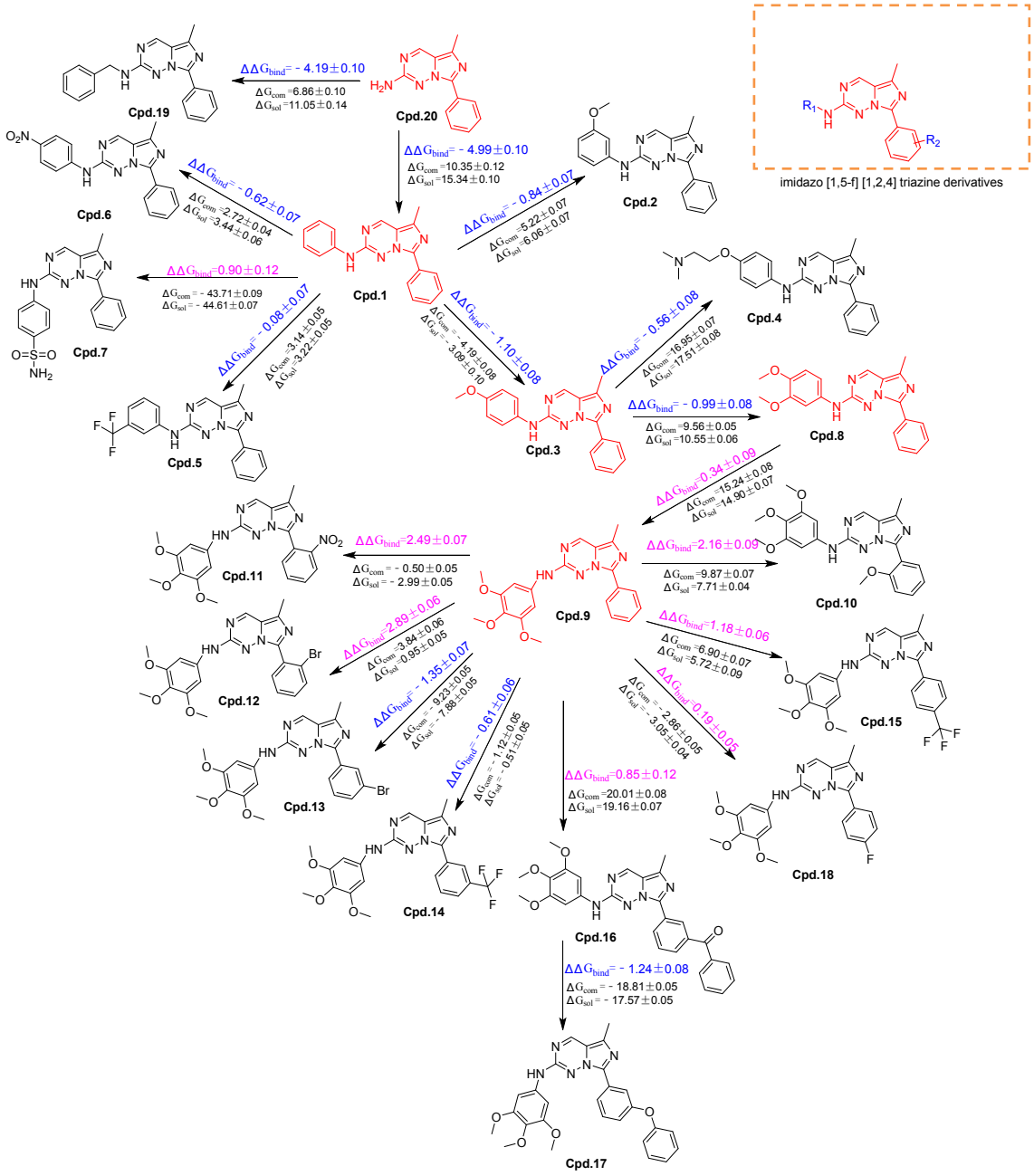
Electronic Supplementary Material (ESI) for MedChemComm.

Supplementary data

Assessing the performance of docking scoring function, FEP, MM-GBSA, and QM/MM-GBSA approaches on a series of PLK1 inhibitors

Chunlan Pu, Guoyi Yan, Jianyou Shi and Rui Li.

Part 1. Figure S1. The computational details of each mutation and calculated results.



Part 2. The sdf files of the small molecules and pdb files of the MD structures used in the assessments.

(1) Ligand1.mol2

@<TRIPOS>MOLECULE
P12A
38 41 1
SMALL
USER_CHARGES

@<TRIPOS>ATOM

1	N1	-42.7518	12.1376	18.0624	N.2	1 SUB -0.5000
2	C2	-44.0619	12.1993	17.6891	C.ar	1 SUB 0.7000
3	N3	-44.5298	12.5419	16.4641	N.2	1 SUB -0.2500
4	N4	-43.5801	12.9237	15.6247	N.pl3	1 SUB 0.0490
5	C5	-42.2419	12.9690	15.8983	C.ar	1 SUB 0.1413
6	C6	-41.8117	12.5347	17.1660	C.ar	1 SUB -0.1053
7	C7	-43.7897	13.4190	14.3678	C.ar	1 SUB 0.3530
8	N8	-42.5850	13.7858	13.8714	N.2	1 SUB -0.5630
9	C9	-41.5929	13.5187	14.8327	C.ar	1 SUB 0.1319
10	N10	-45.0088	11.9035	18.6841	N.pl3	1 SUB -0.7800
11	C11	-40.1574	13.8763	14.6403	C.3	1 SUB -0.0519
12	C12	-45.0982	13.6103	13.7441	C.ar	1 SUB 0.0000
13	C13	-46.1451	12.6823	13.9611	C.ar	1 SUB -0.1150
14	C14	-47.4416	12.9416	13.4814	C.ar	1 SUB -0.1150
15	C15	-47.6911	14.1252	12.7675	C.ar	1 SUB -0.1150
16	C16	-46.6487	15.0383	12.5151	C.ar	1 SUB -0.1150
17	C17	-45.3539	14.7829	13.0054	C.ar	1 SUB -0.1150
18	C18	-46.4153	11.8927	18.5790	C.ar	1 SUB 0.2000
19	C19	-47.1374	12.7672	17.7245	C.ar	1 SUB -0.1150
20	C20	-48.5353	12.6706	17.5962	C.ar	1 SUB -0.1150
21	C21	-49.2452	11.7417	18.3730	C.ar	1 SUB -0.1150
22	C22	-48.5504	10.9318	19.2911	C.ar	1 SUB -0.1150
23	C23	-47.1438	10.9859	19.3779	C.ar	1 SUB -0.1150
24	H24	-40.7695	12.5430	17.4521	H	1 SUB 0.1150
25	H25	-44.6190	11.6208	19.5760	H	1 SUB 0.3800
26	H26	-39.7942	14.4973	15.4618	H	1 SUB 0.0600
27	H27	-39.5400	12.9772	14.6134	H	1 SUB 0.0600
28	H28	-40.0044	14.4390	13.7182	H	1 SUB 0.0600
29	H29	-45.9715	11.7703	14.5101	H	1 SUB 0.1150
30	H30	-48.2430	12.2409	13.6606	H	1 SUB 0.1150
31	H31	-48.6828	14.3253	12.3914	H	1 SUB 0.1150
32	H32	-46.8501	15.9406	11.9569	H	1 SUB 0.1150

```
      33 H33          -44.5656    15.5016    12.8363 H     1 SUB       0.1150
      34 H34          -46.6439    13.5264    17.1400 H     1 SUB       0.1150
      35 H35          -49.0607    13.3138    16.9069 H     1 SUB       0.1150
      36 H36          -50.3179    11.6645    18.2796 H     1 SUB       0.1150
      37 H37          -49.0956    10.2255    19.8990 H     1 SUB       0.1150
      38 H38          -46.6261    10.3206    20.0535 H     1 SUB       0.1150
@<TRIPOS>BOND
      1     1     2 ar
      2     1     6 ar
      3     2     3 ar
      4     2    10 1
      5     3     4 ar
      6     4     5 ar
      7     4     7 ar
      8     5     6 ar
      9     5     9 ar
     10     6    24 1
     11     7     8 ar
     12     7    12 1
     13     8     9 ar
     14     9    11 1
     15    10    18 1
     16    10    25 1
     17    11    26 1
     18    11    27 1
     19    11    28 1
     20    12    13 ar
     21    12    17 ar
     22    13    14 ar
     23    13    29 1
     24    14    15 ar
     25    14    30 1
     26    15    16 ar
     27    15    31 1
     28    16    17 ar
     29    16    32 1
     30    17    33 1
     31    18    19 ar
     32    18    23 ar
     33    19    20 ar
     34    19    34 1
     35    20    21 ar
     36    20    35 1
     37    21    22 ar
```

```
     38     21     36 1
     39     22     23 ar
     40     22     37 1
     41     23     38 1
@<TRIPOS>SUBSTRUCTURE
      1 SUB            1 GROUP                 0          ****       0 ROOT
```

(2) Ligand2.mol2

```
@<TRIPOS>MOLECULE
P12B
42    45     1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
      1 N1          -42.7534    12.1407    18.1672 N.2         1 SUB          -
0.5000
      2 C2          -44.0394    12.2669    17.7481 C.ar        1 SUB
0.7000
      3 N3          -44.4576    12.6233    16.5050 N.2         1 SUB          -
0.2500
      4 N4          -43.4583    12.9483    15.6932 N.pl3       1 SUB
0.0490
      5 C5          -42.1302    12.9421    16.0204 C.ar        1 SUB
0.1413
      6 C6          -41.7692    12.5023    17.3047 C.ar        1 SUB          -
0.1053
      7 C7          -43.5890    13.4193    14.4162 C.ar        1 SUB
0.3530
      8 N8          -42.3499    13.7287    13.9661 N.2         1 SUB          -
0.5630
      9 C9          -41.4123    13.4439    14.9750 C.ar        1 SUB
0.1319
     10 N10         -45.0255    12.0332    18.7133 N.pl3       1 SUB          -
0.7800
     11 C11         -39.9518    13.7341    14.8402 C.3         1 SUB          -
0.0519
     12 C12         -44.8555    13.6299    13.7205 C.ar        1 SUB
0.0000
     13 C13         -45.0488    14.7919    12.9450 C.ar        1 SUB          -
0.1150
     14 C14         -46.3129    15.0604    12.3863 C.ar        1 SUB          -
0.1150
     15 C15         -47.3822    14.1713    12.6073 C.ar        1 SUB          -
```

0.1150
16 C16 -47.1932 12.9976 13.3544 C.ar 1 SUB -
0.1150
17 C17 -45.9282 12.7234 13.8990 C.ar 1 SUB -
0.1150
18 C18 -46.4011 12.2221 18.5287 C.ar 1 SUB
0.2000
19 C19 -47.2975 11.2003 18.8848 C.ar 1 SUB -
0.1150
20 C20 -48.6695 11.3404 18.6033 C.ar 1 SUB -
0.1150
21 C21 -49.1494 12.4992 17.9672 C.ar 1 SUB -
0.1150
22 C22 -48.2778 13.5607 17.6575 C.ar 1 SUB
0.0850
23 C23 -46.9018 13.4184 17.9639 C.ar 1 SUB -
0.1150
24 O24 -48.8362 14.6913 17.0998 O.3 1 SUB -
0.2850
25 C25 -47.9633 15.7451 16.7146 C.3 1 SUB
0.1100
26 H26 -40.7420 12.4738 17.6327 H 1 SUB
0.1150
27 H27 -44.7044 11.6977 19.6142 H 1 SUB
0.3800
28 H28 -39.5808 14.2719 15.7122 H 1 SUB
0.0600
29 H29 -39.3771 12.8133 14.7596 H 1 SUB
0.0600
30 H30 -39.7491 14.3552 13.9701 H 1 SUB
0.0600
31 H31 -44.2384 15.4934 12.8085 H 1 SUB
0.1150
32 H32 -46.4698 15.9573 11.8053 H 1 SUB
0.1150
33 H33 -48.3529 14.3848 12.1936 H 1 SUB
0.1150
34 H34 -48.0160 12.3133 13.5088 H 1 SUB
0.1150
35 H35 -45.7979 11.8184 14.4736 H 1 SUB
0.1150
36 H36 -46.9319 10.2868 19.3337 H 1 SUB
0.1150
37 H37 -49.3535 10.5412 18.8474 H 1 SUB

```
0.1150
     38 H38        -50.2013    12.5829    17.7371 H          1 SUB
0.1150
     39 H39        -46.2017    14.2085    17.7399 H          1 SUB
0.1150
     40 H40        -47.2275    15.4069    15.9824 H          1 SUB
0.0300
     41 H41        -48.5443    16.5424    16.2489 H          1 SUB
0.0300
     42 H42        -47.4473    16.1751    17.5742 H          1 SUB
0.0300
@<TRIPOS>BOND
     1     1     2 ar
     2     1     6 ar
     3     2     3 ar
     4     2    10 1
     5     3     4 ar
     6     4     5 ar
     7     4     7 ar
     8     5     6 ar
     9     5     9 ar
    10     6    26 1
    11     7     8 ar
    12     7    12 1
    13     8     9 ar
    14     9    11 1
    15    10    18 1
    16    10    27 1
    17    11    28 1
    18    11    29 1
    19    11    30 1
    20    12    13 ar
    21    12    17 ar
    22    13    14 ar
    23    13    31 1
    24    14    15 ar
    25    14    32 1
    26    15    16 ar
    27    15    33 1
    28    16    17 ar
    29    16    34 1
    30    17    35 1
    31    18    19 ar
    32    18    23 ar
```

```
    33    19    20 ar
    34    19    36 1
    35    20    21 ar
    36    20    37 1
    37    21    22 ar
    38    21    38 1
    39    22    23 ar
    40    22    24 1
    41    23    39 1
    42    24    25 1
    43    25    40 1
    44    25    41 1
    45    25    42 1
@<TRIPOS>SUBSTRUCTURE
     1 SUB          1 GROUP             0        ****     0 ROOT
```

(3) Ligand3.mol2

```
@<TRIPOS>MOLECULE
P12C
42    45     1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
      1 N1         -42.6829    12.1276    17.9673 N.2        1 SUB         -
0.5000
      2 C2         -44.0153    12.1795    17.6890 C.ar       1 SUB
0.7000
      3 N3         -44.5788    12.5775    16.5172 N.2        1 SUB         -
0.2500
      4 N4         -43.6777    12.9988    15.6262 N.pl3      1 SUB
0.0490
      5 C5         -42.3199    13.0417    15.8177 C.ar       1 SUB
0.1413
      6 C6         -41.8061    12.5684    17.0344 C.ar       1 SUB         -
0.1053
      7 C7         -43.9461    13.5194    14.3872 C.ar       1 SUB
0.3530
      8 N8         -42.7714    13.8991    13.8340 N.2        1 SUB         -
0.5630
      9 C9         -41.7293    13.6143    14.7294 C.ar       1 SUB
0.1319
     10 N10        -44.8359    11.8102    18.7670 N.pl3      1 SUB         -
0.7800
```

11	C11	-40.3055	13.9671	14.4519	C.3	1	SUB	-0.0519
12	C12	-45.2634	13.6964	13.7900	C.ar	1	SUB	0.0000
13	C13	-45.5543	14.8753	13.0720	C.ar	1	SUB	-0.1150
14	C14	-46.8482	15.0871	12.5604	C.ar	1	SUB	-0.1150
15	C15	-47.8526	14.1229	12.7693	C.ar	1	SUB	-0.1150
16	C16	-47.5632	12.9393	13.4676	C.ar	1	SUB	-0.1150
17	C17	-46.2697	12.7214	13.9696	C.ar	1	SUB	-0.1150
18	C18	-46.2189	11.5692	18.8497	C.ar	1	SUB	0.2000
19	C19	-47.1826	12.0514	17.9315	C.ar	1	SUB	-0.1150
20	C20	-48.5497	11.7579	18.0990	C.ar	1	SUB	-0.1150
21	C21	-48.9920	10.9951	19.2062	C.ar	1	SUB	0.0850
22	C22	-48.0343	10.5337	20.1300	C.ar	1	SUB	-0.1150
23	C23	-46.6663	10.8160	19.9544	C.ar	1	SUB	-0.1150
24	O24	-50.3111	10.6847	19.4555	O.3	1	SUB	-0.2850
25	C25	-51.2890	11.1522	18.5378	C.3	1	SUB	0.1100
26	H26	-40.7479	12.5691	17.2515	H	1	SUB	0.1150
27	H27	-44.3301	11.6339	19.6279	H	1	SUB	0.3800
28	H28	-40.2070	14.5391	13.5290	H	1	SUB	0.0600
29	H29	-39.8916	14.5733	15.2579	H	1	SUB	0.0600
30	H30	-39.6934	13.0693	14.3709	H	1	SUB	0.0600
31	H31	-44.7915	15.6268	12.9283	H	1	SUB	0.1150
32	H32	-47.0751	15.9906	12.0136	H	1	SUB	0.1150

```
      33 H33        -48.8447    14.2819    12.3754 H          1 SUB
0.1150
      34 H34        -48.3316    12.1945    13.6119 H          1 SUB
0.1150
      35 H35        -46.0612    11.8043    14.5007 H          1 SUB
0.1150
      36 H36        -46.9169    12.6616    17.0851 H          1 SUB
0.1150
      37 H37        -49.2403    12.1399    17.3619 H          1 SUB
0.1150
      38 H38        -48.3496     9.9547    20.9846 H          1 SUB
0.1150
      39 H39        -45.9564    10.4455    20.6800 H          1 SUB
0.1150
      40 H40        -51.1309    10.7314    17.5443 H          1 SUB
0.0300
      41 H41        -51.2923    12.2418    18.4738 H          1 SUB
0.0300
      42 H42        -52.2774    10.8389    18.8741 H          1 SUB
0.0300
@<TRIPOS>BOND
     1     1     2 ar
     2     1     6 ar
     3     2     3 ar
     4     2    10 1
     5     3     4 ar
     6     4     5 ar
     7     4     7 ar
     8     5     6 ar
     9     5     9 ar
    10     6    26 1
    11     7     8 ar
    12     7    12 1
    13     8     9 ar
    14     9    11 1
    15    10    18 1
    16    10    27 1
    17    11    28 1
    18    11    29 1
    19    11    30 1
    20    12    13 ar
    21    12    17 ar
    22    13    14 ar
    23    13    31 1
```

```
    24    14    15 ar
    25    14    32 1
    26    15    16 ar
    27    15    33 1
    28    16    17 ar
    29    16    34 1
    30    17    35 1
    31    18    19 ar
    32    18    23 ar
    33    19    20 ar
    34    19    36 1
    35    20    21 ar
    36    20    37 1
    37    21    22 ar
    38    21    24 1
    39    22    23 ar
    40    22    38 1
    41    23    39 1
    42    24    25 1
    43    25    40 1
    44    25    41 1
    45    25    42 1
@<TRIPOS>SUBSTRUCTURE
     1 SUB          1 GROUP             0        ****     0 ROOT
```

(4) Ligand4.mol2

```
@<TRIPOS>MOLECULE
P12D
53    56     1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
      1 N1         -42.7007    12.1372    17.9684 N.2        1 SUB         -
0.5000
      2 C2         -44.0329    12.1811    17.6869 C.ar       1 SUB
0.7000
      3 N3         -44.5953    12.5712    16.5123 N.2        1 SUB         -
0.2500
      4 N4         -43.6908    12.9904    15.6197 N.pl3      1 SUB
0.0490
      5 C5         -42.3326    13.0350    15.8124 C.ar       1 SUB
0.1413
      6 C6         -41.8199    12.5690    17.0321 C.ar       1 SUB         -
```

0.1053
7 C7 -43.9568 13.5089 14.3791 C.ar 1 SUB
0.3530
8 N8 -42.7810 13.8842 13.8241 N.2 1 SUB -
0.5630
9 C9 -41.7411 13.6062 14.7241 C.ar 1 SUB
0.1319
10 N10 -44.8540 11.8080 18.7628 N.pl3 1 SUB -
0.7800
11 C11 -40.3184 13.9647 14.4519 C.3 1 SUB -
0.0519
12 C12 -45.2743 13.6871 13.7816 C.ar 1 SUB
0.0000
13 C13 -45.5604 14.8653 13.0618 C.ar 1 SUB -
0.1150
14 C14 -46.8529 15.0813 12.5490 C.ar 1 SUB -
0.1150
15 C15 -47.8593 14.1235 12.7673 C.ar 1 SUB -
0.1150
16 C16 -47.5785 12.9405 13.4713 C.ar 1 SUB -
0.1150
17 C17 -46.2846 12.7173 13.9674 C.ar 1 SUB -
0.1150
18 C18 -46.2387 11.5780 18.8516 C.ar 1 SUB
0.2000
19 C19 -47.1991 12.0916 17.9499 C.ar 1 SUB -
0.1150
20 C20 -48.5688 11.8130 18.1178 C.ar 1 SUB -
0.1150
21 C21 -49.0200 11.0320 19.2099 C.ar 1 SUB
0.0850
22 C22 -48.0637 10.5405 20.1189 C.ar 1 SUB -
0.1150
23 C23 -46.6928 10.8117 19.9442 C.ar 1 SUB -
0.1150
24 O24 -50.3440 10.7378 19.4578 O.3 1 SUB -
0.2850
25 C25 -51.3178 11.2054 18.5304 C.3 1 SUB
0.1400
26 C26 -52.7281 10.7927 18.9922 C.3 1 SUB
0.0900
27 N27 -52.9278 9.3411 19.0388 N.3 1 SUB -
0.6300
28 C28 -52.9310 8.7622 17.6961 C.3 1 SUB

0.0300
29 C29 -54.2174 9.0637 19.6613 C.3 1 SUB
0.0300
30 H30 -40.7622 12.5757 17.2519 H 1 SUB
0.1150
31 H31 -44.3454 11.6267 19.6220 H 1 SUB
0.3800
32 H32 -39.9128 14.5740 15.2604 H 1 SUB
0.0600
33 H33 -40.2172 14.5388 13.5293 H 1 SUB
0.0600
34 H34 -39.7001 13.0725 14.3728 H 1 SUB
0.0600
35 H35 -44.7936 15.6122 12.9158 H 1 SUB
0.1150
36 H36 -47.0749 15.9822 11.9982 H 1 SUB
0.1150
37 H37 -48.8512 14.2852 12.3749 H 1 SUB
0.1150
38 H38 -48.3512 12.2006 13.6242 H 1 SUB
0.1150
39 H39 -46.0796 11.8013 14.5024 H 1 SUB
0.1150
40 H40 -46.9288 12.7170 17.1148 H 1 SUB
0.1150
41 H41 -49.2541 12.2223 17.3917 H 1 SUB
0.1150
42 H42 -48.3787 9.9449 20.9609 H 1 SUB
0.1150
43 H43 -45.9833 10.4176 20.6575 H 1 SUB
0.1150
44 H44 -51.2798 12.2952 18.4873 H 1 SUB
0.0300
45 H45 -51.1055 10.8376 17.5274 H 1 SUB
0.0300
46 H46 -52.8962 11.2094 19.9862 H 1 SUB
0.0600
47 H47 -53.4741 11.2443 18.3366 H 1 SUB
0.0600
48 H48 -53.1551 7.6954 17.7361 H 1 SUB
0.0600
49 H49 -53.6795 9.2382 17.0551 H 1 SUB
0.0600
50 H50 -51.9569 8.8656 17.2158 H 1 SUB

```
0.0600
     51 H51         -54.3871     7.9869    19.7293 H          1 SUB
0.0600
     52 H52         -55.0390     9.5033    19.0900 H          1 SUB
0.0600
     53 H53         -54.2541     9.4668    20.6760 H          1 SUB
0.0600
@<TRIPOS>BOND
     1     1     2 ar
     2     1     6 ar
     3     2     3 ar
     4     2    10 1
     5     3     4 ar
     6     4     5 ar
     7     4     7 ar
     8     5     6 ar
     9     5     9 ar
    10     6    30 1
    11     7     8 ar
    12     7    12 1
    13     8     9 ar
    14     9    11 1
    15    10    18 1
    16    10    31 1
    17    11    32 1
    18    11    33 1
    19    11    34 1
    20    12    13 ar
    21    12    17 ar
    22    13    14 ar
    23    13    35 1
    24    14    15 ar
    25    14    36 1
    26    15    16 ar
    27    15    37 1
    28    16    17 ar
    29    16    38 1
    30    17    39 1
    31    18    19 ar
    32    18    23 ar
    33    19    20 ar
    34    19    40 1
    35    20    21 ar
    36    20    41 1
```

```
    37    21    22 ar
    38    21    24 1
    39    22    23 ar
    40    22    42 1
    41    23    43 1
    42    24    25 1
    43    25    26 1
    44    25    44 1
    45    25    45 1
    46    26    27 1
    47    26    46 1
    48    26    47 1
    49    27    28 1
    50    27    29 1
    51    28    48 1
    52    28    49 1
    53    28    50 1
    54    29    51 1
    55    29    52 1
    56    29    53 1
@<TRIPOS>SUBSTRUCTURE
     1 SUB          1 GROUP             0        ****     0 ROOT
```

(5) Ligand5.mol2

```
@<TRIPOS>MOLECULE
P12E
41    44     1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
      1 N1         -42.8284    12.1367    18.1989 N.2        1 SUB         -
0.5000
      2 C2         -44.1014    12.2102    17.8018 C.ar       1 SUB
0.7000
      3 N3         -44.4477    12.4157    16.5344 N.2        1 SUB         -
0.2500
      4 N4         -43.4811    12.8813    15.7197 N.pl3      1 SUB
0.0490
      5 C5         -42.1869    12.9029    16.0773 C.ar       1 SUB
0.1413
      6 C6         -41.8579    12.4665    17.3273 C.ar       1 SUB         -
0.1053
      7 C7         -43.6945    13.4520    14.5001 C.ar       1 SUB
```

0.3530
8 N8 -42.4506 13.7497 13.9887 N.2 1 SUB -
0.5630
9 C9 -41.5232 13.4641 14.9372 C.ar 1 SUB
0.1319
10 N10 -45.0656 12.0665 18.7500 N.pl3 1 SUB -
0.7800
11 C11 -40.0485 13.7454 14.7891 C.3 1 SUB -
0.0519
12 C12 -45.0239 13.6980 13.8881 C.ar 1 SUB
0.0000
13 C13 -45.2483 14.8174 13.1069 C.ar 1 SUB -
0.1150
14 C14 -46.4547 14.9932 12.4409 C.ar 1 SUB -
0.1150
15 C15 -47.4572 14.0439 12.5600 C.ar 1 SUB -
0.1150
16 C16 -47.2579 12.9469 13.3874 C.ar 1 SUB -
0.1150
17 C17 -46.0478 12.7866 14.0550 C.ar 1 SUB -
0.1150
18 C18 -46.3944 12.1246 18.4542 C.ar 1 SUB
0.2000
19 C19 -47.2951 11.1884 18.9562 C.ar 1 SUB -
0.1150
20 C20 -48.6497 11.3211 18.7002 C.ar 1 SUB -
0.1150
21 C21 -49.1092 12.3613 17.9062 C.ar 1 SUB -
0.1150
22 C22 -48.2100 13.2700 17.3425 C.ar 1 SUB
0.1500
23 C23 -46.8545 13.1366 17.6229 C.ar 1 SUB -
0.1150
24 C -48.5766 14.3290 16.5104 C.3 1 SUB
0.4500
25 F -47.9767 14.1407 15.3044 F 1 SUB -
0.2000
26 F -48.1169 15.4799 17.0706 F 1 SUB -
0.2000
27 F -49.9259 14.3950 16.3533 F 1 SUB -
0.2000
28 H26 -40.8212 12.4131 17.6267 H 1 SUB
0.1150
29 H27 -44.7757 11.8670 19.6866 H 1 SUB

```
0.3800
      30 H28        -39.6664    14.2466    15.6798 H          1 SUB
0.0600
      31 H29        -39.5034    12.8116    14.6582 H          1 SUB
0.0600
      32 H30        -39.8693    14.3939    13.9316 H          1 SUB
0.0600
      33 H31        -44.4824    15.5718    12.9920 H          1 SUB
0.1150
      34 H32        -46.6117    15.8658    11.8253 H          1 SUB
0.1150
      35 H33        -48.3778    14.1667    12.0142 H          1 SUB
0.1150
      36 H34        -48.0394    12.2104    13.5029 H          1 SUB
0.1150
      37 H35        -45.9041    11.9131    14.6748 H          1 SUB
0.1150
      38 H36        -46.9551    10.3665    19.5692 H          1 SUB
0.1150
      39 H37        -49.3475    10.6133    19.1225 H          1 SUB
0.1150
      40 H38        -50.1715    12.4303    17.7338 H          1 SUB
0.1150
      41 H39        -46.1537    13.8422    17.2008 H          1 SUB
0.1150
@<TRIPOS>BOND
     1     1     2 ar
     2     1     6 ar
     3     2     3 ar
     4     2    10 1
     5     3     4 ar
     6     4     5 ar
     7     4     7 ar
     8     5     6 ar
     9     5     9 ar
    10     6    28 1
    11     7     8 ar
    12     7    12 1
    13     8     9 ar
    14     9    11 1
    15    10    18 1
    16    10    29 1
    17    11    30 1
    18    11    31 1
```

```
     19    11    32 1
     20    12    13 ar
     21    12    17 ar
     22    13    14 ar
     23    13    33 1
     24    14    15 ar
     25    14    34 1
     26    15    16 ar
     27    15    35 1
     28    16    17 ar
     29    16    36 1
     30    17    37 1
     31    18    19 ar
     32    18    23 ar
     33    19    20 ar
     34    19    38 1
     35    20    21 ar
     36    20    39 1
     37    21    22 ar
     38    21    40 1
     39    22    23 ar
     40    22    24 1
     41    23    41 1
     42    24    25 1
     43    24    26 1
     44    24    27 1
@<TRIPOS>SUBSTRUCTURE
      1 SUB          1 GROUP             0        ****     0 ROOT
```

(6) Ligand6.mol2

```
@<TRIPOS>MOLECULE
P12F
40    43     1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
       1 N1         -42.7516    12.1398    18.0793 N.2        1 SUB         -
0.5000
       2 C2         -44.0705    12.1633    17.7435 C.ar       1 SUB
0.7000
       3 N3         -44.5843    12.5221    16.5412 N.2        1 SUB         -
0.2500
       4 N4         -43.6628    12.9242    15.6729 N.pl3      1 SUB
```

0.0490
5 C5 -42.3142 12.9870 15.9107 C.ar 1 SUB
0.1413
6 C6 -41.8434 12.5625 17.1658 C.ar 1 SUB -
0.1053
7 C7 -43.9020 13.3981 14.4100 C.ar 1 SUB
0.3530
8 N8 -42.7125 13.7689 13.8813 N.2 1 SUB -
0.5630
9 C9 -41.6938 13.5249 14.8204 C.ar 1 SUB
0.1319
10 N10 -44.9489 11.7785 18.7673 N.pl3 1 SUB -
0.7800
11 C11 -40.2639 13.8764 14.5719 C.3 1 SUB -
0.0519
12 C12 -45.2147 13.5520 13.7850 C.ar 1 SUB
0.0000
13 C13 -46.2534 12.6287 14.0492 C.ar 1 SUB -
0.1150
14 H13 -46.0759 11.7475 14.6465 H 1 SUB
0.1150
15 C14 -47.5515 12.8588 13.5632 C.ar 1 SUB -
0.1150
16 C15 -47.8083 13.9867 12.7674 C.ar 1 SUB -
0.1150
17 H15 -48.8022 14.1471 12.3769 H 1 SUB
0.1150
18 C16 -46.7715 14.8869 12.4566 C.ar 1 SUB -
0.1150
19 H16 -46.9794 15.7480 11.8395 H 1 SUB
0.1150
20 C17 -45.4777 14.6753 12.9732 C.ar 1 SUB -
0.1150
21 H17 -44.6966 15.3902 12.7640 H 1 SUB
0.1150
22 C18 -46.3496 11.6536 18.7648 C.ar 1 SUB
0.2000
23 C19 -47.2040 12.3842 17.9022 C.ar 1 SUB -
0.1150
24 C20 -48.5977 12.2132 17.9480 C.ar 1 SUB -
0.1150
25 H20 -49.2219 12.7823 17.2725 H 1 SUB
0.1150
26 C21 -49.1830 11.3427 18.8885 C.ar 1 SUB

```
0.0900
      27 C22         -48.3406    10.6237    19.7688 C.ar       1 SUB         -
0.1150
      28 H22         -48.7633     9.9496    20.4987 H          1 SUB
0.1150
      29 C23         -46.9393    10.7791    19.7023 C.ar       1 SUB         -
0.1150
      30 H31         -40.7939    12.5808    17.4221 H          1 SUB
0.1150
      31 H32         -44.4883    11.5334    19.6363 H          1 SUB
0.3800
      32 H33         -39.8610    14.4716    15.3938 H          1 SUB
0.0600
      33 H34         -39.6540    12.9763    14.4852 H          1 SUB
0.0600
      34 H35         -40.1530    14.4622    13.6594 H          1 SUB
0.0600
      35 H37         -48.3422    12.1568    13.7839 H          1 SUB
0.1150
      36 H40         -46.8275    13.1043    17.1958 H          1 SUB
0.1150
      37 H41         -46.3157    10.2163    20.3835 H          1 SUB
0.1150
      38 N           -50.6499    11.2349    18.9720 N.pl3      1 SUB
0.6500
      39 O           -51.3103    11.4734    17.9676 O.co2      1 SUB         -
0.3700
      40 O           -51.1418    10.9413    20.0573 O.co2      1 SUB         -
0.3700
@<TRIPOS>BOND
     1    1    2 ar
     2    1    6 ar
     3    2    3 ar
     4    2   10 1
     5    3    4 ar
     6    4    5 ar
     7    4    7 ar
     8    5    6 ar
     9    5    9 ar
    10    6   30 1
    11    7    8 ar
    12    7   12 1
    13    8    9 ar
    14    9   11 1
```

```
     15    10    22 1
     16    10    31 1
     17    11    32 1
     18    11    33 1
     19    11    34 1
     20    12    13 ar
     21    12    20 ar
     22    13    14 1
     23    13    15 ar
     24    15    16 ar
     25    15    35 1
     26    16    17 1
     27    16    18 ar
     28    18    19 1
     29    18    20 ar
     30    20    21 1
     31    22    23 ar
     32    22    29 ar
     33    23    24 ar
     34    23    36 1
     35    24    25 1
     36    24    26 ar
     37    26    27 ar
     38    26    38 1
     39    27    28 1
     40    27    29 ar
     41    29    37 1
     42    38    39 1
     43    38    40 2
@<TRIPOS>SUBSTRUCTURE
      1 SUB          1 GROUP              0        ****     0 ROOT
```

(7) Ligand7.mol2

```
@<TRIPOS>MOLECULE
P12G
43    46     1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
       1 N1          -42.7523    12.1405    18.0369 N.2        1 SUB         -
0.5000
       2 C2          -44.0761    12.1942    17.7188 C.ar       1 SUB
0.7000
```

3	N3	-44.6033	12.5466	16.5181	N.2	1	SUB	-0.2500
4	N4	-43.6780	12.9293	15.6369	N.pl3	1	SUB	0.0490
5	C5	-42.3262	12.9664	15.8602	C.ar	1	SUB	0.1413
6	C6	-41.8474	12.5394	17.1082	C.ar	1	SUB	-0.1053
7	C7	-43.9178	13.4177	14.3801	C.ar	1	SUB	0.3530
8	N8	-42.7276	13.7581	13.8340	N.2	1	SUB	-0.5630
9	C9	-41.7078	13.4912	14.7624	C.ar	1	SUB	0.1319
10	N10	-44.9491	11.8604	18.7659	N.pl3	1	SUB	-0.7800
11	C11	-40.2759	13.8131	14.4963	C.3	1	SUB	-0.0519
12	C12	-45.2256	13.6148	13.7672	C.ar	1	SUB	0.0000
13	C13	-45.4776	14.7894	13.0274	C.ar	1	SUB	-0.1150
14	C14	-46.7667	15.0422	12.5279	C.ar	1	SUB	-0.1150
15	C15	-47.8081	14.1253	12.7670	C.ar	1	SUB	-0.1150
16	C16	-47.5557	12.9414	13.4805	C.ar	1	SUB	-0.1150
17	C17	-46.2661	12.6816	13.9690	C.ar	1	SUB	-0.1150
18	C18	-46.3476	11.7170	18.7596	C.ar	1	SUB	0.2000
19	C19	-47.2059	12.5068	17.9563	C.ar	1	SUB	-0.1150
20	C20	-48.5979	12.2921	17.9580	C.ar	1	SUB	-0.1150
21	C21	-49.1544	11.2974	18.7873	C.ar	1	SUB	0.1567
22	C22	-48.3164	10.5409	19.6308	C.ar	1	SUB	-0.1150
23	C23	-46.9212	10.7545	19.6180	C.ar	1	SUB	-0.1150
24	S24	-50.9177	10.9421	18.7642	S.o2	1	SUB	0.8327

```
      25 O25         -51.5128   11.3396   20.0470 O.2        1 SUB         -
0.4680
      26 O26         -51.0976    9.5685   18.2742 O.2        1 SUB         -
0.4680
      27 N27         -51.5534   11.9908   17.5673 N.pl3      1 SUB         -
0.7678
      28 H28         -40.7938   12.5402   17.3491 H          1 SUB
0.1150
      29 H29         -44.4850   11.6219   19.6341 H          1 SUB
0.3800
      30 H30         -39.8413   14.3718   15.3268 H          1 SUB
0.0600
      31 H31         -39.6896   12.9033   14.3701 H          1 SUB
0.0600
      32 H32         -40.1645   14.4238   13.6001 H          1 SUB
0.0600
      33 H33         -44.6860   15.5060   12.8640 H          1 SUB
0.1150
      34 H34         -46.9626   15.9431   11.9665 H          1 SUB
0.1150
      35 H35         -48.7958   14.3170   12.3762 H          1 SUB
0.1150
      36 H36         -48.3516   12.2310   13.6437 H          1 SUB
0.1150
      37 H37         -46.0885   11.7685   14.5193 H          1 SUB
0.1150
      38 H38         -46.8181   13.2909   17.3227 H          1 SUB
0.1150
      39 H39         -49.2181   12.8941   17.3129 H          1 SUB
0.1150
      40 H40         -48.7402    9.7779   20.2657 H          1 SUB
0.1150
      41 H41         -46.2891   10.1490   20.2509 H          1 SUB
0.1150
      42 H42         -52.5701   11.9428   17.5488 H          1 SUB
0.3572
      43 H43         -51.1856   11.7414   16.6403 H          1 SUB
0.3572
@<TRIPOS>BOND
      1     1     2 ar
      2     1     6 ar
      3     2     3 ar
      4     2    10 1
      5     3     4 ar
```

```
     6     4     5 ar
     7     4     7 ar
     8     5     6 ar
     9     5     9 ar
    10     6    28 1
    11     7     8 ar
    12     7    12 1
    13     8     9 ar
    14     9    11 1
    15    10    18 1
    16    10    29 1
    17    11    30 1
    18    11    31 1
    19    11    32 1
    20    12    13 ar
    21    12    17 ar
    22    13    14 ar
    23    13    33 1
    24    14    15 ar
    25    14    34 1
    26    15    16 ar
    27    15    35 1
    28    16    17 ar
    29    16    36 1
    30    17    37 1
    31    18    19 ar
    32    18    23 ar
    33    19    20 ar
    34    19    38 1
    35    20    21 ar
    36    20    39 1
    37    21    22 ar
    38    21    24 1
    39    22    23 ar
    40    22    40 1
    41    23    41 1
    42    24    25 2
    43    24    26 2
    44    24    27 1
    45    27    42 1
    46    27    43 1
@<TRIPOS>SUBSTRUCTURE
     1 SUB           1 GROUP              0         ****      0 ROOT
```

(8) Ligand8.mol2

@<TRIPOS>MOLECULE
P12H
46 49 1
SMALL
USER_CHARGES

@<TRIPOS>ATOM
1 N1 -42.5990 12.1411 17.9669 N.2 1 SUB -
0.5000
2 C2 -43.9315 12.1655 17.6871 C.ar 1 SUB
0.7000
3 N3 -44.5091 12.5428 16.5156 N.2 1 SUB -
0.2500
4 N4 -43.6208 12.9750 15.6183 N.pl3 1 SUB
0.0490
5 C5 -42.2629 13.0432 15.8063 C.ar 1 SUB
0.1413
6 C6 -41.7351 12.5897 17.0257 C.ar 1 SUB -
0.1053
7 C7 -43.9040 13.4895 14.3794 C.ar 1 SUB
0.3530
8 N8 -42.7357 13.8828 13.8201 N.2 1 SUB -
0.5630
9 C9 -41.6857 13.6196 14.7132 C.ar 1 SUB
0.1319
10 N10 -44.7382 11.7825 18.7663 N.pl3 1 SUB -
0.7800
11 C11 -40.2671 13.9940 14.4348 C.3 1 SUB -
0.0519
12 C12 -45.2282 13.6619 13.7889 C.ar 1 SUB
0.0000
13 C13 -46.2543 12.7151 14.0117 C.ar 1 SUB -
0.1150
14 C14 -47.5508 12.9406 13.5160 C.ar 1 SUB -
0.1150
15 C15 -47.8228 14.1036 12.7763 C.ar 1 SUB -
0.1150
16 C16 -46.8006 15.0384 12.5241 C.ar 1 SUB -
0.1150
17 C17 -45.5059 14.8191 13.0307 C.ar 1 SUB -
0.1150
18 C18 -46.1166 11.5269 18.8586 C.ar 1 SUB
0.2000

19	C19	-47.0943	12.0431	17.9787	C.ar	1	SUB	-0.1150
20	C20	-48.4549	11.7471	18.1753	C.ar	1	SUB	-0.1150
21	C21	-48.8718	10.9408	19.2631	C.ar	1	SUB	0.0850
22	C22	-47.9017	10.4229	20.1520	C.ar	1	SUB	0.0850
23	C23	-46.5339	10.7258	19.9393	C.ar	1	SUB	-0.1150
24	O24	-50.1914	10.6275	19.5135	O.3	1	SUB	-0.2850
25	C25	-51.1760	11.0870	18.5988	C.3	1	SUB	0.1100
26	O26	-48.3518	9.6378	21.1949	O.3	1	SUB	-0.2850
27	C27	-47.3854	9.0075	22.0248	C.3	1	SUB	0.1100
28	H28	-40.6763	12.6114	17.2383	H	1	SUB	0.1150
29	H29	-44.2239	11.6170	19.6245	H	1	SUB	0.3800
30	H30	-39.8735	14.6329	15.2262	H	1	SUB	0.0600
31	H31	-40.1684	14.5406	13.4961	H	1	SUB	0.0600
32	H32	-39.6350	13.1072	14.3867	H	1	SUB	0.0600
33	H33	-46.0605	11.8126	14.5728	H	1	SUB	0.1150
34	H34	-48.3346	12.2192	13.6953	H	1	SUB	0.1150
35	H35	-48.8149	14.2690	12.3836	H	1	SUB	0.1150
36	H36	-47.0146	15.9274	11.9486	H	1	SUB	0.1150
37	H37	-44.7311	15.5516	12.8533	H	1	SUB	0.1150
38	H38	-46.8437	12.6890	17.1531	H	1	SUB	0.1150
39	H39	-49.1618	12.1602	17.4720	H	1	SUB	0.1150
40	H40	-45.7737	10.3474	20.6053	H	1	SUB	0.1150

```
      41 H41         -51.0024    10.6920    17.5965 H          1 SUB
0.0300
      42 H42         -51.2091    12.1768    18.5598 H          1 SUB
0.0300
      43 H43         -52.1569    10.7393    18.9217 H          1 SUB
0.0300
      44 H44         -46.7486     8.3314    21.4518 H          1 SUB
0.0300
      45 H45         -47.8921     8.4174    22.7880 H          1 SUB
0.0300
      46 H46         -46.7629     9.7383    22.5390 H          1 SUB
0.0300
@<TRIPOS>BOND
      1     1     2 ar
      2     1     6 ar
      3     2     3 ar
      4     2    10 1
      5     3     4 ar
      6     4     5 ar
      7     4     7 ar
      8     5     6 ar
      9     5     9 ar
     10     6    28 1
     11     7     8 ar
     12     7    12 1
     13     8     9 ar
     14     9    11 1
     15    10    18 1
     16    10    29 1
     17    11    30 1
     18    11    31 1
     19    11    32 1
     20    12    13 ar
     21    12    17 ar
     22    13    14 ar
     23    13    33 1
     24    14    15 ar
     25    14    34 1
     26    15    16 ar
     27    15    35 1
     28    16    17 ar
     29    16    36 1
     30    17    37 1
     31    18    19 ar
```

```
    32    18    23 ar
    33    19    20 ar
    34    19    38 1
    35    20    21 ar
    36    20    39 1
    37    21    22 ar
    38    21    24 1
    39    22    23 ar
    40    22    26 1
    41    23    40 1
    42    24    25 1
    43    25    41 1
    44    25    42 1
    45    25    43 1
    46    26    27 1
    47    27    44 1
    48    27    45 1
    49    27    46 1
@<TRIPOS>SUBSTRUCTURE
     1 SUB          1 GROUP             0        ****     0 ROOT
```

(9) Ligand9.mol2

```
@<TRIPOS>MOLECULE
P12I
50    53     1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
      1 N1         -42.6154    12.1402    17.9671 N.2        1 SUB         -
0.5000
      2 C2         -43.9520    12.1389    17.7020 C.ar       1 SUB
0.7000
      3 N3         -44.5552    12.5434    16.5517 N.2        1 SUB         -
0.2500
      4 N4         -43.6889    13.0339    15.6608 N.p13      1 SUB
0.0490
      5 C5         -42.3284    13.1209    15.8318 C.ar       1 SUB
0.1413
      6 C6         -41.7742    12.6388    17.0285 C.ar       1 SUB         -
0.1053
      7 C7         -43.9979    13.5886    14.4449 C.ar       1 SUB
0.3530
      8 N8         -42.8479    14.0135    13.8786 N.2        1 SUB         -
```

0.5630
9 C9 -41.7788 13.7321 14.7410 C.ar 1 SUB
0.1319
10 N10 -44.7289 11.6638 18.7673 N.pl3 1 SUB -
0.7800
11 C11 -40.3764 14.1173 14.4130 C.3 1 SUB -
0.0519
12 C12 -45.3206 13.7567 13.8604 C.ar 1 SUB
0.0000
13 C13 -45.6415 14.9611 13.1983 C.ar 1 SUB -
0.1150
14 C14 -46.9285 15.1548 12.6609 C.ar 1 SUB -
0.1150
15 C15 -47.8951 14.1395 12.7788 C.ar 1 SUB -
0.1150
16 C16 -47.5761 12.9350 13.4243 C.ar 1 SUB -
0.1150
17 C17 -46.2940 12.7409 13.9671 C.ar 1 SUB -
0.1150
18 C18 -46.1102 11.4541 18.8982 C.ar 1 SUB
0.2000
19 C19 -47.0934 12.1379 18.1495 C.ar 1 SUB -
0.1150
20 C20 -48.4718 11.8922 18.3638 C.ar 1 SUB
0.0850
21 C21 -48.8594 10.9409 19.3346 C.ar 1 SUB
0.0850
22 C22 -47.8937 10.2868 20.1306 C.ar 1 SUB
0.0850
23 C23 -46.5218 10.5460 19.8920 C.ar 1 SUB -
0.1150
24 O24 -50.1866 10.6647 19.5541 O.3 1 SUB -
0.2850
25 C25 -50.8319 9.9970 18.4768 C.3 1 SUB
0.1100
26 O26 -48.3486 9.4212 21.1081 O.3 1 SUB -
0.2850
27 C27 -47.3793 8.7782 21.9245 C.3 1 SUB
0.1100
28 O28 -49.4756 12.5783 17.7128 O.3 1 SUB -
0.2850
29 C29 -49.1178 13.5012 16.6955 C.3 1 SUB
0.1100
30 H30 -40.7119 12.6763 17.2267 H 1 SUB

```
0.1150
      31 H31        -44.1944    11.4356    19.5964 H          1 SUB
0.3800
      32 H32        -39.7109    13.2542    14.4595 H          1 SUB
0.0600
      33 H33        -40.0003    14.8667    15.1116 H          1 SUB
0.0600
      34 H34        -40.3283    14.5401    13.4103 H          1 SUB
0.0600
      35 H35        -44.9029    15.7435    13.1085 H          1 SUB
0.1150
      36 H36        -47.1760    16.0783    12.1583 H          1 SUB
0.1150
      37 H37        -48.8835    14.2800    12.3700 H          1 SUB
0.1150
      38 H38        -48.3193    12.1529    13.5009 H          1 SUB
0.1150
      39 H39        -46.0632    11.8073    14.4597 H          1 SUB
0.1150
      40 H40        -46.7943    12.8849    17.4357 H          1 SUB
0.1150
      41 H41        -45.7551    10.0532    20.4686 H          1 SUB
0.1150
      42 H42        -51.8560     9.7583    18.7634 H          1 SUB
0.0300
      43 H43        -50.8814    10.5960    17.5684 H          1 SUB
0.0300
      44 H44        -50.3294     9.0566    18.2462 H          1 SUB
0.0300
      45 H45        -46.7564     9.4979    22.4567 H          1 SUB
0.0300
      46 H46        -47.8827     8.1677    22.6752 H          1 SUB
0.0300
      47 H47        -46.7419     8.1168    21.3366 H          1 SUB
0.0300
      48 H48        -48.5188    13.0170    15.9256 H          1 SUB
0.0300
      49 H49        -48.5684    14.3521    17.1008 H          1 SUB
0.0300
      50 H50        -50.0198    13.8798    16.2175 H          1 SUB
0.0300
@<TRIPOS>BOND
      1     1     2 ar
      2     1     6 ar
```

3	2	3	ar
4	2	10	1
5	3	4	ar
6	4	5	ar
7	4	7	ar
8	5	6	ar
9	5	9	ar
10	6	30	1
11	7	8	ar
12	7	12	1
13	8	9	ar
14	9	11	1
15	10	18	1
16	10	31	1
17	11	32	1
18	11	33	1
19	11	34	1
20	12	13	ar
21	12	17	ar
22	13	14	ar
23	13	35	1
24	14	15	ar
25	14	36	1
26	15	16	ar
27	15	37	1
28	16	17	ar
29	16	38	1
30	17	39	1
31	18	19	ar
32	18	23	ar
33	19	20	ar
34	19	40	1
35	20	21	ar
36	20	28	1
37	21	22	ar
38	21	24	1
39	22	23	ar
40	22	26	1
41	23	41	1
42	24	25	1
43	25	42	1
44	25	43	1
45	25	44	1
46	26	27	1

```
    47    27    45 1
    48    27    46 1
    49    27    47 1
    50    28    29 1
    51    29    48 1
    52    29    49 1
    53    29    50 1
@<TRIPOS>SUBSTRUCTURE
     1 SUB          1 GROUP             0        ****     0 ROOT
```

(10) Ligand10.mol2

```
@<TRIPOS>MOLECULE
P15A
54   57    1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
      1 N1         -42.5735   12.1408   17.9674 N.2        1 SUB         -
0.5000
      2 C2         -43.9057   12.1945   17.6923 C.ar       1 SUB
0.7000
      3 N3         -44.4833   12.6182   16.5320 N.2        1 SUB         -
0.2500
      4 N4         -43.5839   13.0576   15.6425 N.pl3      1 SUB
0.0490
      5 C5         -42.2228   13.0869   15.8311 C.ar       1 SUB
0.1413
      6 C6         -41.7034   12.5979   17.0382 C.ar       1 SUB         -
0.1053
      7 C7         -43.8484   13.5988   14.4072 C.ar       1 SUB
0.3530
      8 N8         -42.6644   13.9474   13.8506 N.2        1 SUB         -
0.5630
      9 C9         -41.6269   13.6564   14.7463 C.ar       1 SUB
0.1319
     10 N10        -44.7028   11.7757   18.7668 N.pl3      1 SUB         -
0.7800
     11 C11        -40.1997   13.9948   14.4718 C.3        1 SUB         -
0.0519
     12 C12        -45.1675   13.7973   13.8051 C.ar       1 SUB
0.0000
     13 C13        -46.1274   12.7664   13.9095 C.ar       1 SUB         -
0.1150
```

```
      14 H13       -45.8784   11.8328   14.3919 H         1 SUB
0.1150
      15 C14       -47.4192   12.9410   13.3897 C.ar      1 SUB       -
0.1150
      16 C15       -47.7621   14.1451   12.7624 C.ar      1 SUB       -
0.1150
      17 C16       -46.8124   15.1737   12.6368 C.ar      1 SUB       -
0.1150
      18 H16       -47.1217   16.0806   12.1406 H         1 SUB
0.1150
      19 C17       -45.5020   15.0141   13.1546 C.ar      1 SUB
0.0850
      20 O         -44.5388   15.9994   13.0716 O.3       1 SUB       -
0.2850
      21 C         -44.8326   17.1835   12.3416 C.3       1 SUB
0.1100
      22 H1        -45.6291   17.7570   12.8185 H         1 SUB
0.0300
      23 H2        -45.1127   16.9600   11.3096 H         1 SUB
0.0300
      24 H3        -43.9466   17.8183   12.3086 H         1 SUB
0.0300
      25 C18       -46.0800   11.5224   18.8592 C.ar      1 SUB
0.2000
      26 C19       -46.4880   10.6059   19.8453 C.ar      1 SUB       -
0.1150
      27 C20       -47.8573   10.3159   20.0558 C.ar      1 SUB
0.0850
      28 C21       -48.8261   10.9541   19.2486 C.ar      1 SUB
0.0850
      29 C22       -48.4391   11.9150   18.2813 C.ar      1 SUB
0.0850
      30 C23       -47.0607   12.1812   18.0868 C.ar      1 SUB       -
0.1150
      31 O24       -50.1505   10.6615   19.4695 O.3       1 SUB       -
0.2850
      32 C25       -50.8228   10.0627   18.3689 C.3       1 SUB
0.1100
      33 O26       -49.4390   12.5939   17.6150 O.3       1 SUB       -
0.2850
      34 C27       -49.0783   13.5397   16.6211 C.3       1 SUB
0.1100
      35 O28       -48.3099    9.4392   21.0215 O.3       1 SUB       -
0.2850
```

```
      36 C29         -47.3454     8.8180    21.8618 C.3         1 SUB
0.1100
      37 H           -48.7574    14.2758    12.3692 H           1 SUB
0.1150
      38 H31         -40.6438    12.5946    17.2494 H           1 SUB
0.1150
      39 H32         -44.1788    11.5636    19.6091 H           1 SUB
0.3800
      40 H33         -39.7863    14.6099    15.2718 H           1 SUB
0.0600
      41 H34         -39.5940    13.0916    14.4044 H           1 SUB
0.0600
      42 H35         -40.0937    14.5544    13.5425 H           1 SUB
0.0600
      43 H37         -48.1477    12.1485    13.4761 H           1 SUB
0.1150
      44 H40         -45.7202    10.1305    20.4373 H           1 SUB
0.1150
      45 H41         -46.7560    12.9331    17.3800 H           1 SUB
0.1150
      46 H42         -51.0256    10.7674    17.5654 H           1 SUB
0.0300
      47 H43         -51.7843     9.6784    18.7055 H           1 SUB
0.0300
      48 H44         -50.2565     9.2218    17.9693 H           1 SUB
0.0300
      49 H45         -49.9793    13.9257    16.1445 H           1 SUB
0.0300
      50 H46         -48.5371    14.3849    17.0468 H           1 SUB
0.0300
      51 H47         -48.4724    13.0750    15.8474 H           1 SUB
0.0300
      52 H48         -46.6781     8.1696    21.2910 H           1 SUB
0.0300
      53 H49         -46.7555     9.5562    22.4050 H           1 SUB
0.0300
      54 H50         -47.8514     8.2008    22.6032 H           1 SUB
0.0300
@<TRIPOS>BOND
      1     1     2 ar
      2     1     6 ar
      3     2     3 ar
      4     2    10 1
      5     3     4 ar
```

6	4	5	ar
7	4	7	ar
8	5	6	ar
9	5	9	ar
10	6	38	1
11	7	8	ar
12	7	12	1
13	8	9	ar
14	9	11	1
15	10	25	1
16	10	39	1
17	11	40	1
18	11	41	1
19	11	42	1
20	12	13	ar
21	12	19	ar
22	13	14	1
23	13	15	ar
24	15	16	ar
25	15	43	1
26	16	17	ar
27	16	37	1
28	17	18	1
29	17	19	ar
30	19	20	1
31	20	21	1
32	21	22	1
33	21	23	1
34	21	24	1
35	25	26	ar
36	25	30	ar
37	26	27	ar
38	26	44	1
39	27	28	ar
40	27	35	1
41	28	29	ar
42	28	31	1
43	29	30	ar
44	29	33	1
45	30	45	1
46	31	32	1
47	32	46	1
48	32	47	1
49	32	48	1

```
     50    33    34 1
     51    34    49 1
     52    34    50 1
     53    34    51 1
     54    35    36 1
     55    36    52 1
     56    36    53 1
     57    36    54 1
@<TRIPOS>SUBSTRUCTURE
      1 SUB          1 GROUP             0        ****     0 ROOT
```

(11) Ligand11.mol2

```
@<TRIPOS>MOLECULE
P15B
52    55     1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
       1 N1         -42.5782    12.1411    17.9673 N.2        1 SUB         -
0.5000
       2 C2         -43.9068    12.1905    17.6792 C.ar       1 SUB
0.7000
       3 N3         -44.4745    12.5494    16.4940 N.2        1 SUB         -
0.2500
       4 N4         -43.5741    12.9374    15.5830 N.pl3      1 SUB
0.0490
       5 C5         -42.2163    12.9922    15.7905 C.ar       1 SUB
0.1413
       6 C6         -41.7044    12.5639    17.0252 C.ar       1 SUB         -
0.1053
       7 C7         -43.8317    13.3991    14.3102 C.ar       1 SUB
0.3530
       8 N8         -42.6419    13.7527    13.7689 N.2        1 SUB         -
0.5630
       9 C9         -41.6148    13.5361    14.6975 C.ar       1 SUB
0.1319
      10 N10        -44.7204    11.8528    18.7672 N.pl3      1 SUB         -
0.7800
      11 C11        -40.1945    13.9283    14.4553 C.3        1 SUB         -
0.0519
      12 C12        -45.1530    13.5466    13.6767 C.ar       1 SUB
0.0000
      13 C13        -46.1844    12.6359    14.0156 C.ar       1 SUB         -
```

0.1150
14 H13 -45.9848 11.7806 14.6432 H 1 SUB
0.1150
15 C14 -47.5023 12.8306 13.5682 C.ar 1 SUB -
0.1150
16 C15 -47.8120 13.9366 12.7674 C.ar 1 SUB -
0.1150
17 C16 -46.7909 14.8129 12.3668 C.ar 1 SUB -
0.1150
18 C17 -45.4604 14.6164 12.7881 C.ar 1 SUB
0.0900
19 C18 -46.0991 11.6133 18.8458 C.ar 1 SUB
0.2000
20 C19 -47.0675 12.2706 18.0552 C.ar 1 SUB -
0.1150
21 C20 -48.4494 12.0172 18.2453 C.ar 1 SUB
0.0850
22 C21 -48.8484 11.0671 19.2191 C.ar 1 SUB
0.0850
23 C22 -47.8897 10.4340 20.0411 C.ar 1 SUB
0.0850
24 C23 -46.5187 10.7113 19.8373 C.ar 1 SUB -
0.1150
25 O24 -50.1753 10.7950 19.4508 O.3 1 SUB -
0.2850
26 C25 -50.8565 10.1784 18.3673 C.3 1 SUB
0.1100
27 O26 -48.3503 9.5701 21.0144 O.3 1 SUB -
0.2850
28 C27 -47.3928 8.9392 21.8539 C.3 1 SUB
0.1100
29 O28 -49.4425 12.6943 17.5677 O.3 1 SUB -
0.2850
30 C29 -49.0812 13.7978 16.7524 C.3 1 SUB
0.1100
31 H -48.8249 14.0999 12.4300 H 1 SUB
0.1150
32 H31 -40.6467 12.5794 17.2455 H 1 SUB
0.1150
33 H32 -44.2121 11.6742 19.6274 H 1 SUB
0.3800
34 H33 -39.8109 14.5199 15.2870 H 1 SUB
0.0600
35 H34 -39.5589 13.0477 14.3674 H 1 SUB

```
0.0600
      36 H35         -40.0904    14.5344    13.5549 H          1 SUB
0.0600
      37 H37         -48.2824    12.1408    13.8532 H          1 SUB
0.1150
      38 H38         -47.0325    15.6397    11.7143 H          1 SUB
0.1150
      39 H40         -46.7489    13.0087    17.3391 H          1 SUB
0.1150
      40 H41         -45.7582    10.2393    20.4409 H          1 SUB
0.1150
      41 H42         -51.0710    10.8767    17.5599 H          1 SUB
0.0300
      42 H43         -51.8110     9.7881    18.7190 H          1 SUB
0.0300
      43 H44         -50.2874     9.3384    17.9676 H          1 SUB
0.0300
      44 H45         -47.9060     8.3438    22.6085 H          1 SUB
0.0300
      45 H46         -46.7477     8.2676    21.2844 H          1 SUB
0.0300
      46 H47         -46.7788     9.6702    22.3800 H          1 SUB
0.0300
      47 H48         -48.5791    14.5747    17.3304 H          1 SUB
0.0300
      48 H49         -48.4366    13.4907    15.9332 H          1 SUB
0.0300
      49 H50         -49.9799    14.2331    16.3160 H          1 SUB
0.0300
      50 N           -44.4476    15.5470    12.2785 N.pl3      1 SUB
0.6500
      51 O           -44.4221    16.6707    12.7632 O.co2      1 SUB          -
0.3700
      52 O           -43.7370    15.1669    11.3524 O.co2      1 SUB          -
0.3700
@<TRIPOS>BOND
      1     1     2 ar
      2     1     6 ar
      3     2     3 ar
      4     2    10 1
      5     3     4 ar
      6     4     5 ar
      7     4     7 ar
      8     5     6 ar
```

9	5	9	ar
10	6	32	1
11	7	8	ar
12	7	12	1
13	8	9	ar
14	9	11	1
15	10	19	1
16	10	33	1
17	11	34	1
18	11	35	1
19	11	36	1
20	12	13	ar
21	12	18	ar
22	13	14	1
23	13	15	ar
24	15	16	ar
25	15	37	1
26	16	17	ar
27	16	31	1
28	17	18	ar
29	17	38	1
30	18	50	1
31	19	20	ar
32	19	24	ar
33	20	21	ar
34	20	39	1
35	21	22	ar
36	21	29	1
37	22	23	ar
38	22	25	1
39	23	24	ar
40	23	27	1
41	24	40	1
42	25	26	1
43	26	41	1
44	26	42	1
45	26	43	1
46	27	28	1
47	28	44	1
48	28	45	1
49	28	46	1
50	29	30	1
51	30	47	1
52	30	48	1

```
    53    30    49 1
    54    50    51 1
    55    50    52 2
@<TRIPOS>SUBSTRUCTURE
     1 SUB          1 GROUP             0        ****     0 ROOT
```

(12) Ligand12.mol2

```
@<TRIPOS>MOLECULE
P15C
50    53     1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
      1 N1         -42.7105    12.1948    17.9674 N.2        1 SUB         -
0.5000
      2 C2         -44.0401    12.2666    17.6847 C.ar       1 SUB
0.7000
      3 N3         -44.6117    12.6459    16.5074 N.2        1 SUB         -
0.2500
      4 N4         -43.7118    13.0208    15.5927 N.pl3      1 SUB
0.0490
      5 C5         -42.3510    13.0374    15.7817 C.ar       1 SUB
0.1413
      6 C6         -41.8366    12.5969    17.0135 C.ar       1 SUB         -
0.1053
      7 C7         -43.9747    13.4948    14.3279 C.ar       1 SUB
0.3530
      8 N8         -42.7883    13.7922    13.7559 N.2        1 SUB         -
0.5630
      9 C9         -41.7549    13.5494    14.6686 C.ar       1 SUB
0.1319
     10 N10        -44.8540    11.9169    18.7673 N.pl3      1 SUB         -
0.7800
     11 C11        -40.3390    13.8894    14.3704 C.3        1 SUB         -
0.0519
     12 C12        -45.2929    13.6704    13.7134 C.ar       1 SUB
0.0000
     13 C13        -46.2887    12.7024    13.9774 C.ar       1 SUB         -
0.1150
     14 H13        -46.0624    11.8191    14.5553 H          1 SUB
0.1150
     15 C14        -47.6002    12.8743    13.5107 C.ar       1 SUB         -
0.1150
```

16	C15	-47.9384	14.0114	12.7672	C.ar	1	SUB	-0.1150
17	C16	-46.9477	14.9566	12.4492	C.ar	1	SUB	-0.1150
18	C17	-45.6254	14.7933	12.9057	C.ar	1	SUB	0.2000
19	BR	-44.3629	16.1283	12.3894	Br	1	SUB	-0.2000
20	C18	-46.2341	11.6841	18.8456	C.ar	1	SUB	0.2000
21	C19	-46.6582	10.8044	19.8554	C.ar	1	SUB	-0.1150
22	C20	-48.0306	10.5400	20.0662	C.ar	1	SUB	0.0850
23	C21	-48.9856	11.1621	19.2310	C.ar	1	SUB	0.0850
24	C22	-48.5833	12.0941	18.2429	C.ar	1	SUB	0.0850
25	C23	-47.2008	12.3338	18.0446	C.ar	1	SUB	-0.1150
26	O24	-50.3134	10.8924	19.4552	O.3	1	SUB	-0.2850
27	C25	-50.9736	10.2517	18.3733	C.3	1	SUB	0.1100
28	O26	-49.5757	12.7722	17.5673	O.3	1	SUB	-0.2850
29	C27	-49.2052	13.8079	16.6723	C.3	1	SUB	0.1100
30	O28	-48.4986	9.7135	21.0668	O.3	1	SUB	-0.2850
31	C29	-47.5468	9.0402	21.8801	C.3	1	SUB	0.1100
32	H	-48.9486	14.1410	12.4096	H	1	SUB	0.1150
33	H31	-40.7751	12.5802	17.2183	H	1	SUB	0.1150
34	H32	-44.3424	11.7146	19.6202	H	1	SUB	0.3800
35	H33	-39.9370	14.5667	15.1241	H	1	SUB	0.0600
36	H34	-39.7173	12.9942	14.3675	H	1	SUB	0.0600
37	H35	-40.2586	14.3899	13.4063	H	1	SUB	0.0600

```
      38 H37        -48.3541    12.1364    13.7324 H          1 SUB
0.1150
      39 H38        -47.2072    15.8153    11.8475 H          1 SUB
0.1150
      40 H40        -45.9001    10.3450    20.4721 H          1 SUB
0.1150
      41 H41        -46.8836    13.0622    17.3197 H          1 SUB
0.1150
      42 H42        -51.2101    10.9432    17.5655 H          1 SUB
0.0300
      43 H43        -51.9132     9.8276    18.7232 H          1 SUB
0.0300
      44 H44        -50.3731     9.4341    17.9711 H          1 SUB
0.0300
      45 H45        -50.0996    14.2293    16.2136 H          1 SUB
0.0300
      46 H46        -48.6802    14.6150    17.1861 H          1 SUB
0.0300
      47 H47        -48.5792    13.4274    15.8707 H          1 SUB
0.0300
      48 H48        -46.9294     8.3610    21.2894 H          1 SUB
0.0300
      49 H49        -46.9054     9.7413    22.4130 H          1 SUB
0.0300
      50 H50        -48.0687     8.4477    22.6306 H          1 SUB
0.0300
@<TRIPOS>BOND
     1     1     2 ar
     2     1     6 ar
     3     2     3 ar
     4     2    10 1
     5     3     4 ar
     6     4     5 ar
     7     4     7 ar
     8     5     6 ar
     9     5     9 ar
    10     6    33 1
    11     7     8 ar
    12     7    12 1
    13     8     9 ar
    14     9    11 1
    15    10    20 1
    16    10    34 1
    17    11    35 1
```

```
     18    11    36 1
     19    11    37 1
     20    12    13 ar
     21    12    18 ar
     22    13    14 1
     23    13    15 ar
     24    15    16 ar
     25    15    38 1
     26    16    17 ar
     27    16    32 1
     28    17    18 ar
     29    17    39 1
     30    18    19 1
     31    20    21 ar
     32    20    25 ar
     33    21    22 ar
     34    21    40 1
     35    22    23 ar
     36    22    30 1
     37    23    24 ar
     38    23    26 1
     39    24    25 ar
     40    24    28 1
     41    25    41 1
     42    26    27 1
     43    27    42 1
     44    27    43 1
     45    27    44 1
     46    28    29 1
     47    29    45 1
     48    29    46 1
     49    29    47 1
     50    30    31 1
     51    31    48 1
     52    31    49 1
     53    31    50 1
@<TRIPOS>SUBSTRUCTURE
      1 SUB          1 GROUP              0        ****     0 ROOT
```

(13) Ligand13.mol2

```
@<TRIPOS>MOLECULE
P15D
50    53     1
SMALL
USER_CHARGES
```

@<TRIPOS>ATOM
1 N1 -42.7509 11.9025 17.9673 N.2 1 SUB -0.5000
2 C2 -44.0840 12.0164 17.7189 C.ar 1 SUB 0.7000
3 N3 -44.6704 12.5366 16.6063 N.2 1 SUB -0.2500
4 N4 -43.7770 12.9817 15.7214 N.pl3 1 SUB 0.0490
5 C5 -42.4134 12.9472 15.8678 C.ar 1 SUB 0.1413
6 C6 -41.8844 12.3771 17.0376 C.ar 1 SUB -0.1053
7 C7 -44.0574 13.6052 14.5350 C.ar 1 SUB 0.3530
8 N8 -42.8873 13.9459 13.9566 N.2 1 SUB -0.5630
9 C9 -41.8321 13.5406 14.7843 C.ar 1 SUB 0.1319
10 N10 -44.8724 11.5297 18.7672 N.pl3 1 SUB -0.7800
11 C11 -40.4076 13.8031 14.4276 C.3 1 SUB -0.0519
12 C12 -45.3761 13.9214 14.0100 C.ar 1 SUB 0.0000
13 C13 -46.3913 12.9409 13.9648 C.ar 1 SUB -0.1150
14 H13 -46.1890 11.9283 14.2876 H 1 SUB 0.1150
15 C14 -47.6752 13.2818 13.5019 C.ar 1 SUB -0.1150
16 C15 -47.9536 14.6032 13.1123 C.ar 1 SUB -0.1150
17 C16 -46.9372 15.5758 13.1257 C.ar 1 SUB 0.2000
18 C17 -45.6484 15.2350 13.5727 C.ar 1 SUB -0.1150
19 H17 -44.8734 15.9870 13.6019 H 1 SUB 0.1150
20 C18 -46.2585 11.3653 18.9116 C.ar 1 SUB 0.2000
21 C19 -46.6752 10.5383 19.9707 C.ar 1 SUB -

0.1150
22 C20 -48.0459 10.3309 20.2409 C.ar 1 SUB
0.0850
23 C21 -49.0193 10.9412 19.4155 C.ar 1 SUB
0.0850
24 C22 -48.6176 11.8252 18.3752 C.ar 1 SUB
0.0850
25 C23 -47.2359 12.0145 18.1260 C.ar 1 SUB -
0.1150
26 O24 -50.3392 10.6926 19.7290 O.3 1 SUB -
0.2850
27 C25 -51.2628 10.5592 18.6562 C.3 1 SUB
0.1100
28 O26 -49.5942 12.5356 17.7079 O.3 1 SUB -
0.2850
29 C27 -49.2083 13.4587 16.7037 C.3 1 SUB
0.1100
30 O28 -48.4950 9.5590 21.2945 O.3 1 SUB -
0.2850
31 C29 -47.5344 8.9784 22.1665 C.3 1 SUB
0.1100
32 H -48.9421 14.8673 12.7688 H 1 SUB
0.1150
33 H31 -40.8190 12.3212 17.2159 H 1 SUB
0.1150
34 H32 -44.3337 11.2164 19.5587 H 1 SUB
0.3800
35 H33 -39.9273 14.4434 15.1693 H 1 SUB
0.0600
36 H34 -39.8425 12.8714 14.3692 H 1 SUB
0.0600
37 H35 -40.3487 14.3050 13.4616 H 1 SUB
0.0600
38 H37 -48.4566 12.5382 13.4639 H 1 SUB
0.1150
39 BR -47.3035 17.3501 12.5446 Br 1 SUB -
0.2000
40 H40 -45.9165 10.0710 20.5771 H 1 SUB
0.1150
41 H41 -46.9296 12.7047 17.3621 H 1 SUB
0.1150
42 H42 -51.7166 11.5191 18.4119 H 1 SUB
0.0300
43 H43 -52.0675 9.8894 18.9584 H 1 SUB

```
0.0300
     44 H44         -50.8037    10.1390    17.7604 H          1 SUB
0.0300
     45 H45         -50.1006    13.8996    16.2566 H          1 SUB
0.0300
     46 H46         -48.5992    14.2696    17.1031 H          1 SUB
0.0300
     47 H47         -48.6651    12.9478    15.9125 H          1 SUB
0.0300
     48 H48         -46.9038     8.2556    21.6453 H          1 SUB
0.0300
     49 H49         -46.9017     9.7385    22.6271 H          1 SUB
0.0300
     50 H50         -48.0468     8.4523    22.9714 H          1 SUB
0.0300
@<TRIPOS>BOND
     1     1     2 ar
     2     1     6 ar
     3     2     3 ar
     4     2    10 1
     5     3     4 ar
     6     4     5 ar
     7     4     7 ar
     8     5     6 ar
     9     5     9 ar
    10     6    33 1
    11     7     8 ar
    12     7    12 1
    13     8     9 ar
    14     9    11 1
    15    10    20 1
    16    10    34 1
    17    11    35 1
    18    11    36 1
    19    11    37 1
    20    12    13 ar
    21    12    18 ar
    22    13    14 1
    23    13    15 ar
    24    15    16 ar
    25    15    38 1
    26    16    17 ar
    27    16    32 1
    28    17    18 ar
```

```
    29    17    39 1
    30    18    19 1
    31    20    21 ar
    32    20    25 ar
    33    21    22 ar
    34    21    40 1
    35    22    23 ar
    36    22    30 1
    37    23    24 ar
    38    23    26 1
    39    24    25 ar
    40    24    28 1
    41    25    41 1
    42    26    27 1
    43    27    42 1
    44    27    43 1
    45    27    44 1
    46    28    29 1
    47    29    45 1
    48    29    46 1
    49    29    47 1
    50    30    31 1
    51    31    48 1
    52    31    49 1
    53    31    50 1
@<TRIPOS>SUBSTRUCTURE
     1 SUB          1 GROUP             0        ****     0 ROOT
```

(14) Ligand14.mol2

```
@<TRIPOS>MOLECULE
P15E
53    56     1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
      1 N1         -42.7438    12.1003    17.9673 N.2        1 SUB         -
0.5000
      2 C2         -44.0723    12.1960    17.6926 C.ar       1 SUB
0.7000
      3 N3         -44.6370    12.6464    16.5369 N.2        1 SUB         -
0.2500
      4 N4         -43.7275    13.0739    15.6579 N.pl3      1 SUB
0.0490
```

5	C5	-42.3683	13.0632	15.8393	C.ar	1	SUB	0.1413
6	C6	-41.8610	12.5397	17.0378	C.ar	1	SUB	-0.1053
7	C7	-43.9868	13.6745	14.4545	C.ar	1	SUB	0.3530
8	N8	-42.8063	14.0255	13.8986	N.2	1	SUB	-0.5630
9	C9	-41.7665	13.6527	14.7647	C.ar	1	SUB	0.1319
10	N10	-44.8799	11.8034	18.7660	N.pl3	1	SUB	-0.7800
11	C11	-40.3311	13.9535	14.4790	C.3	1	SUB	-0.0519
12	C12	-45.3043	13.9752	13.9149	C.ar	1	SUB	0.0000
13	C13	-46.2880	12.9689	13.8116	C.ar	1	SUB	-0.1150
14	H13	-46.0559	11.9481	14.0823	H	1	SUB	0.1150
15	C14	-47.5840	13.2993	13.3732	C.ar	1	SUB	-0.1150
16	C15	-47.9058	14.6347	13.0694	C.ar	1	SUB	-0.1150
17	C16	-46.9215	15.6441	13.1491	C.ar	1	SUB	0.1500
18	C17	-45.6182	15.3026	13.5623	C.ar	1	SUB	-0.1150
19	H17	-44.8601	16.0701	13.6398	H	1	SUB	0.1150
20	C18	-46.2673	11.6192	18.8663	C.ar	1	SUB	0.2000
21	C19	-47.2223	12.2842	18.0616	C.ar	1	SUB	-0.1150
22	C20	-48.6094	12.0778	18.2594	C.ar	1	SUB	0.0850
23	C21	-49.0349	11.1693	19.2586	C.ar	1	SUB	0.0850
24	C22	-48.0956	10.5403	20.1045	C.ar	1	SUB	0.0850
25	C23	-46.7164	10.7671	19.8900	C.ar	1	SUB	-0.1150
26	O24	-50.3694	10.9283	19.4790	O.3	1	SUB	-0.2850

27	C25	-51.0317	10.2767	18.4031	C.3	1	SUB	0.1100
28	O26	-48.5853	9.7411	21.1188	O.3	1	SUB	-0.2850
29	C27	-47.6506	9.0520	21.9381	C.3	1	SUB	0.1100
30	O28	-49.5847	12.7684	17.5678	O.3	1	SUB	-0.2850
31	C29	-49.1842	13.6958	16.5699	C.3	1	SUB	0.1100
32	H	-48.9130	14.8782	12.7668	H	1	SUB	0.1150
33	H31	-40.7999	12.5105	17.2484	H	1	SUB	0.1150
34	H32	-44.3529	11.5608	19.5984	H	1	SUB	0.3800
35	H33	-39.8828	14.5222	15.2938	H	1	SUB	0.0600
36	H34	-39.7596	13.0336	14.3673	H	1	SUB	0.0600
37	H35	-40.2211	14.5403	13.5659	H	1	SUB	0.0600
38	H37	-48.3437	12.5325	13.3014	H	1	SUB	0.1150
39	C	-47.2446	17.0903	12.8001	C.3	1	SUB	0.4500
40	F	-46.6970	17.9052	13.6999	F	1	SUB	-0.2000
41	F	-48.5575	17.3132	12.7819	F	1	SUB	-0.2000
42	F	-46.7419	17.3788	11.6003	F	1	SUB	-0.2000
43	H40	-46.8909	12.9973	17.3279	H	1	SUB	0.1150
44	H41	-45.9714	10.2968	20.5152	H	1	SUB	0.1150
45	H42	-51.2263	10.9491	17.5667	H	1	SUB	0.0300
46	H43	-51.9959	9.9054	18.7472	H	1	SUB	0.0300
47	H44	-50.4581	9.4204	18.0404	H	1	SUB	0.0300
48	H45	-48.1853	8.4789	22.6944	H	1	SUB	0.0300

```
      49 H46        -47.0498     8.3531    21.3550 H          1 SUB
0.0300
      50 H47        -46.9912     9.7409    22.4638 H          1 SUB
0.0300
      51 H48        -48.6377    14.5389    17.0000 H          1 SUB
0.0300
      52 H49        -48.5671    13.2109    15.8152 H          1 SUB
0.0300
      53 H50        -50.0672    14.0890    16.0658 H          1 SUB
0.0300
@<TRIPOS>BOND
      1     1     2 ar
      2     1     6 ar
      3     2     3 ar
      4     2    10 1
      5     3     4 ar
      6     4     5 ar
      7     4     7 ar
      8     5     6 ar
      9     5     9 ar
     10     6    33 1
     11     7     8 ar
     12     7    12 1
     13     8     9 ar
     14     9    11 1
     15    10    20 1
     16    10    34 1
     17    11    35 1
     18    11    36 1
     19    11    37 1
     20    12    13 ar
     21    12    18 ar
     22    13    14 1
     23    13    15 ar
     24    15    16 ar
     25    15    38 1
     26    16    17 ar
     27    16    32 1
     28    17    18 ar
     29    17    39 1
     30    18    19 1
     31    20    21 ar
     32    20    25 ar
     33    21    22 ar
```

```
    34    21    43 1
    35    22    23 ar
    36    22    30 1
    37    23    24 ar
    38    23    26 1
    39    24    25 ar
    40    24    28 1
    41    25    44 1
    42    26    27 1
    43    27    45 1
    44    27    46 1
    45    27    47 1
    46    28    29 1
    47    29    48 1
    48    29    49 1
    49    29    50 1
    50    30    31 1
    51    31    51 1
    52    31    52 1
    53    31    53 1
    54    39    40 1
    55    39    41 1
    56    39    42 1
@<TRIPOS>SUBSTRUCTURE
     1 SUB          1 GROUP              0        ****     0 ROOT
```

(15) Ligand15.mol2

```
@<TRIPOS>MOLECULE
P15F
   53     56      1 0 0
SMALL
USER_CHARGES


@<TRIPOS>ATOM
      1 N1           -43.075100    12.338700    17.478100 N.2       1 SUBUNIT
0.0000
      2 C2           -44.394001    12.584600    17.519400 C.2       1 SUBUNIT
0.0000
      3 N3           -45.069500    13.108400    16.495001 N.2       1 SUBUNIT
0.0000
      4 N4           -44.366699    13.476300    15.406600 N.pl3     1 SUBUNIT
0.0000
      5 C5           -43.043999    13.253800    15.304400 C.2       1 SUBUNIT
```

0.0000
6 C6 -42.398602 12.666300 16.359100 C.2 1 SUBUNIT
0.0000
7 C7 -44.884899 14.116300 14.313300 C.2 1 SUBUNIT
0.0000
8 N8 -43.843300 14.254600 13.425200 N.2 1 SUBUNIT
0.0000
9 C9 -42.718601 13.763200 14.001100 C.2 1 SUBUNIT
0.0000
10 N10 -45.035801 12.281900 18.686399 N.pl3 1 SUBUNIT
0.0000
11 C11 -41.367298 13.784500 13.329100 C.3 1 SUBUNIT
0.0000
12 C12 -46.285801 14.580600 14.125100 C.2 1 SUBUNIT
0.0000
13 C13 -47.159901 13.890000 13.310500 C.2 1 SUBUNIT
0.0000
14 C14 -48.474201 14.320200 13.145900 C.2 1 SUBUNIT
0.0000
15 C15 -48.948200 15.455500 13.804100 C.2 1 SUBUNIT
0.0000
16 C16 -48.058300 16.153000 14.613100 C.2 1 SUBUNIT
0.0000
17 C17 -46.748402 15.716000 14.761400 C.2 1 SUBUNIT
0.0000
18 C18 -46.348202 11.900900 18.796000 C.2 1 SUBUNIT
0.0000
19 C19 -47.396900 12.533300 18.125401 C.2 1 SUBUNIT
0.0000
20 C20 -48.715401 12.121600 18.308399 C.2 1 SUBUNIT
0.0000
21 C21 -48.986198 11.092900 19.206600 C.2 1 SUBUNIT
0.0000
22 C22 -47.962898 10.493900 19.933701 C.2 1 SUBUNIT
0.0000
23 C23 -46.643700 10.893600 19.707899 C.2 1 SUBUNIT
0.0000
24 O24 -50.293598 10.692500 19.444599 O.3 1 SUBUNIT
0.0000
25 C25 -50.802502 9.932800 18.365000 C.3 1 SUBUNIT
0.0000
26 O26 -48.346699 9.511800 20.850500 O.3 1 SUBUNIT
0.0000
27 C27 -47.319000 9.002000 21.679300 C.3 1 SUBUNIT

0.0000
28 O28 -49.811501 12.729800 17.693800 O.3 1 SUBUNIT
0.0000
29 C29 -49.526600 13.671900 16.677999 C.3 1 SUBUNIT
0.0000
30 C30 -50.366600 15.949800 13.637200 C.3 1 SUBUNIT
0.0000
31 F31 -50.342300 16.922501 12.744300 F 1 SUBUNIT
0.0000
32 F32 -51.150700 14.968600 13.230800 F 1 SUBUNIT
0.0000
33 F33 -50.791401 16.407700 14.804200 F 1 SUBUNIT
0.0000
34 H34 -41.337299 12.470800 16.297800 H 1 SUBUNIT
0.0000
35 H35 -44.457401 12.179100 19.496201 H 1 SUBUNIT
0.0000
36 H36 -41.470699 13.602200 12.259600 H 1 SUBUNIT
0.0000
37 H37 -40.887798 14.751200 13.476800 H 1 SUBUNIT
0.0000
38 H38 -40.725300 13.014300 13.755700 H 1 SUBUNIT
0.0000
39 H39 -46.832100 13.001600 12.787600 H 1 SUBUNIT
0.0000
40 H40 -49.116699 13.756500 12.492800 H 1 SUBUNIT
0.0000
41 H41 -48.370602 17.050400 15.127300 H 1 SUBUNIT
0.0000
42 H42 -46.107700 16.311600 15.386800 H 1 SUBUNIT
0.0000
43 H43 -47.205898 13.382700 17.493799 H 1 SUBUNIT
0.0000
44 H44 -45.824402 10.438900 20.243999 H 1 SUBUNIT
0.0000
45 H45 -51.804501 9.578900 18.603800 H 1 SUBUNIT
0.0000
46 H46 -50.174400 9.061500 18.177000 H 1 SUBUNIT
0.0000
47 H47 -50.874001 10.525800 17.454399 H 1 SUBUNIT
0.0000
48 H48 -46.841599 9.804100 22.240700 H 1 SUBUNIT
0.0000
49 H49 -47.741699 8.307000 22.405100 H 1 SUBUNIT

```
0.0000
     50 H50          -46.576199    8.459600   21.093300 H         1 SUBUNIT
0.0000
     51 H51          -48.885399   13.237900   15.909500 H         1 SUBUNIT
0.0000
     52 H52          -49.056900   14.565700   17.090000 H         1 SUBUNIT
0.0000
     53 H53          -50.456799   13.974300   16.198601 H         1 SUBUNIT
0.0000
@<TRIPOS>BOND
     1     1     2 1
     2     1     6 2
     3     2     3 2
     4     2    10 1
     5     3     4 1
     6     4     5 1
     7     4     7 1
     8     5     6 1
     9     5     9 2
    10     6    34 1
    11     7     8 2
    12     7    12 1
    13     8     9 1
    14     9    11 1
    15    10    18 1
    16    10    35 1
    17    11    36 1
    18    11    37 1
    19    11    38 1
    20    12    13 2
    21    12    17 1
    22    13    14 1
    23    13    39 1
    24    14    15 2
    25    14    40 1
    26    15    16 1
    27    15    30 1
    28    16    17 2
    29    16    41 1
    30    17    42 1
    31    18    19 2
    32    18    23 1
    33    19    20 1
    34    19    43 1
```

```
    35    20    21 2
    36    20    28 1
    37    21    22 1
    38    21    24 1
    39    22    23 2
    40    22    26 1
    41    23    44 1
    42    24    25 1
    43    25    45 1
    44    25    46 1
    45    25    47 1
    46    26    27 1
    47    27    48 1
    48    27    49 1
    49    27    50 1
    50    28    29 1
    51    29    51 1
    52    29    52 1
    53    29    53 1
    54    30    31 1
    55    30    32 1
    56    30    33 1
@<TRIPOS>SUBSTRUCTURE
     1 SUB          1 GROUP             0        ****     0 ROOT
```

(16) Ligand16.mol2

```
@<TRIPOS>MOLECULE
P15G
62    66     1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
      1 N1         -42.8050    12.0856    17.9695 N.2        1 SUB         -
0.5000
      2 C2         -44.1800    12.1061    17.7980 C.ar       1 SUB
0.7000
      3 N3         -44.7736    12.4311    16.6836 N.2        1 SUB         -
0.2500
      4 N4         -43.9623    12.8079    15.6765 N.pl3      1 SUB
0.0490
      5 C5         -42.6123    12.8335    15.7716 C.ar       1 SUB
0.1413
      6 C6         -42.0392    12.4513    16.9933 C.ar       1 SUB         -
```

0.1053
7 C7 -44.2876 13.2617 14.4106 C.ar 1 SUB
0.3530
8 N8 -43.1835 13.5296 13.7252 N.2 1 SUB -
0.5630
9 C9 -42.1348 13.3043 14.5788 C.ar 1 SUB
0.1319
10 N10 -44.8802 11.7200 18.9126 N.pl3 1 SUB -
0.7800
11 C11 -40.7487 13.6114 14.1839 C.3 1 SUB -
0.0519
12 C12 -45.6368 13.5705 13.9438 C.ar 1 SUB
0.0000
13 C13 -46.6481 12.6073 13.8393 C.ar 1 SUB -
0.1150
14 H13 -46.4569 11.5673 14.0892 H 1 SUB
0.1150
15 C14 -47.9241 12.9772 13.4135 C.ar 1 SUB -
0.1150
16 C15 -48.1941 14.3119 13.1077 C.ar 1 SUB -
0.1150
17 C16 -47.1895 15.2831 13.1988 C.ar 1 SUB -
0.1150
18 C -47.5177 16.6964 12.8847 C.2 1 SUB
0.7000
19 O -48.6816 17.0831 12.8606 O.2 1 SUB -
0.4700
20 C -46.5036 17.7238 12.6335 C.ar 1 SUB -
0.1150
21 C17 -45.9126 14.9030 13.6007 C.ar 1 SUB -
0.1150
22 H17 -45.1108 15.6359 13.6663 H 1 SUB
0.1150
23 C18 -46.2603 11.5348 19.0857 C.ar 1 SUB
0.2000
24 C19 -46.7038 10.7184 20.1358 C.ar 1 SUB -
0.1150
25 C20 -48.0656 10.4455 20.3101 C.ar 1 SUB
0.0850
26 C21 -49.0086 10.9607 19.4069 C.ar 1 SUB
0.0850
27 C22 -48.5892 11.8354 18.3876 C.ar 1 SUB
0.0850
28 C23 -47.2185 12.0797 18.2204 C.ar 1 SUB -

0.1150
29 O24 -50.3240 10.6026 19.6321 O.3 1 SUB -
0.2850
30 C25 -51.0685 10.4319 18.4219 C.3 1 SUB
0.1100
31 O26 -49.5650 12.4251 17.6250 O.3 1 SUB -
0.2850
32 C27 -49.1649 13.4691 16.7364 C.3 1 SUB
0.1100
33 O28 -48.5223 9.6071 21.3038 O.3 1 SUB -
0.2850
34 C29 -47.4629 8.9141 21.9722 C.3 1 SUB
0.1100
35 H -49.1968 14.5974 12.7985 H 1 SUB
0.1150
36 H31 -40.9453 12.4617 17.1119 H 1 SUB
0.1150
37 H32 -44.2988 11.5572 19.7336 H 1 SUB
0.3800
38 H33 -40.3027 14.3250 14.8831 H 1 SUB
0.0600
39 H34 -40.1425 12.7021 14.1830 H 1 SUB
0.0600
40 H35 -40.7167 14.0582 13.1861 H 1 SUB
0.0600
41 H37 -48.7154 12.2305 13.3400 H 1 SUB
0.1150
42 H40 -45.9669 10.2611 20.7889 H 1 SUB
0.1150
43 H41 -46.8764 12.7314 17.4227 H 1 SUB
0.1150
44 H42 -51.6102 11.3485 18.1739 H 1 SUB
0.0300
45 H43 -51.8126 9.6486 18.5924 H 1 SUB
0.0300
46 H44 -50.4322 10.1140 17.5944 H 1 SUB
0.0300
47 H45 -50.0687 13.8873 16.2844 H 1 SUB
0.0300
48 H46 -48.6552 14.2738 17.2754 H 1 SUB
0.0300
49 H47 -48.5414 13.0784 15.9295 H 1 SUB
0.0300
50 H48 -47.1496 8.0399 21.3933 H 1 SUB

```
0.0300
      51 H49        -46.6124    9.5728   22.1792 H         1 SUB
0.0300
      52 H50        -47.8546    8.5573   22.9294 H         1 SUB
0.0300
      53 C          -46.5473   18.9518   13.2936 C.ar      1 SUB        -
0.1150
      54 H          -47.3868   19.2346   13.9120 H         1 SUB
0.1150
      55 C          -45.4807   19.8375   13.1577 C.ar      1 SUB        -
0.1150
      56 H          -45.4957   20.7931   13.6774 H         1 SUB
0.1150
      57 C          -44.3949   19.5071   12.3490 C.ar      1 SUB        -
0.1150
      58 H          -43.5776   20.2148   12.2373 H         1 SUB
0.1150
      59 C          -44.3642   18.2800   11.6892 C.ar      1 SUB        -
0.1150
      60 H          -43.5224   18.0049   11.0645 H         1 SUB
0.1150
      61 C          -45.4148   17.3804   11.8343 C.ar      1 SUB        -
0.1150
      62 H          -45.3737   16.4113   11.3423 H         1 SUB
0.1150
@<TRIPOS>BOND
     1    1    2 ar
     2    1    6 ar
     3    2    3 ar
     4    2   10 1
     5    3    4 ar
     6    4    5 ar
     7    4    7 ar
     8    5    6 ar
     9    5    9 ar
    10    6   36 1
    11    7    8 ar
    12    7   12 1
    13    8    9 ar
    14    9   11 1
    15   10   23 1
    16   10   37 1
    17   11   38 1
    18   11   39 1
```

19	11	40	1
20	12	13	ar
21	12	21	ar
22	13	14	1
23	13	15	ar
24	15	16	ar
25	15	41	1
26	16	17	ar
27	16	35	1
28	17	18	1
29	17	21	ar
30	18	19	2
31	18	20	1
32	20	53	ar
33	20	61	ar
34	21	22	1
35	23	24	ar
36	23	28	ar
37	24	25	ar
38	24	42	1
39	25	26	ar
40	25	33	1
41	26	27	ar
42	26	29	1
43	27	28	ar
44	27	31	1
45	28	43	1
46	29	30	1
47	30	44	1
48	30	45	1
49	30	46	1
50	31	32	1
51	32	47	1
52	32	48	1
53	32	49	1
54	33	34	1
55	34	50	1
56	34	51	1
57	34	52	1
58	53	54	1
59	53	55	ar
60	55	56	1
61	55	57	ar
62	57	58	1

```
    63    57    59 ar
    64    59    60 1
    65    59    61 ar
    66    61    62 1
@<TRIPOS>SUBSTRUCTURE
     1 SUB          1 GROUP             0        ****     0 ROOT
```

(17) Ligand17.mol2

```
@<TRIPOS>MOLECULE
P15H
61    65     1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
      1 N1         -42.7521    11.9465    17.9671 N.2        1 SUB         -
0.5000
      2 C2         -44.1304    12.0450    17.8573 C.ar       1 SUB
0.7000
      3 N3         -44.7525    12.4307    16.7768 N.2        1 SUB         -
0.2500
      4 N4         -43.9693    12.7751    15.7328 N.pl3      1 SUB
0.0490
      5 C5         -42.6175    12.7029    15.7663 C.ar       1 SUB
0.1413
      6 C6         -42.0143    12.2784    16.9590 C.ar       1 SUB         -
0.1053
      7 C7         -44.3172    13.2733    14.4863 C.ar       1 SUB
0.3530
      8 N8         -43.2244    13.4403    13.7484 N.2        1 SUB         -
0.5630
      9 C9         -42.1593    13.1355    14.5527 C.ar       1 SUB
0.1319
     10 N10        -44.8017    11.6678    18.9945 N.pl3      1 SUB         -
0.7800
     11 C11        -40.7727    13.3307    14.0936 C.3        1 SUB         -
0.0519
     12 C12        -45.6538    13.7035    14.0656 C.ar       1 SUB
0.0000
     13 C13        -46.7002    12.8187    13.7814 C.ar       1 SUB         -
0.1150
     14 H13        -46.5496    11.7443    13.8412 H          1 SUB
0.1150
     15 C14        -47.9598    13.3043    13.4171 C.ar       1 SUB         -
```

0.1150
16 C15 -48.1799 14.6793 13.3441 C.ar 1 SUB -
0.1150
17 C16 -47.1453 15.5760 13.6128 C.ar 1 SUB
0.0850
18 O -47.4324 16.9113 13.4352 O.3 1 SUB -
0.1700
19 C -46.3989 17.7687 13.1446 C.ar 1 SUB
0.0850
20 C17 -45.8860 15.0862 13.9522 C.ar 1 SUB -
0.1150
21 H17 -45.0623 15.7742 14.1331 H 1 SUB
0.1150
22 C18 -46.1580 11.3512 19.1708 C.ar 1 SUB
0.2000
23 C19 -47.0943 11.8360 18.2462 C.ar 1 SUB -
0.1150
24 C20 -48.4662 11.6213 18.4303 C.ar 1 SUB
0.0850
25 C21 -48.9266 10.9415 19.5699 C.ar 1 SUB
0.0850
26 C22 -47.9970 10.3820 20.4653 C.ar 1 SUB
0.0850
27 C23 -46.6307 10.6257 20.2709 C.ar 1 SUB -
0.1150
28 O24 -50.2966 10.8205 19.6969 O.3 1 SUB -
0.2850
29 C25 -50.9185 10.2971 18.5182 C.3 1 SUB
0.1100
30 O26 -48.4836 9.6035 21.4846 O.3 1 SUB -
0.2850
31 C27 -47.5517 8.7497 22.1483 C.3 1 SUB
0.1100
32 O28 -49.4106 12.1337 17.5675 O.3 1 SUB -
0.2850
33 C29 -48.9787 13.3378 16.9231 C.3 1 SUB
0.1100
34 H -49.1604 15.0560 13.0702 H 1 SUB
0.1150
35 H31 -40.9160 12.2267 17.0287 H 1 SUB
0.1150
36 H32 -44.2162 11.6247 19.8273 H 1 SUB
0.3800
37 H33 -40.2230 13.9667 14.7952 H 1 SUB

0.0600
38 H34 -40.2588 12.3684 14.0240 H 1 SUB
0.0600
39 H35 -40.7515 13.8164 13.1129 H 1 SUB
0.0600
40 H37 -48.7697 12.6130 13.1986 H 1 SUB
0.1150
41 H40 -46.7412 12.4271 17.4070 H 1 SUB
0.1150
42 H41 -45.9035 10.2263 20.9700 H 1 SUB
0.1150
43 H42 -51.2787 11.1105 17.8825 H 1 SUB
0.0300
44 H43 -51.7907 9.7151 18.8293 H 1 SUB
0.0300
45 H44 -50.2507 9.6323 17.9675 H 1 SUB
0.0300
46 H45 -48.1118 8.1143 22.8401 H 1 SUB
0.0300
47 H46 -47.0307 8.1029 21.4347 H 1 SUB
0.0300
48 H47 -46.8408 9.3286 22.7393 H 1 SUB
0.0300
49 H48 -49.1263 14.1999 17.5811 H 1 SUB
0.0300
50 H49 -47.9364 13.2705 16.5914 H 1 SUB
0.0300
51 H50 -49.6058 13.4818 16.0380 H 1 SUB
0.0300
52 C -45.3621 17.3093 12.3284 C.ar 1 SUB -
0.1150
53 H -45.3150 16.2699 12.0146 H 1 SUB
0.1150
54 C -44.3474 18.1786 11.9297 C.ar 1 SUB -
0.1150
55 H -43.5391 17.8122 11.2965 H 1 SUB
0.1150
56 C -44.3595 19.5052 12.3587 C.ar 1 SUB -
0.1150
57 H -43.5526 20.1716 12.0643 H 1 SUB
0.1150
58 C -45.4014 19.9634 13.1675 C.ar 1 SUB -
0.1150
59 H -45.4139 20.9943 13.5069 H 1 SUB

```
0.1150
     60 C          -46.4285    19.1009    13.5587 C.ar       1 SUB         -
0.1150
     61 H          -47.2404    19.4712    14.1826 H          1 SUB
0.1150
@<TRIPOS>BOND
     1    1    2 ar
     2    1    6 ar
     3    2    3 ar
     4    2   10 1
     5    3    4 ar
     6    4    5 ar
     7    4    7 ar
     8    5    6 ar
     9    5    9 ar
    10    6   35 1
    11    7    8 ar
    12    7   12 1
    13    8    9 ar
    14    9   11 1
    15   10   22 1
    16   10   36 1
    17   11   37 1
    18   11   38 1
    19   11   39 1
    20   12   13 ar
    21   12   20 ar
    22   13   14 1
    23   13   15 ar
    24   15   16 ar
    25   15   40 1
    26   16   17 ar
    27   16   34 1
    28   17   18 1
    29   17   20 ar
    30   18   19 1
    31   19   52 ar
    32   19   60 ar
    33   20   21 1
    34   22   23 ar
    35   22   27 ar
    36   23   24 ar
    37   23   41 1
    38   24   25 ar
```

```
     39    24    32 1
     40    25    26 ar
     41    25    28 1
     42    26    27 ar
     43    26    30 1
     44    27    42 1
     45    28    29 1
     46    29    43 1
     47    29    44 1
     48    29    45 1
     49    30    31 1
     50    31    46 1
     51    31    47 1
     52    31    48 1
     53    32    33 1
     54    33    49 1
     55    33    50 1
     56    33    51 1
     57    52    53 1
     58    52    54 ar
     59    54    55 1
     60    54    56 ar
     61    56    57 1
     62    56    58 ar
     63    58    59 1
     64    58    60 ar
     65    60    61 1
@<TRIPOS>SUBSTRUCTURE
      1 SUB          1 GROUP             0        ****     0 ROOT
```

(18) Ligand18.mol2

```
@<TRIPOS>MOLECULE
P15i
50    53     1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
      1 N1         -42.6346    12.1407    17.9664 N.2        1 SUB         -
0.5000
      2 C2         -43.9721    12.1405    17.7047 C.ar       1 SUB
0.7000
      3 N3         -44.5848    12.5537    16.5614 N.2        1 SUB         -
0.2500
```

4	N4	-43.7242	13.0440	15.6703	N.pl3	1	SUB	0.0490
5	C5	-42.3625	13.1178	15.8208	C.ar	1	SUB	0.1413
6	C6	-41.8009	12.6270	17.0138	C.ar	1	SUB	-0.1053
7	C7	-44.0549	13.6292	14.4790	C.ar	1	SUB	0.3530
8	N8	-42.9151	14.0492	13.8893	N.2	1	SUB	-0.5630
9	C9	-41.8286	13.7351	14.7239	C.ar	1	SUB	0.1319
10	N10	-44.7472	11.6640	18.7674	N.pl3	1	SUB	-0.7800
11	C11	-40.4265	14.1110	14.3756	C.3	1	SUB	-0.0519
12	C12	-45.4084	13.8463	13.9961	C.ar	1	SUB	0.0000
13	C13	-46.2992	12.7608	13.8658	C.ar	1	SUB	-0.1150
14	C14	-47.6457	12.9928	13.5322	C.ar	1	SUB	-0.1150
15	C15	-48.1122	14.3126	13.3650	C.ar	1	SUB	0.2200
16	C16	-47.2153	15.3935	13.4525	C.ar	1	SUB	-0.1150
17	C17	-45.8609	15.1606	13.7585	C.ar	1	SUB	-0.1150
18	C18	-46.1287	11.4522	18.8930	C.ar	1	SUB	0.2000
19	C19	-46.5331	10.5431	19.8884	C.ar	1	SUB	-0.1150
20	C20	-47.9024	10.2798	20.1294	C.ar	1	SUB	0.0850
21	C21	-48.8735	10.9361	19.3415	C.ar	1	SUB	0.0850
22	C22	-48.4921	11.8879	18.3674	C.ar	1	SUB	0.0850
23	C23	-47.1145	12.1353	18.1459	C.ar	1	SUB	-0.1150
24	O24	-50.1991	10.6613	19.5661	O.3	1	SUB	-0.2850
25	C25	-50.8378	9.9803	18.4925	C.3	1	SUB	0.1100

```
      26 O26       -49.5040   12.5743   17.7312 O.3       1 SUB       -
0.2850
      27 C27       -49.1548   13.5302   16.7451 C.3       1 SUB
0.1100
      28 O28       -48.3502    9.4103   21.1044 O.3       1 SUB       -
0.2850
      29 C29       -47.3784    8.7859   21.9356 C.3       1 SUB
0.1100
      30 F30       -49.4309   14.5408   13.1678 F         1 SUB       -
0.2200
      31 H31       -40.7363   12.6542   17.2025 H         1 SUB
0.1150
      32 H32       -44.2132   11.4379   19.5974 H         1 SUB
0.3800
      33 H33       -40.0870   14.9530   14.9793 H         1 SUB
0.0600
      34 H34       -39.7422   13.2806   14.5490 H         1 SUB
0.0600
      35 H35       -40.3515   14.4015   13.3267 H         1 SUB
0.0600
      36 H36       -45.9573   11.7519   14.0500 H         1 SUB
0.1150
      37 H37       -48.3351   12.1640   13.4557 H         1 SUB
0.1150
      38 H38       -47.5752   16.4009   13.3147 H         1 SUB
0.1150
      39 H39       -45.1820   15.9948   13.8656 H         1 SUB
0.1150
      40 H40       -45.7637   10.0523   20.4635 H         1 SUB
0.1150
      41 H41       -46.8194   12.8866   17.4334 H         1 SUB
0.1150
      42 H42       -50.8572   10.5587   17.5698 H         1 SUB
0.0300
      43 H43       -51.8717    9.7696   18.7637 H         1 SUB
0.0300
      44 H44       -50.3494    9.0268   18.2881 H         1 SUB
0.0300
      45 H45       -50.0607   13.9196   16.2807 H         1 SUB
0.0300
      46 H46       -48.6066   14.3701   17.1739 H         1 SUB
0.0300
      47 H47       -48.5573   13.0656   15.9662 H         1 SUB
0.0300
```

```
      48 H48         -46.7368     8.1166    21.3605 H          1 SUB
0.0300
      49 H49         -46.7629     9.5215    22.4546 H          1 SUB
0.0300
      50 H50         -47.8815     8.1901    22.6962 H          1 SUB
0.0300
@<TRIPOS>BOND
      1     1     2 ar
      2     1     6 ar
      3     2     3 ar
      4     2    10 1
      5     3     4 ar
      6     4     5 ar
      7     4     7 ar
      8     5     6 ar
      9     5     9 ar
     10     6    31 1
     11     7     8 ar
     12     7    12 1
     13     8     9 ar
     14     9    11 1
     15    10    18 1
     16    10    32 1
     17    11    33 1
     18    11    34 1
     19    11    35 1
     20    12    13 ar
     21    12    17 ar
     22    13    14 ar
     23    13    36 1
     24    14    15 ar
     25    14    37 1
     26    15    16 ar
     27    15    30 1
     28    16    17 ar
     29    16    38 1
     30    17    39 1
     31    18    19 ar
     32    18    23 ar
     33    19    20 ar
     34    19    40 1
     35    20    21 ar
     36    20    28 1
     37    21    22 ar
```

```
     38    21    24 1
     39    22    23 ar
     40    22    26 1
     41    23    41 1
     42    24    25 1
     43    25    42 1
     44    25    43 1
     45    25    44 1
     46    26    27 1
     47    27    45 1
     48    27    46 1
     49    27    47 1
     50    28    29 1
     51    29    48 1
     52    29    49 1
     53    29    50 1
@<TRIPOS>SUBSTRUCTURE
      1 SUB          1 GROUP             0        ****     0 ROOT
```

(19) Ligand19.mol2

```
@<TRIPOS>MOLECULE
P2
41    44     1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
       1 N1         -42.6266    12.1417    17.9674 N.2        1 SUB         -
0.5000
       2 C2         -43.9519    12.1568    17.6573 C.ar       1 SUB
0.7000
       3 N3         -44.4982    12.4583    16.4503 N.2        1 SUB         -
0.2500
       4 N4         -43.5980    12.8762    15.5631 N.pl3      1 SUB
0.0490
       5 C5         -42.2470    12.9637    15.7781 C.ar       1 SUB
0.1413
       6 C6         -41.7434    12.5490    17.0233 C.ar       1 SUB         -
0.1053
       7 C7         -43.8716    13.3909    14.3221 C.ar       1 SUB
0.3530
       8 N8         -42.6971    13.7906    13.7789 N.2        1 SUB         -
0.5630
       9 C9         -41.6587    13.5413    14.6916 C.ar       1 SUB
```

0.1319
10 N10 -44.8175 11.9182 18.7347 N.pl3 1 SUB -
0.7800
11 C11 -40.2448 13.9527 14.4450 C.3 1 SUB -
0.0519
12 C12 -45.1979 13.5830 13.7355 C.ar 1 SUB
0.0000
13 C13 -46.2528 12.6817 14.0109 C.ar 1 SUB -
0.1150
14 C14 -47.5521 12.9406 13.5464 C.ar 1 SUB -
0.1150
15 C15 -47.8011 14.0825 12.7684 C.ar 1 SUB -
0.1150
16 C16 -46.7544 14.9728 12.4613 C.ar 1 SUB -
0.1150
17 C17 -45.4562 14.7263 12.9477 C.ar 1 SUB -
0.1150
18 C18 -46.2701 11.8274 18.5722 C.3 1 SUB
0.1950
19 C -47.0140 13.0194 17.9666 C.ar 1 SUB -
0.1150
20 H183 -46.4833 10.9460 17.9679 H 1 SUB
0.0600
21 H182 -46.7016 11.6320 19.5537 H 1 SUB
0.0600
22 H28 -40.6909 12.5932 17.2608 H 1 SUB
0.1150
23 H29 -44.4231 11.8352 19.6672 H 1 SUB
0.3800
24 H30 -39.8718 14.5623 15.2682 H 1 SUB
0.0600
25 H31 -39.5971 13.0798 14.3687 H 1 SUB
0.0600
26 H32 -40.1497 14.5418 13.5321 H 1 SUB
0.0600
27 H33 -46.0840 11.7879 14.5927 H 1 SUB
0.1150
28 H34 -48.3511 12.2518 13.7718 H 1 SUB
0.1150
29 H35 -48.7955 14.2693 12.3938 H 1 SUB
0.1150
30 H36 -46.9539 15.8496 11.8622 H 1 SUB
0.1150
31 H37 -44.6631 15.4290 12.7343 H 1 SUB

```
0.1150
      32 C          -46.4721    14.3262    17.9675 C.ar       1 SUB         -
0.1150
      33 H          -45.4913    14.5146    18.3772 H          1 SUB
0.1150
      34 C          -47.1866    15.3971    17.3971 C.ar       1 SUB         -
0.1150
      35 H          -46.7608    16.3907    17.3916 H          1 SUB
0.1150
      36 C          -48.4455    15.1701    16.8094 C.ar       1 SUB         -
0.1150
      37 H          -48.9825    15.9887    16.3521 H          1 SUB
0.1150
      38 C          -48.9920    13.8723    16.8047 C.ar       1 SUB         -
0.1150
      39 H          -49.9515    13.6877    16.3450 H          1 SUB
0.1150
      40 C          -48.2825    12.8057    17.3873 C.ar       1 SUB         -
0.1150
      41 H          -48.7092    11.8136    17.3705 H          1 SUB
0.1150
@<TRIPOS>BOND
     1    1    2 ar
     2    1    6 ar
     3    2    3 ar
     4    2   10 1
     5    3    4 ar
     6    4    5 ar
     7    4    7 ar
     8    5    6 ar
     9    5    9 ar
    10    6   22 1
    11    7    8 ar
    12    7   12 1
    13    8    9 ar
    14    9   11 1
    15   10   18 1
    16   10   23 1
    17   11   24 1
    18   11   25 1
    19   11   26 1
    20   12   13 ar
    21   12   17 ar
    22   13   14 ar
```

```
    23    13    27 1
    24    14    15 ar
    25    14    28 1
    26    15    16 ar
    27    15    29 1
    28    16    17 ar
    29    16    30 1
    30    17    31 1
    31    18    19 1
    32    18    20 1
    33    18    21 1
    34    19    32 ar
    35    19    40 ar
    36    32    33 1
    37    32    34 ar
    38    34    35 1
    39    34    36 ar
    40    36    37 1
    41    36    38 ar
    42    38    39 1
    43    38    40 ar
    44    40    41 1
@<TRIPOS>SUBSTRUCTURE
     1 SUB          1 GROUP             0        ****     0 ROOT
```

(20) Ligand20.mol2

```
@<TRIPOS>MOLECULE
P11
28    30     1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
      1 N1         -43.1531    11.9965    18.4696 N.2        1 SUB         -
0.5000
      2 C2         -44.4669    12.1591    18.0579 C.ar       1 SUB
0.6800
      3 N3         -44.8193    12.4218    16.8328 N.2        1 SUB         -
0.2500
      4 N4         -43.8166    12.5970    15.9498 N.pl3      1 SUB
0.0490
      5 C5         -42.5095    12.4851    16.2814 C.ar       1 SUB
0.1413
      6 C6         -42.1984    12.1685    17.6134 C.ar       1 SUB         -
```

0.1053
7 C7 -43.8752 12.9329 14.6061 C.ar 1 SUB
0.3530
8 N8 -42.6453 13.0171 14.1103 N.2 1 SUB -
0.5630
9 C9 -41.7883 12.7742 15.1552 C.ar 1 SUB
0.1319
10 N10 -45.3844 11.9913 19.0613 N.pl3 1 SUB -
0.9000
11 C11 -40.3287 12.8844 14.9875 C.3 1 SUB -
0.0519
12 C12 -45.1024 13.2594 13.8721 C.ar 1 SUB
0.0000
13 C13 -46.3014 12.5599 14.0628 C.ar 1 SUB -
0.1150
14 C14 -47.4659 12.9412 13.3930 C.ar 1 SUB -
0.1150
15 C15 -47.4421 14.0191 12.5135 C.ar 1 SUB -
0.1150
16 C16 -46.2536 14.7107 12.2958 C.ar 1 SUB -
0.1150
17 C17 -45.0889 14.3277 12.9632 C.ar 1 SUB -
0.1150
18 H26 -41.1465 12.0629 17.9194 H 1 SUB
0.1150
19 H27 -44.9646 11.7907 19.9676 H 1 SUB
0.3600
20 H101 -46.3816 12.0599 18.9164 H 1 SUB
0.3600
21 H28 -39.9188 13.6248 15.6809 H 1 SUB
0.0600
22 H29 -39.8493 11.9227 15.1879 H 1 SUB
0.0600
23 H30 -40.0749 13.2007 13.9715 H 1 SUB
0.0600
24 H31 -46.3448 11.7152 14.7436 H 1 SUB
0.1150
25 H32 -48.3936 12.4064 13.5722 H 1 SUB
0.1150
26 H33 -48.3473 14.3301 11.9997 H 1 SUB
0.1150
27 H34 -46.2366 15.5569 11.6155 H 1 SUB
0.1150
28 H35 -44.1678 14.8817 12.7877 H 1 SUB

```
0.1150
@<TRIPOS>BOND
     1    1    2 ar
     2    1    6 ar
     3    2    3 ar
     4    2   10 1
     5    3    4 ar
     6    4    5 ar
     7    4    7 ar
     8    5    6 ar
     9    5    9 ar
    10    6   18 1
    11    7    8 ar
    12    7   12 1
    13    8    9 ar
    14    9   11 1
    15   10   19 1
    16   10   20 1
    17   11   21 1
    18   11   22 1
    19   11   23 1
    20   12   13 ar
    21   12   17 ar
    22   13   14 ar
    23   13   24 1
    24   14   15 ar
    25   14   25 1
    26   15   16 ar
    27   15   26 1
    28   16   17 ar
    29   16   27 1
    30   17   28 1
@<TRIPOS>SUBSTRUCTURE
     1 SUB         1 GROUP             0       ****    0 ROOT
```

(21) Protein.pdb

```
REMARK   Accelrys Discovery Studio PDB file
REMARK   Created:  Wed Jun 22 14:16:30 中国标准时间 2016
CRYST1   66.593   66.593  154.110  90.00  90.00 120.00 P3221
ATOM      1  N   ALA A  37     -54.071   2.229  -5.927  1.00 45.42
N1+
ATOM      2  CA  ALA A  37     -54.286   2.976  -4.649  1.00 45.50
C
ATOM      3  C   ALA A  37     -53.007   3.130  -3.816  1.00 45.46
C
```

```
ATOM      4  O   ALA A  37     -52.869   4.101  -3.070  1.00 45.43
O
ATOM      5  CB  ALA A  37     -55.387   2.313  -3.829  1.00 45.57
C
ATOM      6  N   LYS A  38     -52.083   2.173  -3.966  1.00 45.50
N
ATOM      7  CA  LYS A  38     -50.795   2.094  -3.221  1.00 45.24
C
ATOM      8  C   LYS A  38     -50.918   2.129  -1.702  1.00 45.11
C
ATOM      9  O   LYS A  38     -51.364   3.117  -1.115  1.00 45.30
O
ATOM     10  CB  LYS A  38     -49.754   3.120  -3.704  1.00 45.27
C
ATOM     11  CG  LYS A  38     -49.191   2.874  -5.116  1.00 46.00
C
ATOM     12  CD  LYS A  38     -48.662   1.442  -5.314  1.00 45.97
C
ATOM     13  CE  LYS A  38     -48.294   1.181  -6.778  1.00 45.60
C
ATOM     14  NZ  LYS A  38     -48.538  -0.250  -7.169  1.00 46.17
N1+
ATOM     15  N   GLU A  39     -50.486   1.042  -1.073  1.00 44.78
N
ATOM     16  CA  GLU A  39     -50.681   0.844   0.352  1.00 44.31
C
ATOM     17  C   GLU A  39     -49.333   0.738   1.040  1.00 44.07
C
ATOM     18  O   GLU A  39     -48.385   0.189   0.469  1.00 43.74
O
ATOM     19  CB  GLU A  39     -51.506  -0.425   0.581  1.00 44.45
C
ATOM     20  CG  GLU A  39     -52.357  -0.416   1.844  1.00 44.99
C
ATOM     21  CD  GLU A  39     -53.699  -1.121   1.658  1.00 45.69
C
ATOM     22  OE1 GLU A  39     -54.383  -1.384   2.673  1.00 45.56
O
ATOM     23  OE2 GLU A  39     -54.075  -1.410   0.499  1.00 45.87
O
ATOM     24  N   ILE A  40     -49.251   1.271   2.259  1.00 43.56
N
ATOM     25  CA  ILE A  40     -48.021   1.235   3.047  1.00 43.47
C
```

```
ATOM     26  C   ILE A  40     -47.769  -0.169   3.613  1.00 43.63
C
ATOM     27  O   ILE A  40     -48.677  -0.765   4.190  1.00 43.62
O
ATOM     28  CB  ILE A  40     -48.052   2.276   4.219  1.00 43.41
C
ATOM     29  CG1 ILE A  40     -48.285   3.696   3.687  1.00 42.89
C
ATOM     30  CG2 ILE A  40     -46.774   2.190   5.066  1.00 42.82
C
ATOM     31  CD1 ILE A  40     -48.477   4.751   4.763  1.00 43.39
C
ATOM     32  N   PRO A  41     -46.537  -0.699   3.448  1.00 43.85
N
ATOM     33  CA  PRO A  41     -46.133  -1.975   4.044  1.00 44.48
C
ATOM     34  C   PRO A  41     -46.383  -2.051   5.552  1.00 45.34
C
ATOM     35  O   PRO A  41     -46.294  -1.035   6.247  1.00 45.59
O
ATOM     36  CB  PRO A  41     -44.627  -2.030   3.765  1.00 44.07
C
ATOM     37  CG  PRO A  41     -44.421  -1.189   2.606  1.00 44.06
C
ATOM     38  CD  PRO A  41     -45.452  -0.111   2.637  1.00 43.85
C
ATOM     39  N   GLU A  42     -46.720  -3.242   6.043  1.00 46.15
N
ATOM     40  CA  GLU A  42     -46.893  -3.466   7.472  1.00 47.04
C
ATOM     41  C   GLU A  42     -45.548  -3.709   8.153  1.00 47.34
C
ATOM     42  O   GLU A  42     -45.375  -3.405   9.338  1.00 47.79
O
ATOM     43  CB  GLU A  42     -47.853  -4.631   7.734  1.00 46.80
C
ATOM     44  CG  GLU A  42     -49.357  -4.334   7.267  1.00 47.51
C
ATOM     45  CD  GLU A  42     -50.253  -5.545   7.894  1.00 47.57
C
ATOM     46  OE1 GLU A  42     -49.756  -6.806   7.953  1.00 49.63
O
ATOM     47  OE2 GLU A  42     -51.453  -5.226   8.240  1.00 48.22
O
```

```
ATOM     48  N   VAL A  43     -44.618  -4.289   7.406  1.00 48.02
N
ATOM     49  CA  VAL A  43     -43.219  -4.400   7.820  1.00 48.82
C
ATOM     50  C   VAL A  43     -42.346  -3.583   6.859  1.00 48.66
C
ATOM     51  O   VAL A  43     -42.410  -3.758   5.630  1.00 48.92
O
ATOM     52  CB  VAL A  43     -42.742  -5.878   7.876  1.00 49.02
C
ATOM     53  CG1 VAL A  43     -41.252  -5.976   8.238  1.00 50.22
C
ATOM     54  CG2 VAL A  43     -43.592  -6.686   8.852  1.00 49.32
C
ATOM     55  N   LEU A  44     -41.541  -2.677   7.415  1.00 48.75
N
ATOM     56  CA  LEU A  44     -40.682  -1.798   6.593  1.00 48.66
C
ATOM     57  C   LEU A  44     -39.264  -2.325   6.649  1.00 49.07
C
ATOM     58  O   LEU A  44     -38.669  -2.414   7.725  1.00 49.30
O
ATOM     59  CB  LEU A  44     -40.700  -0.352   7.112  1.00 48.44
C
ATOM     60  CG  LEU A  44     -41.996   0.300   7.609  1.00 47.48
C
ATOM     61  CD1 LEU A  44     -41.667   1.556   8.369  1.00 46.91
C
ATOM     62  CD2 LEU A  44     -42.932   0.609   6.463  1.00 46.29
C
ATOM     63  N   VAL A  45     -38.719  -2.674   5.494  1.00 49.90
N
ATOM     64  CA  VAL A  45     -37.401  -3.301   5.444  1.00 50.61
C
ATOM     65  C   VAL A  45     -36.375  -2.360   4.843  1.00 50.22
C
ATOM     66  O   VAL A  45     -36.581  -1.814   3.770  1.00 50.55
O
ATOM     67  CB  VAL A  45     -37.426  -4.671   4.677  1.00 50.93
C
ATOM     68  CG1 VAL A  45     -36.082  -5.386   4.791  1.00 51.89
C
ATOM     69  CG2 VAL A  45     -38.540  -5.566   5.211  1.00 49.21
C
```

```
ATOM     70  N   ASP A  46     -35.273  -2.166   5.554  1.00 50.63
N
ATOM     71  CA  ASP A  46     -34.140  -1.392   5.031  1.00 51.25
C
ATOM     72  C   ASP A  46     -33.089  -2.371   4.484  1.00 51.45
C
ATOM     73  O   ASP A  46     -32.352  -2.981   5.258  1.00 51.22
O
ATOM     74  CB  ASP A  46     -33.560  -0.520   6.153  1.00 51.26
C
ATOM     75  CG  ASP A  46     -32.361   0.315   5.716  1.00 52.05
C
ATOM     76  OD1 ASP A  46     -31.849   0.166   4.587  1.00 51.22
O
ATOM     77  OD2 ASP A  46     -31.922   1.150   6.534  1.00 54.26
O
ATOM     78  N   PRO A  47     -32.986  -2.494   3.145  1.00 51.87
N
ATOM     79  CA  PRO A  47     -32.168  -3.567   2.570  1.00 51.98
C
ATOM     80  C   PRO A  47     -30.665  -3.375   2.842  1.00 52.12
C
ATOM     81  O   PRO A  47     -29.909  -4.343   2.880  1.00 52.17
O
ATOM     82  CB  PRO A  47     -32.470  -3.454   1.074  1.00 52.13
C
ATOM     83  CG  PRO A  47     -32.775  -1.982   0.858  1.00 52.52
C
ATOM     84  CD  PRO A  47     -33.566  -1.622   2.101  1.00 52.19
C
ATOM     85  N   ARG A  48     -30.255  -2.127   3.043  1.00 51.36
N
ATOM     86  CA  ARG A  48     -28.867  -1.774   3.299  1.00 50.92
C
ATOM     87  C   ARG A  48     -28.460  -2.161   4.722  1.00 50.96
C
ATOM     88  O   ARG A  48     -27.459  -2.857   4.928  1.00 50.67
O
ATOM     89  CB  ARG A  48     -28.683  -0.276   3.082  1.00 50.63
C
ATOM     90  CG  ARG A  48     -27.317   0.120   2.601  1.00 50.62
C
ATOM     91  CD  ARG A  48     -27.304   1.570   2.158  1.00 52.35
C
```

```
ATOM     92  NE  ARG A  48     -27.992   1.785   0.883  1.00 52.13
N
ATOM     93  CZ  ARG A  48     -27.379   2.029  -0.268  1.00 52.15
C
ATOM     94  NH1 ARG A  48     -26.052   2.097  -0.327  1.00 52.73
N
ATOM     95  NH2 ARG A  48     -28.094   2.214  -1.368  1.00 53.32
N
ATOM     96  N   SER A  49     -29.250  -1.721   5.699  1.00 50.74
N
ATOM     97  CA  SER A  49     -28.917  -1.935   7.103  1.00 50.82
C
ATOM     98  C   SER A  49     -29.386  -3.295   7.611  1.00 50.99
C
ATOM     99  O   SER A  49     -28.934  -3.748   8.658  1.00 51.33
O
ATOM    100  CB  SER A  49     -29.494  -0.806   7.966  1.00 50.61
C
ATOM    101  OG  SER A  49     -30.899  -0.930   8.087  1.00 49.39
O
ATOM    102  N   ARG A  50     -30.285  -3.936   6.863  1.00 51.30
N
ATOM    103  CA  ARG A  50     -30.894  -5.228   7.231  1.00 51.96
C
ATOM    104  C   ARG A  50     -31.831  -5.127   8.441  1.00 52.14
C
ATOM    105  O   ARG A  50     -32.141  -6.124   9.097  1.00 52.28
O
ATOM    106  CB  ARG A  50     -29.832  -6.320   7.437  1.00 51.96
C
ATOM    107  CG  ARG A  50     -29.239  -6.871   6.130  1.00 52.76
C
ATOM    108  CD  ARG A  50     -28.145  -7.918   6.365  1.00 52.62
C
ATOM    109  NE  ARG A  50     -28.559  -8.995   7.265  1.00 54.06
N
ATOM    110  CZ  ARG A  50     -27.902 -10.146   7.417  1.00 54.94
C
ATOM    111  NH1 ARG A  50     -26.792 -10.383   6.720  1.00 54.95
N
ATOM    112  NH2 ARG A  50     -28.356 -11.069   8.263  1.00 54.80
N
ATOM    113  N   ARG A  51     -32.281  -3.912   8.725  1.00 52.28
N
```

```
ATOM    114  CA  ARG A  51      -33.182  -3.659   9.841  1.00 52.79
C
ATOM    115  C   ARG A  51      -34.622  -3.681   9.359  1.00 52.33
C
ATOM    116  O   ARG A  51      -34.933  -3.181   8.278  1.00 52.81
O
ATOM    117  CB  ARG A  51      -32.860  -2.317  10.490  1.00 53.24
C
ATOM    118  CG  ARG A  51      -31.517  -2.282  11.194  1.00 56.49
C
ATOM    119  CD  ARG A  51      -31.343  -0.990  11.993  1.00 63.16
C
ATOM    120  NE  ARG A  51      -29.968  -0.843  12.476  1.00 67.62
N
ATOM    121  CZ  ARG A  51      -29.117   0.108  12.080  1.00 69.60
C
ATOM    122  NH1 ARG A  51      -29.486   1.039  11.199  1.00 69.50
N
ATOM    123  NH2 ARG A  51      -27.888   0.134  12.586  1.00 70.97
N
ATOM    124  N   ARG A  52      -35.497  -4.280  10.157  1.00 51.47
N
ATOM    125  CA  ARG A  52      -36.910  -4.374   9.821  1.00 51.01
C
ATOM    126  C   ARG A  52      -37.702  -3.674  10.916  1.00 50.28
C
ATOM    127  O   ARG A  52      -37.360  -3.772  12.092  1.00 49.77
O
ATOM    128  CB  ARG A  52      -37.358  -5.844   9.707  1.00 51.12
C
ATOM    129  CG  ARG A  52      -36.557  -6.693   8.711  1.00 51.38
C
ATOM    130  CD  ARG A  52      -37.254  -8.030   8.422  1.00 52.65
C
ATOM    131  NE  ARG A  52      -37.865  -8.575   9.631  1.00 56.84
N
ATOM    132  CZ  ARG A  52      -39.017  -9.244   9.672  1.00 58.90
C
ATOM    133  NH1 ARG A  52      -39.705  -9.467   8.552  1.00 60.79
N
ATOM    134  NH2 ARG A  52      -39.480  -9.691  10.837  1.00 58.63
N
ATOM    135  N   TYR A  53      -38.754  -2.974  10.515  1.00 49.50
N
```

```
ATOM    136  CA  TYR A  53      -39.547  -2.174  11.430  1.00 49.44
C
ATOM    137  C   TYR A  53      -41.006  -2.565  11.245  1.00 49.58
C
ATOM    138  O   TYR A  53      -41.524  -2.560  10.135  1.00 50.32
O
ATOM    139  CB  TYR A  53      -39.348  -0.678  11.165  1.00 49.13
C
ATOM    140  CG  TYR A  53      -37.922  -0.160  11.308  1.00 48.06
C
ATOM    141  CD1 TYR A  53      -37.445   0.316  12.532  1.00 47.04
C
ATOM    142  CD2 TYR A  53      -37.075  -0.091  10.204  1.00 48.56
C
ATOM    143  CE1 TYR A  53      -36.151   0.810  12.655  1.00 46.65
C
ATOM    144  CE2 TYR A  53      -35.781   0.399  10.314  1.00 46.45
C
ATOM    145  CZ  TYR A  53      -35.324   0.844  11.544  1.00 47.82
C
ATOM    146  OH  TYR A  53      -34.039   1.327  11.655  1.00 47.94
O
ATOM    147  N   VAL A  54      -41.652  -2.959  12.332  1.00 49.13
N
ATOM    148  CA  VAL A  54      -43.061  -3.304  12.285  1.00 49.14
C
ATOM    149  C   VAL A  54      -43.827  -2.008  12.459  1.00 48.94
C
ATOM    150  O   VAL A  54      -43.555  -1.247  13.400  1.00 48.41
O
ATOM    151  CB  VAL A  54      -43.442  -4.316  13.380  1.00 48.72
C
ATOM    152  CG1 VAL A  54      -44.943  -4.518  13.423  1.00 49.63
C
ATOM    153  CG2 VAL A  54      -42.737  -5.659  13.139  1.00 48.76
C
ATOM    154  N   ARG A  55      -44.758  -1.746  11.542  1.00 48.88
N
ATOM    155  CA  ARG A  55      -45.564  -0.523  11.594  1.00 49.87
C
ATOM    156  C   ARG A  55      -46.640  -0.622  12.674  1.00 49.76
C
ATOM    157  O   ARG A  55      -47.449  -1.570  12.679  1.00 50.93
O
```

ATOM 158 CB ARG A 55 -46.194 -0.253 10.220 1.00 50.19
C
ATOM 159 CG ARG A 55 -47.092 0.984 10.183 1.00 49.82
C
ATOM 160 CD ARG A 55 -47.313 1.466 8.762 1.00 49.97
C
ATOM 161 NE ARG A 55 -47.940 0.473 7.881 1.00 52.93
N
ATOM 162 CZ ARG A 55 -49.249 0.235 7.788 1.00 52.04
C
ATOM 163 NH1 ARG A 55 -50.116 0.890 8.546 1.00 53.86
N
ATOM 164 NH2 ARG A 55 -49.689 -0.673 6.933 1.00 49.05
N
ATOM 165 N GLY A 56 -46.646 0.340 13.593 1.00 49.91
N
ATOM 166 CA GLY A 56 -47.601 0.337 14.693 1.00 49.93
C
ATOM 167 C GLY A 56 -48.626 1.450 14.598 1.00 49.60
C
ATOM 168 O GLY A 56 -49.119 1.774 13.512 1.00 49.73
O
ATOM 169 N ARG A 57 -48.911 2.046 15.750 1.00 48.65
N
ATOM 170 CA ARG A 57 -49.964 3.038 15.922 1.00 48.42
C
ATOM 171 C ARG A 57 -49.799 4.296 15.053 1.00 47.49
C
ATOM 172 O ARG A 57 -48.702 4.850 14.940 1.00 46.32
O
ATOM 173 CB ARG A 57 -50.075 3.359 17.418 1.00 49.27
C
ATOM 174 CG ARG A 57 -50.314 4.799 17.804 1.00 53.02
C
ATOM 175 CD ARG A 57 -50.832 4.831 19.243 1.00 60.20
C
ATOM 176 NE ARG A 57 -51.227 6.171 19.679 1.00 64.47
N
ATOM 177 CZ ARG A 57 -50.560 6.899 20.570 1.00 67.61
C
ATOM 178 NH1 ARG A 57 -49.448 6.437 21.142 1.00 67.57
N
ATOM 179 NH2 ARG A 57 -51.018 8.098 20.902 1.00 70.47
N

ATOM 180 N PHE A 58 -50.894 4.699 14.413 1.00 46.46
N
ATOM 181 CA PHE A 58 -50.918 5.890 13.572 1.00 46.14
C
ATOM 182 C PHE A 58 -50.783 7.133 14.451 1.00 45.60
C
ATOM 183 O PHE A 58 -51.496 7.272 15.441 1.00 45.38
O
ATOM 184 CB PHE A 58 -52.211 5.934 12.742 1.00 46.36
C
ATOM 185 CG PHE A 58 -52.376 7.190 11.912 1.00 46.97
C
ATOM 186 CD1 PHE A 58 -51.467 7.512 10.909 1.00 46.57
C
ATOM 187 CD2 PHE A 58 -53.467 8.037 12.119 1.00 47.84
C
ATOM 188 CE1 PHE A 58 -51.633 8.682 10.134 1.00 47.92
C
ATOM 189 CE2 PHE A 58 -53.641 9.199 11.354 1.00 47.05
C
ATOM 190 CZ PHE A 58 -52.724 9.516 10.354 1.00 47.01
C
ATOM 191 N LEU A 59 -49.873 8.031 14.089 1.00 44.06
N
ATOM 192 CA LEU A 59 -49.608 9.226 14.907 1.00 44.39
C
ATOM 193 C LEU A 59 -50.262 10.483 14.326 1.00 44.52
C
ATOM 194 O LEU A 59 -50.505 11.451 15.048 1.00 43.30
O
ATOM 195 CB LEU A 59 -48.085 9.462 15.076 1.00 43.68
C
ATOM 196 CG LEU A 59 -47.173 8.395 15.705 1.00 44.77
C
ATOM 197 CD1 LEU A 59 -45.720 8.845 15.774 1.00 44.72
C
ATOM 198 CD2 LEU A 59 -47.663 7.991 17.094 1.00 47.21
C
ATOM 199 N GLY A 60 -50.527 10.476 13.020 1.00 45.46
N
ATOM 200 CA GLY A 60 -51.111 11.640 12.362 1.00 47.20
C
ATOM 201 C GLY A 60 -50.408 11.952 11.058 1.00 49.22
C

```
ATOM    202  O   GLY A  60     -49.439  11.299  10.704  1.00 48.49
O
ATOM    203  N   LYS A  61     -50.904  12.949  10.334  1.00 51.12
N
ATOM    204  CA  LYS A  61     -50.199  13.418   9.150  1.00 54.35
C
ATOM    205  C   LYS A  61     -49.237  14.533   9.555  1.00 55.62
C
ATOM    206  O   LYS A  61     -49.519  15.302  10.483  1.00 56.25
O
ATOM    207  CB  LYS A  61     -51.166  13.906   8.062  1.00 54.14
C
ATOM    208  CG  LYS A  61     -52.138  12.824   7.569  1.00 55.26
C
ATOM    209  CD  LYS A  61     -53.103  13.305   6.473  1.00 55.95
C
ATOM    210  CE  LYS A  61     -53.304  12.204   5.396  1.00 58.35
C
ATOM    211  NZ  LYS A  61     -54.226  12.539   4.238  1.00 57.72
N1+
ATOM    212  N   GLY A  62     -48.088  14.576   8.884  1.00 56.69
N
ATOM    213  CA  GLY A  62     -47.215  15.751   8.886  1.00 58.67
C
ATOM    214  C   GLY A  62     -46.894  16.137   7.444  1.00 59.57
C
ATOM    215  O   GLY A  62     -45.948  15.613   6.862  1.00 60.50
O
ATOM    216  N   GLY A  63     -47.697  17.024   6.856  1.00 60.10
N
ATOM    217  CA  GLY A  63     -47.522  17.421   5.452  1.00 60.36
C
ATOM    218  C   GLY A  63     -47.878  16.327   4.460  1.00 60.42
C
ATOM    219  O   GLY A  63     -48.969  15.774   4.502  1.00 61.50
O
ATOM    220  N   PHE A  64     -46.946  16.005   3.568  1.00 60.41
N
ATOM    221  CA  PHE A  64     -47.114  14.887   2.634  1.00 59.71
C
ATOM    222  C   PHE A  64     -47.010  13.530   3.318  1.00 58.13
C
ATOM    223  O   PHE A  64     -47.096  12.506   2.655  1.00 58.31
O
```

ATOM 224 CB PHE A 64 -46.019 14.900 1.555 1.00 60.39
C
ATOM 225 CG PHE A 64 -46.148 15.998 0.548 1.00 62.24
C
ATOM 226 CD1 PHE A 64 -47.283 16.805 0.495 1.00 63.93
C
ATOM 227 CD2 PHE A 64 -45.129 16.203 -0.382 1.00 63.42
C
ATOM 228 CE1 PHE A 64 -47.391 17.819 -0.459 1.00 65.23
C
ATOM 229 CE2 PHE A 64 -45.227 17.209 -1.340 1.00 64.67
C
ATOM 230 CZ PHE A 64 -46.367 18.015 -1.385 1.00 63.83
C
ATOM 231 N ALA A 65 -46.791 13.517 4.627 1.00 55.65
N
ATOM 232 CA ALA A 65 -46.388 12.296 5.287 1.00 53.50
C
ATOM 233 C ALA A 65 -47.514 11.750 6.146 1.00 51.81
C
ATOM 234 O ALA A 65 -48.279 12.516 6.731 1.00 51.28
O
ATOM 235 CB ALA A 65 -45.115 12.527 6.115 1.00 53.47
C
ATOM 236 N LYS A 66 -47.629 10.426 6.172 1.00 49.61
N
ATOM 237 CA LYS A 66 -48.383 9.743 7.200 1.00 48.83
C
ATOM 238 C LYS A 66 -47.368 9.209 8.195 1.00 48.21
C
ATOM 239 O LYS A 66 -46.375 8.594 7.789 1.00 46.42
O
ATOM 240 CB LYS A 66 -49.232 8.602 6.608 1.00 49.03
C
ATOM 241 CG LYS A 66 -50.370 9.090 5.730 1.00 50.88
C
ATOM 242 CD LYS A 66 -51.366 7.968 5.433 1.00 55.28
C
ATOM 243 CE LYS A 66 -52.564 8.476 4.637 1.00 56.76
C
ATOM 244 NZ LYS A 66 -53.747 7.586 4.864 1.00 58.82
N1+
ATOM 245 N CYS A 67 -47.609 9.443 9.493 1.00 47.16
N

```
ATOM    246  CA  CYS A  67     -46.632   9.049  10.512  1.00 46.46
C
ATOM    247  C   CYS A  67     -47.132   7.949  11.451  1.00 46.18
C
ATOM    248  O   CYS A  67     -48.290   7.927  11.794  1.00 44.43
O
ATOM    249  CB  CYS A  67     -46.219  10.264  11.316  1.00 46.65
C
ATOM    250  SG  CYS A  67     -45.649  11.629  10.267  1.00 46.88
S
ATOM    251  N   PHE A  68     -46.222   7.079  11.892  1.00 45.61
N
ATOM    252  CA  PHE A  68     -46.579   5.903  12.690  1.00 46.42
C
ATOM    253  C   PHE A  68     -45.511   5.622  13.734  1.00 46.42
C
ATOM    254  O   PHE A  68     -44.322   5.927  13.526  1.00 45.88
O
ATOM    255  CB  PHE A  68     -46.702   4.650  11.811  1.00 45.22
C
ATOM    256  CG  PHE A  68     -47.752   4.742  10.734  1.00 46.23
C
ATOM    257  CD1 PHE A  68     -47.448   5.263   9.486  1.00 47.92
C
ATOM    258  CD2 PHE A  68     -49.027   4.232  10.942  1.00 47.86
C
ATOM    259  CE1 PHE A  68     -48.430   5.334   8.472  1.00 47.15
C
ATOM    260  CE2 PHE A  68     -50.008   4.311   9.950  1.00 48.04
C
ATOM    261  CZ  PHE A  68     -49.701   4.869   8.710  1.00 45.99
C
ATOM    262  N   GLU A  69     -45.930   5.049  14.856  1.00 46.14
N
ATOM    263  CA  GLU A  69     -44.989   4.376  15.740  1.00 46.83
C
ATOM    264  C   GLU A  69     -44.431   3.213  14.923  1.00 46.50
C
ATOM    265  O   GLU A  69     -45.198   2.507  14.260  1.00 46.52
O
ATOM    266  CB  GLU A  69     -45.710   3.844  17.004  1.00 46.97
C
ATOM    267  CG  GLU A  69     -46.207   4.976  17.895  1.00 47.48
C
```

ATOM 268 CD GLU A 69 -46.472 4.572 19.359 1.00 48.19
C
ATOM 269 OE1 GLU A 69 -46.473 5.481 20.210 1.00 52.07
O
ATOM 270 OE2 GLU A 69 -46.664 3.373 19.661 1.00 49.65
O
ATOM 271 N ILE A 70 -43.107 3.033 14.912 1.00 45.69
N
ATOM 272 CA ILE A 70 -42.524 1.840 14.258 1.00 45.30
C
ATOM 273 C ILE A 70 -41.520 1.195 15.189 1.00 46.13
C
ATOM 274 O ILE A 70 -40.780 1.898 15.880 1.00 47.46
O
ATOM 275 CB ILE A 70 -41.853 2.140 12.867 1.00 44.90
C
ATOM 276 CG1 ILE A 70 -40.650 3.095 13.017 1.00 44.83
C
ATOM 277 CG2 ILE A 70 -42.913 2.567 11.818 1.00 43.40
C
ATOM 278 CD1 ILE A 70 -39.867 3.376 11.726 1.00 43.45
C
ATOM 279 N SER A 71 -41.489 -0.131 15.239 1.00 45.88
N
ATOM 280 CA SER A 71 -40.589 -0.786 16.177 1.00 45.67
C
ATOM 281 C SER A 71 -39.645 -1.728 15.456 1.00 45.24
C
ATOM 282 O SER A 71 -40.072 -2.499 14.608 1.00 46.13
O
ATOM 283 CB SER A 71 -41.370 -1.518 17.290 1.00 45.90
C
ATOM 284 OG SER A 71 -42.030 -2.650 16.779 1.00 46.89
O
ATOM 285 N ASP A 72 -38.363 -1.648 15.800 1.00 44.71
N
ATOM 286 CA ASP A 72 -37.328 -2.515 15.242 1.00 44.52
C
ATOM 287 C ASP A 72 -37.626 -3.953 15.702 1.00 44.86
C
ATOM 288 O ASP A 72 -37.785 -4.196 16.900 1.00 44.21
O
ATOM 289 CB ASP A 72 -35.962 -2.026 15.744 1.00 44.40
C

```
ATOM    290  CG  ASP A  72      -34.797  -2.820  15.196  1.00 44.20
C
ATOM    291  OD1 ASP A  72      -33.784  -2.186  14.828  1.00 44.09
O
ATOM    292  OD2 ASP A  72      -34.866  -4.064  15.154  1.00 40.46
O
ATOM    293  N   ALA A  73      -37.711  -4.893  14.759  1.00 45.06
N
ATOM    294  CA  ALA A  73      -38.121  -6.268  15.082  1.00 45.96
C
ATOM    295  C   ALA A  73      -37.079  -7.029  15.900  1.00 46.55
C
ATOM    296  O   ALA A  73      -37.398  -8.043  16.546  1.00 46.52
O
ATOM    297  CB  ALA A  73      -38.452  -7.028  13.815  1.00 46.29
C
ATOM    298  N   ASP A  74      -35.835  -6.551  15.855  1.00 47.00
N
ATOM    299  CA  ASP A  74      -34.728  -7.178  16.580  1.00 47.62
C
ATOM    300  C   ASP A  74      -34.548  -6.580  17.984  1.00 47.23
C
ATOM    301  O   ASP A  74      -34.537  -7.313  18.971  1.00 47.09
O
ATOM    302  CB  ASP A  74      -33.429  -7.095  15.765  1.00 48.00
C
ATOM    303  CG  ASP A  74      -33.454  -7.989  14.521  1.00 51.14
C
ATOM    304  OD1 ASP A  74      -33.734  -9.201  14.663  1.00 53.44
O
ATOM    305  OD2 ASP A  74      -33.184  -7.488  13.396  1.00 53.83
O
ATOM    306  N   THR A  75      -34.429  -5.254  18.071  1.00 46.59
N
ATOM    307  CA  THR A  75      -34.176  -4.582  19.348  1.00 46.18
C
ATOM    308  C   THR A  75      -35.460  -4.163  20.070  1.00 45.84
C
ATOM    309  O   THR A  75      -35.421  -3.822  21.255  1.00 45.70
O
ATOM    310  CB  THR A  75      -33.350  -3.316  19.151  1.00 46.29
C
ATOM    311  OG1 THR A  75      -34.175  -2.344  18.515  1.00 46.03
O
```

```
ATOM    312  CG2 THR A  75     -32.124  -3.593  18.279  1.00 46.69
C
ATOM    313  N   LYS A  76     -36.585  -4.185  19.357  1.00 45.33
N
ATOM    314  CA  LYS A  76     -37.903  -3.813  19.916  1.00 45.42
C
ATOM    315  C   LYS A  76     -38.029  -2.321  20.227  1.00 45.60
C
ATOM    316  O   LYS A  76     -39.048  -1.866  20.748  1.00 44.75
O
ATOM    317  CB  LYS A  76     -38.260  -4.634  21.164  1.00 45.25
C
ATOM    318  CG  LYS A  76     -37.985  -6.130  21.072  1.00 45.70
C
ATOM    319  CD  LYS A  76     -38.663  -6.788  19.890  1.00 45.79
C
ATOM    320  CE  LYS A  76     -38.378  -8.259  19.904  1.00 45.63
C
ATOM    321  NZ  LYS A  76     -38.947  -8.915  18.716  1.00 47.95
N1+
ATOM    322  N   GLU A  77     -36.990  -1.566  19.899  1.00 46.20
N
ATOM    323  CA  GLU A  77     -37.018  -0.116  20.059  1.00 46.95
C
ATOM    324  C   GLU A  77     -38.098   0.548  19.213  1.00 46.28
C
ATOM    325  O   GLU A  77     -38.336   0.157  18.072  1.00 45.18
O
ATOM    326  CB  GLU A  77     -35.669   0.450  19.675  1.00 47.88
C
ATOM    327  CG  GLU A  77     -34.857   0.933  20.843  1.00 51.77
C
ATOM    328  CD  GLU A  77     -33.944   2.064  20.427  1.00 57.98
C
ATOM    329  OE1 GLU A  77     -32.930   1.769  19.742  1.00 58.39
O
ATOM    330  OE2 GLU A  77     -34.263   3.240  20.765  1.00 60.06
O
ATOM    331  N   VAL A  78     -38.729   1.578  19.773  1.00 46.41
N
ATOM    332  CA  VAL A  78     -39.800   2.289  19.082  1.00 45.64
C
ATOM    333  C   VAL A  78     -39.335   3.667  18.612  1.00 46.14
C
```

```
ATOM    334  O   VAL A  78     -38.672   4.431  19.349  1.00 45.75
O
ATOM    335  CB  VAL A  78     -41.098   2.366  19.951  1.00 46.18
C
ATOM    336  CG1 VAL A  78     -42.251   2.947  19.155  1.00 45.67
C
ATOM    337  CG2 VAL A  78     -41.496   0.963  20.440  1.00 44.99
C
ATOM    338  N   PHE A  79     -39.694   3.967  17.369  1.00 45.39
N
ATOM    339  CA  PHE A  79     -39.344   5.209  16.733  1.00 45.70
C
ATOM    340  C   PHE A  79     -40.633   5.815  16.174  1.00 44.59
C
ATOM    341  O   PHE A  79     -41.706   5.206  16.221  1.00 44.78
O
ATOM    342  CB  PHE A  79     -38.334   4.950  15.597  1.00 45.21
C
ATOM    343  CG  PHE A  79     -37.058   4.285  16.052  1.00 45.72
C
ATOM    344  CD1 PHE A  79     -36.943   2.910  16.037  1.00 47.12
C
ATOM    345  CD2 PHE A  79     -35.980   5.046  16.494  1.00 46.70
C
ATOM    346  CE1 PHE A  79     -35.760   2.271  16.457  1.00 48.74
C
ATOM    347  CE2 PHE A  79     -34.785   4.423  16.917  1.00 49.08
C
ATOM    348  CZ  PHE A  79     -34.684   3.036  16.894  1.00 48.08
C
ATOM    349  N   ALA A  80     -40.515   7.007  15.641  1.00 43.65
N
ATOM    350  CA  ALA A  80     -41.625   7.645  14.948  1.00 43.93
C
ATOM    351  C   ALA A  80     -41.233   7.530  13.494  1.00 44.47
C
ATOM    352  O   ALA A  80     -40.194   8.056  13.101  1.00 45.15
O
ATOM    353  CB  ALA A  80     -41.721   9.113  15.354  1.00 44.73
C
ATOM    354  N   GLY A  81     -42.027   6.821  12.706  1.00 44.45
N
ATOM    355  CA  GLY A  81     -41.746   6.687  11.272  1.00 46.95
C
```

```
ATOM    356  C   GLY A  81      -42.496   7.759  10.506  1.00 47.82
C
ATOM    357  O   GLY A  81      -43.688   7.944  10.712  1.00 47.58
O
ATOM    358  N   LYS A  82      -41.795   8.474   9.634  1.00 47.15
N
ATOM    359  CA  LYS A  82      -42.436   9.403   8.736  1.00 48.13
C
ATOM    360  C   LYS A  82      -42.403   8.779   7.334  1.00 47.90
C
ATOM    361  O   LYS A  82      -41.326   8.448   6.806  1.00 48.07
O
ATOM    362  CB  LYS A  82      -41.677  10.712   8.779  1.00 48.75
C
ATOM    363  CG  LYS A  82      -42.384  11.901   8.184  1.00 52.15
C
ATOM    364  CD  LYS A  82      -41.582  13.123   8.558  1.00 54.85
C
ATOM    365  CE  LYS A  82      -42.037  14.351   7.839  1.00 58.12
C
ATOM    366  NZ  LYS A  82      -41.105  15.475   8.217  1.00 59.22
N1+
ATOM    367  N   ILE A  83      -43.587   8.575   6.753  1.00 47.63
N
ATOM    368  CA  ILE A  83      -43.720   7.812   5.509  1.00 47.45
C
ATOM    369  C   ILE A  83      -44.295   8.681   4.385  1.00 47.40
C
ATOM    370  O   ILE A  83      -45.425   9.152   4.481  1.00 46.82
O
ATOM    371  CB  ILE A  83      -44.600   6.526   5.730  1.00 47.52
C
ATOM    372  CG1 ILE A  83      -43.994   5.673   6.860  1.00 47.98
C
ATOM    373  CG2 ILE A  83      -44.771   5.749   4.401  1.00 45.70
C
ATOM    374  CD1 ILE A  83      -44.765   4.365   7.194  1.00 47.39
C
ATOM    375  N   VAL A  84      -43.502   8.905   3.332  1.00 47.31
N
ATOM    376  CA  VAL A  84      -43.891   9.839   2.272  1.00 46.79
C
ATOM    377  C   VAL A  84      -44.081   9.094   0.970  1.00 46.57
C
```

```
ATOM    378  O   VAL A  84     -43.159   8.436   0.497  1.00 46.46
O
ATOM    379  CB  VAL A  84     -42.862  10.991   2.088  1.00 47.43
C
ATOM    380  CG1 VAL A  84     -43.344  11.972   1.020  1.00 47.72
C
ATOM    381  CG2 VAL A  84     -42.624  11.730   3.405  1.00 47.70
C
ATOM    382  N   PRO A  85     -45.286   9.179   0.389  1.00 46.30
N
ATOM    383  CA  PRO A  85     -45.458   8.452  -0.848  1.00 46.34
C
ATOM    384  C   PRO A  85     -44.788   9.195  -1.987  1.00 45.93
C
ATOM    385  O   PRO A  85     -44.948  10.421  -2.131  1.00 45.15
O
ATOM    386  CB  PRO A  85     -46.977   8.391  -1.046  1.00 45.73
C
ATOM    387  CG  PRO A  85     -47.546   9.452  -0.169  1.00 46.66
C
ATOM    388  CD  PRO A  85     -46.498   9.915   0.801  1.00 46.44
C
ATOM    389  N   LYS A  86     -44.069   8.437  -2.802  1.00 45.66
N
ATOM    390  CA  LYS A  86     -43.375   9.006  -3.956  1.00 46.27
C
ATOM    391  C   LYS A  86     -44.334   9.544  -5.004  1.00 45.29
C
ATOM    392  O   LYS A  86     -43.939  10.328  -5.844  1.00 45.35
O
ATOM    393  CB  LYS A  86     -42.391   7.999  -4.553  1.00 45.55
C
ATOM    394  CG  LYS A  86     -41.121   7.894  -3.714  1.00 47.84
C
ATOM    395  CD  LYS A  86     -40.212   6.808  -4.254  1.00 46.70
C
ATOM    396  CE  LYS A  86     -38.902   6.743  -3.488  1.00 47.48
C
ATOM    397  NZ  LYS A  86     -37.970   5.768  -4.163  1.00 48.10
N1+
ATOM    398  N   SER A  87     -45.596   9.121  -4.931  1.00 45.00
N
ATOM    399  CA  SER A  87     -46.644   9.601  -5.827  1.00 44.94
C
```

ATOM 400 C SER A 87 -46.934 11.066 -5.567 1.00 44.64
C
ATOM 401 O SER A 87 -47.480 11.749 -6.422 1.00 45.26
O
ATOM 402 CB SER A 87 -47.922 8.767 -5.674 1.00 45.32
C
ATOM 403 OG SER A 87 -48.583 9.083 -4.459 1.00 45.64
O
ATOM 404 N LEU A 88 -46.556 11.545 -4.387 1.00 45.00
N
ATOM 405 CA LEU A 88 -46.617 12.977 -4.074 1.00 45.23
C
ATOM 406 C LEU A 88 -45.281 13.691 -4.292 1.00 44.71
C
ATOM 407 O LEU A 88 -45.150 14.866 -3.944 1.00 45.05
O
ATOM 408 CB LEU A 88 -47.133 13.208 -2.633 1.00 45.50
C
ATOM 409 CG LEU A 88 -48.571 12.744 -2.304 1.00 46.88
C
ATOM 410 CD1 LEU A 88 -48.986 13.105 -0.874 1.00 47.72
C
ATOM 411 CD2 LEU A 88 -49.595 13.328 -3.281 1.00 49.58
C
ATOM 412 N LEU A 89 -44.293 12.987 -4.864 1.00 43.65
N
ATOM 413 CA LEU A 89 -42.946 13.560 -5.097 1.00 42.59
C
ATOM 414 C LEU A 89 -42.568 13.474 -6.575 1.00 42.28
C
ATOM 415 O LEU A 89 -41.435 13.154 -6.924 1.00 41.61
O
ATOM 416 CB LEU A 89 -41.878 12.869 -4.231 1.00 42.17
C
ATOM 417 CG LEU A 89 -41.990 12.949 -2.698 1.00 43.34
C
ATOM 418 CD1 LEU A 89 -41.036 11.984 -2.017 1.00 42.54
C
ATOM 419 CD2 LEU A 89 -41.745 14.383 -2.197 1.00 43.53
C
ATOM 420 N LEU A 90 -43.543 13.751 -7.437 1.00 41.22
N
ATOM 421 CA LEU A 90 -43.383 13.635 -8.890 1.00 42.23
C

```
ATOM    422  C   LEU A  90      -42.502  14.739  -9.488  1.00 41.61
C
ATOM    423  O   LEU A  90      -41.908  14.537 -10.543  1.00 41.58
O
ATOM    424  CB  LEU A  90      -44.762  13.646  -9.576  1.00 41.55
C
ATOM    425  CG  LEU A  90      -45.452  12.356 -10.017  1.00 43.78
C
ATOM    426  CD1 LEU A  90      -45.278  11.210  -9.053  1.00 44.46
C
ATOM    427  CD2 LEU A  90      -46.951  12.623 -10.285  1.00 43.15
C
ATOM    428  N   LYS A  91      -42.418  15.889  -8.810  1.00 40.93
N
ATOM    429  CA  LYS A  91      -41.679  17.035  -9.326  1.00 41.23
C
ATOM    430  C   LYS A  91      -40.254  17.052  -8.781  1.00 40.77
C
ATOM    431  O   LYS A  91      -40.059  16.904  -7.575  1.00 39.98
O
ATOM    432  CB  LYS A  91      -42.408  18.339  -8.972  1.00 40.98
C
ATOM    433  CG  LYS A  91      -43.821  18.406  -9.557  1.00 42.25
C
ATOM    434  CD  LYS A  91      -44.451  19.806  -9.431  1.00 42.98
C
ATOM    435  CE  LYS A  91      -44.719  20.185  -7.984  1.00 42.12
C
ATOM    436  NZ  LYS A  91      -45.820  21.186  -7.896  1.00 43.81
N1+
ATOM    437  N   PRO A  92      -39.245  17.193  -9.660  1.00 41.35
N
ATOM    438  CA  PRO A  92      -37.876  17.258  -9.115  1.00 41.81
C
ATOM    439  C   PRO A  92      -37.709  18.234  -7.930  1.00 42.23
C
ATOM    440  O   PRO A  92      -36.982  17.927  -7.010  1.00 43.06
O
ATOM    441  CB  PRO A  92      -37.045  17.699 -10.326  1.00 41.61
C
ATOM    442  CG  PRO A  92      -37.788  17.035 -11.484  1.00 41.43
C
ATOM    443  CD  PRO A  92      -39.243  17.230 -11.141  1.00 41.36
C
```

```
ATOM    444  N   HIS A  93      -38.373  19.386  -7.968  1.00 42.49
N
ATOM    445  CA  HIS A  93      -38.300  20.375  -6.887  1.00 42.84
C
ATOM    446  C   HIS A  93      -38.784  19.769  -5.563  1.00 42.97
C
ATOM    447  O   HIS A  93      -38.191  20.016  -4.527  1.00 42.70
O
ATOM    448  CB  HIS A  93      -39.120  21.616  -7.285  1.00 43.07
C
ATOM    449  CG  HIS A  93      -39.114  22.735  -6.285  1.00 42.22
C
ATOM    450  ND1 HIS A  93      -37.989  23.117  -5.583  1.00 44.56
N
ATOM    451  CD2 HIS A  93      -40.089  23.610  -5.930  1.00 42.99
C
ATOM    452  CE1 HIS A  93      -38.282  24.153  -4.812  1.00 43.97
C
ATOM    453  NE2 HIS A  93      -39.544  24.485  -5.020  1.00 41.38
N
ATOM    454  N   GLN A  94      -39.837  18.947  -5.589  1.00 43.87
N
ATOM    455  CA  GLN A  94      -40.273  18.274  -4.353  1.00 43.54
C
ATOM    456  C   GLN A  94      -39.244  17.288  -3.830  1.00 43.98
C
ATOM    457  O   GLN A  94      -39.005  17.217  -2.613  1.00 43.11
O
ATOM    458  CB  GLN A  94      -41.632  17.580  -4.516  1.00 44.79
C
ATOM    459  CG  GLN A  94      -42.748  18.514  -4.895  1.00 45.48
C
ATOM    460  CD  GLN A  94      -43.992  17.769  -5.400  1.00 49.82
C
ATOM    461  OE1 GLN A  94      -43.918  16.907  -6.294  1.00 46.88
O
ATOM    462  NE2 GLN A  94      -45.145  18.121  -4.838  1.00 49.69
N
ATOM    463  N   ARG A  95      -38.648  16.508  -4.728  1.00 43.86
N
ATOM    464  CA  ARG A  95      -37.638  15.538  -4.323  1.00 44.81
C
ATOM    465  C   ARG A  95      -36.415  16.230  -3.728  1.00 45.34
C
```

```
ATOM    466  O   ARG A  95     -35.824  15.736  -2.754  1.00 46.05
O
ATOM    467  CB  ARG A  95     -37.226  14.655  -5.510  1.00 44.51
C
ATOM    468  CG  ARG A  95     -38.355  13.778  -5.979  1.00 46.37
C
ATOM    469  CD  ARG A  95     -38.080  13.291  -7.380  1.00 50.20
C
ATOM    470  NE  ARG A  95     -37.449  11.965  -7.352  1.00 55.65
N
ATOM    471  CZ  ARG A  95     -38.122  10.817  -7.272  1.00 55.46
C
ATOM    472  NH1 ARG A  95     -39.454  10.811  -7.212  1.00 54.31
N
ATOM    473  NH2 ARG A  95     -37.461   9.677  -7.261  1.00 53.99
N
ATOM    474  N   GLU A  96     -36.035  17.359  -4.323  1.00 45.39
N
ATOM    475  CA  GLU A  96     -34.887  18.122  -3.852  1.00 46.33
C
ATOM    476  C   GLU A  96     -35.143  18.688  -2.446  1.00 46.18
C
ATOM    477  O   GLU A  96     -34.256  18.660  -1.604  1.00 46.59
O
ATOM    478  CB  GLU A  96     -34.548  19.218  -4.853  1.00 47.12
C
ATOM    479  CG  GLU A  96     -33.789  18.650  -6.043  1.00 50.00
C
ATOM    480  CD  GLU A  96     -33.829  19.548  -7.260  1.00 55.49
C
ATOM    481  OE1 GLU A  96     -33.550  19.030  -8.377  1.00 56.73
O
ATOM    482  OE2 GLU A  96     -34.142  20.756  -7.098  1.00 56.34
O
ATOM    483  N   LYS A  97     -36.367  19.143  -2.180  1.00 45.68
N
ATOM    484  CA  LYS A  97     -36.754  19.610  -0.842  1.00 45.73
C
ATOM    485  C   LYS A  97     -36.733  18.477   0.195  1.00 46.45
C
ATOM    486  O   LYS A  97     -36.212  18.636   1.313  1.00 46.64
O
ATOM    487  CB  LYS A  97     -38.125  20.326  -0.884  1.00 44.90
C
```

```
ATOM    488  CG  LYS A  97      -38.068  21.685  -1.658  1.00 45.90
C
ATOM    489  CD  LYS A  97      -39.353  22.533  -1.546  1.00 45.58
C
ATOM    490  CE  LYS A  97      -40.445  21.993  -2.457  1.00 46.49
C
ATOM    491  NZ  LYS A  97      -41.671  22.852  -2.547  1.00 48.17
N1+
ATOM    492  N   MET A  98      -37.261  17.320  -0.183  1.00 45.83
N
ATOM    493  CA  MET A  98      -37.225  16.150   0.680  1.00 46.23
C
ATOM    494  C   MET A  98      -35.786  15.676   0.939  1.00 45.32
C
ATOM    495  O   MET A  98      -35.444  15.312   2.081  1.00 45.14
O
ATOM    496  CB  MET A  98      -38.064  15.045   0.052  1.00 47.22
C
ATOM    497  CG  MET A  98      -37.924  13.668   0.665  1.00 51.32
C
ATOM    498  SD  MET A  98      -39.285  13.157   1.719  1.00 59.46
S
ATOM    499  CE  MET A  98      -38.780  13.890   3.273  1.00 60.30
C
ATOM    500  N   SER A  99      -34.967  15.674  -0.111  0.50 44.95
N
ATOM    501  CA  SER A  99      -33.551  15.316  -0.020  0.50 44.46
C
ATOM    502  C   SER A  99      -32.788  16.217   0.951  0.50 44.21
C
ATOM    503  O   SER A  99      -32.030  15.737   1.801  0.50 44.39
O
ATOM    504  CB  SER A  99      -32.905  15.412  -1.402  0.50 44.88
C
ATOM    505  OG  SER A  99      -31.540  15.043  -1.357  0.50 44.49
O
ATOM    506  N   MET A 100      -32.965  17.525   0.801  1.00 43.97
N
ATOM    507  CA  MET A 100      -32.313  18.504   1.666  1.00 43.19
C
ATOM    508  C   MET A 100      -32.722  18.379   3.145  1.00 41.97
C
ATOM    509  O   MET A 100      -31.852  18.495   4.028  1.00 44.38
O
```

```
ATOM    510  CB  MET A 100     -32.554  19.914   1.120  1.00 44.64
C
ATOM    511  CG  MET A 100     -31.931  21.015   1.926  1.00 46.17
C
ATOM    512  SD  MET A 100     -30.133  20.991   1.819  1.00 51.04
S
ATOM    513  CE  MET A 100     -29.806  21.620   0.171  1.00 53.90
C
ATOM    514  N   GLU A 101     -34.007  18.163   3.435  1.00 37.59
N
ATOM    515  CA  GLU A 101     -34.454  17.894   4.803  1.00 35.03
C
ATOM    516  C   GLU A 101     -33.652  16.727   5.410  1.00 33.17
C
ATOM    517  O   GLU A 101     -33.116  16.831   6.513  1.00 32.12
O
ATOM    518  CB  GLU A 101     -35.963  17.526   4.863  1.00 33.90
C
ATOM    519  CG  GLU A 101     -36.386  17.150   6.302  1.00 35.73
C
ATOM    520  CD  GLU A 101     -37.888  16.879   6.510  1.00 36.35
C
ATOM    521  OE1 GLU A 101     -38.228  16.397   7.618  1.00 40.98
O
ATOM    522  OE2 GLU A 101     -38.694  17.112   5.587  1.00 34.01
O
ATOM    523  N   ILE A 102     -33.626  15.604   4.698  1.00 30.18
N
ATOM    524  CA  ILE A 102     -32.865  14.441   5.136  1.00 30.07
C
ATOM    525  C   ILE A 102     -31.381  14.753   5.292  1.00 28.62
C
ATOM    526  O   ILE A 102     -30.813  14.455   6.304  1.00 28.48
O
ATOM    527  CB  ILE A 102     -33.080  13.222   4.190  1.00 29.83
C
ATOM    528  CG1 ILE A 102     -34.551  12.759   4.274  1.00 29.40
C
ATOM    529  CG2 ILE A 102     -32.047  12.111   4.514  1.00 30.91
C
ATOM    530  CD1 ILE A 102     -35.012  11.961   3.005  1.00 30.71
C
ATOM    531  N   SER A 103     -30.774  15.373   4.288  1.00 29.98
N
```

```
ATOM    532  CA  SER A 103     -29.369  15.769   4.331  1.00 31.20
C
ATOM    533  C   SER A 103     -29.016  16.647   5.562  1.00 30.77
C
ATOM    534  O   SER A 103     -27.986  16.449   6.210  1.00 31.47
O
ATOM    535  CB  SER A 103     -29.009  16.472   3.026  1.00 31.23
C
ATOM    536  OG  SER A 103     -27.778  17.170   3.111  1.00 35.90
O
ATOM    537  N   ILE A 104     -29.872  17.603   5.893  1.00 28.85
N
ATOM    538  CA  ILE A 104     -29.599  18.458   7.049  1.00 26.91
C
ATOM    539  C   ILE A 104     -29.833  17.689   8.338  1.00 26.73
C
ATOM    540  O   ILE A 104     -28.973  17.667   9.210  1.00 25.30
O
ATOM    541  CB  ILE A 104     -30.424  19.750   7.007  1.00 27.62
C
ATOM    542  CG1 ILE A 104     -29.952  20.656   5.872  1.00 27.83
C
ATOM    543  CG2 ILE A 104     -30.319  20.511   8.364  1.00 27.71
C
ATOM    544  CD1 ILE A 104     -30.946  21.771   5.526  1.00 24.09
C
ATOM    545  N   HIS A 105     -30.993  17.031   8.473  1.00 26.03
N
ATOM    546  CA  HIS A 105     -31.348  16.430   9.754  1.00 25.65
C
ATOM    547  C   HIS A 105     -30.402  15.257  10.076  1.00 27.61
C
ATOM    548  O   HIS A 105     -30.049  15.019  11.244  1.00 27.48
O
ATOM    549  CB  HIS A 105     -32.823  15.960   9.733  1.00 25.89
C
ATOM    550  CG  HIS A 105     -33.417  15.709  11.095  1.00 25.32
C
ATOM    551  ND1 HIS A 105     -34.777  15.506  11.289  1.00 23.24
N
ATOM    552  CD2 HIS A 105     -32.845  15.648  12.321  1.00 21.60
C
ATOM    553  CE1 HIS A 105     -35.007  15.310  12.579  1.00 22.08
C
```

```
ATOM    554  NE2 HIS A 105     -33.855  15.400  13.232  1.00 22.44
N
ATOM    555  N   ARG A 106     -29.998  14.500   9.063  1.00 28.75
N
ATOM    556  CA  ARG A 106     -29.112  13.353   9.338  1.00 30.49
C
ATOM    557  C   ARG A 106     -27.739  13.801   9.865  1.00 30.45
C
ATOM    558  O   ARG A 106     -27.035  13.024  10.511  1.00 31.80
O
ATOM    559  CB  ARG A 106     -28.937  12.492   8.087  1.00 31.24
C
ATOM    560  CG  ARG A 106     -27.741  12.884   7.272  1.00 35.90
C
ATOM    561  CD  ARG A 106     -27.882  12.513   5.806  1.00 44.21
C
ATOM    562  NE  ARG A 106     -27.738  11.087   5.577  1.00 50.36
N
ATOM    563  CZ  ARG A 106     -27.235  10.560   4.457  1.00 55.04
C
ATOM    564  NH1 ARG A 106     -26.808  11.340   3.465  1.00 56.61
N
ATOM    565  NH2 ARG A 106     -27.153   9.243   4.334  1.00 55.96
N
ATOM    566  N   SER A 107     -27.358  15.040   9.588  1.00 31.71
N
ATOM    567  CA  SER A 107     -26.053  15.571  10.020  1.00 31.47
C
ATOM    568  C   SER A 107     -26.021  16.077  11.461  1.00 32.34
C
ATOM    569  O   SER A 107     -24.983  16.535  11.927  1.00 32.33
O
ATOM    570  CB  SER A 107     -25.595  16.676   9.081  1.00 32.51
C
ATOM    571  OG  SER A 107     -26.246  17.924   9.309  1.00 33.94
O
ATOM    572  N   LEU A 108     -27.149  16.008  12.171  1.00 31.95
N
ATOM    573  CA  LEU A 108     -27.261  16.696  13.460  1.00 31.92
C
ATOM    574  C   LEU A 108     -27.411  15.679  14.567  1.00 31.44
C
ATOM    575  O   LEU A 108     -28.023  14.635  14.355  1.00 31.79
O
```

```
ATOM    576  CB  LEU A 108     -28.471  17.642  13.475  1.00 30.99
C
ATOM    577  CG  LEU A 108     -28.616  18.723  12.392  1.00 32.29
C
ATOM    578  CD1 LEU A 108     -30.040  19.251  12.439  1.00 31.03
C
ATOM    579  CD2 LEU A 108     -27.632  19.893  12.537  1.00 30.57
C
ATOM    580  N   ALA A 109     -26.848  15.984  15.740  1.00 31.08
N
ATOM    581  CA  ALA A 109     -27.014  15.140  16.942  1.00 30.38
C
ATOM    582  C   ALA A 109     -26.849  15.995  18.178  1.00 30.88
C
ATOM    583  O   ALA A 109     -25.771  16.588  18.418  1.00 30.65
O
ATOM    584  CB  ALA A 109     -26.027  13.956  16.949  1.00 31.69
C
ATOM    585  N   HIS A 110     -27.933  16.141  18.936  1.00 29.09
N
ATOM    586  CA  HIS A 110     -27.909  17.054  20.077  1.00 29.22
C
ATOM    587  C   HIS A 110     -29.083  16.748  20.976  1.00 29.60
C
ATOM    588  O   HIS A 110     -30.142  16.344  20.492  1.00 29.81
O
ATOM    589  CB  HIS A 110     -27.895  18.532  19.632  1.00 28.02
C
ATOM    590  CG  HIS A 110     -27.737  19.505  20.765  1.00 29.94
C
ATOM    591  ND1 HIS A 110     -28.802  19.939  21.529  1.00 29.28
N
ATOM    592  CD2 HIS A 110     -26.640  20.133  21.259  1.00 29.13
C
ATOM    593  CE1 HIS A 110     -28.365  20.775  22.460  1.00 30.44
C
ATOM    594  NE2 HIS A 110     -27.056  20.913  22.315  1.00 30.34
N
ATOM    595  N   GLN A 111     -28.874  16.922  22.280  1.00 29.61
N
ATOM    596  CA  GLN A 111     -29.873  16.613  23.293  1.00 31.21
C
ATOM    597  C   GLN A 111     -31.219  17.265  22.981  1.00 28.79
C
```

ATOM 598 O GLN A 111 -32.268 16.669 23.255 1.00 29.84
O
ATOM 599 CB GLN A 111 -29.390 17.070 24.674 1.00 30.64
C
ATOM 600 CG GLN A 111 -30.273 16.566 25.831 1.00 34.74
C
ATOM 601 CD GLN A 111 -29.777 17.100 27.182 1.00 36.40
C
ATOM 602 OE1 GLN A 111 -29.184 18.186 27.261 1.00 41.82
O
ATOM 603 NE2 GLN A 111 -30.030 16.348 28.244 1.00 42.52
N
ATOM 604 N HIS A 112 -31.179 18.471 22.407 1.00 26.89
N
ATOM 605 CA HIS A 112 -32.424 19.215 22.128 1.00 25.24
C
ATOM 606 C HIS A 112 -32.818 19.282 20.668 1.00 24.13
C
ATOM 607 O HIS A 112 -33.493 20.208 20.256 1.00 24.69
O
ATOM 608 CB HIS A 112 -32.402 20.578 22.830 1.00 25.76
C
ATOM 609 CG HIS A 112 -32.309 20.447 24.318 1.00 25.92
C
ATOM 610 ND1 HIS A 112 -33.204 19.697 25.047 1.00 24.11
N
ATOM 611 CD2 HIS A 112 -31.375 20.886 25.199 1.00 25.56
C
ATOM 612 CE1 HIS A 112 -32.844 19.700 26.323 1.00 26.79
C
ATOM 613 NE2 HIS A 112 -31.744 20.428 26.440 1.00 25.44
N
ATOM 614 N VAL A 113 -32.382 18.287 19.885 1.00 24.11
N
ATOM 615 CA VAL A 113 -32.765 18.161 18.487 1.00 23.46
C
ATOM 616 C VAL A 113 -33.310 16.749 18.327 1.00 24.10
C
ATOM 617 O VAL A 113 -32.742 15.782 18.873 1.00 22.75
O
ATOM 618 CB VAL A 113 -31.588 18.418 17.512 1.00 23.88
C
ATOM 619 CG1 VAL A 113 -31.988 18.082 16.047 1.00 24.75
C

```
ATOM    620  CG2 VAL A 113     -31.094  19.854  17.612  1.00 24.74
C
ATOM    621  N   VAL A 114     -34.415  16.617  17.603  1.00 23.09
N
ATOM    622  CA  VAL A 114     -35.008  15.306  17.371  1.00 25.24
C
ATOM    623  C   VAL A 114     -33.934  14.350  16.781  1.00 26.43
C
ATOM    624  O   VAL A 114     -33.246  14.710  15.826  1.00 25.91
O
ATOM    625  CB  VAL A 114     -36.204  15.400  16.391  1.00 25.68
C
ATOM    626  CG1 VAL A 114     -36.570  14.006  15.834  1.00 24.10
C
ATOM    627  CG2 VAL A 114     -37.371  16.021  17.084  1.00 25.56
C
ATOM    628  N   GLY A 115     -33.789  13.165  17.380  1.00 26.42
N
ATOM    629  CA  GLY A 115     -32.830  12.175  16.882  1.00 27.60
C
ATOM    630  C   GLY A 115     -33.202  11.648  15.507  1.00 28.59
C
ATOM    631  O   GLY A 115     -34.356  11.246  15.268  1.00 27.24
O
ATOM    632  N   PHE A 116     -32.227  11.634  14.602  1.00 29.34
N
ATOM    633  CA  PHE A 116     -32.414  11.076  13.265  1.00 30.48
C
ATOM    634  C   PHE A 116     -31.821   9.655  13.298  1.00 32.94
C
ATOM    635  O   PHE A 116     -30.631   9.491  13.571  1.00 33.43
O
ATOM    636  CB  PHE A 116     -31.670  11.943  12.212  1.00 30.62
C
ATOM    637  CG  PHE A 116     -32.001  11.584  10.787  1.00 29.95
C
ATOM    638  CD1 PHE A 116     -33.079  12.189  10.134  1.00 30.16
C
ATOM    639  CD2 PHE A 116     -31.277  10.584  10.110  1.00 30.70
C
ATOM    640  CE1 PHE A 116     -33.421  11.851   8.813  1.00 31.36
C
ATOM    641  CE2 PHE A 116     -31.606  10.229   8.785  1.00 29.99
C
```

```
ATOM    642  CZ  PHE A 116     -32.676  10.858   8.138  1.00 30.95
C
ATOM    643  N   HIS A 117     -32.634   8.636  13.042  1.00 34.27
N
ATOM    644  CA  HIS A 117     -32.135   7.265  13.158  1.00 37.05
C
ATOM    645  C   HIS A 117     -32.083   6.490  11.826  1.00 37.84
C
ATOM    646  O   HIS A 117     -31.728   5.312  11.815  1.00 39.78
O
ATOM    647  CB  HIS A 117     -32.929   6.508  14.226  1.00 37.37
C
ATOM    648  CG  HIS A 117     -32.753   7.087  15.603  1.00 40.80
C
ATOM    649  ND1 HIS A 117     -31.622   6.862  16.366  1.00 42.80
N
ATOM    650  CD2 HIS A 117     -33.533   7.933  16.326  1.00 40.62
C
ATOM    651  CE1 HIS A 117     -31.726   7.525  17.507  1.00 43.77
C
ATOM    652  NE2 HIS A 117     -32.870   8.192  17.504  1.00 39.95
N
ATOM    653  N   GLY A 118     -32.432   7.128  10.719  1.00 37.20
N
ATOM    654  CA  GLY A 118     -32.259   6.484   9.422  1.00 37.42
C
ATOM    655  C   GLY A 118     -33.283   6.896   8.402  1.00 36.84
C
ATOM    656  O   GLY A 118     -34.296   7.502   8.720  1.00 36.58
O
ATOM    657  N   PHE A 119     -33.019   6.560   7.151  1.00 36.23
N
ATOM    658  CA  PHE A 119     -34.021   6.723   6.125  1.00 36.43
C
ATOM    659  C   PHE A 119     -33.746   5.679   5.036  1.00 36.42
C
ATOM    660  O   PHE A 119     -32.613   5.221   4.871  1.00 35.13
O
ATOM    661  CB  PHE A 119     -33.997   8.130   5.523  1.00 37.10
C
ATOM    662  CG  PHE A 119     -32.958   8.294   4.477  1.00 38.63
C
ATOM    663  CD1 PHE A 119     -33.296   8.198   3.132  1.00 39.98
C
```

ATOM 664 CD2 PHE A 119 -31.622 8.458 4.840 1.00 40.72
C
ATOM 665 CE1 PHE A 119 -32.319 8.287 2.151 1.00 41.44
C
ATOM 666 CE2 PHE A 119 -30.622 8.563 3.865 1.00 41.89
C
ATOM 667 CZ PHE A 119 -30.980 8.462 2.515 1.00 41.56
C
ATOM 668 N PHE A 120 -34.783 5.310 4.309 1.00 36.08
N
ATOM 669 CA PHE A 120 -34.609 4.344 3.247 1.00 37.53
C
ATOM 670 C PHE A 120 -35.848 4.443 2.399 1.00 38.21
C
ATOM 671 O PHE A 120 -36.775 5.196 2.717 1.00 37.49
O
ATOM 672 CB PHE A 120 -34.303 2.917 3.799 1.00 37.65
C
ATOM 673 CG PHE A 120 -35.290 2.435 4.809 1.00 37.85
C
ATOM 674 CD1 PHE A 120 -36.346 1.626 4.421 1.00 35.78
C
ATOM 675 CD2 PHE A 120 -35.179 2.813 6.145 1.00 39.15
C
ATOM 676 CE1 PHE A 120 -37.289 1.198 5.341 1.00 39.86
C
ATOM 677 CE2 PHE A 120 -36.137 2.391 7.085 1.00 39.78
C
ATOM 678 CZ PHE A 120 -37.184 1.586 6.679 1.00 37.68
C
ATOM 679 N GLU A 121 -35.854 3.758 1.267 1.00 39.29
N
ATOM 680 CA GLU A 121 -36.953 3.919 0.353 1.00 41.46
C
ATOM 681 C GLU A 121 -37.244 2.624 -0.394 1.00 42.61
C
ATOM 682 O GLU A 121 -36.418 1.710 -0.430 1.00 42.76
O
ATOM 683 CB GLU A 121 -36.671 5.084 -0.621 1.00 41.27
C
ATOM 684 CG GLU A 121 -35.339 4.992 -1.366 1.00 42.50
C
ATOM 685 CD GLU A 121 -34.948 6.310 -2.030 1.00 42.05
C

ATOM 686 OE1 GLU A 121 -35.749 6.859 -2.812 1.00 41.68
O
ATOM 687 OE2 GLU A 121 -33.833 6.800 -1.764 1.00 44.29
O
ATOM 688 N ASP A 122 -38.449 2.525 -0.927 1.00 43.70
N
ATOM 689 CA ASP A 122 -38.714 1.523 -1.947 1.00 45.50
C
ATOM 690 C ASP A 122 -39.202 2.261 -3.198 1.00 46.24
C
ATOM 691 O ASP A 122 -38.982 3.477 -3.323 1.00 46.41
O
ATOM 692 CB ASP A 122 -39.648 0.411 -1.435 1.00 45.07
C
ATOM 693 CG ASP A 122 -41.018 0.898 -1.065 1.00 46.49
C
ATOM 694 OD1 ASP A 122 -41.394 2.015 -1.447 1.00 49.09
O
ATOM 695 OD2 ASP A 122 -41.755 0.141 -0.395 1.00 48.99
O
ATOM 696 N ASN A 123 -39.853 1.567 -4.126 1.00 46.87
N
ATOM 697 CA ASN A 123 -40.249 2.240 -5.358 1.00 46.62
C
ATOM 698 C ASN A 123 -41.460 3.128 -5.151 1.00 45.47
C
ATOM 699 O ASN A 123 -41.689 4.044 -5.944 1.00 45.58
O
ATOM 700 CB ASN A 123 -40.422 1.254 -6.525 1.00 47.99
C
ATOM 701 CG ASN A 123 -39.090 0.638 -6.976 1.00 51.22
C
ATOM 702 OD1 ASN A 123 -39.012 -0.564 -7.246 1.00 56.31
O
ATOM 703 ND2 ASN A 123 -38.034 1.464 -7.056 1.00 54.58
N
ATOM 704 N ASP A 124 -42.182 2.902 -4.048 1.00 44.15
N
ATOM 705 CA ASP A 124 -43.399 3.664 -3.730 1.00 42.41
C
ATOM 706 C ASP A 124 -43.341 4.676 -2.547 1.00 40.52
C
ATOM 707 O ASP A 124 -44.161 5.603 -2.505 1.00 39.25
O

ATOM 708 CB ASP A 124 -44.564 2.708 -3.484 1.00 43.32
C
ATOM 709 CG ASP A 124 -44.724 1.685 -4.591 1.00 46.32
C
ATOM 710 OD1 ASP A 124 -44.402 0.504 -4.328 1.00 51.12
O
ATOM 711 OD2 ASP A 124 -45.147 2.070 -5.709 1.00 47.72
O
ATOM 712 N PHE A 125 -42.415 4.493 -1.603 1.00 38.63
N
ATOM 713 CA PHE A 125 -42.333 5.370 -0.400 1.00 37.80
C
ATOM 714 C PHE A 125 -40.918 5.767 0.014 1.00 36.85
C
ATOM 715 O PHE A 125 -39.955 5.029 -0.226 1.00 37.71
O
ATOM 716 CB PHE A 125 -43.031 4.724 0.829 1.00 37.56
C
ATOM 717 CG PHE A 125 -44.469 4.358 0.602 1.00 37.94
C
ATOM 718 CD1 PHE A 125 -44.823 3.052 0.264 1.00 39.30
C
ATOM 719 CD2 PHE A 125 -45.461 5.304 0.721 1.00 37.67
C
ATOM 720 CE1 PHE A 125 -46.152 2.705 0.044 1.00 39.02
C
ATOM 721 CE2 PHE A 125 -46.817 4.982 0.490 1.00 39.61
C
ATOM 722 CZ PHE A 125 -47.162 3.684 0.154 1.00 38.42
C
ATOM 723 N VAL A 126 -40.801 6.925 0.672 1.00 34.80
N
ATOM 724 CA VAL A 126 -39.604 7.277 1.425 1.00 33.76
C
ATOM 725 C VAL A 126 -39.949 7.044 2.900 1.00 33.07
C
ATOM 726 O VAL A 126 -40.998 7.466 3.347 1.00 32.95
O
ATOM 727 CB VAL A 126 -39.184 8.771 1.206 1.00 33.34
C
ATOM 728 CG1 VAL A 126 -37.889 9.091 1.961 1.00 35.08
C
ATOM 729 CG2 VAL A 126 -39.016 9.053 -0.285 1.00 34.08
C

ATOM 730 N PHE A 127 -39.074 6.364 3.624 1.00 32.05
N
ATOM 731 CA PHE A 127 -39.260 6.083 5.039 1.00 31.82
C
ATOM 732 C PHE A 127 -38.171 6.799 5.823 1.00 31.38
C
ATOM 733 O PHE A 127 -36.982 6.560 5.601 1.00 31.02
O
ATOM 734 CB PHE A 127 -39.174 4.570 5.330 1.00 32.62
C
ATOM 735 CG PHE A 127 -40.082 3.731 4.468 1.00 33.09
C
ATOM 736 CD1 PHE A 127 -39.559 3.007 3.397 1.00 35.65
C
ATOM 737 CD2 PHE A 127 -41.442 3.675 4.722 1.00 34.97
C
ATOM 738 CE1 PHE A 127 -40.386 2.235 2.588 1.00 35.84
C
ATOM 739 CE2 PHE A 127 -42.289 2.895 3.932 1.00 35.40
C
ATOM 740 CZ PHE A 127 -41.755 2.174 2.862 1.00 35.77
C
ATOM 741 N VAL A 128 -38.580 7.646 6.763 1.00 30.16
N
ATOM 742 CA VAL A 128 -37.644 8.350 7.645 1.00 30.12
C
ATOM 743 C VAL A 128 -37.861 7.916 9.101 1.00 30.17
C
ATOM 744 O VAL A 128 -38.990 7.896 9.583 1.00 30.36
O
ATOM 745 CB VAL A 128 -37.798 9.885 7.478 1.00 30.56
C
ATOM 746 CG1 VAL A 128 -36.726 10.613 8.254 1.00 31.33
C
ATOM 747 CG2 VAL A 128 -37.688 10.248 5.988 1.00 30.77
C
ATOM 748 N VAL A 129 -36.785 7.547 9.772 1.00 29.37
N
ATOM 749 CA VAL A 129 -36.863 7.000 11.126 1.00 30.20
C
ATOM 750 C VAL A 129 -36.367 8.030 12.139 1.00 29.49
C
ATOM 751 O VAL A 129 -35.191 8.401 12.163 1.00 30.05
O

```
ATOM    752  CB  VAL A 129     -36.092   5.669  11.265  1.00 30.19
C
ATOM    753  CG1 VAL A 129     -36.244   5.100  12.677  1.00 33.23
C
ATOM    754  CG2 VAL A 129     -36.597   4.653  10.221  1.00 29.48
C
ATOM    755  N   LEU A 130     -37.282   8.473  12.990  1.00 28.18
N
ATOM    756  CA  LEU A 130     -36.958   9.543  13.926  1.00 27.92
C
ATOM    757  C   LEU A 130     -37.205   9.178  15.372  1.00 28.37
C
ATOM    758  O   LEU A 130     -37.958   8.253  15.652  1.00 28.61
O
ATOM    759  CB  LEU A 130     -37.785  10.772  13.569  1.00 27.00
C
ATOM    760  CG  LEU A 130     -37.687  11.333  12.147  1.00 26.88
C
ATOM    761  CD1 LEU A 130     -38.784  12.371  11.896  1.00 27.31
C
ATOM    762  CD2 LEU A 130     -36.309  11.912  11.887  1.00 27.72
C
ATOM    763  N   GLU A 131     -36.585   9.924  16.285  1.00 28.39
N
ATOM    764  CA  GLU A 131     -36.803   9.777  17.731  1.00 29.36
C
ATOM    765  C   GLU A 131     -38.291   9.895  18.045  1.00 30.02
C
ATOM    766  O   GLU A 131     -38.919  10.849  17.637  1.00 29.27
O
ATOM    767  CB  GLU A 131     -36.006  10.853  18.467  1.00 29.71
C
ATOM    768  CG  GLU A 131     -36.206  10.861  19.958  1.00 30.18
C
ATOM    769  CD  GLU A 131     -35.232  11.715  20.695  1.00 33.38
C
ATOM    770  OE1 GLU A 131     -35.155  11.526  21.923  1.00 37.02
O
ATOM    771  OE2 GLU A 131     -34.560  12.589  20.098  1.00 32.87
O
ATOM    772  N   LEU A 132     -38.892   8.899  18.702  1.00 29.88
N
ATOM    773  CA  LEU A 132     -40.288   9.044  19.109  1.00 29.50
C
```

```
ATOM    774  C   LEU A 132     -40.337   9.950  20.338  1.00 29.47
C
ATOM    775  O   LEU A 132     -39.594   9.718  21.301  1.00 29.26
O
ATOM    776  CB  LEU A 132     -40.945   7.697  19.474  1.00 29.70
C
ATOM    777  CG  LEU A 132     -42.427   7.741  19.898  1.00 29.46
C
ATOM    778  CD1 LEU A 132     -43.392   8.051  18.731  1.00 31.36
C
ATOM    779  CD2 LEU A 132     -42.829   6.402  20.575  1.00 31.33
C
ATOM    780  N   CYS A 133     -41.206  10.967  20.292  1.00 28.20
N
ATOM    781  CA  CYS A 133     -41.337  11.943  21.384  1.00 28.30
C
ATOM    782  C   CYS A 133     -42.717  11.757  21.984  1.00 28.61
C
ATOM    783  O   CYS A 133     -43.694  12.222  21.440  1.00 28.23
O
ATOM    784  CB  CYS A 133     -41.161  13.361  20.848  1.00 26.53
C
ATOM    785  SG  CYS A 133     -39.443  13.626  20.228  1.00 27.89
S
ATOM    786  N   ARG A 134     -42.775  11.041  23.093  1.00 30.22
N
ATOM    787  CA  ARG A 134     -44.035  10.480  23.555  1.00 31.99
C
ATOM    788  C   ARG A 134     -44.992  11.508  24.162  1.00 31.37
C
ATOM    789  O   ARG A 134     -46.173  11.200  24.345  1.00 31.12
O
ATOM    790  CB  ARG A 134     -43.792   9.315  24.524  1.00 32.43
C
ATOM    791  CG  ARG A 134     -43.069   8.112  23.878  1.00 34.50
C
ATOM    792  CD  ARG A 134     -42.963   6.931  24.866  1.00 36.22
C
ATOM    793  NE  ARG A 134     -42.472   5.682  24.247  1.00 40.61
N
ATOM    794  CZ  ARG A 134     -43.259   4.750  23.697  1.00 45.20
C
ATOM    795  NH1 ARG A 134     -44.581   4.903  23.659  1.00 46.62
N
```

```
ATOM    796  NH2 ARG A 134     -42.724   3.643  23.181  1.00 47.74
N
ATOM    797  N   ARG A 135     -44.523  12.728  24.424  1.00 30.07
N
ATOM    798  CA  ARG A 135     -45.437  13.761  24.934  1.00 29.57
C
ATOM    799  C   ARG A 135     -45.824  14.791  23.868  1.00 28.98
C
ATOM    800  O   ARG A 135     -46.249  15.902  24.177  1.00 29.24
O
ATOM    801  CB  ARG A 135     -44.908  14.389  26.227  1.00 29.13
C
ATOM    802  CG  ARG A 135     -44.763  13.420  27.379  1.00 33.22
C
ATOM    803  CD  ARG A 135     -46.121  12.909  27.813  1.00 39.18
C
ATOM    804  NE  ARG A 135     -46.020  12.002  28.947  1.00 44.19
N
ATOM    805  CZ  ARG A 135     -47.060  11.663  29.705  1.00 47.62
C
ATOM    806  NH1 ARG A 135     -46.896  10.835  30.728  1.00 48.66
N
ATOM    807  NH2 ARG A 135     -48.262  12.158  29.437  1.00 44.45
N
ATOM    808  N   ARG A 136     -45.723  14.374  22.602  1.00 28.07
N
ATOM    809  CA  ARG A 136     -46.088  15.192  21.456  1.00 26.69
C
ATOM    810  C   ARG A 136     -45.257  16.470  21.385  1.00 27.10
C
ATOM    811  O   ARG A 136     -44.036  16.369  21.411  1.00 26.71
O
ATOM    812  CB  ARG A 136     -47.610  15.385  21.398  1.00 26.96
C
ATOM    813  CG  ARG A 136     -48.309  13.983  21.369  1.00 27.72
C
ATOM    814  CD  ARG A 136     -49.846  14.051  21.223  1.00 27.18
C
ATOM    815  NE  ARG A 136     -50.255  14.647  19.957  1.00 28.17
N
ATOM    816  CZ  ARG A 136     -51.519  14.961  19.658  1.00 30.96
C
ATOM    817  NH1 ARG A 136     -52.486  14.742  20.550  1.00 34.99
N
```

```
ATOM    818  NH2 ARG A 136     -51.820  15.508  18.488  1.00 30.10
N
ATOM    819  N   SER A 137     -45.900  17.638  21.325  1.00 26.30
N
ATOM    820  CA  SER A 137     -45.221  18.916  21.135  1.00 25.34
C
ATOM    821  C   SER A 137     -45.750  19.990  22.076  1.00 25.22
C
ATOM    822  O   SER A 137     -46.739  19.767  22.821  1.00 24.51
O
ATOM    823  CB  SER A 137     -45.342  19.364  19.677  1.00 24.74
C
ATOM    824  OG  SER A 137     -46.597  19.973  19.379  1.00 24.80
O
ATOM    825  N   LEU A 138     -45.087  21.138  22.070  1.00 23.97
N
ATOM    826  CA  LEU A 138     -45.520  22.281  22.852  1.00 24.77
C
ATOM    827  C   LEU A 138     -46.855  22.849  22.352  1.00 25.06
C
ATOM    828  O   LEU A 138     -47.482  23.649  23.051  1.00 26.22
O
ATOM    829  CB  LEU A 138     -44.460  23.398  22.814  1.00 24.03
C
ATOM    830  CG  LEU A 138     -43.165  23.131  23.599  1.00 24.00
C
ATOM    831  CD1 LEU A 138     -42.199  24.319  23.442  1.00 20.39
C
ATOM    832  CD2 LEU A 138     -43.512  22.951  25.066  1.00 27.07
C
ATOM    833  N   LEU A 139     -47.227  22.520  21.119  1.00 25.39
N
ATOM    834  CA  LEU A 139     -48.535  22.946  20.579  1.00 26.44
C
ATOM    835  C   LEU A 139     -49.658  22.338  21.408  1.00 26.95
C
ATOM    836  O   LEU A 139     -50.587  23.031  21.786  1.00 28.20
O
ATOM    837  CB  LEU A 139     -48.700  22.532  19.102  1.00 25.47
C
ATOM    838  CG  LEU A 139     -50.035  22.960  18.450  1.00 27.77
C
ATOM    839  CD1 LEU A 139     -50.074  24.477  18.455  1.00 26.09
C
```

ATOM 840 CD2 LEU A 139 -50.169 22.429 17.007 1.00 28.20
C
ATOM 841 N GLU A 140 -49.575 21.042 21.680 1.00 28.76
N
ATOM 842 CA GLU A 140 -50.599 20.375 22.491 1.00 30.88
C
ATOM 843 C GLU A 140 -50.555 20.829 23.936 1.00 31.21
C
ATOM 844 O GLU A 140 -51.582 20.871 24.610 1.00 30.65
O
ATOM 845 CB GLU A 140 -50.454 18.855 22.443 1.00 30.51
C
ATOM 846 CG GLU A 140 -50.825 18.235 21.104 1.00 31.52
C
ATOM 847 CD GLU A 140 -49.816 18.582 19.999 1.00 35.01
C
ATOM 848 OE1 GLU A 140 -48.578 18.455 20.223 1.00 32.54
O
ATOM 849 OE2 GLU A 140 -50.274 18.976 18.907 1.00 35.14
O
ATOM 850 N LEU A 141 -49.358 21.119 24.435 1.00 30.82
N
ATOM 851 CA LEU A 141 -49.256 21.710 25.772 1.00 31.31
C
ATOM 852 C LEU A 141 -49.966 23.071 25.804 1.00 31.19
C
ATOM 853 O LEU A 141 -50.794 23.351 26.708 1.00 32.87
O
ATOM 854 CB LEU A 141 -47.776 21.857 26.188 1.00 31.11
C
ATOM 855 CG LEU A 141 -47.535 22.533 27.537 1.00 32.80
C
ATOM 856 CD1 LEU A 141 -47.931 21.566 28.636 1.00 31.88
C
ATOM 857 CD2 LEU A 141 -46.084 23.009 27.702 1.00 30.20
C
ATOM 858 N HIS A 142 -49.649 23.912 24.838 1.00 30.60
N
ATOM 859 CA HIS A 142 -50.217 25.258 24.756 1.00 32.21
C
ATOM 860 C HIS A 142 -51.764 25.235 24.636 1.00 32.64
C
ATOM 861 O HIS A 142 -52.435 26.043 25.258 1.00 32.52
O

```
ATOM    862  CB  HIS A 142     -49.620  26.021  23.578  1.00 32.25
C
ATOM    863  CG  HIS A 142     -50.516  27.097  23.027  1.00 33.85
C
ATOM    864  ND1 HIS A 142     -50.511  28.390  23.515  1.00 33.04
N
ATOM    865  CD2 HIS A 142     -51.448  27.069  22.034  1.00 37.54
C
ATOM    866  CE1 HIS A 142     -51.395  29.114  22.841  1.00 36.42
C
ATOM    867  NE2 HIS A 142     -51.984  28.333  21.945  1.00 38.61
N
ATOM    868  N   LYS A 143     -52.306  24.306  23.856  1.00 33.01
N
ATOM    869  CA  LYS A 143     -53.768  24.181  23.696  1.00 34.89
C
ATOM    870  C   LYS A 143     -54.448  23.828  25.041  1.00 35.58
C
ATOM    871  O   LYS A 143     -55.568  24.282  25.334  1.00 37.06
O
ATOM    872  CB  LYS A 143     -54.098  23.115  22.657  1.00 34.35
C
ATOM    873  CG  LYS A 143     -53.829  23.510  21.231  1.00 35.75
C
ATOM    874  CD  LYS A 143     -53.954  22.296  20.332  1.00 38.58
C
ATOM    875  CE  LYS A 143     -54.176  22.713  18.875  1.00 41.31
C
ATOM    876  NZ  LYS A 143     -54.188  21.539  17.932  1.00 44.24
N1+
ATOM    877  N   ARG A 144     -53.767  23.022  25.845  1.00 36.21
N
ATOM    878  CA  ARG A 144     -54.232  22.649  27.180  1.00 37.35
C
ATOM    879  C   ARG A 144     -53.986  23.704  28.262  1.00 37.21
C
ATOM    880  O   ARG A 144     -54.858  23.945  29.099  1.00 38.51
O
ATOM    881  CB  ARG A 144     -53.607  21.312  27.586  1.00 38.00
C
ATOM    882  CG  ARG A 144     -53.998  20.775  28.956  1.00 42.82
C
ATOM    883  CD  ARG A 144     -55.525  20.694  29.087  1.00 46.95
C
```

```
ATOM    884  NE  ARG A 144     -55.946  20.260  30.411  1.00 51.32
N
ATOM    885  CZ  ARG A 144     -56.159  18.987  30.735  1.00 54.67
C
ATOM    886  NH1 ARG A 144     -55.986  18.037  29.823  1.00 56.61
N
ATOM    887  NH2 ARG A 144     -56.550  18.664  31.965  1.00 55.41
N
ATOM    888  N   ARG A 145     -52.820  24.335  28.272  1.00 35.74
N
ATOM    889  CA  ARG A 145     -52.430  25.163  29.408  1.00 35.61
C
ATOM    890  C   ARG A 145     -52.573  26.643  29.146  1.00 35.75
C
ATOM    891  O   ARG A 145     -52.660  27.415  30.101  1.00 36.97
O
ATOM    892  CB  ARG A 145     -50.982  24.883  29.844  1.00 35.15
C
ATOM    893  CG  ARG A 145     -50.748  23.490  30.475  1.00 34.28
C
ATOM    894  CD  ARG A 145     -51.073  23.484  32.013  1.00 33.59
C
ATOM    895  NE  ARG A 145     -50.598  24.731  32.631  1.00 34.92
N
ATOM    896  CZ  ARG A 145     -49.348  24.931  33.037  1.00 33.73
C
ATOM    897  NH1 ARG A 145     -48.480  23.949  32.948  1.00 31.83
N
ATOM    898  NH2 ARG A 145     -48.975  26.107  33.549  1.00 34.09
N
ATOM    899  N   LYS A 146     -52.558  27.034  27.870  1.00 35.49
N
ATOM    900  CA  LYS A 146     -52.480  28.423  27.439  1.00 35.28
C
ATOM    901  C   LYS A 146     -51.246  29.074  28.070  1.00 34.92
C
ATOM    902  O   LYS A 146     -50.178  28.455  28.043  1.00 34.67
O
ATOM    903  CB  LYS A 146     -53.808  29.169  27.691  1.00 36.90
C
ATOM    904  CG  LYS A 146     -54.920  28.655  26.771  1.00 39.40
C
ATOM    905  CD  LYS A 146     -54.532  28.908  25.285  1.00 42.89
C
```

ATOM 906 CE LYS A 146 -55.150 27.879 24.334 1.00 44.58
C
ATOM 907 NZ LYS A 146 -55.043 28.307 22.886 1.00 43.71
N1+
ATOM 908 N ALA A 147 -51.346 30.283 28.618 1.00 33.81
N
ATOM 909 CA ALA A 147 -50.165 30.926 29.194 1.00 32.77
C
ATOM 910 C ALA A 147 -49.550 30.058 30.287 1.00 32.69
C
ATOM 911 O ALA A 147 -50.237 29.521 31.152 1.00 32.53
O
ATOM 912 CB ALA A 147 -50.480 32.311 29.716 1.00 33.26
C
ATOM 913 N LEU A 148 -48.236 29.897 30.237 1.00 31.89
N
ATOM 914 CA LEU A 148 -47.546 29.051 31.208 1.00 30.85
C
ATOM 915 C LEU A 148 -47.065 29.947 32.330 1.00 30.88
C
ATOM 916 O LEU A 148 -47.029 31.166 32.178 1.00 30.03
O
ATOM 917 CB LEU A 148 -46.326 28.377 30.545 1.00 31.31
C
ATOM 918 CG LEU A 148 -46.579 27.435 29.371 1.00 30.98
C
ATOM 919 CD1 LEU A 148 -45.243 26.830 28.952 1.00 29.83
C
ATOM 920 CD2 LEU A 148 -47.586 26.333 29.739 1.00 28.76
C
ATOM 921 N THR A 149 -46.661 29.354 33.448 1.00 30.40
N
ATOM 922 CA THR A 149 -45.971 30.143 34.478 1.00 31.15
C
ATOM 923 C THR A 149 -44.602 30.549 33.964 1.00 31.87
C
ATOM 924 O THR A 149 -44.065 29.910 33.026 1.00 31.37
O
ATOM 925 CB THR A 149 -45.793 29.345 35.770 1.00 31.70
C
ATOM 926 OG1 THR A 149 -44.869 28.270 35.543 1.00 32.24
O
ATOM 927 CG2 THR A 149 -47.117 28.774 36.205 1.00 30.02
C

ATOM 928 N GLU A 150 -44.020 31.586 34.566 1.00 31.23
N
ATOM 929 CA GLU A 150 -42.753 32.097 34.106 1.00 33.24
C
ATOM 930 C GLU A 150 -41.599 31.073 34.207 1.00 33.15
C
ATOM 931 O GLU A 150 -40.786 31.011 33.290 1.00 32.64
O
ATOM 932 CB GLU A 150 -42.405 33.402 34.814 1.00 33.64
C
ATOM 933 CG GLU A 150 -41.465 34.301 34.081 1.00 37.88
C
ATOM 934 CD GLU A 150 -41.376 35.679 34.738 1.00 42.00
C
ATOM 935 OE1 GLU A 150 -41.342 35.724 35.983 1.00 44.39
O
ATOM 936 OE2 GLU A 150 -41.334 36.704 34.021 1.00 44.81
O
ATOM 937 N PRO A 151 -41.505 30.311 35.320 1.00 33.50
N
ATOM 938 CA PRO A 151 -40.436 29.276 35.409 1.00 34.00
C
ATOM 939 C PRO A 151 -40.572 28.160 34.371 1.00 33.91
C
ATOM 940 O PRO A 151 -39.556 27.693 33.856 1.00 33.64
O
ATOM 941 CB PRO A 151 -40.600 28.715 36.828 1.00 33.73
C
ATOM 942 CG PRO A 151 -41.311 29.795 37.588 1.00 34.30
C
ATOM 943 CD PRO A 151 -42.261 30.401 36.584 1.00 34.07
C
ATOM 944 N GLU A 152 -41.802 27.744 34.056 1.00 35.02
N
ATOM 945 CA GLU A 152 -42.023 26.816 32.930 1.00 35.72
C
ATOM 946 C GLU A 152 -41.540 27.416 31.616 1.00 36.14
C
ATOM 947 O GLU A 152 -40.874 26.732 30.827 1.00 35.32
O
ATOM 948 CB GLU A 152 -43.497 26.471 32.776 1.00 36.31
C
ATOM 949 CG GLU A 152 -44.039 25.558 33.852 1.00 35.88
C

```
ATOM    950  CD  GLU A 152     -45.526  25.352  33.677  1.00 37.59
C
ATOM    951  OE1 GLU A 152     -46.314  26.291  33.970  1.00 35.82
O
ATOM    952  OE2 GLU A 152     -45.911  24.255  33.228  1.00 35.00
O
ATOM    953  N   ALA A 153     -41.869  28.691  31.373  1.00 35.81
N
ATOM    954  CA  ALA A 153     -41.402  29.345  30.151  1.00 36.18
C
ATOM    955  C   ALA A 153     -39.862  29.408  30.097  1.00 36.37
C
ATOM    956  O   ALA A 153     -39.287  29.142  29.061  1.00 37.44
O
ATOM    957  CB  ALA A 153     -42.044  30.749  29.975  1.00 35.96
C
ATOM    958  N   ARG A 154     -39.208  29.746  31.201  1.00 35.55
N
ATOM    959  CA  ARG A 154     -37.732  29.763  31.252  1.00 35.58
C
ATOM    960  C   ARG A 154     -37.169  28.393  30.943  1.00 35.75
C
ATOM    961  O   ARG A 154     -36.218  28.286  30.178  1.00 34.66
O
ATOM    962  CB  ARG A 154     -37.203  30.182  32.632  1.00 34.40
C
ATOM    963  CG  ARG A 154     -37.360  31.663  32.933  1.00 35.87
C
ATOM    964  CD  ARG A 154     -36.586  32.120  34.204  1.00 35.59
C
ATOM    965  NE  ARG A 154     -37.228  33.310  34.721  1.00 39.87
N
ATOM    966  CZ  ARG A 154     -38.186  33.299  35.639  1.00 39.82
C
ATOM    967  NH1 ARG A 154     -38.747  34.435  36.011  1.00 38.57
N
ATOM    968  NH2 ARG A 154     -38.564  32.154  36.203  1.00 39.42
N
ATOM    969  N   TYR A 155     -37.771  27.366  31.561  1.00 36.02
N
ATOM    970  CA  TYR A 155     -37.379  25.970  31.389  1.00 35.12
C
ATOM    971  C   TYR A 155     -37.389  25.532  29.929  1.00 36.06
C
```

ATOM 972 O TYR A 155 -36.420 24.962 29.441 1.00 35.67
O
ATOM 973 CB TYR A 155 -38.307 25.058 32.197 1.00 35.71
C
ATOM 974 CG TYR A 155 -38.057 23.587 31.926 1.00 36.08
C
ATOM 975 CD1 TYR A 155 -37.077 22.864 32.638 1.00 35.87
C
ATOM 976 CD2 TYR A 155 -38.759 22.940 30.921 1.00 34.99
C
ATOM 977 CE1 TYR A 155 -36.848 21.514 32.339 1.00 36.79
C
ATOM 978 CE2 TYR A 155 -38.563 21.602 30.614 1.00 37.55
C
ATOM 979 CZ TYR A 155 -37.607 20.896 31.323 1.00 38.60
C
ATOM 980 OH TYR A 155 -37.417 19.587 30.990 1.00 40.84
O
ATOM 981 N TYR A 156 -38.515 25.747 29.251 1.00 34.85
N
ATOM 982 CA TYR A 156 -38.653 25.340 27.855 1.00 34.79
C
ATOM 983 C TYR A 156 -37.839 26.226 26.952 1.00 34.22
C
ATOM 984 O TYR A 156 -37.162 25.731 26.059 1.00 34.00
O
ATOM 985 CB TYR A 156 -40.124 25.400 27.404 1.00 33.98
C
ATOM 986 CG TYR A 156 -41.029 24.321 28.025 1.00 34.85
C
ATOM 987 CD1 TYR A 156 -40.730 22.961 27.877 1.00 35.82
C
ATOM 988 CD2 TYR A 156 -42.158 24.670 28.750 1.00 37.11
C
ATOM 989 CE1 TYR A 156 -41.549 21.970 28.455 1.00 35.79
C
ATOM 990 CE2 TYR A 156 -42.991 23.689 29.311 1.00 36.45
C
ATOM 991 CZ TYR A 156 -42.670 22.337 29.135 1.00 36.84
C
ATOM 992 OH TYR A 156 -43.463 21.369 29.717 1.00 35.41
O
ATOM 993 N LEU A 157 -37.897 27.532 27.169 1.00 34.30
N

```
ATOM    994  CA  LEU A 157     -37.172  28.440  26.296  1.00 34.67
C
ATOM    995  C   LEU A 157     -35.677  28.127  26.392  1.00 35.55
C
ATOM    996  O   LEU A 157     -34.948  28.267  25.396  1.00 37.02
O
ATOM    997  CB  LEU A 157     -37.468  29.887  26.689  1.00 35.78
C
ATOM    998  CG  LEU A 157     -38.830  30.380  26.198  1.00 35.55
C
ATOM    999  CD1 LEU A 157     -39.275  31.685  26.879  1.00 37.93
C
ATOM   1000  CD2 LEU A 157     -38.826  30.522  24.652  1.00 37.10
C
ATOM   1001  N   ARG A 158     -35.198  27.734  27.578  1.00 34.27
N
ATOM   1002  CA  ARG A 158     -33.729  27.448  27.727  1.00 34.75
C
ATOM   1003  C   ARG A 158     -33.295  26.325  26.801  1.00 34.77
C
ATOM   1004  O   ARG A 158     -32.269  26.405  26.138  1.00 36.69
O
ATOM   1005  CB  ARG A 158     -33.369  27.059  29.154  1.00 34.14
C
ATOM   1006  CG  ARG A 158     -31.857  26.776  29.375  1.00 34.53
C
ATOM   1007  CD  ARG A 158     -31.535  26.418  30.821  1.00 35.30
C
ATOM   1008  NE  ARG A 158     -30.337  25.569  30.912  1.00 40.84
N
ATOM   1009  CZ  ARG A 158     -30.318  24.248  30.694  1.00 42.37
C
ATOM   1010  NH1 ARG A 158     -31.441  23.580  30.373  1.00 42.84
N
ATOM   1011  NH2 ARG A 158     -29.174  23.593  30.799  1.00 44.09
N
ATOM   1012  N   GLN A 159     -34.099  25.283  26.761  1.00 34.71
N
ATOM   1013  CA  GLN A 159     -33.847  24.115  25.931  1.00 35.11
C
ATOM   1014  C   GLN A 159     -34.038  24.390  24.443  1.00 35.95
C
ATOM   1015  O   GLN A 159     -33.239  23.934  23.638  1.00 36.97
O
```

ATOM 1016 CB GLN A 159 -34.749 22.974 26.396 1.00 34.89
C
ATOM 1017 CG GLN A 159 -34.559 22.621 27.899 1.00 34.29
C
ATOM 1018 CD GLN A 159 -35.222 21.307 28.259 1.00 38.96
C
ATOM 1019 OE1 GLN A 159 -36.000 20.778 27.482 1.00 38.67
O
ATOM 1020 NE2 GLN A 159 -34.913 20.777 29.429 1.00 37.62
N
ATOM 1021 N ILE A 160 -35.059 25.160 24.071 1.00 35.84
N
ATOM 1022 CA ILE A 160 -35.179 25.641 22.682 1.00 36.02
C
ATOM 1023 C ILE A 160 -33.923 26.398 22.263 1.00 34.78
C
ATOM 1024 O ILE A 160 -33.344 26.168 21.181 1.00 33.45
O
ATOM 1025 CB ILE A 160 -36.408 26.541 22.571 1.00 37.75
C
ATOM 1026 CG1 ILE A 160 -37.667 25.744 22.855 1.00 37.06
C
ATOM 1027 CG2 ILE A 160 -36.518 27.246 21.162 1.00 39.16
C
ATOM 1028 CD1 ILE A 160 -38.922 26.662 23.083 1.00 37.63
C
ATOM 1029 N VAL A 161 -33.460 27.285 23.141 1.00 34.49
N
ATOM 1030 CA VAL A 161 -32.256 28.087 22.848 1.00 33.84
C
ATOM 1031 C VAL A 161 -31.010 27.244 22.727 1.00 35.21
C
ATOM 1032 O VAL A 161 -30.233 27.466 21.792 1.00 36.64
O
ATOM 1033 CB VAL A 161 -32.064 29.288 23.867 1.00 34.70
C
ATOM 1034 CG1 VAL A 161 -30.663 29.974 23.696 1.00 34.31
C
ATOM 1035 CG2 VAL A 161 -33.148 30.319 23.623 1.00 33.24
C
ATOM 1036 N LEU A 162 -30.788 26.286 23.645 1.00 34.90
N
ATOM 1037 CA LEU A 162 -29.636 25.370 23.527 1.00 34.94
C

```
ATOM   1038  C   LEU A 162     -29.628  24.568  22.208  1.00 36.43
C
ATOM   1039  O   LEU A 162     -28.575  24.416  21.576  1.00 36.11
O
ATOM   1040  CB  LEU A 162     -29.572  24.402  24.708  1.00 34.56
C
ATOM   1041  CG  LEU A 162     -29.234  25.077  26.043  1.00 32.76
C
ATOM   1042  CD1 LEU A 162     -29.478  24.087  27.202  1.00 35.75
C
ATOM   1043  CD2 LEU A 162     -27.768  25.670  26.104  1.00 36.44
C
ATOM   1044  N   GLY A 163     -30.777  24.031  21.822  1.00 36.44
N
ATOM   1045  CA  GLY A 163     -30.922  23.363  20.519  1.00 37.95
C
ATOM   1046  C   GLY A 163     -30.653  24.291  19.344  1.00 38.67
C
ATOM   1047  O   GLY A 163     -29.896  23.955  18.444  1.00 39.44
O
ATOM   1048  N   CYS A 164     -31.220  25.486  19.367  1.00 39.52
N
ATOM   1049  CA  CYS A 164     -30.944  26.451  18.307  1.00 39.20
C
ATOM   1050  C   CYS A 164     -29.479  26.911  18.301  1.00 39.04
C
ATOM   1051  O   CYS A 164     -28.906  27.135  17.229  1.00 40.00
O
ATOM   1052  CB  CYS A 164     -31.912  27.632  18.375  1.00 39.84
C
ATOM   1053  SG  CYS A 164     -32.011  28.567  16.822  1.00 43.06
S
ATOM   1054  N   GLN A 165     -28.865  27.049  19.478  1.00 37.20
N
ATOM   1055  CA  GLN A 165     -27.446  27.409  19.545  1.00 36.52
C
ATOM   1056  C   GLN A 165     -26.625  26.395  18.787  1.00 35.65
C
ATOM   1057  O   GLN A 165     -25.706  26.755  18.051  1.00 35.46
O
ATOM   1058  CB  GLN A 165     -26.937  27.456  20.989  1.00 36.37
C
ATOM   1059  CG  GLN A 165     -27.123  28.802  21.632  1.00 39.90
C
```

```
ATOM   1060  CD  GLN A 165     -26.784  28.833  23.103  1.00 43.37
C
ATOM   1061  OE1 GLN A 165     -27.139  29.797  23.793  1.00 49.40
O
ATOM   1062  NE2 GLN A 165     -26.100  27.802  23.599  1.00 44.36
N
ATOM   1063  N   TYR A 166     -26.933  25.124  19.015  1.00 34.75
N
ATOM   1064  CA  TYR A 166     -26.309  24.007  18.305  1.00 35.08
C
ATOM   1065  C   TYR A 166     -26.529  24.101  16.776  1.00 35.14
C
ATOM   1066  O   TYR A 166     -25.598  23.892  15.992  1.00 33.73
O
ATOM   1067  CB  TYR A 166     -26.865  22.669  18.824  1.00 36.05
C
ATOM   1068  CG  TYR A 166     -26.369  21.476  18.004  1.00 36.93
C
ATOM   1069  CD1 TYR A 166     -25.079  20.999  18.160  1.00 38.43
C
ATOM   1070  CD2 TYR A 166     -27.188  20.867  17.052  1.00 40.50
C
ATOM   1071  CE1 TYR A 166     -24.619  19.900  17.391  1.00 39.27
C
ATOM   1072  CE2 TYR A 166     -26.732  19.787  16.275  1.00 35.04
C
ATOM   1073  CZ  TYR A 166     -25.477  19.331  16.449  1.00 39.07
C
ATOM   1074  OH  TYR A 166     -25.087  18.275  15.688  1.00 38.55
O
ATOM   1075  N   LEU A 167     -27.749  24.441  16.355  1.00 34.16
N
ATOM   1076  CA  LEU A 167     -28.069  24.530  14.924  1.00 34.17
C
ATOM   1077  C   LEU A 167     -27.198  25.610  14.324  1.00 35.16
C
ATOM   1078  O   LEU A 167     -26.526  25.389  13.313  1.00 36.10
O
ATOM   1079  CB  LEU A 167     -29.581  24.870  14.706  1.00 33.90
C
ATOM   1080  CG  LEU A 167     -30.601  23.793  15.127  1.00 32.63
C
ATOM   1081  CD1 LEU A 167     -32.027  24.161  14.650  1.00 30.06
C
```

```
ATOM   1082  CD2 LEU A 167     -30.140  22.421  14.527  1.00 31.93
C
ATOM   1083  N   HIS A 168     -27.176  26.782  14.950  1.00 35.71
N
ATOM   1084  CA  HIS A 168     -26.478  27.944  14.362  1.00 35.96
C
ATOM   1085  C   HIS A 168     -25.000  27.782  14.342  1.00 36.97
C
ATOM   1086  O   HIS A 168     -24.306  28.225  13.407  1.00 36.53
O
ATOM   1087  CB  HIS A 168     -26.872  29.224  15.112  1.00 36.43
C
ATOM   1088  CG  HIS A 168     -28.284  29.652  14.837  1.00 34.58
C
ATOM   1089  ND1 HIS A 168     -28.751  30.908  15.140  1.00 35.50
N
ATOM   1090  CD2 HIS A 168     -29.320  28.993  14.246  1.00 35.72
C
ATOM   1091  CE1 HIS A 168     -30.024  31.007  14.775  1.00 38.50
C
ATOM   1092  NE2 HIS A 168     -30.387  29.862  14.213  1.00 35.66
N
ATOM   1093  N   ARG A 169     -24.475  27.152  15.381  1.00 38.23
N
ATOM   1094  CA  ARG A 169     -23.072  26.859  15.342  1.00 39.13
C
ATOM   1095  C   ARG A 169     -22.699  25.806  14.280  1.00 38.53
C
ATOM   1096  O   ARG A 169     -21.544  25.696  13.877  1.00 38.14
O
ATOM   1097  CB  ARG A 169     -22.532  26.596  16.744  1.00 40.20
C
ATOM   1098  CG  ARG A 169     -22.468  25.182  17.243  1.00 43.16
C
ATOM   1099  CD  ARG A 169     -21.934  25.183  18.697  1.00 42.08
C
ATOM   1100  NE  ARG A 169     -20.668  25.895  18.811  1.00 49.21
N
ATOM   1101  CZ  ARG A 169     -20.457  27.037  19.481  1.00 50.03
C
ATOM   1102  NH1 ARG A 169     -21.438  27.682  20.123  1.00 53.85
N
ATOM   1103  NH2 ARG A 169     -19.248  27.553  19.473  1.00 44.80
N
```

ATOM 1104 N ASN A 170 -23.680 25.061 13.787 1.00 38.24
N
ATOM 1105 CA ASN A 170 -23.418 24.153 12.677 1.00 37.67
C
ATOM 1106 C ASN A 170 -23.968 24.726 11.372 1.00 36.77
C
ATOM 1107 O ASN A 170 -24.154 24.004 10.390 1.00 35.71
O
ATOM 1108 CB ASN A 170 -23.988 22.778 12.961 1.00 37.92
C
ATOM 1109 CG ASN A 170 -23.197 22.045 13.987 1.00 40.01
C
ATOM 1110 OD1 ASN A 170 -22.119 21.533 13.701 1.00 40.34
O
ATOM 1111 ND2 ASN A 170 -23.695 22.029 15.210 1.00 40.91
N
ATOM 1112 N ARG A 171 -24.157 26.043 11.379 1.00 35.74
N
ATOM 1113 CA ARG A 171 -24.568 26.831 10.210 1.00 36.07
C
ATOM 1114 C ARG A 171 -25.899 26.412 9.612 1.00 35.97
C
ATOM 1115 O ARG A 171 -26.105 26.514 8.412 1.00 36.72
O
ATOM 1116 CB ARG A 171 -23.426 26.901 9.155 1.00 36.54
C
ATOM 1117 CG ARG A 171 -22.198 27.535 9.724 1.00 39.78
C
ATOM 1118 CD ARG A 171 -21.289 28.079 8.647 1.00 46.54
C
ATOM 1119 NE ARG A 171 -20.195 27.179 8.285 1.00 53.21
N
ATOM 1120 CZ ARG A 171 -19.045 27.063 8.960 1.00 57.03
C
ATOM 1121 NH1 ARG A 171 -18.846 27.743 10.093 1.00 58.79
N
ATOM 1122 NH2 ARG A 171 -18.093 26.242 8.519 1.00 58.25
N
ATOM 1123 N VAL A 172 -26.809 25.939 10.457 1.00 35.11
N
ATOM 1124 CA VAL A 172 -28.150 25.570 10.009 1.00 35.55
C
ATOM 1125 C VAL A 172 -29.124 26.591 10.541 1.00 35.72
C

```
ATOM   1126  O   VAL A 172     -29.098  26.871  11.747  1.00 35.01
O
ATOM   1127  CB  VAL A 172     -28.541  24.155  10.551  1.00 35.68
C
ATOM   1128  CG1 VAL A 172     -29.998  23.896  10.334  1.00 36.45
C
ATOM   1129  CG2 VAL A 172     -27.669  23.034   9.852  1.00 34.33
C
ATOM   1130  N   ILE A 173     -29.981  27.120   9.650  1.00 34.61
N
ATOM   1131  CA  ILE A 173     -31.091  27.964  10.037  1.00 35.12
C
ATOM   1132  C   ILE A 173     -32.338  27.108   9.908  1.00 35.12
C
ATOM   1133  O   ILE A 173     -32.596  26.518   8.865  1.00 37.00
O
ATOM   1134  CB  ILE A 173     -31.279  29.191   9.129  1.00 33.87
C
ATOM   1135  CG1 ILE A 173     -29.911  29.843   8.811  1.00 35.03
C
ATOM   1136  CG2 ILE A 173     -32.230  30.191   9.791  1.00 34.49
C
ATOM   1137  CD1 ILE A 173     -30.026  30.784   7.600  1.00 35.15
C
ATOM   1138  N   HIS A 174     -33.101  27.000  10.979  1.00 35.03
N
ATOM   1139  CA  HIS A 174     -34.231  26.078  10.955  1.00 33.98
C
ATOM   1140  C   HIS A 174     -35.377  26.667  10.111  1.00 34.46
C
ATOM   1141  O   HIS A 174     -35.945  26.004   9.237  1.00 34.79
O
ATOM   1142  CB  HIS A 174     -34.722  25.868  12.393  1.00 35.77
C
ATOM   1143  CG  HIS A 174     -35.839  24.879  12.496  1.00 33.57
C
ATOM   1144  ND1 HIS A 174     -37.153  25.201  12.232  1.00 37.02
N
ATOM   1145  CD2 HIS A 174     -35.829  23.571  12.845  1.00 34.66
C
ATOM   1146  CE1 HIS A 174     -37.913  24.126  12.422  1.00 36.76
C
ATOM   1147  NE2 HIS A 174     -37.135  23.132  12.834  1.00 35.62
N
```

ATOM 1148 N ARG A 175 -35.700 27.927 10.379 1.00 33.63
N
ATOM 1149 CA ARG A 175 -36.703 28.719 9.606 1.00 35.15
C
ATOM 1150 C ARG A 175 -38.178 28.403 9.867 1.00 35.99
C
ATOM 1151 O ARG A 175 -39.081 29.091 9.328 1.00 35.95
O
ATOM 1152 CB ARG A 175 -36.397 28.748 8.093 1.00 35.34
C
ATOM 1153 CG ARG A 175 -34.968 29.223 7.801 1.00 33.79
C
ATOM 1154 CD ARG A 175 -34.815 29.743 6.363 1.00 35.61
C
ATOM 1155 NE ARG A 175 -35.088 28.679 5.408 1.00 35.31
N
ATOM 1156 CZ ARG A 175 -34.908 28.751 4.097 1.00 37.40
C
ATOM 1157 NH1 ARG A 175 -34.420 29.846 3.548 1.00 35.96
N
ATOM 1158 NH2 ARG A 175 -35.218 27.701 3.326 1.00 34.43
N
ATOM 1159 N ASP A 176 -38.451 27.417 10.718 1.00 36.84
N
ATOM 1160 CA ASP A 176 -39.870 27.030 10.977 1.00 37.82
C
ATOM 1161 C ASP A 176 -40.048 26.694 12.456 1.00 38.39
C
ATOM 1162 O ASP A 176 -40.743 25.750 12.814 1.00 38.94
O
ATOM 1163 CB ASP A 176 -40.264 25.835 10.080 1.00 38.36
C
ATOM 1164 CG ASP A 176 -41.812 25.614 9.961 1.00 41.89
C
ATOM 1165 OD1 ASP A 176 -42.219 24.505 9.540 1.00 46.39
O
ATOM 1166 OD2 ASP A 176 -42.605 26.515 10.273 1.00 41.32
O
ATOM 1167 N LEU A 177 -39.370 27.427 13.337 1.00 38.65
N
ATOM 1168 CA LEU A 177 -39.485 27.119 14.760 1.00 38.34
C
ATOM 1169 C LEU A 177 -40.851 27.569 15.235 1.00 38.19
C

ATOM 1170 O LEU A 177 -41.216 28.747 15.098 1.00 39.41
O
ATOM 1171 CB LEU A 177 -38.357 27.794 15.578 1.00 38.03
C
ATOM 1172 CG LEU A 177 -36.923 27.290 15.423 1.00 38.53
C
ATOM 1173 CD1 LEU A 177 -36.027 28.288 16.219 1.00 36.35
C
ATOM 1174 CD2 LEU A 177 -36.803 25.882 15.957 1.00 36.47
C
ATOM 1175 N LYS A 178 -41.633 26.617 15.744 1.00 38.22
N
ATOM 1176 CA LYS A 178 -43.013 26.874 16.151 1.00 37.70
C
ATOM 1177 C LYS A 178 -43.407 25.845 17.165 1.00 36.65
C
ATOM 1178 O LYS A 178 -42.758 24.797 17.282 1.00 36.36
O
ATOM 1179 CB LYS A 178 -44.005 26.885 14.968 1.00 38.04
C
ATOM 1180 CG LYS A 178 -44.181 25.547 14.240 1.00 37.32
C
ATOM 1181 CD LYS A 178 -45.171 25.624 13.089 1.00 39.20
C
ATOM 1182 CE LYS A 178 -45.274 24.272 12.382 1.00 40.53
C
ATOM 1183 NZ LYS A 178 -46.315 24.344 11.295 1.00 45.01
N1+
ATOM 1184 N LEU A 179 -44.503 26.095 17.883 1.00 36.56
N
ATOM 1185 CA LEU A 179 -44.865 25.174 18.954 1.00 35.61
C
ATOM 1186 C LEU A 179 -44.973 23.723 18.466 1.00 35.35
C
ATOM 1187 O LEU A 179 -44.506 22.828 19.141 1.00 36.24
O
ATOM 1188 CB LEU A 179 -46.148 25.617 19.618 1.00 35.45
C
ATOM 1189 CG LEU A 179 -46.073 27.002 20.271 1.00 34.51
C
ATOM 1190 CD1 LEU A 179 -47.475 27.261 20.876 1.00 40.08
C
ATOM 1191 CD2 LEU A 179 -45.046 27.092 21.328 1.00 38.47
C

ATOM 1192 N GLY A 180 -45.518 23.530 17.271 1.00 33.21
N
ATOM 1193 CA GLY A 180 -45.769 22.196 16.682 1.00 33.80
C
ATOM 1194 C GLY A 180 -44.537 21.379 16.295 1.00 35.22
C
ATOM 1195 O GLY A 180 -44.639 20.151 16.092 1.00 34.70
O
ATOM 1196 N ASN A 181 -43.376 21.993 16.130 0.50 34.86
N
ATOM 1197 CA ASN A 181 -42.209 21.151 15.873 0.50 36.19
C
ATOM 1198 C ASN A 181 -41.184 21.227 16.999 0.50 36.03
C
ATOM 1199 O ASN A 181 -40.010 20.851 16.815 0.50 35.93
O
ATOM 1200 CB ASN A 181 -41.584 21.423 14.488 0.50 36.70
C
ATOM 1201 CG ASN A 181 -41.281 22.867 14.278 0.50 38.02
C
ATOM 1202 OD1 ASN A 181 -41.060 23.586 15.247 0.50 41.02
O
ATOM 1203 ND2 ASN A 181 -41.281 23.322 13.009 0.50 38.29
N
ATOM 1204 N LEU A 182 -41.638 21.693 18.167 1.00 34.74
N
ATOM 1205 CA LEU A 182 -40.837 21.628 19.388 1.00 35.27
C
ATOM 1206 C LEU A 182 -41.421 20.467 20.160 1.00 34.94
C
ATOM 1207 O LEU A 182 -42.406 20.629 20.924 1.00 33.46
O
ATOM 1208 CB LEU A 182 -40.959 22.943 20.143 1.00 35.56
C
ATOM 1209 CG LEU A 182 -40.414 24.165 19.386 1.00 36.77
C
ATOM 1210 CD1 LEU A 182 -40.773 25.478 20.102 1.00 37.01
C
ATOM 1211 CD2 LEU A 182 -38.909 24.065 19.156 1.00 38.54
C
ATOM 1212 N PHE A 183 -40.852 19.280 19.929 1.00 34.97
N
ATOM 1213 CA PHE A 183 -41.408 18.036 20.485 1.00 35.33
C

ATOM 1214 C PHE A 183 -40.965 17.789 21.936 1.00 36.09
C
ATOM 1215 O PHE A 183 -39.943 18.296 22.373 1.00 35.98
O
ATOM 1216 CB PHE A 183 -41.040 16.830 19.597 1.00 35.13
C
ATOM 1217 CG PHE A 183 -41.594 16.919 18.207 1.00 34.18
C
ATOM 1218 CD1 PHE A 183 -40.879 17.552 17.202 1.00 36.13
C
ATOM 1219 CD2 PHE A 183 -42.866 16.441 17.923 1.00 36.21
C
ATOM 1220 CE1 PHE A 183 -41.409 17.687 15.925 1.00 36.14
C
ATOM 1221 CE2 PHE A 183 -43.383 16.562 16.641 1.00 37.06
C
ATOM 1222 CZ PHE A 183 -42.636 17.195 15.649 1.00 36.37
C
ATOM 1223 N LEU A 184 -41.720 16.972 22.661 1.00 36.53
N
ATOM 1224 CA LEU A 184 -41.389 16.662 24.053 1.00 36.82
C
ATOM 1225 C LEU A 184 -41.248 15.170 24.258 1.00 36.78
C
ATOM 1226 O LEU A 184 -42.147 14.413 23.911 1.00 36.79
O
ATOM 1227 CB LEU A 184 -42.476 17.217 24.987 1.00 36.68
C
ATOM 1228 CG LEU A 184 -42.606 18.742 25.038 1.00 38.37
C
ATOM 1229 CD1 LEU A 184 -43.912 19.251 25.758 1.00 36.45
C
ATOM 1230 CD2 LEU A 184 -41.378 19.345 25.672 1.00 36.98
C
ATOM 1231 N ASN A 185 -40.129 14.730 24.839 1.00 36.84
N
ATOM 1232 CA ASN A 185 -40.006 13.351 25.217 1.00 36.63
C
ATOM 1233 C ASN A 185 -40.695 13.094 26.549 1.00 36.96
C
ATOM 1234 O ASN A 185 -41.321 13.996 27.102 1.00 35.69
O
ATOM 1235 CB ASN A 185 -38.538 12.806 25.153 1.00 36.43
C

```
ATOM   1236  CG  ASN A 185     -37.613  13.333  26.277  1.00 37.40
C
ATOM   1237  OD1 ASN A 185     -36.410  12.996  26.293  1.00 40.43
O
ATOM   1238  ND2 ASN A 185     -38.145  14.111  27.207  1.00 31.10
N
ATOM   1239  N   GLU A 186     -40.598  11.856  27.037  1.00 37.35
N
ATOM   1240  CA  GLU A 186     -41.249  11.435  28.292  1.00 39.05
C
ATOM   1241  C   GLU A 186     -40.883  12.319  29.494  1.00 39.10
C
ATOM   1242  O   GLU A 186     -41.682  12.488  30.424  1.00 39.63
O
ATOM   1243  CB  GLU A 186     -40.878   9.988  28.610  1.00 39.43
C
ATOM   1244  CG  GLU A 186     -41.864   8.949  28.083  1.00 44.32
C
ATOM   1245  CD  GLU A 186     -41.216   7.570  27.813  1.00 49.84
C
ATOM   1246  OE1 GLU A 186     -41.684   6.562  28.389  1.00 51.46
O
ATOM   1247  OE2 GLU A 186     -40.247   7.495  27.008  1.00 53.32
O
ATOM   1248  N   ASP A 187     -39.662  12.837  29.486  1.00 38.87
N
ATOM   1249  CA  ASP A 187     -39.131  13.642  30.589  1.00 39.24
C
ATOM   1250  C   ASP A 187     -39.422  15.136  30.396  1.00 39.46
C
ATOM   1251  O   ASP A 187     -38.838  15.957  31.100  1.00 40.09
O
ATOM   1252  CB  ASP A 187     -37.612  13.467  30.696  1.00 38.99
C
ATOM   1253  CG  ASP A 187     -37.190  12.062  31.152  1.00 41.44
C
ATOM   1254  OD1 ASP A 187     -37.943  11.409  31.899  1.00 39.72
O
ATOM   1255  OD2 ASP A 187     -36.077  11.623  30.760  1.00 44.32
O
ATOM   1256  N   LEU A 188     -40.315  15.468  29.456  1.00 38.95
N
ATOM   1257  CA  LEU A 188     -40.602  16.868  29.041  1.00 39.12
C
```

ATOM 1258 C LEU A 188 -39.350 17.622 28.630 1.00 39.11
C
ATOM 1259 O LEU A 188 -39.207 18.823 28.903 1.00 39.90
O
ATOM 1260 CB LEU A 188 -41.406 17.648 30.112 1.00 39.27
C
ATOM 1261 CG LEU A 188 -42.723 16.973 30.520 1.00 41.54
C
ATOM 1262 CD1 LEU A 188 -43.499 17.809 31.538 1.00 37.85
C
ATOM 1263 CD2 LEU A 188 -43.568 16.726 29.294 1.00 43.11
C
ATOM 1264 N GLU A 189 -38.429 16.916 27.977 1.00 38.23
N
ATOM 1265 CA GLU A 189 -37.312 17.574 27.323 1.00 39.00
C
ATOM 1266 C GLU A 189 -37.651 17.951 25.871 1.00 37.95
C
ATOM 1267 O GLU A 189 -38.229 17.138 25.128 1.00 37.66
O
ATOM 1268 CB GLU A 189 -36.107 16.654 27.298 1.00 39.06
C
ATOM 1269 CG GLU A 189 -35.625 16.228 28.659 1.00 44.45
C
ATOM 1270 CD GLU A 189 -34.239 15.666 28.543 1.00 52.49
C
ATOM 1271 OE1 GLU A 189 -34.096 14.457 28.236 1.00 55.76
O
ATOM 1272 OE2 GLU A 189 -33.286 16.456 28.698 1.00 58.17
O
ATOM 1273 N VAL A 190 -37.263 19.159 25.480 1.00 35.81
N
ATOM 1274 CA VAL A 190 -37.570 19.684 24.155 1.00 35.57
C
ATOM 1275 C VAL A 190 -36.636 19.098 23.124 1.00 36.06
C
ATOM 1276 O VAL A 190 -35.404 19.055 23.325 1.00 33.72
O
ATOM 1277 CB VAL A 190 -37.471 21.238 24.103 1.00 36.36
C
ATOM 1278 CG1 VAL A 190 -37.718 21.765 22.681 1.00 38.10
C
ATOM 1279 CG2 VAL A 190 -38.540 21.877 25.023 1.00 35.15
C

ATOM 1280 N LYS A 191 -37.243 18.686 22.008 1.00 36.68
N
ATOM 1281 CA LYS A 191 -36.548 18.198 20.826 1.00 36.56
C
ATOM 1282 C LYS A 191 -37.057 18.996 19.592 1.00 37.01
C
ATOM 1283 O LYS A 191 -38.218 18.899 19.201 1.00 37.09
O
ATOM 1284 CB LYS A 191 -36.786 16.694 20.640 1.00 35.73
C
ATOM 1285 CG LYS A 191 -36.557 15.855 21.900 1.00 36.89
C
ATOM 1286 CD LYS A 191 -35.113 15.755 22.247 1.00 37.80
C
ATOM 1287 CE LYS A 191 -34.914 14.868 23.490 1.00 37.00
C
ATOM 1288 NZ LYS A 191 -33.534 14.367 23.452 1.00 39.63
N1+
ATOM 1289 N ILE A 192 -36.197 19.848 19.052 1.00 36.71
N
ATOM 1290 CA ILE A 192 -36.489 20.588 17.828 1.00 36.85
C
ATOM 1291 C ILE A 192 -36.561 19.594 16.691 1.00 35.96
C
ATOM 1292 O ILE A 192 -35.630 18.783 16.498 1.00 35.13
O
ATOM 1293 CB ILE A 192 -35.345 21.604 17.509 1.00 36.74
C
ATOM 1294 CG1 ILE A 192 -35.288 22.690 18.611 1.00 37.62
C
ATOM 1295 CG2 ILE A 192 -35.552 22.256 16.146 1.00 36.67
C
ATOM 1296 CD1 ILE A 192 -34.078 23.670 18.487 1.00 38.54
C
ATOM 1297 N GLY A 193 -37.643 19.648 15.939 1.00 35.07
N
ATOM 1298 CA GLY A 193 -37.826 18.730 14.818 1.00 36.01
C
ATOM 1299 C GLY A 193 -38.302 19.453 13.579 1.00 37.10
C
ATOM 1300 O GLY A 193 -38.347 20.701 13.540 1.00 37.81
O
ATOM 1301 N ASP A 194 -38.697 18.659 12.592 1.00 36.81
N

```
ATOM   1302  CA  ASP A 194     -39.208  19.143  11.287  1.00 37.81
C
ATOM   1303  C   ASP A 194     -38.261  20.110  10.583  1.00 37.68
C
ATOM   1304  O   ASP A 194     -38.483  21.307  10.575  1.00 38.80
O
ATOM   1305  CB  ASP A 194     -40.609  19.742  11.340  1.00 37.07
C
ATOM   1306  CG  ASP A 194     -41.228  19.848   9.930  1.00 40.54
C
ATOM   1307  OD1 ASP A 194     -40.476  19.809   8.925  1.00 39.35
O
ATOM   1308  OD2 ASP A 194     -42.458  19.893   9.805  1.00 45.91
O
ATOM   1309  N   PHE A 195     -37.244  19.551   9.955  1.00 37.52
N
ATOM   1310  CA  PHE A 195     -36.257  20.316   9.208  1.00 37.95
C
ATOM   1311  C   PHE A 195     -36.677  20.583   7.739  1.00 38.69
C
ATOM   1312  O   PHE A 195     -35.856  20.861   6.862  1.00 38.73
O
ATOM   1313  CB  PHE A 195     -34.911  19.597   9.369  1.00 38.41
C
ATOM   1314  CG  PHE A 195     -34.306  19.848  10.731  1.00 38.31
C
ATOM   1315  CD1 PHE A 195     -34.614  19.032  11.798  1.00 37.37
C
ATOM   1316  CD2 PHE A 195     -33.537  21.004  10.961  1.00 39.30
C
ATOM   1317  CE1 PHE A 195     -34.096  19.295  13.093  1.00 36.34
C
ATOM   1318  CE2 PHE A 195     -32.998  21.269  12.260  1.00 40.37
C
ATOM   1319  CZ  PHE A 195     -33.294  20.402  13.314  1.00 38.05
C
ATOM   1320  N   GLY A 196     -37.981  20.584   7.509  1.00 38.17
N
ATOM   1321  CA  GLY A 196     -38.515  20.739   6.155  1.00 38.43
C
ATOM   1322  C   GLY A 196     -38.228  22.068   5.499  1.00 38.32
C
ATOM   1323  O   GLY A 196     -38.221  22.145   4.265  1.00 38.50
O
```

ATOM 1324 N LEU A 197 -38.029 23.118 6.298 1.00 36.71
N
ATOM 1325 CA LEU A 197 -37.730 24.464 5.741 1.00 37.31
C
ATOM 1326 C LEU A 197 -36.308 24.920 6.029 1.00 37.52
C
ATOM 1327 O LEU A 197 -35.944 26.042 5.676 1.00 38.08
O
ATOM 1328 CB LEU A 197 -38.723 25.557 6.227 1.00 36.17
C
ATOM 1329 CG LEU A 197 -40.198 25.407 5.832 1.00 39.30
C
ATOM 1330 CD1 LEU A 197 -41.016 26.593 6.337 1.00 37.08
C
ATOM 1331 CD2 LEU A 197 -40.357 25.283 4.313 1.00 37.37
C
ATOM 1332 N ALA A 198 -35.507 24.062 6.670 1.00 36.43
N
ATOM 1333 CA ALA A 198 -34.167 24.447 7.080 1.00 36.87
C
ATOM 1334 C ALA A 198 -33.243 24.595 5.896 1.00 37.31
C
ATOM 1335 O ALA A 198 -33.473 24.000 4.823 1.00 36.99
O
ATOM 1336 CB ALA A 198 -33.568 23.431 8.093 1.00 37.12
C
ATOM 1337 N THR A 199 -32.167 25.360 6.114 1.00 37.81
N
ATOM 1338 CA THR A 199 -31.168 25.605 5.100 1.00 37.28
C
ATOM 1339 C THR A 199 -29.796 25.733 5.751 1.00 38.44
C
ATOM 1340 O THR A 199 -29.676 26.068 6.919 1.00 38.53
O
ATOM 1341 CB THR A 199 -31.504 26.867 4.290 1.00 37.34
C
ATOM 1342 OG1 THR A 199 -30.613 27.007 3.172 1.00 37.09
O
ATOM 1343 CG2 THR A 199 -31.455 28.097 5.156 1.00 35.99
C
ATOM 1344 N LYS A 200 -28.771 25.430 4.977 1.00 38.81
N
ATOM 1345 CA LYS A 200 -27.399 25.557 5.417 1.00 40.58
C

ATOM 1346 C LYS A 200 -26.761 26.818 4.827 1.00 40.10
C
ATOM 1347 O LYS A 200 -26.841 27.054 3.634 1.00 39.55
O
ATOM 1348 CB LYS A 200 -26.622 24.317 4.987 1.00 41.80
C
ATOM 1349 CG LYS A 200 -26.224 23.412 6.149 1.00 46.88
C
ATOM 1350 CD LYS A 200 -24.813 23.760 6.597 1.00 51.90
C
ATOM 1351 CE LYS A 200 -23.940 22.533 6.904 1.00 55.61
C
ATOM 1352 NZ LYS A 200 -24.358 21.812 8.152 1.00 59.18
N1+
ATOM 1353 N VAL A 201 -26.159 27.625 5.692 1.00 39.76
N
ATOM 1354 CA VAL A 201 -25.401 28.805 5.316 1.00 41.09
C
ATOM 1355 C VAL A 201 -24.044 28.325 4.809 1.00 41.39
C
ATOM 1356 O VAL A 201 -23.264 27.747 5.553 1.00 41.03
O
ATOM 1357 CB VAL A 201 -25.257 29.722 6.541 1.00 41.25
C
ATOM 1358 CG1 VAL A 201 -24.245 30.834 6.327 1.00 41.78
C
ATOM 1359 CG2 VAL A 201 -26.628 30.271 6.966 1.00 43.13
C
ATOM 1360 N GLU A 202 -23.780 28.552 3.523 1.00 42.37
N
ATOM 1361 CA GLU A 202 -22.637 27.932 2.857 1.00 43.09
C
ATOM 1362 C GLU A 202 -21.366 28.788 2.904 1.00 43.48
C
ATOM 1363 O GLU A 202 -20.268 28.300 2.625 1.00 42.73
O
ATOM 1364 CB GLU A 202 -23.000 27.581 1.406 1.00 43.42
C
ATOM 1365 CG GLU A 202 -24.142 26.574 1.239 1.00 47.89
C
ATOM 1366 CD GLU A 202 -23.729 25.148 1.559 1.00 54.49
C
ATOM 1367 OE1 GLU A 202 -22.527 24.904 1.816 1.00 58.28
O

```
ATOM   1368  OE2 GLU A 202     -24.604  24.255   1.540  1.00 58.85
O
ATOM   1369  N   TYR A 203     -21.535  30.070   3.233  1.00 43.74
N
ATOM   1370  CA  TYR A 203     -20.452  31.032   3.258  1.00 44.06
C
ATOM   1371  C   TYR A 203     -20.845  32.219   4.124  1.00 44.69
C
ATOM   1372  O   TYR A 203     -22.027  32.543   4.268  1.00 44.61
O
ATOM   1373  CB  TYR A 203     -20.029  31.474   1.835  1.00 43.61
C
ATOM   1374  CG  TYR A 203     -21.086  32.199   1.025  1.00 42.18
C
ATOM   1375  CD1 TYR A 203     -21.207  33.589   1.084  1.00 41.58
C
ATOM   1376  CD2 TYR A 203     -21.949  31.499   0.171  1.00 40.97
C
ATOM   1377  CE1 TYR A 203     -22.159  34.269   0.328  1.00 40.06
C
ATOM   1378  CE2 TYR A 203     -22.912  32.160  -0.574  1.00 40.68
C
ATOM   1379  CZ  TYR A 203     -23.018  33.548  -0.487  1.00 43.50
C
ATOM   1380  OH  TYR A 203     -23.986  34.211  -1.223  1.00 44.31
O
ATOM   1381  N   ASP A 204     -19.830  32.843   4.706  1.00 45.94
N
ATOM   1382  CA  ASP A 204     -19.971  34.001   5.593  1.00 46.69
C
ATOM   1383  C   ASP A 204     -20.658  35.202   4.961  1.00 46.32
C
ATOM   1384  O   ASP A 204     -20.161  35.775   3.980  1.00 46.12
O
ATOM   1385  CB  ASP A 204     -18.591  34.453   6.069  1.00 46.90
C
ATOM   1386  CG  ASP A 204     -18.330  34.106   7.517  1.00 48.80
C
ATOM   1387  OD1 ASP A 204     -19.084  33.301   8.103  1.00 50.58
O
ATOM   1388  OD2 ASP A 204     -17.351  34.642   8.065  1.00 52.86
O
ATOM   1389  N   GLY A 205     -21.772  35.593   5.566  1.00 45.47
N
```

```
ATOM   1390  CA  GLY A 205     -22.514  36.759   5.141  1.00 45.17
C
ATOM   1391  C   GLY A 205     -23.567  36.431   4.103  1.00 45.01
C
ATOM   1392  O   GLY A 205     -24.198  37.343   3.573  1.00 46.06
O
ATOM   1393  N   GLU A 206     -23.741  35.143   3.796  1.00 43.65
N
ATOM   1394  CA  GLU A 206     -24.728  34.716   2.798  1.00 43.15
C
ATOM   1395  C   GLU A 206     -26.090  35.158   3.272  1.00 42.50
C
ATOM   1396  O   GLU A 206     -26.419  34.951   4.436  1.00 42.57
O
ATOM   1397  CB  GLU A 206     -24.734  33.194   2.633  1.00 42.55
C
ATOM   1398  CG  GLU A 206     -25.789  32.725   1.637  1.00 42.64
C
ATOM   1399  CD  GLU A 206     -25.893  31.219   1.488  1.00 43.01
C
ATOM   1400  OE1 GLU A 206     -25.181  30.479   2.198  1.00 41.97
O
ATOM   1401  OE2 GLU A 206     -26.710  30.786   0.640  1.00 44.12
O
ATOM   1402  N   ARG A 207     -26.864  35.779   2.392  1.00 42.80
N
ATOM   1403  CA  ARG A 207     -28.261  36.089   2.691  1.00 43.97
C
ATOM   1404  C   ARG A 207     -29.124  35.182   1.814  1.00 44.08
C
ATOM   1405  O   ARG A 207     -28.990  35.204   0.603  1.00 43.54
O
ATOM   1406  CB  ARG A 207     -28.584  37.567   2.409  1.00 44.58
C
ATOM   1407  CG  ARG A 207     -27.670  38.630   3.097  1.00 47.86
C
ATOM   1408  CD  ARG A 207     -27.550  38.481   4.630  1.00 52.79
C
ATOM   1409  NE  ARG A 207     -28.788  38.809   5.335  1.00 56.87
N
ATOM   1410  CZ  ARG A 207     -28.924  38.848   6.664  1.00 60.49
C
ATOM   1411  NH1 ARG A 207     -27.884  38.600   7.461  1.00 60.43
N
```

ATOM 1412 NH2 ARG A 207 -30.112 39.140 7.204 1.00 61.30
N
ATOM 1413 N LYS A 208 -29.980 34.366 2.423 1.00 44.12
N
ATOM 1414 CA LYS A 208 -30.940 33.571 1.675 1.00 44.87
C
ATOM 1415 C LYS A 208 -32.042 34.483 1.106 1.00 45.38
C
ATOM 1416 O LYS A 208 -32.555 35.341 1.818 1.00 44.24
O
ATOM 1417 CB LYS A 208 -31.530 32.484 2.600 1.00 45.66
C
ATOM 1418 CG LYS A 208 -30.466 31.643 3.328 1.00 46.81
C
ATOM 1419 CD LYS A 208 -29.684 30.816 2.335 1.00 47.56
C
ATOM 1420 CE LYS A 208 -28.820 29.781 3.022 1.00 47.08
C
ATOM 1421 NZ LYS A 208 -28.148 28.935 1.989 1.00 48.62
N1+
ATOM 1422 N LYS A 209 -32.388 34.312 -0.173 1.00 45.98
N
ATOM 1423 CA LYS A 209 -33.361 35.194 -0.836 1.00 47.32
C
ATOM 1424 C LYS A 209 -34.729 34.540 -0.999 1.00 47.81
C
ATOM 1425 O LYS A 209 -35.709 35.227 -1.305 1.00 48.47
O
ATOM 1426 CB LYS A 209 -32.862 35.637 -2.214 1.00 47.72
C
ATOM 1427 CG LYS A 209 -31.602 36.521 -2.218 1.00 50.99
C
ATOM 1428 CD LYS A 209 -31.731 37.794 -1.351 1.00 53.87
C
ATOM 1429 CE LYS A 209 -32.458 38.943 -2.075 1.00 56.66
C
ATOM 1430 NZ LYS A 209 -32.256 40.279 -1.393 1.00 55.16
N1+
ATOM 1431 N VAL A 210 -34.781 33.223 -0.795 1.00 47.28
N
ATOM 1432 CA VAL A 210 -35.945 32.404 -1.073 1.00 47.93
C
ATOM 1433 C VAL A 210 -36.243 31.511 0.123 1.00 47.37
C

```
ATOM   1434  O   VAL A 210     -35.317  30.954   0.711  1.00 47.05
O
ATOM   1435  CB  VAL A 210     -35.687  31.515  -2.356  1.00 48.38
C
ATOM   1436  CG1 VAL A 210     -36.584  30.300  -2.422  1.00 50.09
C
ATOM   1437  CG2 VAL A 210     -35.829  32.349  -3.621  1.00 49.19
C
ATOM   1438  N   LEU A 211     -37.527  31.400   0.476  1.00 46.41
N
ATOM   1439  CA  LEU A 211     -38.023  30.422   1.443  1.00 46.32
C
ATOM   1440  C   LEU A 211     -39.265  29.802   0.848  1.00 46.67
C
ATOM   1441  O   LEU A 211     -40.331  30.440   0.843  1.00 46.33
O
ATOM   1442  CB  LEU A 211     -38.406  31.086   2.786  1.00 46.69
C
ATOM   1443  CG  LEU A 211     -38.491  30.175   4.029  1.00 47.65
C
ATOM   1444  CD1 LEU A 211     -38.646  30.989   5.318  1.00 49.43
C
ATOM   1445  CD2 LEU A 211     -39.596  29.176   3.949  1.00 49.96
C
ATOM   1446  N   CYS A 212     -39.143  28.579   0.344  1.00 46.05
N
ATOM   1447  CA  CYS A 212     -40.260  27.922  -0.285  1.00 47.40
C
ATOM   1448  C   CYS A 212     -41.035  27.125   0.761  1.00 49.13
C
ATOM   1449  O   CYS A 212     -40.739  25.955   1.041  1.00 49.50
O
ATOM   1450  CB  CYS A 212     -39.810  27.041  -1.454  1.00 47.31
C
ATOM   1451  SG  CYS A 212     -41.217  26.298  -2.228  1.00 44.73
S
ATOM   1452  N   GLY A 213     -42.011  27.801   1.344  1.00 49.20
N
ATOM   1453  CA  GLY A 213     -42.857  27.256   2.361  1.00 51.35
C
ATOM   1454  C   GLY A 213     -43.530  28.408   3.071  1.00 52.31
C
ATOM   1455  O   GLY A 213     -43.276  29.571   2.745  1.00 51.59
O
```

```
ATOM   1456  N   THR A 214     -44.387  28.059   4.033  1.00 53.01
N
ATOM   1457  CA  THR A 214     -45.143  29.004   4.851  1.00 54.77
C
ATOM   1458  C   THR A 214     -44.869  28.723   6.331  1.00 54.87
C
ATOM   1459  O   THR A 214     -45.589  27.939   6.965  1.00 55.16
O
ATOM   1460  CB  THR A 214     -46.655  28.862   4.593  1.00 55.23
C
ATOM   1461  OG1 THR A 214     -46.896  28.903   3.177  1.00 56.49
O
ATOM   1462  CG2 THR A 214     -47.426  29.974   5.274  1.00 56.67
C
ATOM   1463  N   PRO A 215     -43.818  29.349   6.893  1.00 54.52
N
ATOM   1464  CA  PRO A 215     -43.572  29.159   8.321  1.00 54.60
C
ATOM   1465  C   PRO A 215     -44.645  29.883   9.133  1.00 54.78
C
ATOM   1466  O   PRO A 215     -45.337  30.774   8.594  1.00 54.54
O
ATOM   1467  CB  PRO A 215     -42.201  29.807   8.543  1.00 54.62
C
ATOM   1468  CG  PRO A 215     -41.724  30.265   7.219  1.00 54.41
C
ATOM   1469  CD  PRO A 215     -42.854  30.268   6.276  1.00 54.97
C
ATOM   1470  N   ASN A 216     -44.804  29.476  10.399  1.00 54.53
N
ATOM   1471  CA  ASN A 216     -45.797  30.061  11.296  1.00 54.45
C
ATOM   1472  C   ASN A 216     -45.343  31.459  11.732  1.00 54.25
C
ATOM   1473  O   ASN A 216     -45.945  32.491  11.364  1.00 52.65
O
ATOM   1474  CB  ASN A 216     -46.027  29.143  12.505  1.00 54.79
C
ATOM   1475  CG  ASN A 216     -47.329  29.451  13.264  1.00 57.81
C
ATOM   1476  OD1 ASN A 216     -47.340  29.514  14.491  1.00 58.79
O
ATOM   1477  ND2 ASN A 216     -48.425  29.616  12.537  1.00 59.62
N
```

ATOM 1478 N TYR A 217 -44.225 31.475 12.451 1.00 53.24
N
ATOM 1479 CA TYR A 217 -43.673 32.680 13.050 1.00 53.87
C
ATOM 1480 C TYR A 217 -42.644 33.335 12.111 1.00 53.54
C
ATOM 1481 O TYR A 217 -41.411 33.343 12.395 1.00 54.82
O
ATOM 1482 CB TYR A 217 -43.040 32.309 14.405 1.00 54.17
C
ATOM 1483 CG TYR A 217 -44.038 31.854 15.470 1.00 54.19
C
ATOM 1484 CD1 TYR A 217 -45.231 32.540 15.672 1.00 55.30
C
ATOM 1485 CD2 TYR A 217 -43.768 30.777 16.297 1.00 53.54
C
ATOM 1486 CE1 TYR A 217 -46.132 32.146 16.661 1.00 54.43
C
ATOM 1487 CE2 TYR A 217 -44.677 30.376 17.292 1.00 50.17
C
ATOM 1488 CZ TYR A 217 -45.834 31.062 17.462 1.00 55.51
C
ATOM 1489 OH TYR A 217 -46.721 30.671 18.441 1.00 55.48
O
ATOM 1490 N ILE A 218 -43.138 33.851 10.983 1.00 51.93
N
ATOM 1491 CA ILE A 218 -42.282 34.352 9.895 1.00 49.77
C
ATOM 1492 C ILE A 218 -41.688 35.750 10.159 1.00 47.79
C
ATOM 1493 O ILE A 218 -42.411 36.713 10.364 1.00 46.89
O
ATOM 1494 CB ILE A 218 -43.055 34.335 8.550 1.00 50.60
C
ATOM 1495 CG1 ILE A 218 -42.143 34.728 7.380 1.00 49.08
C
ATOM 1496 CG2 ILE A 218 -44.322 35.218 8.640 1.00 51.17
C
ATOM 1497 CD1 ILE A 218 -42.740 34.397 5.998 1.00 50.90
C
ATOM 1498 N ALA A 219 -40.361 35.834 10.135 1.00 46.25
N
ATOM 1499 CA ALA A 219 -39.609 37.080 10.337 1.00 44.02
C

ATOM 1500 C ALA A 219 -39.912 38.123 9.258 1.00 42.96
C
ATOM 1501 O ALA A 219 -40.151 37.762 8.100 1.00 42.45
O
ATOM 1502 CB ALA A 219 -38.093 36.747 10.384 1.00 43.88
C
ATOM 1503 N PRO A 220 -39.902 39.431 9.618 1.00 42.53
N
ATOM 1504 CA PRO A 220 -40.281 40.441 8.611 1.00 42.60
C
ATOM 1505 C PRO A 220 -39.376 40.475 7.378 1.00 43.12
C
ATOM 1506 O PRO A 220 -39.839 40.851 6.291 1.00 42.67
O
ATOM 1507 CB PRO A 220 -40.183 41.781 9.373 1.00 42.63
C
ATOM 1508 CG PRO A 220 -39.317 41.481 10.597 1.00 41.32
C
ATOM 1509 CD PRO A 220 -39.558 40.033 10.925 1.00 41.51
C
ATOM 1510 N GLU A 221 -38.101 40.125 7.544 1.00 43.03
N
ATOM 1511 CA GLU A 221 -37.144 40.212 6.427 1.00 44.39
C
ATOM 1512 C GLU A 221 -37.373 39.109 5.390 1.00 45.11
C
ATOM 1513 O GLU A 221 -37.001 39.258 4.223 1.00 44.84
O
ATOM 1514 CB GLU A 221 -35.687 40.205 6.913 1.00 44.20
C
ATOM 1515 CG GLU A 221 -35.273 38.962 7.659 1.00 42.94
C
ATOM 1516 CD GLU A 221 -35.448 39.091 9.164 1.00 41.81
C
ATOM 1517 OE1 GLU A 221 -36.310 39.873 9.610 1.00 43.26
O
ATOM 1518 OE2 GLU A 221 -34.714 38.415 9.906 1.00 40.95
O
ATOM 1519 N VAL A 222 -37.985 38.008 5.819 1.00 46.11
N
ATOM 1520 CA VAL A 222 -38.417 36.971 4.887 1.00 47.89
C
ATOM 1521 C VAL A 222 -39.580 37.526 4.054 1.00 49.78
C

ATOM 1522 O VAL A 222 -39.557 37.456 2.823 1.00 50.23
O
ATOM 1523 CB VAL A 222 -38.836 35.703 5.627 1.00 47.59
C
ATOM 1524 CG1 VAL A 222 -39.395 34.642 4.653 1.00 47.67
C
ATOM 1525 CG2 VAL A 222 -37.655 35.159 6.452 1.00 46.59
C
ATOM 1526 N LEU A 223 -40.576 38.092 4.747 1.00 51.82
N
ATOM 1527 CA LEU A 223 -41.810 38.604 4.139 1.00 53.24
C
ATOM 1528 C LEU A 223 -41.553 39.677 3.122 1.00 54.18
C
ATOM 1529 O LEU A 223 -42.227 39.736 2.088 1.00 54.75
O
ATOM 1530 CB LEU A 223 -42.746 39.167 5.199 1.00 53.02
C
ATOM 1531 CG LEU A 223 -43.608 38.149 5.935 1.00 53.77
C
ATOM 1532 CD1 LEU A 223 -44.289 38.782 7.124 1.00 52.72
C
ATOM 1533 CD2 LEU A 223 -44.624 37.574 4.976 1.00 55.04
C
ATOM 1534 N SER A 224 -40.584 40.535 3.422 1.00 55.62
N
ATOM 1535 CA SER A 224 -40.286 41.671 2.569 1.00 56.61
C
ATOM 1536 C SER A 224 -39.356 41.252 1.435 1.00 56.97
C
ATOM 1537 O SER A 224 -39.055 42.050 0.540 1.00 57.54
O
ATOM 1538 CB SER A 224 -39.668 42.801 3.386 1.00 56.61
C
ATOM 1539 OG SER A 224 -38.337 42.472 3.746 1.00 58.92
O
ATOM 1540 N LYS A 225 -38.903 40.001 1.478 1.00 57.26
N
ATOM 1541 CA LYS A 225 -38.041 39.431 0.433 1.00 57.23
C
ATOM 1542 C LYS A 225 -36.794 40.304 0.232 1.00 56.90
C
ATOM 1543 O LYS A 225 -36.473 40.732 -0.884 1.00 56.54
O

ATOM 1544 CB LYS A 225 -38.828 39.212 -0.876 1.00 57.61
C
ATOM 1545 CG LYS A 225 -40.165 38.438 -0.715 1.00 57.89
C
ATOM 1546 CD LYS A 225 -40.885 38.264 -2.064 1.00 57.77
C
ATOM 1547 CE LYS A 225 -42.064 37.273 -1.989 1.00 59.03
C
ATOM 1548 NZ LYS A 225 -43.314 37.879 -1.410 1.00 60.23
N1+
ATOM 1549 N LYS A 226 -36.093 40.558 1.340 1.00 56.60
N
ATOM 1550 CA LYS A 226 -34.895 41.419 1.335 1.00 56.51
C
ATOM 1551 C LYS A 226 -33.582 40.663 1.652 1.00 54.97
C
ATOM 1552 O LYS A 226 -32.501 41.270 1.710 1.00 55.65
O
ATOM 1553 CB LYS A 226 -35.094 42.605 2.295 1.00 56.63
C
ATOM 1554 CG LYS A 226 -36.091 43.647 1.772 1.00 58.37
C
ATOM 1555 CD LYS A 226 -35.977 44.996 2.509 1.00 58.02
C
ATOM 1556 CE LYS A 226 -37.142 45.919 2.148 1.00 59.87
C
ATOM 1557 NZ LYS A 226 -36.799 47.366 2.300 1.00 60.59
N1+
ATOM 1558 N GLY A 227 -33.682 39.347 1.827 1.00 52.73
N
ATOM 1559 CA GLY A 227 -32.544 38.517 2.225 1.00 49.84
C
ATOM 1560 C GLY A 227 -32.533 38.281 3.728 1.00 47.83
C
ATOM 1561 O GLY A 227 -32.672 39.218 4.505 1.00 47.49
O
ATOM 1562 N HIS A 228 -32.368 37.027 4.137 1.00 45.54
N
ATOM 1563 CA HIS A 228 -32.421 36.675 5.548 1.00 44.10
C
ATOM 1564 C HIS A 228 -31.352 35.656 5.929 1.00 43.66
C
ATOM 1565 O HIS A 228 -30.781 35.003 5.066 1.00 43.40
O

```
ATOM   1566  CB  HIS A 228     -33.813  36.121   5.914  1.00 42.75
C
ATOM   1567  CG  HIS A 228     -34.213  34.893   5.150  1.00 41.96
C
ATOM   1568  ND1 HIS A 228     -33.993  33.612   5.620  1.00 43.03
N
ATOM   1569  CD2 HIS A 228     -34.857  34.752   3.967  1.00 38.94
C
ATOM   1570  CE1 HIS A 228     -34.497  32.736   4.763  1.00 41.58
C
ATOM   1571  NE2 HIS A 228     -35.019  33.404   3.749  1.00 43.99
N
ATOM   1572  N   SER A 229     -31.109  35.520   7.230  1.00 43.15
N
ATOM   1573  CA  SER A 229     -30.107  34.574   7.743  1.00 42.68
C
ATOM   1574  C   SER A 229     -30.530  34.086   9.143  1.00 42.16
C
ATOM   1575  O   SER A 229     -31.724  34.000   9.439  1.00 41.97
O
ATOM   1576  CB  SER A 229     -28.738  35.246   7.766  1.00 42.90
C
ATOM   1577  OG  SER A 229     -27.729  34.323   8.132  1.00 44.85
O
ATOM   1578  N   PHE A 230     -29.555  33.784   9.997  1.00 40.94
N
ATOM   1579  CA  PHE A 230     -29.795  33.226  11.333  1.00 41.10
C
ATOM   1580  C   PHE A 230     -30.793  33.968  12.214  1.00 40.75
C
ATOM   1581  O   PHE A 230     -31.453  33.358  13.046  1.00 41.40
O
ATOM   1582  CB  PHE A 230     -28.480  33.139  12.103  1.00 40.84
C
ATOM   1583  CG  PHE A 230     -27.471  32.237  11.469  1.00 42.28
C
ATOM   1584  CD1 PHE A 230     -27.631  30.856  11.495  1.00 41.99
C
ATOM   1585  CD2 PHE A 230     -26.356  32.769  10.831  1.00 43.02
C
ATOM   1586  CE1 PHE A 230     -26.688  30.026  10.889  1.00 39.79
C
ATOM   1587  CE2 PHE A 230     -25.401  31.941  10.237  1.00 42.74
C
```

```
ATOM   1588  CZ  PHE A 230     -25.564  30.571  10.273  1.00 43.58
C
ATOM   1589  N   GLU A 231     -30.899  35.277  12.024  1.00 40.40
N
ATOM   1590  CA  GLU A 231     -31.711  36.123  12.896  1.00 40.33
C
ATOM   1591  C   GLU A 231     -33.174  35.761  12.800  1.00 38.75
C
ATOM   1592  O   GLU A 231     -33.922  36.084  13.692  1.00 38.80
O
ATOM   1593  CB  GLU A 231     -31.565  37.605  12.548  1.00 40.48
C
ATOM   1594  CG  GLU A 231     -30.152  38.109  12.480  1.00 41.43
C
ATOM   1595  CD  GLU A 231     -29.547  38.024  11.090  1.00 44.97
C
ATOM   1596  OE1 GLU A 231     -30.100  37.339  10.205  1.00 46.71
O
ATOM   1597  OE2 GLU A 231     -28.491  38.648  10.887  1.00 46.65
O
ATOM   1598  N   VAL A 232     -33.602  35.129  11.719  1.00 38.84
N
ATOM   1599  CA  VAL A 232     -35.023  34.731  11.637  1.00 39.60
C
ATOM   1600  C   VAL A 232     -35.421  33.735  12.728  1.00 40.08
C
ATOM   1601  O   VAL A 232     -36.607  33.631  13.074  1.00 40.68
O
ATOM   1602  CB  VAL A 232     -35.463  34.180  10.238  1.00 40.06
C
ATOM   1603  CG1 VAL A 232     -34.916  35.018   9.114  1.00 40.28
C
ATOM   1604  CG2 VAL A 232     -35.073  32.702  10.042  1.00 38.84
C
ATOM   1605  N   ASP A 233     -34.457  32.962  13.225  1.00 40.63
N
ATOM   1606  CA  ASP A 233     -34.751  31.927  14.212  1.00 40.59
C
ATOM   1607  C   ASP A 233     -34.913  32.583  15.580  1.00 40.88
C
ATOM   1608  O   ASP A 233     -35.705  32.138  16.421  1.00 41.87
O
ATOM   1609  CB  ASP A 233     -33.662  30.881  14.272  1.00 40.72
C
```

ATOM 1610 CG ASP A 233 -33.813 29.782 13.219 1.00 41.12
C
ATOM 1611 OD1 ASP A 233 -34.881 29.644 12.593 1.00 41.34
O
ATOM 1612 OD2 ASP A 233 -32.809 29.060 13.015 1.00 39.49
O
ATOM 1613 N VAL A 234 -34.218 33.685 15.764 1.00 39.77
N
ATOM 1614 CA VAL A 234 -34.317 34.487 16.996 1.00 39.85
C
ATOM 1615 C VAL A 234 -35.661 35.241 16.987 1.00 39.33
C
ATOM 1616 O VAL A 234 -36.291 35.358 18.017 1.00 39.18
O
ATOM 1617 CB VAL A 234 -33.134 35.482 17.154 1.00 39.98
C
ATOM 1618 CG1 VAL A 234 -33.304 36.387 18.413 1.00 39.46
C
ATOM 1619 CG2 VAL A 234 -31.824 34.726 17.334 1.00 41.68
C
ATOM 1620 N TRP A 235 -36.095 35.733 15.826 1.00 39.30
N
ATOM 1621 CA TRP A 235 -37.454 36.276 15.706 1.00 39.20
C
ATOM 1622 C TRP A 235 -38.472 35.236 16.172 1.00 39.34
C
ATOM 1623 O TRP A 235 -39.333 35.531 16.973 1.00 40.14
O
ATOM 1624 CB TRP A 235 -37.763 36.700 14.273 1.00 39.67
C
ATOM 1625 CG TRP A 235 -39.256 37.058 14.044 1.00 40.40
C
ATOM 1626 CD1 TRP A 235 -40.256 36.190 13.734 1.00 40.20
C
ATOM 1627 CD2 TRP A 235 -39.864 38.356 14.155 1.00 40.14
C
ATOM 1628 NE1 TRP A 235 -41.459 36.867 13.614 1.00 40.86
N
ATOM 1629 CE2 TRP A 235 -41.238 38.199 13.868 1.00 39.72
C
ATOM 1630 CE3 TRP A 235 -39.377 39.636 14.459 1.00 39.85
C
ATOM 1631 CZ2 TRP A 235 -42.135 39.266 13.879 1.00 40.12
C

```
ATOM   1632  CZ3 TRP A 235     -40.268  40.717  14.457  1.00 42.68
C
ATOM   1633  CH2 TRP A 235     -41.636  40.529  14.168  1.00 42.08
C
ATOM   1634  N   SER A 236     -38.388  34.029  15.632  1.00 39.00
N
ATOM   1635  CA  SER A 236     -39.355  32.982  15.952  1.00 39.14
C
ATOM   1636  C   SER A 236     -39.364  32.629  17.448  1.00 38.64
C
ATOM   1637  O   SER A 236     -40.415  32.503  18.042  1.00 39.97
O
ATOM   1638  CB  SER A 236     -39.058  31.740  15.123  1.00 38.04
C
ATOM   1639  OG  SER A 236     -39.133  32.018  13.721  1.00 40.89
O
ATOM   1640  N   ILE A 237     -38.205  32.416  18.043  1.00 38.41
N
ATOM   1641  CA  ILE A 237     -38.114  32.255  19.508  1.00 39.62
C
ATOM   1642  C   ILE A 237     -38.775  33.433  20.279  1.00 41.04
C
ATOM   1643  O   ILE A 237     -39.483  33.238  21.298  1.00 40.13
O
ATOM   1644  CB  ILE A 237     -36.657  32.058  19.926  1.00 39.93
C
ATOM   1645  CG1 ILE A 237     -36.132  30.796  19.225  1.00 38.65
C
ATOM   1646  CG2 ILE A 237     -36.518  31.955  21.446  1.00 41.20
C
ATOM   1647  CD1 ILE A 237     -34.676  30.504  19.459  1.00 41.02
C
ATOM   1648  N   GLY A 238     -38.534  34.660  19.801  1.00 41.54
N
ATOM   1649  CA  GLY A 238     -39.292  35.822  20.302  1.00 41.61
C
ATOM   1650  C   GLY A 238     -40.785  35.531  20.323  1.00 42.37
C
ATOM   1651  O   GLY A 238     -41.487  35.869  21.297  1.00 42.43
O
ATOM   1652  N   CYS A 239     -41.299  34.938  19.240  1.00 42.29
N
ATOM   1653  CA  CYS A 239     -42.742  34.792  19.094  1.00 41.64
C
```

```
ATOM   1654  C   CYS A 239     -43.190  33.673  19.995  1.00 41.99
C
ATOM   1655  O   CYS A 239     -44.255  33.769  20.582  1.00 40.86
O
ATOM   1656  CB  CYS A 239     -43.153  34.461  17.659  1.00 42.77
C
ATOM   1657  SG  CYS A 239     -43.039  35.804  16.455  1.00 45.20
S
ATOM   1658  N   ILE A 240     -42.376  32.606  20.081  1.00 40.55
N
ATOM   1659  CA  ILE A 240     -42.627  31.502  20.994  1.00 41.29
C
ATOM   1660  C   ILE A 240     -42.672  31.953  22.468  1.00 42.33
C
ATOM   1661  O   ILE A 240     -43.602  31.617  23.195  1.00 42.46
O
ATOM   1662  CB  ILE A 240     -41.583  30.355  20.777  1.00 41.80
C
ATOM   1663  CG1 ILE A 240     -41.845  29.707  19.397  1.00 41.32
C
ATOM   1664  CG2 ILE A 240     -41.673  29.312  21.903  1.00 42.33
C
ATOM   1665  CD1 ILE A 240     -40.642  28.932  18.807  1.00 40.08
C
ATOM   1666  N   MET A 241     -41.672  32.719  22.911  1.00 41.87
N
ATOM   1667  CA  MET A 241     -41.705  33.353  24.241  1.00 41.44
C
ATOM   1668  C   MET A 241     -42.990  34.148  24.536  1.00 41.33
C
ATOM   1669  O   MET A 241     -43.574  33.980  25.615  1.00 40.36
O
ATOM   1670  CB  MET A 241     -40.491  34.266  24.426  1.00 41.26
C
ATOM   1671  CG  MET A 241     -40.485  34.977  25.748  1.00 41.54
C
ATOM   1672  SD  MET A 241     -38.837  35.561  26.106  1.00 42.58
S
ATOM   1673  CE  MET A 241     -39.133  36.349  27.692  1.00 38.82
C
ATOM   1674  N   TYR A 242     -43.403  35.021  23.605  1.00 40.13
N
ATOM   1675  CA  TYR A 242     -44.646  35.761  23.736  1.00 40.97
C
```

```
ATOM   1676  C   TYR A 242     -45.781  34.761  23.894  1.00 40.84
C
ATOM   1677  O   TYR A 242     -46.581  34.890  24.801  1.00 41.32
O
ATOM   1678  CB  TYR A 242     -44.899  36.708  22.532  1.00 40.35
C
ATOM   1679  CG  TYR A 242     -46.167  37.581  22.600  1.00 39.59
C
ATOM   1680  CD1 TYR A 242     -47.436  37.030  22.431  1.00 38.47
C
ATOM   1681  CD2 TYR A 242     -46.080  38.969  22.769  1.00 38.23
C
ATOM   1682  CE1 TYR A 242     -48.616  37.837  22.499  1.00 37.13
C
ATOM   1683  CE2 TYR A 242     -47.208  39.763  22.808  1.00 39.39
C
ATOM   1684  CZ  TYR A 242     -48.477  39.198  22.664  1.00 38.53
C
ATOM   1685  OH  TYR A 242     -49.589  39.994  22.700  1.00 41.47
O
ATOM   1686  N   THR A 243     -45.849  33.768  23.006  1.00 41.15
N
ATOM   1687  CA  THR A 243     -46.950  32.813  23.031  1.00 41.36
C
ATOM   1688  C   THR A 243     -46.958  32.031  24.333  1.00 41.43
C
ATOM   1689  O   THR A 243     -48.004  31.811  24.931  1.00 41.32
O
ATOM   1690  CB  THR A 243     -46.872  31.842  21.814  1.00 40.86
C
ATOM   1691  OG1 THR A 243     -46.889  32.625  20.611  1.00 42.13
O
ATOM   1692  CG2 THR A 243     -48.095  30.881  21.793  1.00 42.35
C
ATOM   1693  N   LEU A 244     -45.787  31.605  24.775  1.00 40.35
N
ATOM   1694  CA  LEU A 244     -45.703  30.869  26.033  1.00 41.50
C
ATOM   1695  C   LEU A 244     -46.149  31.684  27.237  1.00 41.52
C
ATOM   1696  O   LEU A 244     -46.811  31.153  28.114  1.00 43.37
O
ATOM   1697  CB  LEU A 244     -44.289  30.283  26.255  1.00 40.43
C
```

ATOM 1698 CG LEU A 244 -43.836 29.161 25.300 1.00 41.27
C
ATOM 1699 CD1 LEU A 244 -42.474 28.659 25.740 1.00 42.25
C
ATOM 1700 CD2 LEU A 244 -44.857 28.015 25.196 1.00 41.57
C
ATOM 1701 N LEU A 245 -45.852 32.983 27.262 1.00 41.65
N
ATOM 1702 CA LEU A 245 -46.182 33.800 28.446 1.00 40.65
C
ATOM 1703 C LEU A 245 -47.525 34.496 28.393 1.00 41.59
C
ATOM 1704 O LEU A 245 -48.125 34.777 29.451 1.00 40.42
O
ATOM 1705 CB LEU A 245 -45.097 34.846 28.680 1.00 40.99
C
ATOM 1706 CG LEU A 245 -43.679 34.381 29.029 1.00 41.18
C
ATOM 1707 CD1 LEU A 245 -42.684 35.524 28.843 1.00 43.62
C
ATOM 1708 CD2 LEU A 245 -43.630 33.876 30.467 1.00 40.63
C
ATOM 1709 N VAL A 246 -47.983 34.800 27.179 1.00 41.76
N
ATOM 1710 CA VAL A 246 -49.230 35.524 26.978 1.00 43.06
C
ATOM 1711 C VAL A 246 -50.419 34.581 26.723 1.00 43.26
C
ATOM 1712 O VAL A 246 -51.536 34.901 27.099 1.00 42.27
O
ATOM 1713 CB VAL A 246 -49.087 36.595 25.856 1.00 43.13
C
ATOM 1714 CG1 VAL A 246 -50.407 37.314 25.594 1.00 42.96
C
ATOM 1715 CG2 VAL A 246 -47.968 37.599 26.198 1.00 43.03
C
ATOM 1716 N GLY A 247 -50.189 33.435 26.087 1.00 44.09
N
ATOM 1717 CA GLY A 247 -51.294 32.510 25.808 1.00 45.25
C
ATOM 1718 C GLY A 247 -51.844 32.609 24.395 1.00 45.87
C
ATOM 1719 O GLY A 247 -52.737 31.854 24.016 1.00 46.57
O

ATOM 1720 N LYS A 248 -51.302 33.535 23.607 1.00 46.03
N
ATOM 1721 CA LYS A 248 -51.652 33.678 22.200 1.00 46.38
C
ATOM 1722 C LYS A 248 -50.440 34.267 21.494 1.00 44.94
C
ATOM 1723 O LYS A 248 -49.619 34.918 22.144 1.00 44.23
O
ATOM 1724 CB LYS A 248 -52.883 34.598 22.014 1.00 46.55
C
ATOM 1725 CG LYS A 248 -52.720 35.943 22.641 1.00 46.98
C
ATOM 1726 CD LYS A 248 -53.775 36.953 22.203 1.00 50.49
C
ATOM 1727 CE LYS A 248 -53.500 38.316 22.896 1.00 56.44
C
ATOM 1728 NZ LYS A 248 -52.140 38.877 22.501 1.00 57.58
N1+
ATOM 1729 N PRO A 249 -50.326 34.045 20.170 1.00 44.90
N
ATOM 1730 CA PRO A 249 -49.224 34.564 19.366 1.00 44.86
C
ATOM 1731 C PRO A 249 -49.340 36.074 19.228 1.00 44.76
C
ATOM 1732 O PRO A 249 -50.455 36.585 19.310 1.00 44.46
O
ATOM 1733 CB PRO A 249 -49.433 33.896 18.005 1.00 45.46
C
ATOM 1734 CG PRO A 249 -50.441 32.854 18.225 1.00 46.65
C
ATOM 1735 CD PRO A 249 -51.276 33.292 19.339 1.00 45.23
C
ATOM 1736 N PRO A 250 -48.204 36.776 19.054 1.00 45.24
N
ATOM 1737 CA PRO A 250 -48.194 38.239 19.014 1.00 45.81
C
ATOM 1738 C PRO A 250 -48.913 38.890 17.841 1.00 47.10
C
ATOM 1739 O PRO A 250 -49.482 39.980 18.014 1.00 47.42
O
ATOM 1740 CB PRO A 250 -46.695 38.590 19.003 1.00 45.71
C
ATOM 1741 CG PRO A 250 -46.008 37.369 18.531 1.00 44.73
C

```
ATOM   1742  CD  PRO A 250     -46.839  36.213  18.969  1.00 44.54
C
ATOM   1743  N   PHE A 251     -48.905  38.263  16.669  1.00 48.17
N
ATOM   1744  CA  PHE A 251     -49.490  38.959  15.476  1.00 48.89
C
ATOM   1745  C   PHE A 251     -50.755  38.339  14.878  1.00 49.70
C
ATOM   1746  O   PHE A 251     -51.096  38.581  13.716  1.00 50.33
O
ATOM   1747  CB  PHE A 251     -48.440  39.128  14.376  1.00 47.77
C
ATOM   1748  CG  PHE A 251     -47.178  39.819  14.839  1.00 48.30
C
ATOM   1749  CD1 PHE A 251     -47.067  41.194  14.785  1.00 45.90
C
ATOM   1750  CD2 PHE A 251     -46.110  39.077  15.332  1.00 46.87
C
ATOM   1751  CE1 PHE A 251     -45.889  41.823  15.205  1.00 47.55
C
ATOM   1752  CE2 PHE A 251     -44.942  39.684  15.762  1.00 46.00
C
ATOM   1753  CZ  PHE A 251     -44.822  41.070  15.685  1.00 45.00
C
ATOM   1754  N   GLU A 252     -51.456  37.552  15.662  1.00 50.33
N
ATOM   1755  CA  GLU A 252     -52.635  36.854  15.187  1.00 50.38
C
ATOM   1756  C   GLU A 252     -53.720  37.786  14.689  1.00 49.78
C
ATOM   1757  O   GLU A 252     -53.998  38.797  15.323  1.00 49.31
O
ATOM   1758  CB  GLU A 252     -53.173  35.994  16.321  1.00 51.27
C
ATOM   1759  CG  GLU A 252     -53.918  34.780  15.844  1.00 55.59
C
ATOM   1760  CD  GLU A 252     -54.229  33.840  16.977  1.00 60.66
C
ATOM   1761  OE1 GLU A 252     -54.861  34.293  17.962  1.00 60.52
O
ATOM   1762  OE2 GLU A 252     -53.831  32.652  16.876  1.00 63.70
O
ATOM   1763  N   THR A 253     -54.301  37.451  13.530  1.00 48.64
N
```

```
ATOM   1764  CA  THR A 253     -55.522  38.069  13.005  1.00 48.24
C
ATOM   1765  C   THR A 253     -56.359  36.946  12.340  1.00 48.11
C
ATOM   1766  O   THR A 253     -55.961  35.769  12.378  1.00 48.96
O
ATOM   1767  CB  THR A 253     -55.236  39.160  11.944  1.00 48.11
C
ATOM   1768  OG1 THR A 253     -54.716  38.537  10.770  1.00 47.55
O
ATOM   1769  CG2 THR A 253     -54.241  40.217  12.446  1.00 48.86
C
ATOM   1770  N   SER A 254     -57.488  37.316  11.740  0.50 47.74
N
ATOM   1771  CA  SER A 254     -58.328  36.359  11.030  0.50 47.41
C
ATOM   1772  C   SER A 254     -57.899  36.128   9.570  0.50 47.09
C
ATOM   1773  O   SER A 254     -58.539  35.362   8.854  0.50 47.20
O
ATOM   1774  CB  SER A 254     -59.803  36.762  11.126  0.50 47.34
C
ATOM   1775  OG  SER A 254     -60.224  36.739  12.482  0.50 47.44
O
ATOM   1776  N   CYS A 255     -56.807  36.769   9.148  1.00 46.55
N
ATOM   1777  CA  CYS A 255     -56.275  36.589   7.788  1.00 47.11
C
ATOM   1778  C   CYS A 255     -54.772  36.626   7.839  1.00 48.17
C
ATOM   1779  O   CYS A 255     -54.200  37.582   8.333  1.00 48.21
O
ATOM   1780  CB  CYS A 255     -56.774  37.686   6.855  1.00 45.78
C
ATOM   1781  SG  CYS A 255     -56.178  37.581   5.137  1.00 44.51
S
ATOM   1782  N   LEU A 256     -54.157  35.575   7.305  1.00 49.94
N
ATOM   1783  CA  LEU A 256     -52.706  35.428   7.212  1.00 51.46
C
ATOM   1784  C   LEU A 256     -52.027  36.650   6.586  1.00 50.34
C
ATOM   1785  O   LEU A 256     -50.961  37.084   7.044  1.00 50.46
O
```

ATOM 1786 CB LEU A 256 -52.394 34.205 6.355 1.00 52.62
C
ATOM 1787 CG LEU A 256 -50.918 33.874 6.199 1.00 54.35
C
ATOM 1788 CD1 LEU A 256 -50.343 33.466 7.566 1.00 60.03
C
ATOM 1789 CD2 LEU A 256 -50.738 32.781 5.132 1.00 55.07
C
ATOM 1790 N LYS A 257 -52.644 37.202 5.540 1.00 49.23
N
ATOM 1791 CA LYS A 257 -52.094 38.376 4.877 1.00 48.52
C
ATOM 1792 C LYS A 257 -52.138 39.628 5.759 1.00 47.69
C
ATOM 1793 O LYS A 257 -51.250 40.480 5.670 1.00 47.16
O
ATOM 1794 CB LYS A 257 -52.744 38.613 3.510 1.00 49.11
C
ATOM 1795 CG LYS A 257 -52.530 37.496 2.495 1.00 49.28
C
ATOM 1796 CD LYS A 257 -51.056 37.200 2.228 1.00 54.51
C
ATOM 1797 CE LYS A 257 -50.842 36.308 1.002 1.00 55.19
C
ATOM 1798 NZ LYS A 257 -51.442 34.942 1.196 1.00 58.04
N1+
ATOM 1799 N GLU A 258 -53.160 39.744 6.603 1.00 47.07
N
ATOM 1800 CA GLU A 258 -53.230 40.846 7.573 1.00 47.59
C
ATOM 1801 C GLU A 258 -52.167 40.629 8.646 1.00 47.89
C
ATOM 1802 O GLU A 258 -51.602 41.587 9.160 1.00 48.40
O
ATOM 1803 CB GLU A 258 -54.608 40.951 8.222 1.00 47.18
C
ATOM 1804 CG GLU A 258 -55.765 41.260 7.226 1.00 50.10
C
ATOM 1805 CD GLU A 258 -55.903 42.739 6.901 1.00 53.64
C
ATOM 1806 OE1 GLU A 258 -55.088 43.537 7.418 1.00 55.78
O
ATOM 1807 OE2 GLU A 258 -56.839 43.112 6.144 1.00 55.79
O

ATOM 1808 N THR A 259 -51.903 39.370 8.982 1.00 48.19
N
ATOM 1809 CA THR A 259 -50.848 39.037 9.949 1.00 48.68
C
ATOM 1810 C THR A 259 -49.492 39.493 9.417 1.00 49.80
C
ATOM 1811 O THR A 259 -48.719 40.159 10.135 1.00 50.16
O
ATOM 1812 CB THR A 259 -50.921 37.547 10.317 1.00 48.21
C
ATOM 1813 OG1 THR A 259 -52.112 37.360 11.080 1.00 50.00
O
ATOM 1814 CG2 THR A 259 -49.723 37.062 11.159 1.00 47.57
C
ATOM 1815 N TYR A 260 -49.232 39.190 8.143 1.00 50.04
N
ATOM 1816 CA TYR A 260 -47.994 39.600 7.488 1.00 50.57
C
ATOM 1817 C TYR A 260 -47.831 41.111 7.496 1.00 50.54
C
ATOM 1818 O TYR A 260 -46.731 41.638 7.707 1.00 49.83
O
ATOM 1819 CB TYR A 260 -47.961 39.086 6.045 1.00 52.04
C
ATOM 1820 CG TYR A 260 -47.855 37.593 5.921 1.00 52.77
C
ATOM 1821 CD1 TYR A 260 -47.542 36.800 7.026 1.00 52.46
C
ATOM 1822 CD2 TYR A 260 -48.036 36.974 4.690 1.00 55.42
C
ATOM 1823 CE1 TYR A 260 -47.421 35.419 6.905 1.00 55.08
C
ATOM 1824 CE2 TYR A 260 -47.928 35.601 4.555 1.00 54.68
C
ATOM 1825 CZ TYR A 260 -47.603 34.832 5.664 1.00 56.37
C
ATOM 1826 OH TYR A 260 -47.489 33.461 5.529 1.00 56.86
O
ATOM 1827 N LEU A 261 -48.929 41.813 7.247 1.00 50.27
N
ATOM 1828 CA LEU A 261 -48.913 43.262 7.307 1.00 50.15
C
ATOM 1829 C LEU A 261 -48.492 43.725 8.674 1.00 49.92
C

ATOM 1830 O LEU A 261 -47.606 44.567 8.799 1.00 49.56
O
ATOM 1831 CB LEU A 261 -50.278 43.848 6.957 1.00 50.42
C
ATOM 1832 CG LEU A 261 -50.277 44.642 5.666 1.00 52.79
C
ATOM 1833 CD1 LEU A 261 -49.937 43.726 4.486 1.00 55.38
C
ATOM 1834 CD2 LEU A 261 -51.638 45.296 5.480 1.00 53.43
C
ATOM 1835 N ARG A 262 -49.115 43.160 9.705 1.00 49.89
N
ATOM 1836 CA ARG A 262 -48.769 43.530 11.062 1.00 50.75
C
ATOM 1837 C ARG A 262 -47.309 43.291 11.391 1.00 50.89
C
ATOM 1838 O ARG A 262 -46.674 44.158 11.988 1.00 51.07
O
ATOM 1839 CB ARG A 262 -49.638 42.799 12.055 1.00 51.36
C
ATOM 1840 CG ARG A 262 -51.025 43.309 12.068 1.00 52.22
C
ATOM 1841 CD ARG A 262 -51.563 43.121 13.418 1.00 54.93
C
ATOM 1842 NE ARG A 262 -52.983 43.428 13.429 1.00 59.45
N
ATOM 1843 CZ ARG A 262 -53.792 43.075 14.416 1.00 60.28
C
ATOM 1844 NH1 ARG A 262 -55.083 43.394 14.362 1.00 58.86
N
ATOM 1845 NH2 ARG A 262 -53.296 42.391 15.448 1.00 59.47
N
ATOM 1846 N ILE A 263 -46.786 42.126 11.000 1.00 50.86
N
ATOM 1847 CA ILE A 263 -45.375 41.754 11.222 1.00 51.32
C
ATOM 1848 C ILE A 263 -44.443 42.764 10.581 1.00 52.93
C
ATOM 1849 O ILE A 263 -43.512 43.261 11.217 1.00 53.24
O
ATOM 1850 CB ILE A 263 -45.073 40.320 10.672 1.00 51.76
C
ATOM 1851 CG1 ILE A 263 -45.711 39.259 11.578 1.00 48.15
C

ATOM 1852 CG2 ILE A 263 -43.555 40.084 10.561 1.00 51.58
C
ATOM 1853 CD1 ILE A 263 -45.826 37.823 10.943 1.00 50.47
C
ATOM 1854 N LYS A 264 -44.712 43.091 9.320 1.00 54.15
N
ATOM 1855 CA LYS A 264 -43.914 44.067 8.601 1.00 55.68
C
ATOM 1856 C LYS A 264 -43.946 45.412 9.303 1.00 55.51
C
ATOM 1857 O LYS A 264 -42.946 46.113 9.344 1.00 55.93
O
ATOM 1858 CB LYS A 264 -44.390 44.173 7.150 1.00 55.77
C
ATOM 1859 CG LYS A 264 -43.994 42.943 6.294 1.00 57.65
C
ATOM 1860 CD LYS A 264 -44.797 42.861 4.975 1.00 58.03
C
ATOM 1861 CE LYS A 264 -44.301 43.868 3.938 1.00 65.13
C
ATOM 1862 NZ LYS A 264 -43.636 43.206 2.747 1.00 69.15
N1+
ATOM 1863 N LYS A 265 -45.093 45.755 9.876 1.00 55.97
N
ATOM 1864 CA LYS A 265 -45.282 47.051 10.540 1.00 56.16
C
ATOM 1865 C LYS A 265 -44.913 46.974 12.016 1.00 55.77
C
ATOM 1866 O LYS A 265 -45.065 47.957 12.746 1.00 55.41
O
ATOM 1867 CB LYS A 265 -46.739 47.514 10.430 1.00 56.49
C
ATOM 1868 CG LYS A 265 -47.202 47.966 9.048 1.00 58.66
C
ATOM 1869 CD LYS A 265 -48.561 48.630 9.162 1.00 61.79
C
ATOM 1870 CE LYS A 265 -49.492 48.206 8.042 1.00 63.76
C
ATOM 1871 NZ LYS A 265 -50.857 48.775 8.235 1.00 65.37
N1+
ATOM 1872 N ASN A 266 -44.451 45.799 12.447 1.00 55.35
N
ATOM 1873 CA ASN A 266 -44.190 45.489 13.861 1.00 55.15
C

```
ATOM   1874  C   ASN A 266     -45.356  45.814  14.806  1.00 54.34
C
ATOM   1875  O   ASN A 266     -45.153  46.275  15.925  1.00 54.59
O
ATOM   1876  CB  ASN A 266     -42.881  46.146  14.352  1.00 56.13
C
ATOM   1877  CG  ASN A 266     -42.287  45.441  15.573  1.00 57.26
C
ATOM   1878  OD1 ASN A 266     -42.036  46.077  16.605  1.00 59.84
O
ATOM   1879  ND2 ASN A 266     -42.073  44.124  15.466  1.00 57.64
N
ATOM   1880  N   GLU A 267     -46.574  45.548  14.360  1.00 53.53
N
ATOM   1881  CA  GLU A 267     -47.768  45.874  15.146  1.00 53.11
C
ATOM   1882  C   GLU A 267     -48.193  44.764  16.116  1.00 52.76
C
ATOM   1883  O   GLU A 267     -48.982  43.879  15.765  1.00 52.56
O
ATOM   1884  CB  GLU A 267     -48.924  46.247  14.217  1.00 53.06
C
ATOM   1885  CG  GLU A 267     -49.060  47.744  14.027  1.00 54.52
C
ATOM   1886  CD  GLU A 267     -50.103  48.136  12.993  1.00 55.75
C
ATOM   1887  OE1 GLU A 267     -50.416  47.323  12.102  1.00 55.99
O
ATOM   1888  OE2 GLU A 267     -50.606  49.277  13.071  1.00 57.48
O
ATOM   1889  N   TYR A 268     -47.639  44.812  17.327  1.00 51.81
N
ATOM   1890  CA  TYR A 268     -48.019  43.918  18.430  1.00 50.93
C
ATOM   1891  C   TYR A 268     -47.933  44.741  19.708  1.00 50.63
C
ATOM   1892  O   TYR A 268     -47.319  45.813  19.719  1.00 50.53
O
ATOM   1893  CB  TYR A 268     -47.110  42.675  18.508  1.00 50.44
C
ATOM   1894  CG  TYR A 268     -45.720  42.937  19.061  1.00 50.42
C
ATOM   1895  CD1 TYR A 268     -44.719  43.476  18.258  1.00 49.79
C
```

ATOM 1896 CD2 TYR A 268 -45.402 42.623 20.389 1.00 50.71
C
ATOM 1897 CE1 TYR A 268 -43.434 43.713 18.765 1.00 50.54
C
ATOM 1898 CE2 TYR A 268 -44.121 42.850 20.909 1.00 46.97
C
ATOM 1899 CZ TYR A 268 -43.155 43.398 20.094 1.00 50.09
C
ATOM 1900 OH TYR A 268 -41.912 43.660 20.599 1.00 50.49
O
ATOM 1901 N SER A 269 -48.556 44.252 20.772 1.00 50.35
N
ATOM 1902 CA SER A 269 -48.364 44.835 22.097 1.00 50.79
C
ATOM 1903 C SER A 269 -48.288 43.732 23.150 1.00 50.51
C
ATOM 1904 O SER A 269 -48.859 42.647 22.979 1.00 50.22
O
ATOM 1905 CB SER A 269 -49.476 45.836 22.423 1.00 51.28
C
ATOM 1906 OG SER A 269 -50.739 45.208 22.366 1.00 53.58
O
ATOM 1907 N ILE A 270 -47.547 44.007 24.216 1.00 50.26
N
ATOM 1908 CA ILE A 270 -47.330 43.049 25.279 1.00 50.37
C
ATOM 1909 C ILE A 270 -48.257 43.487 26.404 1.00 51.21
C
ATOM 1910 O ILE A 270 -48.257 44.661 26.785 1.00 50.37
O
ATOM 1911 CB ILE A 270 -45.830 43.029 25.726 1.00 50.84
C
ATOM 1912 CG1 ILE A 270 -44.921 42.642 24.552 1.00 50.93
C
ATOM 1913 CG2 ILE A 270 -45.586 42.014 26.846 1.00 49.94
C
ATOM 1914 CD1 ILE A 270 -43.446 42.823 24.810 1.00 50.28
C
ATOM 1915 N PRO A 271 -49.086 42.557 26.913 1.00 51.58
N
ATOM 1916 CA PRO A 271 -50.003 42.851 28.023 1.00 52.24
C
ATOM 1917 C PRO A 271 -49.278 43.354 29.279 1.00 52.73
C

```
ATOM   1918  O   PRO A 271     -48.148  42.969  29.532  1.00 52.71
O
ATOM   1919  CB  PRO A 271     -50.682  41.507  28.288  1.00 52.42
C
ATOM   1920  CG  PRO A 271     -50.458  40.698  27.047  1.00 51.77
C
ATOM   1921  CD  PRO A 271     -49.198  41.168  26.441  1.00 51.42
C
ATOM   1922  N   LYS A 272     -49.933  44.215  30.062  1.00 53.19
N
ATOM   1923  CA  LYS A 272     -49.259  44.893  31.176  1.00 53.60
C
ATOM   1924  C   LYS A 272     -48.838  43.962  32.321  1.00 53.37
C
ATOM   1925  O   LYS A 272     -47.967  44.317  33.135  1.00 53.12
O
ATOM   1926  CB  LYS A 272     -50.118  46.042  31.723  1.00 54.04
C
ATOM   1927  CG  LYS A 272     -50.656  47.030  30.674  1.00 55.70
C
ATOM   1928  CD  LYS A 272     -49.562  47.913  30.058  1.00 58.03
C
ATOM   1929  CE  LYS A 272     -50.113  49.294  29.671  1.00 58.37
C
ATOM   1930  NZ  LYS A 272     -50.425  50.130  30.876  1.00 59.16
N1+
ATOM   1931  N   HIS A 273     -49.458  42.784  32.385  1.00 53.08
N
ATOM   1932  CA  HIS A 273     -49.164  41.816  33.443  1.00 52.45
C
ATOM   1933  C   HIS A 273     -47.884  41.015  33.200  1.00 51.99
C
ATOM   1934  O   HIS A 273     -47.370  40.377  34.122  1.00 51.22
O
ATOM   1935  CB  HIS A 273     -50.355  40.886  33.682  1.00 52.99
C
ATOM   1936  CG  HIS A 273     -50.658  39.986  32.529  1.00 53.96
C
ATOM   1937  ND1 HIS A 273     -51.475  40.364  31.489  1.00 56.15
N
ATOM   1938  CD2 HIS A 273     -50.258  38.723  32.252  1.00 54.73
C
ATOM   1939  CE1 HIS A 273     -51.570  39.373  30.621  1.00 55.54
C
```

ATOM 1940 NE2 HIS A 273 -50.838 38.366 31.059 1.00 56.12
N
ATOM 1941 N ILE A 274 -47.372 41.049 31.968 1.00 51.20
N
ATOM 1942 CA ILE A 274 -46.065 40.471 31.676 1.00 51.16
C
ATOM 1943 C ILE A 274 -45.002 41.291 32.396 1.00 51.35
C
ATOM 1944 O ILE A 274 -45.042 42.527 32.399 1.00 51.07
O
ATOM 1945 CB ILE A 274 -45.780 40.407 30.148 1.00 50.98
C
ATOM 1946 CG1 ILE A 274 -46.831 39.546 29.427 1.00 50.66
C
ATOM 1947 CG2 ILE A 274 -44.349 39.909 29.843 1.00 50.77
C
ATOM 1948 CD1 ILE A 274 -47.147 38.184 30.072 1.00 49.90
C
ATOM 1949 N ASN A 275 -44.069 40.595 33.029 1.00 51.68
N
ATOM 1950 CA ASN A 275 -43.053 41.246 33.827 1.00 52.28
C
ATOM 1951 C ASN A 275 -42.070 42.010 32.933 1.00 52.02
C
ATOM 1952 O ASN A 275 -41.750 41.544 31.841 1.00 52.63
O
ATOM 1953 CB ASN A 275 -42.373 40.210 34.716 1.00 52.75
C
ATOM 1954 CG ASN A 275 -43.303 39.694 35.825 1.00 55.66
C
ATOM 1955 OD1 ASN A 275 -44.157 40.432 36.338 1.00 57.26
O
ATOM 1956 ND2 ASN A 275 -43.138 38.426 36.199 1.00 57.40
N
ATOM 1957 N PRO A 276 -41.625 43.204 33.369 1.00 51.54
N
ATOM 1958 CA PRO A 276 -40.752 44.061 32.552 1.00 50.77
C
ATOM 1959 C PRO A 276 -39.517 43.354 31.987 1.00 50.14
C
ATOM 1960 O PRO A 276 -39.151 43.597 30.841 1.00 49.94
O
ATOM 1961 CB PRO A 276 -40.348 45.173 33.519 1.00 51.14
C

ATOM 1962 CG PRO A 276 -41.496 45.264 34.463 1.00 51.52
C
ATOM 1963 CD PRO A 276 -41.927 43.825 34.669 1.00 51.62
C
ATOM 1964 N VAL A 277 -38.891 42.483 32.775 1.00 49.30
N
ATOM 1965 CA VAL A 277 -37.715 41.721 32.327 1.00 48.76
C
ATOM 1966 C VAL A 277 -38.039 40.807 31.135 1.00 48.53
C
ATOM 1967 O VAL A 277 -37.303 40.788 30.140 1.00 48.51
O
ATOM 1968 CB VAL A 277 -37.062 40.961 33.505 1.00 48.69
C
ATOM 1969 CG1 VAL A 277 -35.965 40.020 33.027 1.00 50.79
C
ATOM 1970 CG2 VAL A 277 -36.490 41.964 34.524 1.00 48.59
C
ATOM 1971 N ALA A 278 -39.140 40.069 31.236 1.00 47.81
N
ATOM 1972 CA ALA A 278 -39.618 39.224 30.140 1.00 47.94
C
ATOM 1973 C ALA A 278 -39.973 40.091 28.935 1.00 47.62
C
ATOM 1974 O ALA A 278 -39.491 39.842 27.835 1.00 48.25
O
ATOM 1975 CB ALA A 278 -40.834 38.403 30.576 1.00 47.21
C
ATOM 1976 N ALA A 279 -40.791 41.118 29.164 1.00 47.18
N
ATOM 1977 CA ALA A 279 -41.267 42.012 28.110 1.00 46.81
C
ATOM 1978 C ALA A 279 -40.090 42.644 27.375 1.00 46.94
C
ATOM 1979 O ALA A 279 -40.107 42.805 26.158 1.00 46.79
O
ATOM 1980 CB ALA A 279 -42.181 43.104 28.715 1.00 47.24
C
ATOM 1981 N SER A 280 -39.055 42.988 28.122 1.00 47.31
N
ATOM 1982 CA SER A 280 -37.847 43.544 27.535 1.00 47.88
C
ATOM 1983 C SER A 280 -37.206 42.578 26.548 1.00 47.38
C

ATOM 1984 O SER A 280 -36.877 42.977 25.438 1.00 47.82
O
ATOM 1985 CB SER A 280 -36.852 43.904 28.610 1.00 47.15
C
ATOM 1986 OG SER A 280 -36.265 45.135 28.268 1.00 51.62
O
ATOM 1987 N LEU A 281 -37.051 41.315 26.953 1.00 47.72
N
ATOM 1988 CA LEU A 281 -36.450 40.295 26.100 1.00 47.13
C
ATOM 1989 C LEU A 281 -37.300 40.028 24.855 1.00 48.27
C
ATOM 1990 O LEU A 281 -36.763 39.949 23.746 1.00 49.42
O
ATOM 1991 CB LEU A 281 -36.193 39.001 26.880 1.00 47.13
C
ATOM 1992 CG LEU A 281 -35.511 37.836 26.109 1.00 46.93
C
ATOM 1993 CD1 LEU A 281 -34.236 38.253 25.372 1.00 45.44
C
ATOM 1994 CD2 LEU A 281 -35.224 36.644 27.007 1.00 46.66
C
ATOM 1995 N ILE A 282 -38.608 39.840 25.031 1.00 48.11
N
ATOM 1996 CA ILE A 282 -39.522 39.745 23.881 1.00 47.43
C
ATOM 1997 C ILE A 282 -39.301 40.907 22.892 1.00 48.71
C
ATOM 1998 O ILE A 282 -39.145 40.686 21.689 1.00 48.82
O
ATOM 1999 CB ILE A 282 -41.015 39.704 24.324 1.00 48.00
C
ATOM 2000 CG1 ILE A 282 -41.339 38.428 25.103 1.00 47.07
C
ATOM 2001 CG2 ILE A 282 -41.957 39.794 23.108 1.00 45.89
C
ATOM 2002 CD1 ILE A 282 -42.661 38.512 25.916 1.00 45.63
C
ATOM 2003 N GLN A 283 -39.314 42.141 23.398 1.00 48.83
N
ATOM 2004 CA GLN A 283 -39.076 43.328 22.577 1.00 49.97
C
ATOM 2005 C GLN A 283 -37.766 43.302 21.803 1.00 50.27
C

ATOM 2006 O GLN A 283 -37.752 43.667 20.630 1.00 50.71
O
ATOM 2007 CB GLN A 283 -39.092 44.593 23.434 1.00 50.09
C
ATOM 2008 CG GLN A 283 -40.475 45.071 23.744 1.00 53.22
C
ATOM 2009 CD GLN A 283 -40.462 46.260 24.678 1.00 57.24
C
ATOM 2010 OE1 GLN A 283 -40.744 47.392 24.272 1.00 60.01
O
ATOM 2011 NE2 GLN A 283 -40.114 46.017 25.937 1.00 59.07
N
ATOM 2012 N LYS A 284 -36.674 42.916 22.476 1.00 50.21
N
ATOM 2013 CA LYS A 284 -35.350 42.780 21.861 1.00 50.48
C
ATOM 2014 C LYS A 284 -35.381 41.820 20.679 1.00 50.63
C
ATOM 2015 O LYS A 284 -34.797 42.091 19.620 1.00 50.01
O
ATOM 2016 CB LYS A 284 -34.341 42.230 22.877 1.00 50.59
C
ATOM 2017 CG LYS A 284 -33.851 43.215 23.965 1.00 52.34
C
ATOM 2018 CD LYS A 284 -33.126 42.415 25.083 1.00 51.92
C
ATOM 2019 CE LYS A 284 -33.031 43.217 26.391 1.00 57.82
C
ATOM 2020 NZ LYS A 284 -32.967 42.306 27.587 1.00 57.99
N1+
ATOM 2021 N MET A 285 -36.045 40.687 20.874 1.00 49.93
N
ATOM 2022 CA MET A 285 -36.047 39.638 19.877 1.00 51.55
C
ATOM 2023 C MET A 285 -36.979 39.974 18.713 1.00 51.87
C
ATOM 2024 O MET A 285 -36.750 39.535 17.594 1.00 52.82
O
ATOM 2025 CB MET A 285 -36.457 38.301 20.502 1.00 50.41
C
ATOM 2026 CG MET A 285 -35.395 37.701 21.435 1.00 49.77
C
ATOM 2027 SD MET A 285 -35.774 35.964 21.743 1.00 54.63
S

ATOM 2028 CE MET A 285 -36.653 36.168 23.270 1.00 47.15
C
ATOM 2029 N LEU A 286 -38.041 40.730 18.989 1.00 52.12
N
ATOM 2030 CA LEU A 286 -39.053 41.008 17.967 1.00 51.91
C
ATOM 2031 C LEU A 286 -38.803 42.331 17.248 1.00 52.25
C
ATOM 2032 O LEU A 286 -39.731 42.960 16.794 1.00 54.56
O
ATOM 2033 CB LEU A 286 -40.478 40.951 18.544 1.00 50.80
C
ATOM 2034 CG LEU A 286 -41.017 39.557 18.920 1.00 49.27
C
ATOM 2035 CD1 LEU A 286 -42.462 39.564 19.436 1.00 50.00
C
ATOM 2036 CD2 LEU A 286 -40.902 38.584 17.769 1.00 50.25
C
ATOM 2037 N GLN A 287 -37.558 42.744 17.117 1.00 52.47
N
ATOM 2038 CA GLN A 287 -37.253 43.987 16.392 1.00 52.08
C
ATOM 2039 C GLN A 287 -37.331 43.741 14.886 1.00 51.55
C
ATOM 2040 O GLN A 287 -37.016 42.636 14.401 1.00 49.00
O
ATOM 2041 CB GLN A 287 -35.882 44.496 16.788 1.00 52.52
C
ATOM 2042 CG GLN A 287 -35.867 45.111 18.191 1.00 56.01
C
ATOM 2043 CD GLN A 287 -34.482 45.396 18.686 1.00 58.13
C
ATOM 2044 OE1 GLN A 287 -34.027 46.535 18.662 1.00 59.77
O
ATOM 2045 NE2 GLN A 287 -33.792 44.357 19.146 1.00 58.34
N
ATOM 2046 N THR A 288 -37.778 44.759 14.153 1.00 51.02
N
ATOM 2047 CA THR A 288 -37.958 44.642 12.702 1.00 51.78
C
ATOM 2048 C THR A 288 -36.591 44.407 12.031 1.00 52.22
C
ATOM 2049 O THR A 288 -36.437 43.507 11.179 1.00 52.08
O

ATOM 2050 CB THR A 288 -38.685 45.885 12.116 1.00 51.66
C
ATOM 2051 OG1 THR A 288 -40.019 45.945 12.636 1.00 51.00
O
ATOM 2052 CG2 THR A 288 -38.768 45.811 10.605 1.00 52.52
C
ATOM 2053 N ASP A 289 -35.612 45.190 12.471 1.00 52.26
N
ATOM 2054 CA ASP A 289 -34.232 45.159 11.977 1.00 52.63
C
ATOM 2055 C ASP A 289 -33.489 43.945 12.536 1.00 51.98
C
ATOM 2056 O ASP A 289 -33.187 43.929 13.730 1.00 51.76
O
ATOM 2057 CB ASP A 289 -33.520 46.447 12.411 1.00 52.57
C
ATOM 2058 CG ASP A 289 -32.080 46.553 11.893 1.00 54.18
C
ATOM 2059 OD1 ASP A 289 -31.521 45.552 11.398 1.00 56.06
O
ATOM 2060 OD2 ASP A 289 -31.497 47.658 11.974 1.00 56.07
O
ATOM 2061 N PRO A 290 -33.153 42.949 11.673 1.00 51.77
N
ATOM 2062 CA PRO A 290 -32.563 41.696 12.174 1.00 51.45
C
ATOM 2063 C PRO A 290 -31.243 41.921 12.884 1.00 51.32
C
ATOM 2064 O PRO A 290 -30.901 41.158 13.786 1.00 51.19
O
ATOM 2065 CB PRO A 290 -32.340 40.870 10.904 1.00 51.40
C
ATOM 2066 CG PRO A 290 -32.292 41.873 9.801 1.00 50.55
C
ATOM 2067 CD PRO A 290 -33.284 42.923 10.203 1.00 51.68
C
ATOM 2068 N THR A 291 -30.516 42.968 12.498 1.00 51.55
N
ATOM 2069 CA THR A 291 -29.220 43.230 13.099 1.00 52.02
C
ATOM 2070 C THR A 291 -29.374 43.786 14.516 1.00 52.32
C
ATOM 2071 O THR A 291 -28.380 43.902 15.238 1.00 52.25
O

ATOM 2072 CB THR A 291 -28.353 44.215 12.262 1.00 52.25
C
ATOM 2073 OG1 THR A 291 -29.023 45.474 12.152 1.00 52.79
O
ATOM 2074 CG2 THR A 291 -28.082 43.656 10.863 1.00 52.72
C
ATOM 2075 N ALA A 292 -30.606 44.143 14.896 1.00 51.52
N
ATOM 2076 CA ALA A 292 -30.864 44.772 16.194 1.00 51.23
C
ATOM 2077 C ALA A 292 -31.134 43.725 17.255 1.00 50.68
C
ATOM 2078 O ALA A 292 -30.962 43.975 18.452 1.00 50.53
O
ATOM 2079 CB ALA A 292 -32.044 45.719 16.100 1.00 51.66
C
ATOM 2080 N ARG A 293 -31.594 42.566 16.802 1.00 49.43
N
ATOM 2081 CA ARG A 293 -31.937 41.436 17.668 1.00 48.53
C
ATOM 2082 C ARG A 293 -30.695 40.848 18.294 1.00 48.43
C
ATOM 2083 O ARG A 293 -29.603 40.967 17.722 1.00 48.17
O
ATOM 2084 CB ARG A 293 -32.590 40.351 16.827 1.00 48.23
C
ATOM 2085 CG ARG A 293 -33.852 40.792 16.200 1.00 46.88
C
ATOM 2086 CD ARG A 293 -34.431 39.724 15.315 1.00 45.02
C
ATOM 2087 NE ARG A 293 -35.284 40.366 14.321 1.00 46.42
N
ATOM 2088 CZ ARG A 293 -35.538 39.904 13.098 1.00 48.81
C
ATOM 2089 NH1 ARG A 293 -35.024 38.747 12.696 1.00 45.01
N
ATOM 2090 NH2 ARG A 293 -36.304 40.632 12.274 1.00 47.97
N
ATOM 2091 N PRO A 294 -30.840 40.214 19.471 1.00 48.13
N
ATOM 2092 CA PRO A 294 -29.730 39.464 20.056 1.00 48.15
C
ATOM 2093 C PRO A 294 -29.439 38.267 19.188 1.00 47.43
C

ATOM 2094 O PRO A 294 -30.350 37.757 18.542 1.00 47.31
O
ATOM 2095 CB PRO A 294 -30.306 38.951 21.385 1.00 47.69
C
ATOM 2096 CG PRO A 294 -31.453 39.834 21.649 1.00 49.45
C
ATOM 2097 CD PRO A 294 -32.027 40.174 20.332 1.00 48.48
C
ATOM 2098 N THR A 295 -28.195 37.797 19.186 1.00 45.80
N
ATOM 2099 CA THR A 295 -27.902 36.554 18.491 1.00 44.93
C
ATOM 2100 C THR A 295 -28.175 35.399 19.426 1.00 45.12
C
ATOM 2101 O THR A 295 -28.257 35.574 20.644 1.00 44.98
O
ATOM 2102 CB THR A 295 -26.450 36.475 18.070 1.00 45.30
C
ATOM 2103 OG1 THR A 295 -25.645 36.482 19.247 1.00 42.21
O
ATOM 2104 CG2 THR A 295 -26.081 37.660 17.178 1.00 46.34
C
ATOM 2105 N ILE A 296 -28.271 34.194 18.881 1.00 45.27
N
ATOM 2106 CA ILE A 296 -28.671 33.072 19.693 1.00 45.78
C
ATOM 2107 C ILE A 296 -27.782 32.907 20.931 1.00 46.95
C
ATOM 2108 O ILE A 296 -28.257 32.496 21.988 1.00 47.97
O
ATOM 2109 CB ILE A 296 -28.787 31.734 18.861 1.00 45.30
C
ATOM 2110 CG1 ILE A 296 -29.669 30.713 19.599 1.00 43.16
C
ATOM 2111 CG2 ILE A 296 -27.401 31.176 18.492 1.00 45.02
C
ATOM 2112 CD1 ILE A 296 -31.227 30.987 19.528 1.00 40.32
C
ATOM 2113 N ASN A 297 -26.500 33.239 20.806 1.00 48.49
N
ATOM 2114 CA ASN A 297 -25.549 32.999 21.893 1.00 49.36
C
ATOM 2115 C ASN A 297 -25.694 33.986 23.056 1.00 49.35
C

```
ATOM   2116  O   ASN A 297     -25.123  33.783  24.123  1.00 50.13
O
ATOM   2117  CB  ASN A 297     -24.108  32.968  21.359  1.00 50.21
C
ATOM   2118  CG  ASN A 297     -23.706  31.618  20.757  1.00 52.58
C
ATOM   2119  OD1 ASN A 297     -22.550  31.418  20.405  1.00 57.89
O
ATOM   2120  ND2 ASN A 297     -24.639  30.696  20.655  1.00 56.10
N
ATOM   2121  N   GLU A 298     -26.478  35.041  22.869  1.00 49.22
N
ATOM   2122  CA  GLU A 298     -26.621  36.066  23.895  1.00 50.33
C
ATOM   2123  C   GLU A 298     -27.825  35.824  24.803  1.00 50.47
C
ATOM   2124  O   GLU A 298     -27.924  36.409  25.895  1.00 50.84
O
ATOM   2125  CB  GLU A 298     -26.815  37.432  23.247  1.00 50.39
C
ATOM   2126  CG  GLU A 298     -25.656  37.966  22.477  1.00 52.45
C
ATOM   2127  CD  GLU A 298     -25.937  39.363  21.991  1.00 54.86
C
ATOM   2128  OE1 GLU A 298     -26.420  39.519  20.855  1.00 53.30
O
ATOM   2129  OE2 GLU A 298     -25.694  40.307  22.774  1.00 57.36
O
ATOM   2130  N   LEU A 299     -28.750  35.003  24.321  1.00 49.09
N
ATOM   2131  CA  LEU A 299     -30.065  34.865  24.916  1.00 49.12
C
ATOM   2132  C   LEU A 299     -30.032  34.386  26.349  1.00 48.48
C
ATOM   2133  O   LEU A 299     -30.682  34.992  27.190  1.00 48.53
O
ATOM   2134  CB  LEU A 299     -30.960  33.958  24.058  1.00 48.00
C
ATOM   2135  CG  LEU A 299     -31.400  34.607  22.741  1.00 49.14
C
ATOM   2136  CD1 LEU A 299     -32.341  33.678  21.956  1.00 49.27
C
ATOM   2137  CD2 LEU A 299     -32.096  35.947  23.000  1.00 49.88
C
```

ATOM 2138 N LEU A 300 -29.277 33.322 26.623 1.00 47.73
N
ATOM 2139 CA LEU A 300 -29.239 32.726 27.965 1.00 48.08
C
ATOM 2140 C LEU A 300 -28.564 33.570 29.010 1.00 48.50
C
ATOM 2141 O LEU A 300 -28.702 33.308 30.205 1.00 48.47
O
ATOM 2142 CB LEU A 300 -28.592 31.346 27.945 1.00 47.54
C
ATOM 2143 CG LEU A 300 -29.463 30.303 27.216 1.00 48.62
C
ATOM 2144 CD1 LEU A 300 -28.944 28.895 27.435 1.00 48.46
C
ATOM 2145 CD2 LEU A 300 -30.924 30.409 27.620 1.00 47.57
C
ATOM 2146 N ASN A 301 -27.800 34.560 28.548 1.00 49.17
N
ATOM 2147 CA ASN A 301 -27.186 35.544 29.423 1.00 49.24
C
ATOM 2148 C ASN A 301 -28.125 36.699 29.763 1.00 49.13
C
ATOM 2149 O ASN A 301 -27.759 37.594 30.532 1.00 49.01
O
ATOM 2150 CB ASN A 301 -25.940 36.078 28.755 1.00 50.03
C
ATOM 2151 CG ASN A 301 -24.925 34.994 28.505 1.00 51.93
C
ATOM 2152 OD1 ASN A 301 -24.473 34.326 29.440 1.00 52.66
O
ATOM 2153 ND2 ASN A 301 -24.563 34.805 27.234 1.00 53.75
N
ATOM 2154 N ASP A 302 -29.334 36.668 29.204 1.00 48.76
N
ATOM 2155 CA ASP A 302 -30.320 37.698 29.493 1.00 47.92
C
ATOM 2156 C ASP A 302 -30.782 37.636 30.923 1.00 47.65
C
ATOM 2157 O ASP A 302 -30.951 36.561 31.467 1.00 46.90
O
ATOM 2158 CB ASP A 302 -31.547 37.615 28.595 1.00 47.23
C
ATOM 2159 CG ASP A 302 -32.339 38.903 28.629 1.00 48.18
C

ATOM 2160 OD1 ASP A 302 -31.914 39.865 27.939 1.00 45.32
O
ATOM 2161 OD2 ASP A 302 -33.339 38.976 29.392 1.00 47.81
O
ATOM 2162 N GLU A 303 -31.029 38.809 31.503 1.00 47.04
N
ATOM 2163 CA GLU A 303 -31.590 38.923 32.835 1.00 48.08
C
ATOM 2164 C GLU A 303 -32.794 37.984 33.040 1.00 47.39
C
ATOM 2165 O GLU A 303 -32.966 37.435 34.127 1.00 47.78
O
ATOM 2166 CB GLU A 303 -31.958 40.395 33.142 1.00 47.45
C
ATOM 2167 CG GLU A 303 -32.547 40.599 34.535 1.00 49.71
C
ATOM 2168 CD GLU A 303 -32.786 42.062 34.901 1.00 50.05
C
ATOM 2169 OE1 GLU A 303 -32.668 42.949 34.011 1.00 51.94
O
ATOM 2170 OE2 GLU A 303 -33.080 42.317 36.097 1.00 51.86
O
ATOM 2171 N PHE A 304 -33.586 37.760 31.992 1.00 47.50
N
ATOM 2172 CA PHE A 304 -34.739 36.825 32.064 1.00 47.58
C
ATOM 2173 C PHE A 304 -34.357 35.431 32.530 1.00 48.78
C
ATOM 2174 O PHE A 304 -35.129 34.778 33.237 1.00 49.54
O
ATOM 2175 CB PHE A 304 -35.431 36.700 30.705 1.00 47.17
C
ATOM 2176 CG PHE A 304 -36.596 35.749 30.699 1.00 46.01
C
ATOM 2177 CD1 PHE A 304 -37.773 36.077 31.350 1.00 46.17
C
ATOM 2178 CD2 PHE A 304 -36.509 34.520 30.036 1.00 46.81
C
ATOM 2179 CE1 PHE A 304 -38.881 35.202 31.333 1.00 45.49
C
ATOM 2180 CE2 PHE A 304 -37.592 33.628 30.024 1.00 46.21
C
ATOM 2181 CZ PHE A 304 -38.805 33.998 30.673 1.00 46.77
C

ATOM 2182 N PHE A 305 -33.176 34.965 32.131 1.00 49.26
N
ATOM 2183 CA PHE A 305 -32.730 33.648 32.553 1.00 50.36
C
ATOM 2184 C PHE A 305 -31.900 33.692 33.818 1.00 51.36
C
ATOM 2185 O PHE A 305 -32.103 32.872 34.707 1.00 52.95
O
ATOM 2186 CB PHE A 305 -31.985 32.917 31.418 1.00 50.48
C
ATOM 2187 CG PHE A 305 -32.879 32.592 30.241 1.00 49.46
C
ATOM 2188 CD1 PHE A 305 -33.679 31.453 30.246 1.00 49.84
C
ATOM 2189 CD2 PHE A 305 -32.929 33.454 29.140 1.00 49.00
C
ATOM 2190 CE1 PHE A 305 -34.542 31.177 29.133 1.00 50.95
C
ATOM 2191 CE2 PHE A 305 -33.732 33.185 28.041 1.00 50.17
C
ATOM 2192 CZ PHE A 305 -34.553 32.046 28.030 1.00 48.51
C
ATOM 2193 N THR A 306 -30.988 34.657 33.911 1.00 51.43
N
ATOM 2194 CA THR A 306 -29.965 34.634 34.955 1.00 51.35
C
ATOM 2195 C THR A 306 -30.476 35.085 36.320 1.00 51.68
C
ATOM 2196 O THR A 306 -29.895 34.717 37.341 1.00 51.29
O
ATOM 2197 CB THR A 306 -28.727 35.475 34.563 1.00 51.47
C
ATOM 2198 OG1 THR A 306 -29.118 36.838 34.398 1.00 50.25
O
ATOM 2199 CG2 THR A 306 -28.123 34.969 33.255 1.00 51.78
C
ATOM 2200 N SER A 307 -31.562 35.857 36.346 1.00 50.96
N
ATOM 2201 CA SER A 307 -32.108 36.347 37.610 1.00 51.05
C
ATOM 2202 C SER A 307 -33.478 35.757 37.947 1.00 49.88
C
ATOM 2203 O SER A 307 -34.193 36.294 38.784 1.00 49.81
O

ATOM 2204 CB SER A 307 -32.249 37.876 37.573 1.00 51.63
C
ATOM 2205 OG SER A 307 -33.402 38.199 36.789 1.00 53.13
O
ATOM 2206 N GLY A 308 -33.864 34.676 37.293 1.00 49.15
N
ATOM 2207 CA GLY A 308 -35.136 34.032 37.615 1.00 48.31
C
ATOM 2208 C GLY A 308 -34.923 32.554 37.904 1.00 48.05
C
ATOM 2209 O GLY A 308 -33.854 31.999 37.600 1.00 48.74
O
ATOM 2210 N TYR A 309 -35.936 31.922 38.490 1.00 46.60
N
ATOM 2211 CA TYR A 309 -35.899 30.496 38.783 1.00 46.17
C
ATOM 2212 C TYR A 309 -36.104 29.648 37.532 1.00 45.38
C
ATOM 2213 O TYR A 309 -37.090 29.825 36.806 1.00 42.73
O
ATOM 2214 CB TYR A 309 -36.951 30.149 39.832 1.00 46.10
C
ATOM 2215 CG TYR A 309 -37.104 28.663 40.092 1.00 46.04
C
ATOM 2216 CD1 TYR A 309 -36.018 27.898 40.498 1.00 46.19
C
ATOM 2217 CD2 TYR A 309 -38.344 28.036 39.961 1.00 44.57
C
ATOM 2218 CE1 TYR A 309 -36.149 26.531 40.751 1.00 47.22
C
ATOM 2219 CE2 TYR A 309 -38.485 26.677 40.210 1.00 46.92
C
ATOM 2220 CZ TYR A 309 -37.378 25.934 40.615 1.00 46.50
C
ATOM 2221 OH TYR A 309 -37.501 24.584 40.873 1.00 48.19
O
ATOM 2222 N ILE A 310 -35.154 28.744 37.270 1.00 45.44
N
ATOM 2223 CA ILE A 310 -35.285 27.782 36.187 1.00 46.07
C
ATOM 2224 C ILE A 310 -35.337 26.379 36.805 1.00 45.61
C
ATOM 2225 O ILE A 310 -34.305 25.875 37.306 1.00 45.05
O

ATOM 2226 CB ILE A 310 -34.109 27.872 35.153 1.00 47.37
C
ATOM 2227 CG1 ILE A 310 -33.903 29.306 34.662 1.00 47.35
C
ATOM 2228 CG2 ILE A 310 -34.331 26.920 33.964 1.00 48.90
C
ATOM 2229 CD1 ILE A 310 -32.712 29.469 33.733 1.00 46.84
C
ATOM 2230 N PRO A 311 -36.523 25.737 36.771 1.00 44.91
N
ATOM 2231 CA PRO A 311 -36.604 24.378 37.334 1.00 45.19
C
ATOM 2232 C PRO A 311 -35.598 23.428 36.659 1.00 44.86
C
ATOM 2233 O PRO A 311 -35.307 23.574 35.463 1.00 43.75
O
ATOM 2234 CB PRO A 311 -38.043 23.939 37.057 1.00 45.55
C
ATOM 2235 CG PRO A 311 -38.740 25.077 36.374 1.00 45.47
C
ATOM 2236 CD PRO A 311 -37.816 26.242 36.256 1.00 45.53
C
ATOM 2237 N ALA A 312 -35.057 22.486 37.416 1.00 45.12
N
ATOM 2238 CA ALA A 312 -34.157 21.482 36.844 1.00 45.66
C
ATOM 2239 C ALA A 312 -34.952 20.513 35.973 1.00 46.38
C
ATOM 2240 O ALA A 312 -34.422 19.949 35.005 1.00 46.02
O
ATOM 2241 CB ALA A 312 -33.399 20.726 37.955 1.00 45.45
C
ATOM 2242 N ARG A 313 -36.224 20.335 36.339 1.00 47.03
N
ATOM 2243 CA ARG A 313 -37.158 19.444 35.647 1.00 47.84
C
ATOM 2244 C ARG A 313 -38.601 19.873 35.957 1.00 46.88
C
ATOM 2245 O ARG A 313 -38.847 20.621 36.897 1.00 46.36
O
ATOM 2246 CB ARG A 313 -36.906 17.971 36.010 1.00 47.96
C
ATOM 2247 CG ARG A 313 -37.135 17.618 37.474 1.00 49.99
C

ATOM 2248 CD ARG A 313 -36.480 16.294 37.870 1.00 51.15
C
ATOM 2249 NE ARG A 313 -35.048 16.225 37.535 1.00 57.80
N
ATOM 2250 CZ ARG A 313 -34.042 16.652 38.306 1.00 58.95
C
ATOM 2251 NH1 ARG A 313 -34.276 17.202 39.499 1.00 58.95
N
ATOM 2252 NH2 ARG A 313 -32.786 16.524 37.875 1.00 58.55
N
ATOM 2253 N LEU A 314 -39.539 19.438 35.127 1.00 46.48
N
ATOM 2254 CA LEU A 314 -40.955 19.682 35.364 1.00 46.28
C
ATOM 2255 C LEU A 314 -41.634 18.358 35.696 1.00 46.40
C
ATOM 2256 O LEU A 314 -41.323 17.351 35.095 1.00 46.78
O
ATOM 2257 CB LEU A 314 -41.605 20.312 34.125 1.00 45.90
C
ATOM 2258 CG LEU A 314 -41.032 21.692 33.765 1.00 44.43
C
ATOM 2259 CD1 LEU A 314 -41.730 22.238 32.519 1.00 43.55
C
ATOM 2260 CD2 LEU A 314 -41.158 22.627 34.927 1.00 41.29
C
ATOM 2261 N PRO A 315 -42.558 18.361 36.658 1.00 46.60
N
ATOM 2262 CA PRO A 315 -43.362 17.160 36.923 1.00 46.64
C
ATOM 2263 C PRO A 315 -44.345 16.882 35.774 1.00 46.75
C
ATOM 2264 O PRO A 315 -44.826 17.823 35.156 1.00 46.61
O
ATOM 2265 CB PRO A 315 -44.118 17.518 38.203 1.00 46.74
C
ATOM 2266 CG PRO A 315 -44.187 19.017 38.207 1.00 46.87
C
ATOM 2267 CD PRO A 315 -42.915 19.490 37.536 1.00 46.52
C
ATOM 2268 N ILE A 316 -44.642 15.615 35.492 1.00 46.76
N
ATOM 2269 CA ILE A 316 -45.589 15.278 34.400 1.00 47.00
C

```
ATOM   2270  C   ILE A 316     -46.910  16.036  34.533  1.00 46.95
C
ATOM   2271  O   ILE A 316     -47.562  16.343  33.526  1.00 47.29
O
ATOM   2272  CB  ILE A 316     -45.839  13.740  34.240  1.00 46.62
C
ATOM   2273  CG1 ILE A 316     -44.709  13.085  33.445  1.00 46.66
C
ATOM   2274  CG2 ILE A 316     -47.116  13.455  33.462  1.00 47.02
C
ATOM   2275  CD1 ILE A 316     -44.615  13.513  31.983  1.00 45.96
C
ATOM   2276  N   THR A 317     -47.279  16.368  35.770  1.00 46.62
N
ATOM   2277  CA  THR A 317     -48.524  17.103  36.031  1.00 46.66
C
ATOM   2278  C   THR A 317     -48.600  18.451  35.304  1.00 46.50
C
ATOM   2279  O   THR A 317     -49.696  18.953  35.071  1.00 45.65
O
ATOM   2280  CB  THR A 317     -48.792  17.306  37.543  1.00 46.13
C
ATOM   2281  OG1 THR A 317     -47.733  18.075  38.118  1.00 47.12
O
ATOM   2282  CG2 THR A 317     -48.894  15.955  38.261  1.00 47.25
C
ATOM   2283  N   CYS A 318     -47.428  18.991  34.934  0.50 46.70
N
ATOM   2284  CA  CYS A 318     -47.296  20.282  34.229  0.50 47.11
C
ATOM   2285  C   CYS A 318     -47.909  20.289  32.839  0.50 47.30
C
ATOM   2286  O   CYS A 318     -48.069  21.345  32.229  0.50 47.83
O
ATOM   2287  CB  CYS A 318     -45.831  20.707  34.121  0.50 46.45
C
ATOM   2288  SG  CYS A 318     -45.132  21.302  35.656  0.50 48.14
S
ATOM   2289  N   LEU A 319     -48.249  19.106  32.350  1.00 47.54
N
ATOM   2290  CA  LEU A 319     -48.939  18.945  31.075  1.00 47.91
C
ATOM   2291  C   LEU A 319     -50.390  19.375  31.200  1.00 47.70
C
```

```
ATOM   2292  O   LEU A 319     -51.017  19.709  30.204  1.00 47.76
O
ATOM   2293  CB  LEU A 319     -48.886  17.487  30.600  1.00 47.92
C
ATOM   2294  CG  LEU A 319     -47.536  16.929  30.159  1.00 48.45
C
ATOM   2295  CD1 LEU A 319     -47.619  15.428  29.961  1.00 48.60
C
ATOM   2296  CD2 LEU A 319     -47.026  17.621  28.891  1.00 51.42
C
ATOM   2297  N   THR A 320     -50.924  19.371  32.423  1.00 47.70
N
ATOM   2298  CA  THR A 320     -52.335  19.688  32.621  1.00 47.63
C
ATOM   2299  C   THR A 320     -52.621  20.686  33.750  1.00 47.84
C
ATOM   2300  O   THR A 320     -53.666  21.331  33.734  1.00 48.13
O
ATOM   2301  CB  THR A 320     -53.190  18.410  32.888  1.00 48.39
C
ATOM   2302  OG1 THR A 320     -52.766  17.798  34.112  1.00 47.96
O
ATOM   2303  CG2 THR A 320     -53.076  17.411  31.738  1.00 48.55
C
ATOM   2304  N   ILE A 321     -51.714  20.790  34.727  1.00 47.51
N
ATOM   2305  CA  ILE A 321     -51.951  21.583  35.944  1.00 47.99
C
ATOM   2306  C   ILE A 321     -50.800  22.548  36.172  1.00 47.38
C
ATOM   2307  O   ILE A 321     -49.658  22.131  36.138  1.00 46.82
O
ATOM   2308  CB  ILE A 321     -52.124  20.670  37.202  1.00 47.78
C
ATOM   2309  CG1 ILE A 321     -53.320  19.728  37.017  1.00 47.93
C
ATOM   2310  CG2 ILE A 321     -52.289  21.492  38.497  1.00 48.47
C
ATOM   2311  CD1 ILE A 321     -53.324  18.521  37.951  1.00 49.12
C
ATOM   2312  N   PRO A 322     -51.099  23.838  36.426  1.00 47.63
N
ATOM   2313  CA  PRO A 322     -50.014  24.799  36.645  1.00 47.94
C
```

ATOM 2314 C PRO A 322 -49.143 24.417 37.855 1.00 48.02
C
ATOM 2315 O PRO A 322 -49.673 24.100 38.916 1.00 48.24
O
ATOM 2316 CB PRO A 322 -50.766 26.105 36.925 1.00 48.01
C
ATOM 2317 CG PRO A 322 -52.137 25.900 36.359 1.00 47.83
C
ATOM 2318 CD PRO A 322 -52.429 24.469 36.539 1.00 47.47
C
ATOM 2319 N PRO A 323 -47.810 24.416 37.704 1.00 48.89
N
ATOM 2320 CA PRO A 323 -47.028 24.127 38.908 1.00 49.31
C
ATOM 2321 C PRO A 323 -46.927 25.353 39.810 1.00 49.58
C
ATOM 2322 O PRO A 323 -46.960 26.484 39.337 1.00 49.83
O
ATOM 2323 CB PRO A 323 -45.660 23.721 38.353 1.00 49.08
C
ATOM 2324 CG PRO A 323 -45.564 24.439 37.045 1.00 49.81
C
ATOM 2325 CD PRO A 323 -46.961 24.633 36.523 1.00 48.36
C
ATOM 2326 N ARG A 324 -46.799 25.120 41.106 1.00 50.39
N
ATOM 2327 CA ARG A 324 -46.596 26.207 42.061 1.00 50.67
C
ATOM 2328 C ARG A 324 -45.135 26.277 42.526 1.00 50.14
C
ATOM 2329 O ARG A 324 -44.702 27.267 43.126 1.00 49.87
O
ATOM 2330 CB ARG A 324 -47.551 26.060 43.246 1.00 51.14
C
ATOM 2331 CG ARG A 324 -48.913 26.763 43.048 1.00 54.44
C
ATOM 2332 CD ARG A 324 -49.813 25.984 42.082 1.00 59.59
C
ATOM 2333 NE ARG A 324 -50.758 26.823 41.331 1.00 63.59
N
ATOM 2334 CZ ARG A 324 -51.699 26.353 40.507 1.00 64.58
C
ATOM 2335 NH1 ARG A 324 -51.858 25.036 40.322 1.00 63.14
N

```
ATOM   2336  NH2 ARG A 324     -52.497  27.207  39.871  1.00 65.67
N
ATOM   2337  N   PHE A 325     -44.367  25.233  42.237  1.00 49.66
N
ATOM   2338  CA  PHE A 325     -42.956  25.208  42.607  1.00 49.47
C
ATOM   2339  C   PHE A 325     -42.761  25.494  44.092  1.00 50.12
C
ATOM   2340  O   PHE A 325     -41.925  26.329  44.476  1.00 50.13
O
ATOM   2341  CB  PHE A 325     -42.145  26.195  41.748  1.00 48.88
C
ATOM   2342  CG  PHE A 325     -42.223  25.917  40.279  1.00 48.24
C
ATOM   2343  CD1 PHE A 325     -42.968  26.745  39.435  1.00 47.46
C
ATOM   2344  CD2 PHE A 325     -41.568  24.813  39.739  1.00 46.32
C
ATOM   2345  CE1 PHE A 325     -43.051  26.482  38.069  1.00 46.10
C
ATOM   2346  CE2 PHE A 325     -41.639  24.537  38.378  1.00 47.23
C
ATOM   2347  CZ  PHE A 325     -42.380  25.365  37.537  1.00 46.92
C
ATOM   2348  N   SER A 326     -43.542  24.805  44.920  0.50 50.20
N
ATOM   2349  CA  SER A 326     -43.451  24.931  46.367  0.50 50.56
C
ATOM   2350  C   SER A 326     -42.192  24.252  46.911  0.50 50.95
C
ATOM   2351  O   SER A 326     -41.755  23.223  46.393  0.50 50.53
O
ATOM   2352  CB  SER A 326     -44.715  24.372  47.026  0.50 50.54
C
ATOM   2353  OG  SER A 326     -45.820  25.244  46.816  0.50 50.22
O
ATOM   2354  N   ILE A 327     -41.626  24.845  47.959  1.00 51.36
N
ATOM   2355  CA  ILE A 327     -40.351  24.417  48.526  1.00 53.24
C
ATOM   2356  C   ILE A 327     -40.401  23.052  49.215  1.00 54.79
C
ATOM   2357  O   ILE A 327     -39.469  22.277  49.093  1.00 55.49
O
```

ATOM 2358 CB ILE A 327 -39.731 25.522 49.442 1.00 52.98
C
ATOM 2359 CG1 ILE A 327 -38.361 25.946 48.908 1.00 53.41
C
ATOM 2360 CG2 ILE A 327 -39.666 25.113 50.895 1.00 53.24
C
ATOM 2361 CD1 ILE A 327 -38.451 26.837 47.667 1.00 53.03
C
ATOM 2362 N ALA A 328 -41.478 22.743 49.919 1.00 56.60
N
ATOM 2363 CA ALA A 328 -41.631 21.401 50.467 1.00 58.86
C
ATOM 2364 C ALA A 328 -43.089 20.988 50.354 1.00 60.53
C
ATOM 2365 O ALA A 328 -43.953 21.862 50.213 1.00 60.80
O
ATOM 2366 CB ALA A 328 -41.145 21.342 51.920 1.00 58.50
C
ATOM 2367 N PRO A 329 -43.374 19.660 50.398 1.00 62.28
N
ATOM 2368 CA PRO A 329 -44.777 19.200 50.350 1.00 63.09
C
ATOM 2369 C PRO A 329 -45.439 19.112 51.734 1.00 63.69
C
ATOM 2370 O PRO A 329 -44.791 18.710 52.710 1.00 63.82
O
ATOM 2371 CB PRO A 329 -44.668 17.811 49.704 1.00 63.17
C
ATOM 2372 CG PRO A 329 -43.283 17.313 50.089 1.00 62.85
C
ATOM 2373 CD PRO A 329 -42.431 18.521 50.468 1.00 62.49
C
ATOM 2374 N SER A 330 -46.720 19.483 51.806 1.00 64.29
N
ATOM 2375 CA SER A 330 -47.479 19.442 53.066 1.00 64.62
C
ATOM 2376 C SER A 330 -48.296 18.157 53.194 1.00 64.60
C
ATOM 2377 O SER A 330 -48.861 17.870 54.251 1.00 64.35
O
ATOM 2378 CB SER A 330 -48.396 20.667 53.192 1.00 64.80
C
ATOM 2379 OG SER A 330 -47.668 21.874 53.035 1.00 65.47
O

```
TER     2380        SER A 330
END
```