Table S1. Details of the PDB file, contact distance, atoms involved and geometric parameters describing Trp-aromatic interaction

| PDB CODE | Resolution | R factor | | TRP | Partner | | | Shortest Contact | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Theta (T-P) | Phi | D | Dxy | Dz | | | | | | |
| | | | | Res.No. | Res | Res.No. | | Trp Atom | Partner Atom | Distance (Angstrom) |
| 153l | 1.60 | 0.15 | | 84 | PHE | 91 | | CZ2 | CD1 | 3.68 |
| 22.88 | 39.06 | 5.22 | 2.03 | 4.81 | | | | | | |
| 153l | 1.60 | 0.15 | | 107 | TYR | 48 | | CH2 | OH | 3.71 |
| 42.97 | 88.17 | 7.39 | 5.04 | -5.41 | | | | | | |
| 153l | 1.60 | 0.15 | | 134 | PHE | 131 | | CE2 | CG | 3.57 |
| 34.74 | 29.76 | 4.26 | 2.43 | -3.50 | | | | | | |
| 153l | 1.60 | 0.15 | | 134 | TYR | 157 | | CZ3 | CD1 | 3.99 |
| 19.74 | 99.72 | 5.67 | 1.91 | 5.34 | | | | | | |
| 193l | 1.33 | 0.18 | | 108 | TRP | 28 | | CH2 | CZ3 | 3.85 |
| 39.71 | 96.12 | 7.37 | 4.71 | 5.67 | | | | | | |
| 193l | 1.33 | 0.18 | | 28 | TRP | 108 | | CZ3 | CH2 | 3.85 |
| 69.19 | 114.63 | 7.37 | 6.89 | 2.62 | | | | | | |
| 193l | 1.33 | 0.18 | | 111 | TYR | 23 | | CZ2 | CE1 | 3.80 |
| 36.88 | 35.57 | 5.95 | 3.57 | -4.76 | | | | | | |
| 193l | 1.33 | 0.18 | | 123 | PHE | 34 | | CZ2 | CZ | 3.73 |
| 56.32 | 31.11 | 6.00 | 4.99 | -3.33 | | | | | | |
| 1ade | 2.00 | 0.20 | | 309 A | TYR | 372 A | | CD1 | CE1 | 3.38 |
| 64.05 | -87.82 | 5.72 | 5.14 | -2.51 | | | | | | |
| 1ade | 2.00 | 0.20 | | 365 A | TYR | 347 A | | CZ3 | OH | 3.91 |
| 42.30 | 102.10 | 6.45 | 4.34 | 4.77 | | | | | | |
| 1amp | 1.80 | 0.16 | | 13 | PHE | 137 | | CZ3 | CD1 | 3.63 |
| 84.09 | 105.50 | 7.07 | 7.03 | -0.73 | | | | | | |
| 1amp | 1.80 | 0.16 | | 48 | PHE | 32 | | CG | CZ | 3.95 |
| 33.16 | -136.72 | 5.91 | 3.23 | -4.95 | | | | | | |
| 1amp | 1.80 | 0.16 | | 233 | TYR | 148 | | NE1 | OH | 2.91 |
| 79.10 | -21.25 | 6.30 | 6.19 | 1.19 | | | | | | |
| 1amp | 1.80 | 0.16 | | 233 | TYR | 238 | | CE3 | CD2 | 3.59 |
| 85.81 | 149.10 | 6.48 | 6.46 | -0.47 | | | | | | |
| 1aoz | 1.90 | 0.20 | | 8 A | TYR | 6 A | | NE1 | CD2 | 3.97 |
| 50.49 | -1.98 | 5.80 | 4.47 | -3.69 | | | | | | |
| 1aoz | 1.90 | 0.20 | | 8 A | TRP | 61 A | | CZ3 | CH2 | 3.95 |
| 64.53 | 103.81 | 8.41 | 7.59 | -3.62 | | | | | | |
| 1aoz | 1.90 | 0.20 | | 61 A | TRP | 8 A | | CH2 | CZ3 | 3.95 |
| 87.09 | 84.84 | 8.41 | 8.40 | -0.43 | | | | | | |
| 1aoz | 1.90 | 0.20 | | 8 A | TYR | 103 A | | CH2 | CZ | 3.51 |
| 68.40 | 81.43 | 6.07 | 5.64 | 2.24 | | | | | | |
| 1aoz | 1.90 | 0.20 | | 15 A | PHE | 31 A | | NE1 | CD2 | 3.56 |
| 45.92 | -66.43 | 5.87 | 4.22 | 4.08 | | | | | | |
| 1aoz | 1.90 | 0.20 | | 61 A | TYR | 91 A | | NE1 | CD1 | 3.70 |
| 84.32 | -2.66 | 5.17 | 5.14 | 0.51 | | | | | | |
| 1aoz | 1.90 | 0.20 | | 61 A | PHE | 93 A | | CE2 | CE2 | 3.67 |
| 20.55 | -109.74 | 4.69 | 1.64 | -4.39 | | | | | | |
| 1aoz | 1.90 | 0.20 | | 144 A | HIS | 146 A | | NE1 | CD2 | 3.72 |
| 70.92 | -55.38 | 6.36 | 6.01 | -2.08 | | | | | | |
| 1aoz | 1.90 | 0.20 | | 277 A | TYR | 186 A | | NE1 | OH | 3.09 |
| 73.01 | -16.62 | 5.85 | 5.59 | -1.71 | | | | | | |
| 1aoz | 1.90 | 0.20 | | 362 A | HIS | 445 A | | CH2 | CE1 | 3.48 |
| 44.58 | 96.33 | 5.54 | 3.89 | -3.94 | | | | | | |

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 1aoz   1.90      0.20       362 A     HIS  512 A      NE1  CD2      3.71
30.36  -10.53   4.37   2.20  -3.77
 1aoz   1.90      0.20       447 A     PHE  505 A      CE3  CZ       3.73
70.34  157.37   5.15   4.85  -1.73
 1aoz   1.90      0.20       490 A     PHE  464 A      CD2  CD1      3.81
13.31  113.05   5.08   1.15   4.95
 1aoz   1.90      0.20       503 A     HIS  452 A      CD1  CE1      3.47
32.66  -81.30   5.29   2.85  -4.45
 1arb   1.20      0.15        73       PHE   52        CH2  CE1      3.76
58.40   68.11   6.82   5.81   3.57
 1arb   1.20      0.15        73       PHE  127        CD1  CD2      3.31
65.99  -85.35   5.99   5.47  -2.44
 1arb   1.20      0.15       134       TRP  234        CH2  CH2      3.60
38.42   92.61   6.62   4.11   5.19
 1arb   1.20      0.15       234       TRP  134        CH2  CH2      3.60
68.07   97.20   6.62   6.14   2.47
 1arb   1.20      0.15       169       HIS  210        CE2  NE2      3.45
 8.52  119.79   3.53   0.52   3.49
 1arb   1.20      0.15       182       TYR  227        CZ2  OH       3.51
71.44   36.48   7.17   6.80   2.28
 1arb   1.20      0.15       247       TYR   51        CE3  OH       3.80
63.46 -175.98   6.46   5.78  -2.89
 1asu   1.70      0.15       105       HIS  104        CD1  CD2      3.70
48.09  -82.70   6.04   4.49  -4.04
 1asu   1.70      0.15       105       PHE  126        CH2  CD1      3.67
60.65   41.34   6.45   5.62  -3.16
 1asu   1.70      0.15       105       TRP  134        CE3  CZ3      3.97
82.93  165.88   6.91   6.86   0.85
 1asu   1.70      0.15       134       TRP  105        CZ3  CE3      3.97
53.46  115.01   6.91   5.55  -4.11
 1asu   1.70      0.15       134       TRP  138        CZ2  NE1      3.40
35.85   58.10   5.53   3.24   4.48
 1asu   1.70      0.15       138       TRP  134        NE1  CZ2      3.40
71.69  -64.59   5.53   5.25  -1.74
 1asu#  1.70      0.15       138       TYR  194        CZ3  CE2      3.78
83.20   95.74   6.53   6.48  -0.77
 1atl   1.80      0.16        59 A     TRP   81 A      CZ2  CH2      3.80
74.07   14.85   5.62   5.40   1.54
 1atl   1.80      0.16        81 A     TRP   59 A      CH2  CZ2      3.80
30.51   45.46   5.62   2.85  -4.84
 1atl   1.80      0.16        81 A     PHE   78 A      CZ3  CE1      3.76
70.83  145.35   6.41   6.05  -2.10
 1bbp   2.00      0.20        20 D     PHE   18 D      CE3  CE1      3.78
65.53  156.63   6.57   5.98  -2.72
 1bbp   2.00      0.20        20 D     TYR   23 D      CH2  CD1      3.65
36.98   96.00   5.62   3.38  -4.49
 1bbp   2.00      0.20        27 D     TYR   48 D      CD1  CD2      3.42
58.48  -75.66   6.01   5.12  -3.14
 1bbp   2.00      0.20        28 D     PHE  170 D      CE3  CE1      3.47
46.08  170.87   5.42   3.90  -3.76
 1bbp   2.00      0.20        45 D     TYR   60 D      NE1  CD2      3.32
46.50    6.07   4.66   3.38   3.21
 1bbp   2.00      0.20       133 D     PHE  103 D      CE3  CE1      3.92
58.19  150.28   6.68   5.68   3.52
 1bbp   2.00      0.20       133 D     PHE  131 D      CH2  CD2      3.54
60.77   59.17   6.44   5.62  -3.14
 1bam   1.95      0.19        38       TRP  206        CE3  CZ2      3.44
83.37  138.46   5.99   5.95   0.69
 1bam   1.95      0.19       206       TRP   38        CZ2  CE3      3.44
40.01   20.19   5.99   3.85  -4.59
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 1bdm   1.80      0.17      183 B     TYR  277 B      CH2  CE2      3.63
80.12   76.80   6.16   6.07  -1.06
 1bdm   1.80      0.17      183 B     PHE  191 B      CD1  CE2      3.85
61.56  -83.33   6.34   5.58  -3.02
 1bdm   1.80      0.17      183 B     PHE  287 B      CZ3  CD1      3.72
74.02  131.14   7.04   6.77   1.94
 1bdm   1.80      0.17      256 B     TYR  296 B      NE1  CD2      3.60
36.48  -23.55   5.54   3.29  -4.45
 1bec   1.70      0.20       34       PHE   75        CD1  CD2      3.40
73.95  -76.07   5.80   5.57   1.60
 1bec   1.70      0.20      203       PHE  210        CE3  CE2      3.43
81.93  143.75   5.91   5.85   0.83
 1bri   1.90      0.16       71 A     TYR   97 A      CH2  CD1      3.69
65.19   70.31   6.81   6.18  -2.86
 1bri   1.90      0.16       94 A     HIS   18 A      CE2  CD2      3.59
26.84  -14.77   4.71   2.13  -4.20
 1byb   1.90      0.15       55       TYR   72        CD1  OH       3.36
64.76  -93.70   7.95   7.19   3.39
 1byb   1.90      0.15       55       HIS   93        CZ3  NE2      3.48
69.55  103.23   6.06   5.68   2.12
 1byb   1.90      0.15       56       PHE   92        CG   CD1      3.78
29.01 -159.94   5.59   2.71  -4.89
 1byb   1.90      0.15       56       TYR  157        CD1  CE2      3.65
61.39 -100.76   6.11   5.36  -2.92
 1byb   1.90      0.15       69       TYR  157        CH2  CZ       3.99
74.22   62.04   6.42   6.18   1.75
 1byb   1.90      0.15       69       PHE  161        CZ3  CD1      3.63
42.36   98.03   6.29   4.24  -4.65
 1byb   1.90      0.15      110       HIS  146        CE3  CD2      3.80
62.50  147.46   6.46   5.73   2.98
 1byb   1.90      0.15      198       TRP  301        CZ2  CZ2      3.60
80.47   25.48   6.10   6.02  -1.01
 1byb   1.90      0.15      301       TRP  198        CZ2  CZ2      3.60
57.25   -5.37   6.10   5.13  -3.30
 1byb   1.90      0.15      229       PHE  261        CZ3  CG       3.77
85.53  124.27   6.57   6.55   0.51
 1byb   1.90      0.15      265       PHE  217        CD2  CD1      3.80
16.99  137.81   5.25   1.52  -5.02
 1byb   1.90      0.15      265       PHE  262        CZ3  CE1      3.75
77.46  144.27   6.45   6.30  -1.40
 1byb   1.90      0.15      301       HIS  300        CE3  NE2      3.53
86.79  153.22   5.38   5.37  -0.30
 1byb   1.90      0.15      301       TRP  302        CD1  CD1      3.74
83.33 -101.15   7.33   7.28   0.85
 1byb   1.90      0.15      302       TRP  301        CD1  CD1      3.74
57.73  -73.56   7.33   6.20   3.92
 1byb   1.90      0.15      371       TRP  485        CZ3  CH2      3.90
85.04  103.27   8.13   8.10  -0.70
 1byb   1.90      0.15      485       TRP  371        CH2  CZ3      3.90
56.84   71.21   8.13   6.80  -4.45
 1ccr   1.50      0.19       67       TYR   75        CH2  CG       3.59
62.38   70.11   5.64   5.00  -2.62
 1cel   1.81      0.18       16 B     PHE  120 B      CZ3  CE2      3.85
35.08   78.96   5.87   3.37   4.81
 1cel   1.81      0.18       38 B     TYR   82 B      CD1  CE1      3.92
71.92 -107.15   6.80   6.46   2.11
 1cel   1.81      0.18       40 B     HIS   42 B      CD2  CD2      3.47
19.39   76.21   4.35   1.45   4.10
 1cel   1.81      0.18       56 B     TYR   51 B      CD2  CD1      3.81
 7.30  -39.00   5.03   0.62   4.99
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 1cel   1.81      0.18       56 B     TRP  192 B      NE1  CD2      3.45
77.39  -46.31   5.19   5.06   1.13
 1cel   1.81      0.18      192 B     TYR   51 B      CZ2  OH       3.57
47.48   13.15   5.88   4.34   3.97
 1cel   1.81      0.18      192 B     TRP   56 B      CD2  NE1      3.45
9.12  143.01   5.19   0.82   5.12
 1cel   1.81      0.18      216 B     PHE  129 B      CG   CZ       3.65
24.76 -134.58   5.45   2.28   4.95
 1cel   1.81      0.18      216 B     TYR  274 B      CZ2  OH       3.37
65.16   58.26   6.79   6.16  -2.85
 1cel   1.81      0.18      263 B     TYR  321 B      CH2  OH       3.46
72.67   87.96   7.20   6.87  -2.14
 1cel   1.81      0.18      263 B     TYR  330 B      CZ3  CD1      3.52
54.63  139.83   4.86   3.96  -2.81
 1cel   1.81      0.18      367 B     TRP  376 B      CH2  CZ2      3.97
64.62   58.75   7.46   6.74  -3.20
 1cel   1.81      0.18      376 B     TRP  367 B      CZ2  CH2      3.97
85.90   15.16   7.46   7.44   0.53
 1cfb   2.00      0.20      634       TYR  647        NE1  CZ       3.38
64.35  -24.94   4.62   4.16  -2.00
 1cfb   2.00      0.20      681       PHE  655        CE3  CZ       3.65
38.31  120.11   5.81   3.60   4.56
 1cfb   2.00      0.20      734       TYR  749        NE1  CE2      3.44
61.71  -29.33   4.82   4.24  -2.29
 1cfb   2.00      0.20      770       HIS  742        CG   CE1      3.30
31.11 -152.47   4.92   2.55   4.21
 1chm   1.90      0.18      219 B     PHE   62 A      CZ2  CE2      3.72
85.57   32.19   6.69   6.67  -0.52
 1chm   1.90      0.18      219 B     TRP  221 B      NE1  CZ2      3.17
84.49  -46.27   4.81   4.79  -0.46
 1chm   1.90      0.18      221 B     TRP  219 B      CZ2  NE1      3.17
15.81   58.48   4.81   1.31  -4.63
 1chm   1.90      0.18      219 B     PHE  251 B      NE1  CD2      3.40
28.99   -0.45   4.27   2.06   3.74
 1chm   1.90      0.18      219 B     TYR  258 B      CH2  CE1      3.91
60.06   65.07   7.16   6.20   3.57
 1chm   1.90      0.18      219 B     HIS  331 B      CH2  CD2      3.87
23.89   61.71   5.34   2.17  -4.88
 1chm   1.90      0.18      221 B     PHE   62 A      CH2  CE2      3.63
76.52   83.39   7.39   7.19  -1.72
 1chm   1.90      0.18      221 B     HIS  232 B      CZ3  CD2      3.37
66.24   90.09   6.27   5.74   2.53
 1chm   1.90      0.18      221 B     PHE  251 B      CE3  CE2      3.43
47.21  143.79   5.57   4.09  -3.79
 1chm   1.90      0.18      278 B     PHE  266 B      CZ3  CD1      3.65
43.93  133.24   5.95   4.13  -4.29
 1clc   1.90      0.20      220       PHE  244        CE3  CD2      3.81
68.39  165.96   6.27   5.83   2.31
 1clc   1.90      0.20      220       TYR  316        CZ2  OH       3.60
65.91   18.62   6.83   6.24   2.79
 1clc   1.90      0.20      529       HIS  170        CH2  CD2      3.85
65.78   75.40   7.03   6.41  -2.88
 1clc   1.90      0.20      544       TYR  499        CE3  CD2      3.93
89.97  164.51   5.48   5.48   0.00
 1cmb   1.80      0.20      102 A     TYR  104 A      CD1  CD1      3.72
75.96  -78.78   6.90   6.69  -1.67
 1cns   1.91      0.19       82 A     HIS   17 A      NE1  ND1      3.39
33.67    5.72   4.39   2.43   3.66
 1cns   1.91      0.19      158 A     PHE   44 A      CD1  CD1      3.76
41.97  -76.68   5.96   3.98   4.43
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 1ede   1.90      0.16      125       PHE  128        CD2  CD2     3.35
8.59 -120.28   4.65   0.71   4.59
 1ede   1.90      0.16      125       PHE  222        CD2  CE1     3.43
23.97 -132.36   4.03   1.64  -3.68
 1ede   1.90      0.16      175       PHE  172        CD1  CE1     3.80
60.97  -91.59   6.32   5.53   3.07
 1ede   1.90      0.16      175       PHE  190        CZ3  CZ      3.67
24.94  114.59   5.43   2.29  -4.92
 1ede   1.90      0.16      175       TRP  194        CE3  CD2     3.82
72.56  157.74   5.54   5.29  -1.66
 1ede   1.90      0.16      194       TRP  175        CD2  CE3     3.82
6.53  127.65   5.54   0.67  -5.50
 1ede   1.90      0.16      175       HIS  289        CH2  CD2     3.56
48.91   77.63   5.64   4.25   3.71
 1ede   1.90      0.16      175       PHE  290        CH2  CZ      3.47
87.66   81.06   6.99   6.98  -0.28
 1ede   1.90      0.16      194       PHE  190        CD1  CE1     3.47
55.43  -82.25   5.11   4.21  -2.90
 1ede   1.90      0.16      244       PHE  243        CD2  CD2     3.81
2.82  167.95   5.05   0.14   5.05
 1ede   1.90      0.16      244       TRP  248        CZ3  CD2     3.42
72.96  120.36   5.57   5.32   1.63
 1ede   1.90      0.16      248       TRP  244        CD2  CZ3     3.42
23.39 -158.88   5.57   2.20   5.12
 1ede   1.90      0.16      248       PHE  243        CE3  CE2     3.73
70.75  173.76   6.19   5.84   2.04
 1fba   1.90      0.18      147 B     TYR  173 B      CE3  CD1     3.60
47.11 -160.35   4.70   3.44   3.20
 1fba   1.90      0.18      313 B     TYR   58 B      CE3  CD1     3.82
44.18  132.43   6.15   4.29  -4.41
 1fkj   1.70      0.16       59       TYR   26        CH2  CG      3.94
69.09   43.13   6.32   5.90  -2.26
 1fkj   1.70      0.16       59       PHE   48        CZ3  CE1     3.75
82.13  147.93   6.08   6.02  -0.83
 1fkj   1.70      0.16       59       PHE   99        NE1  CG      3.55
85.89  -23.10   4.90   4.89  -0.35
 1fnc   1.70      0.15      182       PHE  186        CE2  CD2     3.58
9.24  -30.89   4.93   0.79   4.87
 1fnc   1.70      0.15      199       PHE  201        CE2  CZ      3.54
32.59  -35.72   4.62   2.48   3.89
 1fnc   1.70      0.15      199       TYR  254        CZ2  CD1     3.74
85.37   23.77   5.55   5.53   0.45
 1fnc   1.70      0.15      259       TYR  299        CH2  CD2     3.73
58.36   69.81   6.43   5.47  -3.37
 1fnc   1.70      0.15      296       TYR  299        CZ3  CD2     3.61
68.64  129.48   6.84   6.37  -2.49
 1fnc   1.70      0.15      296       TRP  309        CH2  CZ3     3.64
79.37   36.36   6.24   6.13  -1.15
 1fnc   1.70      0.15      309       TRP  296        CZ3  CH2     3.64
29.31   64.64   6.24   3.06   5.44
 1gky   2.00      0.17       70       PHE   67        CD1  CD2     3.87
53.86 -120.45   5.92   4.78   3.49
 1gof   1.70      0.18      105       HIS   85        CD2  CE1     3.38
8.49   85.41   3.67   0.51  -3.63
 1gof   1.70      0.18      161       PHE  453        CZ2  CZ      3.88
54.17   32.23   6.64   5.38   3.89
 1gof   1.70      0.18      161       PHE  528        NE1  CD1     3.54
21.02  -15.13   4.95   1.78   4.62
 1gof   1.70      0.18      207       PHE  508        CE3  CE1     3.63
55.47  145.54   6.01   4.95  -3.40
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|---|---|---|---|---|---|---|---|---|---|---|---|
| 1gof | 1.70 | 0.18 | 290 | PHE | 194 | | CZ2 | CE1 | 3.94 | | |
| 80.86 | 29.35 | 6.59 | 6.51 | -1.05 | | | | | | | |
| 1gof | 1.70 | 0.18 | 290 | PHE | 227 | | CH2 | CD2 | 3.68 | | |
| 47.65 | 56.91 | 6.26 | 4.63 | -4.22 | | | | | | | |
| 1gof | 1.70 | 0.18 | 290 | TYR | 272 | | CD1 | CE2 | 3.40 | | |
| 32.01 | -114.83 | 4.08 | 2.17 | -3.46 | | | | | | | |
| 1gof | 1.70 | 0.18 | 290 | TYR | 329 | | CD1 | OH | 3.38 | | |
| 58.53 | -90.64 | 6.41 | 5.47 | 3.35 | | | | | | | |
| 1gox | 2.00 | 0.19 | 33 | TYR | 261 | | CG | CE1 | 3.45 | | |
| 36.65 | -161.20 | 4.93 | 2.94 | -3.96 | | | | | | | |
| 1gpl | 2.00 | 0.17 | 148 A | PHE | 77 A | | CH2 | CE1 | 3.82 | | |
| 51.11 | 100.38 | 6.42 | 5.00 | -4.03 | | | | | | | |
| 1gpl | 2.00 | 0.17 | 158 A | PHE | 145 A | | CH2 | CD2 | 3.89 | | |
| 75.32 | 81.49 | 6.42 | 6.21 | 1.63 | | | | | | | |
| 1gpb | 1.90 | 0.19 | 189 | TYR | 52 | | NE1 | OH | 3.67 | | |
| 64.88 | -7.10 | 7.30 | 6.61 | 3.10 | | | | | | | |
| 1gpb | 1.90 | 0.19 | 215 | TYR | 297 | | CZ3 | OH | 3.77 | | |
| 74.39 | 82.87 | 7.60 | 7.32 | -2.05 | | | | | | | |
| 1gpb | 1.90 | 0.19 | 244 | TYR | 157 | | NE1 | CD1 | 3.38 | | |
| 67.50 | -11.74 | 5.80 | 5.36 | 2.22 | | | | | | | |
| 1gpb | 1.90 | 0.19 | 825 | TYR | 820 | | CZ2 | CD1 | 3.72 | | |
| 42.52 | 33.28 | 5.66 | 3.83 | -4.17 | | | | | | | |
| 1gse | 2.00 | 0.20 | 21 B | TYR | 165 B | | CH2 | CD1 | 4.00 | | |
| 84.35 | 46.85 | 6.81 | 6.78 | -0.67 | | | | | | | |
| 1gse | 2.00 | 0.20 | 21 B | PHE | 197 B | | CD1 | CE2 | 3.29 | | |
| 21.66 | -101.76 | 4.90 | 1.81 | 4.55 | | | | | | | |
| 1han | 1.90 | 0.16 | 19 | PHE | 11 | | CH2 | CD1 | 3.88 | | |
| 58.93 | 78.39 | 5.87 | 5.03 | -3.03 | | | | | | | |
| 1han | 1.90 | 0.16 | 48 | TYR | 8 | | CH2 | CG | 3.42 | | |
| 57.85 | 51.22 | 5.39 | 4.56 | -2.87 | | | | | | | |
| 1han | 1.90 | 0.16 | 272 | HIS | 194 | | CH2 | CD2 | 3.71 | | |
| 51.52 | 46.07 | 6.01 | 4.70 | 3.74 | | | | | | | |
| 1han# | 1.90 | 0.16 | 283 | PHE | 223 | | CD1 | CE1 | 3.96 | | |
| 73.35 | -88.66 | 5.77 | 5.53 | 1.65 | | | | | | | |
| 1hbq | 1.70 | 0.20 | 24 | PHE | 20 | | NE1 | CE2 | 3.72 | | |
| 50.68 | -20.85 | 4.56 | 3.53 | -2.89 | | | | | | | |
| 1hbq | 1.70 | 0.20 | 24 | PHE | 45 | | CD1 | CD1 | 3.78 | | |
| 64.57 | -77.89 | 6.54 | 5.91 | -2.81 | | | | | | | |
| 1hle | 1.95 | 0.18 | 160 A | TYR | 119 A | | CG | OH | 3.40 | | |
| 33.38 | -170.61 | 6.43 | 3.54 | -5.37 | | | | | | | |
| 1hle | 1.95 | 0.18 | 194 A | TYR | 244 A | | CH2 | OH | 3.43 | | |
| 48.02 | 125.14 | 5.24 | 3.90 | 3.50 | | | | | | | |
| 1hpm | 1.70 | 0.20 | 90 | PHE | 68 | | CD1 | CE1 | 3.84 | | |
| 57.20 | -75.26 | 6.22 | 5.23 | 3.37 | | | | | | | |
| 1hpm | 1.70 | 0.20 | 90 | PHE | 92 | | CG | CZ | 3.45 | | |
| 36.39 | -151.34 | 4.77 | 2.83 | 3.84 | | | | | | | |
| 1hsl | 1.89 | 0.20 | 130 A | PHE | 125 A | | CE2 | CE1 | 3.79 | | |
| 12.66 | -18.98 | 5.26 | 1.16 | -5.13 | | | | | | | |
| 1huw | 2.00 | 0.19 | 86 | PHE | 166 | | CD2 | CD1 | 3.69 | | |
| 17.78 | 116.80 | 5.01 | 1.52 | -4.78 | | | | | | | |
| 1hxn | 1.80 | 0.18 | 353 | TRP | 365 | | CG | CE3 | 3.67 | | |
| 22.50 | -149.35 | 5.63 | 2.15 | 5.20 | | | | | | | |
| 1hxn | 1.80 | 0.18 | 365 | TRP | 353 | | CE3 | CG | 3.67 | | |
| 80.77 | 156.23 | 5.63 | 5.56 | -0.90 | | | | | | | |
| 1hxn | 1.80 | 0.18 | 370 | HIS | 372 | | CE3 | CG | 3.94 | | |
| 46.14 | 140.75 | 5.75 | 4.14 | -3.99 | | | | | | | |
| 1ilb# | 2.00 | 0.19 | 120 | PHE | 150 | | CZ2 | CZ | 3.91 | | |
| 50.99 | -2.57 | 5.69 | 4.42 | -3.58 | | | | | | | |
| 1iae | 1.83 | 0.14 | 10 | TYR | 194 | | CD1 | OH | 3.52 | | |
| 87.65 | -111.12 | 7.95 | 7.94 | -0.32 | | | | | | | |

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 1iae   1.83      0.14       65       PHE   58        CZ2  CZ       3.91
46.43   29.83   6.34   4.59  -4.37
 1isc   1.80      0.19       71 A     PHE   75 A      CH2  CD1      3.44
58.50   81.16   5.97   5.09   3.12
 1isc   1.80      0.19       77 A     TYR    9 A      CE3  OH       3.75
59.66  178.03   7.10   6.13  -3.59
 1isc   1.80      0.19       77 A     TYR   27 A      NE1  CD1      3.53
32.93  -34.47   5.61   3.05  -4.71
 1isc   1.80      0.19       77 A     HIS   31 A      NE1  ND1      3.06
84.64  -41.31   5.78   5.75   0.54
 1isc   1.80      0.19       77 A     TYR   76 A      CZ3  CE2      3.59
29.62  123.81   5.38   2.66   4.68
 1isc   1.80      0.19      122 A     TRP  158 A      NE1  NE1      3.74
49.53  -22.64   6.35   4.83   4.12
 1isc   1.80      0.19      158 A     TRP  122 A      NE1  NE1      3.74
66.36  -56.75   6.35   5.82  -2.55
 1isc   1.80      0.19      158 A     PHE  118 B      CH2  CZ       3.82
89.00   53.92   6.40   6.40  -0.11
 1isc   1.80      0.19      124 A     PHE   75 A      CZ3  CD2      3.97
84.66  121.07   6.94   6.91   0.65
 1isc   1.80      0.19      178 A     PHE  106 A      CH2  CE2      3.70
70.43   75.57   6.85   6.45  -2.29
 1isc   1.80      0.19      178 A     PHE  110 A      CZ2  CD1      3.56
64.23   50.62   6.15   5.54   2.67
 1isc   1.80      0.19      183 A     PHE  103 A      CZ2  CE1      3.68
57.55   30.87   6.24   5.27  -3.35
 1knb   1.70      0.16      478       PHE  461        NE1  CE1      3.95
58.19   -9.79   6.30   5.35   3.32
 1knb   1.70      0.16      478       TYR  491        NE1  OH       3.01
58.50  -59.71   6.33   5.40  -3.31
 1knb   1.70      0.16      556       PHE  568        CG   CZ       3.66
25.67 -150.83   5.50   2.38   4.96
 1knb   1.70      0.16      558       TYR  563        CD1  CD2      3.63
47.69 -111.67   5.94   4.39  -4.00
 1knb   1.70      0.16      558       PHE  568        CZ3  CE1      3.54
57.97   97.25   6.11   5.18  -3.24
 1lcp   1.65      0.16      207 A     PHE  229 A      CZ3  CG       3.75
72.65   97.58   6.49   6.19  -1.94
 1lcp   1.65      0.16      207 A     TYR  345 A      CZ2  OH       3.44
85.20   49.34   6.08   6.06   0.51
 1lcp   1.65      0.16      381 A     PHE  482 A      CH2  CE2      3.79
87.57   55.08   7.39   7.38  -0.31
 1lcp   1.65      0.16      383 A     PHE  387 A      CZ2  CD1      3.64
52.78   14.28   5.51   4.39  -3.34
 1lcp   1.65      0.16      398 A     PHE  403 B      CZ3  CZ       3.94
52.82  129.29   6.42   5.12   3.88
 1lct   2.00      0.18        8       TRP   22        CD2  CZ3      3.73
25.60  170.99   6.45   2.79   5.82
 1lct   2.00      0.18       22       TRP    8        CZ3  CD2      3.73
88.62  101.03   6.45   6.45   0.16
 1lct   2.00      0.18        8       PHE  300        CZ2  CE1      3.62
39.49   16.69   5.45   3.47   4.20
 1lct   2.00      0.18       22       PHE  286        CD1  CE2      3.75
55.23 -108.39   6.17   5.07  -3.52
 1lct   2.00      0.18       22       PHE  300        CH2  CZ       3.71
43.17   83.74   6.31   4.32  -4.60
 1lis   1.90      0.19       34       HIS   38        CE2  CD2      3.35
25.50   -7.13   4.31   1.86   3.89
 1lis   1.90      0.19       34       TYR  102        CG   CD2      3.87
20.17 -178.93   5.25   1.80  -4.93
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 1lis   1.90      0.19       62       TYR  133        NE1  CE2      3.49
83.90  -26.96   5.23   5.20   0.56
 1mml   1.80      0.20      185       PHE  156        CZ3  CZ       3.84
65.75  122.49   6.77   6.17  -2.78
 1mml   1.80      0.20      185       PHE  170        NE1  CE1      3.65
48.99  -20.27   5.89   4.44   3.87
 1mml#  1.80      0.20      185       TYR  271        CZ3  OH       3.36
86.89  124.83   8.06   8.05  -0.44
 1mpp   2.00      0.16       39       TYR   75        NE1  OH       2.68
83.75  -17.80   6.43   6.39   0.70
 1mpp   2.00      0.16      190       TYR  125        CZ3  OH       3.49
17.94   52.80   4.86   1.50   4.62
 1mpp   2.00      0.16      190       TYR  313        CD2  CD1      3.68
4.61 -119.39   5.01   0.39  -4.99
 1mrj   1.60      0.17      192       TYR  164        CD1  OH       3.76
62.22  -95.12   6.39   5.65  -2.98
 1msc   2.00      0.20       32       PHE    4        CZ2  CD1      3.87
10.23   19.10   5.22   0.94  -5.14
 1msc   2.00      0.20       32       PHE    7        NE1  CD1      3.61
22.89  -64.33   5.02   1.94   4.63
 1nar   1.80      0.16       58       TYR  116        NE1  OH       2.99
84.02    4.68   6.15   6.12  -0.64
 1nar   1.80      0.16      101       PHE   93        CZ2  CE1      3.69
25.63   39.33   5.43   2.35  -4.90
 1nar   1.80      0.16      101       TYR  131        CZ2  OH       3.70
71.27   26.36   7.44   7.05  -2.39
 1nar   1.80      0.16      261       TYR    8        CE3  CG       3.64
83.81  147.05   5.69   5.66  -0.61
 1nar   1.80      0.16      261       PHE   39        CH2  CE2      3.69
86.80   86.28   7.07   7.06   0.39
 1nba   2.00      0.19       56 A     PHE   63 A      NE1  CD2      3.52
50.92   -5.13   5.54   4.30  -3.49
 1nba   2.00      0.19      111 A     TYR   96 A      CE3  OH       3.34
73.62  159.69   7.67   7.36   2.16
 1nba   2.00      0.19      126 A     HIS   61 A      CD2  CD2      3.51
17.65 -161.90   4.61   1.40  -4.39
 1nba   2.00      0.19      126 A     TYR  125 A      CD2  CD2      3.83
16.83  135.67   5.26   1.54   5.03
 1nba   2.00      0.19      209 A     PHE   23 B      CH2  CE1      3.65
54.52   65.00   6.74   5.49  -3.91
 1nba   2.00      0.19      209 A     TYR  212 B      CZ2  CD2      3.88
77.78   32.54   6.67   6.52  -1.41
 1nfp   1.60      0.17        4       PHE  194        CE3  CE2      3.79
43.94  158.12   6.13   4.26   4.41
 1nfp   1.60      0.17       96       PHE    9        CD1  CZ       3.56
46.67  -87.40   5.81   4.23   3.99
 1nfp   1.60      0.17       96       PHE  131        CD2  CE1      3.50
16.76  131.97   4.82   1.38   4.62
 1nfp   1.60      0.17       96       TYR  152        CH2  CE1      3.36
79.26   37.73   5.78   5.68  -1.08
 1nif   1.60      0.17      265       PHE  270        CD2  CD1      3.79
9.26 -162.44   5.01   0.83   4.94
 1onc   1.70      0.18        3       PHE    6        CZ3  CD2      3.67
76.51  130.93   6.84   6.65  -1.60
 1ora   2.00      0.18       35       TYR  107        CE3  CE1      3.77
53.06 -176.68   5.28   4.22  -3.17
 1ora   2.00      0.18      275       TRP  278        CZ3  CD1      4.00
64.28  133.57   7.72   6.95  -3.35
 1ora   2.00      0.18      278       TRP  275        CD1  CZ3      4.00
76.00 -103.22   7.72   7.49   1.87
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| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 1ora | 2.00 | 0.18 | 278 | TYR | 164 | CE3 | CD1 | 3.34 |
| 49.50 | 124.69 | 5.62 | 4.27 | -3.65 | | | | |
| 1ora | 2.00 | 0.18 | 278 | TYR | 271 | CE3 | OH | 3.52 |
| 65.68 | 161.52 | 6.50 | 5.92 | 2.67 | | | | |
| 1oyc | 2.00 | 0.17 | 97 | PHE | 101 | CE3 | CE1 | 3.71 |
| 61.10 | 180.00 | 5.59 | 4.89 | -2.70 | | | | |
| 1oyc | 2.00 | 0.17 | 112 | PHE | 284 | CZ3 | CE1 | 3.51 |
| 33.65 | 129.40 | 5.61 | 3.11 | -4.67 | | | | |
| 1oyc | 2.00 | 0.17 | 116 | PHE | 74 | CE3 | CE1 | 3.41 |
| 46.77 | 148.64 | 5.44 | 3.96 | 3.73 | | | | |
| 1oyc | 2.00 | 0.17 | 116 | TYR | 82 | CH2 | CE2 | 3.95 |
| 50.63 | 62.77 | 6.73 | 5.20 | 4.27 | | | | |
| 1oyc | 2.00 | 0.17 | 116 | HIS | 191 | CD1 | ND1 | 3.38 |
| 53.73 | -63.51 | 5.61 | 4.52 | -3.32 | | | | |
| 1oyc | 2.00 | 0.17 | 116 | TYR | 196 | NE1 | CD2 | 3.33 |
| 82.10 | -17.66 | 4.75 | 4.70 | 0.65 | | | | |
| 1pbe | 1.90 | 0.16 | 185 | PHE | 208 | CZ2 | CE2 | 3.43 |
| 38.09 | 0.63 | 4.99 | 3.08 | 3.92 | | | | |
| 1pbe | 1.90 | 0.16 | 185 | TYR | 222 | CE3 | CD1 | 3.51 |
| 69.33 | 146.18 | 5.32 | 4.98 | 1.88 | | | | |
| 1pbe | 1.90 | 0.16 | 185 | HIS | 351 | NE1 | NE2 | 2.83 |
| 82.31 | -28.91 | 5.48 | 5.43 | 0.73 | | | | |
| 1pbe | 1.90 | 0.16 | 240 | TYR | 221 | CH2 | CD2 | 3.47 |
| 84.30 | 95.78 | 6.49 | 6.46 | 0.64 | | | | |
| 1pbe | 1.90 | 0.16 | 337 | PHE | 177 | CZ2 | CG | 3.69 |
| 76.21 | 20.90 | 5.63 | 5.47 | -1.34 | | | | |
| 1pbe | 1.90 | 0.16 | 344 | TYR | 181 | CD1 | OH | 3.68 |
| 77.87 | -89.55 | 7.85 | 7.67 | 1.65 | | | | |
| 1pbe | 1.90 | 0.16 | 345 | TYR | 371 | CZ2 | CD1 | 3.68 |
| 51.91 | 15.49 | 5.10 | 4.02 | -3.14 | | | | |
| 1pbn | 2.00 | 0.20 | 16 | HIS | 20 | NE1 | CE1 | 3.61 |
| 15.58 | 8.06 | 4.17 | 1.13 | 4.01 | | | | |
| 1pbn | 2.00 | 0.20 | 16 | PHE | 48 | CZ3 | CD1 | 3.87 |
| 70.79 | 101.03 | 6.75 | 6.37 | 2.22 | | | | |
| 1pbn | 2.00 | 0.20 | 94 | TYR | 5 | CE3 | CD2 | 3.40 |
| 85.07 | 134.77 | 6.14 | 6.12 | 0.53 | | | | |
| 1pbp | 1.90 | 0.15 | 19 | TYR | 16 | CZ3 | CE1 | 3.94 |
| 57.92 | 131.52 | 6.65 | 5.63 | -3.53 | | | | |
| 1pbp | 1.90 | 0.15 | 156 | TRP | 168 | CH2 | CZ3 | 3.56 |
| 86.91 | 44.58 | 7.19 | 7.18 | -0.39 | | | | |
| 1pbp | 1.90 | 0.15 | 168 | TRP | 156 | CZ3 | CH2 | 3.56 |
| 48.55 | 119.00 | 7.19 | 5.39 | 4.76 | | | | |
| 1pbp | 1.90 | 0.15 | 168 | TYR | 104 | CZ3 | CD2 | 3.80 |
| 67.54 | 121.12 | 7.04 | 6.51 | -2.69 | | | | |
| 1pbp | 1.90 | 0.15 | 168 | TYR | 193 | CZ2 | OH | 3.31 |
| 57.09 | 62.51 | 6.75 | 5.67 | -3.67 | | | | |
| 1pbp | 1.90 | 0.15 | 250 | PHE | 224 | CD1 | CE1 | 3.49 |
| 40.70 | -106.92 | 5.73 | 3.74 | 4.34 | | | | |
| 1pbp | 1.90 | 0.15 | 279 | TYR | 23 | CD2 | CD1 | 3.34 |
| 21.47 | -175.70 | 4.68 | 1.72 | -4.35 | | | | |
| 1pbp | 1.90 | 0.15 | 308 | PHE | 70 | CD1 | CE2 | 3.53 |
| 75.77 | -74.00 | 6.52 | 6.32 | -1.60 | | | | |
| 1pbp | 1.90 | 0.15 | 308 | PHE | 72 | CZ2 | CE2 | 3.70 |
| 85.32 | -12.65 | 4.98 | 4.96 | -0.41 | | | | |
| 1pbp | 1.90 | 0.15 | 308 | TYR | 281 | CH2 | CE2 | 3.76 |
| 60.29 | 53.67 | 6.86 | 5.96 | -3.40 | | | | |
| 1pbp | 1.90 | 0.15 | 308 | TYR | 321 | CE3 | CE1 | 3.71 |
| 76.76 | 157.45 | 5.28 | 5.14 | 1.21 | | | | |
| 1pda | 1.76 | 0.19 | 18 | TYR | 22 | CH2 | CD1 | 3.77 |
| 63.34 | 87.24 | 6.48 | 5.79 | 2.91 | | | | |

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 1pgs   1.80      0.17       191       PHE  292        CE3  CD2      3.79
57.45  146.28   6.54   5.51  -3.52
 1pgs   1.80      0.17       282       TYR  161        CE3  CD2      3.78
59.86  170.94   5.37   4.65  -2.69
 1phg   1.60      0.19        42       PHE   26        CD2  CZ       3.72
9.55  171.45   4.85   0.82   4.78
 1phg   1.60      0.19        55       TRP   63        CZ3  NE1      3.34
80.59  148.36   5.12   5.05   0.84
 1phg   1.60      0.19        63       TRP   55        NE1  CZ3      3.34
6.41   15.86   5.12   0.61   5.08
 1phg   1.60      0.19       374       PHE  150        CZ3  CE1      3.58
38.46  101.37   5.96   3.71   4.67
 1phg   1.60      0.19       374       PHE  381        NE1  CE1      3.46
65.60  -35.86   5.16   4.70   2.13
 1pii   2.00      0.17        15       PHE   97        CH2  CE2      3.56
65.25   62.37   6.67   6.06  -2.79
 1pii   2.00      0.17       356       TYR  278        CZ2  CE1      3.63
85.71   49.60   5.67   5.65  -0.42
 1pii   2.00      0.17       391       PHE  389        CD1  CE1      3.73
88.12  -67.17   5.85   5.85   0.19
 1pne   2.00      0.17         3       TYR    6        CE3  CD2      3.52
49.42  131.68   5.42   4.12   3.52
 1pne   2.00      0.17         3       TRP   31        CZ2  CZ3      3.79
9.38  -14.66   5.40   0.88  -5.33
 1pne   2.00      0.17        31       TRP    3        CZ3  CZ2      3.79
66.99  154.33   5.40   4.97   2.11
 1pne   2.00      0.17         3       TYR  139        CZ2  CE1      3.63
84.54   42.80   5.70   5.67   0.54
 1poc   2.00      0.19       128       TYR   96        CZ3  CD2      3.59
47.84   89.74   6.41   4.75   4.30
 1ppn   1.60      0.16        69       TYR   67        NE1  CD1      3.57
48.57   14.67   4.89   3.67  -3.23
 1ppn   1.60      0.16        69       PHE  207        CD1  CE1      3.52
64.33 -117.88   5.61   5.05   2.43
 1ppn   1.60      0.16       177       PHE  141        CH2  CE1      3.72
56.33   86.00   6.69   5.57  -3.71
 1ppn   1.60      0.16       177       HIS  159        NE1  CE1      3.36
48.90   -4.70   4.74   3.57  -3.11
 1ppn   1.60      0.16       177       TRP  181        CE3  NE1      3.53
71.39  149.03   5.36   5.08  -1.71
 1ppn   1.60      0.16       181       TRP  177        NE1  CE3      3.53
8.85  -80.97   5.36   0.84  -5.29
 1ppn   1.60      0.16       181       PHE  141        CZ2  CE1      3.78
69.25   29.43   5.93   5.55  -2.10
 1ppn   1.60      0.16       181       TYR  144        CZ2  CD2      3.71
36.72   48.87   5.79   3.46   4.64
 1rcf   1.40      0.14       120       TYR  125        NE1  OH       2.95
85.49  -49.83   6.80   6.78  -0.53
 1rcf   1.40      0.14       120       TRP  159        CE3  CD1      3.74
38.27  159.14   6.49   4.02   5.09
 1rcf   1.40      0.14       159       TRP  120        CD1  CE3      3.74
52.47  -97.68   6.49   5.15  -3.95
 1rci   2.00      0.19        89       TYR   36        CD1  CG       3.97
81.29 -110.32   6.58   6.50   1.00
 1rec   1.90      0.19        31       PHE   23        CZ3  CE2      3.58
65.93  135.16   5.74   5.24  -2.34
 1rec   1.90      0.19        31       PHE   83        CG   CZ       3.80
15.56 -122.02   5.19   1.38   5.00
 1rec   1.90      0.19        31       TYR   86        NE1  OH       2.98
54.30    1.99   5.44   4.42   3.17
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 1rec   1.90      0.19       104       PHE   73        NE1  CZ       3.72
71.22  -36.64   5.79   5.48  -1.86
 1rec   1.90      0.19       104       PHE  188        CZ3  CE1      3.39
87.86  120.88   6.12   6.12   0.23
 1rva   2.00      0.16       216 A     TYR  110 A      CZ3  CD2      3.62
77.24  137.41   5.98   5.83  -1.32
 1rva   2.00      0.16       216 A     PHE  206 A      NE1  CZ       3.84
70.38  -53.27   6.50   6.12   2.18
 1rva   2.00      0.16       216 A     PHE  212 A      CD1  CE1      3.65
67.87  -88.48   6.37   5.90  -2.40
 1rva   2.00      0.16       216 A     TYR  215 A      NE1  CD1      3.61
16.89  -36.06   4.96   1.45   4.74
 1rva   2.00      0.16       216 A     TYR  219 A      CZ3  CD2      3.44
55.55  105.08   5.28   4.36   2.98
 1rva   2.00      0.16       239 A     TYR  230 A      CE3  CE2      3.71
27.78  145.72   5.27   2.46  -4.66
 1rva   2.00      0.16       239 A     TYR  236 A      CE3  CD1      3.93
77.20  147.06   6.57   6.41  -1.45
 1sac   2.00      0.18        98 A     PHE   33 A      CE3  CE2      3.92
74.53 -178.79   6.19   5.97  -1.65
 1sac   2.00      0.18       185 A     PHE    9 A      CH2  CE2      3.40
68.86   67.61   6.18   5.76  -2.23
 1sac   2.00      0.18       203 A     TYR   40 A      CG   CD2      3.60
18.57 -144.90   4.93   1.58   4.67
 1sat   1.75      0.19        46       TYR  246        CD1  OH       3.39
85.22 -104.93   7.60   7.57  -0.63
 1sat   1.75      0.19       153       TYR   65        CH2  CZ       3.34
69.93   71.20   5.69   5.34   1.95
 1sat   1.75      0.19       153       TYR  135        CD1  CE1      3.46
64.22 -121.93   5.88   5.29  -2.56
 1sat   1.75      0.19       217       TYR  190        NE1  OH       3.72
70.06   -3.91   5.12   4.81   1.75
 1sat   1.75      0.19       217       TYR  199        CD1  CD1      3.76
45.77 -109.66   6.28   4.50  -4.38
 1sbp   1.70      0.18        28       PHE   24        CE3  CZ       3.78
47.35 -179.81   5.55   4.08   3.76
 1sbp   1.70      0.18       112       PHE   99        CD2  CZ       3.56
9.70  109.82   4.82   0.81   4.75
 1sbp   1.70      0.18       112       TYR  143        CD1  CD2      3.37
68.00 -116.42   5.62   5.21  -2.10
 1sbp   1.70      0.18       135       TRP  192        CD1  CH2      3.42
61.82  -86.34   6.90   6.08  -3.26
 1sbp   1.70      0.18       141       TYR  137        CZ3  OH       3.66
69.35  155.56   6.30   5.90   2.22
 1sbp   1.70      0.18       141       PHE  287        CD1  CE1      3.64
50.82 -100.13   6.38   4.95   4.03
 1sbp   1.70      0.18       192       TYR   10        CZ2  CE2      3.77
39.03   27.19   5.60   3.53  -4.35
 1sbp   1.70      0.18       192       TRP  135        CH2  CD1      3.42
57.13   77.06   6.90   5.80   3.74
 1sbp   1.70      0.18       135       TRP  290        CH2  NE1      3.49
32.30   59.97   5.47   2.92   4.62
 1sbp   1.70      0.18       290       TRP  135        NE1  CH2      3.49
88.90   12.50   5.47   5.47   0.10
 1sbp   1.70      0.18       141       HIS  297        CE2  CE1      3.70
10.39  110.70   4.64   0.86   4.56
 1scs   1.60      0.18        40       TYR   67        CZ2  OH       3.54
71.13  -12.06   6.13   5.80   1.98
 1scs   1.60      0.18        40       PHE  197        CZ2  CE2      3.91
69.31   29.10   6.59   6.16  -2.33
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|---|---|---|---|---|---|---|---|---|---|---|---|
| 1scs | 1.60 | 0.18 | | 88 | HIS | 180 | | CE2 | CD2 | 3.51 |
| 29.48 | 18.47 | 3.93 | 1.93 | 3.42 | | | | | | | |
| 1scs | 1.60 | 0.18 | | 109 | PHE | 128 | | CZ2 | CZ | 3.74 |
| 10.81 | 57.63 | 5.00 | 0.95 | 4.91 | | | | | | | |
| 1scs# | 1.60 | 0.18 | | 182 | TYR | 12 | | CZ2 | OH | 3.32 |
| 86.24 | 26.77 | 6.67 | 6.66 | 0.44 | | | | | | | |
| 1scs# | 1.60 | 0.18 | | 182 | TYR | 100 | | NE1 | OH | 2.98 |
| 82.50 | -16.25 | 6.30 | 6.25 | -0.82 | | | | | | | |
| 1scs# | 1.60 | 0.18 | | 182 | HIS | 205 | | CE2 | NE2 | 3.43 |
| 18.68 | 25.22 | 3.67 | 1.18 | -3.47 | | | | | | | |
| 1slt | 1.90 | 0.17 | | 68 A | HIS | 44 A | | CH2 | CG | 3.38 |
| 68.19 | 77.51 | 5.43 | 5.04 | -2.02 | | | | | | | |
| 1sri | 1.65 | 0.17 | | 21 A | PHE | 29 A | | CD1 | CD2 | 3.89 |
| 44.45 | -96.99 | 6.05 | 4.24 | -4.32 | | | | | | | |
| 1sri | 1.65 | 0.17 | | 21 A | TYR | 96 A | | CH2 | CE1 | 3.76 |
| 76.94 | 50.81 | 7.01 | 6.83 | -1.59 | | | | | | | |
| 1sri | 1.65 | 0.17 | | 75 A | PHE | 29 A | | CE2 | CE1 | 3.66 |
| 25.47 | 41.72 | 4.28 | 1.84 | -3.86 | | | | | | | |
| 1sri | 1.65 | 0.17 | | 75 A | TRP | 92 A | | NE1 | CE3 | 3.05 |
| 47.68 | -11.20 | 4.55 | 3.37 | 3.06 | | | | | | | |
| 1sri | 1.65 | 0.17 | | 92 A | TRP | 75 A | | CE3 | NE1 | 3.05 |
| 43.22 | -177.39 | 4.55 | 3.12 | 3.31 | | | | | | | |
| 1sri | 1.65 | 0.17 | | 75 A | PHE | 130 A | | CH2 | CE2 | 3.83 |
| 85.53 | 39.30 | 6.34 | 6.32 | -0.49 | | | | | | | |
| 1sri | 1.65 | 0.17 | | 79 A | TYR | 43 A | | CH2 | CD1 | 3.63 |
| 77.83 | 64.12 | 6.90 | 6.75 | 1.45 | | | | | | | |
| 1sri | 1.65 | 0.17 | | 79 A | TRP | 92 A | | CZ2 | CH2 | 3.89 |
| 74.81 | 20.49 | 7.88 | 7.60 | 2.06 | | | | | | | |
| 1sri | 1.65 | 0.17 | | 92 A | TRP | 79 A | | CH2 | CZ2 | 3.89 |
| 74.64 | 71.27 | 7.88 | 7.60 | -2.09 | | | | | | | |
| 1sri | 1.65 | 0.17 | | 79 A | TYR | 54 A | | CZ3 | CD1 | 3.69 |
| 78.61 | 150.28 | 5.46 | 5.35 | 1.08 | | | | | | | |
| 1sri | 1.65 | 0.17 | | 92 A | TYR | 43 A | | CZ2 | OH | 3.44 |
| 49.38 | 50.93 | 5.42 | 4.11 | 3.53 | | | | | | | |
| 1sri | 1.65 | 0.17 | | 92 A | TRP | 108 A | | NE1 | CD1 | 3.84 |
| 38.76 | -35.59 | 6.14 | 3.85 | -4.79 | | | | | | | |
| 1sri | 1.65 | 0.17 | | 108 A | TRP | 92 A | | CD1 | NE1 | 3.84 |
| 47.81 | -121.26 | 6.14 | 4.55 | 4.12 | | | | | | | |
| 1sri | 1.65 | 0.17 | | 92 A | PHE | 130 A | | NE1 | CZ | 3.86 |
| 40.18 | -54.09 | 6.07 | 3.91 | 4.64 | | | | | | | |
| 1tca | 1.55 | 0.16 | | 52 | PHE | 131 | | CZ2 | CZ | 3.62 |
| 45.79 | -16.33 | 5.16 | 3.70 | -3.60 | | | | | | | |
| 1tca | 1.55 | 0.16 | | 52 | TYR | 234 | | CH2 | CD1 | 3.76 |
| 51.57 | 68.36 | 6.63 | 5.19 | 4.12 | | | | | | | |
| 1tca | 1.55 | 0.16 | | 104 | HIS | 224 | | CZ2 | CD2 | 3.73 |
| 50.90 | -13.20 | 4.97 | 3.86 | 3.13 | | | | | | | |
| 1tca | 1.55 | 0.16 | | 113 | PHE | 117 | | CE2 | CD2 | 3.63 |
| 16.18 | 47.45 | 4.56 | 1.27 | -4.38 | | | | | | | |
| 1tca | 1.55 | 0.16 | | 113 | TYR | 300 | | NE1 | OH | 3.00 |
| 64.61 | -12.17 | 6.10 | 5.51 | -2.61 | | | | | | | |
| 1tml | 1.80 | 0.18 | | 16 | PHE | 274 | | CG | CE2 | 3.91 |
| 37.39 | -142.57 | 5.80 | 3.52 | -4.61 | | | | | | | |
| 1tml | 1.80 | 0.18 | | 41 | TYR | 73 | | CZ3 | CG | 3.92 |
| 88.82 | 130.35 | 6.20 | 6.20 | 0.13 | | | | | | | |
| 1tml | 1.80 | 0.18 | | 97 | TYR | 94 | | CE3 | CE1 | 3.72 |
| 72.53 | 150.89 | 6.15 | 5.87 | -1.85 | | | | | | | |
| 1tml | 1.80 | 0.18 | | 97 | PHE | 101 | | CH2 | CD2 | 3.90 |
| 42.15 | 68.03 | 6.28 | 4.22 | 4.65 | | | | | | | |
| 1tml | 1.80 | 0.18 | | 162 | HIS | 159 | | CE3 | NE2 | 3.36 |
| 63.02 | 161.41 | 4.97 | 4.43 | -2.25 | | | | | | | |

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 1tml   1.80      0.18       162       HIS  163        NE1  NE2      3.55
28.86  -63.66   4.40   2.13   3.85
 1ton   1.80      0.20        51       PHE   89        CZ3  CE1      3.38
85.18   93.50   6.87   6.85   0.58
 1ton   1.80      0.20        51       HIS  107        CE2  CD2      3.42
35.62   26.68   4.06   2.36   3.30
 1ton   1.80      0.20       237       HIS   91        CD2  CD2      3.56
7.66 -174.47   4.61   0.58  -4.57
 1ton#  1.80      0.20       237       TYR  172        CD1  CE1      3.60
68.15  -78.10   6.64   6.16   2.47
 1tph   1.80      0.19        90 1     PHE    7 1      CZ2  CE2      3.86
29.11   58.90   5.84   2.84  -5.10
 1tph   1.80      0.19       191 1     PHE  144 1      CD1  CG       3.49
66.69  -97.71   5.54   5.09  -2.19
 1tph   1.80      0.19       191 1     HIS  195 1      CD1  CE1      3.35
22.81  -38.31   3.75   1.46   3.45
 1trk   2.00      0.16        45 B     PHE   63 B      CZ2  CD2      3.59
72.94  -11.67   4.95   4.73   1.45
 1trk   2.00      0.16        45 B     TYR   83 B      CZ3  CE1      3.96
79.64  106.85   7.46   7.34   1.34
 1trk   2.00      0.16        57 B     TRP  312 B      NE1  CG       3.41
86.34  -34.67   5.47   5.46   0.35
 1trk   2.00      0.16       312 B     TRP   57 B      CG   NE1      3.41
33.41 -143.26   5.47   3.01  -4.57
 1trk   2.00      0.16       212 B     TYR  207 B      CD2  CD2      3.58
6.67  168.03   4.87   0.59  -4.83
 1trk   2.00      0.16       312 B     PHE  316 B      CH2  CD2      3.89
55.36   72.77   6.21   5.11   3.53
 1trk   2.00      0.16       623 B     PHE  591 B      CH2  CE1      3.75
22.91   77.90   5.23   2.03   4.82
 1tsp   2.00      0.18       207       TYR  328        CH2  CE1      3.61
72.54   49.91   6.90   6.58  -2.07
 1tsp   2.00      0.18       315       TYR  377        CZ3  CD2      3.69
55.96   89.41   6.72   5.57  -3.76
 1tys   1.80      0.18        61       PHE   62        CZ3  CE1      3.53
66.20  145.76   6.04   5.53   2.44
 1tys   1.80      0.18        61       TYR   71        CD1  CD2      3.75
67.45 -106.64   6.59   6.09  -2.53
 1tys   1.80      0.18        61       TRP   80        CZ3  NE1      3.65
73.63   90.48   6.67   6.40  -1.88
 1tys   1.80      0.18        80       TRP   61        NE1  CZ3      3.65
40.38  -77.00   6.67   4.32  -5.08
 1tys   1.80      0.18        98       PHE   62        CH2  CD2      3.83
33.42   65.00   5.76   3.18  -4.80
 1tys   1.80      0.18        98       PHE  150        CZ2  CE1      3.71
34.81   11.81   5.45   3.11   4.47
 1tys   1.80      0.18        98       TYR  181        CZ2  OH       3.59
75.33   36.87   7.16   6.93   1.81
 1tys#  1.80      0.18       133       PHE  149        CG   CE2      3.77
46.87  119.21   7.25   5.29  -4.95
 1tys   1.80      0.18       201       HIS   32        CZ3  CD2      3.99
84.40  125.92   7.33   7.30  -0.71
 1udg   1.75      0.20        19       PHE   22        CZ3  CE2      3.88
45.37  120.83   6.25   4.45  -4.39
 1udg   1.75      0.20        32       TRP   71        CZ3  CZ3      3.79
16.15   83.90   6.34   1.77  -6.09
 1udg   1.75      0.20        71       TRP   32        CZ3  CZ3      3.79
69.14  125.83   6.34   5.93  -2.26
 1udg   1.75      0.20        71       PHE   69        CZ2  CD1      3.57
55.62   -3.06   5.74   4.74  -3.24
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 1udg   1.75      0.20      138      TRP  242        CZ2  CE3     3.82
20.85   19.75   5.71   2.03   5.34
 1udg   1.75      0.20      242      TRP  138        CE3  CZ2     3.82
83.05  153.55   5.71   5.67   0.69
 1udg   1.75      0.20      165      PHE   69        CZ3  CZ      3.96
59.97   95.20   7.11   6.15  -3.56
 1udg   1.75      0.20      188      PHE  101        CE3  CZ      3.79
83.43  133.54   6.33   6.29  -0.72
 1udg   1.75      0.20      188      PHE  219        CE2  CZ      3.61
3.92 -145.03   4.86   0.33   4.85
 1udg   1.75      0.20      188      HIS  224        NE1  ND1     3.07
84.68  -43.41   5.77   5.75   0.54
 1udg   1.75      0.20      242      PHE  225        CD2  CD1     3.89
12.52  141.97   5.19   1.14  -5.06
 1vhh   1.70      0.19      129      PHE   74        CH2  CE1     3.68
51.72   78.79   6.52   5.12  -4.04
 1vhh   1.70      0.19      173      PHE   48        NE1  CD2     3.67
67.35    3.98   5.51   5.09   2.12
 1vhh   1.70      0.19      173      TYR  175        CH2  CG      3.68
60.83   72.67   6.24   5.45   3.04
 1vhh   1.70      0.19      173      HIS  183        CZ3  CD2     3.62
87.91  131.46   6.55   6.55   0.24
 1wht   2.00      0.18       49 A    PHE   92 A      CD1  CD1     3.68
59.14 -111.33   6.37   5.47   3.27
 1wht   2.00      0.18       84 A    PHE  411 B      CE3  CG      3.41
42.98  159.87   4.23   2.89   3.09
 1wht   2.00      0.18      126 A    TYR   32 A      NE1  CE1     3.62
83.06  -46.96   5.17   5.13  -0.62
 1wht   2.00      0.18      126 A    PHE  122 A      CD1  CZ      3.53
56.81 -114.57   5.86   4.90  -3.21
 1wht   2.00      0.18      126 A    PHE  130 A      NE1  CE1     3.23
35.53   11.58   4.11   2.39   3.34
 1wht   2.00      0.18      126 A    TYR  133 A      CH2  CD2     3.60
82.43   75.69   6.60   6.54   0.87
 1wht   2.00      0.18      192 A    PHE  189 A      CZ3  CE1     3.90
33.84  121.29   5.93   3.30  -4.92
 1wht   2.00      0.18      193 A    TYR  203 A      CG   CD2     3.26
41.10 -150.43   4.74   3.11  -3.57
 1wht   2.00      0.18      308 B    TYR  147 A      NE1  OH      3.52
27.06  -22.59   5.58   2.54   4.97
 1wht   2.00      0.18      308 B    TYR  151 A      CH2  OH      3.59
56.02   42.57   6.81   5.65   3.80
 1wht   2.00      0.18      331 B    PHE  414 B      CG   CD1     3.41
26.14 -141.51   5.26   2.32  -4.72
 1wht   2.00      0.18      369 B    TRP  380 B      NE1  CG      3.23
65.00  -31.93   5.69   5.16  -2.41
 1wht   2.00      0.18      380 B    TRP  369 B      CG   NE1     3.23
56.18 -126.75   5.69   4.73   3.17
 1wht#  2.00      0.18      193 A    TYR  348 B      CH2  CZ      3.61
83.87   78.65   6.16   6.12  -0.66
 1xnb   1.49      0.17        6      TYR   26        CZ3  CG      3.97
82.94  109.90   7.22   7.17  -0.89
 1xnb   1.49      0.17       30      PHE   36        CD2  CZ      3.50
21.49 -129.51   4.84   1.78  -4.50
 1xnb   1.49      0.17       71      TYR   69        NE1  OH      3.01
54.93  -46.17   5.85   4.79   3.36
 1xnb   1.49      0.17       71      PHE  125        CH2  CE1     3.66
77.15   81.70   6.16   6.01   1.37
 1xnb   1.49      0.17       71      TYR  166        NE1  OH      3.34
74.48  -81.56   6.27   6.04  -1.68
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 1xnb   1.49      0.17      129       TYR   80        CZ3  CG      3.62
38.22   94.87   4.57   2.83   3.59
 1xnb   1.49      0.17      153       TYR  128        CE3  CD2     3.95
34.50  159.44   5.91   3.34   4.87
 1xnb   1.49      0.17      153       PHE  146        CH2  CE1     3.97
48.26   93.12   6.69   4.99  -4.45
 1xnb   1.49      0.17      164       TYR   79        CZ3  OH      3.77
63.97  110.57   7.11   6.39   3.12
 1xnb   1.49      0.17      164       PHE  146        CZ3  CE2     3.95
81.36   89.12   7.61   7.52  -1.14
 1xyl   1.80      0.18       15 A     HIS   53 A      CE3  ND1     3.35
24.50  139.76   4.55   1.89  -4.14
 1xyl   1.80      0.18       15 A     HIS  284 A      CH2  CE1     3.80
58.99   46.84   6.35   5.44   3.27
 1xyl   1.80      0.18      136 A     PHE   93 A      CE3  CE2     3.47
77.49  127.92   5.59   5.46   1.21
 1xyl   1.80      0.18      136 A     PHE  525 B      CH2  CD1     3.67
73.74   68.27   6.27   6.02  -1.75
 1xyl#  1.80      0.18      236 A     PHE  201 A      CZ3  CD1     3.69
61.77   80.08   6.62   5.83  -3.13
 1xyl   1.80      0.18      269 A     PHE  268 A      CD2  CD2     3.74
13.14  125.66   5.01   1.14   4.88
 1xyz   1.40      0.18      600 B     HIS  601 B      CD1  CD2     3.47
51.73  -59.52   5.30   4.16   3.28
 1xyz   1.40      0.18      607 B     PHE  564 B      CZ2  CE1     3.74
52.95   28.19   6.43   5.13  -3.87
 1xyz   1.40      0.18      659 B     PHE  564 B      CZ2  CE2     3.81
86.70   31.94   6.43   6.42  -0.37
 1xyz   1.40      0.18      795 B     TRP  803 B      CD1  NE1     3.73
70.32  -74.90   6.40   6.03   2.15
 1xyz   1.40      0.18      803 B     TRP  795 B      NE1  CD1     3.73
29.20  -53.75   6.40   3.12   5.59
 1xyz   1.40      0.18      803 B     HIS  723 B      CZ2  CE1     3.41
73.11   13.19   4.96   4.75   1.44
 2abk   1.85      0.19      178       PHE  171        CZ3  CD1     3.74
71.74   93.39   7.27   6.90   2.28
 2acq   1.76      0.17       20       TYR   48        CD1  CD1     3.73
63.97 -121.08   5.72   5.14  -2.51
 2acq   1.76      0.17       20       TRP  219        CH2  CH2     3.30
89.42   52.28   7.37   7.37   0.07
 2acq   1.76      0.17      219       TRP   20        CH2  CH2     3.30
60.07   74.67   7.37   6.39   3.68
 2acq   1.76      0.17       79       HIS  110        CE3  CD2     3.59
87.84  135.46   5.96   5.96   0.22
 2acq   1.76      0.17       79       TRP  111        CZ3  CD1     3.58
66.40   94.58   7.52   6.89  -3.01
 2acq   1.76      0.17      111       TRP   79        CD1  CZ3     3.58
70.31  -78.95   7.52   7.08  -2.54
 2acq   1.76      0.17       79       PHE  115        CZ2  CE2     3.90
43.63    3.83   5.97   4.12  -4.32
 2acq   1.76      0.17       79       PHE  121        CD1  CD1     3.84
33.95  -72.08   5.58   3.11   4.63
 2acq   1.76      0.17       79       PHE  122        CZ2  CE1     3.58
83.97   23.27   5.84   5.81   0.61
 2acq   1.76      0.17      111       HIS  110        NE1  ND1     3.60
62.17  -58.36   5.60   4.95   2.62
 2acq   1.76      0.17      111       PHE  311        CZ3  CE2     3.71
85.06  108.68   7.17   7.14   0.62
 2acq   1.76      0.17      295       HIS  187        CE3  NE2     3.93
72.14  144.35   6.55   6.23   2.01
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 2acq   1.76      0.17       295       TYR  189         CE3  CD2      3.87
49.52  156.23   6.42   4.88  -4.17
 2ak3   1.85      0.19       203 B     HIS   28 B       CZ2  CD2      3.69
74.04   20.39   5.66   5.44   1.56
 2ak3   1.85      0.19       203 B     TYR  207 B       CZ2  CD1      3.82
48.44   13.51   5.75   4.30  -3.82
 2alp   1.70      0.13       105       TYR  238         CD1  CG       3.49
73.43  -75.26   5.62   5.39   1.60
 2ayh   1.60      0.14        18       TYR   64         CG   CE2      3.42
46.79 -164.50   5.04   3.67  -3.45
 2ayh   1.60      0.14        34       TYR   24         CD1  CE2      3.39
79.32  -81.85   5.83   5.73  -1.08
 2ayh   1.60      0.14        34       PHE   30         CZ2  CD2      3.81
72.99   27.08   6.32   6.04   1.85
 2ayh   1.60      0.14       103       TYR   94         NE1  CE2      3.54
49.62  -68.13   5.85   4.45  -3.79
 2ayh   1.60      0.14       103       TYR  123         CZ2  CD2      3.48
45.36   19.90   4.55   3.24   3.19
 2ayh   1.60      0.14       151       TYR   72         NE1  CE1      3.52
20.85  -26.31   4.93   1.74   4.61
 2ayh   1.60      0.14       151       TYR   75         CZ3  OH       3.63
85.12  158.06   6.53   6.51  -0.56
 2ayh   1.60      0.14       158       PHE  120         CD1  CD1      3.26
35.43 -113.50   4.33   2.50   3.53
 2ayh   1.60      0.14       158       HIS  166         CZ3  CD2      3.43
53.97  129.47   5.91   4.78   3.48
 2ayh   1.60      0.14       184       PHE   30         CD2  CE2      3.44
11.77  115.93   4.13   0.83   4.05
 2ayh   1.60      0.14       184       TRP  192         CH2  CZ3      3.89
65.59   54.05   8.15   7.42  -3.37
 2ayh   1.60      0.14       192       TRP  184         CZ3  CH2      3.89
62.82   89.58   8.15   7.25   3.72
 2ayh   1.60      0.14       208       PHE    7         CE3  CE1      3.77
39.49 -168.92   5.54   3.52   4.28
 2aza   1.80      0.16        48 A     TYR   15 A       CD1  OH       3.90
81.10  -89.24   6.84   6.76   1.06
 2aza   1.80      0.16        48 A     PHE   97 A       CH2  CE1      3.92
80.18   79.63   7.41   7.30  -1.26
 2aza   1.80      0.16        48 A     TYR  110 A       NE1  CG       3.18
70.55  -34.04   5.20   4.90   1.73
 2bbk   1.75      0.17       127 H     PHE  172 H       CG   CE1      3.69
39.78 -152.96   5.66   3.62  -4.35
 2bbk   1.75      0.17       127 H     TYR  220 H       CH2  CD2      3.78
25.86   80.58   5.62   2.46  -5.05
 2bbk   1.75      0.17       229 H     PHE  172 H       CZ3  CE2      3.64
54.47  100.42   6.38   5.19  -3.71
 2bbk   1.75      0.17       229 H     HIS  182 H       CH2  CG       3.79
38.30   63.96   5.51   3.42   4.32
 2bbk   1.75      0.17       264 H     PHE  299 H       CZ3  CD1      3.87
85.13   79.47   6.31   6.29   0.54
 2bbk   1.75      0.17       269 H     HIS  217 H       NE1  NE2      3.10
15.78  -68.06   4.15   1.12  -3.99
 2bbk   1.75      0.17       291 H     TYR  232 H       CZ3  CE2      3.92
60.75  115.89   7.25   6.33   3.54
 2bbk   1.75      0.17       291 H     HIS  293 H       CE3  CE1      3.87
78.54  151.91   6.41   6.28   1.27
 2bbk   1.75      0.17        26 L     TYR   25 L       NE1  OH       3.65
48.92  -82.29   5.50   4.15  -3.61
 2bbk   1.75      0.17        26 L     TYR   70 L       CH2  CD1      3.41
62.96   68.15   6.30   5.61   2.87
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|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2bbk | 1.75 | 0.17 | | 108 | L | PHE | 110 | L | CZ3 | CE2 | 3.63 | |
| 58.60 | 135.06 | 6.28 | 5.36 | 3.27 | | | | | | | | |
| 2cba | 1.54 | 0.15 | | 5 | | TYR | 7 | | CZ3 | CE2 | 3.92 | |
| 84.71 | 121.09 | 6.97 | 6.94 | -0.64 | | | | | | | | |
| 2cba | 1.54 | 0.15 | | 5 | | TRP | 16 | | CE3 | CZ2 | 3.66 | |
| 53.80 | 163.52 | 5.52 | 4.45 | 3.26 | | | | | | | | |
| 2cba | 1.54 | 0.15 | | 16 | | TRP | 5 | | CZ2 | CE3 | 3.66 | |
| 26.08 | -10.23 | 5.52 | 2.42 | 4.96 | | | | | | | | |
| 2cba | 1.54 | 0.15 | | 16 | | TYR | 7 | | CH2 | CE1 | 3.80 | |
| 86.87 | 29.46 | 6.13 | 6.12 | -0.33 | | | | | | | | |
| 2cba | 1.54 | 0.15 | | 97 | | PHE | 66 | | CH2 | CD1 | 3.94 | |
| 58.21 | 86.61 | 6.80 | 5.78 | -3.58 | | | | | | | | |
| 2cba | 1.54 | 0.15 | | 97 | | PHE | 226 | | CE3 | CD2 | 3.74 | |
| 19.30 | 153.56 | 5.19 | 1.71 | -4.90 | | | | | | | | |
| 2cba | 1.54 | 0.15 | | 123 | | PHE | 131 | | CD1 | CD1 | 3.92 | |
| 46.60 | -108.01 | 6.53 | 4.74 | 4.49 | | | | | | | | |
| 2cba | 1.54 | 0.15 | | 192 | | PHE | 260 | | CE2 | CZ | 3.67 | |
| 30.89 | -21.90 | 5.27 | 2.71 | -4.52 | | | | | | | | |
| 2cba | 1.54 | 0.15 | | 209 | | HIS | 107 | | CE3 | CE1 | 3.60 | |
| 21.23 | 137.81 | 4.90 | 1.77 | -4.57 | | | | | | | | |
| 2cba | 1.54 | 0.15 | | 209 | | HIS | 119 | | CH2 | NE2 | 3.54 | |
| 84.89 | 82.82 | 5.97 | 5.95 | -0.53 | | | | | | | | |
| 2cba | 1.54 | 0.15 | | 209 | | TYR | 194 | | CD1 | OH | 3.57 | |
| 55.03 | -114.38 | 5.67 | 4.64 | -3.25 | | | | | | | | |
| 2ccy | 1.67 | 0.19 | | 58 | A | PHE | 75 | A | CD1 | CE2 | 3.92 | |
| 88.58 | -94.32 | 6.67 | 6.67 | -0.17 | | | | | | | | |
| 2ccy | 1.67 | 0.19 | | 58 | A | PHE | 82 | A | NE1 | CZ | 3.59 | |
| 18.43 | -95.20 | 4.94 | 1.57 | 4.68 | | | | | | | | |
| 2ccy | 1.67 | 0.19 | | 58 | A | TRP | 86 | A | CH2 | CZ2 | 3.49 | |
| 41.19 | 108.46 | 5.82 | 3.83 | 4.38 | | | | | | | | |
| 2ccy | 1.67 | 0.19 | | 86 | A | TRP | 58 | A | CZ2 | CH2 | 3.49 | |
| 73.63 | -3.79 | 5.82 | 5.58 | -1.64 | | | | | | | | |
| 2ccy | 1.67 | 0.19 | | 86 | A | PHE | 82 | A | NE1 | CE2 | 3.46 | |
| 66.90 | -39.03 | 5.31 | 4.88 | 2.08 | | | | | | | | |
| 2cpl | 1.63 | 0.18 | | 121 | | PHE | 60 | | CZ2 | CE1 | 3.84 | |
| 81.81 | 15.44 | 6.14 | 6.08 | 0.88 | | | | | | | | |
| 2ctc | 1.40 | 0.16 | | 63 | | PHE | 192 | | CD1 | CE2 | 3.33 | |
| 54.04 | -81.91 | 4.97 | 4.02 | 2.92 | | | | | | | | |
| 2ctc | 1.40 | 0.16 | | 73 | | TYR | 12 | | CE3 | CG | 3.81 | |
| 79.07 | 167.50 | 5.75 | 5.65 | 1.09 | | | | | | | | |
| 2ctc | 1.40 | 0.16 | | 73 | | PHE | 116 | | NE1 | CE1 | 3.62 | |
| 36.40 | -44.82 | 5.55 | 3.30 | 4.46 | | | | | | | | |
| 2ctc | 1.40 | 0.16 | | 73 | | HIS | 120 | | CH2 | CE1 | 3.49 | |
| 50.50 | 35.18 | 4.83 | 3.72 | 3.08 | | | | | | | | |
| 2ctc | 1.40 | 0.16 | | 81 | | PHE | 82 | | CE3 | CD1 | 3.70 | |
| 83.88 | 148.79 | 6.84 | 6.80 | -0.73 | | | | | | | | |
| 2ctc | 1.40 | 0.16 | | 126 | | PHE | 118 | | CG | CD2 | 3.66 | |
| 20.53 | -167.26 | 5.04 | 1.78 | 4.72 | | | | | | | | |
| 2ctc | 1.40 | 0.16 | | 147 | | TRP | 257 | | CZ3 | CE3 | 3.66 | |
| 84.12 | 147.33 | 6.00 | 5.97 | -0.61 | | | | | | | | |
| 2ctc | 1.40 | 0.16 | | 257 | | TRP | 147 | | CE3 | CZ3 | 3.66 | |
| 37.00 | -178.37 | 6.00 | 3.61 | -4.79 | | | | | | | | |
| 2ctc | 1.40 | 0.16 | | 294 | | PHE | 86 | | CZ3 | CE1 | 3.24 | |
| 55.78 | 95.37 | 6.42 | 5.31 | 3.61 | | | | | | | | |
| 2ctc | 1.40 | 0.16 | | 294 | | PHE | 96 | | CH2 | CD1 | 3.65 | |
| 78.15 | 44.74 | 6.22 | 6.09 | 1.28 | | | | | | | | |
| 2cyp | 1.70 | 0.20 | | 51 | | HIS | 52 | | NE1 | CD2 | 3.24 | |
| 39.85 | -50.14 | 5.05 | 3.23 | -3.88 | | | | | | | | |
| 2cyp | 1.70 | 0.20 | | 51 | | PHE | 158 | | CH2 | CZ | 3.97 | |
| 58.50 | 77.43 | 6.90 | 5.88 | 3.61 | | | | | | | | |

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 2cyp   1.70      0.20      101       PHE   19        CZ3  CE2     3.54
84.83   91.82   6.46   6.43   0.58
 2cyp   1.70      0.20      101       PHE   99        NE1  CD2     3.67
57.09   -9.38   5.94   4.99  -3.22
 2cyp   1.70      0.20      126       PHE   19        CZ3  CD2     3.79
86.56   96.25   6.52   6.51  -0.39
 2cyp   1.70      0.20      126       PHE  284        CE3  CD1     3.94
78.00  143.78   7.08   6.93   1.47
 2cyp   1.70      0.20      126       PHE  286        CE3  CE2     3.70
51.08  162.41   6.00   4.67  -3.77
 2cyp   1.70      0.20      191       HIS  175        CZ2  CG      3.42
41.09   30.95   4.41   2.90   3.32
 2cyp   1.70      0.20      223       TYR  236        NE1  CG      3.51
7.16    7.93   3.67   0.45  -3.64
 2dnj   2.00      0.17      181 A     TRP  194 A      CZ3  CH2     3.76
56.68  104.61   7.25   6.06  -3.98
 2dnj   2.00      0.17      194 A     TRP  181 A      CH2  CZ3     3.76
40.35   91.19   7.25   4.69  -5.53
 2end#  1.45      0.16      128       HIS  107        CD2  CD2     3.18
7.63 -170.12   4.29   0.58   4.25
 2er7   1.60      0.14       39 E     TYR   75 E      NE1  OH      2.83
82.01  -26.55   6.62   6.56   0.92
 2er7   1.60      0.14       39 E     TRP   71 E      CG   CH2     3.61
45.47 -140.66   6.50   4.64   4.56
 2er7   1.60      0.14       71 E     TRP   39 E      CH2  CG      3.61
70.15   75.49   6.50   6.11   2.21
 2er7   1.60      0.14       39 E     PHE  111 E      CZ2  CZ      3.71
87.36   31.82   5.43   5.42   0.25
 2er7   1.60      0.14      190 E     PHE  125 E      CD2  CE1     3.82
13.73   14.48   4.60   1.07   4.47
 2er7   1.60      0.14      190 E     PHE  314 E      CD2  CD2     3.61
6.89 -130.52   4.97   0.61  -4.93
 2er7   1.60      0.14      192 E     PHE  259 E      CH2  CD1     3.91
84.21   50.99   7.01   6.97   0.71
 2er7   1.60      0.14      192 E     PHE  302 E      CZ2  CE2     3.55
60.44   14.37   4.72   4.11  -2.33
 2er7   1.60      0.14      192 E     PHE  323 E      CZ2  CZ      3.79
28.61   51.47   5.28   2.54   4.63
 2er7   1.60      0.14      232 E     TYR  231 E      CD2  CD1     3.65
5.73   87.43   4.86   0.51   4.83
 2er7   1.60      0.14      232 E     TYR  246 E      CD1  CG      3.36
51.36  -94.54   4.85   3.79  -3.03
 2er7   1.60      0.14      232 E     PHE  248 E      CZ3  CD1     3.61
72.53   92.03   6.55   6.25  -1.97
 2fal   1.80      0.15       14       PHE   18        CZ2  CD1     3.43
57.33  -14.26   5.16   4.34  -2.79
 2fal   1.80      0.15       14       PHE   68        CH2  CD2     3.83
69.79   68.46   5.81   5.45  -2.01
 2fal   1.80      0.15       14       PHE  112        CZ3  CZ      3.86
68.28  128.20   7.25   6.73   2.68
 2fal   1.80      0.15       14       TRP  130        CE3  CH2     4.00
52.89  172.17   6.74   5.38   4.06
 2fal   1.80      0.15      130       TRP   14        CH2  CE3     4.00
76.90   49.84   6.74   6.56  -1.53
 2fal   1.80      0.15      130       PHE  112        CE3  CE2     3.61
22.92  132.82   4.90   1.90  -4.52
 2gbp   1.90      0.15      183       TYR   10        CD1  OH      3.91
58.94  -74.35   7.62   6.53  -3.93
 2gbp   1.90      0.15      183       HIS  152        NE1  CD2     3.36
74.89    4.39   4.71   4.55  -1.23
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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2gdm | 1.70 | 0.16 | | 15 | | TYR | 72 | | CD2 | CD2 | 3.63 | | | |
| 33.01 | 175.44 | 4.47 | 2.44 | -3.75 | | | | | | | | | | |
| 2gst | 1.80 | 0.16 | | 7 | A | TRP | 45 | A | CZ2 | CD1 | 3.97 | | | |
| 37.05 | 29.57 | 6.49 | 3.91 | 5.18 | | | | | | | | | | |
| 2gst | 1.80 | 0.16 | | 45 | A | TRP | 7 | A | CD1 | CZ2 | 3.97 | | | |
| 42.12 | -109.50 | 6.49 | 4.35 | 4.82 | | | | | | | | | | |
| 2gst | 1.80 | 0.16 | | 45 | A | TYR | 32 | A | CE3 | CZ | 3.86 | | | |
| 66.32 | 166.30 | 5.53 | 5.06 | 2.22 | | | | | | | | | | |
| 2gst | 1.80 | 0.16 | | 45 | A | TYR | 61 | A | CZ3 | CE2 | 3.67 | | | |
| 65.25 | 100.27 | 7.05 | 6.40 | 2.95 | | | | | | | | | | |
| 2gst | 1.80 | 0.16 | | 146 | A | PHE | 183 | A | CE3 | CE1 | 3.61 | | | |
| 68.07 | 137.35 | 6.52 | 6.05 | 2.44 | | | | | | | | | | |
| 2gst | 1.80 | 0.16 | | 214 | A | PHE | 169 | A | CE3 | CD1 | 3.77 | | | |
| 7.94 | 88.96 | 4.95 | 0.72 | -4.90 | | | | | | | | | | |
| 2gst | 1.80 | 0.16 | | 214 | A | PHE | 208 | A | CE3 | CE2 | 3.98 | | | |
| 77.20 | 145.62 | 7.00 | 6.83 | 1.55 | | | | | | | | | | |
| 2hbg | 1.50 | 0.13 | | 14 | | TRP | 130 | | CE3 | CH2 | 3.95 | | | |
| 75.12 | 165.05 | 7.31 | 7.06 | 1.88 | | | | | | | | | | |
| 2hbg | 1.50 | 0.13 | | 130 | | TRP | 14 | | CH2 | CE3 | 3.95 | | | |
| 77.42 | 43.90 | 7.31 | 7.13 | -1.59 | | | | | | | | | | |
| 2hft | 1.69 | 0.20 | | 14 | | PHE | 100 | | CD2 | CG | 3.90 | | | |
| 24.92 | 176.75 | 4.75 | 2.00 | -4.31 | | | | | | | | | | |
| 2hft | 1.69 | 0.20 | | 25 | | TYR | 34 | | NE1 | CE2 | 3.37 | | | |
| 77.07 | -30.66 | 4.86 | 4.74 | -1.09 | | | | | | | | | | |
| 2hmz | 1.66 | 0.18 | | 10 | A | PHE | 29 | A | CD1 | CE1 | 3.64 | | | |
| 75.08 | -111.06 | 6.35 | 6.14 | 1.63 | | | | | | | | | | |
| 2hmz | 1.66 | 0.18 | | 97 | A | PHE | 55 | A | CH2 | CZ | 3.57 | | | |
| 68.27 | 75.26 | 7.08 | 6.58 | -2.62 | | | | | | | | | | |
| 2hmz | 1.66 | 0.18 | | 97 | A | PHE | 80 | A | CD2 | CD1 | 3.41 | | | |
| 30.12 | 147.46 | 4.16 | 2.08 | -3.60 | | | | | | | | | | |
| 2hmz | 1.66 | 0.18 | | 97 | A | TYR | 93 | A | CD1 | CZ | 3.96 | | | |
| 66.71 | -113.75 | 6.47 | 5.94 | -2.56 | | | | | | | | | | |
| 2hmz | 1.66 | 0.18 | | 97 | A | HIS | 101 | A | CH2 | CG | 3.40 | | | |
| 56.27 | 60.74 | 5.38 | 4.48 | 2.98 | | | | | | | | | | |
| 2hpd# | 2.00 | 0.17 | | 90 | A | PHE | 11 | B | NE1 | CD1 | 3.28 | | | |
| 89.40 | -28.67 | 5.10 | 5.10 | 0.05 | | | | | | | | | | |
| 2hpd | 2.00 | 0.17 | | 96 | A | HIS | 100 | A | CZ2 | ND1 | 3.41 | | | |
| 54.96 | 55.81 | 5.24 | 4.29 | 3.01 | | | | | | | | | | |
| 2hpd | 2.00 | 0.17 | | 130 | A | PHE | 421 | A | CE3 | CE2 | 3.98 | | | |
| 85.56 | 173.30 | 5.83 | 5.81 | 0.45 | | | | | | | | | | |
| 2hpd | 2.00 | 0.17 | | 130 | A | PHE | 423 | A | CZ3 | CE2 | 3.94 | | | |
| 61.21 | 120.63 | 7.11 | 6.23 | 3.43 | | | | | | | | | | |
| 2hpd | 2.00 | 0.17 | | 325 | A | PHE | 275 | A | CD1 | CE1 | 3.75 | | | |
| 51.32 | -120.84 | 5.34 | 4.17 | -3.34 | | | | | | | | | | |
| 2hpd | 2.00 | 0.17 | | 325 | A | PHE | 279 | A | CD1 | CZ | 3.83 | | | |
| 83.80 | -72.56 | 7.09 | 7.05 | 0.77 | | | | | | | | | | |
| 2hts# | 1.83 | 0.19 | | 203 | | HIS | 259 | | CH2 | CD2 | 3.91 | | | |
| 83.15 | 95.14 | 6.97 | 6.92 | -0.83 | | | | | | | | | | |
| 2hts | 1.83 | 0.19 | | 217 | | TRP | 258 | | CZ3 | CH2 | 3.93 | | | |
| 62.71 | 86.14 | 8.09 | 7.19 | 3.71 | | | | | | | | | | |
| 2hts | 1.83 | 0.19 | | 258 | | TRP | 217 | | CH2 | CZ3 | 3.93 | | | |
| 58.30 | 58.85 | 8.09 | 6.88 | -4.25 | | | | | | | | | | |
| 2hts# | 1.83 | 0.19 | | 217 | | HIS | 259 | | CH2 | ND1 | 3.62 | | | |
| 23.64 | 36.03 | 4.02 | 1.60 | -3.69 | | | | | | | | | | |
| 2hts | 1.83 | 0.19 | | 277 | | PHE | 246 | | CD2 | CE2 | 3.58 | | | |
| 7.45 | -150.01 | 4.88 | 0.62 | -4.84 | | | | | | | | | | |
| 2hts | 1.83 | 0.19 | | 277 | | PHE | 279 | | CE3 | CZ | 3.46 | | | |
| 82.22 | 167.46 | 6.02 | 5.96 | -0.81 | | | | | | | | | | |
| 2kau | 2.00 | 0.19 | | 79 | C | HIS | 78 | C | CD1 | NE2 | 3.99 | | | |
| 81.24 | -101.71 | 6.11 | 6.04 | -0.93 | | | | | | | | | | |

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|---|---|---|---|---|---|---|---|---|---|---|
| 2kau# | 2.00 | 0.19 | | 137 C | PHE | 477 C | CE3 | CZ | 3.82 |
| 52.05 | 179.20 | 6.00 | 4.73 | -3.69 | | | | | | |
| 2kau | 2.00 | 0.19 | | 175 C | TYR | 176 C | CZ3 | CE2 | 3.86 |
| 89.82 | 139.90 | 5.89 | 5.89 | -0.02 | | | | | | |
| 2kau# | 2.00 | 0.19 | | 175 C | HIS | 486 C | NE1 | NE2 | 3.89 |
| 54.99 | -10.16 | 5.74 | 4.70 | 3.29 | | | | | | |
| 2kau# | 2.00 | 0.19 | | 222 C | PHE | 45 C | CE2 | CE1 | 3.67 |
| 24.43 | 68.37 | 4.91 | 2.02 | 4.47 | | | | | | |
| 2kau | 2.00 | 0.19 | | 375 C | TYR | 407 C | NE1 | OH | 2.99 |
| 53.59 | -22.18 | 5.94 | 4.78 | 3.53 | | | | | | |
| 2kau | 2.00 | 0.19 | | 375 C | PHE | 440 C | NE1 | CE2 | 3.46 |
| 27.69 | -29.78 | 5.12 | 2.37 | -4.54 | | | | | | |
| 2kau | 2.00 | 0.19 | | 435 C | PHE | 440 C | CG | CD1 | 3.95 |
| 13.16 | -96.57 | 5.04 | 1.16 | -4.91 | | | | | | |
| 2mnr | 1.90 | 0.16 | | 219 | TYR | 137 | CH2 | CE2 | 3.72 |
| 60.56 | 42.37 | 6.06 | 5.28 | 2.98 | | | | | | |
| 2mnr | 1.90 | 0.16 | | 219 | TRP | 315 | CZ3 | CD1 | 3.79 |
| 61.30 | 103.63 | 7.35 | 6.45 | 3.53 | | | | | | |
| 2mnr | 1.90 | 0.16 | | 315 | TRP | 219 | CD1 | CZ3 | 3.79 |
| 41.00 | -81.95 | 7.35 | 4.82 | -5.55 | | | | | | |
| 2mnr | 1.90 | 0.16 | | 249 | TYR | 229 | CD1 | OH | 3.89 |
| 73.57 | -43.08 | 6.43 | 6.17 | 1.82 | | | | | | |
| 2mnr | 1.90 | 0.16 | | 315 | HIS | 314 | CD1 | CD2 | 3.41 |
| 73.72 | -69.90 | 5.27 | 5.06 | 1.48 | | | | | | |
| 2mnr | 1.90 | 0.16 | | 349 | HIS | 48 | NE1 | ND1 | 3.72 |
| 42.36 | -37.34 | 4.63 | 3.12 | 3.42 | | | | | | |
| 2nac | 1.80 | 0.15 | | 237 B | TYR | 219 B | CE3 | CZ | 3.43 |
| 87.76 | 154.20 | 5.50 | 5.50 | 0.22 | | | | | | |
| 2nac | 1.80 | 0.15 | | 310 B | HIS | 319 B | CE3 | ND1 | 3.72 |
| 88.32 | 150.20 | 5.56 | 5.56 | -0.16 | | | | | | |
| 2nac | 1.80 | 0.15 | | 321 B | TYR | 305 B | CH2 | OH | 3.41 |
| 20.56 | 86.30 | 5.06 | 1.77 | 4.74 | | | | | | |
| 2nac | 1.80 | 0.15 | | 321 B | HIS | 319 B | CG | CE1 | 3.41 |
| 30.39 | -151.65 | 5.01 | 2.54 | -4.32 | | | | | | |
| 2olb | 1.40 | 0.18 | | 64 A | PHE | 74 A | CG | CE1 | 3.88 |
| 45.89 | -144.29 | 5.80 | 4.16 | -4.04 | | | | | | |
| 2olb | 1.40 | 0.18 | | 72 A | PHE | 155 A | CG | CD2 | 3.62 |
| 22.90 | -93.12 | 5.00 | 1.94 | -4.61 | | | | | | |
| 2olb | 1.40 | 0.18 | | 72 A | TYR | 156 A | CH2 | CD1 | 3.96 |
| 63.10 | 92.53 | 7.21 | 6.43 | -3.26 | | | | | | |
| 2olb | 1.40 | 0.18 | | 97 A | PHE | 93 A | NE1 | CD1 | 3.84 |
| 50.10 | -31.12 | 6.34 | 4.86 | -4.07 | | | | | | |
| 2olb | 1.40 | 0.18 | | 97 A | PHE | 144 A | CH2 | CE2 | 3.92 |
| 11.80 | 97.84 | 5.16 | 1.08 | -5.05 | | | | | | |
| 2olb | 1.40 | 0.18 | | 179 A | PHE | 44 A | CH2 | CZ | 3.49 |
| 80.59 | 75.91 | 6.88 | 6.79 | -1.12 | | | | | | |
| 2olb | 1.40 | 0.18 | | 211 A | TYR | 210 A | NE1 | CE1 | 3.41 |
| 33.35 | -73.12 | 4.89 | 2.69 | -4.08 | | | | | | |
| 2olb | 1.40 | 0.18 | | 332 A | PHE | 333 A | CZ3 | CD1 | 3.72 |
| 45.21 | 103.64 | 6.54 | 4.64 | -4.61 | | | | | | |
| 2olb | 1.40 | 0.18 | | 382 A | PHE | 361 A | CZ3 | CZ | 3.83 |
| 50.27 | 126.93 | 6.58 | 5.06 | 4.20 | | | | | | |
| 2olb | 1.40 | 0.18 | | 397 A | PHE | 400 A | CE3 | CD2 | 3.91 |
| 60.64 | 136.36 | 6.67 | 5.81 | -3.27 | | | | | | |
| 2olb | 1.40 | 0.18 | | 416 A | TYR | 109 A | CH2 | OH | 3.13 |
| 77.49 | 59.68 | 7.13 | 6.96 | -1.54 | | | | | | |
| 2olb | 1.40 | 0.18 | | 416 A | TYR | 317 A | CG | OH | 3.57 |
| 46.42 | -115.60 | 6.44 | 4.67 | 4.44 | | | | | | |
| 2olb | 1.40 | 0.18 | | 416 A | PHE | 426 A | CD1 | CD2 | 3.51 |
| 88.42 | -84.33 | 5.58 | 5.58 | 0.15 | | | | | | |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 2olb | 1.40 | 0.18 | | 494 A | HIS | 517 A | CG | ND1 | 3.44 | | |
| 17.61 | -177.79 | 3.62 | 1.09 | -3.45 | | | | | | | |
| 2pgd | 2.00 | 0.20 | | 149 | TRP | 172 | CE3 | CE3 | 3.55 | | |
| 35.03 | -152.58 | 5.21 | 2.99 | 4.26 | | | | | | | |
| 2pgd | 2.00 | 0.20 | | 172 | TRP | 149 | CE3 | CE3 | 3.55 | | |
| 66.51 | 176.42 | 5.21 | 4.78 | 2.08 | | | | | | | |
| 2pgd | 2.00 | 0.20 | | 350 | PHE | 181 | CZ3 | CG | 3.88 | | |
| 84.20 | 93.70 | 6.78 | 6.75 | -0.69 | | | | | | | |
| 2pgd | 2.00 | 0.20 | | 361 | PHE | 338 | CZ3 | CE1 | 3.96 | | |
| 63.25 | 111.67 | 6.77 | 6.05 | -3.05 | | | | | | | |
| 2pgd | 2.00 | 0.20 | | 405 | TYR | 429 | CZ3 | CG | 3.98 | | |
| 74.63 | 100.50 | 6.75 | 6.51 | 1.79 | | | | | | | |
| 2phy | 1.40 | 0.19 | | 119 | PHE | 121 | CG | CZ | 3.42 | | |
| 43.76 | -162.99 | 5.17 | 3.58 | -3.73 | | | | | | | |
| 2pia | 2.00 | 0.19 | | 164 | PHE | 141 | CZ3 | CZ | 3.88 | | |
| 84.08 | 123.42 | 7.44 | 7.40 | 0.77 | | | | | | | |
| 2pia | 2.00 | 0.19 | | 184 | HIS | 214 | CZ3 | CE1 | 3.60 | | |
| 81.34 | 92.34 | 6.65 | 6.57 | -1.00 | | | | | | | |
| 2pia | 2.00 | 0.19 | | 215 | PHE | 187 | CZ2 | CD1 | 3.90 | | |
| 35.21 | 3.29 | 5.88 | 3.39 | -4.80 | | | | | | | |
| 2pia | 2.00 | 0.19 | | 215 | HIS | 214 | CD1 | CE1 | 3.52 | | |
| 77.52 | -73.44 | 5.64 | 5.51 | 1.22 | | | | | | | |
| 2prk | 1.50 | 0.17 | | 212 | HIS | 72 | CE3 | CD2 | 3.85 | | |
| 72.32 | 140.11 | 6.63 | 6.56 | 0.96 | | | | | | | |
| 2rn2 | 1.48 | 0.20 | | 81 | TYR | 73 | CZ3 | CE1 | 3.63 | | |
| 87.08 | 104.12 | 6.81 | 6.80 | -0.35 | | | | | | | |
| 2rn2 | 1.48 | 0.20 | | 81 | TRP | 85 | CE3 | CH2 | 3.41 | | |
| 56.50 | -162.84 | 5.66 | 4.72 | 3.12 | | | | | | | |
| 2rn2 | 1.48 | 0.20 | | 85 | TRP | 81 | CH2 | CE3 | 3.41 | | |
| 46.06 | 42.22 | 5.66 | 4.08 | -3.92 | | | | | | | |
| 2rn2 | 1.48 | 0.20 | | 85 | TRP | 90 | CE3 | CZ3 | 3.68 | | |
| 60.47 | -173.99 | 6.66 | 5.80 | 3.28 | | | | | | | |
| 2rn2 | 1.48 | 0.20 | | 90 | TRP | 85 | CZ3 | CE3 | 3.68 | | |
| 66.04 | 140.49 | 6.66 | 6.09 | 2.70 | | | | | | | |
| 2rn2 | 1.48 | 0.20 | | 85 | TRP | 104 | CZ3 | CD1 | 3.62 | | |
| 87.43 | 105.01 | 6.21 | 6.20 | 0.28 | | | | | | | |
| 2rn2 | 1.48 | 0.20 | | 104 | TRP | 85 | CD1 | CZ3 | 3.62 | | |
| 20.43 | -82.49 | 6.21 | 2.16 | -5.82 | | | | | | | |
| 2rn2 | 1.48 | 0.20 | | 104 | TYR | 73 | NE1 | OH | 3.07 | | |
| 72.82 | 2.33 | 5.37 | 5.13 | 1.59 | | | | | | | |
| 2rn2 | 1.48 | 0.20 | | 118 | TRP | 120 | CE3 | CH2 | 3.36 | | |
| 54.16 | -169.65 | 5.74 | 4.65 | -3.36 | | | | | | | |
| 2rn2 | 1.48 | 0.20 | | 120 | TRP | 118 | CH2 | CE3 | 3.36 | | |
| 56.38 | 59.68 | 5.74 | 4.78 | 3.18 | | | | | | | |
| 2scp | 2.00 | 0.18 | | 170 A | TYR | 11 A | CZ2 | CE1 | 3.35 | | |
| 21.31 | -14.41 | 4.50 | 1.64 | -4.19 | | | | | | | |
| 2scp | 2.00 | 0.18 | | 170 A | PHE | 99 A | CH2 | CE2 | 3.62 | | |
| 81.14 | 66.99 | 6.14 | 6.07 | -0.95 | | | | | | | |
| 2scp | 2.00 | 0.18 | | 170 A | PHE | 119 A | CZ3 | CZ | 3.62 | | |
| 60.89 | 114.28 | 6.90 | 6.03 | 3.36 | | | | | | | |
| 2scp | 2.00 | 0.18 | | 170 A | PHE | 157 A | CD1 | CE2 | 3.40 | | |
| 88.06 | -76.54 | 5.57 | 5.57 | -0.19 | | | | | | | |
| 2scp | 2.00 | 0.18 | | 170 A | PHE | 169 A | NE1 | CD2 | 3.41 | | |
| 26.78 | -26.29 | 5.10 | 2.30 | 4.55 | | | | | | | |
| 2sil | 1.60 | 0.17 | | 80 | PHE | 368 | CZ2 | CG | 3.78 | | |
| 86.64 | 28.30 | 6.00 | 5.99 | 0.35 | | | | | | | |
| 2sil | 1.60 | 0.17 | | 121 | TRP | 128 | CZ2 | CE3 | 3.89 | | |
| 68.84 | 42.28 | 6.61 | 6.16 | 2.38 | | | | | | | |
| 2sil | 1.60 | 0.17 | | 128 | TRP | 121 | CE3 | CZ2 | 3.89 | | |
| 58.85 | -173.64 | 6.61 | 5.66 | 3.42 | | | | | | | |

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 2sil   1.60      0.17       121
33.78    8.72   6.47   3.60  -5.38
 2sil   1.60      0.17       140
86.86  -99.48   6.47   6.46   0.35
 2sil   1.60      0.17       140
66.03  119.58   6.37   5.82   2.59
 2sil   1.60      0.17       218
52.56   74.87   6.36   5.05  -3.87
 2sil   1.60      0.17       263
71.96   29.90   6.73   6.40   2.08
 2tgi#  1.80      0.17        32
41.03  -21.08   3.62   2.37  -2.73
 2tgi   1.80      0.17        52
69.73   37.30   7.09   6.65  -2.46
 3bcl#  1.90      0.19       173
57.28  177.45   6.66   5.60   3.60
 3bcl#  1.90      0.19       173
53.88   75.80   6.93   5.60   4.08
 3bcl   1.90      0.19       178
21.82  -94.77   4.09   1.52   3.80
 3bcl   1.90      0.19       178
88.38   56.26   6.01   6.01  -0.17
 3bcl   1.90      0.19       215
65.23  108.20   6.98   6.34  -2.92
 3bcl   1.90      0.19       332
30.27  -34.18   5.26   2.65   4.54
 3bcl   1.90      0.19       340
68.16  149.52   6.34   5.89  -2.36
 3bcl   1.90      0.19       340
19.16   95.23   5.14   1.68  -4.86
 3cla   1.75      0.16        16
 5.01 -111.97   4.65   0.41  -4.63
 3cla   1.75      0.16        16
85.74  106.28   6.67   6.65   0.50
 3cla   1.75      0.16        86
50.64  117.81   6.46   4.99   4.10
 3cla   1.75      0.16       152
64.40   15.60   5.10   4.60   2.20
 3cox   1.80      0.16        46
48.88  174.28   5.23   3.94  -3.44
 3cox   1.80      0.16       164
64.52  104.54   7.27   6.56   3.13
 3cox   1.80      0.16       318
38.89 -104.21   5.49   3.45  -4.27
 3cox   1.80      0.16       318
86.45  114.89   6.77   6.76   0.42
 3cox   1.80      0.16       401
38.73  176.63   6.77   4.24   5.28
 3cox   1.80      0.16       333
47.41   46.81   5.55   4.08   3.76
 3cox   1.80      0.16       351
77.99   -9.42   4.89   4.78   1.02
 3cox   1.80      0.16       440
50.27   27.92   5.43   4.17   3.47
 3dfr   1.70      0.15         5
89.99   39.22   7.60   7.60   0.00
 3dfr   1.70      0.15        21
73.72  165.03   5.48   5.26  -1.54
 3dfr   1.70      0.15       133
74.79   46.26   7.60   7.33   1.99

TRP  140    CZ2  CD1   3.74
TRP  121    CD1  CZ2   3.74
HIS  162    CZ3  CD2   3.76
PHE  191    CH2  CD2   3.45
PHE  209    CZ2  CE2   3.93
HIS   58    NE1  NE2   2.64
TYR    6    CH2  OH    3.43
TYR  118    CG   OH    3.92
PHE  139    CH2  CE1   3.88
PHE  179    CE2  CZ    3.45
PHE  217    CH2  CG    3.91
PHE  217    CZ3  CD1   3.60
HIS  352    NE1  CE1   3.59
TYR  337    CE3  CE1   3.83
HIS  352    CZ3  CD2   3.84
PHE   11    CD2  CE2   3.39
PHE   22    CZ3  CG    3.62
TYR    8    CZ3  CD2   3.77
PHE   96    CZ2  CG    3.60
PHE   56    CE3  CE1   3.61
TYR  171    CZ3  CE2   3.94
PHE  388    CD1  CE2   3.40
TRP  401    CZ3  CD2   3.99
TRP  318    CD2  CZ3   3.99
HIS  331    CZ2  CD2   3.56
TYR  130    CZ2  CE2   3.64
TYR  428    CZ2  OH    3.64
TRP  133    CH2  CH2   3.61
PHE  122    CE3  CD1   3.59
TRP    5    CH2  CH2   3.61
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 3dfr   1.70      0.15      133
77.57  131.38   5.59   5.46  -1.20
 3dfr   1.70      0.15      158
19.23   75.04   5.59   1.84  -5.28
 3est   1.65      0.17       27
72.68   35.91   6.28   6.00  -1.87
 3est   1.65      0.17       27
50.83  151.04   4.52   3.50  -2.86
 3est   1.65      0.17      141
58.84  178.99   5.64   4.83   2.92
 3est   1.65      0.17      172
27.40   67.98   5.76   2.65  -5.11
 3est   1.65      0.17      237
 8.73  -49.61   4.60   0.68  -4.55
 3grs   1.54      0.19       70
 9.80  138.63   5.09   0.89  -5.01
 3grs   1.54      0.19       70
57.30  -50.43   5.17   4.35   2.79
 3grs   1.54      0.19       96
61.51  176.21   6.22   5.47  -2.97
 3pga   2.00      0.17      186 1
30.70   29.61   3.88   1.98  -3.34
 3pga   2.00      0.17      335 1
73.07  -77.10   5.98   5.72   1.74
 3pte   1.60      0.15      233
 7.01  132.78   4.88   0.57   4.85
 3pte   1.60      0.15      271
65.30   21.60   6.05   5.50  -2.53
 3rub   2.00      0.19      214 L
82.24  151.48   5.50   5.45   0.74
 3rub   2.00      0.19      214 L
64.69   99.22   7.09   6.41  -3.03
 3rub   2.00      0.19      385 L
46.13 -163.34   4.66   3.36  -3.23
 3rub   2.00      0.19      462 L
42.94 -102.59   4.66   3.17  -3.41
 3sdh   1.40      0.16       22 B
65.36  160.49   6.99   6.35   2.91
 3sdh   1.40      0.16      135 B
81.43   47.37   6.99   6.91  -1.04
 3sic   1.80      0.18      113 E
83.97   70.46   7.43   7.39   0.78
 3sic   1.80      0.18      241 E
28.57    9.58   3.76   1.79  -3.31
 4enl   1.90      0.15       56
66.60  -40.80   6.10   5.60   2.42
 4gcr   1.47      0.18       68
83.67  -69.99   5.92   5.88  -0.65
 4gcr   1.47      0.18      157
88.61  -78.19   6.50   6.50  -0.16
 5rub   1.70      0.18      184 B
71.26   44.68   6.80   6.44  -2.18
 5rub   1.70      0.18      417 B
21.78  169.40   5.33   1.99  -4.95
 8abp   1.49      0.17       16
88.45  -83.26   5.70   5.70   0.15
 8abp   1.49      0.17       16
78.24   24.58   5.75   5.63  -1.17
 8abp   1.49      0.17       21
78.25  -73.01   6.39   6.26  -1.30
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TRP  158        CZ3  CE2   3.55
TRP  133        CE2  CZ3   3.55
TYR  137        CZ2  CG    3.91
HIS  200        CE3  NE2   3.47
HIS   40        CE3  CE1   3.82
PHE  215        CH2  CE2   3.89
HIS   91        CD2  CD2   3.80
PHE  372        CD2  CD1   3.84
HIS  374        NE1  CE1   3.57
PHE   94        CE3  CE2   3.71
PHE  200 4      CE2  CG    3.46
HIS  306 1      CD1  CG    3.85
PHE  120        CE3  CE2   3.70
TYR  296        CZ2  CD1   3.39
PHE  218 L      CZ3  CD2   3.93
PHE  256 L      CZ3  CD2   3.84
TRP  462 L      CG   CD1   3.30
TRP  385 L      CD1  CG    3.30
TRP  135 B      CE3  CH2   3.62
TRP   22 B      CH2  CE3   3.62
TYR   91 E      CH2  CD2   3.90
HIS  238 E      CZ2  NE2   3.34
TYR   11        NE1  OH    2.75
TYR   55        CD1  CG    3.75
TYR  144        CD1  CG    4.00
PHE  228 B      CZ2  CD1   3.88
PHE  380 B      CG   CD2   3.99
PHE   17        CD1  CE2   3.77
HIS  259        CZ2  ND1   3.64
PHE    7        CD1  CD1   3.60
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 8abp   1.49      0.17      130       HIS  198        CD2  CG      3.70
21.47 -118.28   4.37   1.59   4.07
 8abp   1.49      0.17      199       PHE  221        NE1  CZ      3.38
86.48  -64.36   5.76   5.75  -0.35
 8acn   2.00      0.16      139       PHE   10        CZ2  CE2     3.73
65.36   32.47   5.87   5.34   2.45
 8acn   2.00      0.16      139       HIS   98        CD1  CE1     3.43
47.26  -90.62   5.21   3.83  -3.54
 8acn   2.00      0.16      139       TYR  154        NE1  OH      3.07
67.91   -6.53   5.93   5.50  -2.23
 8acn   2.00      0.16      139       TYR  517        NE1  CD1     3.30
27.78  -11.95   4.78   2.22   4.23
 8acn   2.00      0.16      346       HIS  332        CH2  CE1     3.69
77.12   92.88   6.59   6.42   1.47
 8acn   2.00      0.16      346       HIS  460        CD1  CD2     3.70
58.63  -98.40   6.35   5.42   3.31
 8acn   2.00      0.16      346       PHE  462        CE3  CZ      3.63
41.35  159.80   5.72   3.78   4.29
 8acn   2.00      0.16      547       PHE  739        CD1  CZ      3.74
22.46 -123.98   4.91   1.87  -4.54
 8acn   2.00      0.16      576       PHE  579        CE3  CD2     3.89
58.62  146.95   6.70   5.72   3.49
 8acn   2.00      0.16      630       TYR  623        CD1  CD2     4.00
50.81  -97.65   6.70   5.19   4.24
 8fab   1.80      0.17      185 C     TYR  191 C      CE3  CD1     3.69
82.00  149.96   6.27   6.21  -0.87
 8fab   1.80      0.17       47 D     HIS   35 D      NE1  ND1     3.03
75.39  -37.89   5.70   5.52  -1.44
 8fab   1.80      0.17       47 D     PHE  106 D      CZ2  CE2     3.98
37.50   11.87   5.61   3.41  -4.45
 8fab   1.80      0.17       47 D     PHE  108 D      CD1  CZ      3.80
67.63  -82.74   6.78   6.27  -2.58
 8fab   1.80      0.17       52 D     TYR   53 D      CD1  CE1     3.85
64.13  -84.86   6.63   5.97  -2.89
 8fab   1.80      0.17       52 D     TYR   59 D      CZ3  CE2     3.90
56.47  116.77   6.61   5.51   3.65
 8fab   1.80      0.17      111 D     TYR   35 C      NE1  CE2     3.81
76.26    4.93   5.51   5.35  -1.31
 8fab   1.80      0.17      111 D     TYR   95 D      CE3  CG      3.94
75.01  148.35   6.22   6.01  -1.61
 8fab   1.80      0.17      111 D     PHE  108 D      CZ2  CG      3.95
45.26   33.27   6.00   4.26   4.22
 8tln   1.60      0.17       55 E     PHE   62 E      NE1  CE2     3.93
57.44  -55.18   6.56   5.53   3.53
 8tln   1.60      0.17       55 E     TYR   66 E      CH2  CE2     3.54
68.89   61.67   6.54   6.10  -2.36
 8tln   1.60      0.17       55 E     HIS  105 E      CZ3  CD2     3.99
89.56   85.58   7.26   7.26   0.06
 8tln   1.60      0.17      186 E     PHE  178 E      NE1  CZ      3.62
31.04  -19.28   5.26   2.72   4.50
 8tln   1.60      0.17      186 E     TYR  242 E      CD2  CD1     3.83
13.59 -142.77   5.23   1.24  -5.08
 9rnt   1.50      0.14       59       TYR   68        CH2  CD2     3.88
35.26   75.71   6.27   3.61  -5.12
 ------------------------------------------------
 #, the symmetry-related-residues is indicated by this  sign
```

Table S2. Number of cases with various values of sequence-difference (absolute value) between TRP and the partner residue.

| Residue | Sequence Difference | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 =>15 |
| PHE(302) | 9 | 12 | 13 | 18 | 5 | 3 | 9 | 8 | 0 | 5 | 1 | 2 | 3 | 1 213 |
| TYR(222) | 8 | 6 | 8 | 5 | 6 | 1 | 5 | 2 | 5 | 3 | 1 | 1 | 7 | 1 163 |
| TRP(124) | 2 | 4 | 2 | 8 | 2 | 0 | 2 | 6 | 2 | 0 | 4 | 4 | 6 | 2 80 |
| HIS(93) | 9 | 6 | 2 | 5 | 0 | 0 | 1 | 1 | 1 | 1 | 1 | 2 | 0 | 1 63 |

In parenthesis the number indicates the total number of interacting pairs.
In case of TRP there are 62 residues giving rise to 124 interacting pairs.

Table S3. TYR residues with the hydroxyl group close to TRP ring.

| PDB file | Residue Number TRP | TYR | Closest TRP atom | Distance (A) |
|---|---|---|---|---|
| (A) OH...pi (O atom on the face of the Trp ring) | | | | |
| 1531 | 107 | 48 | CH2 | 3.71 |
| 1aoz | 8 A | 103 A | CH2 | 3.57 |
| 1dsb | 126 A | 122 A | CE3 | 3.43 |
| 1gof | 290 | 272 | NE1 | 3.50 |
| 1gof | 290 | 329 | CD1 | 3.38 |
| 1hle | 160 A | 119 A | CG | 3.40 |
| 1hle | 194 A | 244 A | CH2 | 3.43 |
| 1mpp | 190 | 125 | CZ3 | 3.49 |
| 1pbp | 168 | 193 | CZ2 | 3.31 |
| 1sat | 153 | 65 | CH2 | 3.74 |
| 1sat | 153 | 135 | CG | 3.93 |
| 1sat | 217 | 190 | NE1 | 3.72 |
| 1wht | 308 B | 147 A | NE1 | 3.52 |
| 1wht | 308 B | 151 A | CH2 | 3.59 |
| 2ayh | 18 | 64 | CG | 3.87 |
| 2cba | 209 | 194 | CD1 | 3.57 |
| 2nac | 237 B | 219 B | CE3 | 3.67 |
| 2nac | 321 B | 305 B | CH2 | 3.41 |
| 2olb | 211 A | 210 A | NE1 | 3.60 |
| 2olb | 416 A | 109 A | CH2 | 3.13 |
| 2olb | 416 A | 317 A | CG | 3.57 |
| 3bcl# | 173 | 118 | CG | 3.92 |
| (B) O atom on the edge of Trp ring | | | | |
| 1ade | 309 A | 372 A | CD1 | 3.46 |
| 1ade | 365 A | 347 A | CZ3 | 3.91 |
| 1amp | 233 | 148 | NE1 | 2.91 |

| | | | | | |
|---|---|---|---|---|---|
| 1aoz | 277 | A | 186 | A | NE1 | 3.09 |
| 1arb | 182 | | 227 | | CZ2 | 3.51 |
| 1arb | 247 | | 51 | | CE3 | 3.80 |
| 1byb | 55 | | 72 | | CD1 | 3.36 |
| 1cel | 192 | B | 51 | B | CZ2 | 3.57 |
| 1cel | 216 | B | 274 | B | CZ2 | 3.37 |
| 1cel | 263 | B | 321 | B | CH2 | 3.46 |
| 1cfb | 634 | | 647 | | NE1 | 3.90 |
| 1clc | 220 | | 316 | | CZ2 | 3.60 |
| 1csh | 109 | | 172 | | CH2 | 3.56 |
| 1ede | 59 | | 18 | | CZ3 | 3.44 |
| 1gpb | 189 | | 52 | | NE1 | 3.67 |
| 1gpb | 215 | | 297 | | CZ3 | 3.77 |
| 1iae | 10 | | 194 | | CD1 | 3.52 |
| 1isc | 77 | A | 9 | A | CE3 | 3.75 |
| 1knb | 478 | | 491 | | NE1 | 3.01 |
| 1lcp | 207 | A | 345 | A | CZ2 | 3.44 |
| 1lis | 62 | | 133 | | CZ2 | 3.73 |
| 1mml# | 185 | | 271 | | CZ3 | 3.36 |
| 1mpp | 39 | | 75 | | NE1 | 2.68 |
| 1mrj | 192 | | 164 | | CD1 | 3.76 |
| 1nar | 58 | | 116 | | NE1 | 2.99 |
| 1nar | 101 | | 131 | | CZ2 | 3.70 |
| 1nba | 111 | A | 96 | A | CE3 | 3.34 |
| 1nfp | 96 | | 152 | | CZ2 | 3.83 |
| 1ora | 278 | | 271 | | CE3 | 3.52 |
| 1oyc | 116 | | 196 | | CZ2 | 3.74 |
| 1pbe | 344 | | 181 | | CD1 | 3.68 |
| 1pii | 356 | | 278 | | CZ2 | 3.93 |
| 1rcf | 120 | | 125 | | NE1 | 2.95 |
| 1rec | 31 | | 86 | | NE1 | 2.98 |
| 1sat | 46 | | 246 | | CD1 | 3.39 |
| 1sbp | 141 | | 137 | | CZ3 | 3.66 |
| 1scs | 40 | | 67 | | CZ2 | 3.54 |
| 1scs# | 182 | | 12 | | CZ2 | 3.32 |
| 1scs# | 182 | | 100 | | NE1 | 2.98 |
| 1sri | 92 | A | 43 | A | CZ2 | 3.44 |
| 1tca | 113 | | 300 | | NE1 | 3.00 |
| 1ton# | 237 | | 172 | | CD1 | 3.70 |
| 1tys | 98 | | 181 | | CZ2 | 3.59 |
| 1wht# | 193 | A | 348 | B | CZ3 | 3.68 |
| 1xnb | 71 | | 69 | | NE1 | 3.01 |
| 1xnb | 71 | | 166 | | NE1 | 3.34 |
| 1xnb | 164 | | 79 | | CZ3 | 3.77 |
| 2ayh | 151 | | 75 | | CZ3 | 3.63 |
| 2aza | 48 | A | 15 | A | CD1 | 3.90 |
| 2bbk | 26 | L | 25 | L | NE1 | 3.65 |
| 2er7 | 39 | E | 75 | E | NE1 | 2.83 |
| 2gbp | 183 | | 10 | | CD1 | 3.91 |
| 2kau | 375 | C | 407 | C | NE1 | 2.99 |
| 2mnr | 219 | | 137 | | CZ2 | 3.82 |
| 2mnr | 249 | | 229 | | CD1 | 3.89 |
| 2rn2 | 104 | | 73 | | NE1 | 3.07 |
| 2tgi | 52 | | 6 | | CH2 | 3.43 |
| 3cox | 351 | | 130 | | CZ2 | 3.92 |
| 3cox | 440 | | 428 | | CZ2 | 3.64 |
| 4enl | 56 | | 11 | | NE1 | 2.75 |
| 8acn | 139 | | 154 | | NE1 | 3.07 |

(C) Hydrogen bonding (O atom on the edge as in (B) + at <3.5A from NE1)

| | | | | | |
|---|---|---|---|---|---|
| 1amp | 233 | | 148 | | NE1 | 2.91 |
| 1aoz | 277 | A | 186 | A | NE1 | 3.09 |
| 1knb | 478 | | 491 | | NE1 | 3.01 |
| 1mpp | 39 | | 75 | | NE1 | 2.68 |
| 1nar | 58 | | 116 | | NE1 | 2.99 |
| 1rcf | 120 | | 125 | | NE1 | 2.95 |
| 1rec | 31 | | 86 | | NE1 | 2.98 |
| 1scs# | 182 | | 100 | | NE1 | 2.98 |
| 1tca | 113 | | 300 | | NE1 | 3.00 |
| 1xnb | 71 | | 69 | | NE1 | 3.01 |
| 1xnb | 71 | | 166 | | NE1 | 3.34 |
| 2er7 | 39 | E | 75 | E | NE1 | 2.83 |
| 2kau | 375 | C | 407 | C | NE1 | 2.99 |
| 2rn2 | 104 | | 73 | | NE1 | 3.07 |
| 4enl | 56 | | 11 | | NE1 | 2.75 |
| 8acn | 139 | | 154 | | NE1 | 3.07 |

# Interaction at crystallographic-symmetry-related position