Table S4 reports the coverage of modeled residues in BCL::Fold SSE-only models. The number of amino acids in the native structure (Naa) and the number of amino acids in SSEs (after filtering by size) (NSSE) are used to calculate the relative coverage in %. The coverage relative to the total number of amino acids (COV) is calculated for BCL::Fold models using native SSEs (COVN-SSE) and predicted SSEs (COVP-SSE). The coverage relative to the number of amino acids in SSEs of the native structure (SSE-COV) is also shown for BCL::Fold models using native SSEs (SSE-COVN-SSE) and SSEs from a predicted pool (SSE-COVP-SSE). The latter is typically above 100%, which is attributed to the over-prediction of SSE length which generates longer SSE definitions, that just cross the SSE-length criteria that is used for filtering short SSEs.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **PDB id** | **Naa** | **Nsse** | **COVN-sse** | **COVP-sse** | **SSE-COVN-sse** | **SSE-COVP-sse** |
| 1BGCA | 174 | 108 | 62.1 ± 0.0 | 64.4 ± 2.9 | 100.0 ± 0.0 | 103.7 ± 4.6 |
| 1EYHA | 144 | 107 | 73.2 ± 2.4 | 74.4 ± 2.4 | 98.5 ± 3.2 | 100.2 ± 3.2 |
| 1FQIA | 147 | 90 | 60.4 ± 1.7 | 65.4 ± 2.8 | 98.6 ± 2.8 | 106.8 ± 4.6 |
| 1GAKA | 141 | 96 | 68.1 ± 0.0 | 67.1 ± 2.9 | 100.0 ± 0.0 | 98.5 ± 4.2 |
| 1GYUA | 140 | 63 | 45.0 ± 0.0 | 50.8 ± 3.0 | 100.0 ± 0.0 | 112.9 ± 6.7 |
| 1IAPA | 211 | 123 | 58.2 ± 0.6 | 62.2 ± 1.9 | 99.9 ± 1.0 | 106.7 ± 3.2 |
| 1ICXA | 155 | 103 | 66.1 ± 1.4 | 70.5 ± 2.7 | 99.4 ± 2.1 | 106.2 ± 4.1 |
| 1J27A | 102 | 76 | 74.5 ± 0.2 | 75.4 ± 3.3 | 100.0 ± 0.2 | 101.2 ± 4.5 |
| 1JL1A | 155 | 97 | 60.5 ± 3.5 | 58.4 ± 2.5 | 96.6 ± 5.6 | 93.3 ± 4.0 |
| 1LKIA | 180 | 113 | 62.8 ± 0.1 | 54.7 ± 2.9 | 100.0 ± 0.1 | 87.1 ± 4.6 |
| 1LMIA | 131 | 63 | 47.9 ± 1.0 | 42.5 ± 3.9 | 99.5 ± 2.1 | 88.4 ± 8.1 |
| 1OXJA | 173 | 108 | 62.4 ± 0.3 | 67.6 ± 3.0 | 100.0 ± 0.4 | 108.3 ± 4.8 |
| 1OZ9A | 150 | 101 | 65.8 ± 1.1 | 64.0 ± 3.2 | 97.8 ± 1.6 | 95.1 ± 4.7 |
| 1PBVA | 195 | 128 | 65.6 ± 0.0 | 65.8 ± 1.5 | 100.0 ± 0.0 | 100.3 ± 2.3 |
| 1PKOA | 139 | 58 | 41.7 ± 0.0 | 54.4 ± 3.6 | 100.0 ± 0.0 | 130.3 ± 8.6 |
| 1Q5ZA | 177 | 77 | 43.5 ± 0.0 | 52.4 ± 2.9 | 100.0 ± 0.0 | 120.5 ± 6.6 |
| 1RJ1A | 151 | 113 | 74.8 ± 0.2 | 77.7 ± 2.5 | 100.0 ± 0.2 | 103.8 ± 3.3 |
| 1T3YA | 141 | 83 | 58.7 ± 1.0 | 60.9 ± 2.8 | 99.7 ± 1.6 | 103.4 ± 4.8 |
| 1TP6A | 128 | 94 | 72.1 ± 1.7 | 69.7 ± 3.6 | 98.2 ± 2.3 | 94.9 ± 4.9 |
| 1TQGA | 105 | 88 | 83.8 ± 0.0 | 79.8 ± 3.5 | 100.0 ± 0.0 | 95.2 ± 4.1 |
| 1TZVA | 142 | 97 | 68.3 ± 0.0 | 70.7 ± 2.3 | 100.0 ± 0.0 | 103.5 ± 3.4 |
| 1UAIA | 224 | 114 | 50.8 ± 0.7 | 50.2 ± 2.4 | 99.8 ± 1.3 | 98.7 ± 4.7 |
| 1ULRA | 88 | 55 | 65.9 ± 0.1 | 71.6 ± 3.1 | 105.5 ± 0.1 | 114.6 ± 4.9 |
| 1VINA | 268 | 156 | 58.2 ± 0.2 | 66.8 ± 2.0 | 100.0 ± 0.4 | 114.8 ± 3.4 |
| 1X91A | 153 | 113 | 73.9 ± 0.0 | 73.9 ± 2.7 | 100.0 ± 0.0 | 100.1 ± 3.7 |
| 1XAKA | 83 | 38 | 45.8 ± 0.0 | 47.6 ± 4.8 | 100.0 ± 0.1 | 104.0 ± 10.4 |
| 1XKRA | 206 | 147 | 69.0 ± 1.2 | 68.4 ± 2.4 | 96.7 ± 1.7 | 95.9 ± 3.4 |
| 1XQOA | 256 | 162 | 62.6 ± 1.5 | 63.7 ± 2.6 | 98.9 ± 2.4 | 100.6 ± 4.1 |
| 1Z3XA | 238 | 129 | 53.3 ± 1.2 | 58.0 ± 1.8 | 98.3 ± 2.2 | 107.1 ± 3.4 |
| 2AP3A | 199 | 156 | 78.4 ± 0.0 | 71.4 ± 4.7 | 100.0 ± 0.0 | 91.1 ± 6.0 |
| 2BK8A | 97 | 47 | 48.5 ± 0.0 | 63.6 ± 4.3 | 100.0 ± 0.0 | 131.3 ± 8.9 |
| 2CWRA | 103 | 60 | 57.9 ± 1.3 | 54.7 ± 3.7 | 99.5 ± 2.3 | 93.8 ± 6.3 |
| 2EJXA | 139 | 107 | 75.1 ± 3.3 | 65.8 ± 3.7 | 97.5 ± 4.3 | 85.5 ± 4.7 |
| 2F1SA | 186 | 115 | 60.9 ± 1.5 | 65.3 ± 2.4 | 98.4 ± 2.5 | 105.6 ± 3.9 |
| 2FC3A | 124 | 80 | 63.2 ± 1.9 | 70.8 ± 3.6 | 98.0 ± 2.9 | 109.7 ± 5.5 |
| 2FM9A | 215 | 153 | 71.0 ± 1.0 | 74.1 ± 3.1 | 99.8 ± 1.4 | 104.1 ± 4.3 |
| 2FRGP | 106 | 64 | 60.2 ± 1.0 | 63.3 ± 4.7 | 99.6 ± 1.7 | 104.9 ± 7.8 |
| 2GKGA | 127 | 80 | 59.8 ± 4.0 | 63.8 ± 2.6 | 94.9 ± 6.4 | 101.3 ± 4.2 |
| 2HUJA | 140 | 99 | 70.7 ± 0.0 | 66.6 ± 2.7 | 100.0 ± 0.0 | 94.2 ± 3.8 |
| 2IU1A | 208 | 126 | 60.5 ± 0.6 | 64.1 ± 1.8 | 99.9 ± 0.9 | 105.8 ± 2.9 |
| 2JLIA | 123 | 69 | 56.0 ± 0.6 | 71.4 ± 3.2 | 99.9 ± 1.0 | 127.3 ± 5.8 |
| 2LISA | 136 | 91 | 66.9 ± 0.0 | 63.4 ± 2.6 | 100.0 ± 0.0 | 94.7 ± 3.9 |
| 2OF3A | 266 | 202 | 72.4 ± 2.6 | 73.2 ± 3.0 | 95.4 ± 3.4 | 96.4 ± 4.0 |
| 2OSAA | 202 | 124 | 61.4 ± 0.2 | 60.5 ± 2.4 | 100.0 ± 0.3 | 98.6 ± 3.9 |
| 2QZQA | 152 | 63 | 41.4 ± 0.1 | 50.4 ± 3.1 | 100.0 ± 0.3 | 121.5 ± 7.5 |
| 2R0SA | 285 | 165 | 55.0 ± 3.5 | 54.0 ± 1.9 | 95.0 ± 6.1 | 93.3 ± 3.3 |
| 2RB8A | 104 | 46 | 44.2 ± 0.0 | 51.5 ± 3.5 | 100.0 ± 0.0 | 116.5 ± 7.8 |
| 2RCIA | 204 | 126 | 60.5 ± 1.5 | 63.4 ± 3.3 | 97.9 ± 2.5 | 102.7 ± 5.3 |
| 2V75A | 104 | 65 | 62.5 ± 0.0 | 74.0 ± 3.6 | 100.0 ± 0.0 | 118.5 ± 5.8 |
| 2VQ4A | 106 | 54 | 49.8 ± 2.0 | 62.2 ± 3.2 | 97.7 ± 4.0 | 122.1 ± 6.2 |
| 2WJ5A | 101 | 42 | 41.6 ± 0.0 | 55.4 ± 3.6 | 100.0 ± 0.0 | 133.2 ± 8.6 |
| 2WWEA | 127 | 69 | 52.9 ± 1.9 | 58.8 ± 2.9 | 97.4 ± 3.5 | 108.3 ± 5.2 |
| 2YV8A | 164 | 79 | 48.2 ± 0.1 | 51.4 ± 2.7 | 100.0 ± 0.3 | 106.7 ± 5.5 |
| 2YXFA | 100 | 46 | 46.0 ± 0.0 | 54.9 ± 4.3 | 100.0 ± 0.0 | 119.3 ± 9.2 |
| 2YYOA | 171 | 66 | 38.5 ± 0.4 | 49.6 ± 2.7 | 99.8 ± 1.1 | 128.6 ± 7.1 |
| 2ZCOA | 293 | 205 | 68.1 ± 1.9 | 72.4 ± 2.3 | 97.4 ± 2.7 | 103.5 ± 3.3 |
| 3B5OA | 244 | 169 | 69.3 ± 0.0 | 73.8 ± 3.3 | 100.0 ± 0.0 | 106.6 ± 4.8 |
| 3CTGA | 129 | 68 | 51.2 ± 2.8 | 60.0 ± 3.1 | 97.0 ± 5.4 | 113.9 ± 6.0 |
| 3CX2A | 108 | 53 | 49.1 ± 0.0 | 64.0 ± 4.1 | 100.0 ± 0.0 | 130.4 ± 8.3 |
| 3FH2A | 146 | 100 | 68.5 ± 0.1 | 69.8 ± 1.8 | 100.0 ± 0.2 | 101.9 ± 2.6 |
| 3FHFA | 214 | 147 | 67.2 ± 3.0 | 67.6 ± 2.8 | 97.8 ± 4.4 | 98.5 ± 4.1 |
| 3FRRA | 191 | 141 | 73.6 ± 0.8 | 70.4 ± 1.6 | 99.7 ± 1.1 | 95.4 ± 2.1 |
| 3HVWA | 176 | 109 | 57.7 ± 3.3 | 68.6 ± 2.7 | 93.2 ± 5.4 | 110.8 ± 4.3 |
| 3IV4A | 112 | 77 | 66.6 ± 1.9 | 65.6 ± 2.8 | 96.9 ± 2.7 | 95.4 ± 4.1 |
| 3NE3B | 130 | 81 | 60.7 ± 0.7 | 71.0 ± 4.1 | 97.4 ± 1.1 | 113.9 ± 6.5 |
| 3OIZA | 99 | 63 | 63.5 ± 0.9 | 71.1 ± 3.6 | 99.8 ± 1.4 | 111.7 ± 5.7 |
| avg | 160 | 99 | 60.5 | 64.0 | 99.1 | 106.0 |
| std | 51 | 38 | 10.3 | 8.2 | 1.7 | 11.3 |

**Table S4: Residue coverage of BCL::Fold models relative to the number of amino acids in the native protein structure**