

Distorted geometry

2958850

Main-chain bond lengths

C 1.231 O 0.185 1.046 A Met 1	CA 1.530 CB 0.077 1.453 A Met 1	N 1.458 CA 0.059 1.399 A Met 1	C 1.231 O 0.073 1.158 A Pro 2	N 1.458 CA 0.119 1.577 A Leu 3	C 1.329 N 0.057 1.272 A Leu 3 - A Leu 4
C 1.231 O 0.102 1.129 A Leu 4	CA 1.530 CB 0.120 1.650 A Asp 5	N 1.458 CA 0.149 1.607 A Asp 5	CA 1.525 C 0.080 1.445 A Ser 6	CA 1.530 CB 0.082 1.448 A Ser 6	C 1.329 N 0.063 1.266 A Ser 6 - A Phe 7
C 1.231 O 0.066 1.297 A Val 9	N 1.458 CA 0.059 1.399 A Val 9	N 1.458 CA 0.053 1.405 A Asp 10	C 1.231 O 0.061 1.170 A His 11	CA 1.525 C 0.055 1.580 A Met 14	CA 1.530 CB 0.066 1.464 A Met 14
CA 1.525 C 0.066 1.591 A Ala 15	CA 1.525 C 0.069 1.594 A Ala 16	C 1.341 N 0.126 1.467 A Ala 16 - A Pro 17	C 1.231 O 0.065 1.296 A Ala 18	CA 1.525 C 0.052 1.577 A Ala 18	C 1.329 N 0.074 1.403 A Ala 18 - A Val 19
CA 1.525 C 0.079 1.446 A Val 21	C 1.329 N 0.065 1.264 A Val 21 - A Ala 22	CA 1.521 CB 0.063 1.584 A Ala 22	N 1.458 CA 0.069 1.389 A Ala 22	C 1.329 N 0.119 1.210 A Ala 22 - A Lys 23	CA 1.525 C 0.181 1.706 A Lys 23
CA 1.530 CB 0.051 1.581 A Lys 23	C 1.329 N 0.061 1.268 A Thr 24 - A Met 25	CA 1.525 C 0.080 1.605 A Met 25	C 1.341 N 0.057 1.398 A Thr 27 - A Pro 28	C 1.329 N 0.057 1.386 A Pro 28 - A Asn 29	CA 1.525 C 0.064 1.461 A Asn 29
N 1.458 CA 0.057 1.515 A Asp 31	C 1.329 N 0.053 1.382 A Asp 31 - A Thr 32	C 1.231 O 0.069 1.300 A Thr 32	C 1.329 N 0.051 1.380 A Thr 32 - A Ile 33	CA 1.540 CB 0.054 1.594 A Thr 34	C 1.329 N 0.117 1.446 A Thr 34 - A Val 35
C 1.329 N 0.092 1.237 A Val 35 - A Phe 36	C 1.231 O 0.094 1.324 A Phe 36	N 1.458 CA 0.059 1.399 A Phe 36	N 1.458 CA 0.085 1.373 A Asp 37	C 1.231 O 0.051 1.282 A Leu 38	CA 1.530 CB 0.055 1.585 A Leu 38
N 1.458 CA 0.058 1.400 A Leu 38	CA 1.525 C 0.056 1.469 A Arg 39	CA 1.525 C 0.050 1.575 A Phe 40	N 1.458 CA 0.071 1.529 A Phe 40	C 1.231 O 0.051 1.282 A Cys 41	C 1.329 N 0.065 1.394 A Cys 41 - A Val 42
C 1.231 O 0.053 1.284 A Val 42	CA 1.525 C 0.073 1.452 A Pro 43	N 1.466 CA 0.054 1.412 A Pro 43	N 1.458 CA 0.053 1.405 A Ser 49	C 1.329 N 0.064 1.265 A Ser 49 - A Glu 50	C 1.231 O 0.073 1.304 A Glu 50
CA 1.530 CB 0.062 1.592 A Glu 50	C 1.231 O 0.087 1.318 A Arg 51	C 1.329 N 0.061 1.390 A Arg 51 - A Gly 52	CA 1.516 C 0.052 1.464 A Gly 52	CA 1.540 CB 0.065 1.605 A Ile 53	CA 1.530 CB 0.072 1.602 A His 54

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Main-chain bond lengths (contd)

CA 1.540 CB 0.063 1.477 A Thr 55	C 1.329 N 0.077 1.252 A Thr 55 - A Leu 56	C 1.231 O 0.083 1.148 A Leu 56	CA 1.525 C 0.050 1.475 A Leu 56	N 1.458 CA 0.054 1.404 A Leu 56	CA 1.525 C 0.086 1.439 A Glu 57
CA 1.530 CB 0.066 1.596 A Glu 57	C 1.329 N 0.071 1.400 A Glu 57 - A His 58	CA 1.525 C 0.060 1.465 A His 58	CA 1.530 CB 0.066 1.596 A His 58	C 1.329 N 0.071 1.258 A His 58 - A Leu 59	CA 1.525 C 0.053 1.577 A Leu 59
C 1.329 N 0.057 1.272 A Leu 59 - A Phe 60	CA 1.525 C 0.059 1.465 A Phe 60	N 1.458 CA 0.070 1.388 A Phe 60	C 1.329 N 0.057 1.272 A Phe 63 - A Met 64	N 1.458 CA 0.090 1.368 A Met 64	CA 1.525 C 0.079 1.604 A Leu 68
CA 1.525 C 0.064 1.589 A Asn 69	N 1.458 CA 0.052 1.510 A Asn 69	CA 1.525 C 0.088 1.437 A Glu 74	CA 1.525 C 0.064 1.461 A Ile 75	CA 1.540 CB 0.051 1.591 A Ile 75	C 1.329 N 0.075 1.254 A Ile 75 - A Ile 76
CA 1.525 C 0.140 1.665 A Ile 76	CA 1.540 CB 0.068 1.608 A Ile 76	N 1.458 CA 0.051 1.407 A Ile 76	C 1.329 N 0.135 1.194 A Ile 76 - A Asp 77	CA 1.525 C 0.091 1.616 A Asp 77	C 1.329 N 0.095 1.234 A Asp 77 - A Ile 78
C 1.231 O 0.053 1.283 A Ile 78	CA 1.525 C 0.069 1.594 A Ile 78	C 1.329 N 0.076 1.405 A Ile 78 - A Ser 79	N 1.458 CA 0.055 1.513 A Ser 79	CA 1.525 C 0.146 1.379 A Pro 80	C 1.329 N 0.052 1.277 A Pro 80 - A Met 81
N 1.451 CA 0.064 1.515 A Gly 82	C 1.329 N 0.056 1.385 A Cys 83 - A Arg 84	CA 1.525 C 0.080 1.605 A Arg 84	C 1.231 O 0.060 1.291 A Thr 85	C 1.329 N 0.050 1.379 A Thr 85 - A Gly 86	C 1.231 O 0.059 1.290 A Phe 87
N 1.458 CA 0.079 1.536 A Phe 87	CA 1.525 C 0.081 1.444 A Tyr 88	CA 1.530 CB 0.063 1.593 A Tyr 88	C 1.329 N 0.059 1.270 A Tyr 88 - A Met 89	C 1.231 O 0.088 1.143 A Met 89	CA 1.525 C 0.081 1.444 A Met 89
C 1.329 N 0.102 1.431 A Met 89 - A Ser 90	N 1.458 CA 0.088 1.370 A Ser 90	C 1.329 N 0.075 1.254 A Ser 90 - A Leu 91	CA 1.525 C 0.067 1.458 A Leu 91	N 1.458 CA 0.062 1.395 A Ile 92	C 1.329 N 0.067 1.396 A Ile 92 - A Gly 93
C 1.231 O 0.082 1.149 A Gly 93	N 1.458 CA 0.055 1.403 A Ala 94	C 1.341 N 0.051 1.290 A Ala 94 - A Pro 95	CA 1.525 C 0.053 1.472 A Pro 95	N 1.466 CA 0.063 1.403 A Pro 95	CA 1.525 C 0.057 1.582 A Asp 96
CA 1.530 CB 0.050 1.480 A Asp 96	C 1.329 N 0.050 1.279 A Arg 99 - A Val 100	C 1.329 N 0.050 1.279 A Ala 103 - A Trp 104	C 1.329 N 0.077 1.406 A Trp 104 - A Gln 105	CA 1.525 C 0.057 1.468 A Gln 105	CA 1.540 CB 0.065 1.605 A Val 114

Distorted geometry

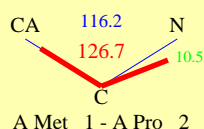
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Main-chain bond lengths (contd)

N 1.458 CA 0.059 1.517 A Val 114	CA 1.525 C 0.061 1.586 A Gln 115	C 1.231 O 0.051 1.282 A Glu 116	N 1.458 CA 0.086 1.544 A Glu 116	CA 1.525 C 0.075 1.450 A Ile 120	CA 1.540 CB 0.051 1.591 A Ile 120
N 1.458 CA 0.067 1.391 A Ile 120	C 1.231 O 0.054 1.176 A Pro 121	CA 1.525 C 0.066 1.591 A Glu 122	N 1.458 CA 0.066 1.523 A Glu 122	N 1.458 CA 0.065 1.523 A Glu 125	C 1.329 N 0.058 1.271 A Glu 125 - A Tyr 126
CA 1.525 C 0.091 1.616 A Cys 128	N 1.451 CA 0.064 1.515 A Gly 129	CA 1.525 C 0.083 1.608 A Thr 130	N 1.458 CA 0.091 1.367 A Met 133	CA 1.525 C 0.055 1.470 A Ser 135	CA 1.530 CB 0.108 1.422 A Ser 135
CA 1.525 C 0.061 1.464 A Ala 141	CA 1.525 C 0.082 1.442 A Arg 144	CA 1.530 CB 0.094 1.624 A His 145	CA 1.525 C 0.058 1.467 A Val 146	CA 1.540 CB 0.080 1.460 A Val 146	N 1.458 CA 0.055 1.403 A Leu 147
C 1.329 N 0.055 1.274 A Leu 147 - A Glu 148	N 1.451 CA 0.083 1.368 A Gly 150	C 1.329 N 0.052 1.277 A Val 153 - A Asn 154	C 1.231 O 0.059 1.172 A Asn 156	C 1.341 N 0.051 1.392 A Leu 161 - A Pro 162	C 1.329 N 0.055 1.274 A Pro 162 - A Glu 163
CA 1.530 CB 0.061 1.590 A Glu 164	C 1.329 N 0.051 1.278 A Glu 164 - A Lys 165	CA 1.530 CB 0.134 1.396 A Lys 165	N 1.458 CA 0.076 1.382 A Lys 165	CA 1.530 CB 0.079 1.451 A Lys 167	CA 1.525 C 0.056 1.581 A Ser 168
CA 1.525 C 0.051 1.576 A Leu 169					

Bonds differing by > 0.05Å from small-molecule values. Values shown: "ideal", difference, actual

Main-chain bond angles

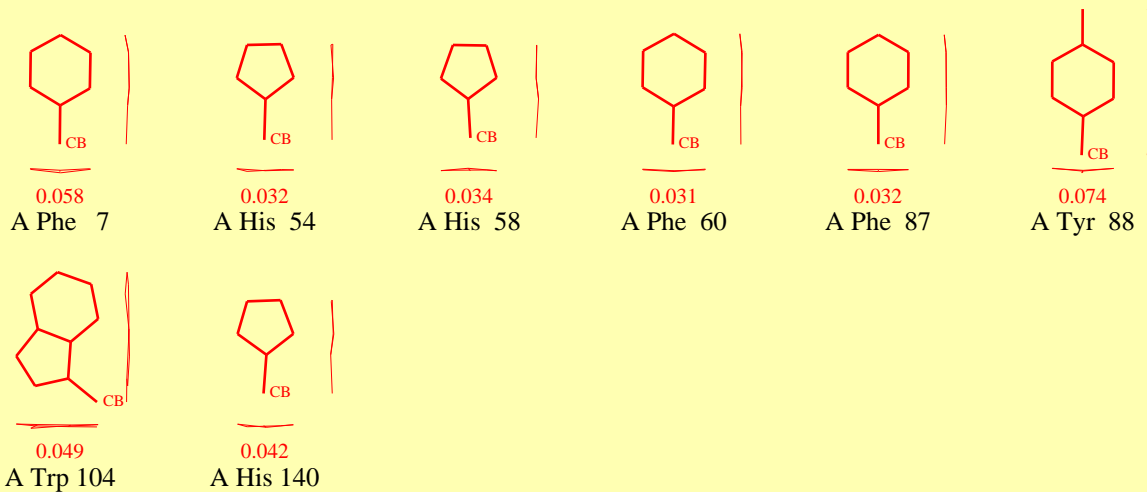


Bond angles differing by > 10.0 degrees from small-molec values. Values shown: "ideal", actual, diff.

Distorted geometry

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Planar groups



Sidechains with RMS dist. from planarity > 0.03A for rings, or > 0.02A otherwise. Value shown is RMS dist.