

xyz coordinates of structure 1

6 0.118832 -1.602850 1.375592
6 -1.149719 -1.578566 0.710477
6 -1.149719 -1.578566 -0.710477
6 0.118832 -1.602850 -1.375592
26 -0.004522 0.012214 0.000000
6 -0.513803 1.151956 1.296349
6 -0.513803 1.151956 -1.296349
6 1.768357 0.243167 0.000000
8 -0.826319 1.870020 2.149222
8 -0.826319 1.870020 -2.149222
8 2.920797 0.358216 0.000000
1 0.899422 -2.280806 1.038127
1 -2.078392 -1.407368 1.251935
1 -2.078392 -1.407368 -1.251935
1 0.128188 -1.416376 -2.448092
1 0.128188 -1.416376 2.448092
1 0.899422 -2.280806 -1.038127

xyz coordinates of structure 2

6 1.190782 -.695329 -1.402765
6 1.757471 -.618157 -.085183
6 1.053816 -1.322799 .931360
6 -.134671 -2.039234 .570196
26 -.260007 -.014268 -.017082
6 .093624 1.708883 -.390393
6 -1.155367 .417904 1.481988
6 -1.607798 -.350738 -1.142111
8 .328009 2.811216 -.658841
8 -1.741204 .670433 2.448632
8 -2.464508 -.599562 -1.881014
1 .848979 -1.647684 -1.802262
1 1.343223 -1.189282 1.973056
1 -.756175 -2.415137 1.381247
1 1.598163 -.025304 -2.159538
1 -.145802 -2.666905 -.318411
6 2.970162 .225703 .233012
1 2.971712 .565865 1.275450
1 3.032983 1.103252 -.420573
1 3.880612 -.367924 .068324

xyz coordinates of structure 2'

6 1.196409 .183955 -1.628867
6 1.778978 -.351940 -.446951
6 1.166336 -1.545026 .074135
6 .050790 -2.098434 -.609357
26 -.261951 -.030810 -.028456
6 -.023600 .595059 1.635220
6 -1.899976 -.686589 .130672
6 -.839617 1.447410 -.813326
8 .100011 1.014005 2.709936
8 -2.973229 -1.116233 .248446
8 -1.206104 2.426541 -1.320646
1 .825786 -.452051 -2.428042
1 1.496078 -1.944793 1.031558
1 -.488611 -2.905976 -.118775

1 1.542635 1.161901 -1.960271
1 -.000097 -2.116981 -1.694929
6 2.950446 .300262 .249811
1 2.957842 .090639 1.325873
1 2.942693 1.387021 .108446
1 3.890375 -.081387 -1.73912

xyz coordinates of structure 3

6 -1.785010 -.709891 -.011755
6 -1.106793 -1.009305 -1.232228
6 .120892 -1.724870 -1.170865
6 .610628 -2.101733 .122087
26 .266229 -.012746 -.006830
6 -.178897 1.636057 -.568564
6 2.000686 .282361 -.370761
6 .223427 .184439 1.768069
8 -.470497 2.703244 -.913041
8 3.127112 .448492 -.584009
8 .184035 .286171 2.922124
1 -1.798701 -1.480550 .757270
1 -1.433041 -.575224 -2.177049
1 .721974 -1.844414 -2.070107
1 1.626169 -2.489365 .180750
1 -.064557 -2.527247 .861320
6 -3.003295 .190527 -.001184
1 -2.957355 .957162 -.784006
1 -3.113232 .701504 .962884
1 -3.918244 -.399236 -.162869

xyz coordinates of structure 4

6 -1.710951 0.558444 -0.642468
6 -1.040165 -0.259083 -1.623034
6 -0.497794 -1.518774 -1.253998
6 -0.577661 -1.961971 0.106721
26 0.264559 -0.015051 -0.018976
6 0.908504 1.568535 -0.576119
6 1.925553 -0.707232 0.087693
6 -0.104504 0.341850 1.689359
8 1.305495 2.598322 -0.927893
8 2.983601 -1.168713 0.181649
8 -0.387004 0.563660 2.791360
1 -0.777869 0.144325 -2.600955
1 0.143610 -2.036467 -1.966318
1 0.053905 -2.805181 0.383077
1 -1.500994 -1.909001 0.668711
1 -1.765093 1.607890 -0.942464
6 -2.959456 0.172758 0.143297
1 -3.845695 0.483211 -0.430274
1 -3.000814 0.692491 1.108285
1 -3.063475 -0.899252 0.323688

xyz coordinates of structure 5

6 -1.057184 -0.471780 -1.750540
6 -1.563112 -1.007743 -0.527921
6 -2.091013 -0.055348 0.465507
6 -2.023445 1.306886 0.279360
26 0.058763 0.009330 0.017142

6 1.553972 -0.817448 -0.605332
6 0.667412 0.054773 1.768046
6 0.664701 1.630505 -0.580396
8 2.488940 -1.340786 -1.007352
8 1.038797 0.079817 2.849501
8 1.063150 2.626701 -0.980121
1 -1.554453 0.367163 -2.230158
1 -2.348078 -0.445285 1.449265
1 -2.200058 1.971748 1.123193
1 -0.544311 -1.142928 -2.436047
1 -1.976260 1.771904 -0.700052
6 -0.856114 -2.062640 0.093744
1 -1.111552 -2.380181 1.101832
1 -0.291526 -2.774078 -0.504769

xyz coordinates of structure 5'

6 -1.147912 .836226 -1.394458
6 -1.600392 -.399361 -.860934
6 -2.638023 -.498176 .185806
6 -3.514195 .476755 .509910
26 .372453 .066850 -1.113486
6 1.949838 -.612664 -.653582
6 .628421 -.786340 1.467664
6 .997700 1.764947 .315428
8 2.934120 -1.030023 -1.063981
8 .716023 -1.301937 2.485728
8 1.402694 2.800258 .578978
1 -1.653228 1.776252 -1.190404
1 -2.718097 -1.466407 .680818
1 -4.279306 .303505 1.263632
1 -.558608 .820075 -2.316872
1 -3.517802 1.454050 .030052
6 -.722047 -1.503379 -1.062764
1 -.914902 -2.447381 -.556912
1 -.184877 -1.592623 -2.007890

xyz coordinates of structure 5ts

6 1.530213 -0.076891 -1.333858
6 1.821876 -0.376078 0.080989
6 1.174731 -1.495525 0.683631
6 0.179810 -2.158309 -0.065039
26 -0.173683 -0.022239 -0.009429
6 -0.132541 1.806950 0.041983
6 -1.338424 -0.126191 1.409639
6 -1.473837 -0.190526 -1.277907
8 -0.109572 2.953278 0.061842
8 -2.053305 -0.209356 2.300298
8 -2.248742 -0.316433 -2.112184
1 1.594998 -0.883710 -2.068763
1 1.340362 -1.708301 1.739146
1 -0.440095 -2.888340 0.450914
1 1.800330 0.903066 -1.728254
1 0.287038 -2.324626 -1.134744
6 2.966911 0.386701 0.451098
1 3.922123 0.149449 -0.021588
1 2.931531 1.289971 1.065591

xyz coordinates of structure 6

6 -1.075708 0.913526 -1.242249
6 -1.562115 -0.367811 -0.810994
6 -2.661708 -0.553366 0.159443
6 -3.639892 0.354690 0.383896
26 0.547613 -0.005390 -0.288741
6 1.456437 1.588439 -0.202104
6 1.879524 -1.241327 0.001950
6 0.148157 0.069336 1.450811
8 2.017965 2.606607 -0.186262
8 2.716078 -2.035026 0.150896
8 -0.141423 0.111404 2.577235
1 -1.540885 1.831492 -0.897055
1 -2.708817 -1.524308 0.651234
1 -4.455491 0.135405 1.067194
1 -0.621869 0.992111 -2.237202
1 -3.678724 1.319365 -0.118088
6 -0.696502 -1.458871 -1.145513
1 -0.880822 -2.453796 -0.750621
1 -0.181454 -1.451709 -2.114587

xyz coordinates of structure 6'

6 .996882 -1.201965 -1.058542
6 1.613457 -0.000027 -0.619632
6 2.656273 -0.000004 .456546
6 3.961335 .000000 .151487
26 -.529130 .000009 -.294056
6 -1.694170 -1.444814 -.216538
6 -1.694055 1.444924 -.216451
6 -.358505 -0.000074 1.491752
8 -2.399519 -2.343028 -.191850
8 -2.399330 2.343193 -.191689
8 -.232020 -0.000124 2.629346
1 1.314937 -2.163706 -.662877
1 2.342857 .000008 1.500501
1 4.713366 .000014 .937435
1 .564700 -1.240421 -2.067955
1 4.320011 -0.000012 -.877122
6 .996913 1.201896 -1.058611
1 1.314994 2.163661 -.663024
1 .564693 1.240288 -2.068013

xyz coordinates of structure 9

6 -0.655742 -1.374935 -1.355161
6 -0.972545 -1.515483 0.038159
6 -1.753230 -0.467029 0.638320
26 0.269273 -0.004025 -0.000869
6 1.925688 -0.257423 -0.653155
6 0.697660 0.795614 1.549976
6 -0.177934 1.461228 -0.939604
8 2.987177 -0.442954 -1.074603
8 0.961004 1.293526 2.561090
8 -0.483630 2.396264 -1.549356
1 -1.380887 -0.944930 -2.041227
1 -1.798884 -0.500726 1.728480
1 0.028163 -2.091416 -1.805976
6 0.140115 -1.949382 0.840296
1 0.033356 -1.982183 1.923301

1 0.840438 -2.670540 0.423723
6 -2.964203 0.184117 0.004661
1 -2.893314 0.260191 -1.085128
1 -3.115316 1.195008 0.402015
1 -3.869916 -0.395688 0.239417

xyz coordinates of structure 11

6 -2.122985 -.522391 .130430
6 -1.443485 -.876872 -1.130593
6 -.409637 -1.830580 -1.013505
6 .085562 -2.150176 .288822
26 .074119 -.017353 .016893
6 -.014569 1.701110 -.667755
6 1.755188 -.132723 -.652768
6 .675632 .266864 1.728309
8 .004174 2.760728 -1.102599
8 2.814924 -.223200 -1.076034
8 1.017717 .420661 2.809671
1 -2.299702 -1.309191 .861733
1 -1.781181 -.501435 -2.094041
1 .146127 -2.120127 -1.904562
1 1.026759 -2.693199 .347777
1 -.586335 -2.355518 1.117592
6 -2.486258 .749723 .475245
1 -2.901280 .954810 1.461126
1 -2.462693 1.580600 -.226261

xyz coordinates of structure 11ts

6 -1.783295 -0.376466 0.006355
6 -1.176954 -1.074256 -1.164551
6 -0.128570 -1.954234 -0.821273
6 0.221462 -2.104698 0.549123
26 0.169774 -0.014708 -0.017295
6 -0.064872 1.637534 -0.746226
6 1.947730 -0.011504 -0.522743
6 0.421572 0.468430 1.712530
8 -0.248655 2.678410 -1.195924
8 3.050841 -0.026447 -0.831843
8 0.525204 0.745886 2.821783
1 -2.190945 -1.224875 0.655794
1 -1.518493 -0.900592 -2.182070
1 0.503402 -2.341857 -1.619542
1 1.170896 -2.578250 0.789383
1 -0.549031 -2.259441 1.303020
6 -3.005243 0.311431 0.108279
1 -3.954617 -0.190947 -0.110315
1 -3.085447 1.318162 0.532306

xyz coordinates of structure 12

6 -1.610408 1.263022 -.608546
6 -1.710965 -.002015 -1.267422
6 -1.605319 -1.267998 -.611401
6 -1.448679 -1.467064 .773103
26 .036081 .000075 -.005059
6 1.145296 1.288317 -.705175
6 1.150572 -1.283791 -.704567
6 .733436 .001194 1.672808

8 1.841646 2.090726 -1.129406
8 1.850121 -2.083772 -1.128122
8 1.152033 .001818 2.738920
1 -1.743318 -.000837 -2.355032
1 -1.426389 -2.116684 -1.272730
1 -1.119382 -2.453948 1.093166
1 -2.012400 -.920361 1.515896
6 -1.455005 1.459902 .776305
1 -1.434687 2.113841 -1.267993
1 -1.129697 2.447408 1.098521
1 -2.016205 .909032 1.517927

xyz coordinates of structure 13

6 -2.108579 0.488772 0.208140
6 -1.498562 0.287051 -1.139711
6 -0.959991 -0.982375 -1.443424
6 -0.684091 -1.892315 -0.382537
26 0.194108 0.008579 0.040276
6 0.668746 1.811138 0.090352
6 1.688143 -0.354038 -0.904757
6 0.934243 -0.636434 1.603764
8 0.994958 2.906536 0.100516
8 2.623873 -0.598229 -1.516690
8 1.357739 -1.054894 2.579780
1 -1.620838 1.040930 -1.916325
1 -0.539475 -1.147709 -2.435500
1 -0.066091 -2.761505 -0.598162
1 -1.398042 -2.024225 0.426020
6 -3.364025 0.189063 0.586417
1 -1.491166 1.000558 0.980577
1 -3.711294 0.391839 1.597579
1 -4.087772 -0.215422 -0.119677

xyz coordinates of structure 14

6 1.326747 1.197728 0.490987
6 2.127450 0.265658 -0.362330
6 1.185765 -0.252278 -1.372891
6 0.198309 0.635963 -1.906851
26 -0.369666 0.017849 0.007334
6 0.006102 -0.962580 1.440605
6 -1.567562 -1.106076 -0.667199
6 -1.433524 1.352518 0.480827
8 0.240338 -1.578151 2.411258
8 -2.351479 -1.847659 -1.128213
8 -2.095543 2.264014 0.812843
1 1.182665 2.198742 0.066232
1 1.371955 -1.218980 -1.845213
1 -0.395223 0.285691 -2.752484
1 1.688264 1.281804 1.521822
1 0.367543 1.712648 -1.905001
6 3.372168 -0.220522 -0.113601
1 3.797592 -1.026689 -0.713409
1 3.959253 0.134603 0.732977

xyz coordinates of structure 14ts

6 1.284146 -0.862152 -1.214720
6 1.851217 -0.558065 0.087917