

20. ENERGY CALCULATIONS AND MOLECULAR DYNAMICS

Table 20.1.3.1. Occurrence of intramolecular hydrogen bonds (%) during the final 1.6 ns of the simulation

The criteria for a hydrogen bond to be present are angle donor–hydrogen–acceptor $\geq 135^\circ$, distance hydrogen–acceptor ≤ 0.25 nm. Hydrogen bonds are shown if they are either present in the X-ray structure or if at least one of the four protein molecules in the unit cell shows the hydrogen bond of interest for at least 50% of the simulation time. The letter h appended to an amino-acid code indicates that the residue is protonated.

Hydrogen bonds		X-ray structure	Molecular dynamics			
Backbone	Backbone		Molecule 1	Molecule 2	Molecule 3	Molecule 4
3Ile H	15Leu O	100	94	94	95	98
4Phe H	65Ser O	100	85	69	87	77
5Val H	13Ile O	100	80	90	87	93
6Lysh H	67Leu O	100	85	82	88	94
7Thr H	11Lysh O	100	65	49	54	62
8Leu H	69Leu O	0	5	52	19	55
10Gly H	7Thr O	100	0	0	0	0
13Ile H	5Val O	100	86	76	70	87
15Leu H	3Ile O	100	87	92	72	82
17Val H	1Met O	100	68	39	79	51
21Asp H	18Glu O	100	68	84	84	90
23Ile H	54Arg O	100	0	74	89	92
24Glu H	52Asp O	100	58	69	63	84
26Val H	22Thr O	100	92	69	78	61
27Lysh H	23Ile O	100	94	97	98	99
28Ala H	24Glu O	100	71	71	84	89
29Lysh H	25Asn O	100	91	79	94	88
30Ile H	26Val O	100	92	76	94	91
31Gln H	27Lysh O	100	85	53	66	93
32Asp H	28Ala O	100	82	27	87	77
33Lysh H	29Lysh O	100	23	13	81	51
33Lysh H	30Ile O	0	59	23	7	19
34Glu H	30Ile O	100	95	54	64	86
35Gly H	31Gln O	100	0	0	0	0
36Ile H	34Glu O	0	62	50	28	35
40Gln H	37Pro O	100	0	0	0	0
41Gln H	37Pro O	0	68	56	72	20
41Gln H	38Pro O	100	14	25	14	50
42Arg H	70Val O	100	82	82	83	88
44Ile H	68Hish O	100	84	96	93	95
45Phe H	48Lysh O	100	20	74	77	91
48Lysh H	45Phe O	100	24	62	59	44
50Leu H	43Leu O	100	29	88	92	85
54Arg H	51GluO	100	20	60	19	69
56Leu H	21Asp O	100	0	90	81	81
57Ser H	19Pro O	100	3	78	86	83
58Asp H	55Thr O	100	0	0	0	0
59Tyr H	55Thr O	100	58	86	92	85
59Tyr H	56Leu O	100	0	0	0	0
60Asn H	57Ser O	100	38	34	60	58
61Ile H	56Leu O	100	67	7	63	56
64Glu H	2Gln O	100	0	42	6	95
65Ser H	62Gln O	100	0	0	0	0
67Leu H	4Phe O	100	69	74	87	70
68Hish H	44Ile O	100	62	68	83	89
69Leu H	6Lysh O	100	79	72	92	90
70Val H	42Arg O	100	91	89	90	91
72Arg H	40Gln O	100	79	59	85	78

20.1. MOLECULAR DYNAMICS: CONVERGENCE OF UBIQUITIN

Table 20.1.3.1. *Occurrence of intramolecular hydrogen bonds (%) during the final 1.6 ns of the simulation (cont.)*

Hydrogen bond		X-ray structure	Molecular dynamics			
Backbone	Side chain		Molecule 1	Molecule 2	Molecule 3	Molecule 4
2Gln H	64Glu OE2	0	63	7	84	0
9Thr H	7Thr OG1	100	0	0	0	0
11Lys H	7Thr OG1	100	0	0	0	0
18Glu H	21Asp OD2	100	80	3	0	0
20Ser H	18Glu OE2	0	0	0	55	0
25Asn H	22Thr OG1	100	31	13	61	38
51Glu H	59Tyr OH	100	46	87	56	76
55Thr H	58Asp OD1	100	29	62	22	75
58Asp H	55Thr OG1	100	53	76	72	86
64Glu H	64Glu OE2	0	55	6	16	0
Hydrogen bond		X-ray structure	Molecular dynamics			
Side chain	Backbone		Molecule 1	Molecule 2	Molecule 3	Molecule 4
29Lys HZ2	16Glu O	100	0	0	0	0
33Lys HZ2	14Thr O	100	0	0	0	0
41Gln HE21	27Lys O	100	81	91	47	71
41Gln HE22	36Ile O	100	90	89	60	83
48Lys HZ3	46Ala O	100	0	0	0	0
Hydrogen bond		X-ray structure	Molecular dynamics			
Side chain	Side chain		Molecule 1	Molecule 2	Molecule 3	Molecule 4
11Lys HZ2	34Glu OE2	100	0	0	0	0
20Ser HG	18Glu OE2	0	0	0	60	0
27Lys HZ2	52Asp OD2	100	0	0	0	0
49Gln HE21	16Glu OE1	100	0	0	0	0
54Arg HH12	58Asp OD1	100	0	0	0	0
55Thr HG1	58Asp OD1	0	44	83	29	86

where the angle brackets indicate a time or a combined time and ensemble average. Molecule 4 was selected because it is the most stable. RMSFs of the $C\alpha$ atoms were calculated directly from the simulation trajectory (Fig. 20.1.3.4*a*) after applying a translational fit using the $C\alpha$ atoms of residues 1–72, which are well defined in the X-ray structure (Fig. 20.1.3.4*b*), and after applying both a rotational and a translational fit on residues 1–72 (Fig. 20.1.3.4*c*). In Fig. 20.1.3.4(*d*), a translational and rotational fit was applied to all $C\alpha$ atoms (residues 1–76). Removal of the overall translational component of motion reduces the positional fluctuations by 0.04 nm on average. Only the RMSFs in the proximity of the end of the large α -helix formed by residues 23–34 are not affected by the

introduction of translational fitting. In contrast, it is exactly this region where the fluctuations are substantially lowered by introducing an additional rotational fit. The regions before residue 27 and after residue 42 are only slightly affected by the removal of overall rotation. These findings suggest that the entire protein translates by about 0.04 nm, while the α -helix region remains close to its initial position, thus rotating relative to the rest of the protein. Inclusion of the four C-terminal residues in the fitting procedure only affects the RMSFs of these residues and residues in the rotating part of the molecule, indicating that these four residues move together with the rest of the molecule. The atom-position fluctuations obtained by applying a full (rotational and transla-

Table 20.1.3.2. *Occurrence of intermolecular hydrogen bonds (%) during the final 1.6 ns of the simulation*

The criteria for a hydrogen bond to be present are: angle donor–hydrogen–acceptor $\geq 135^\circ$, distance hydrogen–acceptor ≤ 0.25 nm. Hydrogen bonds are shown if they are either present in the X-ray structure or if at least one of the four protein molecules in the unit cell shows the hydrogen bond of interest for at least 50% of the simulation time.

Hydrogen bond		X-ray structure	Molecular dynamics			
			Molecules 1–4	Molecules 2–3	Molecules 3–2	Molecules 4–1
6 Lys HZ3	51 Glu OE1	100	0	0	0	0
12 Thr HG1	18 Glu OE1	0	56	57	75	34
49 Gln H	8 Leu O	0	10	34	0	67
68 His HZ2	32 Asp OD2	0	0	0	53 (3–1)	13 (4–2)
71 Leu H	58 Asp O	0	65	0	0	0