Supporting Material

Influence of Protonation, Tautomeric and Stereoisomeric States on Protein-Ligand Docking Results

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This supporting material provides the pdb codes of the complexes taken from the CCDC / ASTEX data set with the corresponding number of protomers and stereoisomers as well as the ones used to extract the active ligands for the virtual screening set. Additionally, new structure files for ligands, where we have found problems in the CCDC / ASTEX data set, are given.

Complexes of the CCDC / ASTEX Data Set

# of protonation states	pdb codes
1	1a28, 1abe, 1abf, 1acl, 1apu, 1bma, 1byb, 1c1e, 1c5c, 1c5x, 1cdg, 1cle, 1coy, 1cqp, 1d3h, 1dbb, 1dbj, 1dmp, 1dwb, 1eed, 1ejn, 1epo, 1f3d, 1fen, 1fkg, 1fki, 1frp, 1hos, 1hpv, 1hvr, 1ibg, 1imb, 1ivq, 1lic, 1mup, 1rob, 1rt2, 1slt, 1snc, 1tdb, 1xid, 1xie, 2cpp, 2gbp, 2mcp, 2tmn, 2yhx, 3cla, 3gpb, 4phv, 5abp, 5cpp, 6rsa
2	1a4g, 1a6w, 1aaq, 1acj, 1ai5, 1apt, 1atl, 1b9v, 1byg, 1c12, 1cbs, 1cvu, 1d0l, 1d4p, 1did, 1dog, 1dwd, 1eap, 1ebg, 1epb, 1ets, 1ett, 1fax, 1fl3, 1hak, 1hfc, 1hri, 1hsb, 1htf, 1lcp, 1ldm, 1lyb, 1mdr, 1mmq, 1mts, 1okl, 1pbd, 1pdz, 1poc, 1ppc, 1pph, 1ppi, 1pso, 1qbu, 1tng, 1tnh, 1tni, 1tnl, 1tyl, 1yee, 25c8, 2ack, 2ctc, 2dbl, 2fox, 2ifb, 2pcp, 2ypi, 4cox, 4lbd, 7tim
4	1a42, 1a4q, 1acm, 1aoe, 1baf, 1cbx, 1cil, 1com, 1cps, 1cx2, 1dg5, 1dwc, 1eoc, 1etr, 1fgi, 1hdc, 1hyt, 1ivb, 1jap, 1kel, 1lyl, 1mbi, 1mcq, 1nco, 1ngp, 1nis, 1okm, 1phd, 1phg, 1ptv, 1qbr, 1rds, 1rne, 1rnt, 1srj, 1tlp, 1trk, 1uvs, 1uvt, 1ydr, 2aad, 2ada, 2cht, 2phh, 2pk4, 2qwk, 2r07, 3erd, 3ert, 3hvt, 3tpi, 4cts, 5er1
8	1a9u,1aco, 1aqw, 1azm, 1c83, 1ckp, 1dd7, 1dr1, 1ei1, 1eta, 1f0r, 1flr, 1glp, 1glq, 1hiv, 1ida, 1lah, 1lna, 1lst, 1mld, 1qcf, 1qpe, 1qpq, 1ukz, 1ulb, 1wap, 1ydt, 2ak3, 2cmd, 2h4n, 2lgs, 2tsc, 3cpa, 4fbp, 6rnt
16	1bbp, 1bl7, 1f0s, 1hsl, 1mrg, 1mrk, 1tmn
32	1b58, 1dhf, 4aah
64	4dfr

Table S1: The 213 complexes of the CCDC / ASTEX data set used for study on protonation states with pdb codes and number of generated protomers.

Complexes Uses in Virtual Screening

active ligands:	1a4q, 1b9t, 1b9v, 1f8b, 1f8c, 1f8d, 1f8e, 1inf, 1inv, 1inw, 1mwe, 1nnc, 2qwi, 2qwj, 2qwk

Table S2: The pdb codes of the complexes, which were used to obtain the active ligands for the virtual screening study.

Subset used for Stereoisomer Study

# of stereoisomers	pdb codes
2	1a42, 1acm, 1cbx, 1cps, 1dd7, 1dhf, 1dwd, 1eap, 1eta, 1ets, 1ett, 1f0r, 1f0s, 1fki, 1hsl, 1hyt, 1kel, 1lah, 1lcp, 1lst, 1lyl, 1mdr, 1mts, 1mup, 1nis, 1poc, 1ppc, 1pph, 1ptv, 1uvs, 1wap, 1ydr, 2ctc, 2lgs, 2tmn, 2tsc, 3cpa, 4dfr, 4lbd
4	1aqw, 1atl, 1bma, 1c12, 1cil, 1dr1, 1fax, 1fkg, 1glp, 1glq, 1hfc, 1jap, 1lna, 1mcq, 1mmq, 1tnl, 3cla

Table S3: The subset of the CCDC / ASTEX data set used for the docking of stereoisomers with number of the stereoisomers per complex and their pdb codes.

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GASTEIGER

@<TRIPOS>DICT

@<TRIPOS>ATOM
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      3 C3         -1.9496   -1.3796    0.3941 C.2       1 PRE221      0.0000
      4 C4         -2.8964   -0.2294    0.1680 C.3       1 PRE221      0.0000
      5 C5         -2.2090    0.9974   -0.3780 C.2       1 PRE221      0.0000
      6 C6         -0.8779    1.1210   -0.4392 C.2       1 PRE221      0.0000
      7 C7          1.1437   -0.2074   -1.0100 C.2       1 PRE221      0.0000
      8 C8          0.7154    0.5497    1.3598 C.3       1 PRE221      0.0000
      9 C1'        -0.3676    0.8271    2.3810 C.2       1 PRE221      0.0000
     10 C2'        -0.9103    2.0387    2.5651 C.2       1 PRE221      0.0000
     11 O4         -3.9004   -0.6819   -0.7579 O.3       1 PRE221      0.0000
     12 UNK(12)     1.1592    0.4898   -2.0616 O.co2     1 PRE221      0.0000
     13 UNK(13)     1.9841   -1.1217   -0.7885 O.co2     1 PRE221      0.0000
     14 O1'        -0.7665   -0.1035    3.0650 O.2       1 PRE221      0.0000
     15 UNK(15)    -1.8198    2.1785    3.4316 O.co2     1 PRE221      0.0000
     16 UNK(16)    -0.5112    3.0121    1.8696 O.co2     1 PRE221      0.0000
     17 H4         -3.3394    0.0138    1.0655 H         1 PRE221      0.0000
     18 H81         1.2425    1.4181    1.1894 H         1 PRE221      0.0000
     19 H82         1.3504   -0.1693    1.7350 H         1 PRE221      0.0000
     20 H2         -0.1163   -2.2007    0.5004 H         1 PRE221      0.0000
     21 H3         -2.2544   -2.3929    0.6292 H         1 PRE221      0.0000
     22 H5         -2.7197    1.8727   -0.7627 H         1 PRE221      0.0000
     23 H6         -0.5785    2.0715   -0.8657 H         1 PRE221      0.0000
     24 H4         -3.7410   -1.6752   -0.9788 H         1 PRE221      0.0000
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GASTEIGER

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      3 C3          27.3483   21.2369   18.1725 C.2       1 S58701      0.0000
      4 C4          28.3940   20.8487   19.2160 C.3       1 S58701      0.0000
      5 C5          24.0831   21.3437   17.0496 C.ar      1 S58701      0.0000
      6 C6          23.3939   20.3298   17.7273 C.ar      1 S58701      0.0000
      7 C7          22.0045   20.2194   17.6418 C.ar      1 S58701      0.0000
      8 C8          21.2752   21.1030   16.8443 C.ar      1 S58701      0.0000
      9 C9          21.9488   22.1327   16.1849 C.ar      1 S58701      0.0000
     10 C10         23.3317   22.2811   16.3263 C.ar      1 S58701      0.0000
     11 C11         26.1173   22.6324   15.1261 C.ar      1 S58701      0.0000
     12 C12         26.5877   23.9258   14.8738 C.ar      1 S58701      0.0000
     13 C13         26.4232   24.5060   13.6128 C.ar      1 S58701      0.0000
     14 C14         25.7936   23.7916   12.5905 C.ar      1 S58701      0.0000
     15 C15         25.3003   22.5097   12.8456 C.ar      1 S58701      0.0000
     16 C16         25.4548   21.9335   14.1103 C.ar      1 S58701      0.0000
     17 N1          25.4337   21.3668   17.1591 N.pl3     1 S58701      0.0000
     18 N2          26.0724   20.8119   18.1918 N.2       1 S58701      0.0000
     19 N3          19.2603   19.3738   16.8689 N.am      1 S58701      0.0000
     20 O1          19.1215   21.3532   15.3618 O.2       1 S58701      0.0000
     21 O2          18.9164   21.6543   17.8415 O.2       1 S58701      0.0000
     22 BR1         25.6129   24.5436   10.9078 Br        1 S58701      0.0000
     23 F1          28.7746   21.9475   19.9223 F         1 S58701      0.0000
     24 F2          29.4805   20.3173   18.5925 F         1 S58701      0.0000
     25 F3          27.8773   19.9254   20.0720 F         1 S58701      0.0000
     26 S1          19.5088   20.9736   16.7057 S.o2      1 S58701      0.0000
     27 H1          28.4299   22.5796   16.7789 H         1 S58701      0.0000
     28 H6          23.9461   19.6172   18.3292 H         1 S58701      0.0000
     29 H7          21.4895   19.4439   18.1973 H         1 S58701      0.0000
     30 H9          21.3941   22.8220   15.5586 H         1 S58701      0.0000
     31 H10         23.8262   23.1313   15.8706 H         1 S58701      0.0000
     32 H12         27.0832   24.4824   15.6610 H         1 S58701      0.0000
     33 H13         26.7843   25.5111   13.4275 H         1 S58701      0.0000
     34 H15         24.7957   21.9600   12.0592 H         1 S58701      0.0000
     35 H16         25.0600   20.9426   14.3037 H         1 S58701      0.0000
     36 H31         18.7243   18.9937   17.7311 H         1 S58701      0.0000
     37 H32         19.6308   18.6881   16.1153 H         1 S58701      0.0000
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     9    4   23 1
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      2 C2          0.0542   -9.2440   -2.3087 C.3       1 BZS807      0.0000
      3 C           0.8189   -9.1359   -0.9609 C.3       1 BZS807      0.0000
      4 C           2.3066   -9.0787   -1.2171 C.2       1 BZS807      0.0000
      5 CB          0.3364   -7.9192   -0.1211 C.3       1 BZS807      0.0000
      6 CG          1.1262   -7.7963    1.1669 C.ar      1 BZS807      0.0000
      7 CD1         0.9765   -8.7086    2.1416 C.ar      1 BZS807      0.0000
      8 CD2         1.9862   -6.7823    1.3666 C.ar      1 BZS807      0.0000
      9 CE1         1.6680   -8.6163    3.2864 C.ar      1 BZS807      0.0000
     10 CE2         2.6794   -6.6817    2.5103 C.ar      1 BZS807      0.0000
     11 CZ          2.5220   -7.6011    3.4724 C.ar      1 BZS807      0.0000
     12 O1          1.4582   -8.0743   -3.8331 O.co2     1 BZS807      0.0000
     13 O2         -0.5071   -7.1695   -3.3421 O.co2     1 BZS807      0.0000
     14 O3          2.8620   -7.9517   -1.3208 O.co2     1 BZS807      0.0000
     15 O4          2.9390  -10.1665   -1.2994 O.co2     1 BZS807      0.0000
     16 HD1         0.2864   -9.5328    2.0020 H         1 BZS807      0.0000
     17 HD2         2.1228   -6.0345    0.5938 H         1 BZS807      0.0000
     18 HE1         1.5366   -9.3625    4.0616 H         1 BZS807      0.0000
     19 HE2         3.3672   -5.8569    2.6572 H         1 BZS807      0.0000
     20 HZ          3.0829   -7.5240    4.3968 H         1 BZS807      0.0000
     21 H21         0.3285  -10.1121   -2.7905 H         1 BZS807      0.0000
     22 H22        -0.9598   -9.2573   -2.1281 H         1 BZS807      0.0000
     23 H           0.6187   -9.9885   -0.4188 H         1 BZS807      0.0000
     24 HB1        -0.6592   -8.0360    0.1157 H         1 BZS807      0.0000
     25 HB2         0.4607   -7.0533   -0.6648 H         1 BZS807      0.0000
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SMALL
GASTEIGER

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      3 O2P        20.5381   36.1239   20.2950 O.co2     1 Q2GP105     0.0000
      4 O3P        18.6103   35.9849   18.8462 O.co2     1 Q2GP105     0.0000
      5 O5'        18.0379   34.9680   24.2023 O.3       1 Q2GP105     0.0000
      6 C5'        18.9898   34.0161   24.7091 C.3       1 Q2GP105     0.0000
      7 C4'        19.4529   33.1296   23.5285 C.3       1 Q2GP105     0.0000
      8 O4'        18.2990   32.4458   23.0131 O.3       1 Q2GP105     0.0000
      9 C3'        20.0079   33.9636   22.3434 C.3       1 Q2GP105     0.0000
     10 O3'        21.2641   33.4205   21.9009 O.3       1 Q2GP105     0.0000
     11 C2'        18.9349   33.7544   21.2585 C.3       1 Q2GP105     0.0000
     12 O2'        19.4477   33.8627   19.9297 O.3       1 Q2GP105     0.0000
     13 C1'        18.4222   32.3418   21.5902 C.3       1 Q2GP105     0.0000
     14 N9         17.1100   32.1200   21.0068 N.pl3     1 Q2GP105     0.0000
     15 C8         16.7680   31.2050   20.0646 C.2       1 Q2GP105     0.0000
     16 N7         15.4341   31.3057   19.8352 N.2       1 Q2GP105     0.0000
     17 C5         14.9532   32.2974   20.6114 C.2       1 Q2GP105     0.0000
     18 C6         13.5928   32.9018   20.8165 C.2       1 Q2GP105     0.0000
     19 O6         12.6166   32.4596   20.2311 O.2       1 Q2GP105     0.0000
     20 N1         13.5641   33.9532   21.6755 N.am      1 Q2GP105     0.0000
     21 C2         14.6877   34.4170   22.3157 C.2       1 Q2GP105     0.0000
     22 N2         14.5820   35.4597   23.0945 N.pl3     1 Q2GP105     0.0000
     23 N3         15.8250   33.8486   22.1622 N.2       1 Q2GP105     0.0000
     24 C4         16.0058   32.8101   21.3310 C.2       1 Q2GP105     0.0000
     25 H8         17.4448   30.5119   19.5782 H         1 Q2GP105     0.0000
     26 H5'1       18.5303   33.4544   25.4400 H         1 Q2GP105     0.0000
     27 H5'2       19.7800   34.5336   25.1198 H         1 Q2GP105     0.0000
     28 H4'        20.1701   32.4648   23.8519 H         1 Q2GP105     0.0000
     29 H3'        20.0795   34.9583   22.6009 H         1 Q2GP105     0.0000
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     32 H1         12.6119   34.4387   21.8563 H         1 Q2GP105     0.0000
     33 H21        15.4558   35.8424   23.6094 H         1 Q2GP105     0.0000
     34 H22        13.6203   35.9427   23.2261 H         1 Q2GP105     0.0000
     35 H5'        17.1240   34.5085   24.0813 H         1 Q2GP105     0.0000
     36 H3'        21.9493   34.1822   21.7953 H         1 Q2GP105     0.0000
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      3 C3          1.0058   -1.1274   -0.1206 C.3       1 NAG401      0.0000
      4 C4         -0.0159    0.0281   -0.0064 C.3       1 NAG401      0.0000
      5 C5         -1.4067   -0.5435    0.3661 C.3       1 NAG401      0.0000
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      6 C6          -2.4149    0.5743    0.3817 C.3       1 NAG401      0.0000
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      8 C8           2.2508   -5.3304   -2.3579 C.3       1 NAG401      0.0000
      9 N2           1.3722   -3.3367   -1.2369 N.am      1 NAG401      0.0000
     10 O3           2.2560   -0.5642   -0.5596 O.3       1 NAG401      0.0000
     11 O4           0.4442    0.9154    1.0350 O.3       1 NAG401      0.0000
     12 O5          -1.8304   -1.5221   -0.6045 O.3       1 NAG401      0.0000
     13 O6          -2.8649    0.9319   -0.8271 O.3       1 NAG401      0.0000
     14 O7           0.5837   -3.9358   -3.2748 O.2       1 NAG401      0.0000
     15 C1           0.3595    2.3107    0.6932 C.3       2 GAL402      0.0000
     16 C2           0.7697    3.1304    1.9397 C.3       2 GAL402      0.0000
     17 C3           0.8463    4.6325    1.5723 C.3       2 GAL402      0.0000
     18 C4           1.7995    4.8154    0.3640 C.3       2 GAL402      0.0000
     19 C5           1.3131    3.9260   -0.8097 C.3       2 GAL402      0.0000
     20 C6           2.2657    4.0218   -2.0276 C.3       2 GAL402      0.0000
     21 O2          -0.1960    2.9649    2.9925 O.3       2 GAL402      0.0000
     22 O3           1.3442    5.3945    2.6849 O.3       2 GAL402      0.0000
     23 O4           3.1348    4.4195    0.7219 O.3       2 GAL402      0.0000
     24 O5           1.2760    2.5499   -0.3928 O.3       2 GAL402      0.0000
     25 O6           1.7938    3.1332   -3.0564 O.3       2 GAL402      0.0000
     26 O1          -0.9009   -3.3417    0.5663 O.3       1 NAG401      0.0000
     27 H1          -1.2861   -3.2924   -1.4180 H         1 NAG401      0.0000
     28 H2           0.3972   -1.7312   -2.0522 H         1 NAG401      0.0000
     29 H3           1.1146   -1.5720    0.8021 H         1 NAG401      0.0000
     30 H4          -0.0785    0.5212   -0.9085 H         1 NAG401      0.0000
     31 H5          -1.3520   -0.9688    1.3026 H         1 NAG401      0.0000
     32 H61         -2.0075    1.4289    0.7875 H         1 NAG401      0.0000
     33 H62         -3.2518    0.3047    0.9182 H         1 NAG401      0.0000
     34 H81          3.2294   -5.0092   -2.3645 H         1 NAG401      0.0000
     35 H82          2.0859   -5.9116   -1.5238 H         1 NAG401      0.0000
     36 H83          2.0661   -5.8859   -3.2053 H         1 NAG401      0.0000
     37 H1          -0.6016    2.5628    0.4218 H         2 GAL402      0.0000
     38 H2           1.6992    2.8167    2.2535 H         2 GAL402      0.0000
     39 H3          -0.0939    4.9585    1.3065 H         2 GAL402      0.0000
     40 H4           1.7813    5.8017    0.0679 H         2 GAL402      0.0000
     41 H5           0.3745    4.2387   -1.0964 H         2 GAL402      0.0000
     42 H61          3.2226    3.7383   -1.7728 H         2 GAL402      0.0000
     43 H62          2.2815    4.9775   -2.4115 H         2 GAL402      0.0000
     44 H2           2.0945   -3.6098   -0.4761 H         1 NAG401      0.0000
     45 H3           2.1553    0.4555   -0.6643 H         1 NAG401      0.0000
     46 H6          -3.5845    0.2634   -1.1372 H         1 NAG401      0.0000
     47 H2          -0.2625    1.9683    3.2438 H         2 GAL402      0.0000
     48 H3           0.6502    6.1077    2.9506 H         2 GAL402      0.0000
     49 H4           3.7297    5.2560    0.8074 H         2 GAL402      0.0000
     50 H6           2.5389    2.4657   -3.3019 H         2 GAL402      0.0000
     51 H1           0.0775   -3.4569    0.8670 H         1 NAG401      0.0000
@<TRIPOS>BOND
     1    1   12 1
     2    1    2 1
     3    1   26 1
     4    2    3 1
     5    2    9 1
     6    3    4 1
     7    3   10 1
     8    4    5 1
     9    4   11 1
    10    5    6 1
    11    5   12 1
    12    6   13 1
    13    7    8 1
    14    7    9 am
    15    7   14 2
    16   11   15 1
    17   15   16 1
    18   15   24 1
```

```
    19   16   17 1
    20   16   21 1
    21   17   18 1
    22   17   22 1
    23   18   23 1
    24   18   19 1
    25   19   24 1
    26   19   20 1
    27   20   25 1
    28    1   27 1
    29    2   28 1
    30    3   29 1
    31    4   30 1
    32    5   31 1
    33    6   32 1
    34    6   33 1
    35    8   34 1
    36    8   35 1
    37    8   36 1
    38   15   37 1
    39   16   38 1
    40   17   39 1
    41   18   40 1
    42   19   41 1
    43   20   42 1
    44   20   43 1
    45    9   44 1
    46   10   45 1
    47   13   46 1
    48   21   47 1
    49   22   48 1
    50   23   49 1
    51   25   50 1
    52   26   51 1
@<TRIPOS>SUBSTRUCTURE
1 NAG401 1
2 GAL402 15
@<TRIPOS>COMMENT
```

```
@<TRIPOS>MOLECULE
Minimised_ligand (1snc) hydrolase (phosphoric diester)
37 38 1
PROTEIN
GASTEIGER

@<TRIPOS>DICT

@<TRIPOS>ATOM
      1 N1         -0.5422    1.3579   -0.5630 N.am      1 PTP143      0.0000
BACKBONE
      2 C2         -0.8718    2.1746    0.4674 C.2       1 PTP143      0.0000
BACKBONE
      3 O2         -0.8363    1.7981    1.6285 O.2       1 PTP143      0.0000
BACKBONE
      4 N3         -1.2407    3.4399    0.1693 N.am      1 PTP143      0.0000
BACKBONE
      5 C4         -1.3022    3.8880   -1.1025 C.2       1 PTP143      0.0000
BACKBONE
      6 O4         -1.6309    5.0386   -1.3517 O.2       1 PTP143      0.0000
BACKBONE
      7 C5         -1.0048    3.0601   -2.1148 C.2       1 PTP143      0.0000
BACKBONE
      8 C5M        -1.0863    3.5653   -3.5412 C.3       1 PTP143      0.0000
```

```
      9 C6          -0.6345    1.7991   -1.8421 C.2       1 PTP143      0.0000
BACKBONE
     10 C1'         -0.0949   -0.0157   -0.2942 C.3       1 PTP143      0.0000
BACKBONE
     11 C2'         -1.2531   -1.0312   -0.3072 C.3       1 PTP143      0.0000
     12 C3'         -0.4994   -2.3717   -0.4465 C.3       1 PTP143      0.0000
     13 O3'         -0.1357   -2.8764    0.8492 O.3       1 PTP143      0.0000
     14 P3'          0.5845   -4.2808    1.1451 P.3       1 PTP143      0.0000
     15 O13          0.4046   -4.6323    2.5822 O.co2     1 PTP143      0.0000
     16 O23          2.0442   -4.2089    0.8586 O.co2     1 PTP143      0.0000
     17 O33         -0.0159   -5.3523    0.3014 O.co2     1 PTP143      0.0000
     18 C4'          0.7497   -1.9691   -1.2756 C.3       1 PTP143      0.0000
     19 O4'          0.7408   -0.5324   -1.3400 O.3       1 PTP143      0.0000
     20 C5'          0.6796   -2.4945   -2.7290 C.3       1 PTP143      0.0000
     21 O5'          1.7861   -1.9650   -3.4704 O.3       1 PTP143      0.0000
     22 P5'          2.0384   -2.1888   -5.0371 P.3       1 PTP143      0.0000
     23 O15          0.7975   -1.8708   -5.7986 O.co2     1 PTP143      0.0000
     24 O25          3.1253   -1.2776   -5.4923 O.co2     1 PTP143      0.0000
     25 O35          2.4429   -3.6010   -5.2894 O.co2     1 PTP143      0.0000
     26 H5M1        -2.0635    3.5251   -3.8644 H         1 PTP143      0.0000
     27 H5M2        -0.7515    4.5385   -3.5804 H         1 PTP143      0.0000
     28 H5M3        -0.4994    2.9757   -4.1483 H         1 PTP143      0.0000
     29 H1'          0.3875   -0.0619    0.6147 H         1 PTP143      0.0000
BACKBONE
     30 H2'1        -1.8829   -0.8699   -1.1061 H         1 PTP143      0.0000
     31 H2'2        -1.7933   -0.9936    0.5690 H         1 PTP143      0.0000
     32 H3'         -1.0707   -3.0478   -0.9732 H         1 PTP143      0.0000
     33 H4'          1.6020   -2.3207   -0.8164 H         1 PTP143      0.0000
     34 H5'1        -0.1890   -2.1905   -3.1916 H         1 PTP143      0.0000
     35 H5'2         0.7408   -3.5223   -2.7550 H         1 PTP143      0.0000
     36 H3          -1.4955    4.1172    0.9764 H         1 PTP143      0.0000
BACKBONE
     37 H6          -0.4075    1.1297   -2.6639 H         1 PTP143      0.0000
BACKBONE
@<TRIPOS>BOND
     1    1    9 1 BACKBONE
     2    1   10 1 BACKBONE
     3    1    2 am BACKBONE
     4    2    3 2 BACKBONE
     5    2    4 am BACKBONE
     6    4    5 am BACKBONE
     7    5    6 2 BACKBONE
     8    5    7 1 BACKBONE
     9    7    9 2
    10    7    8 1
    11   10   11 1
    12   10   19 1
    13   11   12 1
    14   12   18 1
    15   12   13 1
    16   13   14 1
    17   14   17 ar
    18   14   15 ar
    19   14   16 ar
    20   18   19 1
    21   18   20 1
    22   20   21 1
    23   21   22 1
    24   22   24 ar
    25   22   23 ar
    26   22   25 ar
    27    8   26 1
    28    8   27 1
    29    8   28 1
    30   10   29 1 BACKBONE
```

```
    31   11   30 1
    32   11   31 1
    33   12   32 1
    34   18   33 1
    35   20   34 1
    36   20   35 1
    37    4   36 1 BACKBONE
    38    9   37 1 BACKBONE
@<TRIPOS>SUBSTRUCTURE
1 PTP143 1
@<TRIPOS>COMMENT
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```
@<TRIPOS>MOLECULE
Minimised_ligand (1trk) transferase(ketone residues)
43 44 1
SMALL
GASTEIGER

@<TRIPOS>DICT

@<TRIPOS>ATOM
      1 N1'        -4.8929   -3.1905    2.4123 N.ar      1 TPP682      0.0000
      2 C2'        -5.7100   -2.3281    1.7668 C.ar      1 TPP682      0.0000
      3 MC2'       -6.9809   -2.8069    1.0672 C.3       1 TPP682      0.0000
      4 N3'        -5.4072   -1.0181    1.7398 N.ar      1 TPP682      0.0000
      5 C4'        -4.2698   -0.5430    2.2864 C.ar      1 TPP682      0.0000
      6 N4'        -4.1013    0.7933    2.3594 N.pl3     1 TPP682      0.0000
      7 C5'        -3.3014   -1.4401    2.7632 C.ar      1 TPP682      0.0000
      8 C6'        -3.6670   -2.7862    2.8365 C.ar      1 TPP682      0.0000
      9 C7'        -1.8973   -0.9817    3.1972 C.3       1 TPP682      0.0000
     10 N3         -1.1461   -0.2193    2.1945 N.pl3     1 TPP682      0.0000
     11 C2         -0.6921    0.9784    2.4383 C.2       1 TPP682      0.0000
     12 S1          0.2498    1.6508    1.0993 S.3       1 TPP682      0.0000
     13 C5         -0.0663    0.1146    0.2840 C.2       1 TPP682      0.0000
     14 C4         -0.8414   -0.6959    1.0145 C.2       1 TPP682      0.0000
     15 MC4        -1.3360   -2.0374    0.5378 C.3       1 TPP682      0.0000
     16 C6          0.4719   -0.2120   -1.0913 C.3       1 TPP682      0.0000
     17 C7          1.3521    0.8676   -1.7630 C.3       1 TPP682      0.0000
     18 O7          1.4582    0.5886   -3.1692 O.3       1 TPP682      0.0000
     19 PA          1.5900    1.6387   -4.3708 P.3       1 TPP682      0.0000
     20 O1A         0.2258    2.1913   -4.6019 O.co2     1 TPP682      0.0000
     21 O2A         2.0600    0.9224   -5.5912 O.co2     1 TPP682      0.0000
     22 O3A         2.5896    2.8312   -3.9910 O.3       1 TPP682      0.0000
     23 PB          2.6732    3.9847   -5.1004 P.3       1 TPP682      0.0000
     24 O1B         1.3458    4.6376   -5.2781 O.co2     1 TPP682      0.0000
     25 O2B         3.1276    3.4062   -6.3974 O.co2     1 TPP682      0.0000
     26 O3B         3.6313    5.0304   -4.6425 O.co2     1 TPP682      0.0000
     27 ****       -6.8525   -3.8458    0.7317 H         1 TPP682      0.0000
     28 ****       -7.1651   -2.1609    0.2013 H         1 TPP682      0.0000
     29 ****       -7.8319   -2.7294    1.7593 H         1 TPP682      0.0000
     30 ****       -3.3831    1.1890    2.9797 H         1 TPP682      0.0000
     31 ****       -4.7482    1.4229    1.8580 H         1 TPP682      0.0000
     32 ****       -2.9686   -3.5144    3.2317 H         1 TPP682      0.0000
     33 ****       -1.2567   -1.8301    3.4844 H         1 TPP682      0.0000
     34 ****       -2.0197   -0.4160    4.1255 H         1 TPP682      0.0000
     35 ****       -0.8415    1.5700    3.3384 H         1 TPP682      0.0000
     36 ****       -0.8295   -2.3960   -0.3645 H         1 TPP682      0.0000
     37 ****       -2.4083   -1.9603    0.3059 H         1 TPP682      0.0000
     38 ****       -1.2074   -2.8008    1.3063 H         1 TPP682      0.0000
     39 ****       -0.4025   -0.3539   -1.7441 H         1 TPP682      0.0000
     40 ****        1.0467   -1.1510   -1.0554 H         1 TPP682      0.0000
     41 ****        2.3485    0.9085   -1.2892 H         1 TPP682      0.0000
     42 ****        0.8449    1.8365   -1.6633 H         1 TPP682      0.0000
     43 ****       -5.1968   -4.1567    2.5857 H         1 TPP682      0.0000
```

```
@<TRIPOS>BOND
     1    1    8 ar
     2    1   43 1
     3    1    2 ar
     4    2    3 1
     5    2    4 ar
     6    3   29 1
     7    3   27 1
     8    3   28 1
     9    4    5 ar
    10    5    6 1
    11    5    7 ar
    12    6   30 1
    13    6   31 1
    14    7    8 ar
    15    7    9 1
    16    8   32 1
    17    9   33 1
    18    9   10 1
    19    9   34 1
    20   10   11 2
    21   10   14 1
    22   11   35 1
    23   11   12 1
    24   12   13 1
    25   13   16 1
    26   13   14 2
    27   14   15 1
    28   15   38 1
    29   15   36 1
    30   15   37 1
    31   16   17 1
    32   16   40 1
    33   16   39 1
    34   17   18 1
    35   17   41 1
    36   17   42 1
    37   18   19 1
    38   19   20 ar
    39   19   21 ar
    40   19   22 1
    41   22   23 1
    42   23   24 ar
    43   23   25 ar
    44   23   26 ar
@<TRIPOS>SUBSTRUCTURE
1 TPP682 1
@<TRIPOS>COMMENT
```

```
@<TRIPOS>MOLECULE
Minimised_ligand (1yee) catalytic antibody
39 39 1
SMALL
GASTEIGER

@<TRIPOS>DICT

@<TRIPOS>ATOM
      1 N1          4.5807   -2.2894    7.5270 N.pl3     1 PNB551      0.0000
      2 O4          3.4910   -1.8391    7.8128 O.co2     1 PNB551      0.0000
      3 O5          5.5886   -1.6168    7.4909 O.co2     1 PNB551      0.0000
      4 C1          4.9067   -6.4076    6.7964 C.ar      1 PNB551      0.0000
      5 C2          3.6728   -5.8385    7.1291 C.ar      1 PNB551      0.0000
      6 C3          3.5623   -4.4629    7.3517 C.ar      1 PNB551      0.0000
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      7 C4          4.6781   -3.6190    7.2503 C.ar      1 PNB551      0.0000
      8 C5          5.9001   -4.1856    6.8576 C.ar      1 PNB551      0.0000
      9 C6          6.0091   -5.5625    6.6301 C.ar      1 PNB551      0.0000
     10 C7          5.0764   -7.9285    6.6402 C.3       1 PNB551      0.0000
     11 O1          3.9044   -8.6424    6.2229 O.3       1 PNB551      0.0000
     12 P1          3.1866   -8.5694    4.7929 P.3       1 PNB551      0.0000
     13 O2          2.1898   -7.4615    4.7562 O.co2     1 PNB551      0.0000
     14 O3          4.1896   -8.3323    3.7205 O.co2     1 PNB551      0.0000
     15 C8          2.3885  -10.0747    4.5042 C.3       1 PNB551      0.0000
     16 C9          2.1135  -10.9918    5.6674 C.3       1 PNB551      0.0000
     17 C10         1.3277  -12.2722    5.2882 C.3       1 PNB551      0.0000
     18 C11         1.0949  -13.0587    6.5617 C.2       1 PNB551      0.0000
     19 O6          0.0629  -12.8401    7.1745 O.2       1 PNB551      0.0000
     20 N2          2.0430  -13.9468    6.9608 N.am      1 PNB551      0.0000
     21 C12         2.0861  -14.6469    8.1234 C.3       1 PNB551      0.0000
     22 C13         1.2138  -14.4355    9.2964 C.2       1 PNB551      0.0000
     23 O7          1.0268  -15.3966   10.0907 O.co2     1 PNB551      0.0000
     24 O8          0.6903  -13.3088    9.5067 O.co2     1 PNB551      0.0000
     25 H2          2.7950   -6.4687    7.2151 H         1 PNB551      0.0000
     26 H3          2.5958   -4.0438    7.6071 H         1 PNB551      0.0000
     27 H5          6.7702   -3.5521    6.7285 H         1 PNB551      0.0000
     28 H6          6.9604   -5.9801    6.3208 H         1 PNB551      0.0000
     29 H71         5.3580   -8.3381    7.5423 H         1 PNB551      0.0000
     30 H72         5.8001   -8.1236    5.9337 H         1 PNB551      0.0000
     31 H81         2.9450  -10.6589    3.8639 H         1 PNB551      0.0000
     32 H82         1.4553   -9.9141    4.0989 H         1 PNB551      0.0000
     33 H91         1.5715  -10.4605    6.3637 H         1 PNB551      0.0000
     34 H92         3.0204  -11.2636    6.0730 H         1 PNB551      0.0000
     35 H101        1.8710  -12.8436    4.6254 H         1 PNB551      0.0000
     36 H102        0.4213  -12.0251    4.8659 H         1 PNB551      0.0000
     37 H121        3.0604  -14.5148    8.4303 H         1 PNB551      0.0000
     38 H122        1.9546  -15.6182    7.8069 H         1 PNB551      0.0000
     39 H2          2.8613  -14.1168    6.2705 H         1 PNB551      0.0000
@<TRIPOS>BOND
     1    1    2 ar
     2    1    3 ar
     3    1    7 1
     4    4    5 ar
     5    4    9 ar
     6    4   10 1
     7    5    6 ar
     8    6    7 ar
     9    7    8 ar
    10    8    9 ar
    11   10   11 1
    12   11   12 1
    13   12   14 ar
    14   12   13 ar
    15   12   15 1
    16   15   16 1
    17   16   17 1
    18   17   18 1
    19   18   20 am
    20   18   19 2
    21   20   21 1
    22   21   22 1
    23   22   23 ar
    24   22   24 ar
    25    5   25 1
    26    6   26 1
    27    8   27 1
    28    9   28 1
    29   10   29 1
    30   10   30 1
    31   15   31 1
```

```
    32   15   32 1
    33   16   33 1
    34   16   34 1
    35   17   35 1
    36   17   36 1
    37   21   37 1
    38   21   38 1
    39   20   39 1
@<TRIPOS>SUBSTRUCTURE
1 PNB551 1
@<TRIPOS>COMMENT
```

New Ligand Structures with Changed Protonation

```
@<TRIPOS>MOLECULE
Minimised_ligand (1bl7) transferase
45 48 1
SMALL
GASTEIGER

@<TRIPOS>DICT

@<TRIPOS>ATOM
      1 CA1        -0.5554   13.8974   30.9820 C.3       1 SB4800      0.0000
      2 CA2        -2.1018   13.8535   30.8927 C.3       1 SB4800      0.0000
      3 NA3        -2.6081   15.1072   30.2918 N.4       1 SB4800      0.0000
      4 CA4        -2.0746   15.3817   28.9397 C.3       1 SB4800      0.0000
      5 CA5        -0.5299   15.4654   29.0085 C.3       1 SB4800      0.0000
      6 CA6         0.0568   14.1480   29.5826 C.3       1 SB4800      0.0000
      7 C1          5.0562   11.5470   29.0809 C.ar      1 SB4800      0.0000
      8 C2          6.2488   10.8212   29.1487 C.ar      1 SB4800      0.0000
      9 C3          7.1863   11.1138   30.1429 C.ar      1 SB4800      0.0000
     10 C4          6.9493   12.1496   31.0503 C.ar      1 SB4800      0.0000
     11 C5          5.7671   12.8899   30.9685 C.ar      1 SB4800      0.0000
     12 C6          4.8229   12.5863   29.9852 C.ar      1 SB4800      0.0000
     13 FB7         8.3076   10.4024   30.2245 F         1 SB4800      0.0000
     14 CC1         2.3739   10.6140   30.5167 C.ar      1 SB4800      0.0000
     15 CC2         1.8034   11.5960   29.7009 C.ar      1 SB4800      0.0000
     16 NC3         0.8209   11.2357   28.8517 N.ar      1 SB4800      0.0000
     17 CC4         0.3904    9.9599   28.7597 C.ar      1 SB4800      0.0000
     18 NC5         0.9628    8.9913   29.5050 N.ar      1 SB4800      0.0000
     19 CC6         1.9380    9.2934   30.3845 C.ar      1 SB4800      0.0000
     20 N7         -0.6207    9.6637   27.9128 N.pl3     1 SB4800      0.0000
     21 N1          1.5173   14.1275   29.7137 N.pl3     1 SB4800      0.0000
     22 C2          2.2798   15.1798   29.8131 C.2       1 SB4800      0.0000
     23 N3          3.4750   14.8284   29.9330 N.2       1 SB4800      0.0000
     24 C4          3.5522   13.3992   29.8981 C.2       1 SB4800      0.0000
     25 C5          2.2635   13.0371   29.7634 C.2       1 SB4800      0.0000
     26 H1          4.3143   11.3042   28.3288 H         1 SB4800      0.0000
     27 H2          6.4461   10.0328   28.4314 H         1 SB4800      0.0000
     28 H4          7.6813   12.3784   31.8164 H         1 SB4800      0.0000
     29 H5          5.5831   13.6983   31.6669 H         1 SB4800      0.0000
     30 HC1         3.1403   10.8727   31.2384 H         1 SB4800      0.0000
     31 HC6         2.3840    8.5120   30.9891 H         1 SB4800      0.0000
     32 H2          1.9309   16.2060   29.7947 H         1 SB4800      0.0000
     33 HA11       -0.1867   12.9373   31.3723 H         1 SB4800      0.0000
     34 HA12       -0.2536   14.7091   31.6603 H         1 SB4800      0.0000
     35 HA21       -2.5391   13.7482   31.8965 H         1 SB4800      0.0000
     36 HA22       -2.4238   13.0115   30.2623 H         1 SB4800      0.0000
     37 HA31       -2.3305   15.9437   30.9500 H         1 SB4800      0.0000
     38 HA32       -3.7041   15.0414   30.2249 H         1 SB4800      0.0000
     39 HA41       -2.4955   16.3333   28.5829 H         1 SB4800      0.0000
     40 HA42       -2.3858   14.5683   28.2678 H         1 SB4800      0.0000
     41 HA51       -0.2416   16.3052   29.6578 H         1 SB4800      0.0000
     42 HA52       -0.1311   15.6305   27.9967 H         1 SB4800      0.0000
     43 HA6        -0.2548   13.3240   28.9239 H         1 SB4800      0.0000
     44 H71        -0.9587    8.6940   27.8334 H         1 SB4800      0.0000
     45 H72        -1.0532   10.4077   27.3469 H         1 SB4800      0.0000
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     3    2    3 1
     4    3    4 1
     5    4    5 1
     6    5    6 1
     7    6   21 1
```

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     9    7    8 ar
    10    8    9 ar
    11    9   13 1
    12    9   10 ar
    13   10   11 ar
    14   11   12 ar
    15   12   24 1
    16   14   15 ar
    17   14   19 ar
    18   15   25 1
    19   15   16 ar
    20   16   17 ar
    21   17   18 ar
    22   17   20 1
    23   18   19 ar
    24   21   22 1
    25   21   25 1
    26   22   23 2
    27   23   24 1
    28   24   25 2
    29    7   26 1
    30    8   27 1
    31   10   28 1
    32   11   29 1
    33   14   30 1
    34   19   31 1
    35   22   32 1
    36    1   33 1
    37    1   34 1
    38    2   35 1
    39    2   36 1
    40    3   37 1
    41    3   38 1
    42    4   39 1
    43    4   40 1
    44    5   41 1
    45    5   42 1
    46    6   43 1
    47   20   44 1
    48   20   45 1
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@<TRIPOS>COMMENT
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@<TRIPOS>MOLECULE
Minimised_ligand (1d4p) blood clotting
52 55 1
SMALL
GASTEIGER

@<TRIPOS>DICT

@<TRIPOS>ATOM
      1 C1        -23.9656  -31.8371   23.1337 C.ar      1 BPP400      0.0000
      2 C2        -23.2445  -32.9899   22.7886 C.ar      1 BPP400      0.0000
      3 C3        -22.2595  -32.8792   21.8075 C.2       1 BPP400      0.0000
      4 C4        -22.0038  -31.6739   21.1639 C.2       1 BPP400      0.0000
      5 C5        -22.7318  -30.5273   21.4752 C.ar      1 BPP400      0.0000
      6 C6        -23.7105  -30.6249   22.4726 C.ar      1 BPP400      0.0000
      7 C10       -21.3741  -33.8203   21.2884 C.2       1 BPP400      0.0000
      8 C11       -20.5875  -33.1367   20.3598 C.2       1 BPP400      0.0000
      9 N12       -21.0027  -31.8563   20.2833 N.pl3     1 BPP400      0.0000
     10 C13       -25.0137  -31.8625   24.2296 C.2       1 BPP400      0.0000
```

```
     11 N14       -25.1681  -30.7856   24.9491 N.pl3     1 BPP400      0.0000
     12 N15       -25.7580  -32.9048   24.4833 N.pl3     1 BPP400      0.0000
     13 C17       -19.4336  -33.7058   19.5674 C.2       1 BPP400      0.0000
     14 O18       -19.7307  -34.3225   18.5576 O.2       1 BPP400      0.0000
     15 N19       -18.1494  -33.5393   19.9855 N.am      1 BPP400      0.0000
     16 C20       -17.0595  -34.2073   19.2791 C.3       1 BPP400      0.0000
     17 C21       -16.5938  -35.3374   20.2300 C.3       1 BPP400      0.0000
     18 C22       -16.2108  -34.7641   21.6259 C.3       1 BPP400      0.0000
     19 C23       -17.3888  -33.9390   22.2250 C.3       1 BPP400      0.0000
     20 C24       -17.8498  -32.8408   21.2344 C.3       1 BPP400      0.0000
     21 C33       -15.7943  -35.9231   22.5732 C.3       1 BPP400      0.0000
     22 C35       -15.3439  -35.3772   23.9346 C.ar      1 BPP400      0.0000
     23 C38       -16.2147  -35.3886   25.0306 C.ar      1 BPP400      0.0000
     24 C39       -15.7975  -34.8901   26.2678 C.ar      1 BPP400      0.0000
     25 C40       -14.5056  -34.3769   26.4148 C.ar      1 BPP400      0.0000
     26 C41       -13.6325  -34.3640   25.3237 C.ar      1 BPP400      0.0000
     27 C42       -14.0512  -34.8622   24.0868 C.ar      1 BPP400      0.0000
     28 H2        -23.4471  -33.9394   23.2707 H         1 BPP400      0.0000
     29 H5        -22.5468  -29.5904   20.9623 H         1 BPP400      0.0000
     30 H6        -24.2839  -29.7447   22.7401 H         1 BPP400      0.0000
     31 H10       -21.3090  -34.8698   21.5518 H         1 BPP400      0.0000
     32 H12       -20.5973  -31.0991   19.6220 H         1 BPP400      0.0000
     33 H38       -17.2171  -35.7859   24.9192 H         1 BPP400      0.0000
     34 H39       -16.4757  -34.9014   27.1134 H         1 BPP400      0.0000
     35 H40       -14.1814  -33.9894   27.3739 H         1 BPP400      0.0000
     36 H41       -12.6300  -33.9674   25.4367 H         1 BPP400      0.0000
     37 H42       -13.3721  -34.8497   23.2419 H         1 BPP400      0.0000
     38 H201      -16.2532  -33.4853   19.0827 H         1 BPP400      0.0000
     39 H202      -17.4326  -34.6086   18.3253 H         1 BPP400      0.0000
     40 H211      -15.7179  -35.8372   19.7907 H         1 BPP400      0.0000
     41 H212      -17.4101  -36.0651   20.3486 H         1 BPP400      0.0000
     42 H22       -15.3483  -34.0932   21.4993 H         1 BPP400      0.0000
     43 H231      -17.0597  -33.4629   23.1604 H         1 BPP400      0.0000
     44 H232      -18.2339  -34.6116   22.4335 H         1 BPP400      0.0000
     45 H241      -18.7555  -32.3295   21.5924 H         1 BPP400      0.0000
     46 H242      -17.0566  -32.0998   21.0564 H         1 BPP400      0.0000
     47 H331      -14.9626  -36.4836   22.1214 H         1 BPP400      0.0000
     48 H332      -16.6506  -36.5967   22.7252 H         1 BPP400      0.0000
     49 H141      -25.8688  -30.7665   25.7038 H         1 BPP400      0.0000
     50 H142      -24.5893  -29.9543   24.7626 H         1 BPP400      0.0000
     51 H151      -26.4539  -32.8684   25.2418 H         1 BPP400      0.0000
     52 H152      -25.6493  -33.7635   23.9249 H         1 BPP400      0.0000
@<TRIPOS>BOND
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     3    1    2 ar
     4    2    3 ar
     5    3    4 ar
     6    3    7 1
     7    4    5 ar
     8    4    9 1
     9    5    6 ar
    10    7    8 2
    11    8    9 1
    12    8   13 1
    13   10   11 ar
    14   10   12 ar
    15   13   14 2
    16   13   15 am
    17   15   16 1
    18   15   20 1
    19   16   17 1
    20   17   18 1
    21   18   19 1
    22   18   21 1
```

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    23   19   20 1
    24   21   22 1
    25   22   23 ar
    26   22   27 ar
    27   23   24 ar
    28   24   25 ar
    29   25   26 ar
    30   26   27 ar
    31    2   28 1
    32    5   29 1
    33    6   30 1
    34    7   31 1
    35    9   32 1
    36   23   33 1
    37   24   34 1
    38   25   35 1
    39   26   36 1
    40   27   37 1
    41   16   38 1
    42   16   39 1
    43   17   40 1
    44   17   41 1
    45   18   42 1
    46   19   43 1
    47   19   44 1
    48   20   45 1
    49   20   46 1
    50   21   47 1
    51   21   48 1
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    53   11   50 1
    54   12   51 1
    55   12   52 1
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@<TRIPOS>COMMENT
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Minimised_ligand (1d0l) transferase
63 64 1
SMALL
GASTEIGER

@<TRIPOS>DICT

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      3 C3          9.1264   25.1960   14.9191 C.3       1 BLG401      0.0000
      4 C4          8.1927   26.3850   14.5799 C.3       1 BLG401      0.0000
      5 C5          6.7534   25.8661   14.3211 C.3       1 BLG401      0.0000
      6 O5          6.7480   24.8909   13.2577 O.3       1 BLG401      0.0000
      7 O1          7.5415   22.7621   12.5108 O.3       1 BLG401      0.0000
      8 N2          9.7844   22.9334   14.1275 N.am      1 BLG401      0.0000
      9 C7         10.5706   22.3120   13.2163 C.2       1 BLG401      0.0000
     10 O7         10.7157   22.7075   12.0681 O.2       1 BLG401      0.0000
     11 C8         11.2901   21.0570   13.6495 C.3       1 BLG401      0.0000
     12 O3         10.4815   25.6541   15.0582 O.3       1 BLG401      0.0000
     13 O4          8.1159   27.2986   15.6929 O.3       1 BLG401      0.0000
     14 S4          8.9413   28.5568   15.6097 S.o2      1 BLG401      0.0000
     15 O41        10.3356   28.2487   15.2865 O.co2     1 BLG401      0.0000
     16 O42         8.8883   29.2546   16.8960 O.co2     1 BLG401      0.0000
     17 O43         8.3844   29.4281   14.5720 O.co2     1 BLG401      0.0000
     18 C6          5.8122   27.0358   13.9338 C.3       1 BLG401      0.0000
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     19 O6          6.3165   27.7016   12.7636 O.3       1 BLG401      0.0000
     20 CA          6.4429   20.9019   11.4121 C.3       1 BLG401      0.0000
     21 CB          6.2477   22.1835   12.2532 C.3       1 BLG401      0.0000
     22 CG          5.3165   23.0039   11.3359 C.3       1 BLG401      0.0000
     23 CD          4.3407   21.9028   10.8449 C.3       1 BLG401      0.0000
     24 N           5.1378   20.6563   10.7647 N.4       1 BLG401      0.0000
     25 C9          6.9700   19.7174   12.2644 C.3       1 BLG401      0.0000
     26 O9          5.9935   19.3842   13.2662 O.3       1 BLG401      0.0000
     27 C10         3.7541   22.1885    9.4838 C.2       1 BLG401      0.0000
     28 O10         4.5056   22.1086    8.5234 O.2       1 BLG401      0.0000
     29 N3          2.4408   22.5076    9.3716 N.am      1 BLG401      0.0000
     30 C11         1.8420   22.7632    8.0645 C.3       1 BLG401      0.0000
     31 C12         0.3984   22.2017    8.0028 C.3       1 BLG401      0.0000
     32 S           0.4149   20.4366    8.3685 S.o2      1 BLG401      0.0000
     33 O1         -0.9277   19.8892    8.1772 O.co2     1 BLG401      0.0000
     34 O2          1.3444   19.7555    7.4679 O.co2     1 BLG401      0.0000
     35 O3          0.8356   20.2319    9.7549 O.co2     1 BLG401      0.0000
     36 H1          7.1818   23.2726   14.4993 H         1 BLG401      0.0000
     37 H2          9.4166   24.5780   12.8568 H         1 BLG401      0.0000
     38 H3          8.7836   24.7372   15.8582 H         1 BLG401      0.0000
     39 H4          8.5638   26.8950   13.6787 H         1 BLG401      0.0000
     40 H5          6.3769   25.4096   15.2484 H         1 BLG401      0.0000
     41 H81        12.3645   21.2681   13.7547 H         1 BLG401      0.0000
     42 H82        10.8868   20.7179   14.6151 H         1 BLG401      0.0000
     43 H83        11.1431   20.2708   12.8943 H         1 BLG401      0.0000
     44 H61         5.7542   27.7774   14.7441 H         1 BLG401      0.0000
     45 H62         4.8024   26.6664   13.7018 H         1 BLG401      0.0000
     46 HA          7.1901   21.1172   10.6341 H         1 BLG401      0.0000
     47 HB          5.7263   21.9380   13.1901 H         1 BLG401      0.0000
     48 HG1         5.8709   23.4564   10.5005 H         1 BLG401      0.0000
     49 HG2         4.7909   23.7911   11.8963 H         1 BLG401      0.0000
     50 HD          3.5307   21.7856   11.5798 H         1 BLG401      0.0000
     51 H1          4.6120   19.8424   11.2855 H         1 BLG401      0.0000
     52 H2          5.2919   20.3785    9.7116 H         1 BLG401      0.0000
     53 H91         7.9053   19.9855   12.7775 H         1 BLG401      0.0000
     54 H92         7.1359   18.8259   11.6418 H         1 BLG401      0.0000
     55 H111        2.4734   22.2814    7.3034 H         1 BLG401      0.0000
     56 H112        1.8373   23.8511    7.9018 H         1 BLG401      0.0000
     57 H121        0.0277   22.4158    6.9895 H         1 BLG401      0.0000
     58 H122       -0.1869   22.7757    8.7362 H         1 BLG401      0.0000
     59 H2          9.7195   22.5601   15.0529 H         1 BLG401      0.0000
     60 H3          1.8754   22.5686   10.1942 H         1 BLG401      0.0000
     61 H3         10.4932   26.6035   15.0888 H         1 BLG401      0.0000
     62 H6          5.7136   28.3890   12.5059 H         1 BLG401      0.0000
     63 H9          6.0677   18.4632   13.4868 H         1 BLG401      0.0000
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     6    3    4 1
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     8    4    5 1
     9    4   13 1
    10    5    6 1
    11    5   18 1
    12    7   21 1
    13    8    9 am
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    15    9   11 1
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    17   14   15 ar
    18   14   16 ar
    19   14   17 ar
```

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    21   20   25 1
    22   20   24 1
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    25   22   23 1
    26   23   24 1
    27   23   27 1
    28   25   26 1
    29   27   28 2
    30   27   29 am
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    33   31   32 1
    34   32   33 ar
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    36   32   35 ar
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    43   11   42 1
    44   11   43 1
    45   18   44 1
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    57   30   56 1
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    60    8   59 1
    61   29   60 1
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@<TRIPOS>SUBSTRUCTURE
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@<TRIPOS>COMMENT
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