24.687  16.205  1.00  0.00   O
ATOM 119  N   NHE  14   18.280  26.848  15.646  1.00  0.00   N
TER  120   NHE  14
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B3 extended

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ATOM   1 CH3 ACE 1   31.907 40.461 23.519 1.00 0.00   C
ATOM   2 C   ACE 1   31.519 39.316 22.646 1.00 0.00   C
ATOM   3 O   ACE 1   30.714 39.525 21.672 1.00 0.00   O
ATOM   4 N   GLN 2   31.846 38.129 23.180 1.00 0.00   N
ATOM   5 CA  GLN 2   31.472 36.833 22.648 1.00 0.00   C
ATOM   6 CB  GLN 2   32.617 36.244 21.778 1.00 0.00   C
ATOM   7 CG  GLN 2   33.028 37.136 20.605 1.00 0.00   C
ATOM   8 CD  GLN 2   33.494 36.373 19.423 1.00 0.00   C
ATOM   9 OE1 GLN 2   32.737 35.597 18.771 1.00 0.00   O
ATOM  10 NE2 GLN 2   34.787 36.529 18.924 1.00 0.00   N
ATOM  11 C   GLN 2   31.019 35.786 23.705 1.00 0.00   C
ATOM  12 O   GLN 2   31.478 35.828 24.872 1.00 0.00   O
ATOM  13 N   ILE 3   30.185 34.872 23.221 1.00 0.00   N
ATOM  14 CA  ILE 3   29.799 33.688 23.872 1.00 0.00   C
ATOM  15 CB  ILE 3   28.223 33.735 24.121 1.00 0.00   C
ATOM  16 CG2 ILE 3   27.809 34.717 25.214 1.00 0.00   C
ATOM  17 CG1 ILE 3   27.412 33.761 22.757 1.00 0.00   C
ATOM  18 CD1 ILE 3   26.093 33.002 22.733 1.00 0.00   C
ATOM  19 C   ILE 3   30.183 32.293 23.340 1.00 0.00   C
ATOM  20 O   ILE 3   30.542 32.185 22.162 1.00 0.00   O
ATOM  21 N   PHE 4   30.133 31.306 24.241 1.00 0.00   N
ATOM  22 CA  PHE 4   30.585 29.930 24.051 1.00 0.00   C
ATOM  23 CB  PHE 4   31.618 29.535 25.056 1.00 0.00   C
ATOM  24 CG  PHE 4   33.022 30.173 24.876 1.00 0.00   C
ATOM  25 CD1 PHE 4   33.558 31.167 25.726 1.00 0.00   C
ATOM  26 CE1 PHE 4   34.914 31.454 25.702 1.00 0.00   C
ATOM  27 CZ  PHE 4   35.721 30.868 24.663 1.00 0.00   C
ATOM  28 CE2 PHE 4   35.152 29.963 23.709 1.00 0.00   C
ATOM  29 CD2 PHE 4   33.792 29.717 23.800 1.00 0.00   C
ATOM  30 C   PHE 4   29.340 28.965 24.211 1.00 0.00   C
ATOM  31 O   PHE 4   28.373 29.294 24.900 1.00 0.00   O
ATOM  32 N   VAL 5   29.370 27.880 23.433 1.00 0.00   N
ATOM  33 CA  VAL 5   28.225 26.876 23.312 1.00 0.00   C
ATOM  34 CB  VAL 5   28.301 25.944 22.080 1.00 0.00   C
ATOM  35 CG1 VAL 5   28.482 26.818 20.847 1.00 0.00   C
ATOM  36 CG2 VAL 5   29.559 25.029 22.172 1.00 0.00   C
ATOM  37 C   VAL 5   27.961 26.030 24.587 1.00 0.00   C
ATOM  38 O   VAL 5   27.047 25.196 24.648 1.00 0.00   O
ATOM  39 N   LYS 6   28.771 26.261 25.589 1.00 0.00   N
ATOM  40 CA  LYS 6   28.770 25.516 26.887 1.00 0.00   C
ATOM  41 CB  LYS 6   29.712 26.175 27.894 1.00 0.00   C
ATOM  42 CG  LYS 6   29.761 25.308 29.075 1.00 0.00   C
ATOM  43 CD  LYS 6   30.692 25.833 30.143 1.00 0.00   C
ATOM  44 CE  LYS 6   31.027 24.900 31.348 1.00 0.00   C
ATOM  45 NZ  LYS 6   31.910 25.685 32.306 1.00 0.00   N1+
ATOM  46 C   LYS 6   27.401 25.429 27.390 1.00 0.00   C
ATOM  47 O   LYS 6   26.938 24.326 27.714 1.00 0.00   O
ATOM  48 N   THR 7   26.676 26.534 27.386 1.00 0.00   N
ATOM  49 CA  THR 7   25.344 26.749 27.941 1.00 0.00   C
ATOM  50 CB  THR 7   25.127 28.275 28.259 1.00 0.00   C
ATOM  51 CG2 THR 7   26.131 28.858 29.179 1.00 0.00   C
ATOM  52 OG1 THR 7   25.196 29.021 27.073 1.00 0.00   O
ATOM  53 C   THR 7   24.132 26.292 27.015 1.00 0.00   C
ATOM  54 O   THR 7   23.078 25.982 27.513 1.00 0.00   O
ATOM  55 N   LEU 8   24.313 26.250 25.680 1.00 0.00   N
ATOM  56 CA  LEU 8   23.509 25.638 24.651 1.00 0.00   C
ATOM  57 CB  LEU 8   23.945 26.298 23.303 1.00 0.00   C
ATOM  58 CG  LEU 8   23.178 25.711 22.117 1.00 0.00   C
ATOM  59 CD1 LEU 8   21.733 26.250 22.049 1.00 0.00   C
ATOM  60 CD2 LEU 8   23.993 26.138 20.880 1.00 0.00   C
ATOM  61 C   LEU 8   23.574 24.125 24.598 1.00 0.00   C
ATOM  62 O   LEU 8   22.544 23.437 24.463 1.00 0.00   O
ATOM  63 N   THR 9   24.747 23.533 24.655 1.00 0.00   N
ATOM  64 CA  THR 9   24.957 22.112 24.720 1.00 0.00   C
ATOM  65 CB  THR 9   26.480 21.881 24.860 1.00 0.00   C
ATOM  66 CG2 THR 9   26.832 20.429 24.588 1.00 0.00   C
ATOM  67 OG1 THR 9   27.357 22.589 23.969 1.00 0.00   O
ATOM  68 C   THR 9   24.236 21.484 25.960 1.00 0.00   C
ATOM  69 O   THR 9   23.571 20.470 25.840 1.00 0.00   O
ATOM  70 N   GLY 10   24.253 22.238 27.056 1.00 0.00   N
ATOM  71 CA  GLY 10   23.442 21.890 28.193 1.00 0.00   C
ATOM  72 C   GLY 10   21.938 22.086 28.065 1.00 0.00   C
ATOM  73 O   GLY 10   21.197 21.621 28.950 1.00 0.00   O
ATOM  74 N   LYS 11   21.358 22.642 27.010 1.00 0.00   N
ATOM  75 CA  LYS 11   19.977 22.591 26.584 1.00 0.00   C
ATOM  76 CB  LYS 11   19.639 23.959 26.032 1.00 0.00   C
ATOM  77 CG  LYS 11   19.116 24.912 27.153 1.00 0.00   C
ATOM  78 CD  LYS 11   18.953 26.373 26.701 1.00 0.00   C
ATOM  79 CE  LYS 11   18.454 27.297 27.827 1.00 0.00   C
ATOM  80 NZ  LYS 11   16.986 27.060 28.100 1.00 0.00   N1+
ATOM  81 C   LYS 11   19.701 21.495 25.458 1.00 0.00   C
ATOM  82 O   LYS 11   18.545 21.239 25.131 1.00 0.00   O
ATOM  83 N   THR 12   20.733 20.813 24.876 1.00 0.00   N
ATOM  84 CA  THR 12   20.708 20.088 23.671 1.00 0.00   C
ATOM  85 CB  THR 12   21.294 20.710 22.455 1.00 0.00   C
ATOM  86 CG2 THR 12   20.187 21.567 21.741 1.00 0.00   C
ATOM  87 OG1 THR 12   22.483 21.472 22.585 1.00 0.00   O
ATOM  88 C   THR 12   21.225 18.610 23.764 1.00 0.00   C
ATOM  89 O   THR 12   20.779 17.767 23.068 1.00 0.00   O
ATOM  90 N   ILE 13   22.197 18.321 24.657 1.00 0.00   N
ATOM  91 CA  ILE 13   22.849 17.034 24.749 1.00 0.00   C
ATOM  92 CB  ILE 13   24.158 17.181 25.682 1.00 0.00   C
ATOM  93 CG2 ILE 13   23.806 17.390 27.129 1.00 0.00   C
ATOM  94 CG1 ILE 13   25.081 15.971 25.540 1.00 0.00   C
ATOM  95 CD1 ILE 13   25.729 15.791 24.199 1.00 0.00   C
ATOM  96 C   ILE 13   21.926 15.860 25.192 1.00 0.00   C
ATOM  97 O   ILE 13   22.157 14.775 24.744 1.00 0.00   O
ATOM  98 N   THR 14   20.953 16.079 26.096 1.00 0.00   N
ATOM  99 CA  THR 14   19.901 15.165 26.380 1.00 0.00   C
ATOM 100 CB  THR 14   19.333 15.429 27.773 1.00 0.00   C
ATOM 101 CG2 THR 14   20.358 15.067 28.832 1.00 0.00   C
ATOM 102 OG1 THR 14   19.157 16.885 27.959 1.00 0.00   O
ATOM 103 C   THR 14   18.735 15.234 25.478 1.00 0.00   C
ATOM 104 O   THR 14   17.856 14.383 25.642 1.00 0.00   O
ATOM 105 N   LEU 15   18.733 16.126 24.442 1.00 0.00   N
ATOM 106 CA  LEU 15   17.765 16.257 23.330 1.00 0.00   C
ATOM 107 CB  LEU 15   17.460 17.832 22.954 1.00 0.00   C
ATOM 108 CG  LEU 15   16.416 17.938 21.821 1.00 0.00   C
ATOM 109 CD1 LEU 15   15.034 17.389 22.028 1.00 0.00   C
ATOM 110 CD2 LEU 15   16.257 19.396 21.423 1.00 0.00   C
ATOM 111 C   LEU 15   18.311 15.449 22.093 1.00 0.00   C
ATOM 112 O   LEU 15   17.657 14.503 21.647 1.00 0.00   O
ATOM 113 N   GLU 16   19.379 15.979 21.432 1.00 0.00   N
ATOM 114 CA  GLU 16   19.946 15.381 20.205 1.00 0.00   C
ATOM 115 CB  GLU 16   20.482 16.463 19.284 1.00 0.00   C
ATOM 116 CG  GLU 16   19.404 17.475 18.885 1.00 0.00   C
ATOM 117 CD  GLU 16   19.786 18.233 17.584 1.00 0.00   C
ATOM 118 OE1 GLU 16   20.679 19.118 17.696 1.00 0.00   O
ATOM 119 OE2 GLU 16   19.249 17.974 16.480 1.00 0.00   O1-
ATOM 120 C   GLU 16   20.918 14.213 20.528 1.00 0.00   C
ATOM 121 O   GLU 16   21.240 13.487 19.582 1.00 0.00   O
ATOM 122 N   NHE 17   21.422 14.088 21.715 1.00 0.00   N
TER 123   NHE 17
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B3 misfolded

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ATOM   1 CH3 ACE 1   27.711 17.233 34.712 1.00 0.00  C
ATOM   2 C   ACE 1   27.971 18.665 34.241 1.00 0.00  C
ATOM   3 O   ACE 1   28.066 19.582 35.054 1.00 0.00  O
ATOM   4 N   GLN 2   28.083 18.850 32.945 1.00 0.00  N
ATOM   5 CA  GLN 2   28.330 20.164 32.386 1.00 0.00  C
ATOM   6 CB  GLN 2   29.641 20.744 32.907 1.00 0.00  C
ATOM   7 CG  GLN 2   29.863 22.124 32.298 1.00 0.00  C
ATOM   8 CD  GLN 2   31.165 22.738 32.794 1.00 0.00  C
ATOM   9 OE1 GLN 2   31.881 22.128 33.584 1.00 0.00  O
ATOM  10 NE2 GLN 2   31.469 23.952 32.327 1.00 0.00  N
ATOM  11 C   GLN 2   28.417 20.107 30.869 1.00 0.00  C
ATOM  12 O   GLN 2   27.835 20.941 30.179 1.00 0.00  O
ATOM  13 N   ILE 3   29.147 19.118 30.348 1.00 0.00  N
ATOM  14 CA  ILE 3   29.308 18.956 28.917 1.00 0.00  C
ATOM  15 CB  ILE 3   30.192 17.744 28.640 1.00 0.00  C
ATOM  16 CG2 ILE 3   29.540 16.495 29.223 1.00 0.00  C
ATOM  17 CG1 ILE 3   30.360 17.573 27.133 1.00 0.00  C
ATOM  18 CD1 ILE 3   31.244 16.362 26.856 1.00 0.00  C
ATOM  19 C   ILE 3   27.963 18.744 28.236 1.00 0.00  C
ATOM  20 O   ILE 3   27.687 19.348 27.201 1.00 0.00  O
ATOM  21 N   PHE 4   27.126 17.883 28.820 1.00 0.00  N
ATOM  22 CA  PHE 4   25.818 17.596 28.268 1.00 0.00  C
ATOM  23 CB  PHE 4   25.071 16.582 29.128 1.00 0.00  C
ATOM  24 CG  PHE 4   23.692 16.217 28.633 1.00 0.00  C
ATOM  25 CD1 PHE 4   22.913 15.296 29.344 1.00 0.00  C
ATOM  26 CE1 PHE 4   21.634 14.959 28.884 1.00 0.00  C
ATOM  27 CZ  PHE 4   21.134 15.543 27.714 1.00 0.00  C
ATOM  28 CE2 PHE 4   21.912 16.464 27.003 1.00 0.00  C
ATOM  29 CD2 PHE 4   23.191 16.802 27.463 1.00 0.00  C
ATOM  30 C   PHE 4   24.967 18.856 28.190 1.00 0.00  C
ATOM  31 O   PHE 4   24.316 19.107 27.178 1.00 0.00  O
ATOM  32 N   VAL 5   24.974 19.649 29.263 1.00 0.00  N
ATOM  33 CA  VAL 5   24.207 20.877 29.313 1.00 0.00  C
ATOM  34 CB  VAL 5   24.394 21.588 30.649 1.00 0.00  C
ATOM  35 CG1 VAL 5   25.868 21.927 30.842 1.00 0.00  C
ATOM  36 CG2 VAL 5   23.572 22.873 30.660 1.00 0.00  C
ATOM  37 C   VAL 5   24.635 21.836 28.211 1.00 0.00  C
ATOM  38 O   VAL 5   23.794 22.427 27.537 1.00 0.00  O
ATOM  39 N   LYS 6   25.948 21.989 28.029 1.00 0.00  N
ATOM  40 CA  LYS 6   26.483 22.874 27.013 1.00 0.00  C
ATOM  41 CB  LYS 6   28.007 22.861 27.021 1.00 0.00  C
ATOM  42 CG  LYS 6   28.529 23.801 25.940 1.00 0.00  C
ATOM  43 CD  LYS 6   30.054 23.789 25.948 1.00 0.00  C
ATOM  44 CE  LYS 6   30.576 24.729 24.867 1.00 0.00  C
ATOM  45 NZ  LYS 6   32.046 24.717 24.874 1.00 0.00 N1+
ATOM  46 C   LYS 6   26.022 22.454 25.625 1.00 0.00  C
ATOM  47 O   LYS 6   25.614 23.292 24.823 1.00 0.00  O
ATOM  48 N   THR 7   26.086 21.151 25.342 1.00 0.00  N
ATOM  49 CA  THR 7   25.676 20.626 24.055 1.00 0.00  C
ATOM  50 CB  THR 7   25.853 19.112 23.998 1.00 0.00  C
ATOM  51 CG2 THR 7   27.321 18.763 24.222 1.00 0.00  C
ATOM  52 OG1 THR 7   25.056 18.501 25.015 1.00 0.00  O
ATOM  53 C   THR 7   24.211 20.934 23.778 1.00 0.00  C
ATOM  54 O   THR 7   23.860 21.356 22.679 1.00 0.00  O
ATOM  55 N   LEU 8   23.357 20.723 24.781 1.00 0.00  N
ATOM  56 CA  LEU 8   21.937 20.977 24.644 1.00 0.00  C
ATOM  57 CB  LEU 8   21.193 20.652 25.935 1.00 0.00  C
ATOM  58 CG  LEU 8   19.706 20.934 25.750 1.00 0.00  C
ATOM  59 CD1 LEU 8   19.162 20.068 24.618 1.00 0.00  C
ATOM  60 CD2 LEU 8   18.962 20.608 27.041 1.00 0.00  C
ATOM  61 C   LEU 8   21.672 22.439 24.310 1.00 0.00  C
ATOM  62 O   LEU 8   20.870 22.742 23.431 1.00 0.00  O
ATOM  63 N   THR 9   22.351 23.345 25.017 1.00 0.00  N
ATOM  64 CA  THR 9   22.187 24.768 24.794 1.00 0.00  C
ATOM  65 CB  THR 9   23.077 25.576 25.734 1.00 0.00  C
ATOM  66 CG2 THR 9   22.707 25.263 27.180 1.00 0.00  C
ATOM  67 OG1 THR 9   24.447 25.231 25.506 1.00 0.00  O
ATOM  68 C   THR 9   22.555 25.145 23.367 1.00 0.00  C
ATOM  69 O   THR 9   21.837 25.902 22.717 1.00 0.00  O
ATOM  70 N   GLY 10   23.679 24.614 22.878 1.00 0.00  N
ATOM  71 CA  GLY 10   24.137 24.896 21.533 1.00 0.00  C
ATOM  72 C   GLY 10   23.097 24.449 20.514 1.00 0.00  C
ATOM  73 O   GLY 10   22.792 25.178 19.573 1.00 0.00  O
ATOM  74 N   LYS 11   22.552 23.245 20.704 1.00 0.00  N
ATOM  75 CA  LYS 11   21.551 22.707 19.805 1.00 0.00  C
ATOM  76 CB  LYS 11   21.100 21.322 20.254 1.00 0.00  C
ATOM  77 CG  LYS 11   20.049 20.790 19.284 1.00 0.00  C
ATOM  78 CD  LYS 11   19.598 19.405 19.732 1.00 0.00  C
ATOM  79 CE  LYS 11   18.547 18.874 18.762 1.00 0.00  C
ATOM  80 NZ  LYS 11   18.112 17.538 19.193 1.00 0.00 N1+
ATOM  81 C   LYS 11   20.322 23.603 19.755 1.00 0.00  C
ATOM  82 O   LYS 11   19.801 23.886 18.677 1.00 0.00  O
ATOM  83 N   THR 12   19.859 24.050 20.924 1.00 0.00  N
ATOM  84 CA  THR 12   18.696 24.910 21.008 1.00 0.00  C
ATOM  85 CB  THR 12   18.385 25.272 22.457 1.00 0.00  C
ATOM  86 CG2 THR 12   18.109 23.999 23.251 1.00 0.00  C
ATOM  87 OG1 THR 12   19.503 25.957 23.028 1.00 0.00  O
ATOM  88 C   THR 12   18.916 26.207 20.242 1.00 0.00  C
ATOM  89 O   THR 12   18.040 26.651 19.503 1.00 0.00  O
ATOM  90 N   ILE 13   20.091 26.815 20.420 1.00 0.00  N
ATOM  91 CA  ILE 13   20.422 28.054 19.748 1.00 0.00  C
ATOM  92 CB  ILE 13   21.825 28.495 20.154 1.00 0.00  C
ATOM  93 CG2 ILE 13   22.830 27.418 19.758 1.00 0.00  C
ATOM  94 CG1 ILE 13   22.172 29.800 19.446 1.00 0.00  C
ATOM  95 CD1 ILE 13   23.575 30.240 19.851 1.00 0.00  C
ATOM  96 C   ILE 13   20.384 27.885 18.236 1.00 0.00  C
ATOM  97 O   ILE 13   19.834 28.726 17.527 1.00 0.00  O
ATOM  98 N   THR 14   20.970 26.792 17.742 1.00 0.00  N
ATOM  99 CA  THR 14   21.001 26.516 16.320 1.00 0.00  C
ATOM 100 CB  THR 14   21.729 25.208 16.030 1.00 0.00  C
ATOM 101 CG2 THR 14   23.163 25.301 16.540 1.00 0.00  C
ATOM 102 OG1 THR 14   21.058 24.132 16.691 1.00 0.00  O
ATOM 103 C   THR 14   19.593 26.400 15.754 1.00 0.00  C
ATOM 104 O   THR 14   19.297 26.956 14.699 1.00 0.00  O
ATOM 105 N   LEU 15   18.723 25.672 16.459 1.00 0.00  N
ATOM 106 CA  LEU 15   17.353 25.485 16.026 1.00 0.00  C
ATOM 107 CB  LEU 15   16.580 24.617 17.012 1.00 0.00  C
ATOM 108 CG  LEU 15   15.146 24.444 16.522 1.00 0.00  C
ATOM 109 CD1 LEU 15   15.154 23.774 15.151 1.00 0.00  C
ATOM 110 CD2 LEU 15   14.373 23.575 17.507 1.00 0.00  C
ATOM 111 C   LEU 15   16.627 26.818 15.913 1.00 0.00  C
ATOM 112 O   LEU 15   15.927 27.066 14.934 1.00 0.00  O
ATOM 113 N   GLU 16   16.797 27.679 16.920 1.00 0.00  N
ATOM 114 CA  GLU 16   16.160 28.980 16.930 1.00 0.00  C
ATOM 115 CB  GLU 16   16.522 29.758 18.191 1.00 0.00  C
ATOM 116 CG  GLU 16   15.840 31.105 18.163 1.00 0.00  C
ATOM 117 CD  GLU 16   16.202 31.884 19.426 1.00 0.00  C
ATOM 118 OE1 GLU 16   17.225 32.616 19.378 1.00 0.00  O
ATOM 119 OE2 GLU 16   15.450 31.740 20.428 1.00 0.00 O1-
ATOM 120 C   GLU 16   16.593 29.811 15.730 1.00 0.00  C
ATOM 121 O   GLU 16   17.385 29.356 14.909 1.00 0.00  O
ATOM 122 N   NHE 17   16.075 31.035 15.625 1.00 0.00  N
TER 123  NHE 17
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ID1 extended

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ATOM   1  CH3 ACE  1   19.290  14.515  17.295  1.00  0.00   C
ATOM   2  C   ACE  1   20.294  15.592  17.607  1.00  0.00   C
ATOM   3  O   ACE  1   21.149  15.419  18.379  1.00  0.00   O
ATOM   4  N   ILE  2   20.232  16.772  16.895  1.00  0.00   N
ATOM   5  CA  ILE  2   21.240  17.823  16.853  1.00  0.00   C
ATOM   6  CB  ILE  2   21.774  18.003  15.376  1.00  0.00   C
ATOM   7  CG2 ILE  2   22.586  19.332  15.299  1.00  0.00   C
ATOM   8  CG1 ILE  2   22.488  16.784  14.841  1.00  0.00   C
ATOM   9  CD1 ILE  2   22.771  16.820  13.313  1.00  0.00   C
ATOM  10  C   ILE  2   20.474  19.079  17.364  1.00  0.00   C
ATOM  11  O   ILE  2   19.383  19.390  16.928  1.00  0.00   O
ATOM  12  N   ASN  3   21.044  19.793  18.325  1.00  0.00   N
ATOM  13  CA  ASN  3   20.577  21.054  18.905  1.00  0.00   C
ATOM  14  CB  ASN  3   21.358  21.299  20.165  1.00  0.00   C
ATOM  15  CG  ASN  3   20.796  22.226  21.169  1.00  0.00   C
ATOM  16  OD1 ASN  3   20.002  23.094  20.851  1.00  0.00   O
ATOM  17  ND2 ASN  3   21.289  22.154  22.387  1.00  0.00   N
ATOM  18  C   ASN  3   20.617  22.201  17.840  1.00  0.00   C
ATOM  19  O   ASN  3   21.632  22.425  17.212  1.00  0.00   O
ATOM  20  N   TRP  4   19.454  22.827  17.621  1.00  0.00   N
ATOM  21  CA  TRP  4   19.340  23.922  16.684  1.00  0.00   C
ATOM  22  CB  TRP  4   17.970  23.812  15.958  1.00  0.00   C
ATOM  23  CG  TRP  4   16.731  23.695  16.774  1.00  0.00   C
ATOM  24  CD1 TRP  4   15.732  24.602  16.789  1.00  0.00   C
ATOM  25  NE1 TRP  4   14.791  24.197  17.754  1.00  0.00   N
ATOM  26  CE2 TRP  4   15.076  22.954  18.267  1.00  0.00   C
ATOM  27  CZ2 TRP  4   14.525  22.170  19.283  1.00  0.00   C
ATOM  28  CH2 TRP  4   15.103  20.992  19.686  1.00  0.00   C
ATOM  29  CZ3 TRP  4   16.214  20.503  19.023  1.00  0.00   C
ATOM  30  CE3 TRP  4   16.816  21.280  17.969  1.00  0.00   C
ATOM  31  CD2 TRP  4   16.318  22.552  17.628  1.00  0.00   C
ATOM  32  C   TRP  4   19.522  25.336  17.354  1.00  0.00   C
ATOM  33  O   TRP  4   19.795  26.283  16.582  1.00  0.00   O
ATOM  34  N   LEU  5   19.448  25.433  18.695  1.00  0.00   N
ATOM  35  CA  LEU  5   19.331  26.668  19.528  1.00  0.00   C
ATOM  36  CB  LEU  5   18.076  26.369  20.478  1.00  0.00   C
ATOM  37  CG  LEU  5   17.669  27.455  21.471  1.00  0.00   C
ATOM  38  CD1 LEU  5   17.815  28.891  20.982  1.00  0.00   C
ATOM  39  CD2 LEU  5   16.246  27.183  21.987  1.00  0.00   C
ATOM  40  C   LEU  5   20.714  26.985  20.204  1.00  0.00   C
ATOM  41  O   LEU  5   21.211  28.189  20.320  1.00  0.00   O
ATOM  42  N   LYS  6   21.421  25.942  20.781  1.00  0.00   N
ATOM  43  CA  LYS  6   22.623  26.157  21.645  1.00  0.00   C
ATOM  44  CB  LYS  6   22.342  25.783  23.159  1.00  0.00   C
ATOM  45  CG  LYS  6   21.306  26.831  23.679  1.00  0.00   C
ATOM  46  CD  LYS  6   20.890  26.586  25.146  1.00  0.00   C
ATOM  47  CE  LYS  6   20.050  27.860  25.495  1.00  0.00   C
ATOM  48  NZ  LYS  6   19.665  28.108  26.904  1.00  0.00  N1+
ATOM  49  C   LYS  6   23.914  25.517  21.087  1.00  0.00   C
ATOM  50  O   LYS  6   24.673  24.876  21.786  1.00  0.00   O
ATOM  51  N   LEU  7   24.165  25.508  19.823  1.00  0.00   N
ATOM  52  CA  LEU  7   25.184  24.651  19.219  1.00  0.00   C
ATOM  53  CB  LEU  7   24.797  24.451  17.702  1.00  0.00   C
ATOM  54  CG  LEU  7   25.750  23.528  16.877  1.00  0.00   C
ATOM  55  CD1 LEU  7   25.849  22.049  17.329  1.00  0.00   C
ATOM  56  CD2 LEU  7   24.986  23.481  15.505  1.00  0.00   C
ATOM  57  C   LEU  7   26.651  25.033  19.445  1.00  0.00   C
ATOM  58  O   LEU  7   27.604  24.229  19.575  1.00  0.00   O
ATOM  59  N   GLY  8   26.930  26.341  19.717  1.00  0.00   N
ATOM  60  CA  GLY  8   28.161  26.895  20.268  1.00  0.00   C
ATOM  61  C   GLY  8   28.485  26.342  21.703  1.00  0.00   C
ATOM  62  O   GLY  8   29.559  26.698  22.225  1.00  0.00   O
ATOM  63  N   LYS  9   27.596  25.628  22.424  1.00  0.00   N
ATOM  64  CA  LYS  9   27.817  25.042  23.773  1.00  0.00   C
ATOM  65  CB  LYS  9   26.858  25.646  24.741  1.00  0.00   C
ATOM  66  CG  LYS  9   27.420  26.971  25.174  1.00  0.00   C
ATOM  67  CD  LYS  9   26.593  27.540  26.290  1.00  0.00   C
ATOM  68  CE  LYS  9   27.158  28.886  26.884  1.00  0.00   C
ATOM  69  NZ  LYS  9   26.278  29.231  28.021  1.00  0.00  N1+
ATOM  70  C   LYS  9   27.870  23.441  23.846  1.00  0.00   C
ATOM  71  O   LYS  9   28.900  22.867  24.244  1.00  0.00   O
ATOM  72  N   MET  10   26.857  22.854  23.203  1.00  0.00   N
ATOM  73  CA  MET  10   26.578  21.426  22.972  1.00  0.00   C
ATOM  74  CB  MET  10   25.800  20.802  24.165  1.00  0.00   C
ATOM  75  CG  MET  10   26.771  20.407  25.307  1.00  0.00   C
ATOM  76  SD  MET  10   26.354  18.897  26.380  1.00  0.00   S
ATOM  77  CE  MET  10   27.700  17.757  25.967  1.00  0.00   C
ATOM  78  C   MET  10   25.777  21.121  21.655  1.00  0.00   C
ATOM  79  O   MET  10   24.792  21.773  21.267  1.00  0.00   O
ATOM  80  N   VAL  11   26.286  20.093  20.969  1.00  0.00   N
ATOM  81  CA  VAL  11   25.529  19.450  19.837  1.00  0.00   C
ATOM  82  CB  VAL  11   26.534  18.545  18.997  1.00  0.00   C
ATOM  83  CG1 VAL  11   25.862  17.810  17.819  1.00  0.00   C
ATOM  84  CG2 VAL  11   28.007  18.990  18.692  1.00  0.00   C
ATOM  85  C   VAL  11   24.380  18.619  20.252  1.00  0.00   C
ATOM  86  O   VAL  11   23.416  18.699  19.483  1.00  0.00   O
ATOM  87  N   ILE  12   24.369  17.854  21.344  1.00  0.00   N
ATOM  88  CA  ILE  12   23.202  16.970  21.682  1.00  0.00   C
ATOM  89  CB  ILE  12   23.642  15.677  22.393  1.00  0.00   C
ATOM  90  CG2 ILE  12   24.307  15.809  23.771  1.00  0.00   C
ATOM  91  CG1 ILE  12   22.473  14.716  22.483  1.00  0.00   C
ATOM  92  CD1 ILE  12   22.846  13.286  22.808  1.00  0.00   C
ATOM  93  C   ILE  12   22.179  17.848  22.514  1.00  0.00   C
ATOM  94  O   ILE  12   22.517  18.764  23.250  1.00  0.00   O
ATOM  95  N   ASP  13   20.902  17.659  22.168  1.00  0.00   N
ATOM  96  CA  ASP  13   19.772  18.461  22.704  1.00  0.00   C
ATOM  97  CB  ASP  13   18.508  18.190  21.907  1.00  0.00   C
ATOM  98  CG  ASP  13   17.311  19.065  22.261  1.00  0.00   C
ATOM  99  OD1 ASP  13   16.174  18.504  22.313  1.00  0.00   O
ATOM 100  OD2 ASP  13   17.467  20.289  22.515  1.00  0.00  O1-
ATOM 101  C   ASP  13   19.519  17.963  24.171  1.00  0.00   C
ATOM 102  O   ASP  13   19.834  16.872  24.538  1.00  0.00   O
ATOM 103  N   ALA  14   18.872  18.814  24.916  1.00  0.00   N
ATOM 104  CA  ALA  14   18.868  18.670  26.397  1.00  0.00   C
ATOM 105  CB  ALA  14   18.356  19.964  27.047  1.00  0.00   C
ATOM 106  C   ALA  14   18.237  17.346  26.849  1.00  0.00   C
ATOM 107  O   ALA  14   18.666  16.785  27.844  1.00  0.00   O
ATOM 108  N   LEU  15   17.152  16.862  26.128  1.00  0.00   N
ATOM 109  CA  LEU  15   16.374  15.615  26.241  1.00  0.00   C
ATOM 110  CB  LEU  15   14.855  15.929  26.300  1.00  0.00   C
ATOM 111  CG  LEU  15   14.420  16.877  27.418  1.00  0.00   C
ATOM 112  CD1 LEU  15   12.889  16.914  27.299  1.00  0.00   C
ATOM 113  CD2 LEU  15   14.781  16.378  28.853  1.00  0.00   C
ATOM 114  C   LEU  15   16.468  14.671  25.067  1.00  0.00   C
ATOM 115  O   LEU  15   16.804  15.105  24.022  1.00  0.00   O
ATOM 116  N   NHE  16   16.214  13.359  25.169  1.00  0.00   N
TER 117  NHE  16
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ID1 misfolded

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ATOM   1  CH3 ACE  1   26.596  16.649  34.163  1.00  0.00   C
ATOM   2  C   ACE  1   26.968  18.042  33.650  1.00  0.00   C
ATOM   3  O   ACE  1   27.217  18.952  34.439  1.00  0.00   O
ATOM   4  N   ILE  2   27.001  18.202  32.347  1.00  0.00   N
ATOM   5  CA  ILE  2   27.340  19.479  31.749  1.00  0.00   C
ATOM   6  CB  ILE  2   28.743  19.888  32.187  1.00  0.00   C
ATOM   7  CG2 ILE  2   29.745  18.831  31.733  1.00  0.00   C
ATOM   8  CG1 ILE  2   29.100  21.230  31.559  1.00  0.00   C
ATOM   9  CD1 ILE  2   30.502  21.640  31.996  1.00  0.00   C
ATOM  10  C   ILE  2   27.307  19.399  30.230  1.00  0.00   C
ATOM  11  O   ILE  2   26.765  20.282  29.571  1.00  0.00   O
ATOM  12  N   ASN  3   27.891  18.334  29.675  1.00  0.00   N
ATOM  13  CA  ASN  3   27.927  18.143  28.239  1.00  0.00   C
ATOM  14  CB  ASN  3   28.651  16.850  27.875  1.00  0.00   C
ATOM  15  CG  ASN  3   28.689  16.649  26.367  1.00  0.00   C
ATOM  16  OD1 ASN  3   28.175  17.475  25.615  1.00  0.00   O
ATOM  17  ND2 ASN  3   29.300  15.547  25.926  1.00  0.00   N
ATOM  18  C   ASN  3   26.520  18.066  27.661  1.00  0.00   C
ATOM  19  O   ASN  3   26.232  18.686  26.640  1.00  0.00   O
ATOM  20  N   TRP  4   25.645  17.303  28.319  1.00  0.00   N
ATOM  21  CA  TRP  4   24.277  17.148  27.870  1.00  0.00   C
ATOM  22  CB  TRP  4   23.495  16.226  28.799  1.00  0.00   C
ATOM  23  CG  TRP  4   22.053  16.002  28.413  1.00  0.00   C
ATOM  24  CD1 TRP  4   21.154  15.243  29.053  1.00  0.00   C
ATOM  25  NE1 TRP  4   19.928  15.336  28.321  1.00  0.00   N
ATOM  26  CE2 TRP  4   20.108  16.124  27.289  1.00  0.00   C
ATOM  27  CZ2 TRP  4   19.174  16.491  26.312  1.00  0.00   C
ATOM  28  CH2 TRP  4   19.635  17.347  25.321  1.00  0.00   C
ATOM  29  CZ3 TRP  4   20.912  17.786  25.319  1.00  0.00   C
ATOM  30  CE3 TRP  4   21.835  17.404  26.314  1.00  0.00   C
ATOM  31  CD2 TRP  4   21.370  16.541  27.314  1.00  0.00   C
ATOM  32  C   TRP  4   23.556  18.489  27.833  1.00  0.00   C
ATOM  33  O   TRP  4   22.862  18.797  26.867  1.00  0.00   O
ATOM  34  N   LEU  5   23.726  19.287  28.889  1.00  0.00   N
ATOM  35  CA  LEU  5   23.095  20.588  28.974  1.00  0.00   C
ATOM  36  CB  LEU  5   23.454  21.289  30.281  1.00  0.00   C
ATOM  37  CG  LEU  5   22.772  22.652  30.330  1.00  0.00   C
ATOM  38  CD1 LEU  5   21.260  22.467  30.252  1.00  0.00   C
ATOM  39  CD2 LEU  5   23.130  23.352  31.637  1.00  0.00   C
ATOM  40  C   LEU  5   23.536  21.487  27.828  1.00  0.00   C
ATOM  41  O   LEU  5   22.713  22.157  27.207  1.00  0.00   O
ATOM  42  N   LYS  6   24.842  21.501  27.548  1.00  0.00   N
ATOM  43  CA  LYS  6   25.387  22.316  26.480  1.00  0.00   C
ATOM  44  CB  LYS  6   26.898  22.144  26.377  1.00  0.00   C
ATOM  45  CG  LYS  6   27.433  23.015  25.245  1.00  0.00   C
ATOM  46  CD  LYS  6   28.945  22.844  25.142  1.00  0.00   C
ATOM  47  CE  LYS  6   29.479  23.715  24.009  1.00  0.00   C
ATOM  48  NZ  LYS  6   30.936  23.550  23.909  1.00  0.00  N1+
ATOM  49  C   LYS  6   24.783  21.934  25.137  1.00  0.00   C
ATOM  50  O   LYS  6   24.406  22.803  24.353  1.00  0.00   O
ATOM  51  N   LEU  7   24.691  20.629  24.872  1.00  0.00   N
ATOM  52  CA  LEU  7   24.135  20.137  23.627  1.00  0.00   C
ATOM  53  CB  LEU  7   24.150  18.613  23.583  1.00  0.00   C
ATOM  54  CG  LEU  7   23.557  18.137  22.261  1.00  0.00   C
ATOM  55  CD1 LEU  7   24.386  18.687  21.105  1.00  0.00   C
ATOM  56  CD2 LEU  7   23.571  16.613  22.217  1.00  0.00   C
ATOM  57  C   LEU  7   22.693  20.594  23.454  1.00  0.00   C
ATOM  58  O   LEU  7   22.306  21.040  22.376  1.00  0.00   O
ATOM  59  N   GLY  8   21.898  20.482  24.520  1.00  0.00   N
ATOM  60  CA  GLY  8   20.506  20.882  24.483  1.00  0.00   C
ATOM  61  C   GLY  8   20.388  22.361  24.143  1.00  0.00   C
ATOM  62  O   GLY  8   19.564  22.748  23.317  1.00  0.00   O
ATOM  63  N   LYS  9   21.215  23.189  24.785  1.00  0.00   N
ATOM  64  CA  LYS  9   21.202  24.619  24.551  1.00  0.00   C
ATOM  65  CB  LYS  9   22.244  25.326  25.410  1.00  0.00   C
ATOM  66  CG  LYS  9   22.197  26.826  25.134  1.00  0.00   C
ATOM  67  CD  LYS  9   23.239  27.533  25.995  1.00  0.00   C
ATOM  68  CE  LYS  9   23.193  29.033  25.718  1.00  0.00   C
ATOM  69  NZ  LYS  9   24.197  29.714  26.547  1.00  0.00  N1+
ATOM  70  C   LYS  9   21.506  24.938  23.094  1.00  0.00   C
ATOM  71  O   LYS  9   20.835  25.767  22.483  1.00  0.00   O
ATOM  72  N   MET  10  22.523  24.276  22.537  1.00  0.00   N
ATOM  73  CA  MET  10  22.913  24.491  21.158  1.00  0.00   C
ATOM  74  CB  MET  10  24.099  23.611  20.780  1.00  0.00   C
ATOM  75  CG  MET  10  24.477  23.866  19.324  1.00  0.00   C
ATOM  76  SD  MET  10  25.885  22.827  18.859  1.00  0.00   S
ATOM  77  CE  MET  10  26.092  23.328  17.163  1.00  0.00   C
ATOM  78  C   MET  10  21.769  24.164  20.208  1.00  0.00   C
ATOM  79  O   MET  10  21.495  24.919  19.278  1.00  0.00   O
ATOM  80  N   VAL  11  21.101  23.032  20.445  1.00  0.00   N
ATOM  81  CA  VAL  11  19.992  22.610  19.613  1.00  0.00   C
ATOM  82  CB  VAL  11  19.411  21.288  20.103  1.00  0.00   C
ATOM  83  CG1 VAL  11  18.911  21.452  21.536  1.00  0.00   C
ATOM  84  CG2 VAL  11  18.250  20.879  19.204  1.00  0.00   C
ATOM  85  C   VAL  11  18.874  23.642  19.624  1.00  0.00   C
ATOM  86  O   VAL  11  18.325  23.978  18.577  1.00  0.00   O
ATOM  87  N   ILE  12  18.538  24.147  20.814  1.00  0.00   N
ATOM  88  CA  ILE  12  17.489  25.136  20.958  1.00  0.00   C
ATOM  89  CB  ILE  12  17.342  25.512  22.428  1.00  0.00   C
ATOM  90  CG2 ILE  12  18.659  26.087  22.940  1.00  0.00   C
ATOM  91  CG1 ILE  12  16.239  26.554  22.579  1.00  0.00   C
ATOM  92  CD1 ILE  12  16.091  26.928  24.050  1.00  0.00   C
ATOM  93  C   ILE  12  17.812  26.395  20.164  1.00  0.00   C
ATOM  94  O   ILE  12  16.950  26.934  19.472  1.00  0.00   O
ATOM  95  N   ASP  13  19.057  26.862  20.265  1.00  0.00   N
ATOM  96  CA  ASP  13  19.489  28.052  19.559  1.00  0.00   C
ATOM  97  CB  ASP  13  20.953  28.363  19.850  1.00  0.00   C
ATOM  98  CG  ASP  13  21.368  29.620  19.090  1.00  0.00   C
ATOM  99  OD1 ASP  13  21.217  30.724  19.677  1.00  0.00   O
ATOM 100  OD2 ASP  13  21.831  29.465  17.928  1.00  0.00  O1-
ATOM 101  C   ASP  13  19.340  27.880  18.054  1.00  0.00   C
ATOM 102  O   ASP  13  18.850  28.776  17.370  1.00  0.00   O
ATOM 103  N   ALA  14  19.765  26.724  17.539  1.00  0.00   N
ATOM 104  CA  ALA  14  19.677  26.439  16.121  1.00  0.00   C
ATOM 105  CB  ALA  14  20.230  25.054  15.804  1.00  0.00   C
ATOM 106  C   ALA  14  18.234  26.485  15.642  1.00  0.00   C
ATOM 107  O   ALA  14  17.941  27.067  14.598  1.00  0.00   O
ATOM 108  N   LEU  15  17.330  25.867  16.405  1.00  0.00   N
ATOM 109  CA  LEU  15  15.923  25.839  16.056  1.00  0.00   C
ATOM 110  CB  LEU  15  15.116  25.071  17.098  1.00  0.00   C
ATOM 111  CG  LEU  15  13.645  25.064  16.694  1.00  0.00   C
ATOM 112  CD1 LEU  15  13.492  24.391  15.335  1.00  0.00   C
ATOM 113  CD2 LEU  15  12.836  24.296  17.734  1.00  0.00   C
ATOM 114  C   LEU  15  15.352  27.248  15.971  1.00  0.00   C
ATOM 115  O   LEU  15  16.066  28.224  16.186  1.00  0.00   O
ATOM 116  N   NHE  16  14.059  27.349  15.655  1.00  0.00   N
TER  117  NHE  16
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ID2 extended

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ATOM   1  CH3 ACE  1   13.222  26.065  31.411  1.00  0.00   C
ATOM   2  C   ACE  1   14.552  26.714  31.111  1.00  0.00   C
ATOM   3  O   ACE  1   14.553  27.931  31.039  1.00  0.00   O
ATOM   4  N   THR  2   15.678  25.915  30.996  1.00  0.00   N
ATOM   5  CA  THR  2   16.998  26.489  31.117  1.00  0.00   C
ATOM   6  CB  THR  2   17.772  25.953  32.302  1.00  0.00   C
ATOM   7  CG2 THR  2   17.217  26.475  33.624  1.00  0.00   C
ATOM   8  OG1 THR  2   17.722  24.554  32.326  1.00  0.00   O
ATOM   9  C   THR  2   17.865  26.303  29.812  1.00  0.00   C
ATOM  10  O   THR  2   19.035  26.728  29.766  1.00  0.00   O
ATOM  11  N   ARG  3   17.294  25.576  28.836  1.00  0.00   N
ATOM  12  CA  ARG  3   17.885  25.182  27.572  1.00  0.00   C
ATOM  13  CB  ARG  3   16.815  24.603  26.546  1.00  0.00   C
ATOM  14  CG  ARG  3   17.129  24.545  25.064  1.00  0.00   C
ATOM  15  CD  ARG  3   16.049  23.762  24.268  1.00  0.00   C
ATOM  16  NE  ARG  3   16.149  23.956  22.804  1.00  0.00   N
ATOM  17  CZ  ARG  3   15.218  23.928  21.920  1.00  0.00   C
ATOM  18  NH1 ARG  3   14.077  23.420  22.201  1.00  0.00   N
ATOM  19  NH2 ARG  3   15.457  24.172  20.636  1.00  0.00   N1+
ATOM  20  C   ARG  3   18.688  26.255  26.904  1.00  0.00   C
ATOM  21  O   ARG  3   19.667  25.948  26.143  1.00  0.00   O
ATOM  22  N   THR  4   18.323  27.466  27.025  1.00  0.00   N
ATOM  23  CA  THR  4   18.887  28.685  26.440  1.00  0.00   C
ATOM  24  CB  THR  4   18.017  29.900  26.599  1.00  0.00   C
ATOM  25  CG2 THR  4   16.758  29.621  25.755  1.00  0.00   C
ATOM  26  OG1 THR  4   17.703  30.140  27.949  1.00  0.00   O
ATOM  27  C   THR  4   20.275  29.015  26.903  1.00  0.00   C
ATOM  28  O   THR  4   20.959  29.780  26.268  1.00  0.00   O
ATOM  29  N   LYS  5   20.761  28.396  28.041  1.00  0.00   N
ATOM  30  CA  LYS  5   22.203  28.378  28.431  1.00  0.00   C
ATOM  31  CB  LYS  5   22.211  27.615  29.805  1.00  0.00   C
ATOM  32  CG  LYS  5   23.558  27.723  30.610  1.00  0.00   C
ATOM  33  CD  LYS  5   23.450  26.878  31.862  1.00  0.00   C
ATOM  34  CE  LYS  5   24.629  27.098  32.825  1.00  0.00   C
ATOM  35  NZ  LYS  5   24.242  26.493  34.084  1.00  0.00   N1+
ATOM  36  C   LYS  5   23.149  27.648  27.436  1.00  0.00   C
ATOM  37  O   LYS  5   24.301  28.047  27.416  1.00  0.00   O
ATOM  38  N   ILE  6   22.689  26.587  26.722  1.00  0.00   N
ATOM  39  CA  ILE  6   23.528  25.672  25.937  1.00  0.00   C
ATOM  40  CB  ILE  6   23.894  24.424  26.679  1.00  0.00   C
ATOM  41  CG2 ILE  6   24.869  24.742  27.824  1.00  0.00   C
ATOM  42  CG1 ILE  6   22.648  23.565  27.082  1.00  0.00   C
ATOM  43  CD1 ILE  6   22.973  22.344  27.961  1.00  0.00   C
ATOM  44  C   ILE  6   23.013  25.336  24.458  1.00  0.00   C
ATOM  45  O   ILE  6   23.640  24.680  23.647  1.00  0.00   O
ATOM  46  N   ASP  7   21.852  25.897  24.093  1.00  0.00   N
ATOM  47  CA  ASP  7   21.087  25.653  22.851  1.00  0.00   C
ATOM  48  CB  ASP  7   19.771  26.458  22.915  1.00  0.00   C
ATOM  49  CG  ASP  7   18.715  26.129  21.862  1.00  0.00   C
ATOM  50  OD1 ASP  7   18.220  27.031  21.191  1.00  0.00   O
ATOM  51  OD2 ASP  7   18.459  24.927  21.719  1.00  0.00   O1-
ATOM  52  C   ASP  7   21.915  26.000  21.564  1.00  0.00   C
ATOM  53  O   ASP  7   21.654  25.472  20.466  1.00  0.00   O
ATOM  54  N   TRP  8   22.873  26.897  21.686  1.00  0.00   N
ATOM  55  CA  TRP  8   23.740  27.500  20.661  1.00  0.00   C
ATOM  56  CB  TRP  8   24.375  28.799  21.235  1.00  0.00   C
ATOM  57  CG  TRP  8   24.988  28.704  22.611  1.00  0.00   C
ATOM  58  CD1 TRP  8   24.302  28.873  23.796  1.00  0.00   C
ATOM  59  NE1 TRP  8   25.204  28.736  24.869  1.00  0.00   N
ATOM  60  CE2 TRP  8   26.508  28.604  24.468  1.00  0.00   C
ATOM  61  CZ2 TRP  8   27.720  28.626  25.174  1.00  0.00   C
ATOM  62  CH2 TRP  8   28.897  28.381  24.433  1.00  0.00   C
ATOM  63  CZ3 TRP  8   28.883  28.375  23.002  1.00  0.00   C
ATOM  64  CE3 TRP  8   27.612  28.428  22.276  1.00  0.00   C
ATOM  65  CD2 TRP  8   26.394  28.540  23.036  1.00  0.00   C
ATOM  66  C   TRP  8   24.820  26.595  20.048  1.00  0.00   C
ATOM  67  O   TRP  8   25.238  26.937  18.981  1.00  0.00   O
ATOM  68  N   ASN  9   25.169  25.435  20.597  1.00  0.00   N
ATOM  69  CA  ASN  9   26.307  24.535  20.294  1.00  0.00   C
ATOM  70  CB  ASN  9   27.209  24.355  21.513  1.00  0.00   C
ATOM  71  CG  ASN  9   28.647  23.745  21.302  1.00  0.00   C
ATOM  72  OD1 ASN  9   28.811  22.921  20.381  1.00  0.00   O
ATOM  73  ND2 ASN  9   29.622  24.022  22.161  1.00  0.00   N
ATOM  74  C   ASN  9   25.772  23.226  19.765  1.00  0.00   C
ATOM  75  O   ASN  9   24.670  22.820  20.075  1.00  0.00   O
ATOM  76  N   LYS  10   26.376  22.549  18.739  1.00  0.00   N
ATOM  77  CA  LYS  10   25.872  21.387  18.027  1.00  0.00   C
ATOM  78  CB  LYS  10   26.685  21.301  16.726  1.00  0.00   C
ATOM  79  CG  LYS  10   26.429  22.467  15.736  1.00  0.00   C
ATOM  80  CD  LYS  10   24.960  22.724  15.329  1.00  0.00   C
ATOM  81  CE  LYS  10   25.086  23.323  13.904  1.00  0.00   C
ATOM  82  NZ  LYS  10   23.880  23.605  13.058  1.00  0.00   N1+
ATOM  83  C   LYS  10   25.908  20.066  18.812  1.00  0.00   C
ATOM  84  O   LYS  10   25.331  19.126  18.305  1.00  0.00   O
ATOM  85  N   ILE  11   26.463  20.017  20.019  1.00  0.00   N
ATOM  86  CA  ILE  11   26.342  18.857  20.958  1.00  0.00   C
ATOM  87  CB  ILE  11   27.651  17.950  20.966  1.00  0.00   C
ATOM  88  CG2 ILE  11   27.935  17.430  19.542  1.00  0.00   C
ATOM  89  CG1 ILE  11   28.840  18.735  21.601  1.00  0.00   C
ATOM  90  CD1 ILE  11   30.112  17.953  21.669  1.00  0.00   C
ATOM  91  C   ILE  11   26.049  19.145  22.406  1.00  0.00   C
ATOM  92  O   ILE  11   26.286  20.216  22.931  1.00  0.00   O
ATOM  93  N   LEU  12   25.620  18.137  23.159  1.00  0.00   N
ATOM  94  CA  LEU  12   25.164  18.135  24.560  1.00  0.00   C
ATOM  95  CB  LEU  12   26.412  18.148  25.518  1.00  0.00   C
ATOM  96  CG  LEU  12   27.374  16.945  25.295  1.00  0.00   C
ATOM  97  CD1 LEU  12   28.547  16.799  26.319  1.00  0.00   C
ATOM  98  CD2 LEU  12   26.602  15.719  25.527  1.00  0.00   C
ATOM  99  C   LEU  12   24.055  19.205  24.823  1.00  0.00   C
ATOM 100  O   LEU  12   24.036  19.711  25.916  1.00  0.00   O
ATOM 101  N   SER  13   23.197  19.391  23.849  1.00  0.00   N
ATOM 102  CA  SER  13   22.150  20.461  23.861  1.00  0.00   C
ATOM 103  CB  SER  13   22.482  21.594  22.955  1.00  0.00   C
ATOM 104  OG  SER  13   22.939  21.051  21.715  1.00  0.00   O
ATOM 105  C   SER  13   20.741  19.884  23.559  1.00  0.00   C
ATOM 106  O   SER  13   19.835  20.665  23.294  1.00  0.00   O
ATOM 107  N   NHE  14   20.601  18.541  23.322  1.00  0.00   N
TER  108   NHE  14
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ID2 misfolded

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ATOM   1  CH3 ACE  1   23.745  18.437  32.753  1.00  0.00   C
ATOM   2  C   ACE  1   24.121  19.761  32.084  1.00  0.00   C
ATOM   3  O   ACE  1   24.322  20.768  32.761  1.00  0.00   O
ATOM   4  N   THR  2   24.212  19.756  30.774  1.00  0.00   N
ATOM   5  CA  THR  2   24.561  20.953  30.034  1.00  0.00   C
ATOM   6  CB  THR  2   25.934  21.473  30.449  1.00  0.00   C
ATOM   7  CG2 THR  2   25.923  21.804  31.938  1.00  0.00   C
ATOM   8  OG1 THR  2   26.922  20.471  30.191  1.00  0.00   O
ATOM   9  C   THR  2   24.600  20.681  28.538  1.00  0.00   C
ATOM  10  O   THR  2   24.077  21.464  27.748  1.00  0.00   O
ATOM  11  N   ARG  3   25.222  19.566  28.148  1.00  0.00   N
ATOM  12  CA  ARG  3   25.327  19.196  26.751  1.00  0.00   C
ATOM  13  CB  ARG  3   26.084  17.882  26.587  1.00  0.00   C
ATOM  14  CG  ARG  3   26.172  17.529  25.106  1.00  0.00   C
ATOM  15  CD  ARG  3   26.930  16.215  24.942  1.00  0.00   C
ATOM  16  NE  ARG  3   27.035  15.838  23.515  1.00  0.00   N
ATOM  17  CZ  ARG  3   27.649  14.735  23.100  1.00  0.00   C
ATOM  18  NH1 ARG  3   28.217  13.883  23.949  1.00  0.00   N
ATOM  19  NH2 ARG  3   27.685  14.493  21.792  1.00  0.00   N1+
ATOM  20  C   ARG  3   23.950  19.021  26.127  1.00  0.00   C
ATOM  21  O   ARG  3   23.700  19.500  25.023  1.00  0.00   O
ATOM  22  N   THR  4   23.055  18.329  26.837  1.00  0.00   N
ATOM  23  CA  THR  4   21.711  18.093  26.351  1.00  0.00   C
ATOM  24  CB  THR  4   20.899  17.281  27.355  1.00  0.00   C
ATOM  25  CG2 THR  4   21.578  15.935  27.586  1.00  0.00   C
ATOM  26  OG1 THR  4   20.821  17.994  28.593  1.00  0.00   O
ATOM  27  C   THR  4   20.976  19.405  26.113  1.00  0.00   C
ATOM  28  O   THR  4   20.322  19.575  25.086  1.00  0.00   O
ATOM  29  N   LYS  5   21.086  20.333  27.066  1.00  0.00   N
ATOM  30  CA  LYS  5   20.434  21.622  26.956  1.00  0.00   C
ATOM  31  CB  LYS  5   20.723  22.489  28.178  1.00  0.00   C
ATOM  32  CG  LYS  5   20.021  23.834  28.024  1.00  0.00   C
ATOM  33  CD  LYS  5   20.310  24.701  29.246  1.00  0.00   C
ATOM  34  CE  LYS  5   19.609  26.046  29.093  1.00  0.00   C
ATOM  35  NZ  LYS  5   19.888  26.881  30.271  1.00  0.00   N1+
ATOM  36  C   LYS  5   20.916  22.378  25.726  1.00  0.00   C
ATOM  37  O   LYS  5   20.114  22.948  24.990  1.00  0.00   O
ATOM  38  N   ILE  6   22.232  22.381  25.504  1.00  0.00   N
ATOM  39  CA  ILE  6   22.816  23.065  24.367  1.00  0.00   C
ATOM  40  CB  ILE  6   24.330  22.887  24.389  1.00  0.00   C
ATOM  41  CG2 ILE  6   24.668  21.402  24.319  1.00  0.00   C
ATOM  42  CG1 ILE  6   24.944  23.606  23.193  1.00  0.00   C
ATOM  43  CD1 ILE  6   26.459  23.428  23.215  1.00  0.00   C
ATOM  44  C   ILE  6   22.279  22.505  23.058  1.00  0.00   C
ATOM  45  O   ILE  6   21.927  23.261  22.154  1.00  0.00   O
ATOM  46  N   ASP  7   22.217  21.175  22.957  1.00  0.00   N
ATOM  47  CA  ASP  7   21.725  20.520  21.761  1.00  0.00   C
ATOM  48  CB  ASP  7   21.762  19.003  21.912  1.00  0.00   C
ATOM  49  CG  ASP  7   21.237  18.352  20.634  1.00  0.00   C
ATOM  50  OD1 ASP  7   22.078  18.090  19.734  1.00  0.00   O
ATOM  51  OD2 ASP  7   19.999  18.123  20.571  1.00  0.00   O1-
ATOM  52  C   ASP  7   20.287  20.924  21.468  1.00  0.00   C
ATOM  53  O   ASP  7   19.944  21.223  20.326  1.00  0.00   O
ATOM  54  N   TRP  8   19.445  20.932  22.504  1.00  0.00   N
ATOM  55  CA  TRP  8   18.051  21.298  22.355  1.00  0.00   C
ATOM  56  CB  TRP  8   17.318  21.223  23.690  1.00  0.00   C
ATOM  57  CG  TRP  8   15.854  21.587  23.636  1.00  0.00   C
ATOM  58  CD1 TRP  8   14.988  21.604  24.659  1.00  0.00   C
ATOM  59  NE1 TRP  8   13.724  22.010  24.130  1.00  0.00   N
ATOM  60  CE2 TRP  8   13.848  22.223  22.842  1.00  0.00   C
ATOM  61  CZ2 TRP  8   12.862  22.633  21.937  1.00  0.00   C
ATOM  62  CH2 TRP  8   13.271  22.784  20.617  1.00  0.00   C
ATOM  63  CZ3 TRP  8   14.548  22.543  20.253  1.00  0.00   C
ATOM  64  CE3 TRP  8   15.526  22.131  21.183  1.00  0.00   C
ATOM  65  CD2 TRP  8   15.113  21.979  22.513  1.00  0.00   C
ATOM  66  C   TRP  8   17.910  22.718  21.826  1.00  0.00   C
ATOM  67  O   TRP  8   17.115  22.972  20.926  1.00  0.00   O
ATOM  68  N   ASN  9   18.688  23.645  22.390  1.00  0.00   N
ATOM  69  CA  ASN  9   18.648  25.033  21.975  1.00  0.00   C
ATOM  70  CB  ASN  9   19.634  25.875  22.779  1.00  0.00   C
ATOM  71  CG  ASN  9   19.593  27.332  22.344  1.00  0.00   C
ATOM  72  OD1 ASN  9   18.831  27.695  21.449  1.00  0.00   O
ATOM  73  ND2 ASN  9   20.416  28.170  22.978  1.00  0.00   N
ATOM  74  C   ASN  9   19.008  25.175  20.503  1.00  0.00   C
ATOM  75  O   ASN  9   18.343  25.901  19.766  1.00  0.00   O
ATOM  76  N   LYS  10   20.065  24.480  20.076  1.00  0.00   N
ATOM  77  CA  LYS  10   20.508  24.532  18.697  1.00  0.00   C
ATOM  78  CB  LYS  10   21.731  23.647  18.481  1.00  0.00   C
ATOM  79  CG  LYS  10   22.166  23.728  17.021  1.00  0.00   C
ATOM  80  CD  LYS  10   23.389  22.844  16.805  1.00  0.00   C
ATOM  81  CE  LYS  10   23.823  22.925  15.345  1.00  0.00   C
ATOM  82  NZ  LYS  10   25.002  22.073  15.136  1.00  0.00   N1+
ATOM  83  C   LYS  10   19.415  24.053  17.752  1.00  0.00   C
ATOM  84  O   LYS  10   19.162  24.676  16.724  1.00  0.00   O
ATOM  85  N   ILE  11   18.766  22.940  18.104  1.00  0.00   N
ATOM  86  CA  ILE  11   17.705  22.383  17.289  1.00  0.00   C
ATOM  87  CB  ILE  11   17.165  21.121  17.953  1.00  0.00   C
ATOM  88  CG2 ILE  11   16.616  21.467  19.333  1.00  0.00   C
ATOM  89  CG1 ILE  11   16.048  20.534  17.095  1.00  0.00   C
ATOM  90  CD1 ILE  11   15.507  19.272  17.759  1.00  0.00   C
ATOM  91  C   ILE  11   16.561  23.374  17.125  1.00  0.00   C
ATOM  92  O   ILE  11   16.050  23.559  16.023  1.00  0.00   O
ATOM  93  N   LEU  12   16.161  24.014  18.226  1.00  0.00   N
ATOM  94  CA  LEU  12   15.084  24.981  18.201  1.00  0.00   C
ATOM  95  CB  LEU  12   14.832  25.559  19.590  1.00  0.00   C
ATOM  96  CG  LEU  12   13.692  26.570  19.520  1.00  0.00   C
ATOM  97  CD1 LEU  12   12.429  25.879  19.020  1.00  0.00   C
ATOM  98  CD2 LEU  12   13.440  27.147  20.909  1.00  0.00   C
ATOM  99  C   LEU  12   15.408  26.138  17.268  1.00  0.00   C
ATOM 100  O   LEU  12   14.565  26.560  16.480  1.00  0.00   O
ATOM 101  N   SER  13   16.637  26.653  17.358  1.00  0.00   N
ATOM 102  CA  SER  13   17.068  27.758  16.524  1.00  0.00   C
ATOM 103  CB  SER  13   18.510  28.146  16.832  1.00  0.00   C
ATOM 104  OG  SER  13   18.899  29.236  15.992  1.00  0.00   O
ATOM 105  C   SER  13   16.988  27.393  15.048  1.00  0.00   C
ATOM 106  O   SER  13   16.596  26.282  14.701  1.00  0.00   O
ATOM 107  N   NHE  14   17.359  28.328  14.175  1.00  0.00   N
TER  108   NHE  14
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ID3 extended

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ATOM   1  CH3 ACE  1   17.825  17.213  28.169  1.00  0.00   C
ATOM   2  C   ACE  1   18.367  18.323  27.318  1.00  0.00   C
ATOM   3  O   ACE  1   19.273  19.060  27.703  1.00  0.00   O
ATOM   4  N   SER  2   17.788  18.481  26.134  1.00  0.00   N
ATOM   5  CA  SER  2   18.089  19.569  25.113  1.00  0.00   C
ATOM   6  CB  SER  2   17.361  20.849  25.531  1.00  0.00   C
ATOM   7  OG  SER  2   16.024  20.651  25.918  1.00  0.00   O
ATOM   8  C   SER  2   19.528  19.905  24.749  1.00  0.00   C
ATOM   9  O   SER  2   19.853  21.071  24.400  1.00  0.00   O
ATOM  10  N   THR  3   20.431  18.979  24.992  1.00  0.00   N
ATOM  11  CA  THR  3   21.866  19.085  24.794  1.00  0.00   C
ATOM  12  CB  THR  3   22.591  17.842  25.360  1.00  0.00   C
ATOM  13  CG2 THR  3   23.126  18.165  26.781  1.00  0.00   C
ATOM  14  OG1 THR  3   21.627  16.762  25.474  1.00  0.00   O
ATOM  15  C   THR  3   22.215  19.193  23.333  1.00  0.00   C
ATOM  16  O   THR  3   23.247  19.723  22.980  1.00  0.00   O
ATOM  17  N   SER  4   21.266  18.785  22.476  1.00  0.00   N
ATOM  18  CA  SER  4   21.449  18.876  21.020  1.00  0.00   C
ATOM  19  CB  SER  4   21.109  17.517  20.406  1.00  0.00   C
ATOM  20  OG  SER  4   19.802  17.093  20.777  1.00  0.00   O
ATOM  21  C   SER  4   20.653  20.077  20.462  1.00  0.00   C
ATOM  22  O   SER  4   20.945  20.482  19.327  1.00  0.00   O
ATOM  23  N   ARG  5   19.615  20.624  21.178  1.00  0.00   N
ATOM  24  CA  ARG  5   18.691  21.682  20.688  1.00  0.00   C
ATOM  25  CB  ARG  5   17.295  21.468  21.069  1.00  0.00   C
ATOM  26  CG  ARG  5   16.512  20.442  20.216  1.00  0.00   C
ATOM  27  CD  ARG  5   15.100  20.208  20.833  1.00  0.00   C
ATOM  28  NE  ARG  5   14.450  19.116  20.129  1.00  0.00   N
ATOM  29  CZ  ARG  5   13.493  18.323  20.541  1.00  0.00   C
ATOM  30  NH1 ARG  5   12.903  18.431  21.677  1.00  0.00   N
ATOM  31  NH2 ARG  5   13.010  17.245  19.861  1.00  0.00  N1+
ATOM  32  C   ARG  5   19.138  23.092  21.072  1.00  0.00   C
ATOM  33  O   ARG  5   19.426  23.902  20.143  1.00  0.00   O
ATOM  34  N   HIE  6   19.230  23.412  22.374  1.00  0.00   N
ATOM  35  CA  HIE  6   19.394  24.748  22.894  1.00  0.00   C
ATOM  36  CB  HIE  6   18.519  24.806  24.162  1.00  0.00   C
ATOM  37  CG  HIE  6   17.049  24.720  23.999  1.00  0.00   C
ATOM  38  ND1 HIE  6   16.295  23.735  24.717  1.00  0.00   N
ATOM  39  CE1 HIE  6   15.016  24.021  24.611  1.00  0.00   C
ATOM  40  NE2 HIE  6   14.921  25.050  23.709  1.00  0.00   N
ATOM  41  CD2 HIE  6   16.184  25.595  23.404  1.00  0.00   C
ATOM  42  C   HIE  6   20.799  25.127  23.394  1.00  0.00   C
ATOM  43  O   HIE  6   21.086  26.286  23.405  1.00  0.00   O
ATOM  44  N   LYS  7   21.643  24.108  23.745  1.00  0.00   N
ATOM  45  CA  LYS  7   22.960  24.275  24.427  1.00  0.00   C
ATOM  46  CB  LYS  7   23.188  23.232  25.466  1.00  0.00   C
ATOM  47  CG  LYS  7   22.075  23.266  26.560  1.00  0.00   C
ATOM  48  CD  LYS  7   22.225  22.248  27.736  1.00  0.00   C
ATOM  49  CE  LYS  7   20.904  21.978  28.526  1.00  0.00   C
ATOM  50  NZ  LYS  7   21.093  20.949  29.594  1.00  0.00  N1+
ATOM  51  C   LYS  7   24.141  24.523  23.433  1.00  0.00   C
ATOM  52  O   LYS  7   25.279  24.373  23.894  1.00  0.00   O
ATOM  53  N   LYS  8   23.834  24.967  22.184  1.00  0.00   N
ATOM  54  CA  LYS  8   24.843  25.137  21.104  1.00  0.00   C
ATOM  55  CB  LYS  8   24.149  25.197  19.752  1.00  0.00   C
ATOM  56  CG  LYS  8   23.241  23.975  19.346  1.00  0.00   C
ATOM  57  CD  LYS  8   22.740  24.293  17.972  1.00  0.00   C
ATOM  58  CE  LYS  8   23.720  23.958  16.936  1.00  0.00   C
ATOM  59  NZ  LYS  8   23.204  23.661  15.584  1.00  0.00  N1+
ATOM  60  C   LYS  8   25.702  26.401  21.164  1.00  0.00   C
ATOM  61  O   LYS  8   25.267  27.356  21.819  1.00  0.00   O
ATOM  62  N   LEU  9   26.882  26.396  20.613  1.00  0.00   N
ATOM  63  CA  LEU  9   28.032  27.280  21.042  1.00  0.00   C
ATOM  64  CB  LEU  9   29.303  26.952  20.149  1.00  0.00   C
ATOM  65  CG  LEU  9   30.503  27.793  20.655  1.00  0.00   C
ATOM  66  CD1 LEU  9   30.931  27.435  22.109  1.00  0.00   C
ATOM  67  CD2 LEU  9   31.721  27.497  19.770  1.00  0.00   C
ATOM  68  C   LEU  9   27.577  28.760  21.024  1.00  0.00   C
ATOM  69  O   LEU  9   27.792  29.558  21.964  1.00  0.00   O
ATOM  70  N   MET  10  26.896  29.133  19.947  1.00  0.00   N
ATOM  71  CA  MET  10  26.634  30.548  19.704  1.00  0.00   C
ATOM  72  CB  MET  10  26.488  30.744  18.194  1.00  0.00   C
ATOM  73  CG  MET  10  25.200  30.518  17.482  1.00  0.00   C
ATOM  74  SD  MET  10  24.587  28.810  17.748  1.00  0.00   S
ATOM  75  CE  MET  10  23.371  28.664  16.409  1.00  0.00   C
ATOM  76  C   MET  10  25.470  31.133  20.481  1.00  0.00   C
ATOM  77  O   MET  10  25.203  32.311  20.464  1.00  0.00   O
ATOM  78  N   PHE  11  24.745  30.232  21.208  1.00  0.00   N
ATOM  79  CA  PHE  11  23.726  30.528  22.167  1.00  0.00   C
ATOM  80  CB  PHE  11  22.539  29.663  21.832  1.00  0.00   C
ATOM  81  CG  PHE  11  21.243  30.054  22.546  1.00  0.00   C
ATOM  82  CD1 PHE  11  20.920  29.527  23.863  1.00  0.00   C
ATOM  83  CE1 PHE  11  19.755  29.887  24.482  1.00  0.00   C
ATOM  84  CZ  PHE  11  18.859  30.773  23.878  1.00  0.00   C
ATOM  85  CE2 PHE  11  19.090  31.236  22.541  1.00  0.00   C
ATOM  86  CD2 PHE  11  20.331  30.956  21.957  1.00  0.00   C
ATOM  87  C   PHE  11  24.206  30.442  23.606  1.00  0.00   C
ATOM  88  O   PHE  11  23.583  31.042  24.506  1.00  0.00   O
ATOM  89  N   LYS  12  25.365  29.853  23.914  1.00  0.00   N
ATOM  90  CA  LYS  12  25.798  29.491  25.267  1.00  0.00   C
ATOM  91  CB  LYS  12  27.080  28.659  25.129  1.00  0.00   C
ATOM  92  CG  LYS  12  27.297  27.829  26.408  1.00  0.00   C
ATOM  93  CD  LYS  12  28.567  27.006  26.466  1.00  0.00   C
ATOM  94  CE  LYS  12  28.902  26.684  27.946  1.00  0.00   C
ATOM  95  NZ  LYS  12  29.613  25.394  28.181  1.00  0.00  N1+
ATOM  96  C   LYS  12  25.980  30.760  26.136  1.00  0.00   C
ATOM  97  O   LYS  12  25.916  30.586  27.324  1.00  0.00   O
ATOM  98  N   THR  13  26.226  31.953  25.611  1.00  0.00   N
ATOM  99  CA  THR  13  26.376  33.166  26.370  1.00  0.00   C
ATOM 100  CB  THR  13  27.227  34.110  25.537  1.00  0.00   C
ATOM 101  CG2 THR  13  28.649  33.656  25.380  1.00  0.00   C
ATOM 102  OG1 THR  13  26.568  34.274  24.233  1.00  0.00   O
ATOM 103  C   THR  13  25.113  33.969  26.795  1.00  0.00   C
ATOM 104  O   THR  13  25.074  34.910  27.567  1.00  0.00   O
ATOM 105  N   GLU  14  23.939  33.577  26.210  1.00  0.00   N
ATOM 106  CA  GLU  14  22.591  34.079  26.338  1.00  0.00   C
ATOM 107  CB  GLU  14  21.808  34.089  24.957  1.00  0.00   C
ATOM 108  CG  GLU  14  22.294  35.114  23.989  1.00  0.00   C
ATOM 109  CD  GLU  14  21.991  36.521  24.361  1.00  0.00   C
ATOM 110  OE1 GLU  14  22.829  37.437  24.043  1.00  0.00   O
ATOM 111  OE2 GLU  14  20.912  36.883  24.902  1.00  0.00  O1-
ATOM 112  C   GLU  14  21.882  33.337  27.513  1.00  0.00   C
ATOM 113  O   GLU  14  22.346  32.349  28.109  1.00  0.00   O
ATOM 114  N   NHE  15  20.688  33.737  27.917  1.00  0.00   N
TER  115  NHE  15
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ID3 misfolded

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ATOM   1  CH3 ACE  1   27.050  19.552  32.630  1.00  0.00   C
ATOM   2  C   ACE  1   27.280  19.635  31.120  1.00  0.00   C
ATOM   3  O   ACE  1   26.614  20.402  30.428  1.00  0.00   O
ATOM   4  N   SER  2   28.227  18.840  30.616  1.00  0.00   N
ATOM   5  CA  SER  2   28.541  18.826  29.201  1.00  0.00   C
ATOM   6  CB  SER  2   29.657  17.831  28.896  1.00  0.00   C
ATOM   7  OG  SER  2   29.938  17.845  27.494  1.00  0.00   O
ATOM   8  C   SER  2   27.325  18.429  28.375  1.00  0.00   C
ATOM   9  O   SER  2   27.032  19.053  27.357  1.00  0.00   O
ATOM  10  N   THR  3   26.618  17.385  28.815  1.00  0.00   N
ATOM  11  CA  THR  3   25.442  16.910  28.117  1.00  0.00   C
ATOM  12  CB  THR  3   24.826  15.711  28.831  1.00  0.00   C
ATOM  13  CG2 THR  3   25.846  14.579  28.895  1.00  0.00   C
ATOM  14  OG1 THR  3   24.450  16.089  30.159  1.00  0.00   O
ATOM  15  C   THR  3   24.378  17.996  28.032  1.00  0.00   C
ATOM  16  O   THR  3   23.783  18.205  26.977  1.00  0.00   O
ATOM  17  N   SER  4   24.141  18.688  29.148  1.00  0.00   N
ATOM  18  CA  SER  4   23.154  19.748  29.196  1.00  0.00   C
ATOM  19  CB  SER  4   23.085  20.371  30.587  1.00  0.00   C
ATOM  20  OG  SER  4   22.103  21.411  30.594  1.00  0.00   O
ATOM  21  C   SER  4   23.488  20.854  28.206  1.00  0.00   C
ATOM  22  O   SER  4   22.614  21.335  27.489  1.00  0.00   O
ATOM  23  N   ARG  5   24.760  21.258  28.169  1.00  0.00   N
ATOM  24  CA  ARG  5   25.205  22.304  27.269  1.00  0.00   C
ATOM  25  CB  ARG  5   26.698  22.569  27.432  1.00  0.00   C
ATOM  26  CG  ARG  5   27.126  23.672  26.470  1.00  0.00   C
ATOM  27  CD  ARG  5   28.619  23.937  26.632  1.00  0.00   C
ATOM  28  NE  ARG  5   29.072  25.005  25.712  1.00  0.00   N
ATOM  29  CZ  ARG  5   30.332  25.426  25.655  1.00  0.00   C
ATOM  30  NH1 ARG  5   31.283  24.911  26.429  1.00  0.00   N
ATOM  31  NH2 ARG  5   30.628  26.393  24.792  1.00  0.00  N1+
ATOM  32  C   ARG  5   24.956  21.921  25.818  1.00  0.00   C
ATOM  33  O   ARG  5   24.470  22.733  25.033  1.00  0.00   O
ATOM  34  N   HIP  6   25.290  20.679  25.462  1.00  0.00   N
ATOM  35  CA  HIP  6   25.101  20.193  24.109  1.00  0.00   C
ATOM  36  CB  HIP  6   25.565  18.747  23.976  1.00  0.00   C
ATOM  37  CG  HIP  6   25.408  18.151  22.598  1.00  0.00   C
ATOM  38  ND1 HIP  6   25.784  16.844  22.313  1.00  0.00  N1+
ATOM  39  CE1 HIP  6   25.528  16.613  21.039  1.00  0.00   C
ATOM  40  NE2 HIP  6   25.015  17.694  20.504  1.00  0.00   N
ATOM  41  CD2 HIP  6   24.923  18.676  21.441  1.00  0.00   C
ATOM  42  C   HIP  6   23.635  20.251  23.706  1.00  0.00   C
ATOM  43  O   HIP  6   23.308  20.689  22.605  1.00  0.00   O
ATOM  44  N   LYS  7   22.751  19.807  24.601  1.00  0.00   N
ATOM  45  CA  LYS  7   21.326  19.809  24.337  1.00  0.00   C
ATOM  46  CB  LYS  7   20.546  19.251  25.523  1.00  0.00   C
ATOM  47  CG  LYS  7   19.055  19.271  25.205  1.00  0.00   C
ATOM  48  CD  LYS  7   18.275  18.712  26.392  1.00  0.00   C
ATOM  49  CE  LYS  7   16.784  18.732  26.075  1.00  0.00   C
ATOM  50  NZ  LYS  7   16.032  18.194  27.218  1.00  0.00  N1+
ATOM  51  C   LYS  7   20.820  21.220  24.070  1.00  0.00   C
ATOM  52  O   LYS  7   20.056  21.442  23.135  1.00  0.00   O
ATOM  53  N   LYS  8   21.250  22.175  24.898  1.00  0.00   N
ATOM  54  CA  LYS  8   20.841  23.557  24.750  1.00  0.00   C
ATOM  55  CB  LYS  8   21.476  24.436  25.823  1.00  0.00   C
ATOM  56  CG  LYS  8   21.023  25.879  25.632  1.00  0.00   C
ATOM  57  CD  LYS  8   21.658  26.757  26.706  1.00  0.00   C
ATOM  58  CE  LYS  8   21.203  28.201  26.516  1.00  0.00   C
ATOM  59  NZ  LYS  8   21.815  29.047  27.549  1.00  0.00  N1+
ATOM  60  C   LYS  8   21.256  24.109  23.393  1.00  0.00   C
ATOM  61  O   LYS  8   20.467  24.772  22.722  1.00  0.00   O
ATOM  62  N   LEU  9   22.498  23.833  22.989  1.00  0.00   N
ATOM  63  CA  LEU  9   23.011  24.301  21.717  1.00  0.00   C
ATOM  64  CB  LEU  9   24.451  23.846  21.506  1.00  0.00   C
ATOM  65  CG  LEU  9   24.953  24.356  20.160  1.00  0.00   C
ATOM  66  CD1 LEU  9   24.893  25.880  20.140  1.00  0.00   C
ATOM  67  CD2 LEU  9   26.393  23.901  19.948  1.00  0.00   C
ATOM  68  C   LEU  9   22.179  23.764  20.561  1.00  0.00   C
ATOM  69  O   LEU  9   21.836  24.507  19.643  1.00  0.00   O
ATOM  70  N   MET  10  21.856  22.470  20.606  1.00  0.00   N
ATOM  71  CA  MET  10  21.067  21.841  19.566  1.00  0.00   C
ATOM  72  CB  MET  10  20.844  20.363  19.865  1.00  0.00   C
ATOM  73  CG  MET  10  20.013  19.738  18.749  1.00  0.00   C
ATOM  74  SD  MET  10  19.739  17.982  19.089  1.00  0.00   S
ATOM  75  CE  MET  10  18.772  17.537  17.663  1.00  0.00   C
ATOM  76  C   MET  10  19.702  22.501  19.437  1.00  0.00   C
ATOM  77  O   MET  10  19.244  22.778  18.331  1.00  0.00   O
ATOM  78  N   PHE  11  19.050  22.753  20.575  1.00  0.00   N
ATOM  79  CA  PHE  11  17.744  23.378  20.587  1.00  0.00   C
ATOM  80  CB  PHE  11  17.230  23.549  22.013  1.00  0.00   C
ATOM  81  CG  PHE  11  15.869  24.193  22.127  1.00  0.00   C
ATOM  82  CD1 PHE  11  15.297  24.402  23.388  1.00  0.00   C
ATOM  83  CE1 PHE  11  14.036  25.000  23.495  1.00  0.00   C
ATOM  84  CZ  PHE  11  13.346  25.390  22.340  1.00  0.00   C
ATOM  85  CE2 PHE  11  13.918  25.182  21.080  1.00  0.00   C
ATOM  86  CD2 PHE  11  15.180  24.584  20.973  1.00  0.00   C
ATOM  87  C   PHE  11  17.789  24.754  19.940  1.00  0.00   C
ATOM  88  O   PHE  11  16.922  25.097  19.140  1.00  0.00   O
ATOM  89  N   LYS  12  18.805  25.547  20.291  1.00  0.00   N
ATOM  90  CA  LYS  12  18.959  26.881  19.745  1.00  0.00   C
ATOM  91  CB  LYS  12  20.199  27.565  20.312  1.00  0.00   C
ATOM  92  CG  LYS  12  20.326  28.962  19.714  1.00  0.00   C
ATOM  93  CD  LYS  12  21.565  29.647  20.280  1.00  0.00   C
ATOM  94  CE  LYS  12  21.691  31.044  19.684  1.00  0.00   C
ATOM  95  NZ  LYS  12  22.886  31.704  20.230  1.00  0.00  N1+
ATOM  96  C   LYS  12  19.101  26.840  18.230  1.00  0.00   C
ATOM  97  O   LYS  12  18.475  27.626  17.523  1.00  0.00   O
ATOM  98  N   THR  13  19.930  25.918  17.732  1.00  0.00   N
ATOM  99  CA  THR  13  20.151  25.778  16.307  1.00  0.00   C
ATOM 100  CB  THR  13  21.138  24.654  16.013  1.00  0.00   C
ATOM 101  CG2 THR  13  22.472  24.960  16.687  1.00  0.00   C
ATOM 102  OG1 THR  13  20.621  23.421  16.519  1.00  0.00   O
ATOM 103  C   THR  13  18.853  25.459  15.579  1.00  0.00   C
ATOM 104  O   THR  13  18.561  26.044  14.538  1.00  0.00   O
ATOM 105  N   GLU  14  18.071  24.528  16.132  1.00  0.00   N
ATOM 106  CA  GLU  14  16.810  24.135  15.536  1.00  0.00   C
ATOM 107  CB  GLU  14  16.122  23.057  16.367  1.00  0.00   C
ATOM 108  CG  GLU  14  14.814  22.677  15.715  1.00  0.00   C
ATOM 109  CD  GLU  14  14.126  21.597  16.547  1.00  0.00   C
ATOM 110  OE1 GLU  14  13.340  21.983  17.453  1.00  0.00   O
ATOM 111  OE2 GLU  14  14.393  20.398  16.270  1.00  0.00  O1-
ATOM 112  C   GLU  14  15.861  25.320  15.433  1.00  0.00   C
ATOM 113  O   GLU  14  16.204  26.431  15.829  1.00  0.00   O
ATOM 114  N   NHE  15  14.662  25.088  14.899  1.00  0.00   N
TER  115   NHE  15
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