

```
#####  
##          ##  
## Force Field Definition ##  
##          ##  
#####
```

forcefield AMOEBA-NA-2017

|                 |               |
|-----------------|---------------|
| bond-cubic      | -2.55         |
| bond-quartic    | 3.793125      |
| angle-cubic     | -0.014        |
| angle-quartic   | 0.000056      |
| angle-pentic    | -0.0000007    |
| angle-sextic    | 0.000000022   |
| opbendtype      | ALLINGER      |
| opbend-cubic    | -0.014        |
| opbend-quartic  | 0.000056      |
| opbend-pentic   | -0.0000007    |
| opbend-sextic   | 0.000000022   |
| torsionunit     | 0.5           |
| vdwtype         | BUFFERED-14-7 |
| radiusrule      | CUBIC-MEAN    |
| radiustype      | R-MIN         |
| radiussize      | DIAMETER      |
| epsilonrule     | HHG           |
| dielectric      | 1.0           |
| polarization    | MUTUAL        |
| vdw-12-scale    | 0.0           |
| vdw-13-scale    | 0.0           |
| vdw-14-scale    | 1.0           |
| vdw-15-scale    | 1.0           |
| mpole-12-scale  | 0.0           |
| mpole-13-scale  | 0.0           |
| mpole-14-scale  | 0.4           |
| mpole-15-scale  | 0.8           |
| polar-12-scale  | 0.0           |
| polar-13-scale  | 0.0           |
| polar-14-scale  | 1.0           |
| polar-15-scale  | 1.0           |
| polar-14-intra  | 0.5           |
| direct-11-scale | 0.0           |
| direct-12-scale | 1.0           |
| direct-13-scale | 1.0           |
| direct-14-scale | 1.0           |

mutual-11-scale 1.0  
 mutual-12-scale 1.0  
 mutual-13-scale 1.0  
 mutual-14-scale 1.0

|      |    |    |     |                   |   |    |        |   |
|------|----|----|-----|-------------------|---|----|--------|---|
| atom | 1  | 7  | O   | "Ribose O4'       | " | 8  | 15.999 | 2 |
| atom | 2  | 11 | C   | "Ribose C4'       | " | 6  | 12.011 | 4 |
| atom | 3  | 4  | H   | "Ribose H4'       | " | 1  | 1.008  | 1 |
| atom | 4  | 1  | C   | "Ribose C1'       | " | 6  | 12.011 | 4 |
| atom | 5  | 4  | H   | "Ribose H1'       | " | 1  | 1.008  | 1 |
| atom | 6  | 1  | C   | "Ribose C2'       | " | 6  | 12.011 | 4 |
| atom | 7  | 4  | H   | "Ribose H2'1      | " | 1  | 1.008  | 1 |
| atom | 8  | 1  | C   | "Ribose C3'       | " | 6  | 12.011 | 4 |
| atom | 9  | 4  | H   | "Ribose H3'       | " | 1  | 1.008  | 1 |
| atom | 10 | 10 | O   | "Ribose O2'       | " | 8  | 15.999 | 2 |
| atom | 11 | 6  | H   | "Ribose HO'2      | " | 1  | 1.008  | 1 |
| atom | 12 | 8  | O   | "Ribose O3'       | " | 8  | 15.999 | 2 |
| atom | 13 | 6  | H   | "Ribose HO'3      | " | 1  | 1.008  | 1 |
| atom | 16 | 2  | C   | "Ribose C5'       | " | 6  | 12.011 | 4 |
| atom | 17 | 5  | H   | "Ribose H5'       | " | 1  | 1.008  | 1 |
| atom | 19 | 9  | O   | "Ribose O5'       | " | 8  | 15.999 | 2 |
| atom | 20 | 6  | H   | "Ribose HO'5      | " | 1  | 1.008  | 1 |
| atom | 23 | 18 | O   | "Ribose O3'       | " | 8  | 15.999 | 2 |
| atom | 24 | 19 | O   | "Ribose O5'       | " | 8  | 15.999 | 2 |
| atom | 51 | 60 | C   | "deoxyribose C4'  | " | 6  | 12.011 | 4 |
| atom | 52 | 51 | C   | "deoxyribose C3'  | " | 6  | 12.011 | 4 |
| atom | 53 | 51 | C   | "deoxyribose C2'  | " | 6  | 12.011 | 4 |
| atom | 54 | 51 | C   | "deoxyribose C1'  | " | 6  | 12.011 | 4 |
| atom | 55 | 57 | O   | "deoxyribose O4'  | " | 8  | 15.999 | 2 |
| atom | 56 | 54 | H   | "deoxyribose H2'1 | " | 1  | 1.008  | 1 |
| atom | 58 | 54 | H   | "deoxyribose H1'  | " | 1  | 1.008  | 1 |
| atom | 60 | 54 | H   | "deoxyribose H3'  | " | 1  | 1.008  | 1 |
| atom | 61 | 54 | H   | "deoxyribose H4'  | " | 1  | 1.008  | 1 |
| atom | 63 | 52 | C   | "deoxyribose C5'  | " | 6  | 12.011 | 4 |
| atom | 64 | 59 | O   | "deoxyribose O3'  | " | 8  | 15.999 | 2 |
| atom | 65 | 56 | H   | "deoxyribose HO'3 | " | 1  | 1.008  | 1 |
| atom | 66 | 55 | H   | "deoxyribose H5'1 | " | 1  | 1.008  | 1 |
| atom | 68 | 58 | O   | "deoxyribose O5'  | " | 8  | 15.999 | 2 |
| atom | 69 | 56 | H   | "deoxyribose HO'5 | " | 1  | 1.008  | 1 |
| atom | 73 | 69 | O   | "deoxyribose O3'  | " | 8  | 15.999 | 2 |
| atom | 74 | 68 | O   | "deoxyribose O5'  | " | 8  | 15.999 | 2 |
| atom | 36 | 34 | O   | "AMOEBA Water O   | " | 8  | 15.999 | 2 |
| atom | 37 | 35 | H   | "AMOEBA Water H   | " | 1  | 1.008  | 1 |
| atom | 41 | 41 | Na+ | "Sodium Ion Na+   | " | 11 | 22.990 | 0 |

|      |     |     |     |                          |   |    |        |   |
|------|-----|-----|-----|--------------------------|---|----|--------|---|
| atom | 42  | 42  | K+  | "Potassium Ion K+        | " | 19 | 39.098 | 0 |
| atom | 43  | 43  | Mg+ | "Magnesium Ion Mg+2      | " | 12 | 24.305 | 0 |
| atom | 44  | 44  | Cl- | "Chloride Ion Cl-        | " | 17 | 35.453 | 0 |
| atom | 101 | 101 | P   | "R-Phosphodiester P      | " | 15 | 30.974 | 4 |
| atom | 102 | 102 | O   | "R-Phosphodiester OP     | " | 8  | 15.999 | 1 |
| atom | 201 | 219 | C   | "Guanine C2              | " | 6  | 12.011 | 3 |
| atom | 202 | 206 | C   | "Guanine C6              | " | 6  | 12.011 | 3 |
| atom | 203 | 207 | C   | "Guanine C4              | " | 6  | 12.011 | 3 |
| atom | 204 | 205 | C   | "Guanine C8              | " | 6  | 12.011 | 3 |
| atom | 205 | 209 | N   | "Guanine N1              | " | 7  | 14.007 | 3 |
| atom | 206 | 208 | N   | "Guanine N2              | " | 7  | 14.007 | 3 |
| atom | 207 | 207 | C   | "Guanine C5              | " | 6  | 12.011 | 3 |
| atom | 208 | 210 | N   | "Guanine Ribose N9       | " | 7  | 14.007 | 3 |
| atom | 228 | 210 | N   | "Guanine Deoxyribose N9  | " | 7  | 14.007 | 3 |
| atom | 209 | 212 | N   | "Guanine N7              | " | 7  | 14.007 | 2 |
| atom | 210 | 211 | N   | "Guanine N3              | " | 7  | 14.007 | 2 |
| atom | 211 | 218 | H   | "Guanine H1              | " | 1  | 1.008  | 1 |
| atom | 214 | 213 | O   | "Guanine O6              | " | 8  | 15.999 | 1 |
| atom | 215 | 216 | H   | "Guanine H8              | " | 1  | 1.008  | 1 |
| atom | 216 | 217 | H   | "Guanine H21             | " | 1  | 1.008  | 1 |
| atom | 301 | 209 | N   | "Cytosine Ribose N1      | " | 7  | 14.007 | 3 |
| atom | 321 | 209 | N   | "Cytosine Deoxyribose N1 | " | 7  | 14.007 | 3 |
| atom | 302 | 202 | C   | "Cytosine C5             | " | 6  | 12.011 | 3 |
| atom | 303 | 208 | N   | "Cytosine N4             | " | 7  | 14.007 | 3 |
| atom | 304 | 204 | C   | "Cytosine C6             | " | 6  | 12.011 | 3 |
| atom | 305 | 206 | C   | "Cytosine C2             | " | 6  | 12.011 | 3 |
| atom | 306 | 220 | C   | "Cytosine C4             | " | 6  | 12.011 | 3 |
| atom | 307 | 211 | N   | "Cytosine N3             | " | 7  | 14.007 | 2 |
| atom | 308 | 215 | H   | "Cytosine H5             | " | 1  | 1.008  | 1 |
| atom | 309 | 213 | O   | "Cytosine O2             | " | 8  | 15.999 | 1 |
| atom | 312 | 216 | H   | "Cytosine H6             | " | 1  | 1.008  | 1 |
| atom | 313 | 217 | H   | "Cytosine H41            | " | 1  | 1.008  | 1 |
| atom | 401 | 207 | C   | "Adenine C4              | " | 6  | 12.011 | 3 |
| atom | 402 | 205 | C   | "Adenine C8              | " | 6  | 12.011 | 3 |
| atom | 403 | 220 | C   | "Adenine C6              | " | 6  | 12.011 | 3 |
| atom | 404 | 207 | C   | "Adenine C5              | " | 6  | 12.011 | 3 |
| atom | 405 | 310 | N   | "Adenine Ribose N9       | " | 7  | 14.007 | 3 |
| atom | 425 | 310 | N   | "Adenine Deoxyribose N9  | " | 7  | 14.007 | 3 |
| atom | 406 | 208 | N   | "Adenine N6              | " | 7  | 14.007 | 3 |
| atom | 407 | 204 | C   | "Adenine C2              | " | 6  | 12.011 | 3 |
| atom | 408 | 212 | N   | "Adenine N7              | " | 7  | 14.007 | 2 |
| atom | 409 | 211 | N   | "Adenine N3              | " | 7  | 14.007 | 2 |
| atom | 410 | 211 | N   | "Adenine N1              | " | 7  | 14.007 | 2 |
| atom | 413 | 216 | H   | "Adenine H8              | " | 1  | 1.008  | 1 |

|      |     |     |   |          |     |   |   |        |   |
|------|-----|-----|---|----------|-----|---|---|--------|---|
| atom | 414 | 221 | H | "Adenine | H2  | " | 1 | 1.008  | 1 |
| atom | 415 | 217 | H | "Adenine | H61 | " | 1 | 1.008  | 1 |
| atom | 501 | 206 | C | "Uracil  | C2  | " | 6 | 12.011 | 3 |
| atom | 502 | 204 | C | "Uracil  | C6  | " | 6 | 12.011 | 3 |
| atom | 503 | 206 | C | "Uracil  | C4  | " | 6 | 12.011 | 3 |
| atom | 504 | 209 | N | "Uracil  | N3  | " | 7 | 14.007 | 3 |
| atom | 505 | 309 | N | "Uracil  | N1  | " | 7 | 14.007 | 3 |
| atom | 506 | 204 | C | "Uracil  | C5  | " | 6 | 12.011 | 3 |
| atom | 508 | 218 | H | "Uracil  | H3  | " | 1 | 1.008  | 1 |
| atom | 509 | 221 | H | "Uracil  | H5  | " | 1 | 1.008  | 1 |
| atom | 510 | 213 | O | "Uracil  | O2  | " | 8 | 15.999 | 1 |
| atom | 511 | 213 | O | "Uracil  | O4  | " | 8 | 15.999 | 1 |
| atom | 512 | 216 | H | "Uracil  | H6  | " | 1 | 1.008  | 1 |
| atom | 601 | 201 | C | "Thymine | C7  | " | 6 | 12.011 | 4 |
| atom | 602 | 204 | C | "Thymine | C5  | " | 6 | 12.011 | 3 |
| atom | 603 | 206 | C | "Thymine | C4  | " | 6 | 12.011 | 3 |
| atom | 604 | 204 | C | "Thymine | C6  | " | 6 | 12.011 | 3 |
| atom | 605 | 309 | N | "Thymine | N1  | " | 7 | 14.007 | 3 |
| atom | 606 | 209 | N | "Thymine | N3  | " | 7 | 14.007 | 3 |
| atom | 607 | 206 | C | "Thymine | C2  | " | 6 | 12.011 | 3 |
| atom | 608 | 214 | H | "Thymine | H7  | " | 1 | 1.008  | 1 |
| atom | 609 | 213 | O | "Thymine | O2  | " | 8 | 15.999 | 1 |
| atom | 610 | 216 | H | "Thymine | H6  | " | 1 | 1.008  | 1 |
| atom | 611 | 213 | O | "Thymine | O4  | " | 8 | 15.999 | 1 |
| atom | 612 | 218 | H | "Thymine | H3  | " | 1 | 1.008  | 1 |

|     |    |        |        |       |
|-----|----|--------|--------|-------|
| vdw | 1  | 3.8200 | 0.1010 |       |
| vdw | 2  | 3.8200 | 0.1010 |       |
| vdw | 4  | 2.8900 | 0.0240 | 0.920 |
| vdw | 5  | 2.9400 | 0.0240 | 0.920 |
| vdw | 6  | 2.6550 | 0.0135 | 0.910 |
| vdw | 7  | 3.4050 | 0.1120 |       |
| vdw | 8  | 3.4500 | 0.1080 |       |
| vdw | 9  | 3.4500 | 0.1080 |       |
| vdw | 10 | 3.4050 | 0.1120 |       |
| vdw | 11 | 3.8200 | 0.1010 |       |
| vdw | 18 | 3.4050 | 0.1120 |       |
| vdw | 19 | 3.4050 | 0.1120 |       |
| vdw | 34 | 3.4050 | 0.1100 |       |
| vdw | 35 | 2.6550 | 0.0135 | 0.910 |
| vdw | 41 | 3.0200 | 0.2600 |       |
| vdw | 42 | 3.7100 | 0.3500 |       |
| vdw | 43 | 2.9400 | 0.3000 |       |
| vdw | 44 | 4.1300 | 0.3400 |       |

|       |        |        |        |       |
|-------|--------|--------|--------|-------|
| vdw   | 51     | 3.8200 | 0.1010 |       |
| vdw   | 52     | 3.8200 | 0.1010 |       |
| vdw   | 54     | 2.8900 | 0.0240 | 0.920 |
| vdw   | 55     | 2.9400 | 0.0240 | 0.920 |
| vdw   | 56     | 2.6550 | 0.0135 | 0.910 |
| vdw   | 57     | 3.4050 | 0.1120 |       |
| vdw   | 58     | 3.4500 | 0.1080 |       |
| vdw   | 59     | 3.4500 | 0.1080 |       |
| vdw   | 60     | 3.8200 | 0.1010 |       |
| vdw   | 68     | 3.4050 | 0.1120 |       |
| vdw   | 69     | 3.4050 | 0.1120 |       |
| vdw   | 101    | 4.450  | 0.3000 |       |
| vdw   | 102    | 3.400  | 0.1100 |       |
| vdw   | 201    | 3.800  | 0.1010 |       |
| vdw   | 202    | 3.790  | 0.1060 |       |
| vdw   | 204    | 3.740  | 0.1060 |       |
| vdw   | 205    | 3.740  | 0.1060 |       |
| vdw   | 206    | 3.720  | 0.0950 |       |
| vdw   | 207    | 3.720  | 0.1120 |       |
| vdw   | 208    | 3.600  | 0.1240 |       |
| vdw   | 209    | 3.700  | 0.1270 |       |
| vdw   | 210    | 3.700  | 0.1270 |       |
| vdw   | 211    | 3.640  | 0.1270 |       |
| vdw   | 212    | 3.640  | 0.1270 |       |
| vdw   | 213    | 3.350  | 0.1290 |       |
| vdw   | 214    | 2.900  | 0.0250 | 0.91  |
| vdw   | 215    | 3.050  | 0.0290 | 0.91  |
| vdw   | 216    | 2.950  | 0.0290 | 0.92  |
| vdw   | 221    | 3.080  | 0.0290 | 0.92  |
| vdw   | 217    | 2.650  | 0.0200 | 0.88  |
| vdw   | 218    | 2.650  | 0.0200 | 0.89  |
| vdw   | 219    | 3.720  | 0.1060 |       |
| vdw   | 220    | 3.720  | 0.1060 |       |
| vdw   | 309    | 3.700  | 0.1270 |       |
| vdw   | 310    | 3.700  | 0.1270 |       |
| vdwpr | 41 211 | 3.387  | 0.240  |       |
| vdwpr | 41 212 | 3.387  | 0.240  |       |
| vdwpr | 42 211 | 3.676  | 0.290  |       |
| vdwpr | 42 212 | 3.676  | 0.290  |       |
| vdwpr | 43 211 | 3.364  | 0.215  |       |
| vdwpr | 43 212 | 3.364  | 0.215  |       |
| vdwpr | 43 213 | 3.172  | 0.182  |       |

#

# Results of Valence Parameter Fitting

#

|      |     |     |        |        |
|------|-----|-----|--------|--------|
| bond | 34  | 35  | 556.85 | 0.9572 |
| bond | 1   | 1   | 320.00 | 1.5100 |
| bond | 11  | 1   | 320.00 | 1.5100 |
| bond | 7   | 11  | 384.00 | 1.4320 |
| bond | 11  | 2   | 380.00 | 1.5020 |
| bond | 1   | 8   | 384.00 | 1.4100 |
| bond | 2   | 9   | 484.00 | 1.4100 |
| bond | 1   | 18  | 384.00 | 1.4100 |
| bond | 2   | 19  | 484.00 | 1.4100 |
| bond | 1   | 10  | 384.00 | 1.4100 |
| bond | 1   | 4   | 389.50 | 1.0920 |
| bond | 11  | 4   | 389.50 | 1.0920 |
| bond | 2   | 5   | 398.50 | 1.0920 |
| bond | 8   | 6   | 615.50 | 0.9710 |
| bond | 9   | 6   | 615.50 | 0.9710 |
| bond | 18  | 6   | 615.50 | 0.9710 |
| bond | 19  | 6   | 615.50 | 0.9710 |
| bond | 10  | 6   | 615.50 | 0.9710 |
| bond | 7   | 1   | 384.00 | 1.4140 |
| bond | 57  | 51  | 384.00 | 1.4140 |
| bond | 51  | 51  | 320.00 | 1.5100 |
| bond | 60  | 51  | 320.00 | 1.5100 |
| bond | 60  | 57  | 384.00 | 1.4320 |
| bond | 60  | 52  | 380.00 | 1.5020 |
| bond | 51  | 59  | 384.00 | 1.4100 |
| bond | 52  | 58  | 484.00 | 1.4100 |
| bond | 51  | 69  | 384.00 | 1.4100 |
| bond | 52  | 68  | 484.00 | 1.4100 |
| bond | 51  | 54  | 389.50 | 1.0920 |
| bond | 60  | 54  | 389.50 | 1.0920 |
| bond | 52  | 55  | 398.50 | 1.0920 |
| bond | 59  | 56  | 615.50 | 0.9710 |
| bond | 58  | 56  | 615.50 | 0.9710 |
| bond | 69  | 56  | 615.50 | 0.9710 |
| bond | 68  | 56  | 615.50 | 0.9710 |
| bond | 101 | 8   | 320.00 | 1.6060 |
| bond | 101 | 9   | 320.00 | 1.6060 |
| bond | 101 | 102 | 700.00 | 1.4960 |
| bond | 101 | 58  | 320.00 | 1.6060 |

|      |         |        |        |
|------|---------|--------|--------|
| bond | 101 59  | 320.00 | 1.6060 |
| bond | 1 209   | 360.00 | 1.4150 |
| bond | 1 309   | 360.00 | 1.4150 |
| bond | 1 210   | 390.00 | 1.4320 |
| bond | 1 310   | 390.00 | 1.4320 |
| bond | 51 209  | 360.00 | 1.4150 |
| bond | 51 309  | 360.00 | 1.4150 |
| bond | 51 210  | 390.00 | 1.4320 |
| bond | 51 310  | 390.00 | 1.4320 |
| bond | 202 204 | 390.00 | 1.3810 |
| bond | 202 220 | 390.00 | 1.4200 |
| bond | 204 206 | 420.00 | 1.4450 |
| bond | 204 204 | 420.00 | 1.3530 |
| bond | 207 220 | 340.00 | 1.4060 |
| bond | 206 207 | 340.00 | 1.4370 |
| bond | 201 204 | 360.00 | 1.4930 |
| bond | 207 207 | 268.00 | 1.4040 |
| bond | 207 211 | 340.00 | 1.3500 |
| bond | 207 210 | 340.00 | 1.3700 |
| bond | 207 212 | 460.00 | 1.3720 |
| bond | 208 220 | 420.00 | 1.3550 |
| bond | 208 219 | 420.00 | 1.3610 |
| bond | 209 219 | 400.00 | 1.3660 |
| bond | 204 211 | 400.00 | 1.3340 |
| bond | 211 219 | 400.00 | 1.3100 |
| bond | 211 220 | 400.00 | 1.3260 |
| bond | 205 212 | 478.00 | 1.3350 |
| bond | 206 211 | 478.00 | 1.3690 |
| bond | 206 209 | 325.00 | 1.3970 |
| bond | 206 213 | 530.00 | 1.2240 |
| bond | 202 215 | 408.00 | 1.0800 |
| bond | 204 216 | 405.00 | 1.0810 |
| bond | 204 221 | 405.00 | 1.0810 |
| bond | 205 216 | 420.00 | 1.0760 |
| bond | 201 214 | 384.00 | 1.0870 |
| bond | 208 217 | 540.00 | 1.0040 |
| bond | 209 218 | 512.00 | 1.0110 |
| bond | 206 309 | 325.00 | 1.3970 |
| bond | 207 310 | 340.00 | 1.3700 |
| bond | 309 218 | 512.00 | 1.0110 |

|      |     |     |        |        |
|------|-----|-----|--------|--------|
| bond | 205 | 310 | 400.00 | 1.3620 |
| bond | 205 | 210 | 400.00 | 1.3620 |
| bond | 204 | 309 | 400.00 | 1.3420 |
| bond | 204 | 209 | 400.00 | 1.3420 |

|       |    |    |    |       |        |
|-------|----|----|----|-------|--------|
| angle | 35 | 34 | 35 | 48.70 | 108.50 |
|-------|----|----|----|-------|--------|

|       |    |   |   |       |        |
|-------|----|---|---|-------|--------|
| angle | 11 | 7 | 1 | 88.25 | 109.90 |
|-------|----|---|---|-------|--------|

|       |   |   |   |       |        |
|-------|---|---|---|-------|--------|
| angle | 7 | 1 | 1 | 87.95 | 106.58 |
|-------|---|---|---|-------|--------|

|       |   |   |   |       |        |
|-------|---|---|---|-------|--------|
| angle | 1 | 1 | 1 | 60.40 | 101.70 |
|-------|---|---|---|-------|--------|

|       |   |   |   |       |        |
|-------|---|---|---|-------|--------|
| angle | 8 | 1 | 1 | 87.95 | 108.25 |
|-------|---|---|---|-------|--------|

|       |    |   |   |       |        |
|-------|----|---|---|-------|--------|
| angle | 18 | 1 | 1 | 87.95 | 108.25 |
|-------|----|---|---|-------|--------|

|       |    |   |   |       |        |
|-------|----|---|---|-------|--------|
| angle | 11 | 1 | 1 | 60.30 | 102.10 |
|-------|----|---|---|-------|--------|

|       |    |   |   |       |        |
|-------|----|---|---|-------|--------|
| angle | 11 | 1 | 8 | 87.25 | 109.50 |
|-------|----|---|---|-------|--------|

|       |    |   |    |       |        |
|-------|----|---|----|-------|--------|
| angle | 11 | 1 | 18 | 87.25 | 109.50 |
|-------|----|---|----|-------|--------|

|       |   |    |   |       |        |
|-------|---|----|---|-------|--------|
| angle | 7 | 11 | 1 | 87.95 | 105.30 |
|-------|---|----|---|-------|--------|

|       |   |    |   |       |        |
|-------|---|----|---|-------|--------|
| angle | 1 | 11 | 2 | 50.50 | 115.00 |
|-------|---|----|---|-------|--------|

|       |   |    |   |       |        |
|-------|---|----|---|-------|--------|
| angle | 7 | 11 | 2 | 64.50 | 109.20 |
|-------|---|----|---|-------|--------|

|       |   |   |   |       |        |
|-------|---|---|---|-------|--------|
| angle | 1 | 1 | 4 | 38.00 | 111.65 |
|-------|---|---|---|-------|--------|

|       |   |   |   |       |        |
|-------|---|---|---|-------|--------|
| angle | 7 | 1 | 4 | 54.50 | 110.62 |
|-------|---|---|---|-------|--------|

|       |   |    |   |       |        |
|-------|---|----|---|-------|--------|
| angle | 1 | 11 | 4 | 38.00 | 109.25 |
|-------|---|----|---|-------|--------|

|       |   |    |   |       |        |
|-------|---|----|---|-------|--------|
| angle | 2 | 11 | 4 | 39.40 | 108.50 |
|-------|---|----|---|-------|--------|

|       |   |    |   |       |        |
|-------|---|----|---|-------|--------|
| angle | 7 | 11 | 4 | 54.50 | 108.50 |
|-------|---|----|---|-------|--------|

|       |    |   |   |       |        |
|-------|----|---|---|-------|--------|
| angle | 11 | 1 | 4 | 38.00 | 111.30 |
|-------|----|---|---|-------|--------|

|       |   |   |   |       |        |
|-------|---|---|---|-------|--------|
| angle | 8 | 1 | 4 | 54.20 | 111.30 |
|-------|---|---|---|-------|--------|

|       |    |   |   |       |        |
|-------|----|---|---|-------|--------|
| angle | 18 | 1 | 4 | 54.20 | 111.30 |
|-------|----|---|---|-------|--------|

|       |   |   |   |       |        |
|-------|---|---|---|-------|--------|
| angle | 1 | 8 | 6 | 64.50 | 107.65 |
|-------|---|---|---|-------|--------|

|       |   |    |   |       |        |
|-------|---|----|---|-------|--------|
| angle | 1 | 18 | 6 | 64.50 | 107.65 |
|-------|---|----|---|-------|--------|

|       |   |   |   |       |        |
|-------|---|---|---|-------|--------|
| angle | 2 | 9 | 6 | 64.50 | 107.65 |
|-------|---|---|---|-------|--------|

|       |   |    |   |       |        |
|-------|---|----|---|-------|--------|
| angle | 2 | 19 | 6 | 64.50 | 107.65 |
|-------|---|----|---|-------|--------|

|       |   |    |   |       |        |
|-------|---|----|---|-------|--------|
| angle | 1 | 10 | 6 | 63.26 | 104.70 |
|-------|---|----|---|-------|--------|

|       |   |   |    |       |        |
|-------|---|---|----|-------|--------|
| angle | 1 | 1 | 10 | 86.54 | 110.85 |
|-------|---|---|----|-------|--------|

|       |   |   |    |       |        |
|-------|---|---|----|-------|--------|
| angle | 4 | 1 | 10 | 54.20 | 109.90 |
|-------|---|---|----|-------|--------|

|       |    |   |   |       |        |
|-------|----|---|---|-------|--------|
| angle | 11 | 2 | 9 | 75.40 | 108.30 |
|-------|----|---|---|-------|--------|

|       |    |   |    |       |        |
|-------|----|---|----|-------|--------|
| angle | 11 | 2 | 19 | 75.40 | 108.30 |
|-------|----|---|----|-------|--------|

|       |    |   |   |       |        |
|-------|----|---|---|-------|--------|
| angle | 11 | 2 | 5 | 37.35 | 108.65 |
|-------|----|---|---|-------|--------|

|       |   |   |   |       |        |
|-------|---|---|---|-------|--------|
| angle | 9 | 2 | 5 | 51.75 | 110.80 |
|-------|---|---|---|-------|--------|

|       |    |   |   |       |        |
|-------|----|---|---|-------|--------|
| angle | 19 | 2 | 5 | 51.75 | 110.80 |
|-------|----|---|---|-------|--------|

|       |   |   |   |       |        |
|-------|---|---|---|-------|--------|
| angle | 5 | 2 | 5 | 34.20 | 108.38 |
|-------|---|---|---|-------|--------|

|       |    |    |    |       |        |
|-------|----|----|----|-------|--------|
| angle | 60 | 57 | 51 | 88.25 | 109.90 |
|-------|----|----|----|-------|--------|

|       |    |    |    |       |        |
|-------|----|----|----|-------|--------|
| angle | 57 | 51 | 51 | 87.95 | 106.58 |
|-------|----|----|----|-------|--------|

|       |    |    |    |       |        |
|-------|----|----|----|-------|--------|
| angle | 51 | 51 | 51 | 60.40 | 101.70 |
|-------|----|----|----|-------|--------|

|       |    |    |    |       |        |
|-------|----|----|----|-------|--------|
| angle | 59 | 51 | 51 | 87.95 | 110.50 |
|-------|----|----|----|-------|--------|



|       |    |    |    |       |        |
|-------|----|----|----|-------|--------|
| angle | 69 | 51 | 51 | 87.95 | 110.50 |
| angle | 60 | 51 | 51 | 60.30 | 102.10 |
| angle | 60 | 51 | 59 | 87.25 | 109.50 |
| angle | 60 | 51 | 69 | 87.25 | 109.50 |
| angle | 57 | 60 | 51 | 87.95 | 105.30 |
| angle | 51 | 60 | 52 | 50.50 | 115.00 |
| angle | 57 | 60 | 52 | 64.50 | 109.20 |
| angle | 51 | 51 | 54 | 38.00 | 111.65 |
| angle | 57 | 51 | 54 | 54.50 | 110.62 |
| angle | 51 | 60 | 54 | 38.00 | 109.25 |
| angle | 52 | 60 | 54 | 39.40 | 108.50 |
| angle | 57 | 60 | 54 | 54.50 | 108.50 |
| angle | 60 | 51 | 54 | 38.00 | 111.30 |
| angle | 59 | 51 | 54 | 54.20 | 111.30 |
| angle | 69 | 51 | 54 | 54.20 | 111.30 |
| angle | 51 | 59 | 56 | 64.50 | 107.65 |
| angle | 51 | 69 | 56 | 64.50 | 107.65 |
| angle | 52 | 58 | 56 | 64.50 | 107.65 |
| angle | 52 | 68 | 56 | 64.50 | 107.65 |
| angle | 54 | 51 | 54 | 26.23 | 109.30 |
| angle | 60 | 52 | 58 | 75.40 | 108.30 |
| angle | 60 | 52 | 68 | 75.40 | 108.30 |
| angle | 60 | 52 | 55 | 37.35 | 108.65 |
| angle | 58 | 52 | 55 | 51.75 | 110.80 |
| angle | 68 | 52 | 55 | 51.75 | 110.80 |
| angle | 55 | 52 | 55 | 34.20 | 108.38 |

|       |     |     |     |        |        |
|-------|-----|-----|-----|--------|--------|
| angle | 101 | 8   | 1   | 78.00  | 110.00 |
| angle | 101 | 9   | 2   | 78.00  | 110.00 |
| angle | 8   | 101 | 102 | 90.00  | 108.80 |
| angle | 9   | 101 | 102 | 90.00  | 108.80 |
| angle | 102 | 101 | 102 | 125.00 | 122.90 |
| angle | 8   | 101 | 9   | 64.00  | 98.40  |
| angle | 101 | 58  | 52  | 78.00  | 110.00 |
| angle | 51  | 59  | 101 | 78.00  | 110.00 |
| angle | 58  | 101 | 102 | 90.00  | 108.80 |
| angle | 59  | 101 | 102 | 90.00  | 108.80 |
| angle | 59  | 101 | 58  | 64.00  | 98.40  |

|       |   |   |     |       |        |
|-------|---|---|-----|-------|--------|
| angle | 1 | 1 | 209 | 87.95 | 112.80 |
| angle | 1 | 1 | 309 | 87.95 | 112.80 |
| angle | 1 | 1 | 210 | 87.95 | 112.80 |
| angle | 1 | 1 | 310 | 87.95 | 112.80 |
| angle | 4 | 1 | 209 | 54.78 | 106.60 |

|       |   |     |     |       |        |
|-------|---|-----|-----|-------|--------|
| angle | 4 | 1   | 309 | 54.78 | 106.60 |
| angle | 4 | 1   | 210 | 54.78 | 106.60 |
| angle | 4 | 1   | 310 | 54.78 | 106.60 |
| angle | 1 | 209 | 204 | 52.0  | 116.20 |
| angle | 1 | 309 | 204 | 52.0  | 116.20 |
| angle | 1 | 210 | 205 | 58.0  | 125.40 |
| angle | 1 | 310 | 205 | 58.0  | 125.40 |
| angle | 1 | 209 | 206 | 48.0  | 119.00 |
| angle | 1 | 309 | 206 | 48.0  | 119.00 |
| angle | 1 | 210 | 207 | 48.0  | 126.48 |
| angle | 1 | 310 | 207 | 48.0  | 126.48 |
| angle | 7 | 1   | 209 | 49.34 | 106.60 |
| angle | 7 | 1   | 309 | 49.34 | 106.60 |
| angle | 7 | 1   | 210 | 49.34 | 106.60 |
| angle | 7 | 1   | 310 | 49.34 | 106.60 |

|       |    |     |     |       |        |
|-------|----|-----|-----|-------|--------|
| angle | 51 | 51  | 209 | 87.95 | 112.80 |
| angle | 51 | 51  | 309 | 87.95 | 112.80 |
| angle | 51 | 51  | 210 | 87.95 | 112.80 |
| angle | 51 | 51  | 310 | 87.95 | 112.80 |
| angle | 54 | 51  | 209 | 54.78 | 106.60 |
| angle | 54 | 51  | 309 | 54.78 | 106.60 |
| angle | 54 | 51  | 210 | 54.78 | 106.60 |
| angle | 54 | 51  | 310 | 54.78 | 106.60 |
| angle | 51 | 209 | 204 | 52.0  | 116.20 |
| angle | 51 | 309 | 204 | 52.0  | 116.20 |
| angle | 51 | 210 | 205 | 58.0  | 125.40 |
| angle | 51 | 310 | 205 | 58.0  | 125.40 |
| angle | 51 | 209 | 206 | 48.0  | 119.00 |
| angle | 51 | 309 | 206 | 48.0  | 119.00 |
| angle | 51 | 210 | 207 | 48.0  | 126.48 |
| angle | 51 | 310 | 207 | 48.0  | 126.48 |
| angle | 57 | 51  | 209 | 49.34 | 106.60 |
| angle | 57 | 51  | 309 | 49.34 | 106.60 |
| angle | 57 | 51  | 210 | 49.34 | 106.60 |
| angle | 57 | 51  | 310 | 49.34 | 106.60 |

|       |     |     |     |       |        |
|-------|-----|-----|-----|-------|--------|
| angle | 202 | 202 | 220 | 112.0 | 118.66 |
| angle | 204 | 202 | 220 | 112.0 | 116.50 |
| angle | 204 | 202 | 204 | 112.0 | 116.90 |
| angle | 206 | 207 | 207 | 42.0  | 118.49 |
| angle | 207 | 207 | 220 | 42.0  | 115.90 |
| angle | 207 | 207 | 210 | 60.0  | 105.88 |
| angle | 207 | 207 | 211 | 60.0  | 128.40 |

|       |     |     |     |       |        |
|-------|-----|-----|-----|-------|--------|
| angle | 207 | 207 | 212 | 60.0  | 111.38 |
| angle | 207 | 220 | 211 | 60.0  | 119.30 |
| angle | 207 | 220 | 208 | 32.0  | 122.40 |
| angle | 202 | 202 | 208 | 32.0  | 120.63 |
| angle | 202 | 220 | 208 | 32.0  | 119.50 |
| angle | 208 | 219 | 209 | 32.0  | 117.10 |
| angle | 204 | 204 | 206 | 130.0 | 118.99 |
| angle | 202 | 204 | 209 | 130.0 | 120.74 |
| angle | 204 | 204 | 209 | 130.0 | 123.56 |
| angle | 204 | 211 | 204 | 128.0 | 117.03 |
| angle | 204 | 211 | 220 | 128.0 | 118.67 |
| angle | 206 | 211 | 220 | 128.0 | 120.30 |
| angle | 204 | 211 | 207 | 128.0 | 110.86 |
| angle | 207 | 211 | 219 | 128.0 | 111.66 |
| angle | 205 | 212 | 207 | 128.0 | 103.47 |
| angle | 205 | 210 | 207 | 42.0  | 107.20 |
| angle | 212 | 207 | 220 | 90.0  | 132.47 |
| angle | 206 | 207 | 212 | 90.0  | 130.37 |
| angle | 210 | 207 | 211 | 90.0  | 126.37 |
| angle | 210 | 205 | 212 | 130.0 | 113.18 |
| angle | 211 | 206 | 213 | 135.0 | 124.73 |
| angle | 211 | 204 | 211 | 135.0 | 127.90 |
| angle | 208 | 219 | 211 | 135.0 | 119.25 |
| angle | 208 | 220 | 211 | 135.0 | 118.00 |
| angle | 202 | 204 | 211 | 60.0  | 123.28 |
| angle | 202 | 220 | 211 | 60.0  | 122.50 |
| angle | 209 | 206 | 209 | 60.0  | 113.94 |
| angle | 209 | 206 | 211 | 60.0  | 117.24 |
| angle | 209 | 206 | 213 | 60.0  | 120.00 |
| angle | 209 | 219 | 211 | 60.0  | 123.65 |
| angle | 207 | 206 | 213 | 85.0  | 131.17 |
| angle | 204 | 206 | 213 | 85.0  | 126.37 |
| angle | 204 | 206 | 209 | 45.0  | 113.34 |
| angle | 207 | 206 | 209 | 45.0  | 109.14 |
| angle | 206 | 209 | 206 | 125.0 | 128.52 |
| angle | 204 | 209 | 206 | 80.0  | 123.84 |
| angle | 206 | 209 | 219 | 80.0  | 127.19 |
| angle | 201 | 204 | 204 | 28.0  | 123.52 |
| angle | 201 | 204 | 206 | 28.0  | 118.28 |
| angle | 204 | 201 | 214 | 61.4  | 110.61 |
| angle | 214 | 201 | 214 | 34.5  | 109.06 |
| angle | 204 | 202 | 215 | 37.6  | 120.47 |
| angle | 215 | 202 | 220 | 37.6  | 121.50 |
| angle | 202 | 204 | 216 | 32.5  | 121.49 |

|       |     |     |     |      |        |
|-------|-----|-----|-----|------|--------|
| angle | 204 | 204 | 216 | 32.5 | 121.46 |
| angle | 204 | 204 | 221 | 32.5 | 121.46 |
| angle | 206 | 204 | 221 | 32.5 | 116.87 |
| angle | 209 | 204 | 216 | 40.0 | 115.75 |
| angle | 211 | 204 | 221 | 41.2 | 116.07 |
| angle | 210 | 205 | 216 | 41.0 | 121.27 |
| angle | 212 | 205 | 216 | 40.0 | 124.53 |
| angle | 217 | 208 | 219 | 41.5 | 120.00 |
| angle | 217 | 208 | 220 | 41.5 | 120.00 |
| angle | 217 | 208 | 217 | 19.5 | 120.00 |
| angle | 218 | 209 | 219 | 32.8 | 119.77 |
| angle | 204 | 209 | 218 | 32.8 | 120.00 |
| angle | 206 | 209 | 218 | 43.5 | 114.97 |

|       |     |     |     |       |        |
|-------|-----|-----|-----|-------|--------|
| angle | 204 | 309 | 206 | 80.0  | 123.84 |
| angle | 206 | 309 | 206 | 125.0 | 128.52 |
| angle | 205 | 310 | 207 | 42.0  | 107.20 |
| angle | 202 | 204 | 309 | 130.0 | 120.74 |
| angle | 204 | 204 | 309 | 130.0 | 123.56 |
| angle | 208 | 219 | 309 | 32.0  | 117.10 |
| angle | 204 | 206 | 309 | 45.0  | 113.34 |
| angle | 207 | 206 | 309 | 45.0  | 109.14 |
| angle | 209 | 206 | 309 | 60.0  | 113.94 |
| angle | 309 | 206 | 309 | 60.0  | 113.94 |
| angle | 207 | 207 | 310 | 60.0  | 105.88 |
| angle | 310 | 207 | 211 | 90.0  | 126.37 |
| angle | 310 | 205 | 212 | 130.0 | 113.18 |
| angle | 309 | 206 | 213 | 60.0  | 120.00 |
| angle | 309 | 204 | 216 | 40.0  | 115.75 |
| angle | 310 | 205 | 216 | 41.0  | 121.27 |
| angle | 204 | 309 | 218 | 32.8  | 120.00 |
| angle | 206 | 309 | 218 | 43.5  | 114.97 |

ureybrad 35 34 35 -7.60 1.5326

# hydroxyl 5'terminal 3'terminal

|         |    |   |    |   |         |       |         |         |         |       |
|---------|----|---|----|---|---------|-------|---------|---------|---------|-------|
| torsion | 11 | 2 | 19 | 6 | -0.8625 | 0.0 1 | 1.1413  | 180.0 2 | -1.0897 | 0.0 3 |
| torsion | 5  | 2 | 19 | 6 | 0.4033  | 0.0 1 | -0.3030 | 180.0 2 | 0.4283  | 0.0 3 |
| torsion | 1  | 1 | 10 | 6 | -1.0508 | 0.0 1 | 2.6700  | 180.0 2 | 0.0522  | 0.0 3 |
| torsion | 4  | 1 | 10 | 6 | 0.3195  | 0.0 1 | -0.3429 | 180.0 2 | 0.2642  | 0.0 3 |
| torsion | 1  | 1 | 18 | 6 | -1.8073 | 0.0 1 | -0.3831 | 180.0 2 | -0.2626 | 0.0 3 |
| torsion | 11 | 1 | 18 | 6 | 0.4774  | 0.0 1 | -0.1992 | 180.0 2 | 0.6516  | 0.0 3 |
| torsion | 4  | 1 | 18 | 6 | 0.9502  | 0.0 1 | 1.1110  | 180.0 2 | 0.0750  | 0.0 3 |

|         |    |    |    |    |         |       |         |         |         |       |
|---------|----|----|----|----|---------|-------|---------|---------|---------|-------|
| torsion | 55 | 52 | 68 | 56 | 0.6588  | 0.0 1 | 0.9747  | 180.0 2 | -0.4142 | 0.0 3 |
| torsion | 60 | 52 | 68 | 56 | -1.2066 | 0.0 1 | -1.6510 | 180.0 2 | -0.1760 | 0.0 3 |
| torsion | 51 | 51 | 69 | 56 | -0.7272 | 0.0 1 | -0.7079 | 180.0 2 | 0.9736  | 0.0 3 |
| torsion | 54 | 51 | 69 | 56 | -0.2634 | 0.0 1 | -0.4581 | 180.0 2 | 0.4088  | 0.0 3 |
| torsion | 60 | 51 | 69 | 56 | 0.1375  | 0.0 1 | 0.4009  | 180.0 2 | 0.4383  | 0.0 3 |

# v0 and v1 with base

|         |    |   |   |     |         |       |         |         |         |       |
|---------|----|---|---|-----|---------|-------|---------|---------|---------|-------|
| torsion | 11 | 7 | 1 | 210 | 0.2451  | 0.0 1 | -0.3668 | 180.0 2 | 0.3047  | 0.0 3 |
| torsion | 11 | 7 | 1 | 310 | 0.2451  | 0.0 1 | -0.3668 | 180.0 2 | 0.3047  | 0.0 3 |
| torsion | 11 | 7 | 1 | 209 | -0.4444 | 0.0 1 | -1.4574 | 180.0 2 | 1.0514  | 0.0 3 |
| torsion | 11 | 7 | 1 | 309 | -0.4444 | 0.0 1 | -1.4574 | 180.0 2 | 1.0514  | 0.0 3 |
| torsion | 1  | 1 | 1 | 210 | -1.7025 | 0.0 1 | 0.3785  | 180.0 2 | 0.2619  | 0.0 3 |
| torsion | 1  | 1 | 1 | 310 | -1.7025 | 0.0 1 | 0.3785  | 180.0 2 | 0.2619  | 0.0 3 |
| torsion | 1  | 1 | 1 | 209 | 1.3310  | 0.0 1 | -0.4697 | 180.0 2 | -0.5355 | 0.0 3 |
| torsion | 1  | 1 | 1 | 309 | 1.3310  | 0.0 1 | -0.4697 | 180.0 2 | -0.5355 | 0.0 3 |
| torsion | 10 | 1 | 1 | 210 | 0.6769  | 0.0 1 | 0.3576  | 180.0 2 | 1.7806  | 0.0 3 |
| torsion | 10 | 1 | 1 | 310 | 0.6769  | 0.0 1 | 0.3576  | 180.0 2 | 1.7806  | 0.0 3 |
| torsion | 10 | 1 | 1 | 209 | -1.8122 | 0.0 1 | 1.7553  | 180.0 2 | 0.9329  | 0.0 3 |
| torsion | 10 | 1 | 1 | 309 | -1.8122 | 0.0 1 | 1.7553  | 180.0 2 | 0.9329  | 0.0 3 |
| torsion | 4  | 1 | 1 | 210 | -0.1252 | 0.0 1 | 0.0206  | 180.0 2 | -0.0855 | 0.0 3 |
| torsion | 4  | 1 | 1 | 310 | -0.1252 | 0.0 1 | 0.0206  | 180.0 2 | -0.0855 | 0.0 3 |
| torsion | 4  | 1 | 1 | 209 | 0.1510  | 0.0 1 | -0.3180 | 180.0 2 | 0.2288  | 0.0 3 |
| torsion | 4  | 1 | 1 | 309 | 0.1510  | 0.0 1 | -0.3180 | 180.0 2 | 0.2288  | 0.0 3 |

|         |     |    |    |     |         |       |         |         |         |       |
|---------|-----|----|----|-----|---------|-------|---------|---------|---------|-------|
| torsion | 209 | 51 | 57 | 60  | -0.2090 | 0.0 1 | 1.3519  | 180.0 2 | -2.5224 | 0.0 3 |
| torsion | 309 | 51 | 57 | 60  | -0.2090 | 0.0 1 | 1.3519  | 180.0 2 | -2.5224 | 0.0 3 |
| torsion | 210 | 51 | 57 | 60  | -0.2012 | 0.0 1 | -0.6542 | 180.0 2 | -0.7908 | 0.0 3 |
| torsion | 310 | 51 | 57 | 60  | -0.2012 | 0.0 1 | -0.6542 | 180.0 2 | -0.7908 | 0.0 3 |
| torsion | 51  | 51 | 51 | 310 | -0.5831 | 0.0 1 | -0.6158 | 180.0 2 | 0.4111  | 0.0 3 |
| torsion | 54  | 51 | 51 | 310 | 0.4994  | 0.0 1 | -1.0645 | 180.0 2 | -0.0189 | 0.0 3 |
| torsion | 51  | 51 | 51 | 209 | 3.3665  | 0.0 1 | -2.2569 | 180.0 2 | -1.2989 | 0.0 3 |
| torsion | 54  | 51 | 51 | 209 | 1.1185  | 0.0 1 | -0.5524 | 180.0 2 | 1.1401  | 0.0 3 |
| torsion | 51  | 51 | 51 | 210 | -0.5831 | 0.0 1 | -0.6158 | 180.0 2 | 0.4111  | 0.0 3 |
| torsion | 54  | 51 | 51 | 210 | 0.4994  | 0.0 1 | -1.0645 | 180.0 2 | -0.0189 | 0.0 3 |
| torsion | 51  | 51 | 51 | 309 | 3.3665  | 0.0 1 | -2.2569 | 180.0 2 | -1.2989 | 0.0 3 |
| torsion | 54  | 51 | 51 | 309 | 1.1185  | 0.0 1 | -0.5524 | 180.0 2 | 1.1401  | 0.0 3 |

#v0,v1,v2

|         |    |   |   |    |         |       |         |         |         |       |
|---------|----|---|---|----|---------|-------|---------|---------|---------|-------|
| torsion | 1  | 1 | 7 | 11 | -0.3196 | 0.0 1 | -0.2087 | 180.0 2 | 0.3184  | 0.0 3 |
| torsion | 4  | 1 | 7 | 11 | -0.1353 | 0.0 1 | 0.6782  | 180.0 2 | 0.8464  | 0.0 3 |
| torsion | 7  | 1 | 1 | 1  | -0.7340 | 0.0 1 | 0.7791  | 180.0 2 | -1.0582 | 0.0 3 |
| torsion | 7  | 1 | 1 | 10 | 0.0156  | 0.0 1 | -0.9494 | 180.0 2 | 0.6364  | 0.0 3 |
| torsion | 7  | 1 | 1 | 4  | 0.0052  | 0.0 1 | 0.1327  | 180.0 2 | -0.2445 | 0.0 3 |
| torsion | 1  | 1 | 1 | 11 | -0.9404 | 0.0 1 | 1.4895  | 180.0 2 | -1.1430 | 0.0 3 |
| torsion | 10 | 1 | 1 | 11 | -1.2797 | 0.0 1 | 0.4567  | 180.0 2 | 0.9749  | 0.0 3 |
| torsion | 4  | 1 | 1 | 11 | 0.1553  | 0.0 1 | 0.0973  | 180.0 2 | 0.1476  | 0.0 3 |

|         |    |   |   |    |         |       |         |         |         |       |
|---------|----|---|---|----|---------|-------|---------|---------|---------|-------|
| torsion | 8  | 1 | 1 | 1  | 0.5996  | 0.0 1 | -0.5114 | 180.0 2 | -1.8567 | 0.0 3 |
| torsion | 18 | 1 | 1 | 1  | 0.5996  | 0.0 1 | -0.5114 | 180.0 2 | -1.8567 | 0.0 3 |
| torsion | 8  | 1 | 1 | 10 | 0.0443  | 0.0 1 | -1.2079 | 180.0 2 | 1.5299  | 0.0 3 |
| torsion | 18 | 1 | 1 | 10 | 0.0443  | 0.0 1 | -1.2079 | 180.0 2 | 1.5299  | 0.0 3 |
| torsion | 8  | 1 | 1 | 4  | -0.1626 | 0.0 1 | 0.0924  | 180.0 2 | 0.1743  | 0.0 3 |
| torsion | 18 | 1 | 1 | 4  | -0.1626 | 0.0 1 | 0.0924  | 180.0 2 | 0.1743  | 0.0 3 |
| torsion | 4  | 1 | 1 | 1  | -0.0904 | 0.0 1 | -0.3664 | 180.0 2 | 0.1902  | 0.0 3 |
| torsion | 10 | 1 | 1 | 4  | 0.3599  | 0.0 1 | -1.0257 | 180.0 2 | 0.8255  | 0.0 3 |
| torsion | 4  | 1 | 1 | 4  | -0.2443 | 0.0 1 | -0.1030 | 180.0 2 | 0.5367  | 0.0 3 |

|         |    |    |    |    |         |       |         |         |         |       |
|---------|----|----|----|----|---------|-------|---------|---------|---------|-------|
| torsion | 51 | 51 | 57 | 60 | 0.7738  | 0.0 1 | -2.6814 | 180.0 2 | 0.4982  | 0.0 3 |
| torsion | 54 | 51 | 57 | 60 | -1.2524 | 0.0 1 | 1.8924  | 180.0 2 | 0.0589  | 0.0 3 |
| torsion | 57 | 51 | 51 | 51 | 0.0682  | 0.0 1 | -1.0394 | 180.0 2 | -0.1017 | 0.0 3 |
| torsion | 57 | 51 | 51 | 54 | -0.8864 | 0.0 1 | 0.2494  | 180.0 2 | -1.1243 | 0.0 3 |
| torsion | 69 | 51 | 51 | 51 | -0.3539 | 0.0 1 | 0.0075  | 180.0 2 | 0.1288  | 0.0 3 |
| torsion | 69 | 51 | 51 | 54 | -0.5694 | 0.0 1 | 0.0859  | 180.0 2 | -0.3368 | 0.0 3 |
| torsion | 51 | 51 | 51 | 60 | -0.5446 | 0.0 1 | 0.2301  | 180.0 2 | 0.3057  | 0.0 3 |
| torsion | 54 | 51 | 51 | 51 | -0.4644 | 0.0 1 | 0.1587  | 180.0 2 | 0.8960  | 0.0 3 |
| torsion | 54 | 51 | 51 | 60 | 0.0356  | 0.0 1 | -1.4542 | 180.0 2 | 0.0137  | 0.0 3 |
| torsion | 54 | 51 | 51 | 54 | -0.7580 | 0.0 1 | 0.1044  | 180.0 2 | 0.8683  | 0.0 3 |
| torsion | 59 | 51 | 51 | 51 | -0.3539 | 0.0 1 | 0.0075  | 180.0 2 | 0.1288  | 0.0 3 |
| torsion | 59 | 51 | 51 | 54 | -0.5694 | 0.0 1 | 0.0859  | 180.0 2 | -0.3368 | 0.0 3 |

# Ribose Delta C4'-11, C3'-1

|         |   |    |   |    |         |       |         |         |         |       |
|---------|---|----|---|----|---------|-------|---------|---------|---------|-------|
| torsion | 7 | 11 | 1 | 18 | 1.1639  | 0.0 1 | 0.7320  | 180.0 2 | -0.8355 | 0.0 3 |
| torsion | 7 | 11 | 1 | 8  | 1.1639  | 0.0 1 | 0.7320  | 180.0 2 | -0.8355 | 0.0 3 |
| torsion | 7 | 11 | 1 | 1  | -0.7018 | 0.0 1 | -0.3066 | 180.0 2 | 2.8787  | 0.0 3 |
| torsion | 7 | 11 | 1 | 4  | -0.1816 | 0.0 1 | -0.7449 | 180.0 2 | 0.7269  | 0.0 3 |
| torsion | 2 | 11 | 1 | 18 | 1.0898  | 0.0 1 | 3.5490  | 180.0 2 | -1.8335 | 0.0 3 |
| torsion | 2 | 11 | 1 | 8  | 1.0898  | 0.0 1 | 3.5490  | 180.0 2 | -1.8335 | 0.0 3 |
| torsion | 2 | 11 | 1 | 1  | -0.4831 | 0.0 1 | -1.9843 | 180.0 2 | 0.0912  | 0.0 3 |
| torsion | 2 | 11 | 1 | 4  | -0.2647 | 0.0 1 | 0.3598  | 180.0 2 | -0.0391 | 0.0 3 |
| torsion | 4 | 11 | 1 | 18 | 0.0057  | 0.0 1 | -0.1704 | 180.0 2 | -0.1683 | 0.0 3 |
| torsion | 4 | 11 | 1 | 8  | 0.0057  | 0.0 1 | -0.1704 | 180.0 2 | -0.1683 | 0.0 3 |
| torsion | 4 | 11 | 1 | 1  | -0.1897 | 0.0 1 | -0.1006 | 180.0 2 | 0.5427  | 0.0 3 |
| torsion | 4 | 11 | 1 | 4  | 0.0805  | 0.0 1 | -0.0660 | 180.0 2 | 0.4223  | 0.0 3 |

|         |    |    |    |    |         |       |         |         |         |       |
|---------|----|----|----|----|---------|-------|---------|---------|---------|-------|
| torsion | 57 | 60 | 51 | 59 | 0.3860  | 0.0 1 | -0.2471 | 180.0 2 | 0.6173  | 0.0 3 |
| torsion | 57 | 60 | 51 | 69 | 0.3860  | 0.0 1 | -0.2471 | 180.0 2 | 0.6173  | 0.0 3 |
| torsion | 57 | 60 | 51 | 51 | -0.4836 | 0.0 1 | 0.0229  | 180.0 2 | 0.4161  | 0.0 3 |
| torsion | 57 | 60 | 51 | 54 | -0.5619 | 0.0 1 | -0.1530 | 180.0 2 | 0.7195  | 0.0 3 |
| torsion | 52 | 60 | 51 | 59 | 0.3544  | 0.0 1 | 0.5074  | 180.0 2 | -0.2260 | 0.0 3 |
| torsion | 52 | 60 | 51 | 69 | 0.3544  | 0.0 1 | 0.5074  | 180.0 2 | -0.2260 | 0.0 3 |
| torsion | 52 | 60 | 51 | 51 | -0.6093 | 0.0 1 | -1.3990 | 180.0 2 | -0.3256 | 0.0 3 |
| torsion | 52 | 60 | 51 | 54 | -0.3402 | 0.0 1 | -0.2040 | 180.0 2 | 0.0297  | 0.0 3 |

|                              |     |     |    |    |         |      |         |        |         |      |
|------------------------------|-----|-----|----|----|---------|------|---------|--------|---------|------|
| torsion                      | 54  | 60  | 51 | 59 | -0.3670 | 0.01 | -0.1535 | 180.02 | 0.2765  | 0.03 |
| torsion                      | 54  | 60  | 51 | 69 | -0.3670 | 0.01 | -0.1535 | 180.02 | 0.2765  | 0.03 |
| torsion                      | 54  | 60  | 51 | 51 | -0.1504 | 0.01 | 0.0319  | 180.02 | 0.1144  | 0.03 |
| torsion                      | 54  | 60  | 51 | 54 | -0.0561 | 0.01 | -0.2835 | 180.02 | 0.4280  | 0.03 |
| # v4                         |     |     |    |    |         |      |         |        |         |      |
| torsion                      | 1   | 11  | 7  | 1  | -0.5634 | 0.01 | 0.7699  | 180.02 | -0.3217 | 0.03 |
| torsion                      | 2   | 11  | 7  | 1  | -0.7914 | 0.01 | -0.8291 | 180.02 | 1.1013  | 0.03 |
| torsion                      | 4   | 11  | 7  | 1  | -0.1611 | 0.01 | -0.0264 | 180.02 | 0.2770  | 0.03 |
|                              |     |     |    |    |         |      |         |        |         |      |
| torsion                      | 51  | 60  | 57 | 51 | 0.2852  | 0.01 | -1.5117 | 180.02 | -0.2117 | 0.03 |
| torsion                      | 52  | 60  | 57 | 51 | 0.0583  | 0.01 | 0.0000  | 180.02 | 0.0476  | 0.03 |
| torsion                      | 54  | 60  | 57 | 51 | -1.4613 | 0.01 | 1.1453  | 180.02 | 0.3029  | 0.03 |
| # Ribose Alpha P-101, O5'-9  |     |     |    |    |         |      |         |        |         |      |
| torsion                      | 8   | 101 | 9  | 2  | -4.6660 | 0.01 | 6.2820  | 180.02 | 0.9960  | 0.03 |
| torsion                      | 102 | 101 | 9  | 2  | -6.3380 | 0.01 | 6.7880  | 180.02 | 0.3700  | 0.03 |
|                              |     |     |    |    |         |      |         |        |         |      |
| torsion                      | 59  | 101 | 58 | 52 | -4.6660 | 0.01 | 6.2820  | 180.02 | 0.9960  | 0.03 |
| torsion                      | 102 | 101 | 58 | 52 | -6.3380 | 0.01 | 6.7880  | 180.02 | 0.3700  | 0.03 |
| # Ribose Beta C5'-2, O5'-9   |     |     |    |    |         |      |         |        |         |      |
| torsion                      | 101 | 9   | 2  | 11 | 0.0000  | 0.01 | 1.9050  | 180.02 | 0.0000  | 0.03 |
| torsion                      | 101 | 9   | 2  | 5  | 0.0000  | 0.01 | 0.0000  | 180.02 | 0.1200  | 0.03 |
|                              |     |     |    |    |         |      |         |        |         |      |
| torsion                      | 101 | 58  | 52 | 60 | -0.6900 | 0.01 | 0.0000  | 180.02 | -0.1480 | 0.03 |
| torsion                      | 101 | 58  | 52 | 55 | 0.0000  | 0.01 | 0.0000  | 180.02 | 0.1200  | 0.03 |
| # Ribose Gamma C5'-2, C4'-11 |     |     |    |    |         |      |         |        |         |      |
| torsion                      | 9   | 2   | 11 | 7  | 1.3334  | 0.01 | -1.3110 | 180.02 | 0.0000  | 0.03 |
| torsion                      | 19  | 2   | 11 | 7  | 1.3334  | 0.01 | -1.3110 | 180.02 | 0.0000  | 0.03 |
| torsion                      | 9   | 2   | 11 | 1  | -0.4014 | 0.01 | 0.4958  | 180.02 | 2.7144  | 0.03 |
| torsion                      | 19  | 2   | 11 | 1  | -0.4014 | 0.01 | 0.4958  | 180.02 | 2.7144  | 0.03 |
| torsion                      | 9   | 2   | 11 | 4  | 0.0000  | 0.01 | 0.2875  | 180.02 | 0.1324  | 0.03 |
| torsion                      | 19  | 2   | 11 | 4  | 0.0000  | 0.01 | 0.2875  | 180.02 | 0.1324  | 0.03 |
| torsion                      | 5   | 2   | 11 | 7  | 0.0000  | 0.01 | 0.2568  | 180.02 | 0.0963  | 0.03 |
| torsion                      | 5   | 2   | 11 | 1  | 0.0000  | 0.01 | 0.0000  | 180.02 | 0.1364  | 0.03 |
| torsion                      | 5   | 2   | 11 | 4  | 0.0000  | 0.01 | 0.0000  | 180.02 | 0.1332  | 0.03 |
|                              |     |     |    |    |         |      |         |        |         |      |
| torsion                      | 58  | 52  | 60 | 57 | 0.4560  | 0.01 | -1.1660 | 180.02 | 0.0000  | 0.03 |
| torsion                      | 68  | 52  | 60 | 57 | 0.4560  | 0.01 | -1.1660 | 180.02 | 0.0000  | 0.03 |
| torsion                      | 58  | 52  | 60 | 51 | -0.4340 | 0.01 | 0.6300  | 180.02 | 2.3640  | 0.03 |
| torsion                      | 68  | 52  | 60 | 51 | -0.4340 | 0.01 | 0.6300  | 180.02 | 2.3640  | 0.03 |
| torsion                      | 58  | 52  | 60 | 54 | 0.0000  | 0.01 | 0.6540  | 180.02 | 0.1540  | 0.03 |
| torsion                      | 68  | 52  | 60 | 54 | 0.0000  | 0.01 | 0.6540  | 180.02 | 0.1540  | 0.03 |
| torsion                      | 55  | 52  | 60 | 57 | 0.0000  | 0.01 | 0.6070  | 180.02 | 0.0280  | 0.03 |
| torsion                      | 55  | 52  | 60 | 51 | 0.0000  | 0.01 | 0.0000  | 180.02 | 0.1940  | 0.03 |
| torsion                      | 55  | 52  | 60 | 54 | 0.0000  | 0.01 | 0.0000  | 180.02 | 0.3260  | 0.03 |

# Ribose Epsilon O3'-8, C3'-1

torsion 1 1 8 101 -5.4210 0.0 1 0.8555 180.0 2 -2.0901 0.0 3  
torsion 11 1 8 101 0.0599 0.0 1 1.9959 180.0 2 3.8202 0.0 3  
torsion 4 1 8 101 4.4410 0.0 1 -1.1476 180.0 2 -2.2621 0.0 3

torsion 51 51 59 101 -1.5015 0.0 1 0.2227 180.0 2 0.0562 0.0 3  
torsion 54 51 59 101 0.8968 0.0 1 -0.1356 180.0 2 0.1474 0.0 3  
torsion 60 51 59 101 -1.1641 0.0 1 0.5055 180.0 2 0.2392 0.0 3

# Ribose Zeta P-101, O3'-8

torsion 1 8 101 9 -4.6660 0.0 1 6.2820 180.0 2 0.9960 0.0 3  
torsion 1 8 101 102 -6.3380 0.0 1 6.7880 180.0 2 0.3700 0.0 3

torsion 51 59 101 58 -4.6660 0.0 1 6.2820 180.0 2 0.9960 0.0 3  
torsion 51 59 101 102 -6.3380 0.0 1 6.7880 180.0 2 0.3700 0.0 3

# Kai for Adenosine C1'-1, N9-210

torsion 7 1 310 207 0.8713 0.0 1 -0.9386 180.0 2 2.3237 0.0 3  
torsion 7 1 310 205 -1.1473 0.0 1 -1.0816 180.0 2 -0.7501 0.0 3  
torsion 1 1 310 207 -0.6614 0.0 1 0.1858 180.0 2 -1.1674 0.0 3  
torsion 1 1 310 205 0.2332 0.0 1 0.2887 180.0 2 2.7542 0.0 3  
torsion 4 1 310 207 -0.2000 0.0 1 -0.2722 180.0 2 0.7411 0.0 3  
torsion 4 1 310 205 0.1079 0.0 1 -0.2616 180.0 2 -0.4272 0.0 3

torsion 57 51 310 207 0.6480 0.0 1 -0.0882 180.0 2 -0.2331 0.0 3  
torsion 57 51 310 205 -0.7713 0.0 1 -0.2755 180.0 2 1.7577 0.0 3  
torsion 51 51 310 207 -0.2212 0.0 1 1.2575 180.0 2 0.9710 0.0 3  
torsion 51 51 310 205 -1.6754 0.0 1 -0.4008 180.0 2 1.3097 0.0 3  
torsion 54 51 310 207 1.0745 0.0 1 -0.2512 180.0 2 0.3016 0.0 3  
torsion 54 51 310 205 -0.2368 0.0 1 1.2936 180.0 2 -0.1282 0.0 3

# Kai for Guanosine C1'-1, N9-210

torsion 7 1 210 207 0.8713 0.0 1 -0.9386 180.0 2 2.3237 0.0 3  
torsion 7 1 210 205 -1.1473 0.0 1 -1.0816 180.0 2 -0.7501 0.0 3  
torsion 1 1 210 207 -0.6614 0.0 1 0.1858 180.0 2 -1.1674 0.0 3  
torsion 1 1 210 205 0.2332 0.0 1 0.2887 180.0 2 2.7542 0.0 3  
torsion 4 1 210 207 -0.2000 0.0 1 -0.2722 180.0 2 0.7411 0.0 3  
torsion 4 1 210 205 0.1079 0.0 1 -0.2616 180.0 2 -0.4272 0.0 3

torsion 57 51 210 207 0.6480 0.0 1 -0.0882 180.0 2 -0.2331 0.0 3  
torsion 57 51 210 205 -0.7713 0.0 1 -0.2755 180.0 2 1.7577 0.0 3  
torsion 51 51 210 207 -0.2212 0.0 1 1.2575 180.0 2 0.9710 0.0 3  
torsion 51 51 210 205 -1.6754 0.0 1 -0.4008 180.0 2 1.3097 0.0 3  
torsion 54 51 210 207 1.0745 0.0 1 -0.2512 180.0 2 0.3016 0.0 3  
torsion 54 51 210 205 -0.2368 0.0 1 1.2936 180.0 2 -0.1282 0.0 3

# Kai for Uridine C1'-1, N1-309



|         |    |    |     |     |         |     |   |         |       |   |         |     |   |
|---------|----|----|-----|-----|---------|-----|---|---------|-------|---|---------|-----|---|
| torsion | 7  | 1  | 309 | 206 | 3.0680  | 0.0 | 1 | 0.7221  | 180.0 | 2 | 1.3395  | 0.0 | 3 |
| torsion | 7  | 1  | 309 | 204 | -2.3156 | 0.0 | 1 | 0.5960  | 180.0 | 2 | -0.4931 | 0.0 | 3 |
| torsion | 1  | 1  | 309 | 206 | 2.8904  | 0.0 | 1 | 0.8799  | 180.0 | 2 | -0.6047 | 0.0 | 3 |
| torsion | 1  | 1  | 309 | 204 | -2.1630 | 0.0 | 1 | 0.7937  | 180.0 | 2 | 1.4200  | 0.0 | 3 |
| torsion | 4  | 1  | 309 | 206 | -0.9875 | 0.0 | 1 | -0.1860 | 180.0 | 2 | 0.3465  | 0.0 | 3 |
| torsion | 4  | 1  | 309 | 204 | 1.1066  | 0.0 | 1 | -0.1424 | 180.0 | 2 | -0.1781 | 0.0 | 3 |
|         |    |    |     |     |         |     |   |         |       |   |         |     |   |
| torsion | 57 | 51 | 309 | 206 | 4.2998  | 0.0 | 1 | -1.4544 | 180.0 | 2 | -0.0520 | 0.0 | 3 |
| torsion | 57 | 51 | 309 | 204 | -3.1839 | 0.0 | 1 | -2.2337 | 180.0 | 2 | 0.0000  | 0.0 | 3 |
| torsion | 51 | 51 | 309 | 206 | 0.0437  | 0.0 | 1 | 0.5706  | 180.0 | 2 | -0.5156 | 0.0 | 3 |
| torsion | 51 | 51 | 309 | 204 | 0.8187  | 0.0 | 1 | 3.8088  | 180.0 | 2 | 0.6040  | 0.0 | 3 |
| torsion | 54 | 51 | 309 | 206 | -0.9451 | 0.0 | 1 | 2.1213  | 180.0 | 2 | 0.3370  | 0.0 | 3 |
| torsion | 54 | 51 | 309 | 204 | -0.4801 | 0.0 | 1 | -0.6837 | 180.0 | 2 | -0.2819 | 0.0 | 3 |

#

# Kai for Cytidine C1'-1, N1-209

#

|         |   |   |     |     |         |     |   |         |       |   |         |     |   |
|---------|---|---|-----|-----|---------|-----|---|---------|-------|---|---------|-----|---|
| torsion | 7 | 1 | 209 | 206 | 3.0680  | 0.0 | 1 | 0.7221  | 180.0 | 2 | 1.3395  | 0.0 | 3 |
| torsion | 7 | 1 | 209 | 204 | -2.3156 | 0.0 | 1 | 0.5960  | 180.0 | 2 | -0.4931 | 0.0 | 3 |
| torsion | 1 | 1 | 209 | 206 | 2.8904  | 0.0 | 1 | 0.8799  | 180.0 | 2 | -0.6047 | 0.0 | 3 |
| torsion | 1 | 1 | 209 | 204 | -2.1630 | 0.0 | 1 | 0.7937  | 180.0 | 2 | 1.4200  | 0.0 | 3 |
| torsion | 4 | 1 | 209 | 206 | -0.9875 | 0.0 | 1 | -0.1860 | 180.0 | 2 | 0.3465  | 0.0 | 3 |
| torsion | 4 | 1 | 209 | 204 | 1.1066  | 0.0 | 1 | -0.1424 | 180.0 | 2 | -0.1781 | 0.0 | 3 |

#

# Kai for Deoxycytidine C1'-51, N1-209

#

|         |    |    |     |     |         |     |   |         |       |   |         |     |   |
|---------|----|----|-----|-----|---------|-----|---|---------|-------|---|---------|-----|---|
| torsion | 57 | 51 | 209 | 206 | 4.2998  | 0.0 | 1 | -1.4544 | 180.0 | 2 | -0.0520 | 0.0 | 3 |
| torsion | 57 | 51 | 209 | 204 | -3.1839 | 0.0 | 1 | -2.2337 | 180.0 | 2 | 0.0000  | 0.0 | 3 |
| torsion | 51 | 51 | 209 | 206 | 0.0437  | 0.0 | 1 | 0.5706  | 180.0 | 2 | -0.1016 | 0.0 | 3 |
| torsion | 51 | 51 | 209 | 204 | 0.8187  | 0.0 | 1 | 3.8088  | 180.0 | 2 | -0.1104 | 0.0 | 3 |
| torsion | 54 | 51 | 209 | 206 | -0.9451 | 0.0 | 1 | 2.1213  | 180.0 | 2 | 0.3370  | 0.0 | 3 |
| torsion | 54 | 51 | 209 | 204 | -0.4801 | 0.0 | 1 | -0.6837 | 180.0 | 2 | -0.2812 | 0.0 | 3 |

#####

|         |    |     |     |     |        |     |   |         |       |   |        |     |   |
|---------|----|-----|-----|-----|--------|-----|---|---------|-------|---|--------|-----|---|
| torsion | 1  | 209 | 204 | 204 | 0.0000 | 0.0 | 1 | 3.9252  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1  | 209 | 206 | 209 | 0.0000 | 0.0 | 1 | 3.9860  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1  | 209 | 206 | 213 | 0.0000 | 0.0 | 1 | 10.3740 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1  | 209 | 206 | 211 | 0.0000 | 0.0 | 1 | 4.2953  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1  | 209 | 204 | 202 | 0.0000 | 0.0 | 1 | 6.8558  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1  | 209 | 204 | 216 | 0.0000 | 0.0 | 1 | 4.9036  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51 | 209 | 204 | 204 | 0.0000 | 0.0 | 1 | 3.9252  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51 | 209 | 206 | 209 | 0.0000 | 0.0 | 1 | 3.9860  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51 | 209 | 206 | 213 | 0.0000 | 0.0 | 1 | 10.3740 | 180.0 | 2 | 0.0000 | 0.0 | 3 |

|         |     |     |     |     |        |     |   |         |       |   |        |     |   |
|---------|-----|-----|-----|-----|--------|-----|---|---------|-------|---|--------|-----|---|
| torsion | 51  | 209 | 206 | 211 | 0.0000 | 0.0 | 1 | 4.2953  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 209 | 204 | 202 | 0.0000 | 0.0 | 1 | 6.8558  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 209 | 204 | 216 | 0.0000 | 0.0 | 1 | 4.9036  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1   | 309 | 204 | 204 | 0.0000 | 0.0 | 1 | 3.9252  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1   | 309 | 206 | 209 | 0.0000 | 0.0 | 1 | 3.9860  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1   | 309 | 206 | 309 | 0.0000 | 0.0 | 1 | 3.9860  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1   | 209 | 206 | 309 | 0.0000 | 0.0 | 1 | 3.9860  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1   | 309 | 206 | 213 | 0.0000 | 0.0 | 1 | 10.3740 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1   | 309 | 206 | 211 | 0.0000 | 0.0 | 1 | 4.2953  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1   | 309 | 204 | 202 | 0.0000 | 0.0 | 1 | 6.8558  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1   | 309 | 204 | 216 | 0.0000 | 0.0 | 1 | 4.9036  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 309 | 204 | 204 | 0.0000 | 0.0 | 1 | 3.9252  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 309 | 206 | 209 | 0.0000 | 0.0 | 1 | 3.9860  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 309 | 206 | 309 | 0.0000 | 0.0 | 1 | 3.9860  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 209 | 206 | 309 | 0.0000 | 0.0 | 1 | 3.9860  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 309 | 206 | 213 | 0.0000 | 0.0 | 1 | 10.3740 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 309 | 206 | 211 | 0.0000 | 0.0 | 1 | 4.2953  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 309 | 204 | 202 | 0.0000 | 0.0 | 1 | 6.8558  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 309 | 204 | 216 | 0.0000 | 0.0 | 1 | 4.9036  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1   | 210 | 205 | 212 | 0.0000 | 0.0 | 1 | 3.0141  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1   | 210 | 205 | 216 | 0.0000 | 0.0 | 1 | 2.0747  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1   | 210 | 207 | 207 | 0.0000 | 0.0 | 1 | 3.5510  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1   | 210 | 207 | 211 | 0.0000 | 0.0 | 1 | 2.5017  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 210 | 205 | 212 | 0.0000 | 0.0 | 1 | 3.0141  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 210 | 205 | 216 | 0.0000 | 0.0 | 1 | 2.0747  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 210 | 207 | 207 | 0.0000 | 0.0 | 1 | 3.5510  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 210 | 207 | 211 | 0.0000 | 0.0 | 1 | 2.5017  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1   | 310 | 205 | 212 | 0.0000 | 0.0 | 1 | 3.0141  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1   | 310 | 205 | 216 | 0.0000 | 0.0 | 1 | 2.0747  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1   | 310 | 207 | 207 | 0.0000 | 0.0 | 1 | 3.5510  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 1   | 310 | 207 | 211 | 0.0000 | 0.0 | 1 | 2.5017  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 310 | 205 | 212 | 0.0000 | 0.0 | 1 | 3.0141  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 310 | 205 | 216 | 0.0000 | 0.0 | 1 | 2.0747  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 310 | 207 | 207 | 0.0000 | 0.0 | 1 | 3.5510  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 51  | 310 | 207 | 211 | 0.0000 | 0.0 | 1 | 2.5017  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 209 | 206 | 204 | 201 | 0.0000 | 0.0 | 1 | 9.4387  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 213 | 206 | 204 | 201 | 0.0000 | 0.0 | 1 | 4.6447  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 209 | 206 | 204 | 204 | 0.0000 | 0.0 | 1 | 3.8898  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 206 | 209 | 206 | 204 | 0.0000 | 0.0 | 1 | 3.6586  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 213 | 206 | 204 | 204 | 0.0000 | 0.0 | 1 | 3.8721  | 180.0 | 2 | 0.0000 | 0.0 | 3 |

|         |     |     |     |     |        |     |   |         |       |   |        |     |   |
|---------|-----|-----|-----|-----|--------|-----|---|---------|-------|---|--------|-----|---|
| torsion | 204 | 206 | 209 | 218 | 0.0000 | 0.0 | 1 | 3.6657  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 204 | 211 | 220 | 207 | 0.0000 | 0.0 | 1 | 9.5374  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 204 | 211 | 220 | 208 | 0.0000 | 0.0 | 1 | 11.9757 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 206 | 207 | 212 | 205 | 0.0000 | 0.0 | 1 | 3.4413  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 207 | 207 | 210 | 205 | 0.0000 | 0.0 | 1 | 14.1887 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 204 | 211 | 207 | 207 | 0.0000 | 0.0 | 1 | 10.5041 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 219 | 211 | 207 | 207 | 0.0000 | 0.0 | 1 | 7.8605  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 207 | 207 | 212 | 205 | 0.0000 | 0.0 | 1 | 20.1574 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 209 | 219 | 211 | 207 | 0.0000 | 0.0 | 1 | 4.8518  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 208 | 219 | 211 | 207 | 0.0000 | 0.0 | 1 | 16.9078 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 211 | 204 | 211 | 207 | 0.0000 | 0.0 | 1 | 7.2592  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 207 | 211 | 204 | 221 | 0.0000 | 0.0 | 1 | 14.6045 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 207 | 212 | 205 | 216 | 0.0000 | 0.0 | 1 | 7.6499  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 207 | 212 | 205 | 210 | 0.0000 | 0.0 | 1 | 26.3154 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 208 | 219 | 209 | 206 | 0.0000 | 0.0 | 1 | 3.9243  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 207 | 207 | 220 | 208 | 0.0000 | 0.0 | 1 | 9.8846  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 208 | 220 | 207 | 212 | 0.0000 | 0.0 | 1 | 3.7767  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 208 | 219 | 209 | 218 | 0.0000 | 0.0 | 1 | 3.7767  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 209 | 206 | 207 | 207 | 0.0000 | 0.0 | 1 | 7.9802  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 209 | 206 | 207 | 212 | 0.0000 | 0.0 | 1 | 3.8100  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 206 | 207 | 207 | 210 | 0.0000 | 0.0 | 1 | 3.5955  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 212 | 207 | 207 | 210 | 0.0000 | 0.0 | 1 | 12.6346 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 219 | 211 | 207 | 210 | 0.0000 | 0.0 | 1 | 13.8997 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 211 | 204 | 211 | 220 | 0.0000 | 0.0 | 1 | 7.7095  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 211 | 207 | 207 | 206 | 0.0000 | 0.0 | 1 | 3.5397  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 211 | 207 | 207 | 212 | 0.0000 | 0.0 | 1 | 2.7775  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 211 | 207 | 207 | 220 | 0.0000 | 0.0 | 1 | 3.5839  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 211 | 207 | 210 | 205 | 0.0000 | 0.0 | 1 | 3.0308  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 211 | 219 | 209 | 206 | 0.0000 | 0.0 | 1 | 3.8537  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 211 | 219 | 209 | 218 | 0.0000 | 0.0 | 1 | 3.9278  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 211 | 220 | 207 | 207 | 0.0000 | 0.0 | 1 | 4.2558  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 211 | 220 | 207 | 212 | 0.0000 | 0.0 | 1 | 3.7755  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 207 | 210 | 205 | 212 | 0.0000 | 0.0 | 1 | 26.4627 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 207 | 207 | 206 | 213 | 0.0000 | 0.0 | 1 | 6.0510  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 213 | 206 | 207 | 212 | 0.0000 | 0.0 | 1 | 3.8101  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 206 | 209 | 206 | 213 | 0.0000 | 0.0 | 1 | 3.5724  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 204 | 204 | 201 | 214 | 0.0000 | 0.0 | 1 | 2.4000  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 206 | 204 | 201 | 214 | 0.0000 | 0.0 | 1 | 0.2828  | 180.0 | 2 | 0.4939 | 0.0 | 3 |
| torsion | 201 | 204 | 204 | 216 | 0.0000 | 0.0 | 1 | 4.0260  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 206 | 204 | 204 | 216 | 0.0000 | 0.0 | 1 | 3.6824  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 207 | 210 | 205 | 216 | 0.0000 | 0.0 | 1 | 3.5896  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 220 | 211 | 204 | 221 | 0.0000 | 0.0 | 1 | 13.7943 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 220 | 207 | 212 | 205 | 0.0000 | 0.0 | 1 | 3.4849  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 209 | 219 | 208 | 217 | 0.0000 | 0.0 | 1 | 1.0707  | 180.0 | 2 | 0.0000 | 0.0 | 3 |

|         |     |     |     |     |        |     |   |         |       |   |        |     |   |
|---------|-----|-----|-----|-----|--------|-----|---|---------|-------|---|--------|-----|---|
| torsion | 211 | 219 | 208 | 217 | 0.0000 | 0.0 | 1 | 1.3026  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 207 | 220 | 208 | 217 | 0.0000 | 0.0 | 1 | 1.8849  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 211 | 220 | 208 | 217 | 0.0000 | 0.0 | 1 | 0.6219  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 207 | 206 | 209 | 218 | 0.0000 | 0.0 | 1 | 3.8115  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 213 | 206 | 209 | 218 | 0.0000 | 0.0 | 1 | 10.4899 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 219 | 209 | 206 | 207 | 0.0000 | 0.0 | 1 | 3.6487  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 219 | 209 | 206 | 213 | 0.0000 | 0.0 | 1 | 3.7300  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 204 | 209 | 206 | 213 | 0.0000 | 0.0 | 1 | 3.2313  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 204 | 209 | 206 | 211 | 0.0000 | 0.0 | 1 | 3.7741  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 206 | 209 | 204 | 202 | 0.0000 | 0.0 | 1 | 3.9712  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 206 | 209 | 204 | 216 | 0.0000 | 0.0 | 1 | 5.8955  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 209 | 206 | 211 | 220 | 0.0000 | 0.0 | 1 | 3.7982  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 213 | 206 | 211 | 220 | 0.0000 | 0.0 | 1 | 17.6127 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 206 | 211 | 220 | 208 | 0.0000 | 0.0 | 1 | 17.5619 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 206 | 211 | 220 | 202 | 0.0000 | 0.0 | 1 | 3.8561  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 202 | 220 | 208 | 217 | 0.0000 | 0.0 | 1 | 2.0747  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 211 | 220 | 202 | 204 | 0.0000 | 0.0 | 1 | 8.7345  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 211 | 220 | 202 | 215 | 0.0000 | 0.0 | 1 | 4.0425  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 208 | 220 | 202 | 204 | 0.0000 | 0.0 | 1 | 4.7018  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 208 | 220 | 202 | 215 | 0.0000 | 0.0 | 1 | 4.1631  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 220 | 202 | 204 | 209 | 0.0000 | 0.0 | 1 | 8.8842  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 220 | 202 | 204 | 216 | 0.0000 | 0.0 | 1 | 4.7300  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 215 | 202 | 204 | 209 | 0.0000 | 0.0 | 1 | 5.0349  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 215 | 202 | 204 | 216 | 0.0000 | 0.0 | 1 | 3.3113  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 209 | 206 | 204 | 221 | 0.0000 | 0.0 | 1 | 9.1486  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 213 | 206 | 204 | 221 | 0.0000 | 0.0 | 1 | 4.7892  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 216 | 204 | 204 | 221 | 0.0000 | 0.0 | 1 | 3.6987  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
|         |     |     |     |     |        |     |   |         |       |   |        |     |   |
| torsion | 221 | 204 | 204 | 309 | 0.0000 | 0.0 | 1 | 3.9414  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 206 | 309 | 204 | 202 | 0.0000 | 0.0 | 1 | 3.9712  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 207 | 207 | 310 | 205 | 0.0000 | 0.0 | 1 | 14.1887 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 204 | 206 | 309 | 206 | 0.0000 | 0.0 | 1 | 3.6586  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 215 | 202 | 204 | 309 | 0.0000 | 0.0 | 1 | 5.0349  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 201 | 204 | 206 | 309 | 0.0000 | 0.0 | 1 | 9.4387  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 204 | 204 | 206 | 309 | 0.0000 | 0.0 | 1 | 3.8898  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 207 | 207 | 206 | 309 | 0.0000 | 0.0 | 1 | 7.9802  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 207 | 212 | 205 | 310 | 0.0000 | 0.0 | 1 | 26.3154 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 206 | 207 | 207 | 310 | 0.0000 | 0.0 | 1 | 3.5955  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 204 | 309 | 206 | 211 | 0.0000 | 0.0 | 1 | 3.7741  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 205 | 310 | 207 | 211 | 0.0000 | 0.0 | 1 | 3.0308  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 207 | 310 | 205 | 212 | 0.0000 | 0.0 | 1 | 26.4627 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 309 | 206 | 207 | 212 | 0.0000 | 0.0 | 1 | 3.8100  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 310 | 207 | 207 | 212 | 0.0000 | 0.0 | 1 | 3.8100  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 206 | 309 | 206 | 213 | 0.0000 | 0.0 | 1 | 3.5724  | 180.0 | 2 | 0.0000 | 0.0 | 3 |

|         |     |     |     |     |        |     |   |         |       |   |        |     |   |
|---------|-----|-----|-----|-----|--------|-----|---|---------|-------|---|--------|-----|---|
| torsion | 204 | 309 | 206 | 213 | 0.0000 | 0.0 | 1 | 3.2313  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 206 | 309 | 204 | 216 | 0.0000 | 0.0 | 1 | 5.8955  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 207 | 310 | 205 | 216 | 0.0000 | 0.0 | 1 | 3.5896  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 207 | 206 | 309 | 218 | 0.0000 | 0.0 | 1 | 3.8115  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 213 | 206 | 309 | 218 | 0.0000 | 0.0 | 1 | 10.4899 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 204 | 309 | 206 | 209 | 0.0000 | 0.0 | 1 | 3.8556  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 206 | 309 | 204 | 204 | 0.0000 | 0.0 | 1 | 7.1476  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 309 | 206 | 209 | 206 | 0.0000 | 0.0 | 1 | 3.5107  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 309 | 206 | 209 | 218 | 0.0000 | 0.0 | 1 | 3.8689  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 206 | 204 | 204 | 309 | 0.0000 | 0.0 | 1 | 3.9253  | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 201 | 204 | 204 | 309 | 0.0000 | 0.0 | 1 | 10.2722 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 204 | 211 | 207 | 310 | 0.0000 | 0.0 | 1 | 11.4098 | 180.0 | 2 | 0.0000 | 0.0 | 3 |
| torsion | 220 | 207 | 207 | 310 | 0.0000 | 0.0 | 1 | 3.6959  | 180.0 | 2 | 0.0000 | 0.0 | 3 |

|        |     |     |       |
|--------|-----|-----|-------|
| pitors | 202 | 204 | 4.000 |
| pitors | 204 | 204 | 4.000 |
| pitors | 202 | 220 | 4.000 |
| pitors | 207 | 220 | 4.000 |
| pitors | 207 | 207 | 4.000 |
| pitors | 207 | 210 | 6.000 |
| pitors | 205 | 210 | 6.000 |
| pitors | 207 | 310 | 6.000 |
| pitors | 205 | 310 | 6.000 |
| pitors | 204 | 206 | 3.000 |
| pitors | 207 | 206 | 3.000 |
| pitors | 206 | 209 | 3.000 |
| pitors | 204 | 209 | 3.000 |
| pitors | 219 | 209 | 3.000 |
| pitors | 206 | 309 | 3.000 |
| pitors | 204 | 309 | 3.000 |
| pitors | 219 | 309 | 3.000 |
| pitors | 220 | 208 | 6.000 |
| pitors | 219 | 208 | 4.000 |

|         |     |     |    |    |     |     |     |     |     |      |     |     |     |
|---------|-----|-----|----|----|-----|-----|-----|-----|-----|------|-----|-----|-----|
| strtors | 205 | 210 | 1  | 7  | 0.0 | 0.0 | 1.5 | 0.0 | 0.0 | -4.0 | 0.0 | 0.0 | 5.2 |
| strtors | 205 | 310 | 1  | 7  | 0.0 | 0.0 | 1.5 | 0.0 | 0.0 | -4.0 | 0.0 | 0.0 | 5.2 |
| strtors | 204 | 209 | 1  | 7  | 0.0 | 0.0 | 1.5 | 0.0 | 0.0 | -4.0 | 0.0 | 0.0 | 5.2 |
| strtors | 204 | 309 | 1  | 7  | 0.0 | 0.0 | 1.5 | 0.0 | 0.0 | -4.0 | 0.0 | 0.0 | 5.2 |
| strtors | 205 | 210 | 51 | 57 | 0.0 | 0.0 | 1.5 | 0.0 | 0.0 | -4.0 | 0.0 | 0.0 | 5.2 |
| strtors | 205 | 310 | 51 | 57 | 0.0 | 0.0 | 1.5 | 0.0 | 0.0 | -4.0 | 0.0 | 0.0 | 5.2 |
| strtors | 204 | 209 | 51 | 57 | 0.0 | 0.0 | 1.5 | 0.0 | 0.0 | -4.0 | 0.0 | 0.0 | 5.2 |
| strtors | 204 | 309 | 51 | 57 | 0.0 | 0.0 | 1.5 | 0.0 | 0.0 | -4.0 | 0.0 | 0.0 | 5.2 |

|         |     |     |   |   |        |        |         |        |        |         |  |  |  |
|---------|-----|-----|---|---|--------|--------|---------|--------|--------|---------|--|--|--|
| angtors | 205 | 210 | 1 | 7 | 0.0140 | 0.0000 | -0.0580 | 0.0000 | 0.0000 | -0.0110 |  |  |  |
|---------|-----|-----|---|---|--------|--------|---------|--------|--------|---------|--|--|--|

|         |     |     |    |    |        |        |         |        |        |         |
|---------|-----|-----|----|----|--------|--------|---------|--------|--------|---------|
| angtors | 205 | 310 | 1  | 7  | 0.0140 | 0.0000 | -0.0580 | 0.0000 | 0.0000 | -0.0110 |
| angtors | 204 | 209 | 1  | 7  | 0.0140 | 0.0000 | -0.0580 | 0.0000 | 0.0000 | -0.0110 |
| angtors | 204 | 309 | 1  | 7  | 0.0140 | 0.0000 | -0.0580 | 0.0000 | 0.0000 | -0.0110 |
| angtors | 205 | 210 | 51 | 57 | 0.0140 | 0.0000 | -0.0580 | 0.0000 | 0.0000 | -0.0110 |
| angtors | 205 | 310 | 51 | 57 | 0.0140 | 0.0000 | -0.0580 | 0.0000 | 0.0000 | -0.0110 |
| angtors | 204 | 209 | 51 | 57 | 0.0140 | 0.0000 | -0.0580 | 0.0000 | 0.0000 | -0.0110 |
| angtors | 204 | 309 | 51 | 57 | 0.0140 | 0.0000 | -0.0580 | 0.0000 | 0.0000 | -0.0110 |

|         |     |     |    |    |        |         |        |        |        |         |     |     |     |
|---------|-----|-----|----|----|--------|---------|--------|--------|--------|---------|-----|-----|-----|
| strtors | 8   | 101 | 9  | 2  | -4.254 | 0.0     | 0.0    | 0.00   | 1.814  | 0.0     | 0.0 | 0.0 | 0.0 |
| strtors | 9   | 101 | 8  | 1  | -4.254 | 0.0     | 0.0    | 0.00   | 1.814  | 0.0     | 0.0 | 0.0 | 0.0 |
| strtors | 58  | 101 | 59 | 51 | -4.254 | 0.0     | 0.0    | 0.00   | 1.814  | 0.0     | 0.0 | 0.0 | 0.0 |
| strtors | 59  | 101 | 58 | 52 | -4.254 | 0.0     | 0.0    | 0.00   | 1.814  | 0.0     | 0.0 | 0.0 | 0.0 |
| angtors | 102 | 101 | 9  | 2  | 0.0000 | -0.1156 | 0.0000 | 0.0000 | 0.0000 | -0.0112 |     |     |     |
| angtors | 102 | 101 | 8  | 1  | 0.0000 | -0.1156 | 0.0000 | 0.0000 | 0.0000 | -0.0112 |     |     |     |
| angtors | 102 | 101 | 59 | 51 | 0.0000 | -0.1156 | 0.0000 | 0.0000 | 0.0000 | -0.0112 |     |     |     |
| angtors | 102 | 101 | 58 | 52 | 0.0000 | -0.1156 | 0.0000 | 0.0000 | 0.0000 | -0.0112 |     |     |     |

|        |     |   |   |       |       |
|--------|-----|---|---|-------|-------|
| strbnd | 309 | 1 | 7 | 18.70 | 18.70 |
| strbnd | 310 | 1 | 7 | 18.70 | 18.70 |
| strbnd | 209 | 1 | 7 | 18.70 | 18.70 |
| strbnd | 210 | 1 | 7 | 18.70 | 18.70 |
| strbnd | 310 | 1 | 1 | 18.70 | 18.70 |
| strbnd | 310 | 1 | 4 | 11.50 | 11.50 |
| strbnd | 309 | 1 | 1 | 18.70 | 18.70 |
| strbnd | 309 | 1 | 4 | 11.50 | 11.50 |
| strbnd | 210 | 1 | 1 | 18.70 | 18.70 |
| strbnd | 210 | 1 | 4 | 11.50 | 11.50 |
| strbnd | 209 | 1 | 1 | 18.70 | 18.70 |
| strbnd | 209 | 1 | 4 | 11.50 | 11.50 |

|        |     |    |    |       |       |
|--------|-----|----|----|-------|-------|
| strbnd | 309 | 51 | 57 | 18.70 | 18.70 |
| strbnd | 310 | 51 | 57 | 18.70 | 18.70 |
| strbnd | 209 | 51 | 57 | 18.70 | 18.70 |
| strbnd | 210 | 51 | 57 | 18.70 | 18.70 |
| strbnd | 310 | 51 | 51 | 18.70 | 18.70 |
| strbnd | 310 | 51 | 54 | 11.50 | 11.50 |
| strbnd | 309 | 51 | 51 | 18.70 | 18.70 |
| strbnd | 309 | 51 | 54 | 11.50 | 11.50 |
| strbnd | 210 | 51 | 51 | 18.70 | 18.70 |
| strbnd | 210 | 51 | 54 | 11.50 | 11.50 |
| strbnd | 209 | 51 | 51 | 18.70 | 18.70 |
| strbnd | 209 | 51 | 54 | 11.50 | 11.50 |

|        |   |   |    |       |       |
|--------|---|---|----|-------|-------|
| strbnd | 8 | 1 | 11 | 18.70 | 18.70 |
|--------|---|---|----|-------|-------|

|        |    |   |    |       |       |
|--------|----|---|----|-------|-------|
| strbnd | 8  | 1 | 1  | 18.70 | 18.70 |
| strbnd | 8  | 1 | 4  | 11.50 | 11.50 |
| strbnd | 18 | 1 | 11 | 18.70 | 18.70 |
| strbnd | 18 | 1 | 1  | 18.70 | 18.70 |
| strbnd | 18 | 1 | 4  | 11.50 | 11.50 |
| strbnd | 7  | 1 | 1  | 18.70 | 18.70 |
| strbnd | 7  | 1 | 4  | 11.50 | 11.50 |
| strbnd | 11 | 1 | 1  | 18.70 | 18.70 |
| strbnd | 11 | 1 | 4  | 11.50 | 11.50 |
| strbnd | 1  | 1 | 11 | 18.70 | 18.70 |
| strbnd | 1  | 1 | 1  | 18.70 | 18.70 |
| strbnd | 1  | 1 | 4  | 11.50 | 11.50 |
| strbnd | 1  | 1 | 10 | 18.70 | 18.70 |
| strbnd | 4  | 1 | 10 | 11.50 | 11.50 |

|        |    |   |     |       |       |
|--------|----|---|-----|-------|-------|
| strbnd | 5  | 2 | 9   | 11.50 | 11.50 |
| strbnd | 5  | 2 | 19  | 11.50 | 11.50 |
| strbnd | 5  | 2 | 11  | 11.50 | 11.50 |
| strbnd | 9  | 2 | 11  | 18.70 | 18.70 |
| strbnd | 19 | 2 | 11  | 18.70 | 18.70 |
| strbnd | 2  | 9 | 101 | 14.40 | 14.40 |

|        |   |    |    |       |       |
|--------|---|----|----|-------|-------|
| strbnd | 2 | 11 | 7  | 18.70 | 18.70 |
| strbnd | 2 | 11 | 1  | 18.70 | 18.70 |
| strbnd | 2 | 11 | 4  | 11.50 | 11.50 |
| strbnd | 7 | 11 | 1  | 18.70 | 18.70 |
| strbnd | 7 | 11 | 4  | 11.50 | 11.50 |
| strbnd | 1 | 11 | 4  | 11.50 | 11.50 |
| strbnd | 1 | 11 | 10 | 18.70 | 18.70 |

|        |    |    |    |       |       |
|--------|----|----|----|-------|-------|
| strbnd | 59 | 51 | 60 | 18.70 | 18.70 |
| strbnd | 59 | 51 | 51 | 18.70 | 18.70 |
| strbnd | 59 | 51 | 54 | 11.50 | 11.50 |
| strbnd | 69 | 51 | 60 | 18.70 | 18.70 |
| strbnd | 69 | 51 | 51 | 18.70 | 18.70 |
| strbnd | 69 | 51 | 54 | 11.50 | 11.50 |
| strbnd | 57 | 51 | 51 | 18.70 | 18.70 |
| strbnd | 57 | 51 | 54 | 11.50 | 11.50 |
| strbnd | 60 | 51 | 51 | 18.70 | 18.70 |
| strbnd | 60 | 51 | 54 | 11.50 | 11.50 |
| strbnd | 51 | 51 | 60 | 18.70 | 18.70 |
| strbnd | 51 | 51 | 51 | 18.70 | 18.70 |
| strbnd | 51 | 51 | 54 | 11.50 | 11.50 |

|        |     |     |     |       |       |
|--------|-----|-----|-----|-------|-------|
| strbnd | 55  | 52  | 58  | 11.50 | 11.50 |
| strbnd | 55  | 52  | 68  | 11.50 | 11.50 |
| strbnd | 55  | 52  | 60  | 11.50 | 11.50 |
| strbnd | 58  | 52  | 60  | 18.70 | 18.70 |
| strbnd | 68  | 52  | 60  | 18.70 | 18.70 |
| strbnd | 52  | 58  | 101 | 14.40 | 14.40 |
|        |     |     |     |       |       |
| strbnd | 52  | 60  | 57  | 18.70 | 18.70 |
| strbnd | 52  | 60  | 51  | 18.70 | 18.70 |
| strbnd | 52  | 60  | 54  | 11.50 | 11.50 |
| strbnd | 57  | 60  | 51  | 18.70 | 18.70 |
| strbnd | 57  | 60  | 54  | 11.50 | 11.50 |
| strbnd | 51  | 60  | 54  | 11.50 | 11.50 |
|        |     |     |     |       |       |
| strbnd | 207 | 310 | 205 | 14.40 | 14.40 |
| strbnd | 207 | 310 | 1   | 14.40 | 14.40 |
| strbnd | 205 | 310 | 1   | 14.40 | 14.40 |
|        |     |     |     |       |       |
| strbnd | 206 | 209 | 204 | 14.40 | 14.40 |
| strbnd | 206 | 209 | 1   | 14.40 | 14.40 |
| strbnd | 204 | 209 | 1   | 14.40 | 14.40 |
|        |     |     |     |       |       |
| strbnd | 206 | 309 | 204 | 14.40 | 14.40 |
| strbnd | 206 | 309 | 1   | 14.40 | 14.40 |
| strbnd | 204 | 309 | 1   | 14.40 | 14.40 |
|        |     |     |     |       |       |
| strbnd | 207 | 210 | 205 | 14.40 | 14.40 |
| strbnd | 207 | 210 | 1   | 14.40 | 14.40 |
| strbnd | 205 | 210 | 1   | 14.40 | 14.40 |
|        |     |     |     |       |       |
| strbnd | 207 | 310 | 205 | 14.40 | 14.40 |
| strbnd | 207 | 310 | 51  | 14.40 | 14.40 |
| strbnd | 205 | 310 | 51  | 14.40 | 14.40 |
|        |     |     |     |       |       |
| strbnd | 206 | 209 | 204 | 14.40 | 14.40 |
| strbnd | 206 | 209 | 51  | 14.40 | 14.40 |
| strbnd | 204 | 209 | 51  | 14.40 | 14.40 |
|        |     |     |     |       |       |
| strbnd | 206 | 309 | 204 | 14.40 | 14.40 |
| strbnd | 206 | 309 | 51  | 14.40 | 14.40 |
| strbnd | 204 | 309 | 51  | 14.40 | 14.40 |
|        |     |     |     |       |       |
| strbnd | 207 | 210 | 205 | 14.40 | 14.40 |
| strbnd | 207 | 210 | 51  | 14.40 | 14.40 |



strbnd 205 210 51 14.40 14.40

strbnd 202 202 220 18.70 18.70  
strbnd 204 202 220 18.70 18.70  
strbnd 204 202 204 18.70 18.70  
strbnd 206 207 207 18.70 18.70  
strbnd 207 207 220 18.70 18.70  
strbnd 207 207 210 18.70 18.70  
strbnd 207 207 211 18.70 18.70  
strbnd 207 207 212 18.70 18.70  
strbnd 207 220 211 18.70 18.70  
strbnd 207 220 208 18.70 18.70  
strbnd 202 202 208 18.70 18.70  
strbnd 202 220 208 18.70 18.70  
strbnd 208 219 209 18.70 18.70  
strbnd 204 204 206 18.70 18.70  
strbnd 202 204 209 18.70 18.70  
strbnd 204 204 209 18.70 18.70  
strbnd 204 211 204 14.40 14.40  
strbnd 204 211 220 14.40 14.40  
strbnd 206 211 220 14.40 14.40  
strbnd 204 211 207 14.40 14.40  
strbnd 207 211 219 14.40 14.40  
strbnd 205 212 207 14.40 14.40  
strbnd 205 210 207 18.70 18.70  
strbnd 212 207 220 18.70 18.70  
strbnd 206 207 212 18.70 18.70  
strbnd 210 207 211 18.70 18.70  
strbnd 210 205 212 18.70 18.70  
strbnd 211 206 213 18.70 18.70  
strbnd 211 204 211 18.70 18.70  
strbnd 208 219 211 18.70 18.70  
strbnd 208 220 211 18.70 18.70  
strbnd 202 204 211 18.70 18.70  
strbnd 202 220 211 18.70 18.70  
strbnd 209 206 209 18.70 18.70  
strbnd 209 206 211 18.70 18.70  
strbnd 209 206 213 18.70 18.70  
strbnd 209 219 211 18.70 18.70  
strbnd 207 206 213 18.70 18.70  
strbnd 204 206 213 18.70 18.70  
strbnd 204 206 209 18.70 18.70  
strbnd 207 206 209 18.70 18.70  
strbnd 206 209 206 7.20 7.20

|        |     |     |     |       |          |
|--------|-----|-----|-----|-------|----------|
| strbnd | 204 | 209 | 206 | 7.20  | 7.20     |
| strbnd | 206 | 209 | 219 | 7.20  | 7.20     |
| strbnd | 201 | 204 | 204 | 18.70 | 18.70    |
| strbnd | 201 | 204 | 206 | 18.70 | 18.70    |
| strbnd | 204 | 201 | 214 | 11.50 | 11.50    |
| strbnd | 214 | 201 | 214 | 11.50 | 11.50    |
| strbnd | 204 | 202 | 215 | 18.70 | 18.70    |
| strbnd | 215 | 202 | 220 | 18.70 | 18.70    |
| strbnd | 202 | 204 | 216 | 11.50 | 11.50    |
| strbnd | 204 | 204 | 216 | 11.50 | 11.50    |
| strbnd | 204 | 204 | 221 | 18.70 | 18.70    |
| strbnd | 206 | 204 | 221 | 18.70 | 18.70    |
| strbnd | 209 | 204 | 216 | 11.50 | 11.50    |
| strbnd | 211 | 204 | 221 | 18.70 | 18.70    |
| strbnd | 210 | 205 | 216 | 11.50 | 11.50    |
| strbnd | 212 | 205 | 216 | 11.50 | 11.50 // |
| strbnd | 217 | 208 | 219 | 4.30  | 4.30     |
| strbnd | 217 | 208 | 220 | 4.30  | 4.30     |
| strbnd | 217 | 208 | 217 | 4.30  | 4.30     |
| strbnd | 218 | 209 | 219 | 4.30  | 4.30     |
| strbnd | 204 | 209 | 218 | 4.30  | 4.30     |
| strbnd | 206 | 209 | 218 | 4.30  | 4.30     |
| strbnd | 204 | 309 | 206 | 18.70 | 18.70    |
| strbnd | 206 | 309 | 206 | 18.70 | 18.70    |
| strbnd | 205 | 310 | 207 | 18.70 | 18.70    |
| strbnd | 202 | 204 | 309 | 18.70 | 18.70    |
| strbnd | 204 | 204 | 309 | 18.70 | 18.70    |
| strbnd | 208 | 219 | 309 | 18.70 | 18.70    |
| strbnd | 204 | 206 | 309 | 18.70 | 18.70    |
| strbnd | 207 | 206 | 309 | 18.70 | 18.70    |
| strbnd | 209 | 206 | 309 | 18.70 | 18.70    |
| strbnd | 309 | 206 | 309 | 18.70 | 18.70    |
| strbnd | 207 | 207 | 310 | 18.70 | 18.70    |
| strbnd | 310 | 207 | 211 | 18.70 | 18.70    |
| strbnd | 310 | 205 | 212 | 18.70 | 18.70    |
| strbnd | 309 | 206 | 213 | 18.70 | 18.70    |
| strbnd | 309 | 204 | 216 | 11.50 | 11.50    |
| strbnd | 310 | 205 | 216 | 11.50 | 11.50    |
| strbnd | 204 | 309 | 218 | 4.30  | 4.30     |
| strbnd | 206 | 309 | 218 | 4.30  | 4.30     |

|       |     |     |     |     |         |
|-------|-----|-----|-----|-----|---------|
| opbnd | 206 | 204 | 201 | 204 | 8.5038  |
| opbnd | 215 | 202 | 204 | 204 | 13.1715 |
| opbnd | 204 | 204 | 201 | 206 | 8.5038  |

|        |     |     |     |     |         |
|--------|-----|-----|-----|-----|---------|
| opbend | 201 | 204 | 204 | 206 | 8.5038  |
| opbend | 218 | 209 | 206 | 206 | 7.4693  |
| opbend | 212 | 207 | 206 | 207 | 6.9193  |
| opbend | 216 | 204 | 202 | 209 | 10.3143 |
| opbend | 216 | 204 | 204 | 209 | 13.0459 |
| opbend | 213 | 206 | 204 | 209 | 70.6396 |
| opbend | 213 | 206 | 207 | 209 | 70.1557 |
| opbend | 213 | 206 | 209 | 209 | 71.0014 |
| opbend | 211 | 207 | 207 | 210 | 5.8677  |
| opbend | 210 | 207 | 207 | 211 | 5.8677  |
| opbend | 213 | 206 | 209 | 211 | 70.6170 |
| opbend | 207 | 207 | 210 | 211 | 5.8677  |
| opbend | 221 | 204 | 211 | 211 | 10.9555 |
| opbend | 207 | 207 | 206 | 212 | 6.9193  |
| opbend | 206 | 207 | 207 | 212 | 6.9193  |
| opbend | 216 | 205 | 210 | 212 | 8.8783  |
| opbend | 209 | 206 | 204 | 213 | 12.6396 |
| opbend | 209 | 206 | 207 | 213 | 13.1557 |
| opbend | 204 | 206 | 209 | 213 | 12.6396 |
| opbend | 207 | 206 | 209 | 213 | 13.1557 |
| opbend | 209 | 206 | 209 | 213 | 7.5000  |
| opbend | 211 | 206 | 209 | 213 | 12.6170 |
| opbend | 209 | 206 | 211 | 213 | 12.6170 |
| opbend | 204 | 202 | 204 | 215 | 10.3430 |
| opbend | 209 | 204 | 202 | 216 | 10.3143 |
| opbend | 209 | 204 | 204 | 216 | 13.0459 |
| opbend | 202 | 204 | 209 | 216 | 10.3143 |
| opbend | 204 | 204 | 209 | 216 | 13.0459 |
| opbend | 212 | 205 | 210 | 216 | 8.8783  |
| opbend | 211 | 204 | 211 | 221 | 5.9111  |
| opbend | 210 | 205 | 212 | 216 | 8.8783  |
| opbend | 206 | 209 | 206 | 218 | 7.4693  |
| opbend | 218 | 209 | 206 | 219 | 7.0510  |
| opbend | 219 | 209 | 206 | 218 | 7.0510  |
| opbend | 206 | 209 | 219 | 218 | 7.0510  |
| opbend | 207 | 207 | 212 | 220 | 7.9414  |
| opbend | 220 | 207 | 212 | 207 | 7.9414  |
| opbend | 212 | 207 | 220 | 207 | 7.9414  |
| opbend | 204 | 209 | 1   | 206 | 2.1668  |
| opbend | 206 | 209 | 1   | 204 | 2.1668  |
| opbend | 1   | 209 | 206 | 204 | 2.1668  |
| opbend | 204 | 209 | 51  | 206 | 2.1668  |
| opbend | 206 | 209 | 51  | 204 | 2.1668  |
| opbend | 51  | 209 | 206 | 204 | 2.1668  |

|        |     |     |     |     |         |
|--------|-----|-----|-----|-----|---------|
| opbend | 215 | 202 | 220 | 204 | 10.2289 |
| opbend | 204 | 202 | 220 | 215 | 10.2289 |
| opbend | 220 | 202 | 204 | 215 | 10.2289 |
| opbend | 1   | 210 | 205 | 207 | 8.1078  |
| opbend | 207 | 210 | 1   | 205 | 8.1078  |
| opbend | 205 | 210 | 1   | 207 | 8.1078  |
| opbend | 51  | 210 | 205 | 207 | 8.1078  |
| opbend | 207 | 210 | 51  | 205 | 8.1078  |
| opbend | 205 | 210 | 51  | 207 | 8.1078  |
| opbend | 208 | 220 | 207 | 211 | 12.7414 |
| opbend | 207 | 220 | 208 | 211 | 12.7414 |
| opbend | 211 | 220 | 207 | 208 | 12.7414 |
| opbend | 211 | 219 | 208 | 209 | 12.4503 |
| opbend | 208 | 219 | 209 | 211 | 12.4503 |
| opbend | 209 | 219 | 208 | 211 | 12.4503 |
| opbend | 202 | 220 | 208 | 211 | 12.5350 |
| opbend | 208 | 220 | 202 | 211 | 12.5350 |
| opbend | 211 | 220 | 202 | 208 | 12.5350 |
| opbend | 215 | 202 | 204 | 220 | 10.2289 |
| opbend | 204 | 202 | 215 | 220 | 10.2289 |
| opbend | 220 | 202 | 204 | 215 | 10.2289 |
| opbend | 221 | 204 | 204 | 206 | 9.2838  |
| opbend | 204 | 204 | 206 | 221 | 9.2838  |
| opbend | 206 | 204 | 204 | 221 | 9.2838  |

|        |     |     |     |     |         |
|--------|-----|-----|-----|-----|---------|
| opbend | 211 | 219 | 208 | 309 | 12.4503 |
| opbend | 208 | 219 | 309 | 211 | 12.4503 |
| opbend | 309 | 219 | 208 | 211 | 12.4503 |
| opbend | 218 | 309 | 206 | 206 | 7.4693  |
| opbend | 216 | 204 | 202 | 309 | 10.3143 |
| opbend | 216 | 204 | 204 | 309 | 13.0459 |
| opbend | 213 | 206 | 204 | 309 | 70.6396 |
| opbend | 213 | 206 | 207 | 309 | 70.1557 |
| opbend | 213 | 206 | 309 | 209 | 71.0014 |
| opbend | 213 | 206 | 309 | 309 | 71.0014 |
| opbend | 213 | 206 | 209 | 309 | 71.0014 |
| opbend | 211 | 207 | 207 | 310 | 5.8677  |
| opbend | 310 | 207 | 207 | 211 | 5.8677  |
| opbend | 213 | 206 | 309 | 211 | 70.6170 |
| opbend | 207 | 207 | 310 | 211 | 5.8677  |
| opbend | 216 | 205 | 310 | 212 | 8.8783  |
| opbend | 309 | 206 | 204 | 213 | 12.6396 |
| opbend | 309 | 206 | 207 | 213 | 13.1557 |
| opbend | 204 | 206 | 309 | 213 | 12.6396 |

|        |     |     |     |     |         |
|--------|-----|-----|-----|-----|---------|
| opbend | 207 | 206 | 309 | 213 | 13.1557 |
| opbend | 209 | 206 | 309 | 213 | 7.5000  |
| opbend | 309 | 206 | 309 | 213 | 7.5000  |
| opbend | 309 | 206 | 209 | 213 | 7.5000  |
| opbend | 211 | 206 | 309 | 213 | 12.6170 |
| opbend | 309 | 206 | 211 | 213 | 12.6170 |
| opbend | 309 | 204 | 202 | 216 | 10.3143 |
| opbend | 309 | 204 | 204 | 216 | 13.0459 |
| opbend | 202 | 204 | 309 | 216 | 10.3143 |
| opbend | 204 | 204 | 309 | 216 | 13.0459 |
| opbend | 212 | 205 | 310 | 216 | 8.8783  |
| opbend | 310 | 205 | 212 | 216 | 8.8783  |
| opbend | 206 | 309 | 206 | 218 | 7.4693  |
| opbend | 218 | 309 | 206 | 219 | 7.0510  |
| opbend | 219 | 309 | 206 | 218 | 7.0510  |
| opbend | 206 | 309 | 219 | 218 | 7.0510  |
| opbend | 204 | 309 | 1   | 206 | 2.1668  |
| opbend | 206 | 309 | 1   | 204 | 2.1668  |
| opbend | 1   | 309 | 206 | 204 | 2.1668  |
| opbend | 1   | 310 | 205 | 207 | 8.1078  |
| opbend | 207 | 310 | 1   | 205 | 8.1078  |
| opbend | 205 | 310 | 1   | 207 | 8.1078  |
| opbend | 204 | 309 | 51  | 206 | 2.1668  |
| opbend | 206 | 309 | 51  | 204 | 2.1668  |
| opbend | 51  | 309 | 206 | 204 | 2.1668  |
| opbend | 51  | 310 | 205 | 207 | 8.1078  |
| opbend | 207 | 310 | 51  | 205 | 8.1078  |
| opbend | 205 | 310 | 51  | 207 | 8.1078  |

|          |    |        |        |    |       |
|----------|----|--------|--------|----|-------|
| polarize | 1  | 0.8370 | 0.3900 | 2  | 4     |
| polarize | 2  | 1.3340 | 0.3900 | 1  | 3     |
| polarize | 3  | 0.4960 | 0.3900 | 2  |       |
| polarize | 4  | 1.3340 | 0.3900 | 1  | 5     |
| polarize | 5  | 0.4960 | 0.3900 | 4  |       |
| polarize | 6  | 1.3340 | 0.3900 | 7  | 10    |
| polarize | 7  | 0.4960 | 0.3900 | 6  |       |
| polarize | 8  | 1.3340 | 0.3900 | 9  | 12 23 |
| polarize | 9  | 0.4960 | 0.3900 | 8  |       |
| polarize | 10 | 0.8370 | 0.3900 | 6  | 11    |
| polarize | 11 | 0.4960 | 0.3900 | 10 |       |
| polarize | 12 | 0.8370 | 0.3900 | 8  | 101   |
| polarize | 13 | 0.4960 | 0.3900 | 23 |       |
| polarize | 16 | 1.3340 | 0.3900 | 17 | 19 24 |
| polarize | 17 | 0.4960 | 0.3900 | 16 |       |

|          |     |        |        |             |       |
|----------|-----|--------|--------|-------------|-------|
| polarize | 19  | 0.8370 | 0.3900 | 16          | 101   |
| polarize | 20  | 0.4960 | 0.3900 | 24          |       |
| polarize | 23  | 0.8370 | 0.3900 | 8           | 13    |
| polarize | 24  | 0.8370 | 0.3900 | 16          | 20    |
| polarize | 51  | 1.3340 | 0.3900 | 55          | 61    |
| polarize | 52  | 1.3340 | 0.3900 | 60          | 64 73 |
| polarize | 53  | 1.3340 | 0.3900 | 56          |       |
| polarize | 54  | 1.3340 | 0.3900 | 55          | 58    |
| polarize | 55  | 0.8370 | 0.3900 | 51          | 54    |
| polarize | 56  | 0.4960 | 0.3900 | 53          |       |
| polarize | 58  | 0.4960 | 0.3900 | 54          |       |
| polarize | 60  | 0.4960 | 0.3900 | 52          |       |
| polarize | 61  | 0.4960 | 0.3900 | 51          |       |
| polarize | 63  | 1.3340 | 0.3900 | 66          | 68 74 |
| polarize | 64  | 0.8370 | 0.3900 | 52          | 101   |
| polarize | 65  | 0.4960 | 0.3900 | 73          |       |
| polarize | 66  | 0.4960 | 0.3900 | 63          |       |
| polarize | 68  | 0.8370 | 0.3900 | 63          | 101   |
| polarize | 69  | 0.4960 | 0.3900 | 74          |       |
| polarize | 73  | 0.8370 | 0.3900 | 52          | 65    |
| polarize | 74  | 0.8370 | 0.3900 | 63          | 69    |
|          |     |        |        |             |       |
| polarize | 36  | 0.8370 | 0.3900 | 37          |       |
| polarize | 37  | 0.4960 | 0.3900 | 36          |       |
| polarize | 41  | 0.1200 | 0.3900 |             |       |
| polarize | 42  | 0.7800 | 0.3900 |             |       |
| polarize | 43  | 0.0800 | 0.13   |             |       |
| polarize | 44  | 4.0000 | 0.3900 |             |       |
| polarize | 101 | 1.7880 | 0.3900 | 12 19 64 68 | 102   |
| polarize | 102 | 1.7240 | 0.3900 | 101         |       |
| polarize | 201 | 1.7500 | 0.3900 | 205 206     | 210   |
| polarize | 202 | 1.7500 | 0.3900 | 205 207     | 214   |
| polarize | 203 | 2.2500 | 0.3900 | 210 207 208 | 228   |
| polarize | 204 | 1.7500 | 0.3900 | 209 208 215 | 228   |
| polarize | 205 | 1.0730 | 0.3900 | 201 202     | 211   |
| polarize | 206 | 1.4500 | 0.3900 | 201         | 216   |
| polarize | 207 | 2.2500 | 0.3900 | 203 202     | 209   |
| polarize | 208 | 1.0730 | 0.3900 | 203         | 204   |
| polarize | 228 | 1.0730 | 0.3900 | 203         | 204   |
| polarize | 209 | 1.4500 | 0.3900 | 207         | 204   |
| polarize | 210 | 1.4500 | 0.3900 | 201         | 203   |
| polarize | 211 | 0.4960 | 0.3900 | 205         |       |
| polarize | 214 | 1.3000 | 0.3900 | 202         |       |
| polarize | 215 | 0.6960 | 0.3900 | 204         |       |

|          |     |        |                        |
|----------|-----|--------|------------------------|
| polarize | 216 | 0.6960 | 0.3900 206             |
| polarize | 301 | 1.0730 | 0.3900 305 304         |
| polarize | 321 | 1.0730 | 0.3900 305 304         |
| polarize | 302 | 1.7500 | 0.3900 306 304 308     |
| polarize | 303 | 1.4500 | 0.3900 306 313         |
| polarize | 304 | 1.7500 | 0.3900 301 302 312 321 |
| polarize | 305 | 1.7500 | 0.3900 301 309 307 321 |
| polarize | 306 | 1.7500 | 0.3900 307 303 302     |
| polarize | 307 | 1.4500 | 0.3900 305 306         |
| polarize | 308 | 0.6960 | 0.3900 302             |
| polarize | 309 | 1.3000 | 0.3900 305             |
| polarize | 312 | 0.6960 | 0.3900 304             |
| polarize | 313 | 0.6960 | 0.3900 303             |
| polarize | 401 | 1.7500 | 0.3900 409 404 405 425 |
| polarize | 402 | 1.7500 | 0.3900 408 405 413 425 |
| polarize | 403 | 2.2500 | 0.3900 410 404 406     |
| polarize | 404 | 2.2500 | 0.3900 401 403 408     |
| polarize | 405 | 1.0730 | 0.3900 401 402         |
| polarize | 425 | 1.0730 | 0.3900 401 402         |
| polarize | 406 | 1.4500 | 0.3900 403 415         |
| polarize | 407 | 1.7500 | 0.3900 410 409 414     |
| polarize | 408 | 1.4500 | 0.3900 404 402         |
| polarize | 409 | 1.4500 | 0.3900 407 401         |
| polarize | 410 | 1.4500 | 0.3900 407 403         |
| polarize | 413 | 0.6960 | 0.3900 402             |
| polarize | 414 | 0.6960 | 0.3900 407             |
| polarize | 415 | 0.6960 | 0.3900 406             |
| polarize | 501 | 1.7500 | 0.3900 505 510 504     |
| polarize | 502 | 1.7500 | 0.3900 505 506 512     |
| polarize | 503 | 1.7500 | 0.3900 504 511 506     |
| polarize | 504 | 1.0730 | 0.3900 501 503 508     |
| polarize | 505 | 1.0730 | 0.3900 501 502         |
| polarize | 506 | 1.7500 | 0.3900 503 502 509     |
| polarize | 508 | 0.4960 | 0.3900 504             |
| polarize | 509 | 0.6960 | 0.3900 506             |
| polarize | 510 | 1.3000 | 0.3900 501             |
| polarize | 511 | 1.3000 | 0.3900 503             |
| polarize | 512 | 0.6960 | 0.3900 502             |
| polarize | 601 | 1.3340 | 0.3900 602 608         |
| polarize | 602 | 1.7500 | 0.3900 603 604 601     |
| polarize | 603 | 1.7500 | 0.3900 606 611 602     |
| polarize | 604 | 1.7500 | 0.3900 605 602 610     |
| polarize | 605 | 1.0730 | 0.3900 607 604         |
| polarize | 606 | 1.0730 | 0.3900 607 603 612     |

polarize 607 1.7500 0.3900 605 609 606  
 polarize 608 0.4960 0.3900 601  
 polarize 609 1.3000 0.3900 607  
 polarize 610 0.6960 0.3900 604  
 polarize 611 1.3000 0.3900 603  
 polarize 612 0.4960 0.3900 606

#  
 # Results of Electrostatic Potential Fitting  
 #

multipole 4 1 6 0.22509  
 -0.02635 0.00000 0.29464  
 -0.08112  
 0.00000 -0.47377  
 0.09344 0.00000 0.55489

multipole 1 -4 -2 -0.21219  
 0.14040 0.00000 0.44294  
 1.12348  
 0.00000 -0.86617  
 0.03072 0.00000 -0.25731

multipole 2 1 8 -0.04958  
 0.13334 0.00000 0.11242  
 -0.15679  
 0.00000 -0.51619  
 0.33627 0.00000 0.67298

multipole 2 1 23 -0.04958  
 0.13334 0.00000 0.11242  
 -0.15679  
 0.00000 -0.51619  
 0.33627 0.00000 0.67298

multipole 8 12 2 0.20366  
 0.20594 0.00000 0.09319  
 -0.11723  
 0.00000 -0.31762  
 -0.43984 0.00000 0.43485

multipole 8 23 2 0.20366  
 0.20594 0.00000 0.09319  
 -0.11723  
 0.00000 -0.31762  
 -0.43984 0.00000 0.43485

multipole 6 10 4 0.03216  
 0.10990 0.00000 -0.01958  
 0.37889



|           |    |    |    |          |          |          |
|-----------|----|----|----|----------|----------|----------|
|           |    |    |    | 0.00000  | -0.28717 |          |
|           |    |    |    | -0.17655 | 0.00000  | -0.09172 |
| multipole | 3  | 2  | 1  | 0.05304  |          |          |
|           |    |    |    | 0.02860  | 0.00000  | -0.02198 |
|           |    |    |    | -0.05851 |          |          |
|           |    |    |    | 0.00000  | 0.07881  |          |
|           |    |    |    | -0.01698 | 0.00000  | -0.02030 |
| multipole | 5  | 4  | 1  | 0.01372  |          |          |
|           |    |    |    | -0.00919 | 0.00000  | -0.08228 |
|           |    |    |    | -0.07774 |          |          |
|           |    |    |    | 0.00000  | 0.12514  |          |
|           |    |    |    | -0.03924 | 0.00000  | -0.04740 |
| multipole | 7  | 6  | 10 | 0.02686  |          |          |
|           |    |    |    | 0.00928  | 0.00000  | -0.08296 |
|           |    |    |    | 0.06542  |          |          |
|           |    |    |    | 0.00000  | 0.05572  |          |
|           |    |    |    | -0.06717 | 0.00000  | -0.12114 |
| multipole | 9  | 8  | 12 | 0.05807  |          |          |
|           |    |    |    | 0.02182  | 0.00000  | -0.04741 |
|           |    |    |    | -0.01189 |          |          |
|           |    |    |    | 0.00000  | 0.01995  |          |
|           |    |    |    | 0.00147  | 0.00000  | -0.00806 |
| multipole | 9  | 8  | 23 | 0.05807  |          |          |
|           |    |    |    | 0.02182  | 0.00000  | -0.04741 |
|           |    |    |    | -0.01189 |          |          |
|           |    |    |    | 0.00000  | 0.01995  |          |
|           |    |    |    | 0.00147  | 0.00000  | -0.00806 |
| multipole | 10 | 6  | 11 | -0.46715 |          |          |
|           |    |    |    | -0.24005 | 0.00000  | 0.22215  |
|           |    |    |    | -0.23660 |          |          |
|           |    |    |    | 0.00000  | -0.43315 |          |
|           |    |    |    | -0.40748 | 0.00000  | 0.66975  |
| multipole | 11 | 10 | 6  | 0.36314  |          |          |
|           |    |    |    | 0.09447  | 0.00000  | -0.13458 |
|           |    |    |    | 0.10571  |          |          |
|           |    |    |    | 0.00000  | 0.03601  |          |
|           |    |    |    | 0.09130  | 0.00000  | -0.14172 |
| multipole | 12 | 8  | 2  | -0.54322 |          |          |
|           |    |    |    | -0.13139 | 0.00000  | -0.09707 |
|           |    |    |    | 0.25255  |          |          |
|           |    |    |    | 0.00000  | -0.62094 |          |
|           |    |    |    | 0.53908  | 0.00000  | 0.36839  |
| multipole | 13 | 23 | 8  | 0.36509  |          |          |
|           |    |    |    | -0.03477 | 0.00000  | -0.07061 |

|           |    |     |     |          |          |          |  |
|-----------|----|-----|-----|----------|----------|----------|--|
|           |    |     |     | 0.00668  |          |          |  |
|           |    |     |     | 0.00000  | -0.00878 |          |  |
|           |    |     |     | -0.03884 | 0.00000  | 0.00210  |  |
| multipole | 16 | 19  | 2   | 0.21472  |          |          |  |
|           |    |     |     | 0.26025  | 0.00000  | 0.34835  |  |
|           |    |     |     | 0.07978  |          |          |  |
|           |    |     |     | 0.00000  | -0.45645 |          |  |
|           |    |     |     | -0.03790 | 0.00000  | 0.37667  |  |
| multipole | 16 | 24  | 2   | 0.21472  |          |          |  |
|           |    |     |     | 0.26025  | 0.00000  | 0.34835  |  |
|           |    |     |     | 0.07978  |          |          |  |
|           |    |     |     | 0.00000  | -0.45645 |          |  |
|           |    |     |     | -0.03790 | 0.00000  | 0.37667  |  |
| multipole | 17 | 16  | 19  | 0.01769  |          |          |  |
|           |    |     |     | -0.00317 | 0.00000  | -0.11654 |  |
|           |    |     |     | 0.10449  |          |          |  |
|           |    |     |     | 0.00000  | -0.04493 |          |  |
|           |    |     |     | -0.02925 | 0.00000  | -0.05956 |  |
| multipole | 17 | 16  | 24  | 0.01769  |          |          |  |
|           |    |     |     | -0.00317 | 0.00000  | -0.11654 |  |
|           |    |     |     | 0.10449  |          |          |  |
|           |    |     |     | 0.00000  | -0.04493 |          |  |
|           |    |     |     | -0.02925 | 0.00000  | -0.05956 |  |
| multipole | 19 | 16  | 2   | -0.56592 |          |          |  |
|           |    |     |     | -0.32270 | 0.00000  | -0.10112 |  |
|           |    |     |     | 0.42126  |          |          |  |
|           |    |     |     | 0.00000  | -1.13829 |          |  |
|           |    |     |     | 0.05033  | 0.00000  | 0.71703  |  |
| multipole | 20 | 24  | 16  | 0.36475  |          |          |  |
|           |    |     |     | 0.00908  | 0.00000  | -0.09922 |  |
|           |    |     |     | 0.06175  |          |          |  |
|           |    |     |     | 0.00000  | -0.02643 |          |  |
|           |    |     |     | 0.03413  | 0.00000  | -0.03532 |  |
| multipole | 23 | -8  | -13 | -0.53022 |          |          |  |
|           |    |     |     | -0.30181 | 0.00000  | 0.07347  |  |
|           |    |     |     | 0.67028  |          |          |  |
|           |    |     |     | 0.00000  | -0.55976 |          |  |
|           |    |     |     | -0.27623 | 0.00000  | -0.11052 |  |
| multipole | 24 | -16 | -20 | -0.55194 |          |          |  |
|           |    |     |     | -0.28854 | 0.00000  | 0.13115  |  |
|           |    |     |     | 0.52394  |          |          |  |
|           |    |     |     | 0.00000  | -0.49611 |          |  |
|           |    |     |     | -0.53329 | 0.00000  | -0.02783 |  |
| multipole | 54 | 55  | 53  | 0.36158  |          |          |  |

|           |    |     |          |          |          |
|-----------|----|-----|----------|----------|----------|
|           |    |     | 0.07286  | 0.00000  | 0.32523  |
|           |    |     | 0.20365  |          |          |
|           |    |     | 0.00000  | -0.53379 |          |
|           |    |     | -0.16275 | 0.00000  | 0.33014  |
| multipole | 55 | -54 | -51      | -0.20726 |          |
|           |    |     | 0.17196  | 0.00000  | 0.47089  |
|           |    |     | 1.34014  |          |          |
|           |    |     | 0.00000  | -1.03558 |          |
|           |    |     | 0.09226  | 0.00000  | -0.30456 |
| multipole | 51 | 55  | 52       | -0.04092 |          |
|           |    |     | 0.09394  | 0.00000  | 0.14534  |
|           |    |     | -0.08972 |          |          |
|           |    |     | 0.00000  | -0.36979 |          |
|           |    |     | 0.35252  | 0.00000  | 0.45951  |
| multipole | 52 | 64  | 51       | 0.09541  |          |
|           |    |     | 0.23270  | 0.00000  | 0.16242  |
|           |    |     | -0.08206 |          |          |
|           |    |     | 0.00000  | -0.24668 |          |
|           |    |     | -0.05092 | 0.00000  | 0.32874  |
| multipole | 52 | 73  | 51       | 0.09541  |          |
|           |    |     | 0.23270  | 0.00000  | 0.16242  |
|           |    |     | -0.08206 |          |          |
|           |    |     | 0.00000  | -0.24668 |          |
|           |    |     | -0.05092 | 0.00000  | 0.32874  |
| multipole | 53 | 54  | 52       | -0.16585 |          |
|           |    |     | 0.34883  | 0.00000  | 0.32833  |
|           |    |     | 0.52159  |          |          |
|           |    |     | 0.00000  | -0.79855 |          |
|           |    |     | -0.04388 | 0.00000  | 0.27696  |
| multipole | 56 | 53  | 52       | 0.07594  |          |
|           |    |     | -0.00339 | 0.00000  | -0.12482 |
|           |    |     | 0.03839  |          |          |
|           |    |     | 0.00000  | 0.06287  |          |
|           |    |     | -0.06388 | 0.00000  | -0.10126 |
| multipole | 58 | 54  | 55       | -0.02874 |          |
|           |    |     | -0.02540 | 0.00000  | -0.16522 |
|           |    |     | 0.03324  |          |          |
|           |    |     | 0.00000  | 0.05278  |          |
|           |    |     | -0.02045 | 0.00000  | -0.08602 |
| multipole | 60 | 52  | 64       | 0.04534  |          |
|           |    |     | 0.03745  | 0.00000  | -0.06219 |
|           |    |     | 0.05688  |          |          |
|           |    |     | 0.00000  | 0.05897  |          |
|           |    |     | 0.04350  | 0.00000  | -0.11585 |

|           |    |    |    |          |          |          |
|-----------|----|----|----|----------|----------|----------|
| multipole | 60 | 52 | 73 | 0.04534  |          |          |
|           |    |    |    | 0.03745  | 0.00000  | -0.06219 |
|           |    |    |    | 0.05688  |          |          |
|           |    |    |    | 0.00000  | 0.05897  |          |
|           |    |    |    | 0.04350  | 0.00000  | -0.11585 |
| multipole | 61 | 51 | 55 | 0.06371  |          |          |
|           |    |    |    | -0.00143 | 0.00000  | 0.03820  |
|           |    |    |    | -0.07016 |          |          |
|           |    |    |    | 0.00000  | -0.02994 |          |
|           |    |    |    | -0.02128 | 0.00000  | 0.10010  |
| multipole | 63 | 68 | 51 | 0.20884  |          |          |
|           |    |    |    | 0.23256  | 0.00000  | 0.32780  |
|           |    |    |    | 0.07966  |          |          |
|           |    |    |    | 0.00000  | -0.49936 |          |
|           |    |    |    | -0.23651 | 0.00000  | 0.41970  |
| multipole | 63 | 74 | 51 | 0.20884  |          |          |
|           |    |    |    | 0.23256  | 0.00000  | 0.32780  |
|           |    |    |    | 0.07966  |          |          |
|           |    |    |    | 0.00000  | -0.49936 |          |
|           |    |    |    | -0.23651 | 0.00000  | 0.41970  |
| multipole | 64 | 52 | 51 | -0.53633 |          |          |
|           |    |    |    | -0.15241 | 0.00000  | 0.08515  |
|           |    |    |    | -0.15239 |          |          |
|           |    |    |    | 0.00000  | -0.52084 |          |
|           |    |    |    | 0.11305  | 0.00000  | 0.67323  |
| multipole | 65 | 73 | 52 | 0.35299  |          |          |
|           |    |    |    | -0.02338 | 0.00000  | -0.07709 |
|           |    |    |    | 0.08385  |          |          |
|           |    |    |    | 0.00000  | -0.02966 |          |
|           |    |    |    | -0.02571 | 0.00000  | -0.05419 |
| multipole | 66 | 63 | 68 | 0.01484  |          |          |
|           |    |    |    | -0.00257 | 0.00000  | -0.14412 |
|           |    |    |    | 0.09017  |          |          |
|           |    |    |    | 0.00000  | 0.03078  |          |
|           |    |    |    | -0.02370 | 0.00000  | -0.12095 |
| multipole | 66 | 63 | 74 | 0.01484  |          |          |
|           |    |    |    | -0.00257 | 0.00000  | -0.14412 |
|           |    |    |    | 0.09017  |          |          |
|           |    |    |    | 0.00000  | 0.03078  |          |
|           |    |    |    | -0.02370 | 0.00000  | -0.12095 |
| multipole | 68 | 63 | 51 | -0.56353 |          |          |
|           |    |    |    | -0.22239 | 0.00000  | -0.06011 |
|           |    |    |    | 0.38656  |          |          |
|           |    |    |    | 0.00000  | -1.00409 |          |

|           |    |     |     |          |          |          |
|-----------|----|-----|-----|----------|----------|----------|
|           |    |     |     | 0.25289  | 0.00000  | 0.61753  |
| multipole | 69 | 74  | 63  | 0.36821  |          |          |
|           |    |     |     | -0.00780 | 0.00000  | -0.05456 |
|           |    |     |     | 0.01443  |          |          |
|           |    |     |     | 0.00000  | -0.02693 |          |
|           |    |     |     | 0.00842  | 0.00000  | 0.01250  |
| multipole | 73 | -52 | -65 | -0.51852 |          |          |
|           |    |     |     | -0.33062 | 0.00000  | 0.16496  |
|           |    |     |     | 0.59735  |          |          |
|           |    |     |     | 0.00000  | -0.64156 |          |
|           |    |     |     | -0.24661 | 0.00000  | 0.04421  |
| multipole | 74 | -63 | -69 | -0.54572 |          |          |
|           |    |     |     | -0.35421 | 0.00000  | 0.09483  |
|           |    |     |     | 0.77382  |          |          |
|           |    |     |     | 0.00000  | -0.63430 |          |
|           |    |     |     | -0.30271 | 0.00000  | -0.13952 |
| multipole | 36 | -37 | -37 | -0.51966 |          |          |
|           |    |     |     | 0.00000  | 0.00000  | 0.14279  |
|           |    |     |     | 0.37928  |          |          |
|           |    |     |     | 0.00000  | -0.41809 |          |
|           |    |     |     | 0.00000  | 0.00000  | 0.03881  |
| multipole | 37 | 36  | 37  | 0.25983  |          |          |
|           |    |     |     | -0.03859 | 0.00000  | -0.05818 |
|           |    |     |     | -0.03673 |          |          |
|           |    |     |     | 0.00000  | -0.10739 |          |
|           |    |     |     | -0.00203 | 0.00000  | 0.14412  |
| multipole | 41 | 0   | 0   | 1.00000  |          |          |
|           |    |     |     | 0.00000  | 0.00000  | 0.00000  |
|           |    |     |     | 0.00000  |          |          |
|           |    |     |     | 0.00000  | 0.00000  |          |
|           |    |     |     | 0.00000  | 0.00000  | 0.00000  |
| multipole | 42 | 0   | 0   | 1.00000  |          |          |
|           |    |     |     | 0.00000  | 0.00000  | 0.00000  |
|           |    |     |     | 0.00000  |          |          |
|           |    |     |     | 0.00000  | 0.00000  |          |
|           |    |     |     | 0.00000  | 0.00000  | 0.00000  |
| multipole | 43 | 0   | 0   | 2.00000  |          |          |
|           |    |     |     | 0.00000  | 0.00000  | 0.00000  |
|           |    |     |     | 0.00000  |          |          |
|           |    |     |     | 0.00000  | 0.00000  |          |
|           |    |     |     | 0.00000  | 0.00000  | 0.00000  |
| multipole | 44 | 0   | 0   | -1.00000 |          |          |
|           |    |     |     | 0.00000  | 0.00000  | 0.00000  |
|           |    |     |     | 0.00000  |          |          |

|           |     |     |         |          |          |
|-----------|-----|-----|---------|----------|----------|
|           |     |     | 0.00000 | 0.00000  |          |
|           |     |     | 0.00000 | 0.00000  | 0.00000  |
| multipole | 101 | -19 | -12     | 1.70654  |          |
|           |     |     |         | 0.00000  | 0.00000  |
|           |     |     |         |          | -0.01783 |
|           |     |     |         | 0.54887  |          |
|           |     |     |         | 0.00000  | -0.40394 |
|           |     |     |         | 0.00000  | 0.00000  |
|           |     |     |         |          | -0.14493 |
| multipole | 101 | -68 | -64     | 1.70654  |          |
|           |     |     |         | 0.00000  | 0.00000  |
|           |     |     |         |          | -0.01783 |
|           |     |     |         | 0.54887  |          |
|           |     |     |         | 0.00000  | -0.40394 |
|           |     |     |         | 0.00000  | 0.00000  |
|           |     |     |         |          | -0.14493 |
| multipole | 102 | 101 | 102     | -0.97486 |          |
|           |     |     |         | 0.00176  | 0.00000  |
|           |     |     |         |          | -0.07975 |
|           |     |     |         | -0.17391 |          |
|           |     |     |         | 0.00000  | -0.19149 |
|           |     |     |         | -0.01158 | 0.00000  |
|           |     |     |         |          | 0.36540  |
| multipole | 201 | 205 | 206     | 0.81575  |          |
|           |     |     |         | 0.07393  | 0.00000  |
|           |     |     |         |          | -0.07697 |
|           |     |     |         | -1.62256 |          |
|           |     |     |         | 0.00000  | 0.42511  |
|           |     |     |         | 0.47701  | 0.00000  |
|           |     |     |         |          | 1.19745  |
| multipole | 202 | 205 | 207     | 0.91682  |          |
|           |     |     |         | -0.28939 | 0.00000  |
|           |     |     |         |          | -0.03405 |
|           |     |     |         | -0.49481 |          |
|           |     |     |         | 0.00000  | 0.06805  |
|           |     |     |         | 0.30090  | 0.00000  |
|           |     |     |         |          | 0.42676  |
| multipole | 203 | 207 | 208     | 0.25636  |          |
|           |     |     |         | -0.06429 | 0.00000  |
|           |     |     |         |          | -0.39303 |
|           |     |     |         | -0.02366 |          |
|           |     |     |         | 0.00000  | -0.11189 |
|           |     |     |         | -0.68217 | 0.00000  |
|           |     |     |         |          | 0.13555  |
| multipole | 203 | 207 | 228     | 0.25636  |          |
|           |     |     |         | -0.06429 | 0.00000  |
|           |     |     |         |          | -0.39303 |
|           |     |     |         | -0.02366 |          |
|           |     |     |         | 0.00000  | -0.11189 |
|           |     |     |         | -0.68217 | 0.00000  |
|           |     |     |         |          | 0.13555  |
| multipole | 204 | 208 | 209     | 0.33548  |          |
|           |     |     |         | 0.26446  | 0.00000  |
|           |     |     |         |          | 0.19054  |
|           |     |     |         | -0.14954 |          |
|           |     |     |         | 0.00000  | -0.63553 |
|           |     |     |         | -0.24037 | 0.00000  |
|           |     |     |         |          | 0.78507  |
| multipole | 204 | 228 | 209     | 0.33548  |          |
|           |     |     |         | 0.26446  | 0.00000  |
|           |     |     |         |          | 0.19054  |

|           |     |     |     |          |          |          |  |
|-----------|-----|-----|-----|----------|----------|----------|--|
|           |     |     |     | -0.14954 |          |          |  |
|           |     |     |     | 0.00000  | -0.63553 |          |  |
|           |     |     |     | -0.24037 | 0.00000  | 0.78507  |  |
| multipole | 205 | 201 | 202 | -0.46516 |          |          |  |
|           |     |     |     | -0.20039 | 0.00000  | -0.02958 |  |
|           |     |     |     | 0.18319  |          |          |  |
|           |     |     |     | 0.00000  | -0.31924 |          |  |
|           |     |     |     | 0.55206  | 0.00000  | 0.13605  |  |
| multipole | 206 | 201 | 216 | -0.34777 |          |          |  |
|           |     |     |     | 0.00000  | 0.00000  | 0.09810  |  |
|           |     |     |     | -0.22674 |          |          |  |
|           |     |     |     | 0.00000  | -0.22674 |          |  |
|           |     |     |     | 0.00000  | 0.00000  | 0.45348  |  |
| multipole | 207 | 202 | 203 | -0.00139 |          |          |  |
|           |     |     |     | -0.34214 | 0.00000  | -0.25452 |  |
|           |     |     |     | 0.57109  |          |          |  |
|           |     |     |     | 0.00000  | 0.08638  |          |  |
|           |     |     |     | -0.46661 | 0.00000  | -0.65747 |  |
| multipole | 208 | 203 | 204 | -0.13948 |          |          |  |
|           |     |     |     | -0.16345 | 0.00000  | -0.28631 |  |
|           |     |     |     | 0.81099  |          |          |  |
|           |     |     |     | 0.00000  | -0.38335 |          |  |
|           |     |     |     | 0.22009  | 0.00000  | -0.42764 |  |
| multipole | 228 | 203 | 204 | -0.16551 |          |          |  |
|           |     |     |     | -0.15213 | 0.00000  | -0.24822 |  |
|           |     |     |     | 0.87781  |          |          |  |
|           |     |     |     | 0.00000  | -0.04263 |          |  |
|           |     |     |     | 0.16842  | 0.00000  | -0.83518 |  |
| multipole | 209 | 204 | 207 | -0.49075 |          |          |  |
|           |     |     |     | 0.19750  | 0.00000  | 0.34115  |  |
|           |     |     |     | -0.18411 |          |          |  |
|           |     |     |     | 0.00000  | 0.02266  |          |  |
|           |     |     |     | -0.00528 | 0.00000  | 0.16145  |  |
| multipole | 210 | 201 | 203 | -0.68515 |          |          |  |
|           |     |     |     | 0.30301  | 0.00000  | 0.07467  |  |
|           |     |     |     | 0.27482  |          |          |  |
|           |     |     |     | 0.00000  | 0.10098  |          |  |
|           |     |     |     | 0.18985  | 0.00000  | -0.37580 |  |
| multipole | 211 | 205 | 201 | 0.13360  |          |          |  |
|           |     |     |     | -0.01556 | 0.00000  | -0.29570 |  |
|           |     |     |     | 0.16829  |          |          |  |
|           |     |     |     | 0.00000  | 0.14413  |          |  |
|           |     |     |     | -0.17971 | 0.00000  | -0.31242 |  |
| multipole | 214 | 202 | 205 | -0.75414 |          |          |  |

|           |     |     |     |          |          |          |
|-----------|-----|-----|-----|----------|----------|----------|
|           |     |     |     | -0.02651 | 0.00000  | -0.22256 |
|           |     |     |     | -0.25663 |          |          |
|           |     |     |     | 0.00000  | 0.15963  |          |
|           |     |     |     | -0.07481 | 0.00000  | 0.09700  |
| multipole | 215 | 204 | 208 | 0.03471  |          |          |
|           |     |     |     | 0.00549  | 0.00000  | -0.20010 |
|           |     |     |     | 0.02971  |          |          |
|           |     |     |     | 0.00000  | 0.08931  |          |
|           |     |     |     | 0.04294  | 0.00000  | -0.11902 |
| multipole | 215 | 204 | 228 | 0.03471  |          |          |
|           |     |     |     | 0.00549  | 0.00000  | -0.20010 |
|           |     |     |     | 0.02971  |          |          |
|           |     |     |     | 0.00000  | 0.08931  |          |
|           |     |     |     | 0.04294  | 0.00000  | -0.11902 |
| multipole | 216 | 206 | 201 | 0.12326  |          |          |
|           |     |     |     | -0.12194 | 0.00000  | -0.40562 |
|           |     |     |     | 0.04772  |          |          |
|           |     |     |     | 0.00000  | 0.25205  |          |
|           |     |     |     | -0.10563 | 0.00000  | -0.29977 |
| multipole | 301 | 304 | 305 | -0.24104 |          |          |
|           |     |     |     | -0.46930 | 0.00000  | -0.00215 |
|           |     |     |     | -0.63770 |          |          |
|           |     |     |     | 0.00000  | -0.12764 |          |
|           |     |     |     | -0.21639 | 0.00000  | 0.76534  |
| multipole | 321 | 304 | 305 | -0.26707 |          |          |
|           |     |     |     | -0.43500 | 0.00000  | -0.02543 |
|           |     |     |     | -0.80418 |          |          |
|           |     |     |     | 0.00000  | -0.16395 |          |
|           |     |     |     | -0.56679 | 0.00000  | 0.96813  |
| multipole | 302 | 304 | 306 | -0.21855 |          |          |
|           |     |     |     | -0.02433 | 0.00000  | -0.04067 |
|           |     |     |     | 0.07073  |          |          |
|           |     |     |     | 0.00000  | -0.29598 |          |
|           |     |     |     | 0.18324  | 0.00000  | 0.22525  |
| multipole | 303 | 306 | 313 | -0.26774 |          |          |
|           |     |     |     | 0.00000  | 0.00000  | -0.14722 |
|           |     |     |     | -0.20683 |          |          |
|           |     |     |     | 0.00000  | -0.20683 |          |
|           |     |     |     | 0.00000  | 0.00000  | 0.41366  |
| multipole | 304 | 301 | 302 | 0.21574  |          |          |
|           |     |     |     | 0.02713  | 0.00000  | 0.38093  |
|           |     |     |     | -0.32457 |          |          |
|           |     |     |     | 0.00000  | -0.21073 |          |
|           |     |     |     | 0.24767  | 0.00000  | 0.53530  |



|                       |          |          |          |
|-----------------------|----------|----------|----------|
| multipole 304 321 302 | 0.21574  |          |          |
|                       | 0.02713  | 0.00000  | 0.38093  |
|                       | -0.32457 |          |          |
|                       | 0.00000  | -0.21073 |          |
|                       | 0.24767  | 0.00000  | 0.53530  |
| multipole 305 301 307 | 0.99441  |          |          |
|                       | -0.20032 | 0.00000  | -0.07584 |
|                       | 0.26825  |          |          |
|                       | 0.00000  | -0.16618 |          |
|                       | -0.12141 | 0.00000  | -0.10207 |
| multipole 305 321 307 | 0.99441  |          |          |
|                       | -0.20032 | 0.00000  | -0.07584 |
|                       | 0.26825  |          |          |
|                       | 0.00000  | -0.16618 |          |
|                       | -0.12141 | 0.00000  | -0.10207 |
| multipole 306 302 303 | 0.63287  |          |          |
|                       | 0.11720  | 0.00000  | -0.36908 |
|                       | -0.70790 |          |          |
|                       | 0.00000  | -0.09015 |          |
|                       | 0.13248  | 0.00000  | 0.79805  |
| multipole 307 305 306 | -0.72673 |          |          |
|                       | 0.11437  | 0.00000  | 0.27430  |
|                       | -0.36580 |          |          |
|                       | 0.00000  | 0.16860  |          |
|                       | -0.15967 | 0.00000  | 0.19720  |
| multipole 308 302 304 | 0.03287  |          |          |
|                       | -0.02386 | 0.00000  | -0.16869 |
|                       | 0.19235  |          |          |
|                       | 0.00000  | -0.04497 |          |
|                       | -0.11320 | 0.00000  | -0.14738 |
| multipole 309 305 301 | -0.80802 |          |          |
|                       | -0.13691 | 0.00000  | -0.17532 |
|                       | -0.06093 |          |          |
|                       | 0.00000  | -0.00808 |          |
|                       | -0.25644 | 0.00000  | 0.06901  |
| multipole 309 305 321 | -0.80802 |          |          |
|                       | -0.13691 | 0.00000  | -0.17532 |
|                       | -0.06093 |          |          |
|                       | 0.00000  | -0.00808 |          |
|                       | -0.25644 | 0.00000  | 0.06901  |
| multipole 312 304 301 | 0.01925  |          |          |
|                       | 0.00579  | 0.00000  | -0.19218 |
|                       | 0.10120  |          |          |
|                       | 0.00000  | 0.03689  |          |
|                       |          |          |          |

|           |     |     |          |          |          |
|-----------|-----|-----|----------|----------|----------|
|           |     |     | 0.06622  | 0.00000  | -0.13809 |
| multipole | 312 | 304 | 321      | 0.01925  |          |
|           |     |     | 0.00579  | 0.00000  | -0.19218 |
|           |     |     | 0.10120  |          |          |
|           |     |     | 0.00000  | 0.03689  |          |
|           |     |     | 0.06622  | 0.00000  | -0.13809 |
| multipole | 313 | 303 | 306      | 0.11117  |          |
|           |     |     | 0.06785  | 0.00000  | -0.34828 |
|           |     |     | 0.25530  |          |          |
|           |     |     | 0.00000  | 0.00041  |          |
|           |     |     | 0.07371  | 0.00000  | -0.25571 |
| multipole | 401 | 404 | 405      | 0.19705  |          |
|           |     |     | 0.05235  | 0.00000  | -0.55644 |
|           |     |     | -0.17689 |          |          |
|           |     |     | 0.00000  | 0.07507  |          |
|           |     |     | -0.26977 | 0.00000  | 0.10182  |
| multipole | 401 | 404 | 425      | 0.19705  |          |
|           |     |     | 0.05235  | 0.00000  | -0.55644 |
|           |     |     | -0.17689 |          |          |
|           |     |     | 0.00000  | 0.07507  |          |
|           |     |     | -0.26977 | 0.00000  | 0.10182  |
| multipole | 402 | 405 | 408      | 0.35474  |          |
|           |     |     | 0.27278  | 0.00000  | 0.17660  |
|           |     |     | -0.11495 |          |          |
|           |     |     | 0.00000  | -0.52849 |          |
|           |     |     | -0.24464 | 0.00000  | 0.64344  |
| multipole | 402 | 425 | 408      | 0.35474  |          |
|           |     |     | 0.27278  | 0.00000  | 0.17660  |
|           |     |     | -0.11495 |          |          |
|           |     |     | 0.00000  | -0.52849 |          |
|           |     |     | -0.24464 | 0.00000  | 0.64344  |
| multipole | 403 | 404 | 406      | 0.62323  |          |
|           |     |     | 0.04051  | 0.00000  | -0.40121 |
|           |     |     | -0.16700 |          |          |
|           |     |     | 0.00000  | -0.05202 |          |
|           |     |     | 0.14286  | 0.00000  | 0.21902  |
| multipole | 404 | 401 | 403      | 0.11018  |          |
|           |     |     | -0.27451 | 0.00000  | -0.16246 |
|           |     |     | -0.43024 |          |          |
|           |     |     | 0.00000  | 0.15634  |          |
|           |     |     | 0.11274  | 0.00000  | 0.27390  |
| multipole | 405 | 401 | 402      | -0.16574 |          |
|           |     |     | -0.15654 | 0.00000  | -0.29303 |
|           |     |     | 0.81194  |          |          |

|           |     |     |          |          |          |
|-----------|-----|-----|----------|----------|----------|
|           |     |     | 0.00000  | -0.31643 |          |
|           |     |     | -0.09665 | 0.00000  | -0.49551 |
| multipole | 425 | 401 | 402      | -0.19177 |          |
|           |     |     | -0.15102 | 0.00000  | -0.28082 |
|           |     |     | 1.02852  |          |          |
|           |     |     | 0.00000  | 0.19924  |          |
|           |     |     | -0.11670 | 0.00000  | -1.22776 |
| multipole | 406 | 403 | 415      | -0.30216 |          |
|           |     |     | 0.00000  | 0.00000  | -0.23479 |
|           |     |     | -0.18214 |          |          |
|           |     |     | 0.00000  | -0.18214 |          |
|           |     |     | 0.00000  | 0.00000  | 0.36428  |
| multipole | 407 | 409 | 410      | 0.53583  |          |
|           |     |     | 0.46262  | 0.00000  | 0.23806  |
|           |     |     | 0.30445  |          |          |
|           |     |     | 0.00000  | -0.30622 |          |
|           |     |     | 0.27296  | 0.00000  | 0.00177  |
| multipole | 408 | 402 | 404      | -0.50058 |          |
|           |     |     | 0.27961  | 0.00000  | 0.29857  |
|           |     |     | -0.21774 |          |          |
|           |     |     | 0.00000  | -0.20902 |          |
|           |     |     | -0.22060 | 0.00000  | 0.42676  |
| multipole | 409 | 401 | 407      | -0.59923 |          |
|           |     |     | 0.25112  | 0.00000  | -0.03017 |
|           |     |     | 0.05684  |          |          |
|           |     |     | 0.00000  | 0.03677  |          |
|           |     |     | -0.42077 | 0.00000  | -0.09361 |
| multipole | 410 | 403 | 407      | -0.68218 |          |
|           |     |     | 0.26819  | 0.00000  | -0.11771 |
|           |     |     | -0.22542 |          |          |
|           |     |     | 0.00000  | 0.23562  |          |
|           |     |     | -0.49764 | 0.00000  | -0.01020 |
| multipole | 413 | 402 | 405      | 0.03522  |          |
|           |     |     | -0.00715 | 0.00000  | -0.19094 |
|           |     |     | 0.12022  |          |          |
|           |     |     | 0.00000  | -0.00738 |          |
|           |     |     | -0.01223 | 0.00000  | -0.11284 |
| multipole | 413 | 402 | 425      | 0.03522  |          |
|           |     |     | -0.00715 | 0.00000  | -0.19094 |
|           |     |     | 0.12022  |          |          |
|           |     |     | 0.00000  | -0.00738 |          |
|           |     |     | -0.01223 | 0.00000  | -0.11284 |
| multipole | 414 | 407 | 409      | 0.01012  |          |
|           |     |     | 0.00378  | 0.00000  | -0.20885 |

|           |     |     |          |          |
|-----------|-----|-----|----------|----------|
|           |     |     | 0.29328  |          |
|           |     |     | 0.00000  | -0.03702 |
|           |     |     | 0.01627  | 0.00000  |
|           |     |     |          | -0.25626 |
| multipole | 415 | 406 | 403      | 0.11946  |
|           |     |     | 0.10111  | 0.00000  |
|           |     |     |          | -0.36228 |
|           |     |     | 0.30681  |          |
|           |     |     | 0.00000  | 0.00962  |
|           |     |     | 0.09733  | 0.00000  |
|           |     |     |          | -0.31643 |
| multipole | 501 | 504 | 505      | 0.96728  |
|           |     |     | -0.16517 | 0.00000  |
|           |     |     |          | -0.11030 |
|           |     |     | -0.14243 |          |
|           |     |     | 0.00000  | -0.19294 |
|           |     |     | 0.11920  | 0.00000  |
|           |     |     |          | 0.33537  |
| multipole | 502 | 505 | 506      | 0.20155  |
|           |     |     | 0.10244  | 0.00000  |
|           |     |     |          | 0.30074  |
|           |     |     | -0.12081 |          |
|           |     |     | 0.00000  | -0.38422 |
|           |     |     | -0.06545 | 0.00000  |
|           |     |     |          | 0.50503  |
| multipole | 503 | 504 | 506      | 0.85168  |
|           |     |     | -0.22270 | 0.00000  |
|           |     |     |          | -0.07763 |
|           |     |     | -0.00198 |          |
|           |     |     | 0.00000  | -0.01706 |
|           |     |     | -0.28197 | 0.00000  |
|           |     |     |          | 0.01904  |
| multipole | 504 | 501 | 503      | -0.38069 |
|           |     |     | -0.14505 | 0.00000  |
|           |     |     |          | -0.04085 |
|           |     |     | 0.47767  |          |
|           |     |     | 0.00000  | -0.40383 |
|           |     |     | 0.32823  | 0.00000  |
|           |     |     |          | -0.07384 |
| multipole | 505 | 501 | 502      | -0.19639 |
|           |     |     | -0.16349 | 0.00000  |
|           |     |     |          | -0.36007 |
|           |     |     | 0.98907  |          |
|           |     |     | 0.00000  | -1.02460 |
|           |     |     | -0.18271 | 0.00000  |
|           |     |     |          | 0.03553  |
| multipole | 506 | 502 | 503      | -0.30583 |
|           |     |     | -0.17480 | 0.00000  |
|           |     |     |          | -0.07381 |
|           |     |     | -0.09671 |          |
|           |     |     | 0.00000  | -0.36088 |
|           |     |     | 0.02211  | 0.00000  |
|           |     |     |          | 0.45759  |
| multipole | 508 | 504 | 501      | 0.16490  |
|           |     |     | 0.00383  | 0.00000  |
|           |     |     |          | -0.15117 |
|           |     |     | 0.07794  |          |
|           |     |     | 0.00000  | -0.04305 |
|           |     |     | 0.06224  | 0.00000  |
|           |     |     |          | -0.03489 |
| multipole | 509 | 506 | 502      | 0.03819  |

|           |     |     |     |          |          |          |
|-----------|-----|-----|-----|----------|----------|----------|
|           |     |     |     | -0.01137 | 0.00000  | -0.19659 |
|           |     |     |     | 0.13645  |          |          |
|           |     |     |     | 0.00000  | 0.01095  |          |
|           |     |     |     | -0.04797 | 0.00000  | -0.14740 |
| multipole | 510 | 501 | 504 | -0.80827 |          |          |
|           |     |     |     | 0.04828  | 0.00000  | -0.21537 |
|           |     |     |     | -0.20344 |          |          |
|           |     |     |     | 0.00000  | 0.08236  |          |
|           |     |     |     | 0.10174  | 0.00000  | 0.12108  |
| multipole | 511 | 503 | 504 | -0.71662 |          |          |
|           |     |     |     | -0.03231 | 0.00000  | -0.16721 |
|           |     |     |     | -0.47288 |          |          |
|           |     |     |     | 0.00000  | 0.23591  |          |
|           |     |     |     | -0.01906 | 0.00000  | 0.23697  |
| multipole | 512 | 502 | 505 | 0.03960  |          |          |
|           |     |     |     | -0.00001 | 0.00000  | -0.18599 |
|           |     |     |     | 0.07673  |          |          |
|           |     |     |     | 0.00000  | 0.06769  |          |
|           |     |     |     | 0.06469  | 0.00000  | -0.14442 |
| multipole | 601 | 602 | 608 | -0.12472 |          |          |
|           |     |     |     | 0.00000  | 0.00000  | 0.23414  |
|           |     |     |     | -0.16670 |          |          |
|           |     |     |     | 0.00000  | -0.16670 |          |
|           |     |     |     | 0.00000  | 0.00000  | 0.33340  |
| multipole | 602 | 601 | 603 | -0.32491 |          |          |
|           |     |     |     | -0.11852 | 0.00000  | 0.38086  |
|           |     |     |     | 0.04438  |          |          |
|           |     |     |     | 0.00000  | -0.36513 |          |
|           |     |     |     | 0.61277  | 0.00000  | 0.32075  |
| multipole | 603 | 602 | 606 | 0.94792  |          |          |
|           |     |     |     | -0.37385 | 0.00000  | -0.16991 |
|           |     |     |     | 0.27250  |          |          |
|           |     |     |     | 0.00000  | -0.11690 |          |
|           |     |     |     | -0.46630 | 0.00000  | -0.15560 |
| multipole | 604 | 602 | 605 | 0.13457  |          |          |
|           |     |     |     | 0.28512  | 0.00000  | -0.15252 |
|           |     |     |     | 0.24926  |          |          |
|           |     |     |     | 0.00000  | -0.37318 |          |
|           |     |     |     | -0.29476 | 0.00000  | 0.12392  |
| multipole | 605 | 604 | 607 | -0.20596 |          |          |
|           |     |     |     | -0.28927 | 0.00000  | 0.05138  |
|           |     |     |     | -0.61284 |          |          |
|           |     |     |     | 0.00000  | -0.37546 |          |
|           |     |     |     | -0.25749 | 0.00000  | 0.98830  |

|           |     |     |     |          |          |          |
|-----------|-----|-----|-----|----------|----------|----------|
| multipole | 606 | 603 | 607 | -0.37323 |          |          |
|           |     |     |     | -0.03823 | 0.00000  | -0.10180 |
|           |     |     |     | 0.54796  |          |          |
|           |     |     |     | 0.00000  | -0.43130 |          |
|           |     |     |     | 0.23181  | 0.00000  | -0.11666 |
| multipole | 607 | 605 | 606 | 0.96217  |          |          |
|           |     |     |     | -0.16525 | 0.00000  | -0.11314 |
|           |     |     |     | 0.36596  |          |          |
|           |     |     |     | 0.00000  | -0.21822 |          |
|           |     |     |     | -0.05615 | 0.00000  | -0.14774 |
| multipole | 608 | 601 | 602 | 0.07468  |          |          |
|           |     |     |     | 0.01065  | 0.00000  | -0.01558 |
|           |     |     |     | -0.01394 |          |          |
|           |     |     |     | 0.00000  | -0.06177 |          |
|           |     |     |     | 0.02095  | 0.00000  | 0.07571  |
| multipole | 609 | 607 | 605 | -0.81528 |          |          |
|           |     |     |     | -0.05664 | 0.00000  | -0.20927 |
|           |     |     |     | -0.13286 |          |          |
|           |     |     |     | 0.00000  | 0.05238  |          |
|           |     |     |     | -0.06252 | 0.00000  | 0.08048  |
| multipole | 610 | 604 | 602 | 0.03316  |          |          |
|           |     |     |     | 0.00796  | 0.00000  | -0.15603 |
|           |     |     |     | 0.06552  |          |          |
|           |     |     |     | 0.00000  | 0.00785  |          |
|           |     |     |     | -0.01504 | 0.00000  | -0.07337 |
| multipole | 611 | 603 | 602 | -0.79250 |          |          |
|           |     |     |     | -0.09925 | 0.00000  | -0.24004 |
|           |     |     |     | -0.27421 |          |          |
|           |     |     |     | 0.00000  | 0.16551  |          |
|           |     |     |     | -0.12860 | 0.00000  | 0.10870  |
| multipole | 612 | 606 | 603 | 0.16411  |          |          |
|           |     |     |     | 0.00839  | 0.00000  | -0.12442 |
|           |     |     |     | -0.09057 |          |          |
|           |     |     |     | 0.00000  | 0.00294  |          |
|           |     |     |     | 0.00693  | 0.00000  | 0.08763  |

|         |      |     |             |    |
|---------|------|-----|-------------|----|
| biotype | 1001 | O5* | "Adenosine" | 19 |
| biotype | 1002 | C5* | "Adenosine" | 16 |
| biotype | 1003 | H5* | "Adenosine" | 17 |
| biotype | 1004 | H5* | "Adenosine" | 17 |
| biotype | 1005 | C4* | "Adenosine" | 2  |
| biotype | 1006 | H4* | "Adenosine" | 3  |
| biotype | 1007 | O4* | "Adenosine" | 1  |
| biotype | 1008 | C1* | "Adenosine" | 4  |

|         |      |     |             |     |
|---------|------|-----|-------------|-----|
| biotype | 1009 | H1* | "Adenosine" | 5   |
| biotype | 1010 | C3* | "Adenosine" | 8   |
| biotype | 1011 | H3* | "Adenosine" | 9   |
| biotype | 1012 | C2* | "Adenosine" | 6   |
| biotype | 1013 | H2* | "Adenosine" | 7   |
| biotype | 1014 | O2* | "Adenosine" | 10  |
| biotype | 1015 | HO* | "Adenosine" | 11  |
| biotype | 1016 | O3* | "Adenosine" | 12  |
| biotype | 1017 | N9  | "Adenosine" | 405 |
| biotype | 1018 | C4  | "Adenosine" | 401 |
| biotype | 1019 | C5  | "Adenosine" | 404 |
| biotype | 1020 | N7  | "Adenosine" | 408 |
| biotype | 1021 | C8  | "Adenosine" | 402 |
| biotype | 1022 | N3  | "Adenosine" | 409 |
| biotype | 1023 | C2  | "Adenosine" | 407 |
| biotype | 1024 | N1  | "Adenosine" | 410 |
| biotype | 1025 | C6  | "Adenosine" | 403 |
| biotype | 1026 | H2  | "Adenosine" | 414 |
| biotype | 1027 | N6  | "Adenosine" | 406 |
| biotype | 1028 | H61 | "Adenosine" | 415 |
| biotype | 1029 | H62 | "Adenosine" | 415 |
| biotype | 1030 | H8  | "Adenosine" | 413 |
| biotype | 1031 | O5* | "Guanosine" | 19  |
| biotype | 1032 | C5* | "Guanosine" | 16  |
| biotype | 1033 | H5* | "Guanosine" | 17  |
| biotype | 1034 | H5* | "Guanosine" | 17  |
| biotype | 1035 | C4* | "Guanosine" | 2   |
| biotype | 1036 | H4* | "Guanosine" | 3   |
| biotype | 1037 | O4* | "Guanosine" | 1   |
| biotype | 1038 | C1* | "Guanosine" | 4   |
| biotype | 1039 | H1* | "Guanosine" | 5   |
| biotype | 1040 | C3* | "Guanosine" | 8   |
| biotype | 1041 | H3* | "Guanosine" | 9   |
| biotype | 1042 | C2* | "Guanosine" | 6   |
| biotype | 1043 | H2* | "Guanosine" | 7   |
| biotype | 1044 | O2* | "Guanosine" | 10  |
| biotype | 1045 | HO* | "Guanosine" | 11  |
| biotype | 1046 | O3* | "Guanosine" | 12  |
| biotype | 1047 | N9  | "Guanosine" | 208 |
| biotype | 1048 | C4  | "Guanosine" | 203 |
| biotype | 1049 | C5  | "Guanosine" | 207 |
| biotype | 1050 | N7  | "Guanosine" | 209 |
| biotype | 1051 | C8  | "Guanosine" | 204 |
| biotype | 1052 | N3  | "Guanosine" | 210 |

|         |      |     |             |     |
|---------|------|-----|-------------|-----|
| biotype | 1053 | C2  | "Guanosine" | 201 |
| biotype | 1054 | N1  | "Guanosine" | 205 |
| biotype | 1055 | C6  | "Guanosine" | 202 |
| biotype | 1056 | H1  | "Guanosine" | 211 |
| biotype | 1057 | N2  | "Guanosine" | 206 |
| biotype | 1058 | H21 | "Guanosine" | 216 |
| biotype | 1059 | H22 | "Guanosine" | 216 |
| biotype | 1060 | O6  | "Guanosine" | 214 |
| biotype | 1061 | H8  | "Guanosine" | 215 |
| biotype | 1062 | O5* | "Cytidine"  | 19  |
| biotype | 1063 | C5* | "Cytidine"  | 16  |
| biotype | 1064 | H5* | "Cytidine"  | 17  |
| biotype | 1065 | H5* | "Cytidine"  | 17  |
| biotype | 1066 | C4* | "Cytidine"  | 2   |
| biotype | 1067 | H4* | "Cytidine"  | 3   |
| biotype | 1068 | O4* | "Cytidine"  | 1   |
| biotype | 1069 | C1* | "Cytidine"  | 4   |
| biotype | 1070 | H1* | "Cytidine"  | 5   |
| biotype | 1071 | C3* | "Cytidine"  | 8   |
| biotype | 1072 | H3* | "Cytidine"  | 9   |
| biotype | 1073 | C2* | "Cytidine"  | 6   |
| biotype | 1074 | H2* | "Cytidine"  | 7   |
| biotype | 1075 | O2* | "Cytidine"  | 10  |
| biotype | 1076 | HO* | "Cytidine"  | 11  |
| biotype | 1077 | O3* | "Cytidine"  | 12  |
| biotype | 1078 | N1  | "Cytidine"  | 301 |
| biotype | 1079 | C2  | "Cytidine"  | 305 |
| biotype | 1080 | N3  | "Cytidine"  | 307 |
| biotype | 1081 | C4  | "Cytidine"  | 306 |
| biotype | 1082 | C5  | "Cytidine"  | 302 |
| biotype | 1083 | C6  | "Cytidine"  | 304 |
| biotype | 1084 | O2  | "Cytidine"  | 309 |
| biotype | 1085 | N4  | "Cytidine"  | 303 |
| biotype | 1086 | H41 | "Cytidine"  | 313 |
| biotype | 1087 | H42 | "Cytidine"  | 313 |
| biotype | 1088 | H5  | "Cytidine"  | 308 |
| biotype | 1089 | H6  | "Cytidine"  | 312 |
| biotype | 1090 | O5* | "Uridine"   | 19  |
| biotype | 1091 | C5* | "Uridine"   | 16  |
| biotype | 1092 | H5* | "Uridine"   | 17  |
| biotype | 1093 | H5* | "Uridine"   | 17  |
| biotype | 1094 | C4* | "Uridine"   | 2   |
| biotype | 1095 | H4* | "Uridine"   | 3   |
| biotype | 1096 | O4* | "Uridine"   | 1   |



|         |      |     |                      |     |
|---------|------|-----|----------------------|-----|
| biotype | 1097 | C1* | "Uridine"            | 4   |
| biotype | 1098 | H1* | "Uridine"            | 5   |
| biotype | 1099 | C3* | "Uridine"            | 8   |
| biotype | 1100 | H3* | "Uridine"            | 9   |
| biotype | 1101 | C2* | "Uridine"            | 6   |
| biotype | 1102 | H2* | "Uridine"            | 7   |
| biotype | 1103 | O2* | "Uridine"            | 10  |
| biotype | 1104 | HO* | "Uridine"            | 11  |
| biotype | 1105 | O3* | "Uridine"            | 12  |
| biotype | 1106 | N1  | "Uridine"            | 505 |
| biotype | 1107 | C2  | "Uridine"            | 501 |
| biotype | 1108 | N3  | "Uridine"            | 504 |
| biotype | 1109 | C4  | "Uridine"            | 503 |
| biotype | 1110 | C5  | "Uridine"            | 506 |
| biotype | 1111 | C6  | "Uridine"            | 502 |
| biotype | 1112 | O2  | "Uridine"            | 510 |
| biotype | 1113 | H3  | "Uridine"            | 508 |
| biotype | 1114 | O4  | "Uridine"            | 511 |
| biotype | 1115 | H5  | "Uridine"            | 509 |
| biotype | 1116 | H6  | "Uridine"            | 512 |
| biotype | 1230 | P   | "Phosphodiester RNA" | 101 |
| biotype | 1231 | OP  | "Phosphodiester RNA" | 102 |
| biotype | 1232 | O5* | "5'-Hydroxyl RNA"    | 19  |
| biotype | 1233 | H5T | "5'-Hydroxyl RNA"    | 20  |
| biotype | 1237 | O3* | "3'-Hydroxyl RNA"    | 12  |
| biotype | 1238 | H3T | "3'-Hydroxyl RNA"    | 13  |
| biotype | 1117 | O5* | "Deoxyadenosine"     | 68  |
| biotype | 1118 | C5* | "Deoxyadenosine"     | 63  |
| biotype | 1119 | H5* | "Deoxyadenosine"     | 66  |
| biotype | 1120 | H5* | "Deoxyadenosine"     | 66  |
| biotype | 1121 | C4* | "Deoxyadenosine"     | 51  |
| biotype | 1122 | H4* | "Deoxyadenosine"     | 61  |
| biotype | 1123 | O4* | "Deoxyadenosine"     | 55  |
| biotype | 1124 | C1* | "Deoxyadenosine"     | 54  |
| biotype | 1125 | H1* | "Deoxyadenosine"     | 58  |
| biotype | 1126 | C3* | "Deoxyadenosine"     | 52  |
| biotype | 1127 | H3* | "Deoxyadenosine"     | 60  |
| biotype | 1128 | C2* | "Deoxyadenosine"     | 53  |
| biotype | 1129 | H2* | "Deoxyadenosine"     | 56  |
| biotype | 1130 | H2* | "Deoxyadenosine"     | 56  |
| biotype | 1131 | O3* | "Deoxyadenosine"     | 64  |
| biotype | 1132 | N9  | "Deoxyadenosine"     | 425 |
| biotype | 1133 | C4  | "Deoxyadenosine"     | 401 |
| biotype | 1134 | C5  | "Deoxyadenosine"     | 404 |

|         |      |     |                  |     |
|---------|------|-----|------------------|-----|
| biotype | 1135 | N7  | "Deoxyadenosine" | 408 |
| biotype | 1136 | C8  | "Deoxyadenosine" | 402 |
| biotype | 1137 | N3  | "Deoxyadenosine" | 409 |
| biotype | 1138 | C2  | "Deoxyadenosine" | 407 |
| biotype | 1139 | N1  | "Deoxyadenosine" | 410 |
| biotype | 1140 | C6  | "Deoxyadenosine" | 403 |
| biotype | 1141 | H2  | "Deoxyadenosine" | 414 |
| biotype | 1142 | N6  | "Deoxyadenosine" | 406 |
| biotype | 1143 | H61 | "Deoxyadenosine" | 415 |
| biotype | 1144 | H62 | "Deoxyadenosine" | 415 |
| biotype | 1145 | H8  | "Deoxyadenosine" | 413 |
| biotype | 1146 | O5* | "Deoxyguanosine" | 68  |
| biotype | 1147 | C5* | "Deoxyguanosine" | 63  |
| biotype | 1148 | H5* | "Deoxyguanosine" | 66  |
| biotype | 1149 | H5* | "Deoxyguanosine" | 66  |
| biotype | 1150 | C4* | "Deoxyguanosine" | 51  |
| biotype | 1151 | H4* | "Deoxyguanosine" | 61  |
| biotype | 1152 | O4* | "Deoxyguanosine" | 55  |
| biotype | 1153 | C1* | "Deoxyguanosine" | 54  |
| biotype | 1154 | H1* | "Deoxyguanosine" | 58  |
| biotype | 1155 | C3* | "Deoxyguanosine" | 52  |
| biotype | 1156 | H3* | "Deoxyguanosine" | 60  |
| biotype | 1157 | C2* | "Deoxyguanosine" | 53  |
| biotype | 1158 | H2* | "Deoxyguanosine" | 56  |
| biotype | 1159 | H2* | "Deoxyguanosine" | 56  |
| biotype | 1160 | O3* | "Deoxyguanosine" | 64  |
| biotype | 1161 | N9  | "Deoxyguanosine" | 228 |
| biotype | 1162 | C4  | "Deoxyguanosine" | 203 |
| biotype | 1163 | C5  | "Deoxyguanosine" | 207 |
| biotype | 1164 | N7  | "Deoxyguanosine" | 209 |
| biotype | 1165 | C8  | "Deoxyguanosine" | 204 |
| biotype | 1166 | N3  | "Deoxyguanosine" | 210 |
| biotype | 1167 | C2  | "Deoxyguanosine" | 201 |
| biotype | 1168 | N1  | "Deoxyguanosine" | 205 |
| biotype | 1169 | C6  | "Deoxyguanosine" | 202 |
| biotype | 1170 | H1  | "Deoxyguanosine" | 211 |
| biotype | 1171 | N2  | "Deoxyguanosine" | 206 |
| biotype | 1172 | H21 | "Deoxyguanosine" | 216 |
| biotype | 1173 | H22 | "Deoxyguanosine" | 216 |
| biotype | 1174 | O6  | "Deoxyguanosine" | 214 |
| biotype | 1175 | H8  | "Deoxyguanosine" | 215 |
| biotype | 1176 | O5* | "Deoxycytidine"  | 68  |
| biotype | 1177 | C5* | "Deoxycytidine"  | 63  |
| biotype | 1178 | H5* | "Deoxycytidine"  | 66  |

|         |      |     |                  |     |
|---------|------|-----|------------------|-----|
| biotype | 1179 | H5* | "Deoxycytidine"  | 66  |
| biotype | 1180 | C4* | "Deoxycytidine"  | 51  |
| biotype | 1181 | H4* | "Deoxycytidine"  | 61  |
| biotype | 1182 | O4* | "Deoxycytidine"  | 55  |
| biotype | 1183 | C1* | "Deoxycytidine"  | 54  |
| biotype | 1184 | H1* | "Deoxycytidine"  | 58  |
| biotype | 1185 | C3* | "Deoxycytidine"  | 52  |
| biotype | 1186 | H3* | "Deoxycytidine"  | 60  |
| biotype | 1187 | C2* | "Deoxycytidine"  | 53  |
| biotype | 1188 | H2* | "Deoxycytidine"  | 56  |
| biotype | 1189 | H2* | "Deoxycytidine"  | 56  |
| biotype | 1190 | O3* | "Deoxycytidine"  | 64  |
| biotype | 1191 | N1  | "Deoxycytidine"  | 321 |
| biotype | 1192 | C2  | "Deoxycytidine"  | 305 |
| biotype | 1193 | N3  | "Deoxycytidine"  | 307 |
| biotype | 1194 | C4  | "Deoxycytidine"  | 306 |
| biotype | 1195 | C5  | "Deoxycytidine"  | 302 |
| biotype | 1196 | C6  | "Deoxycytidine"  | 304 |
| biotype | 1197 | O2  | "Deoxycytidine"  | 309 |
| biotype | 1198 | N4  | "Deoxycytidine"  | 303 |
| biotype | 1199 | H41 | "Deoxycytidine"  | 313 |
| biotype | 1200 | H42 | "Deoxycytidine"  | 313 |
| biotype | 1201 | H5  | "Deoxycytidine"  | 308 |
| biotype | 1202 | H6  | "Deoxycytidine"  | 312 |
| biotype | 1203 | O5* | "Deoxythymidine" | 68  |
| biotype | 1204 | C5* | "Deoxythymidine" | 63  |
| biotype | 1205 | H5* | "Deoxythymidine" | 66  |
| biotype | 1206 | H5* | "Deoxythymidine" | 66  |
| biotype | 1207 | C4* | "Deoxythymidine" | 51  |
| biotype | 1208 | H4* | "Deoxythymidine" | 61  |
| biotype | 1209 | O4* | "Deoxythymidine" | 55  |
| biotype | 1210 | C1* | "Deoxythymidine" | 54  |
| biotype | 1211 | H1* | "Deoxythymidine" | 58  |
| biotype | 1212 | C3* | "Deoxythymidine" | 52  |
| biotype | 1213 | H3* | "Deoxythymidine" | 60  |
| biotype | 1214 | C2* | "Deoxythymidine" | 53  |
| biotype | 1215 | H2* | "Deoxythymidine" | 56  |
| biotype | 1216 | H2* | "Deoxythymidine" | 56  |
| biotype | 1217 | O3* | "Deoxythymidine" | 64  |
| biotype | 1218 | N1  | "Deoxythymidine" | 605 |
| biotype | 1219 | C2  | "Deoxythymidine" | 607 |
| biotype | 1220 | N3  | "Deoxythymidine" | 606 |
| biotype | 1221 | C4  | "Deoxythymidine" | 603 |
| biotype | 1222 | C5  | "Deoxythymidine" | 602 |

|         |      |     |                      |     |
|---------|------|-----|----------------------|-----|
| biotype | 1223 | C6  | "Deoxythymidine"     | 604 |
| biotype | 1224 | O2  | "Deoxythymidine"     | 609 |
| biotype | 1225 | H3  | "Deoxythymidine"     | 612 |
| biotype | 1226 | O4  | "Deoxythymidine"     | 611 |
| biotype | 1227 | C7  | "Deoxythymidine"     | 601 |
| biotype | 1228 | H7  | "Deoxythymidine"     | 608 |
| biotype | 1229 | H6  | "Deoxythymidine"     | 610 |
| biotype | 1242 | P   | "Phosphodiester DNA" | 101 |
| biotype | 1243 | OP  | "Phosphodiester DNA" | 102 |
| biotype | 1244 | O5* | "5'-Hydroxyl DNA"    | 68  |
| biotype | 1245 | H5T | "5'-Hydroxyl DNA"    | 69  |
| biotype | 1249 | O3* | "3'-Hydroxyl DNA"    | 64  |
| biotype | 1250 | H3T | "3'-Hydroxyl DNA"    | 65  |
| biotype | 2001 | O   | "Water"              | 36  |
| biotype | 2002 | H   | "Water"              | 37  |
| biotype | 2003 | NA  | "Sodium Ion"         | 41  |
| biotype | 2004 | K   | "Potassium Ion"      | 42  |
| biotype | 2005 | MG  | "Magnesium Ion"      | 43  |
| biotype | 2007 | CL  | "Chloride Ion"       | 44  |