**Table 4.2** 13C, 15N, and 1HN chemical shift assignments for LBD derived -synuclein fibrils

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Residue** | **1HN** | **15N** | **13C’** | **13CA** | **13CB** | **13CG** | **13CD** | **13CE** | **13CZ** | **15ND/15NE/15NZ** |
| -- | -- | -- | -- | -- | -- | -- | -- | -- | -- | -- |
| K34 | 7.46 | 125.5 | 174.5 | 56.1 | - | - | - | - | - | - |
| E35 | 8.76 | 121.9 | 176.3 | 53.4 | 35.7 | 35.6 | 183.4 |  |  |  |
| G36 | 8.75 | 117.5 | 173.6 | 48.4 |  |  |  |  |  |  |
| V37 | 7.67 | 118.6 | 172.4 | 60.0 | 35.7 | 21.9/24.5 |  |  |  |  |
| L38 | 8.88 | 127.8 | 173.8 | 52.6 | 47.3 | 27.5 | 25.3/29.0 |  |  |  |
| Y39 | 8.39 | 131.3 | 173.9 | 56.3 | 43.4 | 128.0 | 133.0 | 117.5 | 157.3 |  |
| V40 | 8.76 | 127.1 | 173.8 | 60.0 | 34.4 | 19.9/22.1 |  |  |  |  |
| G41 | 9.08 | 111.6 | 170.2 | 44.7 |  |  |  |  |  |  |
| S42 | 8.94 | 116.9 | 175.4 | 56.5 | 68.7 |  |  |  |  |  |
| K43 | 7.96 | 123.4 | 176.6 | 56.6 | - | - | - | - | - | - |
| -- | -- | -- | -- | -- | -- | -- | -- | -- | -- | -- |
| V49 | - | - | - | - | - |  |  |  |  |  |
| H50 | - | - | 175.8 | 51.7 | 31.5 | 125.1 | 129.4 | 140.3 |  | -/- |
| -- | -- | -- | -- | -- | -- | -- | -- | -- | -- | -- |
| E61 | - | - | 173.1 | - | - | - | - |  |  |  |
| Q62 | 8.15 | 122.6 | 174.3 | 54.5 | - | - | - |  |  | - |
| V63 | 8.96 | 124.6 | 173.9 | 61.2 | 35.5 | 21.1/- |  |  |  |  |
| T64 | 9.32 | 124.8 | 172.3 | 60.8 | 68.5 | 23.4/23.4 |  |  |  |  |
| N65 | 9.61 | 126.5 | 173.0 | 51.9 | 42.0 | 174.4 |  |  |  | 113.9 |
| V66 | 9.32 | 125.0 | 177.0 | 59.9 | 34.4 | 20.9/23.0 |  |  |  |  |
| G67 | 8.83 | 112.6 | 171.9 | 47.4 |  |  |  |  |  |  |
| G68 | 6.07 | 100.7 | 172.1 | 44.4 |  |  |  |  |  |  |
| A69 | 8.74 | 121.8 | 175.0 | 50.0 | 22.1 |  |  |  |  |  |
| V70 | 8.95 | 124.5 | 175.8 | 61.7 | 32.7 | 19.7/21.2 |  |  |  |  |
| V71 | 9.18 | 131.0 | 173.9 | 61.3 | 34.7 | 19.7/22.1 |  |  |  |  |
| T72 | 9.28 | 124.7 | 174.6 | 60.1 | 71.4 | 22.5 |  |  |  |  |
| G73 | 8.96 | 117.8 | 172.1 | 49.0 |  |  |  |  |  |  |
| V74 | 7.73 | 117.6 | 173.8 | 59.4 | 37.4 | 20.3/23.3 |  |  |  |  |
| T75 | 8.86 | 123.4 | 171.8 | 61.7 | 68.8 | 22.9 |  |  |  |  |
| A76\* | 9.55 | 131.2 | 174.2 | 49.7 | 21.7 |  |  |  |  |  |
| V77\* | 8.76 | 122.4 | 172.2 | 60.6 | 36.7 | 20.6/25.1 |  |  |  |  |
| A78 | 9.17 | 130.3 | 175.7 | 50.7 | 23.1 |  |  |  |  |  |
| Q79 | 8.80 | 122.6 | 174.1 | 54.6 | 37.6 | 34.7 | 179.3 |  |  | 112.4 |
| K80 | 8.97 | 126.5 | 173.9 | 54.7 | - | - | - | - | - | - |
| T81 | 8.53 | 124.7 | 172.8 | 61.9 | 69.9 | 21.1 |  |  |  |  |
| V82 | 9.42 | 127.0 | 175.4 | 60.1 | - | -/- |  |  |  |  |
| E83 | 8.93 | 118.3 | 175.9 | 55.3 |  |  |  |  |  |  |
| G84 | 8.96 | 124.4 | 175.0 | 49.8 |  |  |  |  |  |  |
| A85 | 9.13 | 124.7 | 174.5 | 49.9 | - |  |  |  |  |  |
| G86 | 8.86 | 110.3 | 172.5 | 44.2 |  |  |  |  |  |  |
| S87\* | 9.46 | 119.7 | 174.4 | 56.4 | 67.4 |  |  |  |  |  |
| I88\* | 8.96 | 128.2 | 173.2 | 60.1 | 44.4 | 27.8/17.6 | 16.9 |  |  |  |
| A89 | 8.97 | 129.1 | 175.2 | 50.3 | 22.5 |  |  |  |  |  |
| A90 | 9.31 | 126.3 | 174.4 | 49.7 | 22.2 |  |  |  |  |  |
| A91 | 8.73 | 123.7 | 175.4 | 50.3 | 23.2 |  |  |  |  |  |
| T92 | 8.79 | 117.3 | 173.3 | 61.2 | 70.8 | 20.5 |  |  |  |  |
| G93 | - | 116.8 | 170.3 | 44.9 |  |  |  |  |  |  |
| F94 | 9.16 | 129.0 | 173.1 | 56.9 | 43.5 | 137.4 | 131.2 | 129.3 | 140.3 |  |
| V95 | 9.00 | 128.5 | 173.0 | 60.9 | 35.6 | -/- |  |  |  |  |
| K96 | 8.99 | 129.0 | 175.1 | 54.5 | - | - | - | - | - | - |
| -- | -- | -- | -- | -- | -- | -- | -- | -- | -- | -- |

(\*) Two sets of shifts observed for at least one atom in the residue. Primary shift is reported here.