

;;; MARTINI coarse-grained topology

[moleculetype]

;molname exclusions

PMAL 1

[atoms]

| | | | | | | | |
|----|-----|----|-----|-----|----|--------|---|
| 1 | Qa | 1 | MAL | BN0 | 1 | -1.000 | ; |
| 2 | Nda | 1 | MAL | SC1 | 2 | 0.000 | ; |
| 3 | Qd | 1 | MAL | SC2 | 3 | 1.000 | ; |
| 4 | N0 | 2 | MAL | BN0 | 4 | 0.000 | ; |
| 5 | C1 | 2 | MAL | SC1 | 5 | 0.000 | ; |
| 6 | C1 | 2 | MAL | SC2 | 6 | 0.000 | ; |
| 7 | Qa | 3 | MAL | BN0 | 7 | -0.100 | ; |
| 8 | Nda | 3 | MAL | SC1 | 8 | 0.000 | ; |
| 9 | Qd | 3 | MAL | SC2 | 9 | 1.000 | ; |
| 10 | N0 | 4 | MAL | BN0 | 10 | 0.000 | ; |
| 11 | C1 | 4 | MAL | SC1 | 11 | 0.000 | ; |
| 12 | C1 | 4 | MAL | SC2 | 12 | 0.000 | ; |
| 13 | Qa | 5 | MAL | BN0 | 13 | -0.100 | ; |
| 14 | Nda | 5 | MAL | SC1 | 14 | 0.000 | ; |
| 15 | Qd | 5 | MAL | SC2 | 15 | 1.000 | ; |
| 16 | N0 | 6 | MAL | BN0 | 16 | 0.000 | ; |
| 17 | C1 | 6 | MAL | SC1 | 17 | 0.000 | ; |
| 18 | C1 | 6 | MAL | SC2 | 18 | 0.000 | ; |
| 19 | Qa | 7 | MAL | BN0 | 19 | -0.100 | ; |
| 20 | Nda | 7 | MAL | SC1 | 20 | 0.000 | ; |
| 21 | Qd | 7 | MAL | SC2 | 21 | 1.000 | ; |
| 22 | N0 | 8 | MAL | BN0 | 22 | 0.000 | ; |
| 23 | C1 | 8 | MAL | SC1 | 23 | 0.000 | ; |
| 24 | C1 | 8 | MAL | SC2 | 24 | 0.000 | ; |
| 25 | Qa | 9 | MAL | BN0 | 25 | -0.100 | ; |
| 26 | Nda | 9 | MAL | SC1 | 26 | 0.000 | ; |
| 27 | Qd | 9 | MAL | SC2 | 27 | 1.000 | ; |
| 28 | N0 | 10 | MAL | BN0 | 28 | 0.000 | ; |
| 29 | C1 | 10 | MAL | SC1 | 29 | 0.000 | ; |
| 30 | C1 | 10 | MAL | SC2 | 30 | 0.000 | ; |
| 31 | Qa | 11 | MAL | BN0 | 31 | -0.100 | ; |
| 32 | Nda | 11 | MAL | SC1 | 32 | 0.000 | ; |
| 33 | Qd | 11 | MAL | SC2 | 33 | 1.000 | ; |
| 34 | N0 | 12 | MAL | BN0 | 34 | 0.000 | ; |
| 35 | C1 | 12 | MAL | SC1 | 35 | 0.000 | ; |
| 36 | C1 | 12 | MAL | SC2 | 36 | 0.000 | ; |
| 37 | Qa | 13 | MAL | BN0 | 37 | -0.100 | ; |
| 38 | Nda | 13 | MAL | SC1 | 38 | 0.000 | ; |
| 39 | Qd | 13 | MAL | SC2 | 39 | 1.000 | ; |
| 40 | N0 | 14 | MAL | BN0 | 40 | 0.000 | ; |
| 41 | C1 | 14 | MAL | SC1 | 41 | 0.000 | ; |
| 42 | C1 | 14 | MAL | SC2 | 42 | 0.000 | ; |
| 43 | Qa | 15 | MAL | BN0 | 43 | -0.100 | ; |
| 44 | Nda | 15 | MAL | SC1 | 44 | 0.000 | ; |
| 45 | Qd | 15 | MAL | SC2 | 45 | 1.000 | ; |
| 46 | N0 | 16 | MAL | BN0 | 46 | 0.000 | ; |

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|-----|-----|----|-----|-----|-----|--------|---|
| 47 | C1 | 16 | MAL | SC1 | 47 | 0.000 | ; |
| 48 | C1 | 16 | MAL | SC2 | 48 | 0.000 | ; |
| 49 | Qa | 17 | MAL | BN0 | 49 | -0.100 | ; |
| 50 | Nda | 17 | MAL | SC1 | 50 | 0.000 | ; |
| 51 | Qd | 17 | MAL | SC2 | 51 | 1.000 | ; |
| 52 | N0 | 18 | MAL | BN0 | 52 | 0.000 | ; |
| 53 | C1 | 18 | MAL | SC1 | 53 | 0.000 | ; |
| 54 | C1 | 18 | MAL | SC2 | 54 | 0.000 | ; |
| 55 | Qa | 19 | MAL | BN0 | 55 | -0.100 | ; |
| 56 | Nda | 19 | MAL | SC1 | 56 | 0.000 | ; |
| 57 | Qd | 19 | MAL | SC2 | 57 | 1.000 | ; |
| 58 | N0 | 20 | MAL | BN0 | 58 | 0.000 | ; |
| 59 | C1 | 20 | MAL | SC1 | 59 | 0.000 | ; |
| 60 | C1 | 20 | MAL | SC2 | 60 | 0.000 | ; |
| 61 | Qa | 21 | MAL | BN0 | 61 | -0.100 | ; |
| 62 | Nda | 21 | MAL | SC1 | 62 | 0.000 | ; |
| 63 | Qd | 21 | MAL | SC2 | 63 | 1.000 | ; |
| 64 | N0 | 22 | MAL | BN0 | 64 | 0.000 | ; |
| 65 | C1 | 22 | MAL | SC1 | 65 | 0.000 | ; |
| 66 | C1 | 22 | MAL | SC2 | 66 | 0.000 | ; |
| 67 | Qa | 23 | MAL | BN0 | 67 | -0.100 | ; |
| 68 | Nda | 23 | MAL | SC1 | 68 | 0.000 | ; |
| 69 | Qd | 23 | MAL | SC2 | 69 | 1.000 | ; |
| 70 | N0 | 24 | MAL | BN0 | 70 | 0.000 | ; |
| 71 | C1 | 24 | MAL | SC1 | 71 | 0.000 | ; |
| 72 | C1 | 24 | MAL | SC2 | 72 | 0.000 | ; |
| 73 | Qa | 25 | MAL | BN0 | 73 | -0.100 | ; |
| 74 | Nda | 25 | MAL | SC1 | 74 | 0.000 | ; |
| 75 | Qd | 25 | MAL | SC2 | 75 | 1.000 | ; |
| 76 | N0 | 26 | MAL | BN0 | 76 | 0.000 | ; |
| 77 | C1 | 26 | MAL | SC1 | 77 | 0.000 | ; |
| 78 | C1 | 26 | MAL | SC2 | 78 | 0.000 | ; |
| 79 | Qa | 27 | MAL | BN0 | 79 | -0.100 | ; |
| 80 | Nda | 27 | MAL | SC1 | 80 | 0.000 | ; |
| 81 | Qd | 27 | MAL | SC2 | 81 | 1.000 | ; |
| 82 | N0 | 28 | MAL | BN0 | 82 | 0.000 | ; |
| 83 | C1 | 28 | MAL | SC1 | 83 | 0.000 | ; |
| 84 | C1 | 28 | MAL | SC2 | 84 | 0.000 | ; |
| 85 | Qa | 29 | MAL | BN0 | 85 | -0.100 | ; |
| 86 | Nda | 29 | MAL | SC1 | 86 | 0.000 | ; |
| 87 | Qd | 29 | MAL | SC2 | 87 | 1.000 | ; |
| 88 | N0 | 30 | MAL | BN0 | 88 | 0.000 | ; |
| 89 | C1 | 30 | MAL | SC1 | 89 | 0.000 | ; |
| 90 | C1 | 30 | MAL | SC2 | 90 | 0.000 | ; |
| 91 | Qa | 31 | MAL | BN0 | 91 | -0.100 | ; |
| 92 | Nda | 31 | MAL | SC1 | 92 | 0.000 | ; |
| 93 | Qd | 31 | MAL | SC2 | 93 | 1.000 | ; |
| 94 | N0 | 32 | MAL | BN0 | 94 | 0.000 | ; |
| 95 | C1 | 32 | MAL | SC1 | 95 | 0.000 | ; |
| 96 | C1 | 32 | MAL | SC2 | 96 | 0.000 | ; |
| 97 | Qa | 33 | MAL | BN0 | 97 | -0.100 | ; |
| 98 | Nda | 33 | MAL | SC1 | 98 | 0.000 | ; |
| 99 | Qd | 33 | MAL | SC2 | 99 | 1.000 | ; |
| 100 | N0 | 34 | MAL | BN0 | 100 | 0.000 | ; |

| | | | | | | | |
|-----|-----|----|-----|-----|-----|--------|---|
| 101 | C1 | 34 | MAL | SC1 | 101 | 0.000 | ; |
| 102 | C1 | 34 | MAL | SC2 | 102 | 0.000 | ; |
| 103 | Qa | 35 | MAL | BN0 | 103 | -0.100 | ; |
| 104 | Nda | 35 | MAL | SC1 | 104 | 0.000 | ; |
| 105 | Qd | 35 | MAL | SC2 | 105 | 1.000 | ; |
| 106 | N0 | 36 | MAL | BN0 | 106 | 0.000 | ; |
| 107 | C1 | 36 | MAL | SC1 | 107 | 0.000 | ; |
| 108 | C1 | 36 | MAL | SC2 | 108 | 0.000 | ; |
| 109 | Qa | 37 | MAL | BN0 | 109 | -0.100 | ; |
| 110 | Nda | 37 | MAL | SC1 | 110 | 0.000 | ; |
| 111 | Qd | 37 | MAL | SC2 | 111 | 1.000 | ; |
| 112 | N0 | 38 | MAL | BN0 | 112 | 0.000 | ; |
| 113 | C1 | 38 | MAL | SC1 | 113 | 0.000 | ; |
| 114 | C1 | 38 | MAL | SC2 | 114 | 0.000 | ; |
| 115 | Qa | 39 | MAL | BN0 | 115 | -0.100 | ; |
| 116 | Nda | 39 | MAL | SC1 | 116 | 0.000 | ; |
| 117 | Qd | 39 | MAL | SC2 | 117 | 1.000 | ; |
| 118 | N0 | 40 | MAL | BN0 | 118 | 0.000 | ; |
| 119 | C1 | 40 | MAL | SC1 | 119 | 0.000 | ; |
| 120 | C1 | 40 | MAL | SC2 | 120 | 0.000 | ; |
| 121 | Qa | 41 | MAL | BN0 | 121 | -0.100 | ; |
| 122 | Nda | 41 | MAL | SC1 | 122 | 0.000 | ; |
| 123 | Qd | 41 | MAL | SC2 | 123 | 1.000 | ; |
| 124 | N0 | 42 | MAL | BN0 | 124 | 0.000 | ; |
| 125 | C1 | 42 | MAL | SC1 | 125 | 0.000 | ; |
| 126 | C1 | 42 | MAL | SC2 | 126 | 0.000 | ; |
| 127 | Qa | 43 | MAL | BN0 | 127 | -0.100 | ; |
| 128 | Nda | 43 | MAL | SC1 | 128 | 0.000 | ; |
| 129 | Qd | 43 | MAL | SC2 | 129 | 1.000 | ; |
| 130 | N0 | 44 | MAL | BN0 | 130 | 0.000 | ; |
| 131 | C1 | 44 | MAL | SC1 | 131 | 0.000 | ; |
| 132 | C1 | 44 | MAL | SC2 | 132 | 0.000 | ; |
| 133 | Qa | 45 | MAL | BN0 | 133 | -0.100 | ; |
| 134 | Nda | 45 | MAL | SC1 | 134 | 0.000 | ; |
| 135 | Qd | 45 | MAL | SC2 | 135 | 1.000 | ; |
| 136 | N0 | 46 | MAL | BN0 | 136 | 0.000 | ; |
| 137 | C1 | 46 | MAL | SC1 | 137 | 0.000 | ; |
| 138 | C1 | 46 | MAL | SC2 | 138 | 0.000 | ; |
| 139 | Qa | 47 | MAL | BN0 | 139 | -0.100 | ; |
| 140 | Nda | 47 | MAL | SC1 | 140 | 0.000 | ; |
| 141 | Qd | 47 | MAL | SC2 | 141 | 1.000 | ; |
| 142 | N0 | 48 | MAL | BN0 | 142 | 0.000 | ; |
| 143 | C1 | 48 | MAL | SC1 | 143 | 0.000 | ; |
| 144 | C1 | 48 | MAL | SC2 | 144 | 0.000 | ; |
| 145 | Qa | 49 | MAL | BN0 | 145 | -0.100 | ; |
| 146 | Nda | 49 | MAL | SC1 | 146 | 0.000 | ; |
| 147 | Qd | 49 | MAL | SC2 | 147 | 1.000 | ; |
| 148 | N0 | 50 | MAL | BN0 | 148 | 0.000 | ; |
| 149 | C1 | 50 | MAL | SC1 | 149 | 0.000 | ; |
| 150 | C1 | 50 | MAL | SC2 | 150 | 0.000 | ; |
| 151 | Qa | 51 | MAL | BN0 | 151 | -0.100 | ; |
| 152 | Nda | 51 | MAL | SC1 | 152 | 0.000 | ; |
| 153 | Qd | 51 | MAL | SC2 | 153 | 1.000 | ; |
| 154 | N0 | 52 | MAL | BN0 | 154 | 0.000 | ; |

| | | | | | | | |
|-----|-----|----|-----|-----|-----|--------|---|
| 155 | C1 | 52 | MAL | SC1 | 155 | 0.000 | ; |
| 156 | C1 | 52 | MAL | SC2 | 156 | 0.000 | ; |
| 157 | Qa | 53 | MAL | BN0 | 157 | -0.100 | ; |
| 158 | Nda | 53 | MAL | SC1 | 158 | 0.000 | ; |
| 159 | Qd | 53 | MAL | SC2 | 159 | 1.000 | ; |
| 160 | N0 | 54 | MAL | BN0 | 160 | 0.000 | ; |
| 161 | C1 | 54 | MAL | SC1 | 161 | 0.000 | ; |
| 162 | C1 | 54 | MAL | SC2 | 162 | 0.000 | ; |
| 163 | Qa | 55 | MAL | BN0 | 163 | -0.100 | ; |
| 164 | Nda | 55 | MAL | SC1 | 164 | 0.000 | ; |
| 165 | Qd | 55 | MAL | SC2 | 165 | 1.000 | ; |
| 166 | N0 | 56 | MAL | BN0 | 166 | 0.000 | ; |
| 167 | C1 | 56 | MAL | SC1 | 167 | 0.000 | ; |
| 168 | C1 | 56 | MAL | SC2 | 168 | 0.000 | ; |
| 169 | Qa | 57 | MAL | BN0 | 169 | -0.100 | ; |
| 170 | Nda | 57 | MAL | SC1 | 170 | 0.000 | ; |
| 171 | Qd | 57 | MAL | SC2 | 171 | 1.000 | ; |
| 172 | N0 | 58 | MAL | BN0 | 172 | 0.000 | ; |
| 173 | C1 | 58 | MAL | SC1 | 173 | 0.000 | ; |
| 174 | C1 | 58 | MAL | SC2 | 174 | 0.000 | ; |
| 175 | Qa | 59 | MAL | BN0 | 175 | -0.100 | ; |
| 176 | Nda | 59 | MAL | SC1 | 176 | 0.000 | ; |
| 177 | Qd | 59 | MAL | SC2 | 177 | 1.000 | ; |
| 178 | N0 | 60 | MAL | BN0 | 178 | 0.000 | ; |
| 179 | C1 | 60 | MAL | SC1 | 179 | 0.000 | ; |
| 180 | C1 | 60 | MAL | SC2 | 180 | 0.000 | ; |
| 181 | Qa | 61 | MAL | BN0 | 181 | -0.100 | ; |
| 182 | Nda | 61 | MAL | SC1 | 182 | 0.000 | ; |
| 183 | Qd | 61 | MAL | SC2 | 183 | 1.000 | ; |
| 184 | N0 | 62 | MAL | BN0 | 184 | 0.000 | ; |
| 185 | C1 | 62 | MAL | SC1 | 185 | 0.000 | ; |
| 186 | C1 | 62 | MAL | SC2 | 186 | 0.000 | ; |
| 187 | Qa | 63 | MAL | BN0 | 187 | -0.100 | ; |
| 188 | Nda | 63 | MAL | SC1 | 188 | 0.000 | ; |
| 189 | Qd | 63 | MAL | SC2 | 189 | 1.000 | ; |
| 190 | N0 | 64 | MAL | BN0 | 190 | 0.000 | ; |
| 191 | C1 | 64 | MAL | SC1 | 191 | 0.000 | ; |
| 192 | C1 | 64 | MAL | SC2 | 192 | 0.000 | ; |
| 193 | Qa | 65 | MAL | BN0 | 193 | -0.100 | ; |
| 194 | Nda | 65 | MAL | SC1 | 194 | 0.000 | ; |
| 195 | Qd | 65 | MAL | SC2 | 195 | 1.000 | ; |
| 196 | N0 | 66 | MAL | BN0 | 196 | 0.000 | ; |
| 197 | C1 | 66 | MAL | SC1 | 197 | 0.000 | ; |
| 198 | C1 | 66 | MAL | SC2 | 198 | 0.000 | ; |
| 199 | Qa | 67 | MAL | BN0 | 199 | -0.100 | ; |
| 200 | Nda | 67 | MAL | SC1 | 200 | 0.000 | ; |
| 201 | Qd | 67 | MAL | SC2 | 201 | 1.000 | ; |
| 202 | N0 | 68 | MAL | BN0 | 202 | 0.000 | ; |
| 203 | C1 | 68 | MAL | SC1 | 203 | 0.000 | ; |
| 204 | C1 | 68 | MAL | SC2 | 204 | 0.000 | ; |
| 205 | Qa | 69 | MAL | BN0 | 205 | -0.100 | ; |
| 206 | Nda | 69 | MAL | SC1 | 206 | 0.000 | ; |
| 207 | Qd | 69 | MAL | SC2 | 207 | 1.000 | ; |
| 208 | N0 | 70 | MAL | BN0 | 208 | 0.000 | ; |

| | | | | | | | |
|-----|-----|----|-----|-----|-----|--------|---|
| 209 | C1 | 70 | MAL | SC1 | 209 | 0.000 | ; |
| 210 | C1 | 70 | MAL | SC2 | 210 | 0.000 | ; |
| 211 | Qa | 71 | MAL | BN0 | 211 | -0.100 | ; |
| 212 | Nda | 71 | MAL | SC1 | 212 | 0.000 | ; |
| 213 | Qd | 71 | MAL | SC2 | 213 | 1.000 | ; |
| 214 | N0 | 72 | MAL | BN0 | 214 | 0.000 | ; |
| 215 | C1 | 72 | MAL | SC1 | 215 | 0.000 | ; |
| 216 | C1 | 72 | MAL | SC2 | 216 | 0.000 | ; |
| 217 | Qa | 73 | MAL | BN0 | 217 | -0.100 | ; |
| 218 | Nda | 73 | MAL | SC1 | 218 | 0.000 | ; |
| 219 | Qd | 73 | MAL | SC2 | 219 | 1.000 | ; |
| 220 | N0 | 74 | MAL | BN0 | 220 | 0.000 | ; |
| 221 | C1 | 74 | MAL | SC1 | 221 | 0.000 | ; |
| 222 | C1 | 74 | MAL | SC2 | 222 | 0.000 | ; |
| 223 | Qa | 75 | MAL | BN0 | 223 | -0.100 | ; |
| 224 | Nda | 75 | MAL | SC1 | 224 | 0.000 | ; |
| 225 | Qd | 75 | MAL | SC2 | 225 | 1.000 | ; |
| 226 | N0 | 76 | MAL | BN0 | 226 | 0.000 | ; |
| 227 | C1 | 76 | MAL | SC1 | 227 | 0.000 | ; |
| 228 | C1 | 76 | MAL | SC2 | 228 | 0.000 | ; |
| 229 | Qa | 77 | MAL | BN0 | 229 | -0.100 | ; |
| 230 | Nda | 77 | MAL | SC1 | 230 | 0.000 | ; |
| 231 | Qd | 77 | MAL | SC2 | 231 | 1.000 | ; |
| 232 | N0 | 78 | MAL | BN0 | 232 | 0.000 | ; |
| 233 | C1 | 78 | MAL | SC1 | 233 | 0.000 | ; |
| 234 | C1 | 78 | MAL | SC2 | 234 | 0.000 | ; |
| 235 | Qa | 79 | MAL | BN0 | 235 | -0.100 | ; |
| 236 | Nda | 79 | MAL | SC1 | 236 | 0.000 | ; |
| 237 | Qd | 79 | MAL | SC2 | 237 | 1.000 | ; |
| 238 | N0 | 80 | MAL | BN0 | 238 | 0.000 | ; |
| 239 | C1 | 80 | MAL | SC1 | 239 | 0.000 | ; |
| 240 | C1 | 80 | MAL | SC2 | 240 | 0.000 | ; |
| 241 | Qa | 81 | MAL | BN0 | 241 | -0.100 | ; |
| 242 | Nda | 81 | MAL | SC1 | 242 | 0.000 | ; |
| 243 | Qd | 81 | MAL | SC2 | 243 | 1.000 | ; |
| 244 | N0 | 82 | MAL | BN0 | 244 | 0.000 | ; |
| 245 | C1 | 82 | MAL | SC1 | 245 | 0.000 | ; |
| 246 | C1 | 82 | MAL | SC2 | 246 | 0.000 | ; |
| 247 | Qa | 83 | MAL | BN0 | 247 | -0.100 | ; |
| 248 | Nda | 83 | MAL | SC1 | 248 | 0.000 | ; |
| 249 | Qd | 83 | MAL | SC2 | 249 | 1.000 | ; |
| 250 | N0 | 84 | MAL | BN0 | 250 | 0.000 | ; |
| 251 | C1 | 84 | MAL | SC1 | 251 | 0.000 | ; |
| 252 | C1 | 84 | MAL | SC2 | 252 | 0.000 | ; |
| 253 | Qa | 85 | MAL | BN0 | 253 | -0.100 | ; |
| 254 | Nda | 85 | MAL | SC1 | 254 | 0.000 | ; |
| 255 | Qd | 85 | MAL | SC2 | 255 | 1.000 | ; |
| 256 | N0 | 86 | MAL | BN0 | 256 | 0.000 | ; |
| 257 | C1 | 86 | MAL | SC1 | 257 | 0.000 | ; |
| 258 | C1 | 86 | MAL | SC2 | 258 | 0.000 | ; |
| 259 | Qa | 87 | MAL | BN0 | 259 | -0.100 | ; |
| 260 | Nda | 87 | MAL | SC1 | 260 | 0.000 | ; |
| 261 | Qd | 87 | MAL | SC2 | 261 | 1.000 | ; |
| 262 | N0 | 88 | MAL | BN0 | 262 | 0.000 | ; |

| | | | | | | | |
|-----|---------|-----|-----|-----|-------|--------|---|
| 263 | C1 | 88 | MAL | SC1 | 263 | 0.000 | ; |
| 264 | C1 | 88 | MAL | SC2 | 264 | 0.000 | ; |
| 265 | Qa | 89 | MAL | BN0 | 265 | -0.100 | ; |
| 266 | Nda 89 | MAL | SC1 | 266 | 0.000 | ; | |
| 267 | Qd | 89 | MAL | SC2 | 267 | 1.000 | ; |
| 268 | N0 | 90 | MAL | BN0 | 268 | 0.000 | ; |
| 269 | C1 | 90 | MAL | SC1 | 269 | 0.000 | ; |
| 270 | C1 | 90 | MAL | SC2 | 270 | 0.000 | ; |
| 271 | Qa | 91 | MAL | BN0 | 271 | -0.100 | ; |
| 272 | Nda 91 | MAL | SC1 | 272 | 0.000 | ; | |
| 273 | Qd | 91 | MAL | SC2 | 273 | 1.000 | ; |
| 274 | N0 | 92 | MAL | BN0 | 274 | 0.000 | ; |
| 275 | C1 | 92 | MAL | SC1 | 275 | 0.000 | ; |
| 276 | C1 | 92 | MAL | SC2 | 276 | 0.000 | ; |
| 277 | Qa | 93 | MAL | BN0 | 277 | -0.100 | ; |
| 278 | Nda 93 | MAL | SC1 | 278 | 0.000 | ; | |
| 279 | Qd | 93 | MAL | SC2 | 279 | 1.000 | ; |
| 280 | N0 | 94 | MAL | BN0 | 280 | 0.000 | ; |
| 281 | C1 | 94 | MAL | SC1 | 281 | 0.000 | ; |
| 282 | C1 | 94 | MAL | SC2 | 282 | 0.000 | ; |
| 283 | Qa | 95 | MAL | BN0 | 283 | -0.100 | ; |
| 284 | Nda 95 | MAL | SC1 | 284 | 0.000 | ; | |
| 285 | Qd | 95 | MAL | SC2 | 285 | 1.000 | ; |
| 286 | N0 | 96 | MAL | BN0 | 286 | 0.000 | ; |
| 287 | C1 | 96 | MAL | SC1 | 287 | 0.000 | ; |
| 288 | C1 | 96 | MAL | SC2 | 288 | 0.000 | ; |
| 289 | Qa | 97 | MAL | BN0 | 289 | -0.100 | ; |
| 290 | Nda 97 | MAL | SC1 | 290 | 0.000 | ; | |
| 291 | Qd | 97 | MAL | SC2 | 291 | 1.000 | ; |
| 292 | N0 | 98 | MAL | BN0 | 292 | 0.000 | ; |
| 293 | C1 | 98 | MAL | SC1 | 293 | 0.000 | ; |
| 294 | C1 | 98 | MAL | SC2 | 294 | 0.000 | ; |
| 295 | Qa | 99 | MAL | BN0 | 295 | -0.100 | ; |
| 296 | Nda 99 | MAL | SC1 | 296 | 0.000 | ; | |
| 297 | Qd | 99 | MAL | SC2 | 297 | 1.000 | ; |
| 298 | N0 | 100 | MAL | BN0 | 298 | 0.000 | ; |
| 299 | C1 | 100 | MAL | SC1 | 299 | 0.000 | ; |
| 300 | C1 | 100 | MAL | SC2 | 300 | 0.000 | ; |
| 301 | Qa | 101 | MAL | BN0 | 301 | -0.100 | ; |
| 302 | Nda 101 | MAL | SC1 | 302 | 0.000 | ; | |
| 303 | Qd | 101 | MAL | SC2 | 303 | 1.000 | ; |
| 304 | N0 | 102 | MAL | BN0 | 304 | 0.000 | ; |
| 305 | C1 | 102 | MAL | SC1 | 305 | 0.000 | ; |
| 306 | C1 | 102 | MAL | SC2 | 306 | 0.000 | ; |
| 307 | Qa | 103 | MAL | BN0 | 307 | -1.000 | ; |
| 308 | Nda 103 | MAL | SC1 | 308 | 0.000 | ; | |
| 309 | Qd | 103 | MAL | SC2 | 309 | 1.000 | ; |
| 310 | N0 | 104 | MAL | BN0 | 310 | 0.000 | ; |
| 311 | C1 | 104 | MAL | SC1 | 311 | 0.000 | ; |
| 312 | C1 | 104 | MAL | SC2 | 312 | 0.000 | ; |

[bonds]

;backbone-backbone bonds

| | | | | | |
|---|---|---|-------|------|---|
| 1 | 4 | 1 | 0.355 | 3800 | ; |
|---|---|---|-------|------|---|

| | | | | | |
|-----|-----|---|-------|------|---|
| 4 | 7 | 1 | 0.355 | 3800 | ; |
| 7 | 10 | 1 | 0.355 | 3800 | ; |
| 10 | 13 | 1 | 0.355 | 3800 | ; |
| 13 | 16 | 1 | 0.355 | 3800 | ; |
| 16 | 19 | 1 | 0.355 | 3800 | ; |
| 19 | 22 | 1 | 0.355 | 3800 | ; |
| 22 | 25 | 1 | 0.355 | 3800 | ; |
| 25 | 28 | 1 | 0.355 | 3800 | ; |
| 28 | 31 | 1 | 0.355 | 3800 | ; |
| 31 | 34 | 1 | 0.355 | 3800 | ; |
| 34 | 37 | 1 | 0.355 | 3800 | ; |
| 37 | 40 | 1 | 0.355 | 3800 | ; |
| 40 | 43 | 1 | 0.355 | 3800 | ; |
| 43 | 46 | 1 | 0.355 | 3800 | ; |
| 46 | 49 | 1 | 0.355 | 3800 | ; |
| 49 | 52 | 1 | 0.355 | 3800 | ; |
| 52 | 55 | 1 | 0.355 | 3800 | ; |
| 55 | 58 | 1 | 0.355 | 3800 | ; |
| 58 | 61 | 1 | 0.355 | 3800 | ; |
| 61 | 64 | 1 | 0.355 | 3800 | ; |
| 64 | 67 | 1 | 0.355 | 3800 | ; |
| 67 | 70 | 1 | 0.355 | 3800 | ; |
| 70 | 73 | 1 | 0.355 | 3800 | ; |
| 73 | 76 | 1 | 0.355 | 3800 | ; |
| 76 | 79 | 1 | 0.355 | 3800 | ; |
| 79 | 82 | 1 | 0.355 | 3800 | ; |
| 82 | 85 | 1 | 0.355 | 3800 | ; |
| 85 | 88 | 1 | 0.355 | 3800 | ; |
| 88 | 91 | 1 | 0.355 | 3800 | ; |
| 91 | 94 | 1 | 0.355 | 3800 | ; |
| 94 | 97 | 1 | 0.355 | 3800 | ; |
| 97 | 100 | 1 | 0.355 | 3800 | ; |
| 100 | 103 | 1 | 0.355 | 3800 | ; |
| 103 | 106 | 1 | 0.355 | 3800 | ; |
| 106 | 109 | 1 | 0.355 | 3800 | ; |
| 109 | 112 | 1 | 0.355 | 3800 | ; |
| 112 | 115 | 1 | 0.355 | 3800 | ; |
| 115 | 118 | 1 | 0.355 | 3800 | ; |
| 118 | 121 | 1 | 0.355 | 3800 | ; |
| 121 | 124 | 1 | 0.355 | 3800 | ; |
| 124 | 127 | 1 | 0.355 | 3800 | ; |
| 127 | 130 | 1 | 0.355 | 3800 | ; |
| 130 | 133 | 1 | 0.355 | 3800 | ; |
| 133 | 136 | 1 | 0.355 | 3800 | ; |
| 136 | 139 | 1 | 0.355 | 3800 | ; |
| 139 | 142 | 1 | 0.355 | 3800 | ; |
| 142 | 145 | 1 | 0.355 | 3800 | ; |
| 145 | 148 | 1 | 0.355 | 3800 | ; |
| 148 | 151 | 1 | 0.355 | 3800 | ; |
| 151 | 154 | 1 | 0.355 | 3800 | ; |
| 154 | 157 | 1 | 0.355 | 3800 | ; |
| 157 | 160 | 1 | 0.355 | 3800 | ; |
| 160 | 163 | 1 | 0.355 | 3800 | ; |
| 163 | 166 | 1 | 0.355 | 3800 | ; |

| | | | | | |
|---|-----|---|-------|------|---|
| 166 | 169 | 1 | 0.355 | 3800 | ; |
| 169 | 172 | 1 | 0.355 | 3800 | ; |
| 172 | 175 | 1 | 0.355 | 3800 | ; |
| 175 | 178 | 1 | 0.355 | 3800 | ; |
| 178 | 181 | 1 | 0.355 | 3800 | ; |
| 181 | 184 | 1 | 0.355 | 3800 | ; |
| 184 | 187 | 1 | 0.355 | 3800 | ; |
| 187 | 190 | 1 | 0.355 | 3800 | ; |
| 190 | 193 | 1 | 0.355 | 3800 | ; |
| 193 | 196 | 1 | 0.355 | 3800 | ; |
| 196 | 199 | 1 | 0.355 | 3800 | ; |
| 199 | 202 | 1 | 0.355 | 3800 | ; |
| 202 | 205 | 1 | 0.355 | 3800 | ; |
| 205 | 208 | 1 | 0.355 | 3800 | ; |
| 208 | 211 | 1 | 0.355 | 3800 | ; |
| 211 | 214 | 1 | 0.355 | 3800 | ; |
| 214 | 217 | 1 | 0.355 | 3800 | ; |
| 217 | 220 | 1 | 0.355 | 3800 | ; |
| 220 | 223 | 1 | 0.355 | 3800 | ; |
| 223 | 226 | 1 | 0.355 | 3800 | ; |
| 226 | 229 | 1 | 0.355 | 3800 | ; |
| 229 | 232 | 1 | 0.355 | 3800 | ; |
| 232 | 235 | 1 | 0.355 | 3800 | ; |
| 235 | 238 | 1 | 0.355 | 3800 | ; |
| 238 | 241 | 1 | 0.355 | 3800 | ; |
| 241 | 244 | 1 | 0.355 | 3800 | ; |
| 244 | 247 | 1 | 0.355 | 3800 | ; |
| 247 | 250 | 1 | 0.355 | 3800 | ; |
| 250 | 253 | 1 | 0.355 | 3800 | ; |
| 253 | 256 | 1 | 0.355 | 3800 | ; |
| 256 | 259 | 1 | 0.355 | 3800 | ; |
| 259 | 262 | 1 | 0.355 | 3800 | ; |
| 262 | 265 | 1 | 0.355 | 3800 | ; |
| 265 | 268 | 1 | 0.355 | 3800 | ; |
| 268 | 271 | 1 | 0.355 | 3800 | ; |
| 271 | 274 | 1 | 0.355 | 3800 | ; |
| 274 | 277 | 1 | 0.355 | 3800 | ; |
| 277 | 280 | 1 | 0.355 | 3800 | ; |
| 280 | 283 | 1 | 0.355 | 3800 | ; |
| 283 | 286 | 1 | 0.355 | 3800 | ; |
| 286 | 289 | 1 | 0.355 | 3800 | ; |
| 289 | 292 | 1 | 0.355 | 3800 | ; |
| 292 | 295 | 1 | 0.355 | 3800 | ; |
| 295 | 298 | 1 | 0.355 | 3800 | ; |
| 298 | 301 | 1 | 0.355 | 3800 | ; |
| 301 | 304 | 1 | 0.355 | 3800 | ; |
| 304 | 307 | 1 | 0.355 | 3800 | ; |
| 307 | 310 | 1 | 0.355 | 3800 | ; |
| ;backbone-sidechain and sidechain-sidechain bonds | | | | | |
| 1 | 2 | 1 | 0.395 | 4100 | ; |
| 2 | 3 | 1 | 0.485 | 4100 | ; |
| 4 | 5 | 1 | 0.375 | 4100 | ; |
| 5 | 6 | 1 | 0.375 | 4900 | ; |
| 7 | 8 | 1 | 0.395 | 4100 | ; |

| | | | | | |
|----|----|---|-------|------|---|
| 8 | 9 | 1 | 0.485 | 4100 | ; |
| 10 | 11 | 1 | 0.375 | 4100 | ; |
| 11 | 12 | 1 | 0.375 | 4900 | ; |
| 13 | 14 | 1 | 0.395 | 4100 | ; |
| 14 | 15 | 1 | 0.485 | 4100 | ; |
| 16 | 17 | 1 | 0.375 | 4100 | ; |
| 17 | 18 | 1 | 0.375 | 4900 | ; |
| 19 | 20 | 1 | 0.395 | 4100 | ; |
| 20 | 21 | 1 | 0.485 | 4100 | ; |
| 22 | 23 | 1 | 0.375 | 4100 | ; |
| 23 | 24 | 1 | 0.375 | 4900 | ; |
| 25 | 26 | 1 | 0.395 | 4100 | ; |
| 26 | 27 | 1 | 0.485 | 4100 | ; |
| 28 | 29 | 1 | 0.375 | 4100 | ; |
| 29 | 30 | 1 | 0.375 | 4900 | ; |
| 31 | 32 | 1 | 0.395 | 4100 | ; |
| 32 | 33 | 1 | 0.485 | 4100 | ; |
| 34 | 35 | 1 | 0.375 | 4100 | ; |
| 35 | 36 | 1 | 0.375 | 4900 | ; |
| 37 | 38 | 1 | 0.395 | 4100 | ; |
| 38 | 39 | 1 | 0.485 | 4100 | ; |
| 40 | 41 | 1 | 0.375 | 4100 | ; |
| 41 | 42 | 1 | 0.375 | 4900 | ; |
| 43 | 44 | 1 | 0.395 | 4100 | ; |
| 44 | 45 | 1 | 0.485 | 4100 | ; |
| 46 | 47 | 1 | 0.375 | 4100 | ; |
| 47 | 48 | 1 | 0.375 | 4900 | ; |
| 49 | 50 | 1 | 0.395 | 4100 | ; |
| 50 | 51 | 1 | 0.485 | 4100 | ; |
| 52 | 53 | 1 | 0.375 | 4100 | ; |
| 53 | 54 | 1 | 0.375 | 4900 | ; |
| 55 | 56 | 1 | 0.395 | 4100 | ; |
| 56 | 57 | 1 | 0.485 | 4100 | ; |
| 58 | 59 | 1 | 0.375 | 4100 | ; |
| 59 | 60 | 1 | 0.375 | 4900 | ; |
| 61 | 62 | 1 | 0.395 | 4100 | ; |
| 62 | 63 | 1 | 0.485 | 4100 | ; |
| 64 | 65 | 1 | 0.375 | 4100 | ; |
| 65 | 66 | 1 | 0.375 | 4900 | ; |
| 67 | 68 | 1 | 0.395 | 4100 | ; |
| 68 | 69 | 1 | 0.485 | 4100 | ; |
| 70 | 71 | 1 | 0.375 | 4100 | ; |
| 71 | 72 | 1 | 0.375 | 4900 | ; |
| 73 | 74 | 1 | 0.395 | 4100 | ; |
| 74 | 75 | 1 | 0.485 | 4100 | ; |
| 76 | 77 | 1 | 0.375 | 4100 | ; |
| 77 | 78 | 1 | 0.375 | 4900 | ; |
| 79 | 80 | 1 | 0.395 | 4100 | ; |
| 80 | 81 | 1 | 0.485 | 4100 | ; |
| 82 | 83 | 1 | 0.375 | 4100 | ; |
| 83 | 84 | 1 | 0.375 | 4900 | ; |
| 85 | 86 | 1 | 0.395 | 4100 | ; |
| 86 | 87 | 1 | 0.485 | 4100 | ; |
| 88 | 89 | 1 | 0.375 | 4100 | ; |

| | | | | | |
|-----|-----|---|-------|------|---|
| 89 | 90 | 1 | 0.375 | 4900 | ; |
| 91 | 92 | 1 | 0.395 | 4100 | ; |
| 92 | 93 | 1 | 0.485 | 4100 | ; |
| 94 | 95 | 1 | 0.375 | 4100 | ; |
| 95 | 96 | 1 | 0.375 | 4900 | ; |
| 97 | 98 | 1 | 0.395 | 4100 | ; |
| 98 | 99 | 1 | 0.485 | 4100 | ; |
| 100 | 101 | 1 | 0.375 | 4100 | ; |
| 101 | 102 | 1 | 0.375 | 4900 | ; |
| 103 | 104 | 1 | 0.395 | 4100 | ; |
| 104 | 105 | 1 | 0.485 | 4100 | ; |
| 106 | 107 | 1 | 0.375 | 4100 | ; |
| 107 | 108 | 1 | 0.375 | 4900 | ; |
| 109 | 110 | 1 | 0.395 | 4100 | ; |
| 110 | 111 | 1 | 0.485 | 4100 | ; |
| 112 | 113 | 1 | 0.375 | 4100 | ; |
| 113 | 114 | 1 | 0.375 | 4900 | ; |
| 115 | 116 | 1 | 0.395 | 4100 | ; |
| 116 | 117 | 1 | 0.485 | 4100 | ; |
| 118 | 119 | 1 | 0.375 | 4100 | ; |
| 119 | 120 | 1 | 0.375 | 4900 | ; |
| 121 | 122 | 1 | 0.395 | 4100 | ; |
| 122 | 123 | 1 | 0.485 | 4100 | ; |
| 124 | 125 | 1 | 0.375 | 4100 | ; |
| 125 | 126 | 1 | 0.375 | 4900 | ; |
| 127 | 128 | 1 | 0.395 | 4100 | ; |
| 128 | 129 | 1 | 0.485 | 4100 | ; |
| 130 | 131 | 1 | 0.375 | 4100 | ; |
| 131 | 132 | 1 | 0.375 | 4900 | ; |
| 133 | 134 | 1 | 0.395 | 4100 | ; |
| 134 | 135 | 1 | 0.485 | 4100 | ; |
| 136 | 137 | 1 | 0.375 | 4100 | ; |
| 137 | 138 | 1 | 0.375 | 4900 | ; |
| 139 | 140 | 1 | 0.395 | 4100 | ; |
| 140 | 141 | 1 | 0.485 | 4100 | ; |
| 142 | 143 | 1 | 0.375 | 4100 | ; |
| 143 | 144 | 1 | 0.375 | 4900 | ; |
| 145 | 146 | 1 | 0.395 | 4100 | ; |
| 146 | 147 | 1 | 0.485 | 4100 | ; |
| 148 | 149 | 1 | 0.375 | 4100 | ; |
| 149 | 150 | 1 | 0.375 | 4900 | ; |
| 151 | 152 | 1 | 0.395 | 4100 | ; |
| 152 | 153 | 1 | 0.485 | 4100 | ; |
| 154 | 155 | 1 | 0.375 | 4100 | ; |
| 155 | 156 | 1 | 0.375 | 4900 | ; |
| 157 | 158 | 1 | 0.395 | 4100 | ; |
| 158 | 159 | 1 | 0.485 | 4100 | ; |
| 160 | 161 | 1 | 0.375 | 4100 | ; |
| 161 | 162 | 1 | 0.375 | 4900 | ; |
| 163 | 164 | 1 | 0.395 | 4100 | ; |
| 164 | 165 | 1 | 0.485 | 4100 | ; |
| 166 | 167 | 1 | 0.375 | 4100 | ; |
| 167 | 168 | 1 | 0.375 | 4900 | ; |
| 169 | 170 | 1 | 0.395 | 4100 | ; |

| | | | | | |
|-----|-----|---|-------|------|---|
| 170 | 171 | 1 | 0.485 | 4100 | ; |
| 172 | 173 | 1 | 0.375 | 4100 | ; |
| 173 | 174 | 1 | 0.375 | 4900 | ; |
| 175 | 176 | 1 | 0.395 | 4100 | ; |
| 176 | 177 | 1 | 0.485 | 4100 | ; |
| 178 | 179 | 1 | 0.375 | 4100 | ; |
| 179 | 180 | 1 | 0.375 | 4900 | ; |
| 181 | 182 | 1 | 0.395 | 4100 | ; |
| 182 | 183 | 1 | 0.485 | 4100 | ; |
| 184 | 185 | 1 | 0.375 | 4100 | ; |
| 185 | 186 | 1 | 0.375 | 4900 | ; |
| 187 | 188 | 1 | 0.395 | 4100 | ; |
| 188 | 189 | 1 | 0.485 | 4100 | ; |
| 190 | 191 | 1 | 0.375 | 4100 | ; |
| 191 | 192 | 1 | 0.375 | 4900 | ; |
| 193 | 194 | 1 | 0.395 | 4100 | ; |
| 194 | 195 | 1 | 0.485 | 4100 | ; |
| 196 | 197 | 1 | 0.375 | 4100 | ; |
| 197 | 198 | 1 | 0.375 | 4900 | ; |
| 199 | 200 | 1 | 0.395 | 4100 | ; |
| 200 | 201 | 1 | 0.485 | 4100 | ; |
| 202 | 203 | 1 | 0.375 | 4100 | ; |
| 203 | 204 | 1 | 0.375 | 4900 | ; |
| 205 | 206 | 1 | 0.395 | 4100 | ; |
| 206 | 207 | 1 | 0.485 | 4100 | ; |
| 208 | 209 | 1 | 0.375 | 4100 | ; |
| 209 | 210 | 1 | 0.375 | 4900 | ; |
| 211 | 212 | 1 | 0.395 | 4100 | ; |
| 212 | 213 | 1 | 0.485 | 4100 | ; |
| 214 | 215 | 1 | 0.375 | 4100 | ; |
| 215 | 216 | 1 | 0.375 | 4900 | ; |
| 217 | 218 | 1 | 0.395 | 4100 | ; |
| 218 | 219 | 1 | 0.485 | 4100 | ; |
| 220 | 221 | 1 | 0.375 | 4100 | ; |
| 221 | 222 | 1 | 0.375 | 4900 | ; |
| 223 | 224 | 1 | 0.395 | 4100 | ; |
| 224 | 225 | 1 | 0.485 | 4100 | ; |
| 226 | 227 | 1 | 0.375 | 4100 | ; |
| 227 | 228 | 1 | 0.375 | 4900 | ; |
| 229 | 230 | 1 | 0.395 | 4100 | ; |
| 230 | 231 | 1 | 0.485 | 4100 | ; |
| 232 | 233 | 1 | 0.375 | 4100 | ; |
| 233 | 234 | 1 | 0.375 | 4900 | ; |
| 235 | 236 | 1 | 0.395 | 4100 | ; |
| 236 | 237 | 1 | 0.485 | 4100 | ; |
| 238 | 239 | 1 | 0.375 | 4100 | ; |
| 239 | 240 | 1 | 0.375 | 4900 | ; |
| 241 | 242 | 1 | 0.395 | 4100 | ; |
| 242 | 243 | 1 | 0.485 | 4100 | ; |
| 244 | 245 | 1 | 0.375 | 4100 | ; |
| 245 | 246 | 1 | 0.375 | 4900 | ; |
| 247 | 248 | 1 | 0.395 | 4100 | ; |
| 248 | 249 | 1 | 0.485 | 4100 | ; |
| 250 | 251 | 1 | 0.375 | 4100 | ; |

| | | | | | |
|-----|-----|---|-------|------|---|
| 251 | 252 | 1 | 0.375 | 4900 | ; |
| 253 | 254 | 1 | 0.395 | 4100 | ; |
| 254 | 255 | 1 | 0.485 | 4100 | ; |
| 256 | 257 | 1 | 0.375 | 4100 | ; |
| 257 | 258 | 1 | 0.375 | 4900 | ; |
| 259 | 260 | 1 | 0.395 | 4100 | ; |
| 260 | 261 | 1 | 0.485 | 4100 | ; |
| 262 | 263 | 1 | 0.375 | 4100 | ; |
| 263 | 264 | 1 | 0.375 | 4900 | ; |
| 265 | 266 | 1 | 0.395 | 4100 | ; |
| 266 | 267 | 1 | 0.485 | 4100 | ; |
| 268 | 269 | 1 | 0.375 | 4100 | ; |
| 269 | 270 | 1 | 0.375 | 4900 | ; |
| 271 | 272 | 1 | 0.395 | 4100 | ; |
| 272 | 273 | 1 | 0.485 | 4100 | ; |
| 274 | 275 | 1 | 0.375 | 4100 | ; |
| 275 | 276 | 1 | 0.375 | 4900 | ; |
| 277 | 278 | 1 | 0.395 | 4100 | ; |
| 278 | 279 | 1 | 0.485 | 4100 | ; |
| 280 | 281 | 1 | 0.375 | 4100 | ; |
| 281 | 282 | 1 | 0.375 | 4900 | ; |
| 283 | 284 | 1 | 0.395 | 4100 | ; |
| 284 | 285 | 1 | 0.485 | 4100 | ; |
| 286 | 287 | 1 | 0.375 | 4100 | ; |
| 287 | 288 | 1 | 0.375 | 4900 | ; |
| 289 | 290 | 1 | 0.395 | 4100 | ; |
| 290 | 291 | 1 | 0.485 | 4100 | ; |
| 292 | 293 | 1 | 0.375 | 4100 | ; |
| 293 | 294 | 1 | 0.375 | 4900 | ; |
| 295 | 296 | 1 | 0.395 | 4100 | ; |
| 296 | 297 | 1 | 0.485 | 4100 | ; |
| 298 | 299 | 1 | 0.375 | 4100 | ; |
| 299 | 300 | 1 | 0.375 | 4900 | ; |
| 301 | 302 | 1 | 0.395 | 4100 | ; |
| 302 | 303 | 1 | 0.485 | 4100 | ; |
| 304 | 305 | 1 | 0.375 | 4100 | ; |
| 305 | 306 | 1 | 0.375 | 4900 | ; |
| 307 | 308 | 1 | 0.395 | 4100 | ; |
| 308 | 309 | 1 | 0.485 | 4100 | ; |
| 310 | 311 | 1 | 0.375 | 4100 | ; |
| 311 | 312 | 1 | 0.375 | 4900 | ; |

[constraints]
;iso backbone-sidechain

[angles]
;backbone-sidechain-sidechain angles

| | | | | | | |
|----|----|----|---|-----|----|---|
| 1 | 2 | 3 | 2 | 110 | 30 | ; |
| 4 | 5 | 6 | 2 | 160 | 30 | ; |
| 7 | 8 | 9 | 2 | 110 | 30 | ; |
| 10 | 11 | 12 | 2 | 160 | 30 | ; |
| 13 | 14 | 15 | 2 | 110 | 30 | ; |
| 16 | 17 | 18 | 2 | 160 | 30 | ; |
| 19 | 20 | 21 | 2 | 110 | 30 | ; |

| | | | | | | |
|-----|-----|-----|---|-----|----|---|
| 22 | 23 | 24 | 2 | 160 | 30 | ; |
| 25 | 26 | 27 | 2 | 110 | 30 | ; |
| 28 | 29 | 30 | 2 | 160 | 30 | ; |
| 31 | 32 | 33 | 2 | 110 | 30 | ; |
| 34 | 35 | 36 | 2 | 160 | 30 | ; |
| 37 | 38 | 39 | 2 | 110 | 30 | ; |
| 40 | 41 | 42 | 2 | 160 | 30 | ; |
| 43 | 44 | 45 | 2 | 110 | 30 | ; |
| 46 | 47 | 48 | 2 | 160 | 30 | ; |
| 49 | 50 | 51 | 2 | 110 | 30 | ; |
| 52 | 53 | 54 | 2 | 160 | 30 | ; |
| 55 | 56 | 57 | 2 | 110 | 30 | ; |
| 58 | 59 | 60 | 2 | 160 | 30 | ; |
| 61 | 62 | 63 | 2 | 110 | 30 | ; |
| 64 | 65 | 66 | 2 | 160 | 30 | ; |
| 67 | 68 | 69 | 2 | 110 | 30 | ; |
| 70 | 71 | 72 | 2 | 160 | 30 | ; |
| 73 | 74 | 75 | 2 | 110 | 30 | ; |
| 76 | 77 | 78 | 2 | 160 | 30 | ; |
| 79 | 80 | 81 | 2 | 110 | 30 | ; |
| 82 | 83 | 84 | 2 | 160 | 30 | ; |
| 85 | 86 | 87 | 2 | 110 | 30 | ; |
| 88 | 89 | 90 | 2 | 160 | 30 | ; |
| 91 | 92 | 93 | 2 | 110 | 30 | ; |
| 94 | 95 | 96 | 2 | 160 | 30 | ; |
| 97 | 98 | 99 | 2 | 110 | 30 | ; |
| 100 | 101 | 102 | 2 | 160 | 30 | ; |
| 103 | 104 | 105 | 2 | 110 | 30 | ; |
| 106 | 107 | 108 | 2 | 160 | 30 | ; |
| 109 | 110 | 111 | 2 | 110 | 30 | ; |
| 112 | 113 | 114 | 2 | 160 | 30 | ; |
| 115 | 116 | 117 | 2 | 110 | 30 | ; |
| 118 | 119 | 120 | 2 | 160 | 30 | ; |
| 121 | 122 | 123 | 2 | 110 | 30 | ; |
| 124 | 125 | 126 | 2 | 160 | 30 | ; |
| 127 | 128 | 129 | 2 | 110 | 30 | ; |
| 130 | 131 | 132 | 2 | 160 | 30 | ; |
| 133 | 134 | 135 | 2 | 110 | 30 | ; |
| 136 | 137 | 138 | 2 | 160 | 30 | ; |
| 139 | 140 | 141 | 2 | 110 | 30 | ; |
| 142 | 143 | 144 | 2 | 160 | 30 | ; |
| 145 | 146 | 147 | 2 | 110 | 30 | ; |
| 148 | 149 | 150 | 2 | 160 | 30 | ; |
| 151 | 152 | 153 | 2 | 110 | 30 | ; |
| 154 | 155 | 156 | 2 | 160 | 30 | ; |
| 157 | 158 | 159 | 2 | 110 | 30 | ; |
| 160 | 161 | 162 | 2 | 160 | 30 | ; |
| 163 | 164 | 165 | 2 | 110 | 30 | ; |
| 166 | 167 | 168 | 2 | 160 | 30 | ; |
| 169 | 170 | 171 | 2 | 110 | 30 | ; |
| 172 | 173 | 174 | 2 | 160 | 30 | ; |
| 175 | 176 | 177 | 2 | 110 | 30 | ; |
| 178 | 179 | 180 | 2 | 160 | 30 | ; |
| 181 | 182 | 183 | 2 | 110 | 30 | ; |

| | | | | | | |
|-----|-----|-----|---|-----|----|---|
| 184 | 185 | 186 | 2 | 160 | 30 | ; |
| 187 | 188 | 189 | 2 | 110 | 30 | ; |
| 190 | 191 | 192 | 2 | 160 | 30 | ; |
| 193 | 194 | 195 | 2 | 110 | 30 | ; |
| 196 | 197 | 198 | 2 | 160 | 30 | ; |
| 199 | 200 | 201 | 2 | 110 | 30 | ; |
| 202 | 203 | 204 | 2 | 160 | 30 | ; |
| 205 | 206 | 207 | 2 | 110 | 30 | ; |
| 208 | 209 | 210 | 2 | 160 | 30 | ; |
| 211 | 212 | 213 | 2 | 110 | 30 | ; |
| 214 | 215 | 216 | 2 | 160 | 30 | ; |
| 217 | 218 | 219 | 2 | 110 | 30 | ; |
| 220 | 221 | 222 | 2 | 160 | 30 | ; |
| 223 | 224 | 225 | 2 | 110 | 30 | ; |
| 226 | 227 | 228 | 2 | 160 | 30 | ; |
| 229 | 230 | 231 | 2 | 110 | 30 | ; |
| 232 | 233 | 234 | 2 | 160 | 30 | ; |
| 235 | 236 | 237 | 2 | 110 | 30 | ; |
| 238 | 239 | 240 | 2 | 160 | 30 | ; |
| 241 | 242 | 243 | 2 | 110 | 30 | ; |
| 244 | 245 | 246 | 2 | 160 | 30 | ; |
| 247 | 248 | 249 | 2 | 110 | 30 | ; |
| 250 | 251 | 252 | 2 | 160 | 30 | ; |
| 253 | 254 | 255 | 2 | 110 | 30 | ; |
| 256 | 257 | 258 | 2 | 160 | 30 | ; |
| 259 | 260 | 261 | 2 | 110 | 30 | ; |
| 262 | 263 | 264 | 2 | 160 | 30 | ; |
| 265 | 266 | 267 | 2 | 110 | 30 | ; |
| 268 | 269 | 270 | 2 | 160 | 30 | ; |
| 271 | 272 | 273 | 2 | 110 | 30 | ; |
| 274 | 275 | 276 | 2 | 160 | 30 | ; |
| 277 | 278 | 279 | 2 | 110 | 30 | ; |
| 280 | 281 | 282 | 2 | 160 | 30 | ; |
| 283 | 284 | 285 | 2 | 110 | 30 | ; |
| 286 | 287 | 288 | 2 | 160 | 30 | ; |
| 289 | 290 | 291 | 2 | 110 | 30 | ; |
| 292 | 293 | 294 | 2 | 160 | 30 | ; |
| 295 | 296 | 297 | 2 | 110 | 30 | ; |
| 298 | 299 | 300 | 2 | 160 | 30 | ; |
| 301 | 302 | 303 | 2 | 110 | 30 | ; |
| 304 | 305 | 306 | 2 | 160 | 30 | ; |
| 307 | 308 | 309 | 2 | 110 | 30 | ; |
| 310 | 311 | 312 | 2 | 160 | 30 | ; |

;backbone-backbone-sidechain angles

| | | | | | | |
|----|----|----|---|-----|----|---|
| 1 | 4 | 5 | 2 | 5 | 50 | ; |
| 4 | 7 | 8 | 2 | 170 | 20 | ; |
| 7 | 10 | 11 | 2 | 5 | 50 | ; |
| 10 | 13 | 14 | 2 | 170 | 20 | ; |
| 13 | 16 | 17 | 2 | 5 | 50 | ; |
| 16 | 19 | 20 | 2 | 170 | 20 | ; |
| 19 | 22 | 23 | 2 | 5 | 50 | ; |
| 22 | 25 | 26 | 2 | 170 | 20 | ; |
| 25 | 28 | 29 | 2 | 5 | 50 | ; |
| 28 | 31 | 32 | 2 | 170 | 20 | ; |

| | | | | | | |
|-----|-----|-----|---|-----|----|---|
| 31 | 34 | 35 | 2 | 5 | 50 | ; |
| 34 | 37 | 38 | 2 | 170 | 20 | ; |
| 37 | 40 | 41 | 2 | 5 | 50 | ; |
| 40 | 43 | 44 | 2 | 170 | 20 | ; |
| 43 | 46 | 47 | 2 | 5 | 50 | ; |
| 46 | 49 | 50 | 2 | 170 | 20 | ; |
| 49 | 52 | 53 | 2 | 5 | 50 | ; |
| 52 | 55 | 56 | 2 | 170 | 20 | ; |
| 55 | 58 | 59 | 2 | 5 | 50 | ; |
| 58 | 61 | 62 | 2 | 170 | 20 | ; |
| 61 | 64 | 65 | 2 | 5 | 50 | ; |
| 64 | 67 | 68 | 2 | 170 | 20 | ; |
| 67 | 70 | 71 | 2 | 5 | 50 | ; |
| 70 | 73 | 74 | 2 | 170 | 20 | ; |
| 73 | 76 | 77 | 2 | 5 | 50 | ; |
| 76 | 79 | 80 | 2 | 170 | 20 | ; |
| 79 | 82 | 83 | 2 | 5 | 50 | ; |
| 82 | 85 | 86 | 2 | 170 | 20 | ; |
| 85 | 88 | 89 | 2 | 5 | 50 | ; |
| 88 | 91 | 92 | 2 | 170 | 20 | ; |
| 91 | 94 | 95 | 2 | 5 | 50 | ; |
| 94 | 97 | 98 | 2 | 170 | 20 | ; |
| 97 | 100 | 101 | 2 | 5 | 50 | ; |
| 100 | 103 | 104 | 2 | 170 | 20 | ; |
| 103 | 106 | 107 | 2 | 5 | 50 | ; |
| 106 | 109 | 110 | 2 | 170 | 20 | ; |
| 109 | 112 | 113 | 2 | 5 | 50 | ; |
| 112 | 115 | 116 | 2 | 170 | 20 | ; |
| 115 | 118 | 119 | 2 | 5 | 50 | ; |
| 118 | 121 | 122 | 2 | 170 | 20 | ; |
| 121 | 124 | 125 | 2 | 5 | 50 | ; |
| 124 | 127 | 128 | 2 | 170 | 20 | ; |
| 127 | 130 | 131 | 2 | 5 | 50 | ; |
| 130 | 133 | 134 | 2 | 170 | 20 | ; |
| 133 | 136 | 137 | 2 | 5 | 50 | ; |
| 136 | 139 | 140 | 2 | 170 | 20 | ; |
| 139 | 142 | 143 | 2 | 5 | 50 | ; |
| 142 | 145 | 146 | 2 | 170 | 20 | ; |
| 145 | 148 | 149 | 2 | 5 | 50 | ; |
| 148 | 151 | 152 | 2 | 170 | 20 | ; |
| 151 | 154 | 155 | 2 | 5 | 50 | ; |
| 154 | 157 | 158 | 2 | 170 | 20 | ; |
| 157 | 160 | 161 | 2 | 5 | 50 | ; |
| 160 | 163 | 164 | 2 | 170 | 20 | ; |
| 163 | 166 | 167 | 2 | 5 | 50 | ; |
| 166 | 169 | 170 | 2 | 170 | 20 | ; |
| 169 | 172 | 173 | 2 | 5 | 50 | ; |
| 172 | 175 | 176 | 2 | 170 | 20 | ; |
| 175 | 178 | 179 | 2 | 5 | 50 | ; |
| 178 | 181 | 182 | 2 | 170 | 20 | ; |
| 181 | 184 | 185 | 2 | 5 | 50 | ; |
| 184 | 187 | 188 | 2 | 170 | 20 | ; |
| 187 | 190 | 191 | 2 | 5 | 50 | ; |
| 190 | 193 | 194 | 2 | 170 | 20 | ; |

| | | | | | | |
|-----|-----|-----|---|-----|----|---|
| 193 | 196 | 197 | 2 | 5 | 50 | ; |
| 196 | 199 | 200 | 2 | 170 | 20 | ; |
| 199 | 202 | 203 | 2 | 5 | 50 | ; |
| 202 | 205 | 206 | 2 | 170 | 20 | ; |
| 205 | 208 | 209 | 2 | 5 | 50 | ; |
| 208 | 211 | 212 | 2 | 170 | 20 | ; |
| 211 | 214 | 215 | 2 | 5 | 50 | ; |
| 214 | 217 | 218 | 2 | 170 | 20 | ; |
| 217 | 220 | 221 | 2 | 5 | 50 | ; |
| 220 | 223 | 224 | 2 | 170 | 20 | ; |
| 223 | 226 | 227 | 2 | 5 | 50 | ; |
| 226 | 229 | 230 | 2 | 170 | 20 | ; |
| 229 | 232 | 233 | 2 | 5 | 50 | ; |
| 232 | 235 | 236 | 2 | 170 | 20 | ; |
| 235 | 238 | 239 | 2 | 5 | 50 | ; |
| 238 | 241 | 242 | 2 | 170 | 20 | ; |
| 241 | 244 | 245 | 2 | 5 | 50 | ; |
| 244 | 247 | 248 | 2 | 170 | 20 | ; |
| 247 | 250 | 251 | 2 | 5 | 50 | ; |
| 250 | 253 | 254 | 2 | 170 | 20 | ; |
| 253 | 256 | 257 | 2 | 5 | 50 | ; |
| 256 | 259 | 260 | 2 | 170 | 20 | ; |
| 259 | 262 | 263 | 2 | 5 | 50 | ; |
| 262 | 265 | 266 | 2 | 170 | 20 | ; |
| 265 | 268 | 269 | 2 | 5 | 50 | ; |
| 268 | 271 | 272 | 2 | 170 | 20 | ; |
| 271 | 274 | 275 | 2 | 5 | 50 | ; |
| 274 | 277 | 278 | 2 | 170 | 20 | ; |
| 277 | 280 | 281 | 2 | 5 | 50 | ; |
| 280 | 283 | 284 | 2 | 170 | 20 | ; |
| 283 | 286 | 287 | 2 | 5 | 50 | ; |
| 286 | 289 | 290 | 2 | 170 | 20 | ; |
| 289 | 292 | 293 | 2 | 5 | 50 | ; |
| 292 | 295 | 296 | 2 | 170 | 20 | ; |
| 295 | 298 | 299 | 2 | 5 | 50 | ; |
| 298 | 301 | 302 | 2 | 170 | 20 | ; |
| 301 | 304 | 305 | 2 | 5 | 50 | ; |
| 304 | 307 | 308 | 2 | 170 | 20 | ; |
| 307 | 310 | 311 | 2 | 5 | 50 | ; |

;backbone-backbone-backbone angles

| | | | | | | |
|----|----|----|---|-----|----|---|
| 1 | 4 | 7 | 1 | 100 | 30 | ; |
| 4 | 7 | 10 | 1 | 100 | 30 | ; |
| 7 | 10 | 13 | 1 | 100 | 30 | ; |
| 10 | 13 | 16 | 1 | 100 | 30 | ; |
| 13 | 16 | 19 | 1 | 100 | 30 | ; |
| 16 | 19 | 22 | 1 | 100 | 30 | ; |
| 19 | 22 | 25 | 1 | 100 | 30 | ; |
| 22 | 25 | 28 | 1 | 100 | 30 | ; |
| 25 | 28 | 31 | 1 | 100 | 30 | ; |
| 28 | 31 | 34 | 1 | 100 | 30 | ; |
| 31 | 34 | 37 | 1 | 100 | 30 | ; |
| 34 | 37 | 40 | 1 | 100 | 30 | ; |
| 37 | 40 | 43 | 1 | 100 | 30 | ; |
| 40 | 43 | 46 | 1 | 100 | 30 | ; |

| | | | | | | |
|-----|-----|-----|---|-----|----|---|
| 43 | 46 | 49 | 1 | 100 | 30 | ; |
| 46 | 49 | 52 | 1 | 100 | 30 | ; |
| 49 | 52 | 55 | 1 | 100 | 30 | ; |
| 52 | 55 | 58 | 1 | 100 | 30 | ; |
| 55 | 58 | 61 | 1 | 100 | 30 | ; |
| 58 | 61 | 64 | 1 | 100 | 30 | ; |
| 61 | 64 | 67 | 1 | 100 | 30 | ; |
| 64 | 67 | 70 | 1 | 100 | 30 | ; |
| 67 | 70 | 73 | 1 | 100 | 30 | ; |
| 70 | 73 | 76 | 1 | 100 | 30 | ; |
| 73 | 76 | 79 | 1 | 100 | 30 | ; |
| 76 | 79 | 82 | 1 | 100 | 30 | ; |
| 79 | 82 | 85 | 1 | 100 | 30 | ; |
| 82 | 85 | 88 | 1 | 100 | 30 | ; |
| 85 | 88 | 91 | 1 | 100 | 30 | ; |
| 88 | 91 | 94 | 1 | 100 | 30 | ; |
| 91 | 94 | 97 | 1 | 100 | 30 | ; |
| 94 | 97 | 100 | 1 | 100 | 30 | ; |
| 97 | 100 | 103 | 1 | 100 | 30 | ; |
| 100 | 103 | 106 | 1 | 100 | 30 | ; |
| 103 | 106 | 109 | 1 | 100 | 30 | ; |
| 106 | 109 | 112 | 1 | 100 | 30 | ; |
| 109 | 112 | 115 | 1 | 100 | 30 | ; |
| 112 | 115 | 118 | 1 | 100 | 30 | ; |
| 115 | 118 | 121 | 1 | 100 | 30 | ; |
| 118 | 121 | 124 | 1 | 100 | 30 | ; |
| 121 | 124 | 127 | 1 | 100 | 30 | ; |
| 124 | 127 | 130 | 1 | 100 | 30 | ; |
| 127 | 130 | 133 | 1 | 100 | 30 | ; |
| 130 | 133 | 136 | 1 | 100 | 30 | ; |
| 133 | 136 | 139 | 1 | 100 | 30 | ; |
| 136 | 139 | 142 | 1 | 100 | 30 | ; |
| 139 | 142 | 145 | 1 | 100 | 30 | ; |
| 142 | 145 | 148 | 1 | 100 | 30 | ; |
| 145 | 148 | 151 | 1 | 100 | 30 | ; |
| 148 | 151 | 154 | 1 | 100 | 30 | ; |
| 151 | 154 | 157 | 1 | 100 | 30 | ; |
| 154 | 157 | 160 | 1 | 100 | 30 | ; |
| 157 | 160 | 163 | 1 | 100 | 30 | ; |
| 160 | 163 | 166 | 1 | 100 | 30 | ; |
| 163 | 166 | 169 | 1 | 100 | 30 | ; |
| 166 | 169 | 172 | 1 | 100 | 30 | ; |
| 169 | 172 | 175 | 1 | 100 | 30 | ; |
| 172 | 175 | 178 | 1 | 100 | 30 | ; |
| 175 | 178 | 181 | 1 | 100 | 30 | ; |
| 178 | 181 | 184 | 1 | 100 | 30 | ; |
| 181 | 184 | 187 | 1 | 100 | 30 | ; |
| 184 | 187 | 190 | 1 | 100 | 30 | ; |
| 187 | 190 | 193 | 1 | 100 | 30 | ; |
| 190 | 193 | 196 | 1 | 100 | 30 | ; |
| 193 | 196 | 199 | 1 | 100 | 30 | ; |
| 196 | 199 | 202 | 1 | 100 | 30 | ; |
| 199 | 202 | 205 | 1 | 100 | 30 | ; |
| 202 | 205 | 208 | 1 | 100 | 30 | ; |

| | | | | | | |
|-----|-----|-----|---|-----|----|---|
| 205 | 208 | 211 | 1 | 100 | 30 | ; |
| 208 | 211 | 214 | 1 | 100 | 30 | ; |
| 211 | 214 | 217 | 1 | 100 | 30 | ; |
| 214 | 217 | 220 | 1 | 100 | 30 | ; |
| 217 | 220 | 223 | 1 | 100 | 30 | ; |
| 220 | 223 | 226 | 1 | 100 | 30 | ; |
| 223 | 226 | 229 | 1 | 100 | 30 | ; |
| 226 | 229 | 232 | 1 | 100 | 30 | ; |
| 229 | 232 | 235 | 1 | 100 | 30 | ; |
| 232 | 235 | 238 | 1 | 100 | 30 | ; |
| 235 | 238 | 241 | 1 | 100 | 30 | ; |
| 238 | 241 | 244 | 1 | 100 | 30 | ; |
| 241 | 244 | 247 | 1 | 100 | 30 | ; |
| 244 | 247 | 250 | 1 | 100 | 30 | ; |
| 247 | 250 | 253 | 1 | 100 | 30 | ; |
| 250 | 253 | 256 | 1 | 100 | 30 | ; |
| 253 | 256 | 259 | 1 | 100 | 30 | ; |
| 256 | 259 | 262 | 1 | 100 | 30 | ; |
| 259 | 262 | 265 | 1 | 100 | 30 | ; |
| 262 | 265 | 268 | 1 | 100 | 30 | ; |
| 265 | 268 | 271 | 1 | 100 | 30 | ; |
| 268 | 271 | 274 | 1 | 100 | 30 | ; |
| 271 | 274 | 277 | 1 | 100 | 30 | ; |
| 274 | 277 | 280 | 1 | 100 | 30 | ; |
| 277 | 280 | 283 | 1 | 100 | 30 | ; |
| 280 | 283 | 286 | 1 | 100 | 30 | ; |
| 283 | 286 | 289 | 1 | 100 | 30 | ; |
| 286 | 289 | 292 | 1 | 100 | 30 | ; |
| 289 | 292 | 295 | 1 | 100 | 30 | ; |
| 292 | 295 | 298 | 1 | 100 | 30 | ; |
| 295 | 298 | 301 | 1 | 100 | 30 | ; |
| 298 | 301 | 304 | 1 | 100 | 30 | ; |
| 301 | 304 | 307 | 1 | 100 | 30 | ; |
| 304 | 307 | 310 | 1 | 100 | 30 | ; |

[dihedrals]

;proper dihedrals angles

| | | | | | | | |
|----|----|----|----|---|----|-----|---|
| 1 | 4 | 7 | 10 | 1 | 80 | 1.5 | 1 |
| | ; | | | | | | |
| 4 | 7 | 10 | 13 | 1 | 80 | 1.5 | 1 |
| | ; | | | | | | |
| 7 | 10 | 13 | 16 | 1 | 80 | 1.5 | 1 |
| | ; | | | | | | |
| 10 | 13 | 16 | 19 | 1 | 80 | 1.5 | 1 |
| | ; | | | | | | |
| 13 | 16 | 19 | 22 | 1 | 80 | 1.5 | 1 |
| | ; | | | | | | |
| 16 | 19 | 22 | 25 | 1 | 80 | 1.5 | 1 |
| | ; | | | | | | |
| 19 | 22 | 25 | 28 | 1 | 80 | 1.5 | 1 |
| | ; | | | | | | |
| 22 | 25 | 28 | 31 | 1 | 80 | 1.5 | 1 |
| | ; | | | | | | |
| 25 | 28 | 31 | 34 | 1 | 80 | 1.5 | 1 |

| | | | | | | | | |
|-----|---|-----|-----|-----|---|----|-----|---|
| 28 | ; | 31 | 34 | 37 | 1 | 80 | 1.5 | 1 |
| 31 | ; | 34 | 37 | 40 | 1 | 80 | 1.5 | 1 |
| 34 | ; | 37 | 40 | 43 | 1 | 80 | 1.5 | 1 |
| 37 | ; | 40 | 43 | 46 | 1 | 80 | 1.5 | 1 |
| 40 | ; | 43 | 46 | 49 | 1 | 80 | 1.5 | 1 |
| 43 | ; | 46 | 49 | 52 | 1 | 80 | 1.5 | 1 |
| 46 | ; | 49 | 52 | 55 | 1 | 80 | 1.5 | 1 |
| 49 | ; | 52 | 55 | 58 | 1 | 80 | 1.5 | 1 |
| 52 | ; | 55 | 58 | 61 | 1 | 80 | 1.5 | 1 |
| 55 | ; | 58 | 61 | 64 | 1 | 80 | 1.5 | 1 |
| 58 | ; | 61 | 64 | 67 | 1 | 80 | 1.5 | 1 |
| 61 | ; | 64 | 67 | 70 | 1 | 80 | 1.5 | 1 |
| 64 | ; | 67 | 70 | 73 | 1 | 80 | 1.5 | 1 |
| 67 | ; | 70 | 73 | 76 | 1 | 80 | 1.5 | 1 |
| 70 | ; | 73 | 76 | 79 | 1 | 80 | 1.5 | 1 |
| 73 | ; | 76 | 79 | 82 | 1 | 80 | 1.5 | 1 |
| 76 | ; | 79 | 82 | 85 | 1 | 80 | 1.5 | 1 |
| 79 | ; | 82 | 85 | 88 | 1 | 80 | 1.5 | 1 |
| 82 | ; | 85 | 88 | 91 | 1 | 80 | 1.5 | 1 |
| 85 | ; | 88 | 91 | 94 | 1 | 80 | 1.5 | 1 |
| 88 | ; | 91 | 94 | 97 | 1 | 80 | 1.5 | 1 |
| 91 | ; | 94 | 97 | 100 | 1 | 80 | 1.5 | 1 |
| 94 | ; | 97 | 100 | 103 | 1 | 80 | 1.5 | 1 |
| 97 | ; | 100 | 103 | 106 | 1 | 80 | 1.5 | 1 |
| 100 | ; | 103 | 106 | 109 | 1 | 80 | 1.5 | 1 |
| 103 | ; | 106 | 109 | 112 | 1 | 80 | 1.5 | 1 |
| 106 | ; | 109 | 112 | 115 | 1 | 80 | 1.5 | 1 |

| | | | | | | | | |
|-----|---|-----|-----|-----|---|----|-----|---|
| 109 | ; | 112 | 115 | 118 | 1 | 80 | 1.5 | 1 |
| 112 | ; | 115 | 118 | 121 | 1 | 80 | 1.5 | 1 |
| 115 | ; | 118 | 121 | 124 | 1 | 80 | 1.5 | 1 |
| 118 | ; | 121 | 124 | 127 | 1 | 80 | 1.5 | 1 |
| 121 | ; | 124 | 127 | 130 | 1 | 80 | 1.5 | 1 |
| 124 | ; | 127 | 130 | 133 | 1 | 80 | 1.5 | 1 |
| 127 | ; | 130 | 133 | 136 | 1 | 80 | 1.5 | 1 |
| 130 | ; | 133 | 136 | 139 | 1 | 80 | 1.5 | 1 |
| 133 | ; | 136 | 139 | 142 | 1 | 80 | 1.5 | 1 |
| 136 | ; | 139 | 142 | 145 | 1 | 80 | 1.5 | 1 |
| 139 | ; | 142 | 145 | 148 | 1 | 80 | 1.5 | 1 |
| 142 | ; | 145 | 148 | 151 | 1 | 80 | 1.5 | 1 |
| 145 | ; | 148 | 151 | 154 | 1 | 80 | 1.5 | 1 |
| 148 | ; | 151 | 154 | 157 | 1 | 80 | 1.5 | 1 |
| 151 | ; | 154 | 157 | 160 | 1 | 80 | 1.5 | 1 |
| 154 | ; | 157 | 160 | 163 | 1 | 80 | 1.5 | 1 |
| 157 | ; | 160 | 163 | 166 | 1 | 80 | 1.5 | 1 |
| 160 | ; | 163 | 166 | 169 | 1 | 80 | 1.5 | 1 |
| 163 | ; | 166 | 169 | 172 | 1 | 80 | 1.5 | 1 |
| 166 | ; | 169 | 172 | 175 | 1 | 80 | 1.5 | 1 |
| 169 | ; | 172 | 175 | 178 | 1 | 80 | 1.5 | 1 |
| 172 | ; | 175 | 178 | 181 | 1 | 80 | 1.5 | 1 |
| 175 | ; | 178 | 181 | 184 | 1 | 80 | 1.5 | 1 |
| 178 | ; | 181 | 184 | 187 | 1 | 80 | 1.5 | 1 |
| 181 | ; | 184 | 187 | 190 | 1 | 80 | 1.5 | 1 |
| 184 | ; | 187 | 190 | 193 | 1 | 80 | 1.5 | 1 |
| 187 | ; | 190 | 193 | 196 | 1 | 80 | 1.5 | 1 |

| | | | | | | | | |
|-----|---|-----|-----|-----|---|----|-----|---|
| 190 | ; | 193 | 196 | 199 | 1 | 80 | 1.5 | 1 |
| 193 | ; | 196 | 199 | 202 | 1 | 80 | 1.5 | 1 |
| 196 | ; | 199 | 202 | 205 | 1 | 80 | 1.5 | 1 |
| 199 | ; | 202 | 205 | 208 | 1 | 80 | 1.5 | 1 |
| 202 | ; | 205 | 208 | 211 | 1 | 80 | 1.5 | 1 |
| 205 | ; | 208 | 211 | 214 | 1 | 80 | 1.5 | 1 |
| 208 | ; | 211 | 214 | 217 | 1 | 80 | 1.5 | 1 |
| 211 | ; | 214 | 217 | 220 | 1 | 80 | 1.5 | 1 |
| 214 | ; | 217 | 220 | 223 | 1 | 80 | 1.5 | 1 |
| 217 | ; | 220 | 223 | 226 | 1 | 80 | 1.5 | 1 |
| 220 | ; | 223 | 226 | 229 | 1 | 80 | 1.5 | 1 |
| 223 | ; | 226 | 229 | 232 | 1 | 80 | 1.5 | 1 |
| 226 | ; | 229 | 232 | 235 | 1 | 80 | 1.5 | 1 |
| 229 | ; | 232 | 235 | 238 | 1 | 80 | 1.5 | 1 |
| 232 | ; | 235 | 238 | 241 | 1 | 80 | 1.5 | 1 |
| 235 | ; | 238 | 241 | 244 | 1 | 80 | 1.5 | 1 |
| 238 | ; | 241 | 244 | 247 | 1 | 80 | 1.5 | 1 |
| 241 | ; | 244 | 247 | 250 | 1 | 80 | 1.5 | 1 |
| 244 | ; | 247 | 250 | 253 | 1 | 80 | 1.5 | 1 |
| 247 | ; | 250 | 253 | 256 | 1 | 80 | 1.5 | 1 |
| 250 | ; | 253 | 256 | 259 | 1 | 80 | 1.5 | 1 |
| 253 | ; | 256 | 259 | 262 | 1 | 80 | 1.5 | 1 |
| 256 | ; | 259 | 262 | 265 | 1 | 80 | 1.5 | 1 |
| 259 | ; | 262 | 265 | 268 | 1 | 80 | 1.5 | 1 |
| 262 | ; | 265 | 268 | 271 | 1 | 80 | 1.5 | 1 |
| 265 | ; | 268 | 271 | 274 | 1 | 80 | 1.5 | 1 |
| 268 | ; | 271 | 274 | 277 | 1 | 80 | 1.5 | 1 |

```
271      ;      274      277      280      1      80      1.5      1
274      ;      277      280      283      1      80      1.5      1
277      ;      280      283      286      1      80      1.5      1
280      ;      283      286      289      1      80      1.5      1
283      ;      286      289      292      1      80      1.5      1
286      ;      289      292      295      1      80      1.5      1
289      ;      292      295      298      1      80      1.5      1
292      ;      295      298      301      1      80      1.5      1
295      ;      298      301      304      1      80      1.5      1
298      ;      301      304      307      1      80      1.5      1
301      ;      304      307      310      1      80      1.5      1
      ;
```

```
ifdef POSRES
#include "./posre-pmal.itp"
endif
```