



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:06 am GMT

PDB ID : 3HKZ
Title : The X-ray crystal structure of RNA polymerase from Archaea
Authors : Murakami, K.S.
Deposited on : 2009-05-26
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

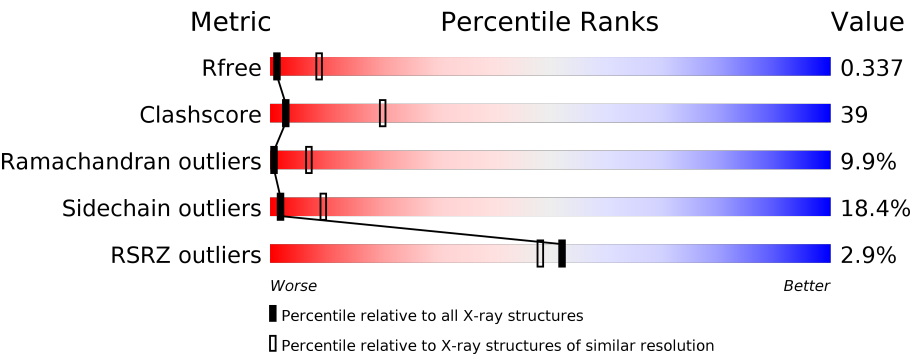
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 100719 | 1679 (3.50-3.30) |
| Clashscore | 112137 | 1832 (3.50-3.30) |
| Ramachandran outliers | 110173 | 1789 (3.50-3.30) |
| Sidechain outliers | 110143 | 1789 (3.50-3.30) |
| RSRZ outliers | 101464 | 1709 (3.50-3.30) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 880 | <div><div></div><div><div></div><div>33%</div><div>46%</div><div>14%</div><div>• 5%</div></div></div> |
| 1 | I | 880 | <div><div></div><div><div></div><div>32%</div><div>48%</div><div>14%</div><div>• 5%</div></div></div> |
| 2 | C | 395 | <div><div></div><div><div></div><div>32%</div><div>43%</div><div>16%</div><div>• 6%</div></div></div> |
| 2 | M | 395 | <div><div></div><div><div></div><div>27%</div><div>44%</div><div>19%</div><div>• 6%</div></div></div> |
| 3 | B | 1124 | <div><div></div><div><div></div><div>32%</div><div>48%</div><div>15%</div><div>• •</div></div></div> |
| 3 | J | 1124 | <div><div></div><div><div></div><div>31%</div><div>49%</div><div>15%</div><div>• •</div></div></div> |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4 | D | 265 | |
| 4 | O | 265 | |
| 5 | E | 180 | |
| 5 | Q | 180 | |
| 6 | F | 113 | |
| 6 | R | 113 | |
| 7 | G | 132 | |
| 7 | S | 132 | |
| 8 | H | 84 | |
| 8 | T | 84 | |
| 9 | K | 95 | |
| 9 | U | 95 | |
| 10 | L | 92 | |
| 10 | V | 92 | |
| 11 | N | 66 | |
| 11 | W | 66 | |
| 12 | P | 48 | |
| 12 | X | 48 | |
| 13 | Y | 104 | |
| 13 | Z | 104 | |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | ZN | B | 2001 | - | - | X | - |
| 14 | ZN | J | 2001 | - | - | X | - |
| 16 | F3S | O | 1001 | - | - | X | - |

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 53072 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit A'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1 | A | 836 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6673 | 4248 | 1178 | 1221 | 26 | | | |
| 1 | I | 836 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6673 | 4248 | 1178 | 1221 | 26 | | | |

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit A''.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | C | 370 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2868 | 1818 | 490 | 551 | 9 | | | |
| 2 | M | 370 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2868 | 1818 | 490 | 551 | 9 | | | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| C | 1 | MET | - | EXPRESSION TAG | UNP P58192 |
| C | 2 | GLU | - | EXPRESSION TAG | UNP P58192 |
| C | 3 | GLY | - | EXPRESSION TAG | UNP P58192 |
| M | 1 | MET | - | EXPRESSION TAG | UNP P58192 |
| M | 2 | GLU | - | EXPRESSION TAG | UNP P58192 |
| M | 3 | GLY | - | EXPRESSION TAG | UNP P58192 |

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3 | B | 1090 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8645 | 5483 | 1529 | 1602 | 31 | | | |
| 3 | J | 1090 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8645 | 5483 | 1529 | 1602 | 31 | | | |

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit D.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4 | D | 264 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2114 | 1355 | 342 | 403 | 14 | | | |
| 4 | O | 264 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2114 | 1355 | 342 | 403 | 14 | | | |

- Molecule 5 is a protein called DNA-directed RNA polymerase, subunit E' (RpoE1).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | E | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1402 | 903 | 236 | 259 | 4 | | | |
| 5 | Q | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1402 | 903 | 236 | 259 | 4 | | | |

- Molecule 6 is a protein called DNA-directed RNA polymerase, subunit F (RpoF).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | F | 89 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 694 | 433 | 115 | 142 | 4 | | | |
| 6 | R | 89 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 694 | 433 | 115 | 142 | 4 | | | |

- Molecule 7 is a protein called DNA-directed RNA polymerase, subunit G (RpoG).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | G | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 884 | 556 | 149 | 174 | 5 | | | |
| 7 | S | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 884 | 556 | 149 | 174 | 5 | | | |

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit H.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 8 | H | 74 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 611 | 397 | 109 | 105 | | | | |
| 8 | T | 74 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 611 | 397 | 109 | 105 | | | | |

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit K.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | K | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 658 | 420 | 121 | 116 | 1 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | U | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 658 | 420 | 121 | 116 | 1 | | | |

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit L.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | L | 92 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 723 | 459 | 121 | 141 | 2 | | | |
| 10 | V | 92 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 723 | 459 | 121 | 141 | 2 | | | |

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit N.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 11 | N | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 514 | 326 | 94 | 88 | 6 | | | |
| 11 | W | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 514 | 326 | 94 | 88 | 6 | | | |

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12 | P | 43 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 346 | 230 | 58 | 53 | 5 | | | |
| 12 | X | 43 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 346 | 230 | 58 | 53 | 5 | | | |

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit 13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 13 | Y | 45 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 391 | 245 | 68 | 77 | 1 | | | |
| 13 | Z | 45 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 391 | 245 | 68 | 77 | 1 | | | |

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 14 | P | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 14 | J | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

Continued on next page...

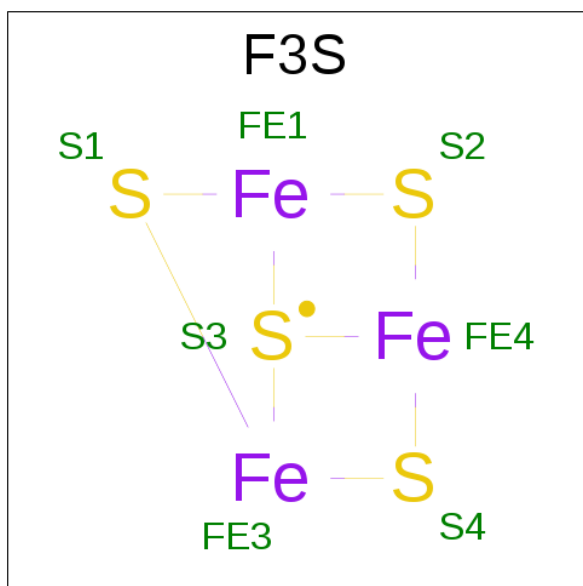
Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 14 | B | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 14 | I | 2 | Total | Zn | 0 | 0 |
| | | | 2 | 2 | | |
| 14 | W | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 14 | A | 2 | Total | Zn | 0 | 0 |
| | | | 2 | 2 | | |
| 14 | N | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 14 | X | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 15 | I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 15 | A | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 16 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 16 | D | 1 | Total | Fe | S | 0 | 0 |
| | | | 7 | 3 | 4 | | |

Continued on next page...

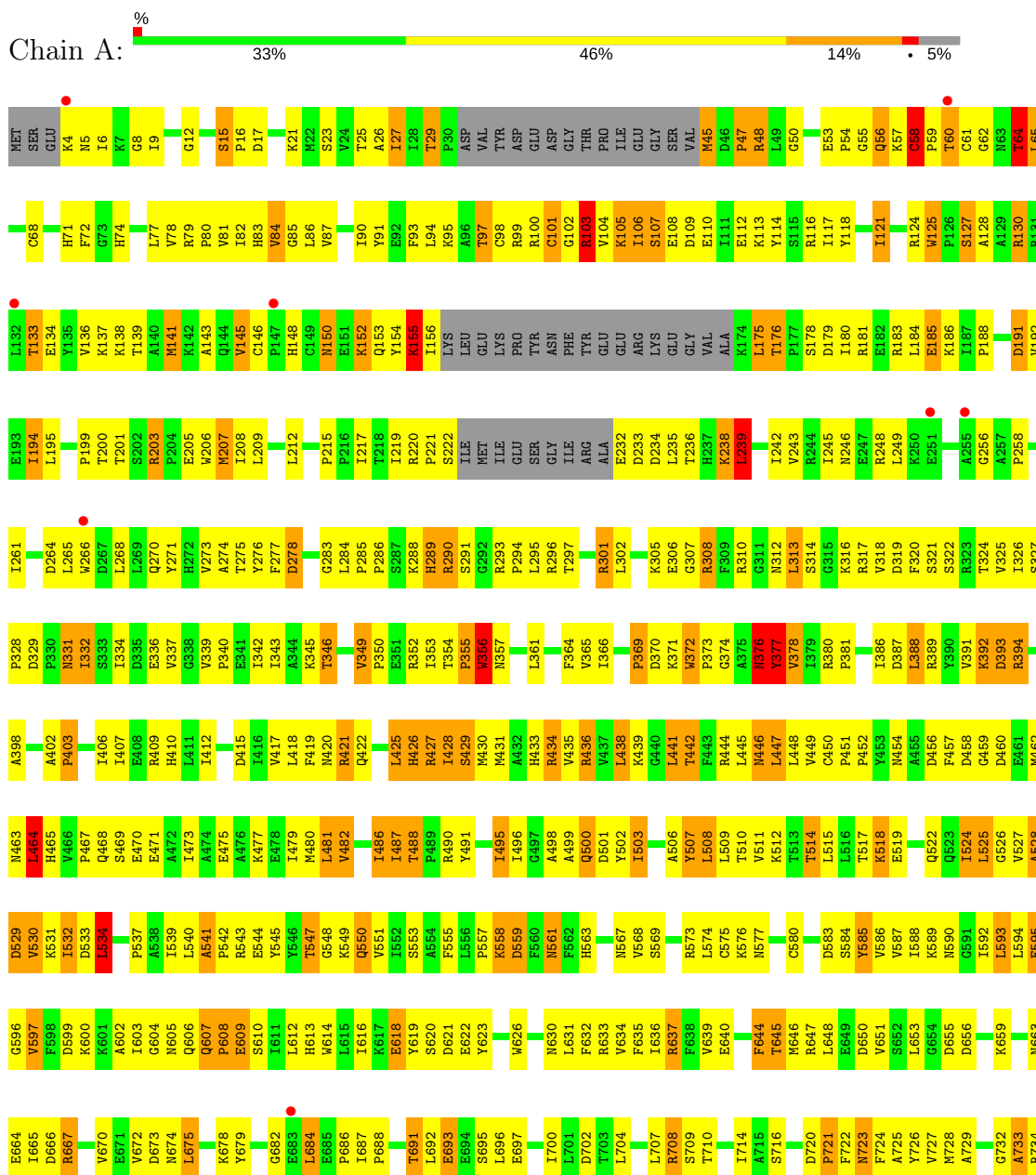
Continued from previous page...

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 16 | O | 1 | Total | Fe | S | 0 | 0 |
| | | | 7 | 3 | 4 | | |

3 Residue-property plots

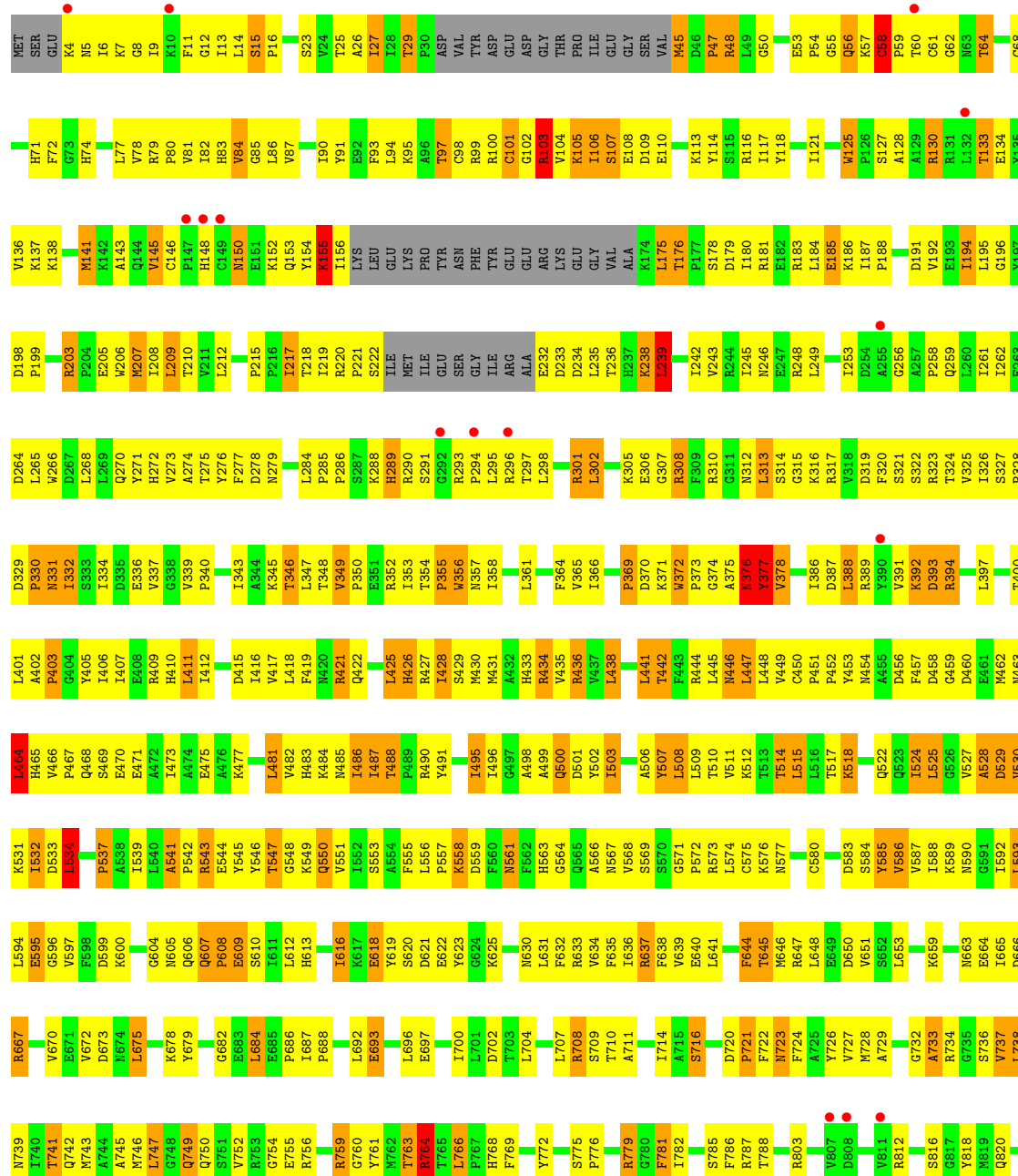
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA-directed RNA polymerase subunit A'



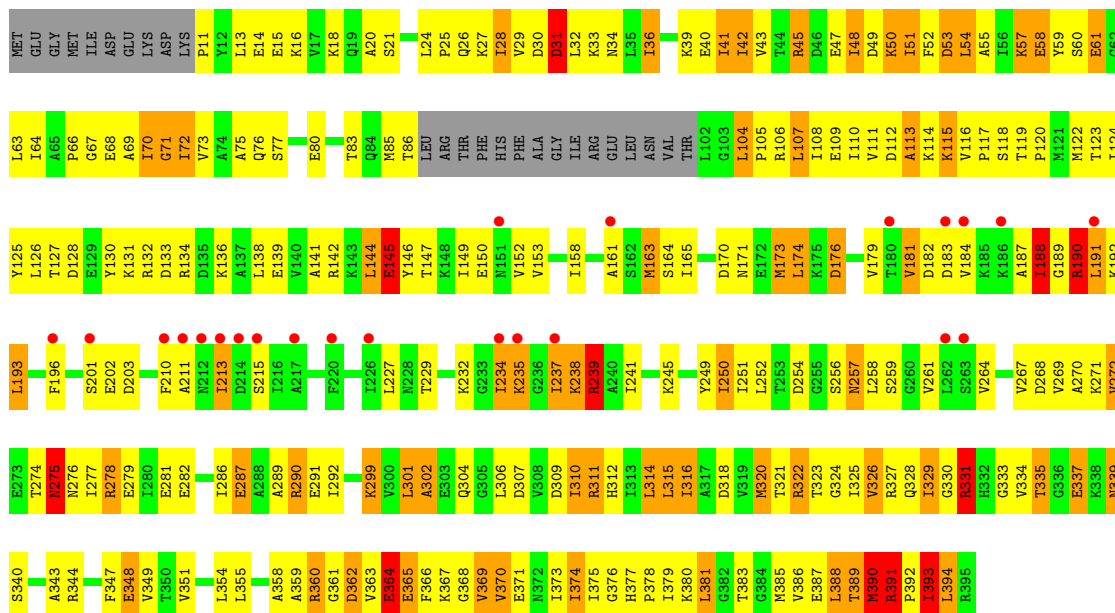


- Molecule 1: DNA-directed RNA polymerase subunit A'

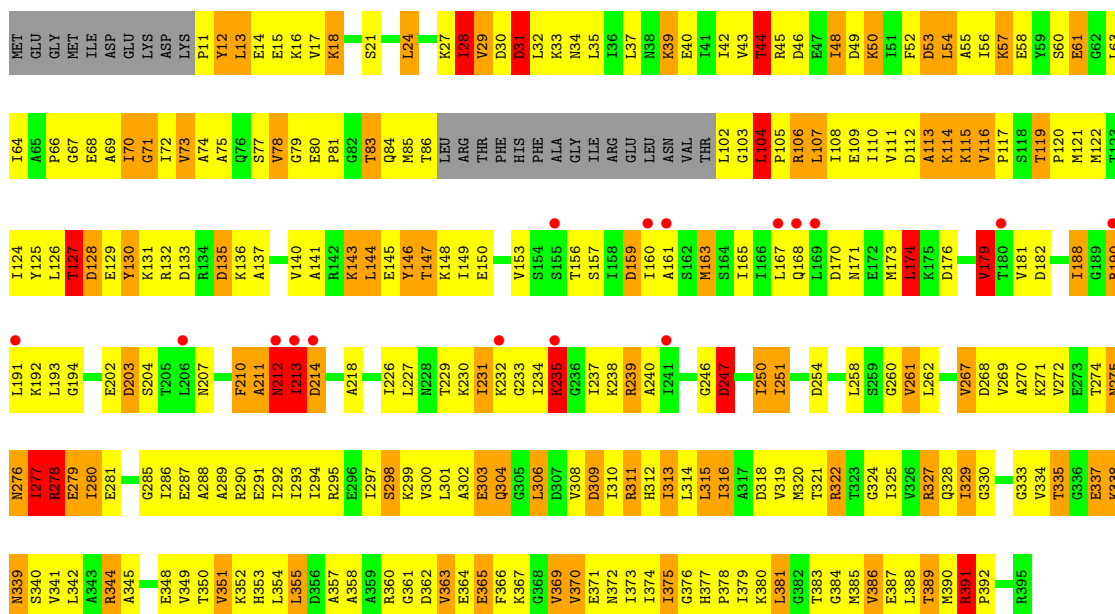




• Molecule 2: DNA-directed RNA polymerase subunit A''



• Molecule 2: DNA-directed RNA polymerase subunit A''



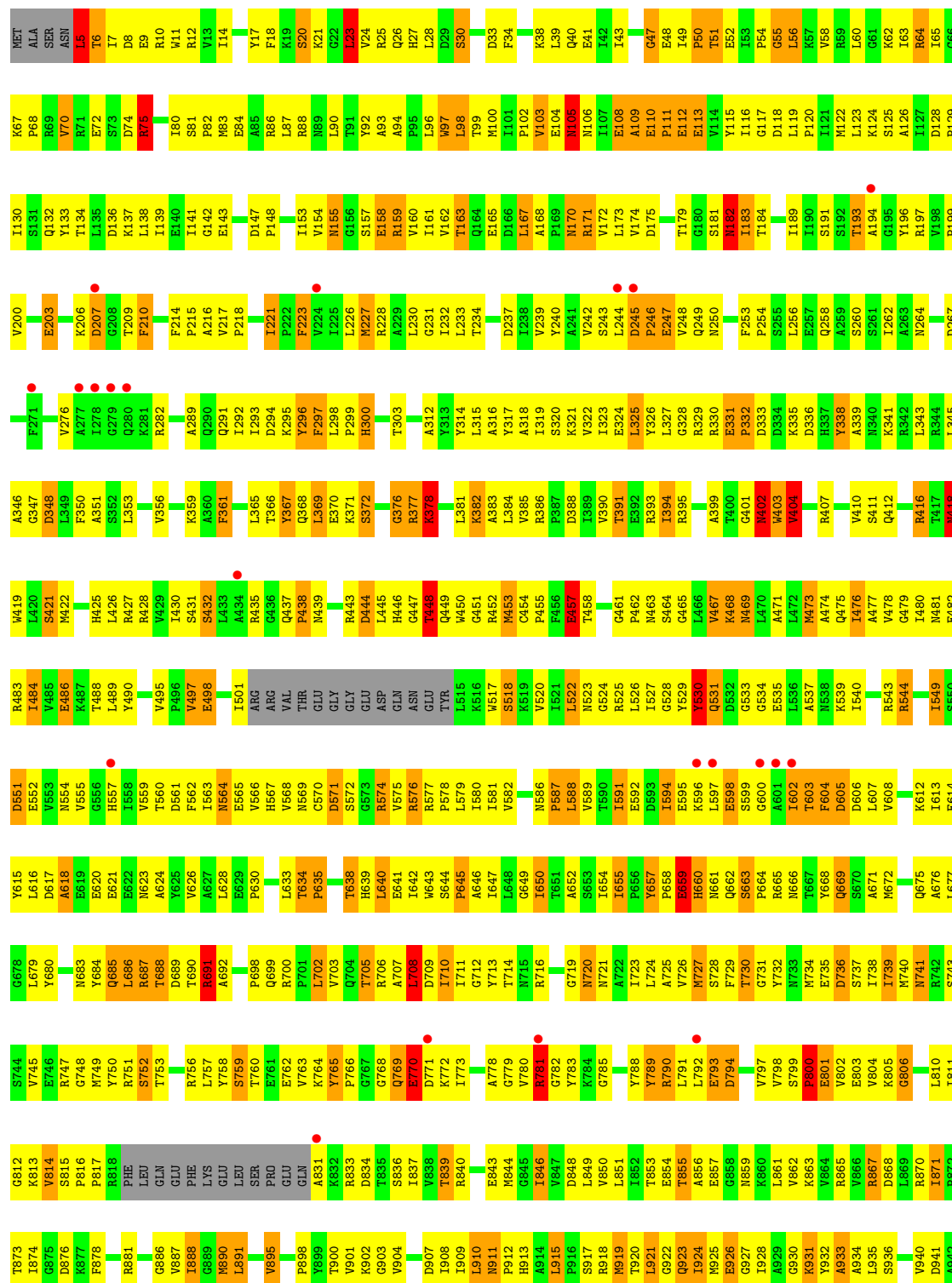
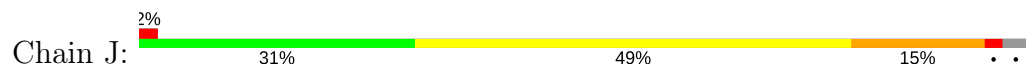
• Molecule 3: DNA-directed RNA polymerase subunit B

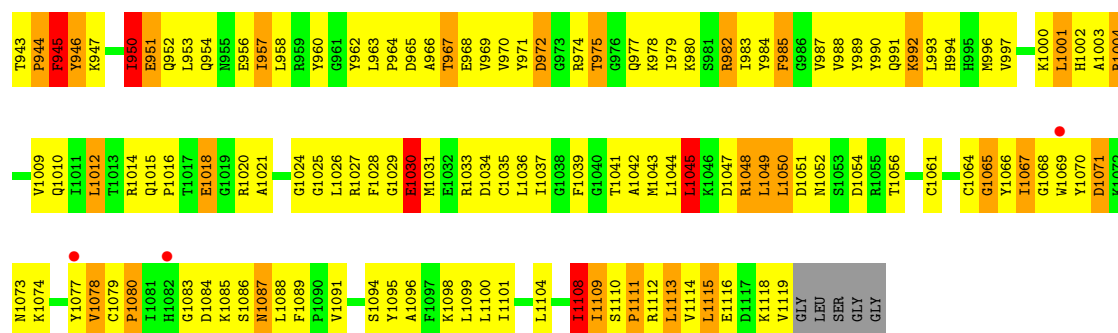


| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| E1018 | G1019 | R1020 | A1021 | G1024 | G1025 | L1026 | F1027 | F1028 | G1029 | E1030 | M1031 | E1032 | R1033 | D1034 | C1035 | L1036 | L1037 | G1038 | F1039 | G1040 | T1041 | L1044 | L1045 | D1046 | L1047 | R1048 | L1049 | L1050 | D1051 | N1052 | S1053 | D1054 | R1055 | T1056 | C1061 | C1064 | G1065 | I1066 | I1067 | G1068 | W1069 | Y1070 | D1071 | K1072 | N1073 | K1074 | V1075 | K1076 | Y1077 | V1078 | C1079 | P1080 | L1081 | H1082 | G1083 | | | |
| P849 | R850 | E851 | Q852 | L853 | Q854 | I857 | L858 | R859 | Y860 | G861 | Y862 | L863 | P864 | D865 | A866 | T867 | Y868 | Y869 | Y870 | Y871 | D872 | G873 | R874 | T875 | G876 | Q877 | K878 | I879 | R882 | D883 | R884 | R885 | R886 | R887 | R888 | R889 | R890 | R891 | R892 | R893 | R894 | R895 | R896 | K1000 | Y1001 | R1002 | R1003 | R1004 | A1005 | V1009 | Q1010 | I1011 | L1012 | T1013 | R1014 | L1015 | H1016 | T1017 |
| P816 | F817 | R818 | P819 | LEU | GLN | GLU | P819 | PHE | LYS | LEU | SER | PRO | GLU | GLN | A831 | R832 | R833 | R834 | T835 | S836 | I837 | R838 | T839 | R840 | E843 | M844 | G845 | R846 | V847 | D848 | L849 | V850 | L851 | T852 | R853 | R854 | T855 | A856 | E857 | G858 | N859 | K860 | V861 | V862 | K863 | V864 | R865 | V866 | D867 | L868 | R869 | R870 | I871 | L872 | P873 | T874 | R875 | G876 |
| R881 | G886 | V887 | I888 | G889 | M890 | L891 | I892 | P893 | Q894 | V895 | P898 | Y899 | T900 | K901 | K902 | K903 | G904 | V904 | D907 | R908 | I909 | L910 | N911 | P912 | H913 | A914 | L915 | P916 | S917 | R918 | M919 | L920 | L921 | R922 | Q923 | I924 | M925 | E926 | G930 | K931 | Y932 | A933 | A934 | L935 | S936 | G937 | V940 | D941 | A942 | T943 | P944 | F945 | Y946 | L947 | T948 | | | |
| P849 | R850 | E851 | Q852 | L853 | Q854 | I857 | L858 | R859 | Y860 | G861 | Y862 | L863 | P864 | D865 | A866 | T867 | Y868 | Y869 | Y870 | Y871 | D872 | G873 | R874 | T875 | G876 | Q877 | K878 | I879 | R882 | D883 | R884 | R885 | R886 | R887 | R888 | R889 | R890 | R891 | R892 | R893 | R894 | R895 | R896 | K1000 | Y1001 | R1002 | R1003 | R1004 | A1005 | V1009 | Q1010 | I1011 | L1012 | T1013 | R1014 | L1015 | H1016 | T1017 |
| E1018 | G1019 | R1020 | A1021 | G1024 | G1025 | L1026 | F1027 | F1028 | G1029 | E1030 | M1031 | E1032 | R1033 | D1034 | C1035 | L1036 | L1037 | G1038 | F1039 | G1040 | T1041 | L1044 | L1045 | D1046 | L1047 | R1048 | L1049 | L1050 | D1051 | N1052 | S1053 | D1054 | R1055 | T1056 | C1061 | C1064 | G1065 | I1066 | I1067 | G1068 | W1069 | Y1070 | D1071 | K1072 | N1073 | K1074 | V1075 | K1076 | Y1077 | V1078 | C1079 | P1080 | L1081 | H1082 | G1083 | | | |
| P68 | R69 | V70 | R71 | E72 | S73 | D74 | R75 | E78 | R79 | G80 | S81 | P82 | M83 | A85 | L87 | R88 | K89 | L90 | T91 | Y92 | A93 | A94 | P95 | L96 | T97 | L98 | T99 | M100 | I101 | P102 | V103 | E104 | N105 | N106 | I107 | E108 | A109 | P110 | P111 | E112 | V113 | V114 | G115 | G117 | D118 | L119 | P120 | T121 | M122 | L123 | K124 | S125 | D128 | P129 | | | | |
| L130 | S131 | Y132 | T133 | L134 | L135 | D136 | K137 | L138 | E139 | L140 | I141 | G142 | E143 | D147 | P148 | L153 | V154 | R155 | G156 | S157 | E158 | R159 | V160 | I161 | V162 | T163 | L167 | M170 | R171 | V172 | L173 | V174 | D175 | S181 | R182 | I183 | T184 | L189 | I190 | S191 | S192 | T193 | A194 | G195 | Y196 | N264 | D267 | Y276 | G279 | E203 | R204 | L205 | | | | | | |
| K206 | D207 | G208 | T209 | F210 | H211 | V212 | S213 | F214 | P215 | A216 | T221 | P222 | F223 | T303 | S304 | D307 | A312 | Y313 | T314 | L315 | A316 | Y317 | A318 | L319 | S320 | K321 | V322 | L323 | E324 | L324 | P245 | P246 | E247 | V248 | Q249 | E331 | P332 | D333 | K334 | K335 | D336 | H337 | E338 | A339 | K340 | K341 | K342 | L343 | R344 | L345 | A346 | G347 | D348 | L349 | A351 | | | |
| S352 | L353 | V356 | K359 | A360 | F361 | L365 | T366 | Y367 | Q368 | L369 | E370 | K371 | S372 | K373 | V374 | R375 | G376 | R377 | K378 | L381 | K382 | A383 | L384 | V385 | S386 | K387 | D388 | L389 | V390 | T391 | E392 | R393 | L394 | R395 | A399 | F253 | P254 | S255 | L256 | E257 | Y258 | Q259 | A260 | S261 | T262 | A263 | N264 | D267 | Y276 | G279 | E203 | R204 | L205 | | | | | |
| H425 | L426 | R427 | R428 | V429 | L430 | S431 | S432 | L433 | A434 | R435 | Q436 | D437 | P438 | N439 | V440 | T441 | A442 | E443 | R444 | D445 | L446 | H447 | G448 | T449 | V450 | G451 | R452 | N453 | C454 | P455 | F456 | E457 | T458 | Q461 | P462 | N463 | S464 | G465 | Y466 | Q467 | D468 | N469 | L470 | A471 | L472 | N473 | A474 | O475 | L476 | A477 | V478 | G479 | L480 | N481 | E482 | R483 | S484 | V485 |
| E486 | K487 | L488 | L489 | Y490 | V495 | F496 | E497 | E498 | I501 | ARG | THR | VAL | GLY | GLY | GLY | GLU | ASP | GLN | ASN | TYR | L515 | K516 | W517 | S518 | V520 | E521 | L522 | G523 | R524 | R525 | L526 | I527 | G528 | Y529 | Q531 | D532 | G533 | G534 | E535 | L536 | A537 | N538 | K539 | I540 | R543 | R544 | I549 | S550 | D551 | E552 | V553 | | | | | | | |
| N554 | V555 | G556 | H557 | L558 | T559 | D561 | S562 | L563 | N564 | E565 | V566 | H567 | V568 | N569 | C570 | D571 | S572 | G573 | R574 | V575 | R576 | R577 | P578 | L579 | I580 | V581 | V582 | N586 | P587 | L588 | V589 | T590 | I591 | E592 | D593 | L594 | E595 | K596 | L597 | E598 | S599 | A601 | I602 | T603 | F604 | D605 | D606 | L607 | V608 | K612 | I613 | E614 | Y615 | L616 | D617 | | | |
| A618 | E619 | E620 | E621 | E622 | G623 | A624 | E625 | A627 | E628 | E629 | P630 | L633 | T634 | P635 | T638 | H639 | E641 | I642 | V643 | S644 | P645 | A646 | L647 | L648 | G649 | L650 | T651 | A652 | S653 | L654 | L655 | P656 | V657 | P658 | E659 | H660 | N661 | O662 | S663 | P664 | R665 | Q669 | S670 | A671 | H672 | Q675 | A676 | L677 | G678 | L679 | V680 | A681 | A682 | | | | | |
| N683 | Y684 | Q685 | L686 | R687 | T688 | D689 | T690 | P691 | P698 | Q699 | R700 | F701 | L702 | V703 | Q704 | T705 | R706 | A707 | L708 | D709 | I710 | R711 | G712 | Y713 | T714 | N715 | R716 | G719 | N720 | R721 | L722 | I723 | L724 | P725 | V726 | M727 | S728 | F729 | T730 | G731 | Y732 | M733 | E734 | L735 | D736 | S737 | I738 | I739 | M740 | N741 | R742 | S743 | T744 | V745 | G748 | M749 | | |
| Y750 | R751 | S752 | T753 | R756 | L757 | Y758 | S759 | T760 | E761 | E762 | V763 | K764 | Y765 | P766 | G767 | G768 | Q769 | E770 | D771 | K772 | I773 | A778 | G779 | V780 | R781 | G782 | Y783 | K784 | G785 | R786 | E787 | Y788 | R789 | R790 | L791 | L792 | E793 | D794 | V797 | V798 | S799 | P800 | E801 | V802 | E803 | V804 | K805 | G806 | V809 | R810 | L811 | T812 | S813 | G814 | R815 | V816 | S817 | |
| P816 | F817 | R818 | P819 | LEU | GLN | GLU | P819 | PHE | LYS | LEU | SER | PRO | GLU | GLN | A831 | R832 | R833 | R834 | T835 | S836 | I837 | R838 | T839 | R840 | E843 | M844 | G845 | R846 | V847 | D848 | L849 | V850 | L851 | T852 | R853 | R854 | T855 | A856 | E857 | G858 | N859 | K860 | V861 | V862 | K863 | V864 | R865 | V866 | D867 | L868 | R869 | R870 | I871 | L872 | P873 | T874 | R875 | G876 |
| R881 | G886 | V887 | I888 | G889 | M890 | L891 | I892 | P893 | Q894 | V895 | P898 | Y899 | T900 | K901 | K902 | K903 | G904 | V904 | D907 | R908 | I909 | L910 | N911 | P912 | H913 | A914 | L915 | P916 | S917 | R918 | M919 | L920 | L921 | R922 | Q923 | I924 | M925 | E926 | G930 | K931 | Y932 | A933 | A934 | L935 | S936 | G937 | V940 | D941 | A942 | T943 | P944 | F945 | Y946 | L947 | T948 | | | |
| P849 | R850 | E851 | Q852 | L853 | Q854 | I857 | L858 | R859 | Y860 | G861 | Y862 | L863 | P864 | D865 | A866 | T867 | Y868 | Y869 | Y870 | Y871 | D872 | G873 | R874 | T875 | G876 | Q877 | K878 | I879 | R882 | D883 | R884 | R885 | R886 | R887 | R888 | R889 | R890 | R891 | R892 | R893 | R894 | R895 | R896 | K1000 | Y1001 | R1002 | R1003 | R1004 | A1005 | V1009 | Q1010 | I1011 | L1012 | T1013 | R1014 | L1015 | H1016 | T1017 |
| E1018 | G1019 | R1020 | A1021 | G1024 | G1025 | L1026 | F1027 | F1028 | G1029 | E1030 | M1031 | E1032 | R1033 | D1034 | C1035 | L1036 | L1037 | G1038 | F1039 | G1040 | T1041 | L1044 | L1045 | D1046 | L1047 | R1048 | L1049 | L1050 | D1051 | N1052 | S1053 | D1054 | R1055 | T1056 | C1061 | C1064 | G1065 | I1066 | I1067 | G1068 | W1069 | Y1070 | D1071 | K1072 | N1073 | K1074 | V1075 | K1076 | Y1077 | V1078 | C1079 | P1080 | L1081 | H1082 | G1083 | | | |

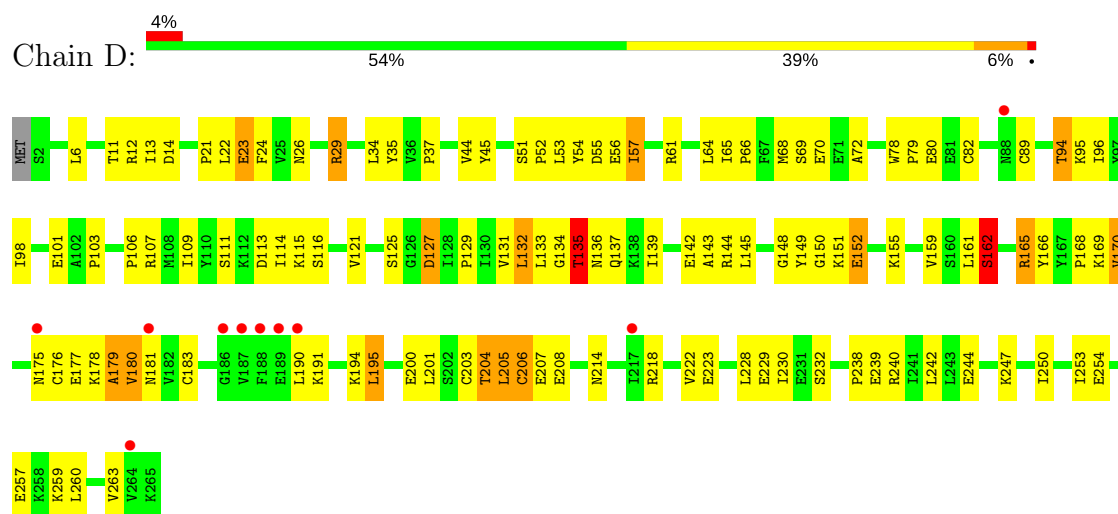


Molecule 3: DNA-directed RNA polymerase subunit B





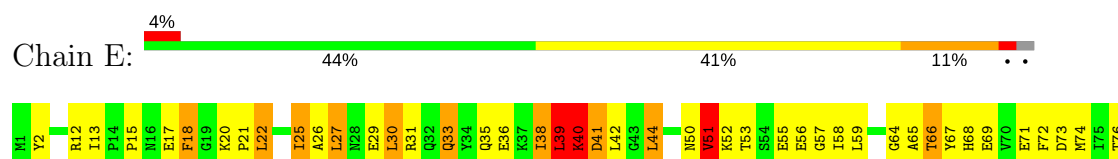
• Molecule 4: DNA-directed RNA polymerase subunit D

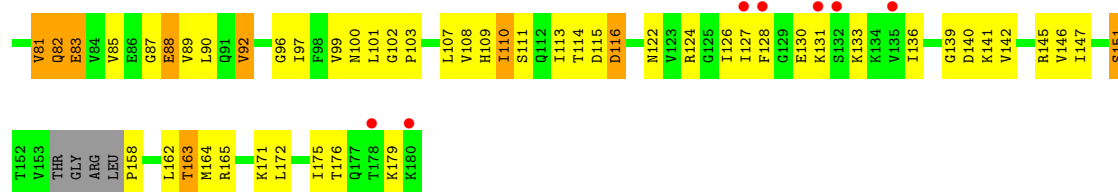


• Molecule 4: DNA-directed RNA polymerase subunit D

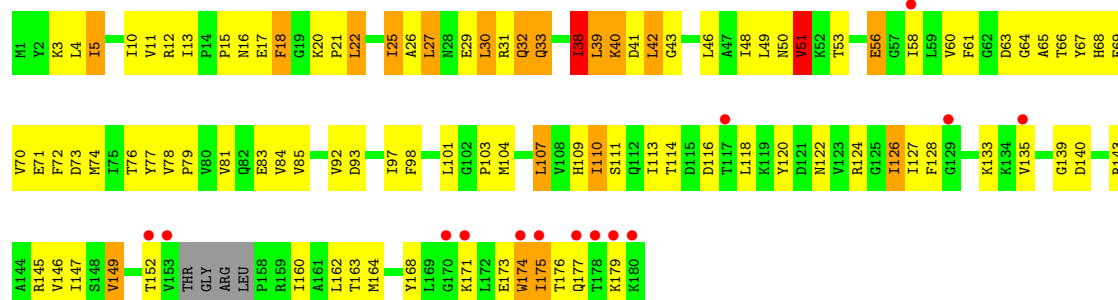


• Molecule 5: DNA-directed RNA polymerase, subunit E' (RpoE1)

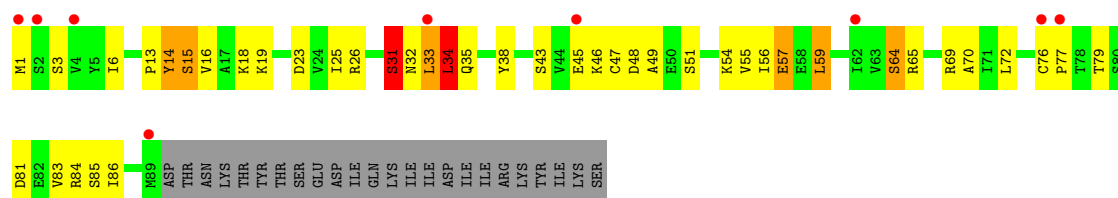




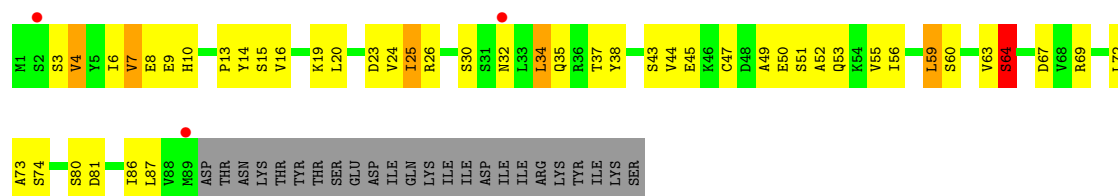
• Molecule 5: DNA-directed RNA polymerase, subunit E' (RpoE1)



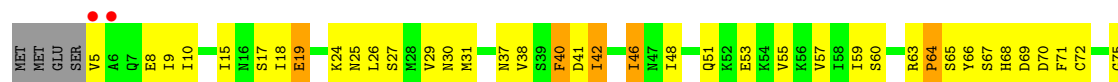
• Molecule 6: DNA-directed RNA polymerase, subunit F (RpoF)

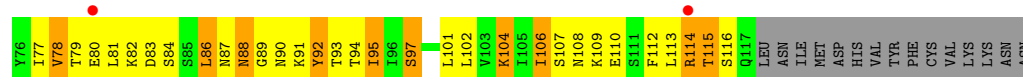


• Molecule 6: DNA-directed RNA polymerase, subunit F (RpoF)

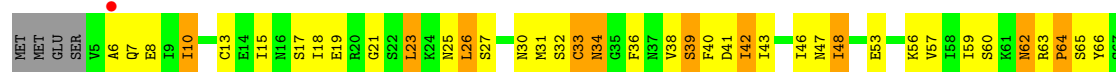


• Molecule 7: DNA-directed RNA polymerase, subunit G (RpoG)

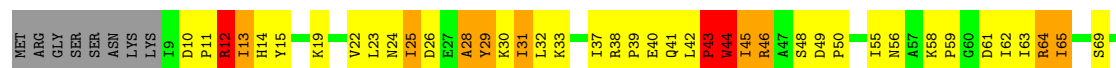




• Molecule 7: DNA-directed RNA polymerase, subunit G (RpoG)



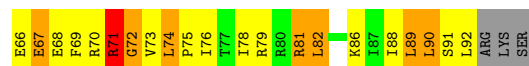
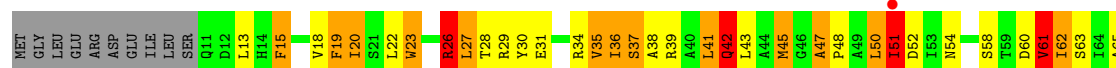
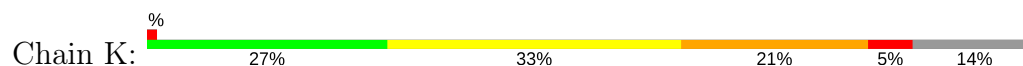
• Molecule 8: DNA-directed RNA polymerase subunit H



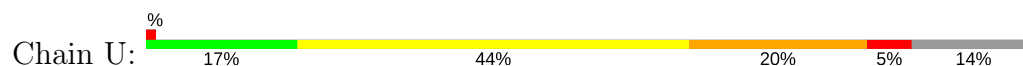
• Molecule 8: DNA-directed RNA polymerase subunit H



• Molecule 9: DNA-directed RNA polymerase subunit K

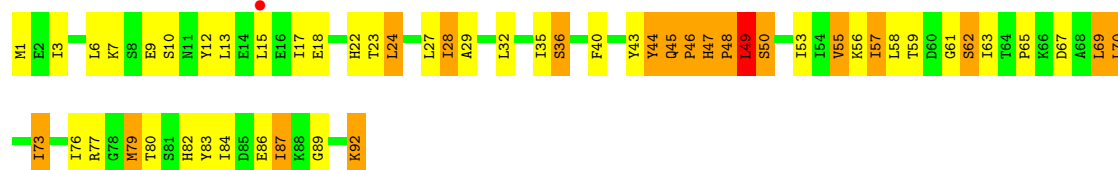


• Molecule 9: DNA-directed RNA polymerase subunit K

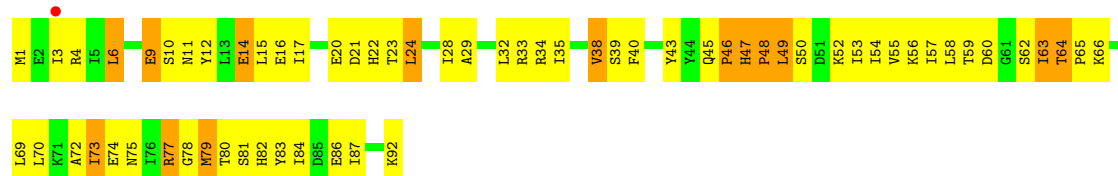




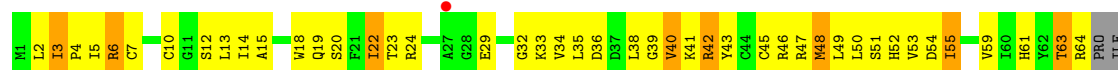
• Molecule 10: DNA-directed RNA polymerase subunit L



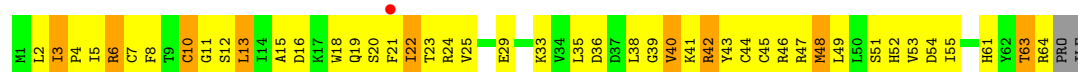
• Molecule 10: DNA-directed RNA polymerase subunit L



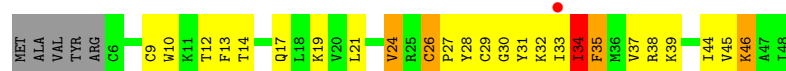
• Molecule 11: DNA-directed RNA polymerase subunit N



• Molecule 11: DNA-directed RNA polymerase subunit N



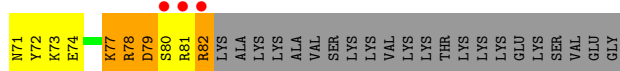
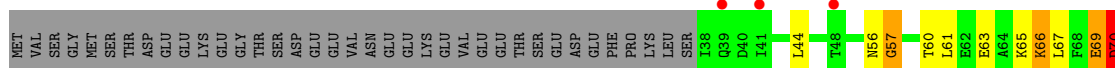
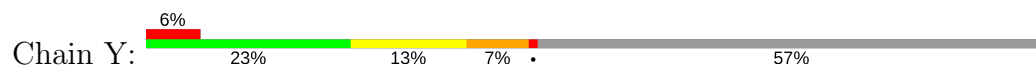
• Molecule 12: DNA-directed RNA polymerase subunit P



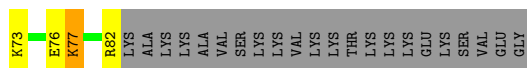
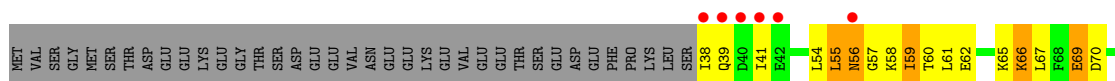
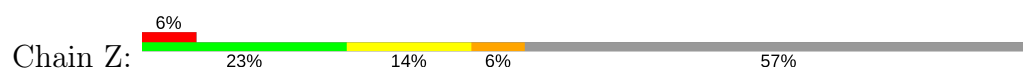
• Molecule 12: DNA-directed RNA polymerase subunit P



- Molecule 13: DNA-directed RNA polymerase subunit 13



- Molecule 13: DNA-directed RNA polymerase subunit 13



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 125.82Å 201.24Å 196.05Å 90.00° 100.92° 90.00° | Depositor |
| Resolution (Å) | 40.00 – 3.40 39.79 – 3.40 | Depositor EDS |
| % Data completeness (in resolution range) | 80.3 (40.00-3.40) 80.3 (39.79-3.40) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.69 (at 3.40Å) | Xtriage |
| Refinement program | REFMAC 5.5.0072 | Depositor |
| R, R_{free} | 0.265 , 0.341 0.264 , 0.337 | Depositor DCC |
| R_{free} test set | 5323 reflections (5.31%) | DCC |
| Wilson B-factor (Å ²) | 76.2 | Xtriage |
| Anisotropy | 0.062 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.26 , 71.4 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.85 | EDS |
| Total number of atoms | 53072 | wwPDB-VP |
| Average B, all atoms (Å ²) | 78.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, F3S, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.60 | 0/6815 | 0.76 | 4/9219 (0.0%) |
| 1 | I | 0.62 | 0/6815 | 0.77 | 5/9219 (0.1%) |
| 2 | C | 0.64 | 0/2892 | 0.85 | 1/3891 (0.0%) |
| 2 | M | 0.66 | 0/2892 | 0.84 | 2/3891 (0.1%) |
| 3 | B | 0.60 | 0/8810 | 0.78 | 7/11921 (0.1%) |
| 3 | J | 0.60 | 0/8810 | 0.79 | 6/11921 (0.1%) |
| 4 | D | 0.49 | 0/2152 | 0.66 | 0/2911 |
| 4 | O | 0.52 | 0/2152 | 0.66 | 0/2911 |
| 5 | E | 0.53 | 0/1423 | 0.72 | 0/1919 |
| 5 | Q | 0.52 | 0/1423 | 0.72 | 0/1919 |
| 6 | F | 0.50 | 0/701 | 0.66 | 1/949 (0.1%) |
| 6 | R | 0.52 | 0/701 | 0.70 | 0/949 |
| 7 | G | 0.63 | 0/895 | 0.78 | 0/1203 |
| 7 | S | 0.68 | 0/895 | 0.75 | 1/1203 (0.1%) |
| 8 | H | 0.54 | 0/625 | 0.77 | 0/848 |
| 8 | T | 0.61 | 0/625 | 0.83 | 1/848 (0.1%) |
| 9 | K | 0.61 | 0/667 | 0.87 | 0/903 |
| 9 | U | 0.70 | 0/667 | 0.95 | 1/903 (0.1%) |
| 10 | L | 0.51 | 0/733 | 0.71 | 1/986 (0.1%) |
| 10 | V | 0.57 | 0/733 | 0.74 | 0/986 |
| 11 | N | 0.51 | 0/523 | 0.74 | 0/705 |
| 11 | W | 0.52 | 0/523 | 0.74 | 0/705 |
| 12 | P | 0.63 | 0/354 | 0.73 | 0/475 |
| 12 | X | 0.65 | 0/354 | 0.70 | 0/475 |
| 13 | Y | 0.71 | 0/395 | 0.73 | 0/527 |
| 13 | Z | 0.67 | 0/395 | 0.75 | 0/527 |
| All | All | 0.60 | 0/53970 | 0.77 | 30/72914 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | M | 0 | 1 |
| 3 | B | 0 | 1 |
| 3 | J | 0 | 1 |
| 7 | G | 0 | 1 |
| 9 | K | 0 | 1 |
| 9 | U | 0 | 1 |
| All | All | 0 | 6 |

There are no bond length outliers.

All (30) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | A | 464 | LEU | CA-CB-CG | 6.85 | 131.04 | 115.30 |
| 1 | I | 239 | LEU | CA-CB-CG | 6.55 | 130.36 | 115.30 |
| 8 | T | 42 | LEU | CA-CB-CG | 6.31 | 129.80 | 115.30 |
| 1 | A | 239 | LEU | CA-CB-CG | 6.30 | 129.79 | 115.30 |
| 1 | I | 464 | LEU | CA-CB-CG | 6.19 | 129.55 | 115.30 |
| 2 | C | 54 | LEU | CA-CB-CG | 6.15 | 129.45 | 115.30 |
| 3 | B | 1045 | LEU | CA-CB-CG | 6.04 | 129.20 | 115.30 |
| 3 | J | 23 | LEU | CA-CB-CG | 6.02 | 129.14 | 115.30 |
| 3 | J | 5 | LEU | CA-CB-CG | 5.89 | 128.85 | 115.30 |
| 3 | B | 571 | ASP | N-CA-C | 5.87 | 126.86 | 111.00 |
| 1 | I | 534 | LEU | CA-CB-CG | 5.86 | 128.77 | 115.30 |
| 3 | B | 5 | LEU | CA-CB-CG | 5.85 | 128.76 | 115.30 |
| 3 | J | 571 | ASP | N-CA-C | 5.84 | 126.77 | 111.00 |
| 3 | J | 1045 | LEU | CA-CB-CG | 5.82 | 128.68 | 115.30 |
| 1 | I | 827 | LEU | CA-CB-CG | 5.80 | 128.64 | 115.30 |
| 3 | J | 522 | LEU | CA-CB-CG | 5.72 | 128.45 | 115.30 |
| 3 | B | 522 | LEU | CA-CB-CG | 5.70 | 128.42 | 115.30 |
| 3 | B | 23 | LEU | CA-CB-CG | 5.59 | 128.15 | 115.30 |
| 1 | A | 534 | LEU | CA-CB-CG | 5.55 | 128.06 | 115.30 |
| 2 | M | 174 | LEU | CA-CB-CG | 5.51 | 127.98 | 115.30 |
| 3 | B | 436 | GLY | N-CA-C | -5.43 | 99.52 | 113.10 |
| 1 | A | 827 | LEU | CA-CB-CG | 5.40 | 127.72 | 115.30 |
| 2 | M | 37 | LEU | CA-CB-CG | 5.28 | 127.44 | 115.30 |
| 10 | L | 49 | LEU | CA-CB-CG | 5.12 | 127.08 | 115.30 |
| 1 | I | 302 | LEU | CA-CB-CG | 5.10 | 127.03 | 115.30 |
| 9 | U | 60 | ASP | N-CA-C | 5.07 | 124.69 | 111.00 |
| 3 | B | 963 | LEU | CA-CB-CG | -5.05 | 103.69 | 115.30 |
| 6 | F | 34 | LEU | CA-CB-CG | 5.05 | 126.91 | 115.30 |
| 7 | S | 26 | LEU | CA-CB-CG | 5.04 | 126.88 | 115.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3 | J | 792 | LEU | CA-CB-CG | 5.01 | 126.82 | 115.30 |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 3 | B | 945 | PHE | Peptide |
| 7 | G | 40 | PHE | Peptide |
| 3 | J | 945 | PHE | Peptide |
| 9 | K | 26 | ARG | Peptide |
| 2 | M | 27 | LYS | Peptide |
| 9 | U | 59 | THR | Peptide |

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 6673 | 0 | 6763 | 612 | 0 |
| 1 | I | 6673 | 0 | 6763 | 619 | 0 |
| 2 | C | 2868 | 0 | 3035 | 277 | 0 |
| 2 | M | 2868 | 0 | 3035 | 331 | 0 |
| 3 | B | 8645 | 0 | 8780 | 817 | 0 |
| 3 | J | 8645 | 0 | 8780 | 862 | 0 |
| 4 | D | 2114 | 0 | 2146 | 120 | 0 |
| 4 | O | 2114 | 0 | 2146 | 122 | 0 |
| 5 | E | 1402 | 0 | 1467 | 80 | 0 |
| 5 | Q | 1402 | 0 | 1467 | 97 | 0 |
| 6 | F | 694 | 0 | 705 | 37 | 0 |
| 6 | R | 694 | 0 | 705 | 29 | 0 |
| 7 | G | 884 | 0 | 888 | 91 | 0 |
| 7 | S | 884 | 0 | 888 | 86 | 0 |
| 8 | H | 611 | 0 | 641 | 49 | 0 |
| 8 | T | 611 | 0 | 641 | 51 | 0 |
| 9 | K | 658 | 0 | 692 | 81 | 0 |
| 9 | U | 658 | 0 | 692 | 92 | 0 |
| 10 | L | 723 | 0 | 749 | 54 | 0 |
| 10 | V | 723 | 0 | 749 | 57 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11 | N | 514 | 0 | 528 | 66 | 0 |
| 11 | W | 514 | 0 | 528 | 69 | 0 |
| 12 | P | 346 | 0 | 375 | 28 | 0 |
| 12 | X | 346 | 0 | 375 | 28 | 0 |
| 13 | Y | 391 | 0 | 389 | 27 | 0 |
| 13 | Z | 391 | 0 | 389 | 13 | 0 |
| 14 | A | 2 | 0 | 0 | 0 | 0 |
| 14 | B | 1 | 0 | 0 | 2 | 0 |
| 14 | I | 2 | 0 | 0 | 0 | 0 |
| 14 | J | 1 | 0 | 0 | 2 | 0 |
| 14 | N | 1 | 0 | 0 | 0 | 0 |
| 14 | P | 1 | 0 | 0 | 0 | 0 |
| 14 | W | 1 | 0 | 0 | 0 | 0 |
| 14 | X | 1 | 0 | 0 | 0 | 0 |
| 15 | A | 1 | 0 | 0 | 0 | 0 |
| 15 | I | 1 | 0 | 0 | 0 | 0 |
| 16 | D | 7 | 0 | 0 | 1 | 0 |
| 16 | O | 7 | 0 | 0 | 6 | 0 |
| All | All | 53072 | 0 | 54316 | 4172 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (4172) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:29:TYR:OH | 13:Y:67:LEU:HD22 | 1.31 | 1.25 |
| 4:D:183:CYS:SG | 16:D:1001:F3S:S2 | 2.42 | 1.17 |
| 6:R:72:LEU:HD21 | 6:R:86:ILE:HD12 | 1.30 | 1.14 |
| 5:Q:147:ILE:HD11 | 5:Q:163:THR:HB | 1.21 | 1.14 |
| 4:D:250:ILE:HD11 | 10:L:84:ILE:HD11 | 1.31 | 1.13 |
| 3:B:581:ILE:HD11 | 3:B:614:GLU:HB2 | 1.16 | 1.13 |
| 3:B:353:LEU:HA | 3:B:404:VAL:HG11 | 1.21 | 1.13 |
| 3:J:353:LEU:HA | 3:J:404:VAL:HG11 | 1.18 | 1.12 |
| 2:M:389:THR:HG23 | 9:U:77:THR:HB | 1.30 | 1.11 |
| 3:J:759:SER:HB2 | 3:J:862:VAL:O | 1.51 | 1.11 |
| 1:A:760:GLY:HA3 | 3:B:447:GLY:HA3 | 1.24 | 1.10 |
| 3:B:88:ARG:HD3 | 3:B:853:THR:HG21 | 1.10 | 1.10 |
| 5:Q:53:THR:HB | 5:Q:71:GLU:H | 1.09 | 1.09 |
| 3:J:922:GLY:HA2 | 3:J:925:MET:HB2 | 1.26 | 1.09 |
| 3:J:581:ILE:HD11 | 3:J:614:GLU:CB | 1.83 | 1.09 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:647:ARG:HH11 | 3:J:965:ASP:HB2 | 0.96 | 1.09 |
| 9:K:90:LEU:HD23 | 9:K:90:LEU:H | 1.09 | 1.09 |
| 2:C:340:SER:HB3 | 2:C:371:GLU:HG2 | 1.14 | 1.08 |
| 3:J:88:ARG:HD3 | 3:J:853:THR:HG21 | 1.09 | 1.08 |
| 2:M:146:TYR:HD2 | 2:M:233:GLY:O | 1.35 | 1.08 |
| 1:I:308:ARG:HH21 | 3:J:1099:LEU:HD13 | 1.16 | 1.08 |
| 1:A:647:ARG:HH11 | 3:B:965:ASP:HB2 | 0.99 | 1.08 |
| 5:E:36:GLU:HG2 | 6:F:34:LEU:HD11 | 1.37 | 1.07 |
| 3:J:26:GLN:O | 3:J:345:LEU:HD23 | 1.55 | 1.06 |
| 5:E:39:LEU:HD11 | 6:F:1:MET:HA | 1.35 | 1.06 |
| 3:B:26:GLN:O | 3:B:345:LEU:HD23 | 1.56 | 1.06 |
| 2:C:55:ALA:HA | 2:C:58:GLU:HG3 | 1.38 | 1.06 |
| 1:A:418:LEU:HD21 | 3:B:1044:LEU:HD21 | 1.35 | 1.06 |
| 1:I:68:CYS:SG | 1:I:71:HIS:NE2 | 2.28 | 1.05 |
| 1:A:532:ILE:HD11 | 10:L:56:LYS:HD3 | 1.39 | 1.05 |
| 3:J:581:ILE:HD11 | 3:J:614:GLU:HB2 | 1.05 | 1.04 |
| 1:A:541:ALA:HB1 | 1:A:542:PRO:HD3 | 1.36 | 1.04 |
| 1:I:760:GLY:HA3 | 3:J:447:GLY:HA3 | 1.09 | 1.04 |
| 3:B:579:LEU:HD12 | 3:B:616:LEU:HD12 | 1.38 | 1.04 |
| 3:B:1033:ARG:NH1 | 3:B:1034:ASP:OD2 | 1.92 | 1.03 |
| 3:J:672:MET:HG2 | 3:J:993:LEU:HD21 | 1.37 | 1.03 |
| 2:M:28:ILE:HG21 | 9:U:14:HIS:CE1 | 1.93 | 1.02 |
| 2:C:55:ALA:HA | 2:C:58:GLU:CG | 1.89 | 1.02 |
| 4:O:175:ASN:HA | 4:O:195:LEU:HD11 | 1.39 | 1.02 |
| 1:A:308:ARG:HH21 | 3:B:1099:LEU:HD13 | 1.14 | 1.02 |
| 3:B:922:GLY:HA2 | 3:B:925:MET:HB2 | 1.39 | 1.01 |
| 2:M:340:SER:CB | 2:M:371:GLU:HG2 | 1.90 | 1.01 |
| 9:U:61:VAL:HG12 | 9:U:62:ILE:H | 1.25 | 1.01 |
| 3:B:38:LYS:HG3 | 3:B:39:LEU:H | 1.18 | 1.00 |
| 2:C:146:TYR:HB2 | 2:C:238:LYS:HD3 | 1.43 | 1.00 |
| 8:H:40:GLU:OE1 | 13:Y:66:LYS:HE2 | 1.61 | 1.00 |
| 3:J:38:LYS:HG3 | 3:J:39:LEU:H | 1.23 | 1.00 |
| 3:J:1113:LEU:HD12 | 3:J:1113:LEU:H | 1.24 | 1.00 |
| 3:J:702:LEU:HD22 | 3:J:933:ALA:HB1 | 1.39 | 1.00 |
| 3:J:569:ASN:HB3 | 3:J:574:ARG:HH22 | 1.22 | 1.00 |
| 5:Q:53:THR:O | 5:Q:70:VAL:HG13 | 1.62 | 1.00 |
| 3:J:650:ILE:HD13 | 3:J:650:ILE:H | 1.25 | 0.99 |
| 3:B:445:LEU:HD21 | 3:B:455:PRO:HA | 1.45 | 0.99 |
| 7:S:63:ARG:HG3 | 7:S:114:ARG:HH22 | 1.25 | 0.99 |
| 1:A:877:GLY:C | 3:J:377:ARG:HH12 | 1.65 | 0.98 |
| 3:J:458:THR:HG21 | 3:J:465:GLY:H | 1.28 | 0.98 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:I:647:ARG:NH1 | 3:J:965:ASP:HB2 | 1.76 | 0.98 |
| 1:A:376:ASN:O | 1:A:377:TYR:HB2 | 1.62 | 0.98 |
| 2:C:391:ARG:HH11 | 2:C:391:ARG:HG2 | 1.26 | 0.98 |
| 12:P:26:CYS:HB2 | 12:P:27:PRO:HD2 | 1.43 | 0.98 |
| 12:X:26:CYS:SG | 12:X:29:CYS:HB2 | 2.02 | 0.98 |
| 1:A:558:LYS:HG3 | 3:J:104:GLU:HB2 | 1.42 | 0.98 |
| 2:C:109:GLU:O | 2:C:113:ALA:HA | 1.63 | 0.98 |
| 2:M:274:THR:HG22 | 2:M:275:ASN:H | 1.27 | 0.97 |
| 12:P:46:LYS:HD2 | 12:P:46:LYS:H | 1.29 | 0.97 |
| 1:A:647:ARG:NH1 | 3:B:965:ASP:HB2 | 1.78 | 0.97 |
| 1:I:331:ASN:O | 1:I:332:ILE:HB | 1.62 | 0.97 |
| 2:M:340:SER:HB3 | 2:M:371:GLU:CG | 1.94 | 0.97 |
| 2:C:340:SER:HB3 | 2:C:371:GLU:CG | 1.94 | 0.97 |
| 1:I:376:ASN:O | 1:I:377:TYR:HB2 | 1.65 | 0.97 |
| 2:M:55:ALA:HA | 2:M:58:GLU:HB2 | 1.47 | 0.97 |
| 2:C:329:ILE:HA | 2:C:334:VAL:HG12 | 1.46 | 0.97 |
| 9:K:45:MET:CE | 9:K:45:MET:HA | 1.95 | 0.97 |
| 2:M:340:SER:HB3 | 2:M:371:GLU:HG2 | 0.98 | 0.97 |
| 2:C:276:ASN:HD22 | 2:C:279:GLU:HB2 | 1.29 | 0.97 |
| 4:D:175:ASN:HA | 4:D:195:LEU:HD11 | 1.43 | 0.96 |
| 6:R:72:LEU:CD2 | 6:R:86:ILE:HD12 | 1.94 | 0.96 |
| 1:A:541:ALA:HB1 | 1:A:542:PRO:CD | 1.94 | 0.96 |
| 2:C:126:LEU:HB2 | 2:C:131:LYS:HG3 | 1.46 | 0.96 |
| 1:I:541:ALA:HB1 | 1:I:542:PRO:HD3 | 1.44 | 0.96 |
| 3:B:581:ILE:HD11 | 3:B:614:GLU:CB | 1.94 | 0.96 |
| 3:B:702:LEU:HD22 | 3:B:933:ALA:HB1 | 1.45 | 0.96 |
| 8:H:43:PRO:O | 8:H:44:TRP:HB2 | 1.63 | 0.96 |
| 3:B:702:LEU:H | 3:B:721:ASN:HD21 | 0.98 | 0.96 |
| 1:I:426:HIS:CE1 | 1:I:428:ILE:HG22 | 2.00 | 0.96 |
| 3:J:579:LEU:HD12 | 3:J:616:LEU:HD12 | 1.45 | 0.96 |
| 3:B:88:ARG:CD | 3:B:853:THR:HG21 | 1.96 | 0.95 |
| 3:J:339:ALA:HB2 | 3:J:618:ALA:HB3 | 1.45 | 0.95 |
| 3:J:88:ARG:CD | 3:J:853:THR:HG21 | 1.95 | 0.95 |
| 5:Q:27:LEU:HB2 | 5:Q:51:VAL:HG11 | 1.48 | 0.95 |
| 1:I:109:ASP:O | 1:I:113:LYS:HG3 | 1.64 | 0.95 |
| 9:U:69:PHE:HA | 9:U:74:LEU:HD11 | 1.47 | 0.95 |
| 3:J:450:TRP:HZ2 | 3:J:641:GLU:OE1 | 1.50 | 0.94 |
| 3:J:104:GLU:O | 3:J:105:ASN:HB2 | 1.63 | 0.94 |
| 3:B:1113:LEU:HD12 | 3:B:1113:LEU:H | 1.28 | 0.94 |
| 3:B:82:PRO:HG2 | 3:B:143:GLU:OE1 | 1.67 | 0.94 |
| 3:J:748:GLY:HA2 | 3:J:751:ARG:HD2 | 1.47 | 0.94 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:P:26:CYS:SG | 12:P:29:CYS:HB2 | 2.07 | 0.94 |
| 3:J:1033:ARG:NH1 | 3:J:1034:ASP:OD2 | 2.00 | 0.94 |
| 3:B:855:THR:HB | 3:B:857:GLU:HG2 | 1.47 | 0.94 |
| 4:O:98:ILE:HD11 | 4:O:114:ILE:HG13 | 1.50 | 0.94 |
| 3:B:650:ILE:H | 3:B:650:ILE:HD13 | 1.32 | 0.94 |
| 1:A:830:LEU:HD23 | 1:A:840:SER:HB3 | 1.47 | 0.94 |
| 3:J:445:LEU:HD21 | 3:J:455:PRO:HA | 1.49 | 0.94 |
| 2:C:237:ILE:HG13 | 2:C:238:LYS:N | 1.82 | 0.93 |
| 2:C:40:GLU:O | 2:C:45:ARG:HG2 | 1.68 | 0.93 |
| 1:A:124:ARG:HH21 | 13:Y:81:ARG:HH12 | 1.17 | 0.93 |
| 3:J:88:ARG:HD3 | 3:J:853:THR:CG2 | 1.98 | 0.93 |
| 9:K:82:LEU:HD23 | 9:K:82:LEU:H | 1.32 | 0.93 |
| 2:M:126:LEU:HB2 | 2:M:131:LYS:HG3 | 1.50 | 0.93 |
| 2:M:70:ILE:CD1 | 2:M:70:ILE:H | 1.82 | 0.93 |
| 3:J:764:LYS:HE2 | 3:J:813:LYS:HE2 | 1.51 | 0.93 |
| 1:A:317:ARG:HA | 3:B:1027:ARG:HA | 1.51 | 0.93 |
| 3:J:702:LEU:H | 3:J:721:ASN:HD21 | 0.94 | 0.93 |
| 2:C:391:ARG:HH11 | 2:C:391:ARG:CG | 1.82 | 0.92 |
| 3:J:855:THR:HB | 3:J:857:GLU:HG2 | 1.51 | 0.92 |
| 3:J:881:ARG:HH11 | 3:J:989:TYR:HB3 | 1.34 | 0.92 |
| 12:X:46:LYS:H | 12:X:46:LYS:HD2 | 1.32 | 0.92 |
| 1:A:595:GLU:HB2 | 7:G:91:LYS:HE2 | 1.52 | 0.92 |
| 1:I:760:GLY:HA3 | 3:J:447:GLY:CA | 1.97 | 0.92 |
| 3:J:854:GLU:HA | 3:J:859:ASN:O | 1.69 | 0.91 |
| 3:B:88:ARG:HD3 | 3:B:853:THR:CG2 | 1.97 | 0.91 |
| 7:S:7:GLN:HG2 | 7:S:8:GLU:H | 1.33 | 0.91 |
| 1:I:541:ALA:HB1 | 1:I:542:PRO:CD | 1.98 | 0.91 |
| 9:K:50:LEU:HD23 | 9:K:74:LEU:HA | 1.52 | 0.91 |
| 1:I:317:ARG:HA | 3:J:1027:ARG:HA | 1.51 | 0.91 |
| 3:B:672:MET:HG2 | 3:B:993:LEU:HD21 | 1.52 | 0.91 |
| 7:G:86:LEU:HD11 | 7:G:89:GLY:O | 1.70 | 0.91 |
| 9:K:34:ARG:O | 9:K:37:SER:HB2 | 1.71 | 0.91 |
| 1:A:365:VAL:HG23 | 1:A:388:LEU:HD11 | 1.51 | 0.91 |
| 1:A:541:ALA:HB2 | 7:G:72:CYS:H | 1.36 | 0.90 |
| 1:A:853:ASP:HB2 | 2:C:311:ARG:HH12 | 1.36 | 0.90 |
| 1:A:308:ARG:NH2 | 3:B:1099:LEU:HD13 | 1.86 | 0.90 |
| 2:C:340:SER:CB | 2:C:371:GLU:HG2 | 2.01 | 0.90 |
| 3:B:104:GLU:O | 3:B:105:ASN:HB2 | 1.71 | 0.90 |
| 3:B:640:LEU:HD22 | 3:B:641:GLU:H | 1.35 | 0.90 |
| 3:B:687:ARG:HG3 | 3:B:687:ARG:HH11 | 1.34 | 0.90 |
| 1:I:594:LEU:HA | 7:S:86:LEU:HD22 | 1.53 | 0.90 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:830:LEU:HD23 | 1:I:840:SER:HB3 | 1.50 | 0.90 |
| 2:M:28:ILE:HG21 | 9:U:14:HIS:HE1 | 1.36 | 0.90 |
| 3:B:854:GLU:HA | 3:B:859:ASN:O | 1.72 | 0.90 |
| 1:A:590:ASN:ND2 | 3:J:377:ARG:HB2 | 1.87 | 0.89 |
| 4:D:96:ILE:HG22 | 4:D:116:SER:HA | 1.54 | 0.89 |
| 9:K:45:MET:HA | 9:K:45:MET:HE2 | 1.55 | 0.89 |
| 2:M:392:PRO:HB2 | 5:Q:22:LEU:HD11 | 1.51 | 0.89 |
| 3:J:418:ASN:HD21 | 3:J:421:SER:H | 1.20 | 0.89 |
| 1:A:872:PHE:HA | 1:A:876:VAL:HB | 1.55 | 0.89 |
| 3:J:98:LEU:HD11 | 3:J:100:MET:HG3 | 1.54 | 0.89 |
| 4:O:96:ILE:HG22 | 4:O:116:SER:HA | 1.54 | 0.89 |
| 1:I:647:ARG:HH11 | 3:J:965:ASP:CB | 1.85 | 0.88 |
| 3:B:569:ASN:HB3 | 3:B:574:ARG:HH22 | 1.39 | 0.88 |
| 3:B:638:THR:HB | 3:B:639:HIS:CD2 | 2.08 | 0.88 |
| 2:C:390:MET:O | 2:C:391:ARG:HB3 | 1.72 | 0.88 |
| 4:D:98:ILE:HD11 | 4:D:114:ILE:HG13 | 1.55 | 0.88 |
| 12:X:26:CYS:HB2 | 12:X:27:PRO:HD2 | 1.54 | 0.88 |
| 1:A:109:ASP:O | 1:A:113:LYS:HG3 | 1.74 | 0.88 |
| 3:B:339:ALA:HB2 | 3:B:618:ALA:HB3 | 1.54 | 0.88 |
| 3:B:640:LEU:CD2 | 3:B:641:GLU:H | 1.86 | 0.88 |
| 3:B:418:ASN:ND2 | 3:B:421:SER:H | 1.71 | 0.88 |
| 3:B:702:LEU:H | 3:B:721:ASN:ND2 | 1.72 | 0.87 |
| 4:D:111:SER:HA | 4:D:114:ILE:HD13 | 1.54 | 0.87 |
| 3:J:82:PRO:HG2 | 3:J:143:GLU:OE1 | 1.74 | 0.87 |
| 3:J:418:ASN:ND2 | 3:J:421:SER:H | 1.72 | 0.87 |
| 1:A:541:ALA:CB | 1:A:542:PRO:CD | 2.52 | 0.87 |
| 3:B:242:VAL:HA | 3:B:316:ALA:HB1 | 1.55 | 0.87 |
| 3:J:638:THR:HB | 3:J:639:HIS:CD2 | 2.10 | 0.87 |
| 1:A:512:LYS:HE2 | 7:G:91:LYS:HE3 | 1.56 | 0.87 |
| 3:B:759:SER:HB2 | 3:B:862:VAL:O | 1.74 | 0.87 |
| 3:B:910:LEU:HD22 | 3:B:911:ASN:N | 1.89 | 0.87 |
| 3:J:1064:CYS:SG | 14:J:2001:ZN:ZN | 1.62 | 0.87 |
| 3:J:560:THR:HG22 | 3:J:562:PHE:H | 1.38 | 0.87 |
| 3:J:242:VAL:HA | 3:J:316:ALA:HB1 | 1.57 | 0.87 |
| 2:C:241:ILE:O | 2:C:251:ILE:HG13 | 1.73 | 0.87 |
| 1:I:823:LEU:HD13 | 2:M:75:ALA:HB1 | 1.56 | 0.87 |
| 5:Q:53:THR:HB | 5:Q:71:GLU:N | 1.88 | 0.87 |
| 1:A:369:PRO:HB3 | 1:A:376:ASN:HB3 | 1.56 | 0.87 |
| 1:I:632:PHE:HA | 1:I:635:PHE:CD1 | 2.10 | 0.87 |
| 3:J:314:TYR:HE2 | 3:J:526:LEU:H | 1.23 | 0.87 |
| 3:B:579:LEU:HD12 | 3:B:616:LEU:CD1 | 2.04 | 0.86 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:O:209:CYS:HG | 16:O:1001:F3S:FE1 | 0.56 | 0.86 |
| 1:A:589:LYS:O | 1:A:592:ILE:HG12 | 1.73 | 0.86 |
| 3:B:560:THR:HG22 | 3:B:562:PHE:H | 1.40 | 0.86 |
| 3:B:595:GLU:HA | 3:B:599:SER:HB3 | 1.56 | 0.86 |
| 4:D:250:ILE:HD11 | 10:L:84:ILE:CD1 | 2.03 | 0.86 |
| 9:K:90:LEU:N | 9:K:90:LEU:HD23 | 1.90 | 0.86 |
| 3:B:314:TYR:HE2 | 3:B:526:LEU:H | 1.21 | 0.86 |
| 3:B:47:GLY:HA2 | 3:B:58:VAL:O | 1.76 | 0.86 |
| 1:I:308:ARG:NH2 | 3:J:1099:LEU:HD13 | 1.91 | 0.86 |
| 2:M:289:ALA:O | 2:M:292:ILE:HG22 | 1.74 | 0.86 |
| 3:J:650:ILE:CD1 | 3:J:650:ILE:H | 1.89 | 0.86 |
| 3:B:98:LEU:HD11 | 3:B:100:MET:HG3 | 1.56 | 0.86 |
| 3:J:851:LEU:HA | 12:X:35:PHE:HB3 | 1.58 | 0.86 |
| 3:J:902:LYS:HB3 | 11:W:42:ARG:HD3 | 1.55 | 0.86 |
| 1:I:875:VAL:O | 1:I:877:GLY:N | 2.08 | 0.85 |
| 3:J:662:GLN:HG2 | 3:J:664:PRO:HD2 | 1.58 | 0.85 |
| 1:A:841:LEU:O | 1:A:843:GLY:N | 2.10 | 0.85 |
| 3:B:183:ILE:HD13 | 3:B:183:ILE:O | 1.76 | 0.85 |
| 3:B:418:ASN:HD21 | 3:B:421:SER:H | 1.16 | 0.85 |
| 1:I:365:VAL:HG23 | 1:I:388:LEU:HD11 | 1.58 | 0.85 |
| 3:J:47:GLY:HA2 | 3:J:58:VAL:O | 1.76 | 0.85 |
| 8:T:42:LEU:HB2 | 8:T:43:PRO:HD2 | 1.55 | 0.85 |
| 4:O:111:SER:HA | 4:O:114:ILE:HD13 | 1.55 | 0.85 |
| 1:I:589:LYS:O | 1:I:592:ILE:HG12 | 1.77 | 0.85 |
| 3:J:640:LEU:HD22 | 3:J:641:GLU:H | 1.42 | 0.85 |
| 3:J:529:TYR:O | 3:J:530:TYR:HB3 | 1.76 | 0.85 |
| 3:J:687:ARG:HH11 | 3:J:687:ARG:HG3 | 1.40 | 0.85 |
| 3:J:702:LEU:H | 3:J:721:ASN:ND2 | 1.73 | 0.85 |
| 3:B:451:GLY:HA3 | 3:B:577:ARG:HH11 | 1.42 | 0.85 |
| 3:B:748:GLY:HA2 | 3:B:751:ARG:HD2 | 1.58 | 0.85 |
| 3:B:662:GLN:HG2 | 3:B:664:PRO:HD2 | 1.57 | 0.85 |
| 2:C:340:SER:HA | 2:C:364:GLU:HG2 | 1.59 | 0.85 |
| 1:I:672:VAL:HG13 | 1:I:700:ILE:HD12 | 1.58 | 0.85 |
| 3:J:958:LEU:HD12 | 3:J:964:PRO:HG3 | 1.59 | 0.84 |
| 2:M:391:ARG:HH22 | 9:U:39:ARG:HH11 | 1.20 | 0.84 |
| 1:A:426:HIS:CE1 | 1:A:428:ILE:HG22 | 2.11 | 0.84 |
| 3:B:497:VAL:HG23 | 3:B:528:GLY:HA2 | 1.60 | 0.84 |
| 3:B:427:ARG:HH11 | 3:B:650:ILE:HD12 | 1.42 | 0.84 |
| 1:A:331:ASN:O | 1:A:332:ILE:HB | 1.76 | 0.84 |
| 3:B:557:HIS:N | 3:B:623:ASN:HD21 | 1.75 | 0.84 |
| 3:J:595:GLU:HA | 3:J:599:SER:HB3 | 1.59 | 0.84 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:875:VAL:O | 1:A:877:GLY:N | 2.10 | 0.84 |
| 7:G:72:CYS:SG | 7:G:114:ARG:HD3 | 2.17 | 0.84 |
| 3:J:702:LEU:N | 3:J:721:ASN:HD21 | 1.74 | 0.84 |
| 5:E:50:ASN:HB2 | 5:E:73:ASP:OD2 | 1.76 | 0.84 |
| 1:I:426:HIS:CD2 | 1:I:490:ARG:HH12 | 1.96 | 0.84 |
| 1:I:667:ARG:O | 1:I:670:VAL:HG22 | 1.77 | 0.84 |
| 2:C:388:LEU:HD11 | 9:K:34:ARG:HG3 | 1.59 | 0.84 |
| 3:B:764:LYS:HE2 | 3:B:813:LYS:HE2 | 1.60 | 0.84 |
| 1:I:547:THR:O | 1:I:550:GLN:HB3 | 1.78 | 0.84 |
| 2:M:72:ILE:N | 2:M:72:ILE:HD12 | 1.91 | 0.84 |
| 13:Z:57:GLY:HA2 | 13:Z:61:LEU:HG | 1.59 | 0.84 |
| 3:J:702:LEU:CD2 | 3:J:933:ALA:HB1 | 2.07 | 0.83 |
| 1:I:412:ILE:O | 1:I:415:ASP:HB2 | 1.78 | 0.83 |
| 1:I:418:LEU:HD21 | 3:J:1044:LEU:HD21 | 1.60 | 0.83 |
| 1:A:672:VAL:HG13 | 1:A:700:ILE:HD12 | 1.57 | 0.83 |
| 1:I:369:PRO:HB3 | 1:I:376:ASN:HB3 | 1.60 | 0.83 |
| 1:A:647:ARG:HH11 | 3:B:965:ASP:CB | 1.89 | 0.83 |
| 4:O:13:ILE:HD11 | 4:O:238:PRO:HB2 | 1.61 | 0.83 |
| 3:B:253:PHE:H | 3:B:254:PRO:HD2 | 1.42 | 0.83 |
| 3:B:958:LEU:HD12 | 3:B:964:PRO:HG3 | 1.59 | 0.83 |
| 2:M:146:TYR:CD2 | 2:M:233:GLY:O | 2.26 | 0.83 |
| 3:J:90:LEU:HD11 | 3:J:856:ALA:H | 1.43 | 0.83 |
| 1:I:220:ARG:NH1 | 1:I:236:THR:HG23 | 1.93 | 0.83 |
| 3:J:451:GLY:HA3 | 3:J:577:ARG:HH11 | 1.41 | 0.83 |
| 3:B:557:HIS:H | 3:B:623:ASN:HD21 | 1.27 | 0.83 |
| 4:O:209:CYS:SG | 16:O:1001:F3S:FE1 | 1.69 | 0.83 |
| 3:J:544:ARG:HH11 | 3:J:544:ARG:HG3 | 1.42 | 0.83 |
| 1:A:324:THR:HG22 | 1:A:325:VAL:H | 1.43 | 0.83 |
| 1:I:541:ALA:CB | 1:I:542:PRO:CD | 2.57 | 0.83 |
| 3:B:870:ARG:NH1 | 3:B:996:MET:HB2 | 1.93 | 0.82 |
| 1:I:872:PHE:HA | 1:I:876:VAL:HB | 1.61 | 0.82 |
| 5:E:53:THR:HG23 | 5:E:55:GLU:HG3 | 1.60 | 0.82 |
| 4:O:13:ILE:CD1 | 4:O:238:PRO:HB2 | 2.10 | 0.82 |
| 3:B:458:THR:HG21 | 3:B:465:GLY:H | 1.44 | 0.82 |
| 3:B:851:LEU:HA | 12:P:35:PHE:HB3 | 1.59 | 0.82 |
| 3:B:881:ARG:HH11 | 3:B:989:TYR:HB3 | 1.45 | 0.82 |
| 3:B:138:LEU:HA | 3:B:141:ILE:HD12 | 1.59 | 0.82 |
| 3:B:450:TRP:HZ2 | 3:B:641:GLU:OE1 | 1.60 | 0.82 |
| 3:B:702:LEU:N | 3:B:721:ASN:HD21 | 1.77 | 0.82 |
| 3:J:890:MET:HE2 | 3:J:891:LEU:H | 1.44 | 0.82 |
| 1:A:733:ALA:HB1 | 3:B:913:HIS:CE1 | 2.15 | 0.82 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:738:ILE:HD11 | 3:J:908:ILE:HG23 | 1.62 | 0.82 |
| 2:M:390:MET:HG3 | 5:Q:56:GLU:HG2 | 1.60 | 0.82 |
| 3:B:529:TYR:O | 3:B:530:TYR:HB3 | 1.79 | 0.81 |
| 5:E:15:PRO:HG2 | 9:K:45:MET:HB3 | 1.60 | 0.81 |
| 9:K:71:ARG:O | 9:K:73:VAL:HG13 | 1.80 | 0.81 |
| 3:B:203:GLU:HA | 3:B:203:GLU:OE1 | 1.76 | 0.81 |
| 1:I:90:ILE:HD11 | 1:I:207:MET:HB2 | 1.61 | 0.81 |
| 3:J:800:PRO:O | 3:J:802:VAL:N | 2.14 | 0.81 |
| 1:A:412:ILE:O | 1:A:415:ASP:HB2 | 1.80 | 0.81 |
| 9:K:28:THR:OG1 | 9:K:31:GLU:HG3 | 1.79 | 0.81 |
| 1:A:220:ARG:NH1 | 1:A:236:THR:HG23 | 1.94 | 0.81 |
| 1:A:491:TYR:HB2 | 1:A:607:GLN:OE1 | 1.81 | 0.81 |
| 1:A:760:GLY:HA3 | 3:B:447:GLY:CA | 2.10 | 0.81 |
| 5:E:36:GLU:HG2 | 6:F:34:LEU:CD1 | 2.10 | 0.81 |
| 5:Q:97:ILE:HD12 | 5:Q:113:ILE:HD11 | 1.62 | 0.81 |
| 2:C:55:ALA:HA | 2:C:58:GLU:CB | 2.09 | 0.81 |
| 3:J:579:LEU:HD12 | 3:J:616:LEU:CD1 | 2.10 | 0.81 |
| 2:M:170:ASP:O | 2:M:174:LEU:HD11 | 1.81 | 0.81 |
| 3:J:569:ASN:HB3 | 3:J:574:ARG:NH2 | 1.95 | 0.81 |
| 3:J:935:LEU:HD12 | 3:J:957:ILE:HG22 | 1.63 | 0.81 |
| 2:M:329:ILE:HA | 2:M:334:VAL:HG12 | 1.60 | 0.81 |
| 5:Q:15:PRO:HG2 | 9:U:45:MET:HB3 | 1.63 | 0.81 |
| 5:E:39:LEU:HD13 | 5:E:42:LEU:H | 1.46 | 0.81 |
| 3:J:138:LEU:HA | 3:J:141:ILE:HD12 | 1.62 | 0.81 |
| 2:C:179:VAL:HG21 | 2:C:232:LYS:HZ2 | 1.44 | 0.81 |
| 2:M:48:ILE:HG12 | 2:M:50:LYS:HE3 | 1.63 | 0.81 |
| 6:F:35:GLN:HA | 6:F:38:TYR:CD1 | 2.16 | 0.80 |
| 3:J:771:ASP:HB2 | 3:J:816:PRO:HD3 | 1.63 | 0.80 |
| 4:D:13:ILE:HD11 | 4:D:238:PRO:HB2 | 1.64 | 0.80 |
| 1:I:79:ARG:HB2 | 1:I:266:TRP:CE3 | 2.17 | 0.80 |
| 3:J:253:PHE:H | 3:J:254:PRO:HD2 | 1.47 | 0.80 |
| 3:J:458:THR:CG2 | 3:J:465:GLY:H | 1.95 | 0.80 |
| 1:I:336:GLU:HA | 1:I:434:ARG:O | 1.82 | 0.80 |
| 2:M:114:LYS:O | 2:M:116:VAL:N | 2.13 | 0.80 |
| 3:B:687:ARG:CG | 3:B:687:ARG:HH11 | 1.94 | 0.80 |
| 3:J:910:LEU:HD22 | 3:J:911:ASN:N | 1.97 | 0.80 |
| 1:I:853:ASP:OD2 | 1:I:864:LYS:HB3 | 1.82 | 0.80 |
| 3:J:813:LYS:H | 3:J:836:SER:HB3 | 1.45 | 0.80 |
| 1:A:647:ARG:HH21 | 3:B:982:ARG:HH12 | 1.26 | 0.80 |
| 3:B:90:LEU:HD11 | 3:B:856:ALA:H | 1.47 | 0.80 |
| 2:C:55:ALA:HA | 2:C:58:GLU:HB2 | 1.64 | 0.80 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:29:ARG:HG3 | 4:D:162:SER:HB3 | 1.63 | 0.80 |
| 4:O:259:LYS:O | 4:O:263:VAL:HG23 | 1.82 | 0.80 |
| 5:E:89:VAL:HG11 | 5:E:92:VAL:HG22 | 1.64 | 0.79 |
| 1:A:547:THR:O | 1:A:550:GLN:HB3 | 1.83 | 0.79 |
| 1:A:733:ALA:HB1 | 3:B:913:HIS:HE1 | 1.47 | 0.79 |
| 1:A:549:LYS:HE2 | 7:G:89:GLY:HA2 | 1.64 | 0.79 |
| 8:H:29:TYR:HA | 8:H:32:LEU:HD12 | 1.61 | 0.79 |
| 1:I:331:ASN:O | 1:I:332:ILE:CB | 2.30 | 0.79 |
| 3:J:450:TRP:CZ2 | 3:J:641:GLU:OE1 | 2.36 | 0.79 |
| 1:A:426:HIS:CD2 | 1:A:490:ARG:HH12 | 1.99 | 0.79 |
| 5:E:87:GLY:O | 5:E:88:GLU:HB2 | 1.81 | 0.79 |
| 6:R:35:GLN:HA | 6:R:38:TYR:CD1 | 2.17 | 0.79 |
| 3:B:539:LYS:O | 3:B:543:ARG:HG3 | 1.83 | 0.79 |
| 3:J:773:ILE:HG12 | 3:J:813:LYS:HG2 | 1.64 | 0.79 |
| 3:J:665:ARG:HG3 | 3:J:920:THR:CG2 | 2.13 | 0.79 |
| 2:M:110:ILE:HD11 | 2:M:277:ILE:HD11 | 1.64 | 0.79 |
| 2:M:61:GLU:O | 2:M:64:ILE:HD12 | 1.83 | 0.79 |
| 3:J:183:ILE:HG12 | 3:J:206:LYS:HB3 | 1.65 | 0.79 |
| 3:J:203:GLU:HA | 3:J:203:GLU:OE1 | 1.82 | 0.79 |
| 1:A:79:ARG:HB2 | 1:A:266:TRP:CE3 | 2.17 | 0.79 |
| 4:D:109:ILE:HD11 | 4:D:133:LEU:HD12 | 1.65 | 0.79 |
| 1:I:491:TYR:HB2 | 1:I:607:GLN:OE1 | 1.83 | 0.79 |
| 9:U:91:SER:O | 9:U:92:LEU:HB2 | 1.82 | 0.79 |
| 8:H:29:TYR:HH | 13:Y:67:LEU:HD22 | 1.48 | 0.79 |
| 1:I:134:GLU:HA | 1:I:137:LYS:HD2 | 1.64 | 0.78 |
| 1:I:353:ILE:HG13 | 1:I:361:LEU:HD23 | 1.65 | 0.78 |
| 1:A:206:TRP:O | 1:A:208:ILE:N | 2.16 | 0.78 |
| 1:A:525:LEU:HD11 | 1:A:530:VAL:HG11 | 1.65 | 0.78 |
| 1:A:61:CYS:SG | 3:B:1070:TYR:HB3 | 2.23 | 0.78 |
| 3:B:702:LEU:CD2 | 3:B:933:ALA:HB1 | 2.12 | 0.78 |
| 1:I:541:ALA:HB2 | 7:S:72:CYS:H | 1.46 | 0.78 |
| 7:G:72:CYS:SG | 7:G:114:ARG:HB3 | 2.22 | 0.78 |
| 1:A:58:CYS:HB2 | 1:A:59:PRO:HD3 | 1.64 | 0.78 |
| 3:J:497:VAL:HG23 | 3:J:528:GLY:HA2 | 1.63 | 0.78 |
| 3:B:850:VAL:O | 12:P:35:PHE:HB2 | 1.84 | 0.78 |
| 1:I:313:LEU:HB3 | 2:M:374:ILE:HG13 | 1.65 | 0.78 |
| 8:T:39:PRO:HB2 | 8:T:80:TYR:HE2 | 1.48 | 0.78 |
| 1:A:353:ILE:HG13 | 1:A:361:LEU:HD23 | 1.64 | 0.78 |
| 1:I:853:ASP:HB2 | 2:M:311:ARG:HH12 | 1.49 | 0.78 |
| 1:A:853:ASP:OD2 | 1:A:864:LYS:HB3 | 1.83 | 0.78 |
| 2:C:70:ILE:HA | 2:C:73:VAL:HG22 | 1.64 | 0.78 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:541:ALA:CB | 7:G:72:CYS:H | 1.96 | 0.78 |
| 1:I:721:PRO:HA | 1:I:726:TYR:HD1 | 1.49 | 0.78 |
| 4:D:13:ILE:CD1 | 4:D:238:PRO:HB2 | 2.13 | 0.78 |
| 1:I:324:THR:HG22 | 1:I:325:VAL:H | 1.47 | 0.78 |
| 3:J:557:HIS:N | 3:J:623:ASN:HD21 | 1.82 | 0.78 |
| 7:S:63:ARG:HG3 | 7:S:114:ARG:NH2 | 1.99 | 0.78 |
| 3:B:38:LYS:HG3 | 3:B:39:LEU:N | 1.98 | 0.77 |
| 2:C:173:MET:HA | 2:C:176:ASP:HB2 | 1.65 | 0.77 |
| 2:C:41:ILE:HB | 2:C:42:ILE:HD12 | 1.64 | 0.77 |
| 7:G:55:VAL:HG23 | 7:G:116:SER:O | 1.84 | 0.77 |
| 3:J:554:ASN:HD21 | 3:J:576:ARG:HH21 | 1.32 | 0.77 |
| 3:J:451:GLY:H | 3:J:647:ILE:HG23 | 1.47 | 0.77 |
| 1:A:301:ARG:O | 1:A:302:LEU:HG | 1.84 | 0.77 |
| 1:A:507:TYR:O | 1:A:508:LEU:HB2 | 1.83 | 0.77 |
| 2:C:391:ARG:NH2 | 9:K:42:GLN:HG2 | 1.98 | 0.77 |
| 2:M:168:GLN:HA | 2:M:204:SER:HA | 1.67 | 0.77 |
| 2:M:345:ALA:HB1 | 2:M:350:THR:HG23 | 1.66 | 0.77 |
| 8:T:24:ASN:O | 8:T:27:GLU:HG2 | 1.84 | 0.77 |
| 1:A:530:VAL:O | 1:A:532:ILE:HG12 | 1.84 | 0.77 |
| 3:B:771:ASP:HB2 | 3:B:816:PRO:HD3 | 1.64 | 0.77 |
| 3:J:853:THR:HG22 | 3:J:854:GLU:H | 1.48 | 0.77 |
| 1:I:647:ARG:HH21 | 3:J:982:ARG:HH12 | 1.33 | 0.77 |
| 3:J:317:TYR:CD2 | 3:J:526:LEU:HD13 | 2.20 | 0.77 |
| 9:K:90:LEU:CD2 | 9:K:90:LEU:H | 1.89 | 0.77 |
| 3:B:935:LEU:HD12 | 3:B:957:ILE:HG22 | 1.66 | 0.77 |
| 1:I:823:LEU:HB3 | 2:M:329:ILE:HD13 | 1.66 | 0.77 |
| 1:A:667:ARG:O | 1:A:670:VAL:HG22 | 1.85 | 0.77 |
| 3:B:962:TYR:OH | 11:N:42:ARG:HD2 | 1.83 | 0.77 |
| 2:C:63:LEU:HD23 | 2:C:63:LEU:O | 1.84 | 0.77 |
| 3:B:1064:CYS:SG | 14:B:2001:ZN:ZN | 1.74 | 0.77 |
| 8:H:25:ILE:HD11 | 8:H:61:ASP:OD1 | 1.85 | 0.77 |
| 1:A:447:LEU:HD13 | 3:B:734:MET:SD | 2.25 | 0.77 |
| 3:B:853:THR:HG22 | 3:B:854:GLU:H | 1.49 | 0.77 |
| 10:V:40:PHE:HB3 | 10:V:58:LEU:HB3 | 1.66 | 0.77 |
| 1:A:336:GLU:HA | 1:A:434:ARG:O | 1.85 | 0.77 |
| 3:B:813:LYS:H | 3:B:836:SER:HB3 | 1.49 | 0.77 |
| 2:C:391:ARG:H | 2:C:392:PRO:HD3 | 1.49 | 0.77 |
| 1:I:378:VAL:O | 1:I:378:VAL:HG22 | 1.85 | 0.77 |
| 3:J:88:ARG:NH1 | 3:J:854:GLU:O | 2.18 | 0.77 |
| 12:X:17:GLN:HB3 | 12:X:19:LYS:HG3 | 1.64 | 0.77 |
| 2:C:329:ILE:HA | 2:C:334:VAL:CG1 | 2.15 | 0.76 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:812:ARG:HE | 2:C:86:THR:HG23 | 1.48 | 0.76 |
| 3:J:758:TYR:O | 3:J:759:SER:HB3 | 1.83 | 0.76 |
| 4:O:29:ARG:HG3 | 4:O:162:SER:HB3 | 1.68 | 0.76 |
| 1:A:697:GLU:OE1 | 1:A:756:ARG:HD3 | 1.85 | 0.76 |
| 1:I:841:LEU:O | 1:I:843:GLY:N | 2.18 | 0.76 |
| 3:J:473:MET:SD | 3:J:474:ALA:N | 2.58 | 0.76 |
| 1:I:308:ARG:HH21 | 3:J:1099:LEU:CD1 | 1.97 | 0.76 |
| 3:J:911:ASN:HD22 | 3:J:913:HIS:H | 1.33 | 0.76 |
| 1:A:134:GLU:HA | 1:A:137:LYS:HD2 | 1.67 | 0.76 |
| 3:B:630:PRO:O | 3:B:633:LEU:HB3 | 1.84 | 0.76 |
| 1:I:58:CYS:HB2 | 1:I:59:PRO:HD3 | 1.66 | 0.76 |
| 3:J:640:LEU:CD2 | 3:J:641:GLU:H | 1.98 | 0.76 |
| 1:I:760:GLY:CA | 3:J:447:GLY:HA3 | 2.04 | 0.76 |
| 1:I:507:TYR:O | 1:I:508:LEU:HB2 | 1.84 | 0.76 |
| 1:I:530:VAL:O | 1:I:532:ILE:HG12 | 1.86 | 0.76 |
| 3:J:992:LYS:HE3 | 3:J:996:MET:SD | 2.25 | 0.76 |
| 2:M:35:LEU:O | 2:M:39:LYS:HE3 | 1.85 | 0.76 |
| 4:O:44:VAL:HA | 4:O:143:ALA:HA | 1.67 | 0.76 |
| 3:J:870:ARG:NH1 | 3:J:996:MET:HB2 | 2.00 | 0.76 |
| 1:A:595:GLU:CB | 7:G:91:LYS:HE2 | 2.15 | 0.76 |
| 3:J:249:GLN:HG3 | 3:J:250:ASN:H | 1.50 | 0.76 |
| 8:H:29:TYR:O | 8:H:33:LYS:HG3 | 1.86 | 0.76 |
| 3:J:569:ASN:CB | 3:J:574:ARG:HH22 | 1.98 | 0.76 |
| 3:J:922:GLY:HA2 | 3:J:925:MET:CB | 2.13 | 0.76 |
| 12:P:26:CYS:HB2 | 12:P:27:PRO:CD | 2.14 | 0.76 |
| 9:K:92:LEU:O | 9:K:92:LEU:HD23 | 1.86 | 0.75 |
| 2:M:179:VAL:HG11 | 2:M:232:LYS:HZ2 | 1.50 | 0.75 |
| 3:J:873:THR:HG22 | 3:J:874:ILE:N | 2.01 | 0.75 |
| 10:L:13:LEU:HB3 | 10:L:57:ILE:HD12 | 1.68 | 0.75 |
| 3:B:588:LEU:HD13 | 3:B:612:LYS:HB3 | 1.67 | 0.75 |
| 3:B:730:THR:HB | 3:B:732:TYR:HD1 | 1.51 | 0.75 |
| 7:G:109:LYS:HZ3 | 3:J:378:LYS:HE3 | 1.51 | 0.75 |
| 3:J:650:ILE:N | 3:J:650:ILE:HD13 | 2.01 | 0.75 |
| 2:M:115:LYS:HD3 | 2:M:278:ARG:HB3 | 1.68 | 0.75 |
| 2:M:60:SER:O | 2:M:63:LEU:HB3 | 1.87 | 0.75 |
| 3:B:317:TYR:CD2 | 3:B:526:LEU:HD13 | 2.22 | 0.75 |
| 1:A:742:GLN:HB2 | 3:B:919:MET:HE3 | 1.69 | 0.75 |
| 1:I:541:ALA:CB | 7:S:72:CYS:H | 1.98 | 0.75 |
| 10:V:59:THR:HG21 | 10:V:65:PRO:HD3 | 1.68 | 0.75 |
| 1:A:130:ARG:HB3 | 1:A:195:LEU:O | 1.87 | 0.75 |
| 1:A:15:SER:HA | 1:A:203:ARG:HH22 | 1.51 | 0.75 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:293:ARG:HH11 | 1:A:296:ARG:NH2 | 1.85 | 0.75 |
| 1:A:308:ARG:HH21 | 3:B:1099:LEU:CD1 | 1.94 | 0.75 |
| 3:B:650:ILE:H | 3:B:650:ILE:CD1 | 2.00 | 0.75 |
| 3:B:773:ILE:HG12 | 3:B:813:LYS:HG2 | 1.69 | 0.75 |
| 2:C:377:HIS:ND1 | 2:C:378:PRO:HD2 | 2.02 | 0.75 |
| 1:I:220:ARG:HH11 | 1:I:236:THR:HG23 | 1.50 | 0.75 |
| 2:M:146:TYR:CE2 | 2:M:235:LYS:HB2 | 2.22 | 0.75 |
| 1:I:326:ILE:HG21 | 1:I:462:MET:HG3 | 1.69 | 0.75 |
| 1:I:324:THR:HG22 | 1:I:325:VAL:N | 2.02 | 0.75 |
| 3:J:539:LYS:O | 3:J:543:ARG:HG3 | 1.87 | 0.75 |
| 3:J:874:ILE:HD12 | 3:J:874:ILE:H | 1.52 | 0.75 |
| 1:A:525:LEU:HD12 | 10:L:56:LYS:HE3 | 1.69 | 0.74 |
| 1:I:234:ASP:OD2 | 1:I:296:ARG:HD3 | 1.85 | 0.74 |
| 3:J:38:LYS:HG3 | 3:J:39:LEU:N | 2.01 | 0.74 |
| 3:B:249:GLN:HG3 | 3:B:250:ASN:H | 1.50 | 0.74 |
| 3:J:427:ARG:HH11 | 3:J:650:ILE:HD12 | 1.53 | 0.74 |
| 3:B:851:LEU:HD12 | 12:P:35:PHE:HD2 | 1.50 | 0.74 |
| 1:A:525:LEU:CD1 | 1:A:530:VAL:HG11 | 2.17 | 0.74 |
| 3:B:591:ILE:HG12 | 3:B:612:LYS:NZ | 2.02 | 0.74 |
| 3:B:800:PRO:O | 3:B:802:VAL:N | 2.20 | 0.74 |
| 3:B:870:ARG:CZ | 3:B:996:MET:SD | 2.75 | 0.74 |
| 2:C:389:THR:HG21 | 9:K:79:ARG:HH11 | 1.52 | 0.74 |
| 1:A:833:GLU:OE2 | 1:A:839:ARG:HB2 | 1.88 | 0.74 |
| 3:B:874:ILE:H | 3:B:874:ILE:HD12 | 1.53 | 0.74 |
| 1:A:632:PHE:HA | 1:A:635:PHE:CD1 | 2.22 | 0.74 |
| 3:B:763:VAL:HG22 | 3:B:770:GLU:HG3 | 1.68 | 0.74 |
| 2:M:30:ASP:O | 2:M:31:ASP:HB3 | 1.87 | 0.74 |
| 10:V:3:ILE:CG2 | 10:V:15:LEU:HD21 | 2.17 | 0.74 |
| 7:G:80:GLU:HG2 | 7:G:81:LEU:H | 1.52 | 0.74 |
| 3:J:972:ASP:OD2 | 3:J:974:ARG:HG2 | 1.87 | 0.74 |
| 1:A:490:ARG:HA | 2:C:312:HIS:HE1 | 1.51 | 0.74 |
| 1:I:206:TRP:O | 1:I:208:ILE:N | 2.20 | 0.74 |
| 3:J:581:ILE:CD1 | 3:J:614:GLU:HB2 | 2.01 | 0.74 |
| 3:J:557:HIS:H | 3:J:623:ASN:HD21 | 1.35 | 0.74 |
| 3:B:1000:LYS:O | 3:B:1001:LEU:HB2 | 1.86 | 0.74 |
| 1:I:470:GLU:O | 1:I:473:ILE:HG12 | 1.88 | 0.74 |
| 2:C:60:SER:O | 2:C:63:LEU:N | 2.20 | 0.74 |
| 1:A:324:THR:HG22 | 1:A:325:VAL:N | 2.02 | 0.74 |
| 3:B:738:ILE:HD11 | 3:B:908:ILE:HG23 | 1.70 | 0.74 |
| 2:C:55:ALA:O | 2:C:58:GLU:HB2 | 1.88 | 0.74 |
| 1:A:594:LEU:HA | 7:G:86:LEU:HD22 | 1.69 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:Q:84:VAL:HG21 | 6:R:86:ILE:HG12 | 1.70 | 0.73 |
| 8:T:65:ILE:HD11 | 8:T:79:ARG:HG2 | 1.68 | 0.73 |
| 3:B:1054:ASP:HB3 | 3:B:1095:TYR:H | 1.53 | 0.73 |
| 3:J:473:MET:SD | 3:J:475:GLN:N | 2.61 | 0.73 |
| 1:I:499:ALA:HB3 | 3:J:734:MET:CE | 2.18 | 0.73 |
| 2:M:70:ILE:CD1 | 2:M:70:ILE:N | 2.49 | 0.73 |
| 1:I:331:ASN:HD22 | 10:V:47:HIS:HB2 | 1.53 | 0.73 |
| 1:A:256:GLY:O | 1:A:258:PRO:HD3 | 1.88 | 0.73 |
| 1:A:541:ALA:HB2 | 7:G:72:CYS:N | 2.04 | 0.73 |
| 3:J:763:VAL:HG22 | 3:J:770:GLU:HG3 | 1.69 | 0.73 |
| 2:M:103:GLY:C | 2:M:105:PRO:HD2 | 2.09 | 0.73 |
| 8:T:29:TYR:HA | 8:T:32:LEU:HD12 | 1.70 | 0.73 |
| 1:A:721:PRO:HA | 1:A:726:TYR:HD1 | 1.51 | 0.73 |
| 3:B:451:GLY:H | 3:B:647:ILE:HG23 | 1.53 | 0.73 |
| 1:I:567:ASN:N | 1:I:599:ASP:OD2 | 2.22 | 0.73 |
| 3:J:687:ARG:HH11 | 3:J:687:ARG:CG | 2.00 | 0.73 |
| 3:J:708:LEU:HD13 | 3:J:713:TYR:HB3 | 1.69 | 0.73 |
| 7:G:30:ASN:O | 7:G:31:MET:HG3 | 1.87 | 0.73 |
| 1:A:98:CYS:HA | 1:A:146:CYS:SG | 2.28 | 0.73 |
| 3:B:700:ARG:O | 11:N:51:SER:HB2 | 1.88 | 0.73 |
| 1:A:859:TYR:HB2 | 2:C:64:ILE:HG12 | 1.71 | 0.73 |
| 3:J:461:GLY:O | 3:J:464:SER:HB3 | 1.89 | 0.73 |
| 2:M:70:ILE:HD12 | 2:M:70:ILE:H | 1.52 | 0.73 |
| 3:B:911:ASN:HD22 | 3:B:913:HIS:H | 1.36 | 0.73 |
| 3:J:345:LEU:HD11 | 3:J:476:ILE:HG13 | 1.69 | 0.73 |
| 11:N:7:CYS:SG | 11:N:48:MET:HG3 | 2.29 | 0.73 |
| 3:J:700:ARG:O | 11:W:51:SER:HB2 | 1.89 | 0.73 |
| 7:G:83:ASP:O | 7:G:93:THR:HA | 1.89 | 0.73 |
| 1:I:245:ILE:HD13 | 1:I:268:LEU:HB3 | 1.71 | 0.73 |
| 3:B:353:LEU:HA | 3:B:404:VAL:CG1 | 2.11 | 0.73 |
| 1:A:846:VAL:HA | 2:C:322:ARG:HE | 1.54 | 0.73 |
| 5:E:179:LYS:HE2 | 6:F:81:ASP:HB2 | 1.70 | 0.73 |
| 1:I:50:GLY:HA2 | 1:I:68:CYS:SG | 2.29 | 0.73 |
| 1:I:828:SER:C | 1:I:830:LEU:H | 1.93 | 0.73 |
| 3:B:210:PHE:HZ | 3:B:323:ILE:HG22 | 1.54 | 0.72 |
| 1:I:301:ARG:O | 1:I:302:LEU:HG | 1.89 | 0.72 |
| 3:J:1067:ILE:HG13 | 3:J:1068:GLY:N | 2.03 | 0.72 |
| 3:J:726:VAL:HG12 | 3:J:912:PRO:HG3 | 1.69 | 0.72 |
| 9:U:50:LEU:HD22 | 9:U:75:PRO:HD3 | 1.71 | 0.72 |
| 1:I:15:SER:HA | 1:I:203:ARG:HH22 | 1.54 | 0.72 |
| 3:J:353:LEU:HA | 3:J:404:VAL:CG1 | 2.10 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:63:LEU:HD12 | 9:U:22:LEU:HD22 | 1.71 | 0.72 |
| 1:A:721:PRO:HA | 1:A:726:TYR:CD1 | 2.24 | 0.72 |
| 2:C:322:ARG:N | 2:C:322:ARG:HH11 | 1.88 | 0.72 |
| 3:J:1047:ASP:HA | 3:J:1051:ASP:HB2 | 1.71 | 0.72 |
| 3:J:161:ILE:HG21 | 3:J:346:ALA:HA | 1.71 | 0.72 |
| 3:B:687:ARG:NH1 | 3:B:687:ARG:HG3 | 2.04 | 0.72 |
| 3:B:88:ARG:NH1 | 3:B:854:GLU:O | 2.22 | 0.72 |
| 3:B:665:ARG:HG3 | 3:B:920:THR:CG2 | 2.19 | 0.72 |
| 1:I:632:PHE:HA | 1:I:635:PHE:HD1 | 1.53 | 0.72 |
| 1:A:90:ILE:HD11 | 1:A:207:MET:HB2 | 1.70 | 0.72 |
| 1:A:220:ARG:HH11 | 1:A:236:THR:HG23 | 1.53 | 0.72 |
| 1:A:507:TYR:HB3 | 1:A:597:VAL:HG13 | 1.71 | 0.72 |
| 3:B:758:TYR:O | 3:B:759:SER:HB3 | 1.88 | 0.72 |
| 2:M:70:ILE:HD13 | 2:M:70:ILE:N | 2.03 | 0.72 |
| 8:T:30:LYS:O | 8:T:33:LYS:HB2 | 1.90 | 0.72 |
| 7:S:7:GLN:HG2 | 7:S:8:GLU:N | 2.04 | 0.72 |
| 5:E:53:THR:HB | 5:E:71:GLU:H | 1.55 | 0.72 |
| 3:J:458:THR:HG21 | 3:J:465:GLY:N | 2.04 | 0.72 |
| 2:M:179:VAL:HG11 | 2:M:232:LYS:NZ | 2.04 | 0.72 |
| 3:B:902:LYS:HB3 | 11:N:42:ARG:HD3 | 1.69 | 0.72 |
| 5:Q:84:VAL:HG22 | 5:Q:145:ARG:HH11 | 1.54 | 0.72 |
| 3:J:805:LYS:HG3 | 3:J:844:MET:HB2 | 1.71 | 0.72 |
| 4:O:11:THR:O | 4:O:238:PRO:HB3 | 1.90 | 0.72 |
| 3:B:890:MET:HE2 | 3:B:891:LEU:H | 1.55 | 0.72 |
| 2:C:237:ILE:HG22 | 2:C:257:ASN:HB2 | 1.72 | 0.72 |
| 2:C:343:ALA:HB2 | 2:C:371:GLU:HG3 | 1.71 | 0.72 |
| 2:C:55:ALA:CA | 2:C:58:GLU:HG3 | 2.19 | 0.72 |
| 5:E:26:ALA:O | 5:E:30:LEU:HB2 | 1.89 | 0.72 |
| 7:G:63:ARG:HG3 | 7:G:114:ARG:HH22 | 1.55 | 0.72 |
| 1:A:558:LYS:HZ3 | 3:J:108:GLU:HG2 | 1.53 | 0.72 |
| 3:B:522:LEU:O | 3:B:525:ARG:HB3 | 1.90 | 0.71 |
| 3:J:873:THR:CG2 | 3:J:874:ILE:N | 2.53 | 0.71 |
| 2:M:179:VAL:HG23 | 2:M:182:ASP:H | 1.55 | 0.71 |
| 1:I:525:LEU:CD1 | 1:I:530:VAL:HG11 | 2.20 | 0.71 |
| 7:S:30:ASN:HA | 7:S:39:SER:HB3 | 1.73 | 0.71 |
| 2:M:391:ARG:NH2 | 9:U:39:ARG:HH11 | 1.88 | 0.71 |
| 4:O:254:GLU:HG2 | 10:V:77:ARG:HH12 | 1.54 | 0.71 |
| 1:A:567:ASN:N | 1:A:599:ASP:OD2 | 2.21 | 0.71 |
| 1:A:502:TYR:CE1 | 1:A:636:ILE:HD11 | 2.24 | 0.71 |
| 3:J:890:MET:HA | 3:J:890:MET:HE3 | 1.72 | 0.71 |
| 2:M:391:ARG:HH22 | 9:U:39:ARG:HD2 | 1.55 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:B:690:THR:HG22 | 3:B:691:ARG:HG3 | 1.71 | 0.71 |
| 1:I:90:ILE:HD11 | 1:I:207:MET:CB | 2.20 | 0.71 |
| 1:I:220:ARG:HA | 1:I:233:ASP:OD1 | 1.91 | 0.71 |
| 1:A:590:ASN:ND2 | 3:J:377:ARG:CB | 2.53 | 0.71 |
| 1:A:446:ASN:ND2 | 1:A:448:LEU:H | 1.89 | 0.71 |
| 3:J:730:THR:HB | 3:J:732:TYR:HD1 | 1.55 | 0.71 |
| 9:K:60:ASP:O | 9:K:61:VAL:O | 2.08 | 0.71 |
| 5:Q:64:GLY:H | 9:U:41:LEU:HD22 | 1.55 | 0.71 |
| 3:B:1070:TYR:O | 3:B:1071:ASP:O | 2.08 | 0.71 |
| 1:I:666:ASP:O | 1:I:670:VAL:HG13 | 1.91 | 0.71 |
| 3:J:739:ILE:CG2 | 3:J:909:ILE:HB | 2.21 | 0.71 |
| 3:J:803:GLU:HB3 | 3:J:805:LYS:NZ | 2.05 | 0.71 |
| 5:Q:135:VAL:H | 5:Q:174:TRP:HZ2 | 1.36 | 0.71 |
| 10:V:4:ARG:HG2 | 10:V:4:ARG:HH11 | 1.56 | 0.71 |
| 1:A:853:ASP:HB2 | 2:C:311:ARG:NH1 | 2.05 | 0.71 |
| 1:A:846:VAL:O | 2:C:322:ARG:NH2 | 2.23 | 0.71 |
| 2:C:327:ARG:HG3 | 2:C:334:VAL:HB | 1.71 | 0.71 |
| 1:I:106:ILE:HG22 | 1:I:107:SER:H | 1.56 | 0.71 |
| 1:I:155:LYS:H | 1:I:155:LYS:HZ1 | 1.37 | 0.71 |
| 2:M:54:LEU:O | 2:M:58:GLU:HG3 | 1.90 | 0.71 |
| 12:X:46:LYS:N | 12:X:46:LYS:HD2 | 2.06 | 0.71 |
| 1:A:446:ASN:HD22 | 1:A:446:ASN:C | 1.94 | 0.71 |
| 1:A:468:GLN:HG3 | 3:B:1052:ASN:HD21 | 1.54 | 0.71 |
| 3:B:805:LYS:HG3 | 3:B:844:MET:HB2 | 1.71 | 0.71 |
| 1:I:595:GLU:CB | 7:S:91:LYS:HE2 | 2.21 | 0.71 |
| 2:M:69:ALA:HB2 | 2:M:381:LEU:HD13 | 1.72 | 0.71 |
| 1:A:234:ASP:OD2 | 1:A:296:ARG:HD3 | 1.91 | 0.71 |
| 3:B:554:ASN:HD21 | 3:B:576:ARG:HH21 | 1.39 | 0.71 |
| 2:C:354:LEU:HD13 | 3:B:1104:LEU:HD21 | 1.73 | 0.71 |
| 1:I:697:GLU:OE1 | 1:I:756:ARG:HD3 | 1.91 | 0.71 |
| 1:A:532:ILE:CD1 | 10:L:56:LYS:HD3 | 2.20 | 0.71 |
| 12:P:17:GLN:HB3 | 12:P:19:LYS:HG3 | 1.73 | 0.71 |
| 1:A:331:ASN:O | 1:A:332:ILE:CB | 2.39 | 0.70 |
| 8:H:46:ARG:HH22 | 13:Y:78:ARG:HH11 | 1.39 | 0.70 |
| 1:I:238:LYS:HD3 | 1:I:276:TYR:HA | 1.73 | 0.70 |
| 8:T:39:PRO:HB2 | 8:T:80:TYR:CE2 | 2.25 | 0.70 |
| 1:A:828:SER:C | 1:A:830:LEU:H | 1.94 | 0.70 |
| 3:B:183:ILE:HB | 3:B:207:ASP:C | 2.11 | 0.70 |
| 7:G:87:ASN:C | 7:G:89:GLY:H | 1.93 | 0.70 |
| 3:J:1000:LYS:O | 3:J:1001:LEU:HB2 | 1.90 | 0.70 |
| 5:E:179:LYS:CE | 6:F:81:ASP:HB2 | 2.21 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:Z:57:GLY:CA | 13:Z:61:LEU:HG | 2.21 | 0.70 |
| 3:B:28:LEU:HG | 3:B:122:MET:HE1 | 1.72 | 0.70 |
| 3:B:458:THR:CG2 | 3:B:465:GLY:H | 2.03 | 0.70 |
| 8:H:29:TYR:OH | 13:Y:67:LEU:CD2 | 2.25 | 0.70 |
| 1:I:589:LYS:HG2 | 1:I:877:GLY:HA2 | 1.73 | 0.70 |
| 3:J:724:LEU:HD12 | 3:J:908:ILE:HG22 | 1.73 | 0.70 |
| 2:M:301:LEU:HA | 2:M:304:GLN:HG3 | 1.71 | 0.70 |
| 9:U:90:LEU:N | 9:U:90:LEU:HD23 | 2.07 | 0.70 |
| 1:A:828:SER:O | 1:A:830:LEU:N | 2.22 | 0.70 |
| 3:B:1004:ARG:HH11 | 3:B:1025:GLY:H | 1.39 | 0.70 |
| 1:I:604:GLY:C | 1:I:606:GLN:H | 1.93 | 0.70 |
| 1:I:742:GLN:HB3 | 3:J:919:MET:HE1 | 1.73 | 0.70 |
| 3:J:1070:TYR:O | 3:J:1071:ASP:O | 2.09 | 0.70 |
| 3:B:1067:ILE:HG13 | 3:B:1068:GLY:N | 2.07 | 0.70 |
| 1:I:525:LEU:HD11 | 1:I:530:VAL:HG11 | 1.71 | 0.70 |
| 1:I:704:LEU:HD22 | 1:I:781:PHE:CE1 | 2.26 | 0.70 |
| 3:J:1095:TYR:CE1 | 3:J:1098:LYS:HD2 | 2.26 | 0.70 |
| 10:L:24:LEU:O | 10:L:28:ILE:HG12 | 1.90 | 0.70 |
| 2:M:377:HIS:ND1 | 2:M:378:PRO:HD2 | 2.07 | 0.70 |
| 12:P:46:LYS:HD2 | 12:P:46:LYS:N | 2.04 | 0.70 |
| 7:S:72:CYS:SG | 7:S:114:ARG:HB3 | 2.31 | 0.70 |
| 1:A:604:GLY:C | 1:A:606:GLN:H | 1.93 | 0.70 |
| 1:I:316:LYS:HE2 | 3:J:1054:ASP:OD2 | 1.91 | 0.70 |
| 1:I:733:ALA:HB1 | 3:J:913:HIS:CE1 | 2.27 | 0.70 |
| 2:M:277:ILE:O | 2:M:279:GLU:N | 2.24 | 0.70 |
| 1:I:827:LEU:HD11 | 2:M:315:LEU:HD13 | 1.73 | 0.70 |
| 1:A:50:GLY:HA2 | 1:A:68:CYS:SG | 2.31 | 0.70 |
| 2:C:276:ASN:HD22 | 2:C:279:GLU:CB | 2.05 | 0.70 |
| 9:K:23:TRP:CE3 | 9:K:23:TRP:HA | 2.27 | 0.70 |
| 1:I:9:ILE:O | 2:M:363:VAL:O | 2.10 | 0.70 |
| 3:B:848:ASP:HB2 | 3:B:867:ARG:H | 1.55 | 0.70 |
| 1:I:594:LEU:CA | 7:S:86:LEU:HD22 | 2.21 | 0.70 |
| 1:I:468:GLN:HG3 | 3:J:1052:ASN:HD21 | 1.56 | 0.70 |
| 3:J:210:PHE:HZ | 3:J:323:ILE:HG22 | 1.56 | 0.70 |
| 5:Q:18:PHE:CE2 | 9:U:42:GLN:HG2 | 2.27 | 0.70 |
| 2:C:269:VAL:HA | 2:C:272:VAL:HG23 | 1.74 | 0.69 |
| 7:G:109:LYS:NZ | 3:J:378:LYS:HE3 | 2.07 | 0.69 |
| 1:I:541:ALA:HB1 | 7:S:71:PHE:HA | 1.73 | 0.69 |
| 11:W:22:ILE:HD13 | 11:W:23:THR:H | 1.56 | 0.69 |
| 1:A:99:ARG:HD2 | 1:A:150:ASN:H | 1.58 | 0.69 |
| 1:I:293:ARG:HH11 | 1:I:296:ARG:NH2 | 1.88 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:J:1004:ARG:HH11 | 3:J:1025:GLY:H | 1.38 | 0.69 |
| 3:B:480:ILE:HG22 | 3:B:481:ASN:N | 2.07 | 0.69 |
| 2:C:69:ALA:HB2 | 2:C:381:LEU:HD22 | 1.73 | 0.69 |
| 5:E:83:GLU:H | 5:E:145:ARG:HG3 | 1.55 | 0.69 |
| 9:K:38:ALA:HB1 | 9:K:42:GLN:HE22 | 1.56 | 0.69 |
| 2:M:70:ILE:HD13 | 2:M:70:ILE:H | 1.57 | 0.69 |
| 1:A:541:ALA:HB1 | 7:G:71:PHE:HA | 1.75 | 0.69 |
| 2:M:86:THR:HA | 2:M:104:LEU:HD12 | 1.74 | 0.69 |
| 3:J:591:ILE:CG1 | 3:J:612:LYS:HZ3 | 2.06 | 0.69 |
| 3:J:812:GLY:HA2 | 3:J:836:SER:HB3 | 1.74 | 0.69 |
| 3:J:70:VAL:HG11 | 3:J:90:LEU:HD23 | 1.75 | 0.69 |
| 3:J:881:ARG:NH1 | 3:J:989:TYR:HB3 | 2.06 | 0.69 |
| 1:A:470:GLU:O | 1:A:473:ILE:HG12 | 1.91 | 0.69 |
| 3:B:800:PRO:HD3 | 3:B:850:VAL:HG23 | 1.74 | 0.69 |
| 1:A:313:LEU:HG | 2:C:374:ILE:HG23 | 1.73 | 0.69 |
| 4:D:111:SER:HA | 4:D:114:ILE:CD1 | 2.22 | 0.69 |
| 1:I:4:LYS:HD2 | 3:J:1089:PHE:HB3 | 1.74 | 0.69 |
| 3:J:181:SER:HB3 | 3:J:183:ILE:HD12 | 1.72 | 0.69 |
| 3:J:930:GLY:HA2 | 11:W:47:ARG:HH22 | 1.58 | 0.69 |
| 3:B:974:ARG:HB2 | 10:L:22:HIS:CD2 | 2.27 | 0.69 |
| 1:A:510:THR:O | 1:A:549:LYS:HG3 | 1.93 | 0.69 |
| 2:C:54:LEU:O | 2:C:58:GLU:N | 2.25 | 0.69 |
| 6:F:81:ASP:O | 6:F:84:ARG:HG2 | 1.92 | 0.69 |
| 1:I:293:ARG:HH11 | 1:I:296:ARG:HH22 | 1.39 | 0.69 |
| 1:I:594:LEU:HA | 7:S:86:LEU:CD2 | 2.22 | 0.69 |
| 1:I:502:TYR:CE1 | 1:I:636:ILE:HD11 | 2.27 | 0.69 |
| 3:J:1015:GLN:NE2 | 3:J:1096:ALA:HB2 | 2.08 | 0.69 |
| 1:A:364:PHE:CE1 | 1:A:409:ARG:HD2 | 2.28 | 0.69 |
| 3:B:890:MET:HE3 | 3:B:890:MET:HA | 1.73 | 0.69 |
| 3:J:1067:ILE:HG13 | 3:J:1068:GLY:H | 1.57 | 0.69 |
| 3:J:10:ARG:HB2 | 3:J:642:ILE:O | 1.91 | 0.69 |
| 2:M:390:MET:HB2 | 5:Q:56:GLU:CG | 2.23 | 0.69 |
| 3:B:602:ILE:CG2 | 3:B:603:THR:H | 2.05 | 0.69 |
| 2:C:237:ILE:HG13 | 2:C:238:LYS:H | 1.57 | 0.69 |
| 3:J:933:ALA:HB3 | 11:W:47:ARG:HH12 | 1.58 | 0.69 |
| 7:S:43:ILE:O | 7:S:46:ILE:HG22 | 1.93 | 0.69 |
| 1:I:541:ALA:HB2 | 7:S:72:CYS:N | 2.08 | 0.69 |
| 10:V:83:TYR:O | 10:V:87:ILE:HB | 1.92 | 0.69 |
| 1:A:446:ASN:HD22 | 1:A:448:LEU:H | 1.38 | 0.69 |
| 3:B:479:GLY:HA2 | 3:B:552:GLU:HB3 | 1.75 | 0.69 |
| 2:C:70:ILE:N | 2:C:70:ILE:HD13 | 2.07 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:67:SER:O | 7:G:69:ASP:N | 2.26 | 0.69 |
| 1:I:696:LEU:O | 1:I:700:ILE:HG12 | 1.93 | 0.69 |
| 3:B:10:ARG:HB2 | 3:B:642:ILE:O | 1.92 | 0.68 |
| 3:B:81:SER:HB3 | 3:B:84:GLU:HG3 | 1.74 | 0.68 |
| 1:I:637:ARG:HD3 | 1:I:640:GLU:CD | 2.13 | 0.68 |
| 3:J:17:TYR:OH | 3:J:474:ALA:HA | 1.93 | 0.68 |
| 2:M:315:LEU:O | 2:M:319:VAL:HG23 | 1.93 | 0.68 |
| 6:R:47:CYS:HB2 | 6:R:52:ALA:HB2 | 1.76 | 0.68 |
| 1:I:852:ASP:HB3 | 8:T:75:VAL:HG21 | 1.76 | 0.68 |
| 3:J:851:LEU:HD12 | 12:X:35:PHE:HD2 | 1.56 | 0.68 |
| 1:A:245:ILE:HD13 | 1:A:268:LEU:HB3 | 1.75 | 0.68 |
| 1:A:293:ARG:HH11 | 1:A:296:ARG:HH22 | 1.39 | 0.68 |
| 3:B:708:LEU:HD13 | 3:B:713:TYR:HB3 | 1.75 | 0.68 |
| 1:I:110:GLU:HG2 | 1:I:113:LYS:HD2 | 1.75 | 0.68 |
| 1:I:11:PHE:HB2 | 2:M:361:GLY:O | 1.93 | 0.68 |
| 2:M:366:PHE:CZ | 2:M:375:ILE:HD12 | 2.28 | 0.68 |
| 11:N:18:TRP:HD1 | 11:N:49:LEU:HD22 | 1.57 | 0.68 |
| 2:M:386:VAL:HG13 | 9:U:34:ARG:HG2 | 1.74 | 0.68 |
| 1:A:491:TYR:HD1 | 1:A:607:GLN:NE2 | 1.92 | 0.68 |
| 3:B:253:PHE:N | 3:B:254:PRO:HD2 | 2.08 | 0.68 |
| 3:B:445:LEU:HD11 | 3:B:455:PRO:CB | 2.23 | 0.68 |
| 2:C:190:ARG:HD3 | 2:C:191:LEU:H | 1.58 | 0.68 |
| 11:N:7:CYS:HB3 | 11:N:45:CYS:SG | 2.33 | 0.68 |
| 3:B:361:PHE:HE1 | 3:B:385:VAL:HG13 | 1.57 | 0.68 |
| 5:E:179:LYS:NZ | 6:F:79:THR:HB | 2.09 | 0.68 |
| 2:M:111:VAL:HG12 | 2:M:329:ILE:HB | 1.75 | 0.68 |
| 4:D:230:ILE:HG13 | 4:D:242:LEU:HD21 | 1.75 | 0.68 |
| 1:I:99:ARG:HD2 | 1:I:150:ASN:H | 1.56 | 0.68 |
| 1:I:68:CYS:SG | 1:I:71:HIS:CE1 | 2.86 | 0.68 |
| 1:I:826:ALA:H | 2:M:335:THR:CG2 | 2.07 | 0.68 |
| 3:J:602:ILE:CG2 | 3:J:603:THR:H | 2.06 | 0.68 |
| 3:J:555:VAL:O | 3:J:620:GLU:HG3 | 1.93 | 0.68 |
| 1:I:733:ALA:HB1 | 3:J:913:HIS:HE1 | 1.59 | 0.68 |
| 3:B:763:VAL:HA | 3:B:770:GLU:HG3 | 1.75 | 0.68 |
| 1:I:325:VAL:O | 1:I:442:THR:HB | 1.94 | 0.68 |
| 3:J:20:SER:O | 3:J:25:ARG:NH2 | 2.24 | 0.68 |
| 1:A:331:ASN:ND2 | 3:B:732:TYR:OH | 2.27 | 0.68 |
| 3:B:17:TYR:OH | 3:B:474:ALA:HA | 1.94 | 0.68 |
| 1:A:595:GLU:HB3 | 7:G:86:LEU:HD13 | 1.76 | 0.68 |
| 8:H:40:GLU:OE1 | 13:Y:66:LYS:CE | 2.39 | 0.68 |
| 1:I:491:TYR:HD1 | 1:I:607:GLN:NE2 | 1.91 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:630:PRO:O | 3:J:633:LEU:HB3 | 1.93 | 0.68 |
| 13:Z:58:LYS:O | 13:Z:59:ILE:HB | 1.94 | 0.68 |
| 1:I:575:CYS:HG | 1:I:580:CYS:CB | 2.06 | 0.68 |
| 1:I:721:PRO:HA | 1:I:726:TYR:CD1 | 2.27 | 0.68 |
| 3:J:591:ILE:HG12 | 3:J:612:LYS:NZ | 2.09 | 0.68 |
| 2:M:117:PRO:O | 2:M:120:PRO:HG3 | 1.92 | 0.68 |
| 1:A:549:LYS:HG2 | 1:A:593:LEU:HD13 | 1.75 | 0.68 |
| 1:I:130:ARG:HB3 | 1:I:195:LEU:O | 1.93 | 0.68 |
| 3:J:926:GLU:HB3 | 3:J:988:VAL:HG22 | 1.76 | 0.68 |
| 2:M:277:ILE:C | 2:M:279:GLU:H | 1.97 | 0.68 |
| 2:M:392:PRO:HD3 | 5:Q:56:GLU:HG3 | 1.75 | 0.68 |
| 1:I:141:MET:HG3 | 1:I:148:HIS:HA | 1.76 | 0.67 |
| 1:I:828:SER:O | 1:I:830:LEU:N | 2.27 | 0.67 |
| 1:I:839:ARG:NH1 | 8:T:37:ILE:HG23 | 2.09 | 0.67 |
| 9:K:82:LEU:CD2 | 9:K:82:LEU:H | 2.07 | 0.67 |
| 3:B:881:ARG:HD2 | 3:B:989:TYR:HD2 | 1.59 | 0.67 |
| 1:I:256:GLY:O | 1:I:258:PRO:HD3 | 1.94 | 0.67 |
| 1:I:328:PRO:HG3 | 1:I:457:PHE:CD1 | 2.30 | 0.67 |
| 3:J:28:LEU:HG | 3:J:122:MET:HE1 | 1.75 | 0.67 |
| 2:M:55:ALA:CA | 2:M:58:GLU:HB2 | 2.22 | 0.67 |
| 1:A:90:ILE:HD11 | 1:A:207:MET:CB | 2.24 | 0.67 |
| 3:B:544:ARG:HH11 | 3:B:544:ARG:HG3 | 1.59 | 0.67 |
| 3:J:759:SER:HB3 | 3:J:863:LYS:HA | 1.76 | 0.67 |
| 4:O:111:SER:HA | 4:O:114:ILE:CD1 | 2.24 | 0.67 |
| 1:A:499:ALA:HB3 | 3:B:734:MET:CE | 2.25 | 0.67 |
| 2:M:109:GLU:O | 2:M:113:ALA:N | 2.28 | 0.67 |
| 4:D:250:ILE:HA | 4:D:253:ILE:HG22 | 1.77 | 0.67 |
| 3:J:537:ALA:HB2 | 3:J:557:HIS:NE2 | 2.09 | 0.67 |
| 3:J:64:ARG:HG2 | 3:J:97:TRP:CD1 | 2.29 | 0.67 |
| 2:M:373:ILE:HG13 | 3:J:1049:LEU:HD13 | 1.75 | 0.67 |
| 3:B:851:LEU:HD12 | 12:P:35:PHE:CD2 | 2.28 | 0.67 |
| 3:J:851:LEU:HD12 | 12:X:35:PHE:CD2 | 2.30 | 0.67 |
| 1:A:490:ARG:HG2 | 1:A:491:TYR:CD2 | 2.30 | 0.67 |
| 2:C:237:ILE:HG22 | 2:C:257:ASN:CB | 2.25 | 0.67 |
| 2:M:355:LEU:HD22 | 3:J:1109:ILE:HD11 | 1.76 | 0.67 |
| 2:M:391:ARG:H | 2:M:392:PRO:HD3 | 1.60 | 0.67 |
| 11:W:18:TRP:HD1 | 11:W:49:LEU:HD22 | 1.58 | 0.67 |
| 3:B:161:ILE:HG21 | 3:B:346:ALA:HA | 1.77 | 0.67 |
| 1:I:426:HIS:CE1 | 1:I:428:ILE:CG2 | 2.77 | 0.67 |
| 11:N:22:ILE:HD13 | 11:N:23:THR:H | 1.58 | 0.67 |
| 5:Q:27:LEU:HB2 | 5:Q:51:VAL:CG1 | 2.22 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:11:THR:O | 4:D:238:PRO:HB3 | 1.94 | 0.67 |
| 2:M:231:ILE:HB | 2:M:234:ILE:HG12 | 1.75 | 0.67 |
| 2:M:237:ILE:HG13 | 2:M:238:LYS:N | 2.10 | 0.67 |
| 2:M:55:ALA:HA | 2:M:58:GLU:CB | 2.21 | 0.67 |
| 9:U:61:VAL:HG12 | 9:U:62:ILE:N | 2.06 | 0.67 |
| 1:A:532:ILE:HD11 | 10:L:56:LYS:CD | 2.22 | 0.67 |
| 3:B:291:GLN:HB3 | 3:B:295:LYS:HE2 | 1.77 | 0.67 |
| 3:B:933:ALA:HB3 | 11:N:47:ARG:HH12 | 1.58 | 0.67 |
| 3:J:38:LYS:HA | 3:J:41:GLU:HG3 | 1.76 | 0.67 |
| 3:J:848:ASP:HB2 | 3:J:867:ARG:H | 1.60 | 0.67 |
| 1:A:589:LYS:HG2 | 1:A:877:GLY:HA2 | 1.77 | 0.67 |
| 3:B:602:ILE:HG23 | 3:B:603:THR:H | 1.59 | 0.67 |
| 6:R:51:SER:O | 6:R:55:VAL:HG23 | 1.94 | 0.67 |
| 3:J:850:VAL:O | 12:X:35:PHE:HB2 | 1.95 | 0.67 |
| 3:B:602:ILE:CG2 | 3:B:603:THR:N | 2.58 | 0.66 |
| 3:J:665:ARG:HG3 | 3:J:920:THR:HG21 | 1.76 | 0.66 |
| 3:J:962:TYR:OH | 11:W:42:ARG:HD2 | 1.95 | 0.66 |
| 1:I:826:ALA:HB2 | 2:M:335:THR:HG23 | 1.77 | 0.66 |
| 5:Q:64:GLY:N | 9:U:41:LEU:HD22 | 2.09 | 0.66 |
| 3:B:457:GLU:HG2 | 3:B:469:ASN:OD1 | 1.96 | 0.66 |
| 3:B:451:GLY:CA | 3:B:577:ARG:HH11 | 2.08 | 0.66 |
| 3:B:934:ALA:O | 11:N:46:ARG:HD3 | 1.95 | 0.66 |
| 3:J:451:GLY:CA | 3:J:577:ARG:HH11 | 2.08 | 0.66 |
| 2:M:159:ASP:HB3 | 2:M:163:MET:HB2 | 1.77 | 0.66 |
| 2:M:391:ARG:HH22 | 9:U:39:ARG:NH1 | 1.93 | 0.66 |
| 2:C:104:LEU:HB3 | 2:C:105:PRO:HD3 | 1.77 | 0.66 |
| 3:J:253:PHE:N | 3:J:254:PRO:HD2 | 2.09 | 0.66 |
| 2:M:104:LEU:HB3 | 2:M:105:PRO:HD3 | 1.76 | 0.66 |
| 2:M:309:ASP:OD2 | 2:M:311:ARG:N | 2.29 | 0.66 |
| 2:M:390:MET:CG | 5:Q:56:GLU:HG2 | 2.25 | 0.66 |
| 1:A:326:ILE:HG21 | 1:A:462:MET:HG3 | 1.77 | 0.66 |
| 1:A:569:SER:HB2 | 1:A:584:SER:OG | 1.95 | 0.66 |
| 1:A:666:ASP:O | 1:A:670:VAL:HG13 | 1.94 | 0.66 |
| 3:B:20:SER:O | 3:B:25:ARG:NH2 | 2.28 | 0.66 |
| 3:B:806:GLY:O | 3:B:839:THR:HB | 1.95 | 0.66 |
| 2:M:261:VAL:O | 2:M:261:VAL:HG12 | 1.96 | 0.66 |
| 1:A:104:VAL:HG12 | 1:A:104:VAL:O | 1.96 | 0.66 |
| 1:I:4:LYS:HD3 | 3:J:1091:VAL:HB | 1.78 | 0.66 |
| 4:O:250:ILE:HA | 4:O:253:ILE:HG22 | 1.78 | 0.66 |
| 1:I:722:PHE:HZ | 7:S:23:LEU:HG | 1.60 | 0.66 |
| 7:S:86:LEU:HD12 | 7:S:91:LYS:CG | 2.26 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:B:26:GLN:O | 3:B:345:LEU:CD2 | 2.40 | 0.66 |
| 4:D:111:SER:CA | 4:D:114:ILE:HD13 | 2.24 | 0.66 |
| 6:F:33:LEU:O | 6:F:34:LEU:HD23 | 1.96 | 0.66 |
| 3:J:602:ILE:HG23 | 3:J:603:THR:H | 1.61 | 0.66 |
| 3:J:702:LEU:HD12 | 11:W:51:SER:HB3 | 1.76 | 0.66 |
| 4:O:109:ILE:HD11 | 4:O:133:LEU:HD12 | 1.77 | 0.66 |
| 3:J:1012:LEU:O | 3:J:1095:TYR:HE2 | 1.79 | 0.66 |
| 2:M:298:SER:O | 2:M:302:ALA:HB2 | 1.96 | 0.66 |
| 3:B:450:TRP:CZ2 | 3:B:641:GLU:OE1 | 2.47 | 0.66 |
| 1:A:549:LYS:CE | 7:G:89:GLY:HA2 | 2.25 | 0.66 |
| 3:J:291:GLN:HB3 | 3:J:295:LYS:HE2 | 1.77 | 0.66 |
| 3:J:448:THR:C | 3:J:450:TRP:H | 1.99 | 0.66 |
| 3:J:522:LEU:O | 3:J:525:ARG:HB3 | 1.95 | 0.66 |
| 2:M:72:ILE:HD12 | 2:M:72:ILE:H | 1.58 | 0.66 |
| 7:S:13:CYS:HA | 7:S:33:CYS:HA | 1.77 | 0.66 |
| 1:I:549:LYS:CE | 7:S:89:GLY:HA2 | 2.26 | 0.66 |
| 1:I:534:LEU:HB2 | 10:V:39:SER:OG | 1.96 | 0.66 |
| 1:A:575:CYS:HG | 1:A:580:CYS:CB | 2.09 | 0.66 |
| 1:A:818:TYR:OH | 2:C:348:GLU:OE2 | 2.12 | 0.66 |
| 4:D:190:LEU:CD2 | 4:D:195:LEU:HA | 2.25 | 0.66 |
| 4:D:259:LYS:O | 4:D:263:VAL:HG23 | 1.96 | 0.66 |
| 4:O:190:LEU:CD2 | 4:O:195:LEU:HA | 2.26 | 0.66 |
| 5:Q:43:GLY:HA3 | 5:Q:78:VAL:HG23 | 1.78 | 0.66 |
| 1:A:106:ILE:HG22 | 1:A:107:SER:H | 1.59 | 0.65 |
| 1:A:239:LEU:HD22 | 1:A:276:TYR:CE1 | 2.31 | 0.65 |
| 3:B:1015:GLN:NE2 | 3:B:1096:ALA:HB2 | 2.11 | 0.65 |
| 3:B:1095:TYR:CE1 | 3:B:1098:LYS:HD2 | 2.30 | 0.65 |
| 5:E:113:ILE:O | 5:E:164:MET:HB2 | 1.96 | 0.65 |
| 1:I:345:LYS:HA | 1:I:410:HIS:CD2 | 2.30 | 0.65 |
| 1:I:353:ILE:HD11 | 1:I:407:ILE:HG23 | 1.78 | 0.65 |
| 3:J:690:THR:HG22 | 3:J:691:ARG:HG3 | 1.77 | 0.65 |
| 2:M:168:GLN:HG2 | 2:M:204:SER:HB3 | 1.78 | 0.65 |
| 3:J:902:LYS:HB3 | 11:W:42:ARG:CD | 2.25 | 0.65 |
| 3:B:569:ASN:HB3 | 3:B:574:ARG:NH2 | 2.09 | 0.65 |
| 1:A:647:ARG:NH2 | 3:B:982:ARG:HH12 | 1.94 | 0.65 |
| 4:D:44:VAL:HA | 4:D:143:ALA:HA | 1.77 | 0.65 |
| 2:M:354:LEU:HD22 | 3:J:1104:LEU:HD21 | 1.77 | 0.65 |
| 1:A:696:LEU:O | 1:A:700:ILE:HG12 | 1.95 | 0.65 |
| 1:A:837:THR:HG22 | 1:A:838:VAL:H | 1.62 | 0.65 |
| 3:B:448:THR:C | 3:B:450:TRP:H | 1.99 | 0.65 |
| 3:B:345:LEU:HD11 | 3:B:476:ILE:HG13 | 1.77 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:591:ILE:CG1 | 3:B:612:LYS:HZ3 | 2.08 | 0.65 |
| 1:I:308:ARG:HG3 | 1:I:312:ASN:HD22 | 1.61 | 0.65 |
| 1:I:27:ILE:HG23 | 1:I:45:MET:HA | 1.78 | 0.65 |
| 1:I:515:LEU:HD13 | 7:S:43:ILE:HD12 | 1.78 | 0.65 |
| 3:J:781:ARG:HD3 | 3:J:782:GLY:H | 1.61 | 0.65 |
| 12:P:24:VAL:O | 12:P:24:VAL:HG13 | 1.96 | 0.65 |
| 1:A:141:MET:HG3 | 1:A:148:HIS:HA | 1.78 | 0.65 |
| 5:E:127:ILE:HB | 5:E:136:ILE:HB | 1.78 | 0.65 |
| 1:I:841:LEU:HD11 | 2:M:339:ASN:HB3 | 1.78 | 0.65 |
| 1:A:590:ASN:HD21 | 3:J:377:ARG:HD2 | 1.61 | 0.65 |
| 3:J:587:PRO:O | 3:J:588:LEU:HD23 | 1.96 | 0.65 |
| 1:A:421:ARG:HB2 | 1:A:462:MET:HE3 | 1.78 | 0.65 |
| 10:L:67:ASP:HA | 10:L:70:LEU:HB2 | 1.77 | 0.65 |
| 5:Q:26:ALA:O | 5:Q:30:LEU:HB2 | 1.97 | 0.65 |
| 2:M:390:MET:CB | 5:Q:56:GLU:HG2 | 2.26 | 0.65 |
| 3:B:739:ILE:CG2 | 3:B:909:ILE:HB | 2.27 | 0.65 |
| 3:J:162:VAL:HG11 | 3:J:412:GLN:NE2 | 2.10 | 0.65 |
| 2:M:288:ALA:HB2 | 8:T:17:VAL:HB | 1.77 | 0.65 |
| 7:S:60:SER:OG | 7:S:64:PRO:HD3 | 1.95 | 0.65 |
| 1:A:827:LEU:HD11 | 2:C:315:LEU:HD12 | 1.79 | 0.65 |
| 1:I:635:PHE:O | 1:I:639:VAL:HG23 | 1.97 | 0.65 |
| 3:J:588:LEU:HD13 | 3:J:612:LYS:HB3 | 1.79 | 0.65 |
| 1:A:749:GLN:H | 1:A:781:PHE:HA | 1.61 | 0.65 |
| 3:B:1047:ASP:HA | 3:B:1051:ASP:HB2 | 1.79 | 0.65 |
| 3:J:147:ASP:OD2 | 3:J:148:PRO:HD2 | 1.97 | 0.65 |
| 3:B:245:ASP:N | 3:B:246:PRO:HD3 | 2.12 | 0.65 |
| 3:B:724:LEU:HD12 | 3:B:908:ILE:HG22 | 1.78 | 0.65 |
| 3:J:602:ILE:CG2 | 3:J:603:THR:N | 2.60 | 0.65 |
| 9:U:91:SER:O | 9:U:92:LEU:CB | 2.44 | 0.65 |
| 1:A:512:LYS:HE2 | 7:G:91:LYS:CE | 2.26 | 0.65 |
| 3:B:552:GLU:HA | 3:B:576:ARG:HH22 | 1.62 | 0.65 |
| 7:G:15:ILE:HD13 | 7:G:53:GLU:HB3 | 1.78 | 0.65 |
| 1:I:764:ARG:HH11 | 1:I:764:ARG:CB | 2.09 | 0.65 |
| 2:M:192:LYS:C | 2:M:194:GLY:H | 2.00 | 0.65 |
| 12:X:26:CYS:HB2 | 12:X:27:PRO:CD | 2.26 | 0.65 |
| 1:A:378:VAL:HG22 | 1:A:378:VAL:O | 1.97 | 0.64 |
| 1:A:378:VAL:HG23 | 1:A:407:ILE:HG22 | 1.80 | 0.64 |
| 2:C:299:LYS:HA | 2:C:302:ALA:HB3 | 1.78 | 0.64 |
| 2:C:390:MET:O | 2:C:391:ARG:CB | 2.45 | 0.64 |
| 5:E:39:LEU:O | 5:E:40:LYS:HB2 | 1.96 | 0.64 |
| 7:G:41:ASP:HB2 | 7:G:90:ASN:HB3 | 1.79 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:354:THR:HB | 1:I:355:PRO:HD2 | 1.78 | 0.64 |
| 1:I:549:LYS:HG2 | 1:I:593:LEU:HD13 | 1.79 | 0.64 |
| 1:I:507:TYR:HB3 | 1:I:597:VAL:HG13 | 1.79 | 0.64 |
| 1:I:750:GLN:HG3 | 1:I:782:ILE:CD1 | 2.27 | 0.64 |
| 3:J:840:ARG:HH11 | 3:J:1021:ALA:HB2 | 1.62 | 0.64 |
| 9:U:61:VAL:CG1 | 9:U:62:ILE:H | 2.05 | 0.64 |
| 1:A:345:LYS:HA | 1:A:410:HIS:CD2 | 2.32 | 0.64 |
| 1:A:4:LYS:HD2 | 3:B:1089:PHE:HB3 | 1.79 | 0.64 |
| 2:C:104:LEU:O | 2:C:108:ILE:HG12 | 1.96 | 0.64 |
| 2:C:69:ALA:CB | 2:C:381:LEU:HD22 | 2.27 | 0.64 |
| 1:A:558:LYS:NZ | 3:J:108:GLU:HG2 | 2.12 | 0.64 |
| 3:J:1064:CYS:HG | 14:J:2001:ZN:ZN | 1.08 | 0.64 |
| 4:O:133:LEU:HD21 | 4:O:139:ILE:HG13 | 1.78 | 0.64 |
| 7:S:83:ASP:O | 7:S:93:THR:HA | 1.98 | 0.64 |
| 3:B:764:LYS:HZ3 | 3:B:814:VAL:H | 1.44 | 0.64 |
| 3:B:577:ARG:HE | 3:B:578:PRO:HD2 | 1.63 | 0.64 |
| 3:B:881:ARG:HD2 | 3:B:989:TYR:CD2 | 2.32 | 0.64 |
| 8:H:78:TYR:O | 8:H:79:ARG:HG2 | 1.98 | 0.64 |
| 1:I:196:GLY:O | 2:M:360:ARG:HG2 | 1.97 | 0.64 |
| 10:V:32:LEU:O | 10:V:32:LEU:HD13 | 1.98 | 0.64 |
| 3:B:28:LEU:HG | 3:B:122:MET:CE | 2.28 | 0.64 |
| 4:D:247:LYS:HA | 4:D:250:ILE:HD12 | 1.78 | 0.64 |
| 3:J:336:ASP:HA | 3:J:341:LYS:HE3 | 1.79 | 0.64 |
| 2:M:328:GLN:O | 2:M:333:GLY:HA3 | 1.98 | 0.64 |
| 2:C:50:LYS:HA | 2:C:53:ASP:HB2 | 1.79 | 0.64 |
| 8:H:42:LEU:HB2 | 8:H:43:PRO:HD2 | 1.78 | 0.64 |
| 5:Q:15:PRO:HG2 | 9:U:45:MET:CB | 2.28 | 0.64 |
| 2:M:68:GLU:HB3 | 9:U:30:TYR:HE1 | 1.62 | 0.64 |
| 12:X:24:VAL:HG13 | 12:X:24:VAL:O | 1.97 | 0.64 |
| 3:B:416:ARG:NH1 | 3:B:687:ARG:NH2 | 2.46 | 0.64 |
| 3:B:900:THR:HG22 | 3:B:970:VAL:HG12 | 1.79 | 0.64 |
| 1:I:647:ARG:O | 1:I:650:ASP:HB2 | 1.96 | 0.64 |
| 1:I:830:LEU:CD2 | 1:I:840:SER:HB3 | 2.24 | 0.64 |
| 3:J:318:ALA:O | 3:J:321:LYS:HB2 | 1.97 | 0.64 |
| 3:J:890:MET:CE | 3:J:891:LEU:H | 2.08 | 0.64 |
| 2:M:150:GLU:HG3 | 2:M:227:LEU:HD22 | 1.78 | 0.64 |
| 2:M:391:ARG:HH21 | 9:U:42:GLN:CG | 2.11 | 0.64 |
| 1:A:678:LYS:HD2 | 1:A:684:LEU:HG | 1.79 | 0.64 |
| 3:B:569:ASN:CB | 3:B:574:ARG:HH22 | 2.10 | 0.64 |
| 3:B:64:ARG:O | 3:B:97:TRP:HB2 | 1.98 | 0.64 |
| 3:B:657:TYR:O | 3:B:660:HIS:HB2 | 1.97 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:1:MET:SD | 6:F:6:ILE:HG12 | 2.37 | 0.64 |
| 7:G:101:LEU:HD12 | 7:G:104:LYS:NZ | 2.12 | 0.64 |
| 1:A:27:ILE:HG23 | 1:A:45:MET:HA | 1.79 | 0.64 |
| 3:B:972:ASP:OD2 | 3:B:974:ARG:HG2 | 1.97 | 0.64 |
| 3:J:246:PRO:C | 3:J:248:VAL:H | 2.02 | 0.64 |
| 3:B:239:VAL:HA | 3:B:253:PHE:HE2 | 1.63 | 0.64 |
| 3:B:116:ILE:HG22 | 3:B:390:VAL:HG21 | 1.79 | 0.64 |
| 1:I:490:ARG:HG2 | 1:I:491:TYR:CD2 | 2.33 | 0.64 |
| 3:J:480:ILE:HG22 | 3:J:481:ASN:N | 2.13 | 0.64 |
| 1:I:549:LYS:HE2 | 7:S:89:GLY:HA2 | 1.80 | 0.64 |
| 8:T:42:LEU:O | 8:T:44:TRP:N | 2.30 | 0.64 |
| 3:B:930:GLY:HA2 | 11:N:47:ARG:HH22 | 1.62 | 0.63 |
| 2:C:311:ARG:HD3 | 2:C:311:ARG:N | 2.14 | 0.63 |
| 2:C:60:SER:O | 2:C:63:LEU:HB3 | 1.98 | 0.63 |
| 3:J:591:ILE:HG12 | 3:J:612:LYS:HZ3 | 1.63 | 0.63 |
| 6:R:23:ASP:O | 6:R:26:ARG:HB2 | 1.97 | 0.63 |
| 2:M:68:GLU:HB3 | 9:U:30:TYR:CE1 | 2.33 | 0.63 |
| 9:U:61:VAL:C | 9:U:63:SER:H | 2.00 | 0.63 |
| 10:V:59:THR:CG2 | 10:V:65:PRO:HD3 | 2.28 | 0.63 |
| 1:I:647:ARG:NH2 | 3:J:982:ARG:HH12 | 1.97 | 0.63 |
| 3:J:591:ILE:HD12 | 3:J:591:ILE:H | 1.61 | 0.63 |
| 1:A:133:THR:HB | 1:A:137:LYS:HZ2 | 1.63 | 0.63 |
| 1:A:156:ILE:HD11 | 1:A:270:GLN:HG2 | 1.80 | 0.63 |
| 1:A:353:ILE:HG13 | 1:A:361:LEU:CD2 | 2.29 | 0.63 |
| 3:B:246:PRO:C | 3:B:248:VAL:H | 2.02 | 0.63 |
| 3:B:537:ALA:HB2 | 3:B:557:HIS:NE2 | 2.13 | 0.63 |
| 3:B:99:THR:O | 3:B:99:THR:HG22 | 1.98 | 0.63 |
| 4:D:131:VAL:HG22 | 4:D:132:LEU:N | 2.13 | 0.63 |
| 8:H:11:PRO:O | 8:H:13:ILE:N | 2.29 | 0.63 |
| 3:J:702:LEU:HB2 | 3:J:721:ASN:ND2 | 2.14 | 0.63 |
| 9:K:41:LEU:O | 9:K:42:GLN:C | 2.36 | 0.63 |
| 3:B:840:ARG:HH11 | 3:B:1021:ALA:HB2 | 1.62 | 0.63 |
| 2:C:321:THR:C | 2:C:322:ARG:HH11 | 2.02 | 0.63 |
| 2:C:33:LYS:O | 2:C:36:ILE:HG22 | 1.99 | 0.63 |
| 1:I:364:PHE:CE1 | 1:I:409:ARG:HD2 | 2.34 | 0.63 |
| 3:J:325:LEU:HD13 | 3:J:330:ARG:H | 1.62 | 0.63 |
| 3:J:638:THR:HB | 3:J:639:HIS:HD2 | 1.62 | 0.63 |
| 3:J:739:ILE:HG12 | 3:J:890:MET:O | 1.98 | 0.63 |
| 1:I:750:GLN:HG3 | 1:I:782:ILE:HD11 | 1.80 | 0.63 |
| 3:J:361:PHE:HE1 | 3:J:385:VAL:HG13 | 1.62 | 0.63 |
| 9:K:74:LEU:N | 9:K:74:LEU:HD12 | 2.14 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:106:ARG:O | 2:M:109:GLU:N | 2.31 | 0.63 |
| 1:I:191:ASP:HA | 1:I:194:ILE:HD11 | 1.81 | 0.63 |
| 5:Q:109:HIS:CD2 | 5:Q:111:SER:H | 2.17 | 0.63 |
| 1:I:512:LYS:HE2 | 7:S:91:LYS:CE | 2.29 | 0.63 |
| 8:T:65:ILE:HD11 | 8:T:79:ARG:CG | 2.28 | 0.63 |
| 3:B:922:GLY:O | 3:B:926:GLU:HB2 | 1.99 | 0.63 |
| 1:I:12:GLY:HA2 | 2:M:358:ALA:O | 1.99 | 0.63 |
| 1:I:503:ILE:HD11 | 1:I:733:ALA:N | 2.12 | 0.63 |
| 3:J:245:ASP:N | 3:J:246:PRO:HD3 | 2.13 | 0.63 |
| 3:J:64:ARG:HG2 | 3:J:97:TRP:CG | 2.33 | 0.63 |
| 1:I:595:GLU:HB2 | 7:S:91:LYS:HE2 | 1.80 | 0.63 |
| 1:A:110:GLU:HG2 | 1:A:113:LYS:HD2 | 1.81 | 0.63 |
| 3:B:683:ASN:O | 3:B:685:GLN:N | 2.32 | 0.63 |
| 2:C:183:ASP:O | 2:C:187:ALA:HB2 | 1.98 | 0.63 |
| 1:I:327:SER:HB2 | 1:I:444:ARG:HD3 | 1.80 | 0.63 |
| 3:J:239:VAL:HA | 3:J:253:PHE:HE2 | 1.63 | 0.63 |
| 3:J:922:GLY:CA | 3:J:925:MET:HB2 | 2.17 | 0.63 |
| 7:S:86:LEU:HD12 | 7:S:91:LYS:HG2 | 1.81 | 0.63 |
| 3:B:249:GLN:HG3 | 3:B:250:ASN:N | 2.14 | 0.63 |
| 6:R:34:LEU:HD22 | 6:R:38:TYR:CE2 | 2.34 | 0.63 |
| 1:A:316:LYS:HD2 | 3:B:1049:LEU:O | 1.99 | 0.62 |
| 3:B:356:VAL:HG11 | 3:B:404:VAL:HG12 | 1.81 | 0.62 |
| 6:F:23:ASP:O | 6:F:26:ARG:HB2 | 1.99 | 0.62 |
| 3:J:296:TYR:O | 3:J:297:PHE:HB2 | 1.99 | 0.62 |
| 2:M:150:GLU:HG3 | 2:M:227:LEU:CD2 | 2.29 | 0.62 |
| 1:I:475:GLU:CD | 2:M:383:THR:HG21 | 2.19 | 0.62 |
| 12:X:37:VAL:HG22 | 12:X:38:ARG:H | 1.63 | 0.62 |
| 3:B:1067:ILE:HG13 | 3:B:1068:GLY:H | 1.64 | 0.62 |
| 3:B:591:ILE:HG12 | 3:B:612:LYS:HZ3 | 1.64 | 0.62 |
| 5:E:179:LYS:HZ3 | 6:F:79:THR:HB | 1.64 | 0.62 |
| 1:I:823:LEU:HD13 | 2:M:75:ALA:CB | 2.27 | 0.62 |
| 2:M:391:ARG:HH21 | 9:U:42:GLN:HG2 | 1.64 | 0.62 |
| 12:P:37:VAL:HG22 | 12:P:38:ARG:H | 1.63 | 0.62 |
| 1:A:587:VAL:HB | 1:A:594:LEU:O | 1.99 | 0.62 |
| 1:A:555:PHE:CD2 | 1:A:631:LEU:HD13 | 2.34 | 0.62 |
| 3:B:1085:LYS:O | 3:B:1086:SER:OG | 2.17 | 0.62 |
| 3:B:700:ARG:N | 11:N:51:SER:O | 2.31 | 0.62 |
| 3:J:738:ILE:CD1 | 3:J:908:ILE:HG23 | 2.29 | 0.62 |
| 3:B:469:ASN:HD22 | 3:B:469:ASN:N | 1.98 | 0.62 |
| 3:B:890:MET:CE | 3:B:891:LEU:H | 2.13 | 0.62 |
| 8:H:25:ILE:HA | 8:H:28:ALA:HB3 | 1.81 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:421:ARG:HB2 | 1:I:462:MET:HE3 | 1.80 | 0.62 |
| 1:I:833:GLU:HG3 | 1:I:839:ARG:HG3 | 1.81 | 0.62 |
| 2:M:338:LYS:HA | 2:M:338:LYS:HE2 | 1.80 | 0.62 |
| 7:S:104:LYS:HB3 | 7:S:104:LYS:NZ | 2.14 | 0.62 |
| 2:M:389:THR:CG2 | 9:U:77:THR:HB | 2.17 | 0.62 |
| 1:A:877:GLY:C | 3:J:377:ARG:NH1 | 2.47 | 0.62 |
| 3:B:1033:ARG:HD2 | 3:B:1037:ILE:HD11 | 1.80 | 0.62 |
| 3:B:1045:LEU:O | 3:B:1049:LEU:HB3 | 1.99 | 0.62 |
| 1:I:483:HIS:CD2 | 1:I:625:LYS:HG3 | 2.35 | 0.62 |
| 3:J:794:ASP:N | 3:J:794:ASP:OD1 | 2.32 | 0.62 |
| 3:J:81:SER:HB3 | 3:J:84:GLU:HG3 | 1.82 | 0.62 |
| 5:Q:143:ARG:CZ | 5:Q:168:TYR:O | 2.48 | 0.62 |
| 6:R:50:GLU:HA | 6:R:53:GLN:HB2 | 1.79 | 0.62 |
| 1:A:865:THR:HG21 | 1:A:870:ARG:NH1 | 2.14 | 0.62 |
| 3:B:1012:LEU:O | 3:B:1095:TYR:HE2 | 1.82 | 0.62 |
| 3:B:60:LEU:HD22 | 3:B:98:LEU:HD21 | 1.80 | 0.62 |
| 3:J:1033:ARG:HD2 | 3:J:1037:ILE:HD11 | 1.80 | 0.62 |
| 3:J:931:LYS:HE2 | 3:J:985:PHE:O | 1.98 | 0.62 |
| 5:Q:83:GLU:O | 5:Q:145:ARG:HA | 1.99 | 0.62 |
| 8:T:12:ARG:HH12 | 8:T:55:ILE:HB | 1.65 | 0.62 |
| 3:B:356:VAL:HG22 | 3:B:393:ARG:HH12 | 1.65 | 0.62 |
| 3:B:473:MET:SD | 3:B:475:GLN:N | 2.72 | 0.62 |
| 3:B:650:ILE:HD13 | 3:B:650:ILE:N | 2.11 | 0.62 |
| 2:C:139:GLU:HA | 2:C:142:ARG:HB2 | 1.80 | 0.62 |
| 7:G:66:TYR:HD1 | 7:G:114:ARG:NH1 | 1.98 | 0.62 |
| 3:J:963:LEU:HD22 | 4:O:208:GLU:HG3 | 1.82 | 0.62 |
| 4:O:175:ASN:HA | 4:O:195:LEU:CD1 | 2.22 | 0.62 |
| 7:S:101:LEU:C | 7:S:103:VAL:H | 2.02 | 0.62 |
| 1:I:834:TYR:CE1 | 9:U:80:ARG:HD3 | 2.34 | 0.62 |
| 11:W:22:ILE:HD13 | 11:W:23:THR:N | 2.14 | 0.62 |
| 1:A:336:GLU:OE1 | 1:A:436:ARG:NH1 | 2.33 | 0.62 |
| 2:C:124:ILE:HG23 | 2:C:272:VAL:HG22 | 1.82 | 0.62 |
| 2:C:125:TYR:HD1 | 2:C:271:LYS:HB3 | 1.64 | 0.62 |
| 2:C:31:ASP:O | 2:C:34:ASN:N | 2.33 | 0.62 |
| 1:I:93:PHE:HB3 | 1:I:184:LEU:HD21 | 1.80 | 0.62 |
| 3:J:881:ARG:HH11 | 3:J:989:TYR:CB | 2.12 | 0.62 |
| 2:C:276:ASN:ND2 | 2:C:279:GLU:HB2 | 2.09 | 0.62 |
| 1:A:475:GLU:CD | 2:C:383:THR:HG21 | 2.20 | 0.62 |
| 1:I:376:ASN:O | 1:I:377:TYR:CB | 2.46 | 0.62 |
| 3:J:707:ALA:O | 3:J:711:ILE:HG13 | 1.99 | 0.62 |
| 1:I:864:LYS:HG3 | 2:M:32:LEU:HD11 | 1.81 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:137:GLN:HE21 | 11:N:63:THR:HG22 | 1.65 | 0.62 |
| 5:Q:31:ARG:C | 5:Q:33:GLN:H | 2.01 | 0.62 |
| 1:A:418:LEU:HD21 | 3:B:1044:LEU:CD2 | 2.20 | 0.62 |
| 3:B:296:TYR:O | 3:B:297:PHE:HB2 | 1.99 | 0.62 |
| 1:I:104:VAL:HG12 | 1:I:104:VAL:O | 2.00 | 0.62 |
| 1:I:98:CYS:HA | 1:I:146:CYS:SG | 2.40 | 0.62 |
| 1:I:11:PHE:HA | 3:J:1110:SER:O | 2.00 | 0.62 |
| 4:O:247:LYS:HA | 4:O:250:ILE:HD12 | 1.81 | 0.62 |
| 1:A:289:HIS:HB2 | 1:A:295:LEU:HD21 | 1.81 | 0.61 |
| 1:A:866:VAL:HG12 | 1:A:869:ASN:H | 1.65 | 0.61 |
| 3:B:702:LEU:HD12 | 11:N:51:SER:HB3 | 1.79 | 0.61 |
| 8:H:29:TYR:HA | 8:H:32:LEU:CD1 | 2.30 | 0.61 |
| 1:I:502:TYR:HE1 | 1:I:636:ILE:HD11 | 1.65 | 0.61 |
| 3:J:806:GLY:O | 3:J:839:THR:HB | 2.00 | 0.61 |
| 3:J:881:ARG:HD2 | 3:J:989:TYR:HD2 | 1.64 | 0.61 |
| 9:K:82:LEU:HD23 | 9:K:82:LEU:N | 2.10 | 0.61 |
| 7:S:15:ILE:HD13 | 7:S:53:GLU:HB3 | 1.80 | 0.61 |
| 1:A:710:THR:O | 1:A:714:ILE:HG12 | 2.00 | 0.61 |
| 3:B:21:LYS:HE2 | 3:B:475:GLN:OE1 | 2.00 | 0.61 |
| 3:B:587:PRO:O | 3:B:588:LEU:HD23 | 2.00 | 0.61 |
| 2:C:125:TYR:CD1 | 2:C:271:LYS:HB3 | 2.36 | 0.61 |
| 2:C:390:MET:HG3 | 5:E:57:GLY:N | 2.16 | 0.61 |
| 3:J:289:ALA:O | 3:J:293:ILE:HG12 | 2.00 | 0.61 |
| 3:J:679:LEU:HD23 | 3:J:716:ARG:HG2 | 1.81 | 0.61 |
| 2:M:49:ASP:O | 2:M:52:PHE:N | 2.32 | 0.61 |
| 4:O:131:VAL:HA | 11:W:2:LEU:HD11 | 1.81 | 0.61 |
| 5:Q:110:ILE:HD13 | 5:Q:113:ILE:HG21 | 1.82 | 0.61 |
| 1:A:506:ALA:HA | 1:A:635:PHE:CE2 | 2.36 | 0.61 |
| 1:A:812:ARG:NE | 2:C:86:THR:HG23 | 2.14 | 0.61 |
| 1:A:833:GLU:HG3 | 1:A:839:ARG:HG3 | 1.82 | 0.61 |
| 1:I:239:LEU:HD22 | 1:I:276:TYR:CE1 | 2.35 | 0.61 |
| 3:J:484:ILE:H | 3:J:484:ILE:HD12 | 1.65 | 0.61 |
| 3:J:764:LYS:HZ1 | 3:J:814:VAL:H | 1.47 | 0.61 |
| 3:J:763:VAL:HA | 3:J:770:GLU:HG3 | 1.83 | 0.61 |
| 10:V:3:ILE:HG23 | 10:V:15:LEU:HD21 | 1.82 | 0.61 |
| 3:B:356:VAL:CG1 | 3:B:404:VAL:HG12 | 2.31 | 0.61 |
| 3:B:683:ASN:C | 3:B:685:GLN:H | 2.04 | 0.61 |
| 7:G:63:ARG:HA | 7:G:114:ARG:NH2 | 2.16 | 0.61 |
| 1:I:426:HIS:HD2 | 1:I:490:ARG:HH12 | 1.45 | 0.61 |
| 1:A:238:LYS:HD3 | 1:A:276:TYR:HA | 1.81 | 0.61 |
| 1:A:827:LEU:HD11 | 2:C:315:LEU:CD1 | 2.30 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:448:THR:O | 3:B:450:TRP:N | 2.33 | 0.61 |
| 2:C:107:LEU:O | 2:C:110:ILE:HG22 | 2.00 | 0.61 |
| 2:C:391:ARG:NH1 | 2:C:391:ARG:CG | 2.50 | 0.61 |
| 7:G:87:ASN:C | 7:G:89:GLY:N | 2.53 | 0.61 |
| 1:I:371:LYS:NZ | 1:I:373:PRO:HD3 | 2.16 | 0.61 |
| 1:I:501:ASP:OD2 | 3:J:913:HIS:CD2 | 2.54 | 0.61 |
| 9:K:50:LEU:HD23 | 9:K:75:PRO:HD3 | 1.83 | 0.61 |
| 2:M:127:THR:OG1 | 2:M:130:TYR:O | 2.19 | 0.61 |
| 2:M:309:ASP:OD2 | 2:M:310:ILE:N | 2.34 | 0.61 |
| 3:B:557:HIS:H | 3:B:623:ASN:ND2 | 1.97 | 0.61 |
| 3:B:739:ILE:HG23 | 3:B:909:ILE:HB | 1.81 | 0.61 |
| 1:A:85:GLY:HA3 | 2:C:355:LEU:CD1 | 2.31 | 0.61 |
| 2:C:270:ALA:HA | 8:H:14:HIS:ND1 | 2.15 | 0.61 |
| 3:J:28:LEU:HG | 3:J:122:MET:CE | 2.30 | 0.61 |
| 3:J:934:ALA:O | 11:W:46:ARG:HD3 | 1.99 | 0.61 |
| 3:J:965:ASP:O | 3:J:967:THR:N | 2.33 | 0.61 |
| 2:M:269:VAL:HA | 2:M:272:VAL:HG23 | 1.81 | 0.61 |
| 2:M:274:THR:HG22 | 2:M:275:ASN:N | 2.09 | 0.61 |
| 2:C:311:ARG:HD3 | 2:C:311:ARG:H | 1.66 | 0.61 |
| 4:D:106:PRO:HA | 4:D:134:GLY:HA2 | 1.81 | 0.61 |
| 6:F:19:LYS:HG3 | 6:F:49:ALA:HB2 | 1.83 | 0.61 |
| 1:I:632:PHE:HA | 1:I:635:PHE:CE1 | 2.35 | 0.61 |
| 3:J:291:GLN:C | 3:J:293:ILE:H | 2.04 | 0.61 |
| 3:J:450:TRP:HZ3 | 3:J:621:GLU:OE2 | 1.84 | 0.61 |
| 4:O:23:GLU:OE1 | 10:V:34:ARG:NH2 | 2.34 | 0.61 |
| 10:V:74:GLU:HA | 10:V:77:ARG:HE | 1.65 | 0.61 |
| 1:A:105:LYS:NZ | 1:A:108:GLU:HB2 | 2.16 | 0.61 |
| 2:C:16:LYS:O | 2:C:20:ALA:HB3 | 2.01 | 0.61 |
| 6:F:14:TYR:HD1 | 6:F:14:TYR:N | 1.98 | 0.61 |
| 1:I:720:ASP:O | 1:I:722:PHE:N | 2.33 | 0.61 |
| 3:B:6:THR:HG22 | 3:B:7:ILE:H | 1.66 | 0.61 |
| 6:F:14:TYR:CD1 | 6:F:14:TYR:N | 2.69 | 0.61 |
| 8:H:49:ASP:OD2 | 8:H:50:PRO:HD2 | 2.01 | 0.61 |
| 3:J:686:LEU:H | 3:J:686:LEU:HD12 | 1.64 | 0.61 |
| 9:K:71:ARG:O | 9:K:72:GLY:C | 2.37 | 0.61 |
| 10:L:7:LYS:HE3 | 10:L:12:TYR:HE2 | 1.65 | 0.61 |
| 4:O:111:SER:CA | 4:O:114:ILE:HD13 | 2.27 | 0.61 |
| 11:W:7:CYS:SG | 11:W:48:MET:HG3 | 2.41 | 0.61 |
| 1:A:176:THR:O | 1:A:180:ILE:HG13 | 2.00 | 0.61 |
| 1:A:191:ASP:HA | 1:A:194:ILE:HD11 | 1.81 | 0.61 |
| 1:A:637:ARG:HD3 | 1:A:640:GLU:CD | 2.20 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:70:ILE:N | 2:C:70:ILE:CD1 | 2.64 | 0.61 |
| 1:I:856:PHE:CE2 | 2:M:73:VAL:HG21 | 2.35 | 0.61 |
| 1:I:866:VAL:HG12 | 1:I:869:ASN:H | 1.65 | 0.61 |
| 3:J:495:VAL:O | 3:J:528:GLY:HA3 | 2.01 | 0.61 |
| 1:I:595:GLU:HB3 | 7:S:91:LYS:HE2 | 1.82 | 0.61 |
| 8:T:12:ARG:NH1 | 8:T:55:ILE:HB | 2.15 | 0.61 |
| 1:A:121:ILE:HG21 | 13:Y:66:LYS:HE3 | 1.81 | 0.60 |
| 3:B:458:THR:HG21 | 3:B:465:GLY:N | 2.15 | 0.60 |
| 1:I:329:ASP:CG | 1:I:332:ILE:HD12 | 2.21 | 0.60 |
| 1:I:856:PHE:HE2 | 2:M:73:VAL:HG21 | 1.65 | 0.60 |
| 3:J:163:THR:HG23 | 3:J:428:ARG:O | 2.01 | 0.60 |
| 3:J:249:GLN:HG3 | 3:J:250:ASN:N | 2.15 | 0.60 |
| 3:J:881:ARG:HD2 | 3:J:989:TYR:CD2 | 2.36 | 0.60 |
| 2:M:104:LEU:HB3 | 2:M:105:PRO:CD | 2.30 | 0.60 |
| 2:M:237:ILE:HG13 | 2:M:238:LYS:H | 1.66 | 0.60 |
| 5:Q:13:ILE:HG23 | 5:Q:25:ILE:HG21 | 1.83 | 0.60 |
| 1:A:506:ALA:HA | 1:A:635:PHE:CD2 | 2.36 | 0.60 |
| 1:A:853:ASP:CB | 2:C:311:ARG:HH12 | 2.12 | 0.60 |
| 1:I:155:LYS:H | 1:I:155:LYS:NZ | 1.99 | 0.60 |
| 3:J:81:SER:O | 3:J:84:GLU:HB2 | 2.01 | 0.60 |
| 1:I:734:ARG:HG3 | 3:J:917:SER:HB3 | 1.82 | 0.60 |
| 1:A:328:PRO:HG3 | 1:A:457:PHE:CD1 | 2.36 | 0.60 |
| 1:A:531:LYS:O | 1:A:532:ILE:HB | 2.00 | 0.60 |
| 1:A:640:GLU:OE1 | 3:B:974:ARG:NH1 | 2.34 | 0.60 |
| 3:B:759:SER:HB3 | 3:B:863:LYS:HA | 1.81 | 0.60 |
| 3:B:873:THR:HG22 | 3:B:874:ILE:N | 2.14 | 0.60 |
| 1:I:58:CYS:CB | 1:I:59:PRO:HD3 | 2.31 | 0.60 |
| 3:J:298:LEU:C | 3:J:300:HIS:H | 2.05 | 0.60 |
| 3:B:160:VAL:O | 3:B:411:SER:HA | 2.02 | 0.60 |
| 1:A:798:HIS:HE2 | 3:B:663:SER:H | 1.50 | 0.60 |
| 3:B:803:GLU:HB3 | 3:B:805:LYS:NZ | 2.16 | 0.60 |
| 8:H:23:LEU:HB2 | 8:H:62:ILE:O | 2.01 | 0.60 |
| 3:J:60:LEU:HD22 | 3:J:98:LEU:HD21 | 1.82 | 0.60 |
| 3:J:87:LEU:HD23 | 3:J:688:THR:CG2 | 2.31 | 0.60 |
| 2:M:303:GLU:O | 2:M:304:GLN:HG2 | 2.01 | 0.60 |
| 3:J:958:LEU:HD21 | 4:O:181:ASN:O | 2.01 | 0.60 |
| 5:Q:110:ILE:O | 5:Q:113:ILE:HG22 | 2.00 | 0.60 |
| 9:U:87:ILE:HG22 | 9:U:87:ILE:O | 2.01 | 0.60 |
| 3:B:707:ALA:O | 3:B:711:ILE:HG13 | 2.01 | 0.60 |
| 3:B:781:ARG:HD3 | 3:B:782:GLY:H | 1.67 | 0.60 |
| 3:J:1004:ARG:NH1 | 3:J:1024:GLY:HA2 | 2.16 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:356:VAL:HG22 | 3:J:393:ARG:HH12 | 1.65 | 0.60 |
| 9:K:41:LEU:O | 9:K:43:LEU:N | 2.34 | 0.60 |
| 3:B:197:ARG:HB2 | 3:B:199:PRO:HD3 | 1.84 | 0.60 |
| 3:B:727:MET:HE1 | 3:B:898:PRO:CG | 2.31 | 0.60 |
| 3:B:741:ASN:OD1 | 3:B:743:SER:N | 2.34 | 0.60 |
| 2:C:392:PRO:HG3 | 5:E:66:THR:HG21 | 1.82 | 0.60 |
| 1:I:531:LYS:O | 1:I:532:ILE:HB | 2.00 | 0.60 |
| 3:J:902:LYS:HB2 | 11:W:42:ARG:NH1 | 2.15 | 0.60 |
| 7:S:80:GLU:CG | 7:S:81:LEU:H | 2.14 | 0.60 |
| 1:A:81:VAL:HG12 | 1:A:270:GLN:HG3 | 1.84 | 0.60 |
| 1:A:859:TYR:CB | 2:C:64:ILE:HG12 | 2.32 | 0.60 |
| 3:B:163:THR:HG23 | 3:B:428:ARG:O | 2.02 | 0.60 |
| 3:J:367:TYR:CD2 | 3:J:367:TYR:C | 2.75 | 0.60 |
| 2:M:286:ILE:HD12 | 8:T:45:ILE:HG13 | 1.84 | 0.60 |
| 1:A:155:LYS:NZ | 1:A:155:LYS:H | 1.99 | 0.60 |
| 1:A:491:TYR:CB | 1:A:607:GLN:OE1 | 2.50 | 0.60 |
| 1:A:71:HIS:ND1 | 3:B:1070:TYR:HE2 | 1.98 | 0.60 |
| 3:B:298:LEU:C | 3:B:300:HIS:H | 2.04 | 0.60 |
| 3:B:40:GLN:HE22 | 3:B:62:LYS:HA | 1.66 | 0.60 |
| 7:G:80:GLU:O | 7:G:81:LEU:HD12 | 2.00 | 0.60 |
| 1:I:847:GLN:HG2 | 2:M:318:ASP:OD1 | 2.02 | 0.60 |
| 3:J:183:ILE:HB | 3:J:207:ASP:C | 2.22 | 0.60 |
| 1:A:376:ASN:O | 1:A:377:TYR:CB | 2.43 | 0.60 |
| 1:A:632:PHE:HA | 1:A:635:PHE:HD1 | 1.63 | 0.60 |
| 1:A:868:VAL:HG22 | 2:C:39:LYS:NZ | 2.17 | 0.60 |
| 3:B:38:LYS:HA | 3:B:41:GLU:HG3 | 1.84 | 0.60 |
| 3:B:555:VAL:O | 3:B:620:GLU:HG3 | 2.00 | 0.60 |
| 3:B:686:LEU:HD12 | 3:B:686:LEU:H | 1.67 | 0.60 |
| 5:E:66:THR:CG2 | 5:E:68:HIS:NE2 | 2.64 | 0.60 |
| 3:J:197:ARG:HB2 | 3:J:199:PRO:HD3 | 1.83 | 0.60 |
| 3:J:971:TYR:CZ | 4:O:165:ARG:HA | 2.37 | 0.60 |
| 9:U:41:LEU:O | 9:U:45:MET:HG2 | 2.01 | 0.60 |
| 1:I:510:THR:O | 1:I:549:LYS:HG3 | 2.02 | 0.60 |
| 3:J:83:MET:HG3 | 3:J:142:GLY:O | 2.01 | 0.60 |
| 1:I:447:LEU:HD13 | 3:J:734:MET:SD | 2.42 | 0.60 |
| 9:K:90:LEU:N | 9:K:90:LEU:CD2 | 2.57 | 0.60 |
| 10:L:1:MET:HA | 10:L:18:GLU:O | 2.01 | 0.60 |
| 2:M:133:ASP:HB2 | 2:M:136:LYS:HG2 | 1.84 | 0.60 |
| 1:A:220:ARG:HA | 1:A:233:ASP:OD1 | 2.02 | 0.59 |
| 1:A:93:PHE:HB3 | 1:A:184:LEU:HD21 | 1.84 | 0.59 |
| 1:I:317:ARG:NH1 | 3:J:1018:GLU:HG3 | 2.17 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:I:446:ASN:HD22 | 1:I:446:ASN:C | 2.05 | 0.59 |
| 1:I:839:ARG:HH12 | 8:T:37:ILE:HG23 | 1.65 | 0.59 |
| 2:M:390:MET:CB | 5:Q:56:GLU:CG | 2.80 | 0.59 |
| 1:A:133:THR:HB | 1:A:137:LYS:NZ | 2.16 | 0.59 |
| 1:A:329:ASP:CG | 1:A:332:ILE:HD12 | 2.22 | 0.59 |
| 1:A:354:THR:HB | 1:A:355:PRO:HD2 | 1.84 | 0.59 |
| 3:B:484:ILE:H | 3:B:484:ILE:HD12 | 1.67 | 0.59 |
| 3:B:881:ARG:HH11 | 3:B:989:TYR:CB | 2.15 | 0.59 |
| 7:G:87:ASN:O | 7:G:89:GLY:N | 2.35 | 0.59 |
| 1:I:355:PRO:O | 1:I:356:TRP:CD1 | 2.55 | 0.59 |
| 3:J:230:LEU:HD13 | 3:J:312:ALA:HA | 1.82 | 0.59 |
| 3:J:75:ARG:H | 3:J:75:ARG:HE | 1.47 | 0.59 |
| 2:M:318:ASP:O | 2:M:322:ARG:CD | 2.50 | 0.59 |
| 1:I:849:ALA:HB2 | 9:U:15:PHE:CD1 | 2.37 | 0.59 |
| 9:U:19:PHE:O | 9:U:20:ILE:C | 2.40 | 0.59 |
| 10:V:72:ALA:HA | 10:V:75:ASN:HB2 | 1.82 | 0.59 |
| 1:A:284:LEU:N | 1:A:285:PRO:HD2 | 2.17 | 0.59 |
| 1:A:450:CYS:HB2 | 1:A:451:PRO:HD3 | 1.84 | 0.59 |
| 1:I:84:VAL:HG11 | 1:I:274:ALA:HB1 | 1.83 | 0.59 |
| 1:I:290:ARG:HD2 | 1:I:291:SER:N | 2.16 | 0.59 |
| 1:I:678:LYS:HD2 | 1:I:684:LEU:HG | 1.84 | 0.59 |
| 1:I:720:ASP:C | 1:I:722:PHE:H | 2.04 | 0.59 |
| 3:J:183:ILE:HD13 | 3:J:183:ILE:O | 2.03 | 0.59 |
| 3:J:479:GLY:HA2 | 3:J:552:GLU:HB3 | 1.84 | 0.59 |
| 3:J:902:LYS:HE2 | 11:W:41:LYS:HB3 | 1.83 | 0.59 |
| 2:M:330:GLY:O | 2:M:335:THR:OG1 | 2.20 | 0.59 |
| 3:B:735:GLU:O | 3:B:736:ASP:C | 2.40 | 0.59 |
| 3:B:799:SER:O | 3:B:800:PRO:O | 2.19 | 0.59 |
| 3:J:1004:ARG:HH12 | 3:J:1016:PRO:HB3 | 1.67 | 0.59 |
| 3:J:1113:LEU:CD1 | 3:J:1113:LEU:H | 2.03 | 0.59 |
| 3:J:448:THR:O | 3:J:450:TRP:N | 2.35 | 0.59 |
| 3:J:577:ARG:HE | 3:J:578:PRO:HD2 | 1.66 | 0.59 |
| 2:M:144:LEU:HA | 2:M:146:TYR:CE2 | 2.37 | 0.59 |
| 4:O:183:CYS:SG | 16:O:1001:F3S:S1 | 3.00 | 0.59 |
| 1:A:558:LYS:HG3 | 3:J:104:GLU:CB | 2.26 | 0.59 |
| 1:A:58:CYS:CB | 1:A:59:PRO:HD3 | 2.29 | 0.59 |
| 3:B:473:MET:SD | 3:B:474:ALA:N | 2.76 | 0.59 |
| 3:B:75:ARG:H | 3:B:75:ARG:HE | 1.50 | 0.59 |
| 2:C:390:MET:HB2 | 5:E:56:GLU:HG2 | 1.85 | 0.59 |
| 1:I:491:TYR:CB | 1:I:607:GLN:OE1 | 2.49 | 0.59 |
| 3:J:315:LEU:O | 3:J:319:ILE:HG12 | 2.02 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:99:THR:O | 3:J:99:THR:HG22 | 2.02 | 0.59 |
| 2:M:309:ASP:C | 2:M:309:ASP:OD2 | 2.41 | 0.59 |
| 2:M:78:VAL:O | 2:M:81:PRO:HD2 | 2.01 | 0.59 |
| 5:Q:110:ILE:HG23 | 5:Q:118:LEU:HB3 | 1.84 | 0.59 |
| 5:Q:53:THR:OG1 | 5:Q:71:GLU:HB2 | 2.03 | 0.59 |
| 1:A:316:LYS:HE2 | 3:B:1054:ASP:OD2 | 2.03 | 0.59 |
| 1:A:502:TYR:HE1 | 1:A:636:ILE:HD11 | 1.66 | 0.59 |
| 3:B:68:PRO:HD3 | 3:B:129:PRO:HG2 | 1.85 | 0.59 |
| 2:C:321:THR:HG22 | 2:C:321:THR:O | 2.02 | 0.59 |
| 4:D:69:SER:HA | 4:D:72:ALA:HB3 | 1.84 | 0.59 |
| 1:I:518:LYS:HE2 | 1:I:544:GLU:HB2 | 1.83 | 0.59 |
| 3:J:700:ARG:N | 11:W:51:SER:O | 2.36 | 0.59 |
| 9:K:45:MET:HE3 | 9:K:45:MET:HA | 1.82 | 0.59 |
| 9:K:54:ASN:HD21 | 9:K:58:SER:HB2 | 1.67 | 0.59 |
| 9:K:74:LEU:HD12 | 9:K:74:LEU:H | 1.65 | 0.59 |
| 2:M:389:THR:HG21 | 9:U:79:ARG:HH11 | 1.67 | 0.59 |
| 6:R:30:SER:OG | 6:R:34:LEU:HB3 | 2.02 | 0.59 |
| 1:A:249:LEU:HB3 | 1:A:266:TRP:CH2 | 2.38 | 0.59 |
| 1:A:720:ASP:O | 1:A:722:PHE:N | 2.33 | 0.59 |
| 4:D:131:VAL:HA | 11:N:2:LEU:HD11 | 1.84 | 0.59 |
| 1:I:659:LYS:O | 1:I:663:ASN:HB2 | 2.02 | 0.59 |
| 1:I:847:GLN:OE1 | 1:I:850:TYR:HA | 2.02 | 0.59 |
| 1:A:878:TRP:N | 3:J:377:ARG:HH12 | 2.00 | 0.59 |
| 9:K:50:LEU:CD2 | 9:K:75:PRO:HD3 | 2.33 | 0.59 |
| 5:E:141:LYS:HB2 | 5:E:172:LEU:HG | 1.85 | 0.59 |
| 1:I:522:GLN:HG2 | 10:V:40:PHE:CE1 | 2.37 | 0.59 |
| 1:I:812:ARG:HE | 2:M:86:THR:HG23 | 1.68 | 0.59 |
| 11:W:18:TRP:CD1 | 11:W:49:LEU:HD22 | 2.38 | 0.59 |
| 1:A:321:SER:O | 1:A:322:SER:HB2 | 2.03 | 0.59 |
| 1:A:530:VAL:HG13 | 1:A:530:VAL:O | 2.02 | 0.59 |
| 1:A:644:PHE:HA | 1:A:724:PHE:CE2 | 2.37 | 0.59 |
| 1:A:750:GLN:HG3 | 1:A:782:ILE:CD1 | 2.32 | 0.59 |
| 1:A:97:THR:HG22 | 1:A:99:ARG:H | 1.67 | 0.59 |
| 3:B:123:LEU:O | 3:B:125:SER:N | 2.36 | 0.59 |
| 7:G:40:PHE:HA | 7:G:92:TYR:HD1 | 1.68 | 0.59 |
| 1:I:826:ALA:H | 2:M:335:THR:HG22 | 1.66 | 0.59 |
| 3:J:900:THR:HG22 | 3:J:970:VAL:HG12 | 1.84 | 0.59 |
| 1:A:569:SER:HB2 | 1:A:584:SER:HG | 1.67 | 0.59 |
| 3:B:730:THR:HB | 3:B:732:TYR:CD1 | 2.36 | 0.59 |
| 2:C:55:ALA:CA | 2:C:58:GLU:HB2 | 2.31 | 0.59 |
| 4:D:51:SER:HB2 | 4:D:52:PRO:HD2 | 1.85 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:508:LEU:O | 1:I:514:THR:HG23 | 2.03 | 0.59 |
| 3:J:325:LEU:HD11 | 3:J:331:GLU:H | 1.67 | 0.59 |
| 2:M:188:ILE:HG23 | 2:M:190:ARG:H | 1.68 | 0.59 |
| 4:O:259:LYS:O | 4:O:263:VAL:CG2 | 2.51 | 0.59 |
| 8:T:59:PRO:HA | 8:T:81:VAL:HB | 1.84 | 0.59 |
| 13:Y:67:LEU:O | 13:Y:71:ASN:ND2 | 2.36 | 0.59 |
| 1:A:752:VAL:C | 1:A:754:GLY:H | 2.06 | 0.58 |
| 3:B:171:ARG:HH22 | 3:B:569:ASN:HD21 | 1.49 | 0.58 |
| 2:C:359:ALA:C | 2:C:361:GLY:H | 2.06 | 0.58 |
| 8:H:31:ILE:HD11 | 9:K:13:LEU:HG | 1.84 | 0.58 |
| 3:J:416:ARG:NH1 | 3:J:687:ARG:NH2 | 2.51 | 0.58 |
| 2:M:202:GLU:O | 2:M:203:ASP:HB2 | 2.03 | 0.58 |
| 1:I:816:SER:OG | 2:M:83:THR:HG22 | 2.02 | 0.58 |
| 5:Q:64:GLY:H | 9:U:41:LEU:CD2 | 2.16 | 0.58 |
| 10:V:6:LEU:HB2 | 10:V:14:GLU:O | 2.03 | 0.58 |
| 1:A:704:LEU:HD22 | 1:A:781:PHE:CE1 | 2.38 | 0.58 |
| 3:B:1069:TRP:CD1 | 3:B:1088:LEU:HD22 | 2.38 | 0.58 |
| 3:B:183:ILE:HG12 | 3:B:206:LYS:HB3 | 1.84 | 0.58 |
| 2:C:268:ASP:OD1 | 2:C:270:ALA:HB3 | 2.03 | 0.58 |
| 1:I:530:VAL:HG13 | 1:I:530:VAL:O | 2.02 | 0.58 |
| 3:J:12:ARG:HH11 | 3:J:596:LYS:HG2 | 1.68 | 0.58 |
| 3:J:193:THR:HG21 | 3:J:197:ARG:H | 1.68 | 0.58 |
| 3:J:325:LEU:HD22 | 3:J:330:ARG:HG3 | 1.85 | 0.58 |
| 4:O:180:VAL:HG21 | 4:O:190:LEU:HG | 1.85 | 0.58 |
| 1:A:491:TYR:HD1 | 1:A:607:GLN:HE22 | 1.49 | 0.58 |
| 1:A:720:ASP:C | 1:A:722:PHE:H | 2.06 | 0.58 |
| 3:B:419:TRP:CZ3 | 3:B:712:GLY:HA3 | 2.38 | 0.58 |
| 3:B:569:ASN:HB3 | 3:B:574:ARG:HH12 | 1.68 | 0.58 |
| 2:C:373:ILE:HG12 | 3:B:1049:LEU:HD13 | 1.85 | 0.58 |
| 6:F:13:PRO:HG2 | 6:F:16:VAL:HG23 | 1.85 | 0.58 |
| 1:I:549:LYS:NZ | 7:S:89:GLY:HA2 | 2.17 | 0.58 |
| 1:I:575:CYS:HG | 1:I:580:CYS:HG | 0.80 | 0.58 |
| 1:I:749:GLN:H | 1:I:781:PHE:HA | 1.69 | 0.58 |
| 3:J:325:LEU:CD1 | 3:J:331:GLU:H | 2.16 | 0.58 |
| 2:M:112:ASP:HA | 2:M:328:GLN:HB3 | 1.86 | 0.58 |
| 4:O:131:VAL:HG22 | 4:O:132:LEU:N | 2.18 | 0.58 |
| 1:I:512:LYS:HE2 | 7:S:91:LYS:HE3 | 1.85 | 0.58 |
| 1:A:48:ARG:HB2 | 1:A:59:PRO:HB3 | 1.84 | 0.58 |
| 2:C:15:GLU:HG3 | 2:C:18:LYS:HD2 | 1.85 | 0.58 |
| 1:I:345:LYS:NZ | 1:I:370:ASP:O | 2.35 | 0.58 |
| 1:I:569:SER:HB2 | 1:I:584:SER:OG | 2.02 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:87:LEU:HD23 | 3:J:688:THR:HG21 | 1.86 | 0.58 |
| 3:J:707:ALA:C | 3:J:709:ASP:H | 2.07 | 0.58 |
| 2:M:70:ILE:O | 2:M:71:GLY:C | 2.41 | 0.58 |
| 4:O:69:SER:HA | 4:O:72:ALA:HB3 | 1.85 | 0.58 |
| 9:U:90:LEU:HD23 | 9:U:90:LEU:H | 1.68 | 0.58 |
| 1:A:301:ARG:HH12 | 1:A:312:ASN:HD21 | 1.52 | 0.58 |
| 1:A:830:LEU:CD2 | 1:A:840:SER:HB3 | 2.26 | 0.58 |
| 3:B:183:ILE:CG1 | 3:B:206:LYS:HB3 | 2.33 | 0.58 |
| 3:B:518:SER:HB3 | 3:B:564:ASN:ND2 | 2.19 | 0.58 |
| 1:I:106:ILE:HG22 | 1:I:107:SER:N | 2.17 | 0.58 |
| 1:I:825:ASN:O | 1:I:826:ALA:C | 2.41 | 0.58 |
| 3:J:160:VAL:O | 3:J:411:SER:HA | 2.03 | 0.58 |
| 4:O:239:GLU:HA | 4:O:242:LEU:HD12 | 1.85 | 0.58 |
| 5:Q:147:ILE:CD1 | 5:Q:163:THR:HB | 2.15 | 0.58 |
| 1:A:155:LYS:HZ1 | 1:A:155:LYS:H | 1.52 | 0.58 |
| 1:A:392:LYS:O | 1:A:394:ARG:HB2 | 2.04 | 0.58 |
| 1:A:509:LEU:O | 1:A:548:GLY:HA3 | 2.03 | 0.58 |
| 3:B:739:ILE:HG12 | 3:B:890:MET:O | 2.03 | 0.58 |
| 2:C:115:LYS:HG3 | 2:C:115:LYS:O | 2.03 | 0.58 |
| 5:E:97:ILE:HD13 | 5:E:136:ILE:HG21 | 1.85 | 0.58 |
| 1:I:83:HIS:HB3 | 1:I:86:LEU:HB2 | 1.86 | 0.58 |
| 1:I:859:TYR:HB2 | 2:M:64:ILE:CG2 | 2.33 | 0.58 |
| 3:J:557:HIS:H | 3:J:623:ASN:ND2 | 2.01 | 0.58 |
| 3:J:992:LYS:CE | 3:J:996:MET:SD | 2.91 | 0.58 |
| 2:M:104:LEU:O | 2:M:108:ILE:HG12 | 2.03 | 0.58 |
| 3:B:227:MET:HE1 | 3:B:232:ILE:HG13 | 1.85 | 0.58 |
| 3:B:873:THR:CG2 | 3:B:874:ILE:N | 2.65 | 0.58 |
| 8:H:46:ARG:NH2 | 13:Y:78:ARG:HH11 | 2.00 | 0.58 |
| 1:I:353:ILE:HG13 | 1:I:361:LEU:CD2 | 2.32 | 0.58 |
| 1:I:803:ARG:HG2 | 3:J:444:ASP:HA | 1.86 | 0.58 |
| 3:J:762:GLU:O | 3:J:764:LYS:HG3 | 2.03 | 0.58 |
| 2:M:277:ILE:C | 2:M:279:GLU:N | 2.57 | 0.58 |
| 2:M:310:ILE:HG22 | 2:M:314:LEU:CD2 | 2.32 | 0.58 |
| 6:R:3:SER:OG | 6:R:4:VAL:N | 2.36 | 0.58 |
| 12:X:26:CYS:HG | 12:X:29:CYS:HB2 | 1.67 | 0.58 |
| 3:B:445:LEU:HD11 | 3:B:455:PRO:HB3 | 1.86 | 0.58 |
| 3:B:794:ASP:N | 3:B:794:ASP:OD1 | 2.31 | 0.58 |
| 1:I:301:ARG:HH12 | 1:I:312:ASN:HD21 | 1.52 | 0.58 |
| 1:I:785:SER:H | 1:I:788:THR:HB | 1.68 | 0.58 |
| 2:M:295:ARG:HA | 2:M:298:SER:HB2 | 1.86 | 0.58 |
| 4:O:98:ILE:CD1 | 4:O:114:ILE:HG13 | 2.30 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:Q:3:LYS:HB2 | 6:R:10:HIS:O | 2.04 | 0.58 |
| 3:B:489:LEU:HD11 | 3:B:568:VAL:HG21 | 1.84 | 0.58 |
| 5:E:108:VAL:HG22 | 5:E:162:LEU:HB2 | 1.85 | 0.58 |
| 1:I:387:ASP:OD2 | 1:I:388:LEU:N | 2.34 | 0.58 |
| 2:M:373:ILE:O | 3:J:1049:LEU:HD11 | 2.04 | 0.58 |
| 3:J:1119:VAL:HG22 | 5:Q:10:ILE:HD13 | 1.85 | 0.58 |
| 2:M:392:PRO:HG3 | 5:Q:68:HIS:HE1 | 1.69 | 0.58 |
| 1:A:589:LYS:O | 1:A:592:ILE:CG1 | 2.49 | 0.58 |
| 3:B:895:VAL:HG11 | 4:D:34:LEU:HD21 | 1.86 | 0.58 |
| 2:C:389:THR:HG21 | 9:K:79:ARG:NH1 | 2.18 | 0.58 |
| 1:I:524:ILE:CG2 | 1:I:634:VAL:HG13 | 2.34 | 0.58 |
| 1:I:97:THR:HG22 | 1:I:99:ARG:H | 1.69 | 0.58 |
| 3:J:1045:LEU:O | 3:J:1049:LEU:HB3 | 2.04 | 0.58 |
| 3:J:376:GLY:O | 3:J:377:ARG:HB3 | 2.02 | 0.58 |
| 9:U:82:LEU:HD12 | 9:U:86:LYS:HB3 | 1.85 | 0.58 |
| 11:W:7:CYS:HB3 | 11:W:45:CYS:SG | 2.44 | 0.58 |
| 3:B:87:LEU:HD23 | 3:B:688:THR:CG2 | 2.34 | 0.57 |
| 3:B:738:ILE:HG23 | 3:B:888:ILE:HA | 1.86 | 0.57 |
| 1:I:289:HIS:HB2 | 1:I:295:LEU:HD21 | 1.86 | 0.57 |
| 3:J:1031:MET:O | 3:J:1034:ASP:HB2 | 2.04 | 0.57 |
| 3:J:457:GLU:HG2 | 3:J:469:ASN:OD1 | 2.04 | 0.57 |
| 3:J:489:LEU:HD11 | 3:J:568:VAL:HG21 | 1.85 | 0.57 |
| 3:J:40:GLN:HE22 | 3:J:62:LYS:HA | 1.69 | 0.57 |
| 3:J:881:ARG:NH1 | 3:J:989:TYR:CB | 2.67 | 0.57 |
| 2:M:103:GLY:HA2 | 2:M:106:ARG:CB | 2.34 | 0.57 |
| 4:O:230:ILE:HG13 | 4:O:242:LEU:HD21 | 1.85 | 0.57 |
| 8:T:19:LYS:HD2 | 8:T:19:LYS:H | 1.69 | 0.57 |
| 1:A:355:PRO:O | 1:A:356:TRP:CD1 | 2.57 | 0.57 |
| 2:C:49:ASP:O | 2:C:52:PHE:N | 2.36 | 0.57 |
| 1:I:4:LYS:HD2 | 3:J:1089:PHE:CB | 2.35 | 0.57 |
| 3:J:324:GLU:O | 3:J:325:LEU:HB2 | 2.04 | 0.57 |
| 1:I:742:GLN:HB2 | 3:J:919:MET:HE3 | 1.86 | 0.57 |
| 2:C:391:ARG:HB3 | 9:K:75:PRO:O | 2.03 | 0.57 |
| 1:A:319:ASP:HB2 | 3:B:1052:ASN:HB3 | 1.86 | 0.57 |
| 2:C:234:ILE:O | 2:C:235:LYS:HG3 | 2.04 | 0.57 |
| 2:C:270:ALA:HA | 8:H:14:HIS:CG | 2.39 | 0.57 |
| 1:I:249:LEU:HB3 | 1:I:266:TRP:CH2 | 2.39 | 0.57 |
| 1:I:477:LYS:O | 1:I:481:LEU:HB2 | 2.03 | 0.57 |
| 1:I:587:VAL:HB | 1:I:594:LEU:O | 2.05 | 0.57 |
| 1:I:865:THR:HG21 | 1:I:870:ARG:NH1 | 2.19 | 0.57 |
| 3:J:922:GLY:O | 3:J:926:GLU:HB2 | 2.02 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:21:SER:O | 2:M:33:LYS:HE3 | 2.04 | 0.57 |
| 3:J:801:GLU:HG3 | 12:X:38:ARG:NH2 | 2.19 | 0.57 |
| 1:A:594:LEU:CA | 7:G:86:LEU:HD22 | 2.33 | 0.57 |
| 1:A:503:ILE:HD11 | 1:A:733:ALA:N | 2.19 | 0.57 |
| 1:A:785:SER:H | 1:A:788:THR:HB | 1.70 | 0.57 |
| 3:B:119:LEU:HD12 | 3:B:120:PRO:HD2 | 1.86 | 0.57 |
| 3:B:14:ILE:HG13 | 3:B:18:PHE:CE2 | 2.40 | 0.57 |
| 3:B:348:ASP:OD2 | 3:B:348:ASP:N | 2.38 | 0.57 |
| 3:B:812:GLY:HA2 | 3:B:836:SER:HB3 | 1.85 | 0.57 |
| 3:J:662:GLN:O | 3:J:663:SER:C | 2.43 | 0.57 |
| 9:K:91:SER:O | 9:K:92:LEU:CB | 2.51 | 0.57 |
| 3:B:853:THR:HG23 | 12:P:32:LYS:O | 2.04 | 0.57 |
| 1:A:327:SER:HB2 | 1:A:444:ARG:HD3 | 1.85 | 0.57 |
| 1:A:477:LYS:O | 1:A:481:LEU:HB2 | 2.05 | 0.57 |
| 1:A:488:THR:HB | 1:A:495:ILE:HB | 1.86 | 0.57 |
| 1:A:555:PHE:HD2 | 1:A:631:LEU:HD13 | 1.69 | 0.57 |
| 3:B:172:VAL:HG22 | 3:B:189:ILE:HD11 | 1.85 | 0.57 |
| 3:B:289:ALA:O | 3:B:293:ILE:HG12 | 2.05 | 0.57 |
| 3:B:64:ARG:HG2 | 3:B:97:TRP:CD1 | 2.39 | 0.57 |
| 3:B:658:PRO:O | 3:B:660:HIS:N | 2.35 | 0.57 |
| 3:J:119:LEU:HD12 | 3:J:120:PRO:HD2 | 1.85 | 0.57 |
| 3:J:210:PHE:CZ | 3:J:323:ILE:HG22 | 2.39 | 0.57 |
| 1:I:637:ARG:NH1 | 3:J:974:ARG:HH22 | 2.02 | 0.57 |
| 2:M:392:PRO:CD | 5:Q:56:GLU:HG3 | 2.34 | 0.57 |
| 1:A:607:GLN:O | 1:A:608:PRO:C | 2.43 | 0.57 |
| 3:B:159:ARG:HD3 | 3:B:399:ALA:HA | 1.86 | 0.57 |
| 3:B:402:ASN:HB2 | 3:B:410:VAL:CG2 | 2.34 | 0.57 |
| 3:B:43:ILE:O | 3:B:43:ILE:HG22 | 2.04 | 0.57 |
| 3:B:495:VAL:O | 3:B:528:GLY:HA3 | 2.04 | 0.57 |
| 2:C:340:SER:HA | 2:C:364:GLU:CG | 2.34 | 0.57 |
| 8:H:63:ILE:CG2 | 8:H:64:ARG:N | 2.67 | 0.57 |
| 3:J:451:GLY:CA | 3:J:577:ARG:NH1 | 2.68 | 0.57 |
| 3:J:6:THR:HG22 | 3:J:7:ILE:H | 1.69 | 0.57 |
| 3:J:943:THR:HG22 | 3:J:944:PRO:HD2 | 1.87 | 0.57 |
| 2:M:61:GLU:C | 2:M:63:LEU:H | 2.06 | 0.57 |
| 5:Q:18:PHE:HE2 | 9:U:42:GLN:HG2 | 1.70 | 0.57 |
| 1:A:490:ARG:HG3 | 2:C:77:SER:HB3 | 1.86 | 0.57 |
| 3:B:68:PRO:HA | 3:B:93:ALA:O | 2.05 | 0.57 |
| 2:C:70:ILE:HA | 2:C:73:VAL:CG2 | 2.33 | 0.57 |
| 1:I:249:LEU:HD22 | 1:I:266:TRP:CE2 | 2.40 | 0.57 |
| 1:I:833:GLU:OE2 | 1:I:839:ARG:HB2 | 2.05 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:702:LEU:HD22 | 3:J:933:ALA:CB | 2.27 | 0.57 |
| 2:M:53:ASP:C | 2:M:55:ALA:H | 2.07 | 0.57 |
| 11:W:6:ARG:HG2 | 11:W:11:GLY:O | 2.05 | 0.57 |
| 1:A:426:HIS:CE1 | 1:A:428:ILE:CG2 | 2.85 | 0.57 |
| 3:B:315:LEU:O | 3:B:319:ILE:HG12 | 2.04 | 0.57 |
| 3:B:367:TYR:CD2 | 3:B:367:TYR:C | 2.77 | 0.57 |
| 3:B:376:GLY:O | 3:B:377:ARG:HB3 | 2.05 | 0.57 |
| 3:B:727:MET:CE | 3:B:898:PRO:HG3 | 2.35 | 0.57 |
| 1:I:426:HIS:O | 1:I:429:SER:HB2 | 2.04 | 0.57 |
| 3:J:26:GLN:O | 3:J:345:LEU:CD2 | 2.42 | 0.57 |
| 2:M:107:LEU:O | 2:M:111:VAL:HG23 | 2.04 | 0.57 |
| 1:A:575:CYS:HG | 1:A:580:CYS:HB3 | 1.70 | 0.57 |
| 1:A:98:CYS:O | 1:A:99:ARG:HB2 | 2.05 | 0.57 |
| 3:B:291:GLN:C | 3:B:293:ILE:H | 2.08 | 0.57 |
| 3:B:116:ILE:HD12 | 3:B:361:PHE:CZ | 2.40 | 0.57 |
| 1:A:803:ARG:HG2 | 3:B:444:ASP:HA | 1.86 | 0.57 |
| 3:B:64:ARG:HG2 | 3:B:97:TRP:CG | 2.39 | 0.57 |
| 1:A:734:ARG:HG3 | 3:B:917:SER:HB3 | 1.85 | 0.57 |
| 2:C:373:ILE:HD13 | 3:B:1033:ARG:HD3 | 1.87 | 0.57 |
| 5:E:88:GLU:H | 5:E:99:VAL:HG13 | 1.68 | 0.57 |
| 6:F:15:SER:HA | 6:F:18:LYS:NZ | 2.19 | 0.57 |
| 7:G:80:GLU:HG2 | 7:G:81:LEU:N | 2.20 | 0.57 |
| 1:I:133:THR:HB | 1:I:137:LYS:HZ2 | 1.70 | 0.57 |
| 1:I:352:ARG:HA | 1:I:406:ILE:HA | 1.86 | 0.57 |
| 1:I:6:ILE:HD11 | 3:J:1091:VAL:HG11 | 1.86 | 0.57 |
| 3:J:1054:ASP:HB3 | 3:J:1095:TYR:H | 1.69 | 0.57 |
| 3:J:197:ARG:HH22 | 3:J:359:LYS:HG2 | 1.70 | 0.57 |
| 3:J:116:ILE:HG22 | 3:J:390:VAL:HG21 | 1.85 | 0.57 |
| 3:J:338:TYR:HB2 | 3:J:448:THR:HG21 | 1.87 | 0.57 |
| 3:J:683:ASN:O | 3:J:685:GLN:N | 2.38 | 0.57 |
| 3:J:82:PRO:HG3 | 3:J:130:ILE:CD1 | 2.35 | 0.57 |
| 5:Q:30:LEU:HD21 | 5:Q:72:PHE:CE1 | 2.40 | 0.57 |
| 1:A:106:ILE:HG22 | 1:A:107:SER:N | 2.20 | 0.57 |
| 2:C:355:LEU:CD2 | 3:B:1109:ILE:HD11 | 2.35 | 0.57 |
| 3:B:291:GLN:O | 3:B:295:LYS:HG2 | 2.05 | 0.57 |
| 4:D:134:GLY:N | 4:D:137:GLN:OE1 | 2.23 | 0.57 |
| 3:J:445:LEU:HD11 | 3:J:455:PRO:CB | 2.34 | 0.57 |
| 2:M:103:GLY:HA3 | 2:M:300:VAL:HG13 | 1.87 | 0.57 |
| 1:A:764:ARG:CB | 1:A:764:ARG:HH11 | 2.18 | 0.56 |
| 1:A:825:ASN:O | 1:A:826:ALA:C | 2.44 | 0.56 |
| 3:B:699:GLN:HB2 | 3:B:720:ASN:HA | 1.87 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:110:ILE:HD11 | 2:C:277:ILE:HD11 | 1.86 | 0.56 |
| 2:C:139:GLU:HG2 | 2:C:142:ARG:HD2 | 1.86 | 0.56 |
| 4:D:101:GLU:O | 4:D:107:ARG:NH1 | 2.36 | 0.56 |
| 4:D:53:LEU:HD22 | 4:D:57:ILE:CG2 | 2.35 | 0.56 |
| 1:A:594:LEU:HA | 7:G:86:LEU:CD2 | 2.33 | 0.56 |
| 1:I:176:THR:O | 1:I:180:ILE:HG13 | 2.04 | 0.56 |
| 1:I:764:ARG:HB2 | 1:I:764:ARG:HH11 | 1.69 | 0.56 |
| 3:J:870:ARG:CZ | 3:J:996:MET:SD | 2.93 | 0.56 |
| 5:Q:42:LEU:HD23 | 5:Q:42:LEU:H | 1.69 | 0.56 |
| 7:S:17:SER:HB2 | 7:S:19:GLU:HG3 | 1.86 | 0.56 |
| 1:A:369:PRO:HA | 1:A:410:HIS:HE1 | 1.70 | 0.56 |
| 3:B:193:THR:HG21 | 3:B:197:ARG:H | 1.70 | 0.56 |
| 4:D:133:LEU:HD21 | 4:D:139:ILE:HG13 | 1.87 | 0.56 |
| 1:I:446:ASN:ND2 | 1:I:448:LEU:H | 2.03 | 0.56 |
| 1:I:853:ASP:HB2 | 2:M:311:ARG:NH1 | 2.20 | 0.56 |
| 3:J:181:SER:O | 3:J:182:ASN:HB2 | 2.06 | 0.56 |
| 3:J:183:ILE:CD1 | 3:J:183:ILE:O | 2.53 | 0.56 |
| 3:J:64:ARG:O | 3:J:97:TRP:HB2 | 2.05 | 0.56 |
| 3:J:739:ILE:HG23 | 3:J:909:ILE:HB | 1.86 | 0.56 |
| 7:S:18:ILE:O | 7:S:18:ILE:HG22 | 2.05 | 0.56 |
| 1:A:749:GLN:N | 1:A:781:PHE:HA | 2.21 | 0.56 |
| 3:B:157:SER:O | 3:B:158:GLU:HB2 | 2.04 | 0.56 |
| 3:B:419:TRP:HZ3 | 3:B:712:GLY:HA3 | 1.70 | 0.56 |
| 3:B:457:GLU:OE1 | 3:B:652:ALA:HB2 | 2.06 | 0.56 |
| 3:B:662:GLN:O | 3:B:663:SER:C | 2.44 | 0.56 |
| 3:B:910:LEU:CD2 | 3:B:911:ASN:N | 2.66 | 0.56 |
| 4:D:94:THR:OG1 | 4:D:95:LYS:N | 2.39 | 0.56 |
| 1:I:116:ARG:HE | 1:I:117:ILE:HG12 | 1.71 | 0.56 |
| 1:I:392:LYS:O | 1:I:394:ARG:HB2 | 2.06 | 0.56 |
| 1:I:512:LYS:HE2 | 7:S:91:LYS:NZ | 2.19 | 0.56 |
| 1:I:870:ARG:NH2 | 2:M:57:LYS:O | 2.38 | 0.56 |
| 2:M:262:LEU:HD23 | 2:M:269:VAL:HG11 | 1.86 | 0.56 |
| 4:O:96:ILE:CG1 | 4:O:143:ALA:HB3 | 2.36 | 0.56 |
| 4:O:51:SER:HB2 | 4:O:52:PRO:HD2 | 1.87 | 0.56 |
| 2:M:390:MET:HB2 | 5:Q:56:GLU:HG2 | 1.87 | 0.56 |
| 3:B:591:ILE:H | 3:B:591:ILE:HD12 | 1.70 | 0.56 |
| 2:C:390:MET:HE1 | 5:E:66:THR:HA | 1.87 | 0.56 |
| 1:I:710:THR:O | 1:I:714:ILE:HG12 | 2.06 | 0.56 |
| 3:J:171:ARG:HH22 | 3:J:569:ASN:HD21 | 1.53 | 0.56 |
| 3:J:710:ILE:H | 3:J:710:ILE:HD13 | 1.69 | 0.56 |
| 5:Q:124:ARG:HE | 5:Q:126:ILE:HD13 | 1.71 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:S:87:ASN:C | 7:S:89:GLY:H | 2.09 | 0.56 |
| 1:A:220:ARG:N | 1:A:221:PRO:HD3 | 2.20 | 0.56 |
| 3:B:1036:LEU:HD22 | 3:B:1041:THR:HG21 | 1.87 | 0.56 |
| 5:E:179:LYS:NZ | 6:F:81:ASP:HB2 | 2.20 | 0.56 |
| 7:G:82:LYS:HB2 | 7:G:95:ILE:HG13 | 1.86 | 0.56 |
| 1:I:557:PRO:HD3 | 1:I:623:TYR:OH | 2.05 | 0.56 |
| 1:I:569:SER:HB2 | 1:I:584:SER:HG | 1.69 | 0.56 |
| 1:I:81:VAL:HG23 | 1:I:209:LEU:HB2 | 1.87 | 0.56 |
| 9:K:23:TRP:HE3 | 9:K:23:TRP:HA | 1.69 | 0.56 |
| 5:Q:113:ILE:O | 5:Q:164:MET:HB2 | 2.05 | 0.56 |
| 1:A:345:LYS:HG2 | 1:A:410:HIS:CD2 | 2.41 | 0.56 |
| 3:B:230:LEU:HD13 | 3:B:312:ALA:HA | 1.88 | 0.56 |
| 3:B:451:GLY:CA | 3:B:577:ARG:NH1 | 2.68 | 0.56 |
| 3:B:81:SER:O | 3:B:84:GLU:HB2 | 2.06 | 0.56 |
| 1:A:816:SER:OG | 2:C:83:THR:HA | 2.06 | 0.56 |
| 9:K:35:VAL:HG22 | 9:K:36:ILE:HD13 | 1.88 | 0.56 |
| 11:N:22:ILE:HD13 | 11:N:23:THR:N | 2.20 | 0.56 |
| 1:A:518:LYS:HE2 | 1:A:544:GLU:HB2 | 1.87 | 0.56 |
| 3:B:544:ARG:HB2 | 3:B:549:ILE:HG22 | 1.88 | 0.56 |
| 2:C:376:GLY:HA2 | 3:B:1049:LEU:HD21 | 1.87 | 0.56 |
| 7:G:79:THR:HG22 | 7:G:80:GLU:H | 1.70 | 0.56 |
| 8:H:40:GLU:HG2 | 8:H:41:GLN:N | 2.20 | 0.56 |
| 1:I:727:VAL:O | 1:I:729:ALA:O | 2.23 | 0.56 |
| 3:J:227:MET:HE1 | 3:J:232:ILE:HG13 | 1.86 | 0.56 |
| 3:J:68:PRO:HD3 | 3:J:129:PRO:HG2 | 1.87 | 0.56 |
| 3:J:765:TYR:CG | 3:J:766:PRO:HD2 | 2.41 | 0.56 |
| 3:J:943:THR:CG2 | 3:J:944:PRO:HD2 | 2.35 | 0.56 |
| 3:J:946:TYR:HD2 | 3:J:947:LYS:H | 1.54 | 0.56 |
| 4:O:253:ILE:HG13 | 10:V:73:ILE:HD13 | 1.88 | 0.56 |
| 8:T:29:TYR:OH | 13:Z:67:LEU:HD13 | 2.05 | 0.56 |
| 3:B:1004:ARG:HH12 | 3:B:1016:PRO:HB3 | 1.70 | 0.56 |
| 1:A:4:LYS:HD3 | 3:B:1091:VAL:HB | 1.88 | 0.56 |
| 3:B:719:GLY:O | 3:B:989:TYR:CE1 | 2.59 | 0.56 |
| 3:B:83:MET:O | 3:B:87:LEU:HD12 | 2.06 | 0.56 |
| 1:I:575:CYS:CB | 1:I:580:CYS:HG | 2.18 | 0.56 |
| 3:J:741:ASN:OD1 | 3:J:743:SER:N | 2.39 | 0.56 |
| 11:N:3:ILE:HG22 | 11:N:4:PRO:HD2 | 1.88 | 0.56 |
| 1:A:563:HIS:HB2 | 1:A:872:PHE:HE2 | 1.70 | 0.56 |
| 2:C:383:THR:HG22 | 3:B:1040:GLY:O | 2.05 | 0.56 |
| 2:C:387:GLU:OE1 | 9:K:81:ARG:HD2 | 2.06 | 0.56 |
| 1:I:220:ARG:N | 1:I:221:PRO:HD3 | 2.21 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:55:GLY:O | 1:I:57:LYS:N | 2.39 | 0.56 |
| 3:J:381:LEU:C | 3:J:383:ALA:H | 2.09 | 0.56 |
| 3:J:402:ASN:HB2 | 3:J:410:VAL:CG2 | 2.36 | 0.56 |
| 2:M:14:GLU:O | 2:M:17:VAL:HG12 | 2.05 | 0.56 |
| 2:M:24:LEU:HD13 | 2:M:33:LYS:HA | 1.88 | 0.56 |
| 2:M:72:ILE:N | 2:M:72:ILE:CD1 | 2.63 | 0.56 |
| 2:M:80:GLU:HB3 | 2:M:81:PRO:HD3 | 1.87 | 0.56 |
| 5:Q:11:VAL:HG12 | 5:Q:12:ARG:H | 1.70 | 0.56 |
| 9:U:33:ALA:O | 9:U:35:VAL:N | 2.39 | 0.56 |
| 10:V:80:THR:O | 10:V:84:ILE:HG12 | 2.05 | 0.56 |
| 1:A:91:TYR:OH | 1:A:153:GLN:O | 2.12 | 0.56 |
| 1:A:15:SER:HA | 1:A:203:ARG:NH2 | 2.19 | 0.56 |
| 1:A:288:LYS:HG2 | 1:A:294:PRO:HA | 1.88 | 0.56 |
| 3:B:43:ILE:HG13 | 3:B:63:ILE:CD1 | 2.36 | 0.56 |
| 2:C:238:LYS:HB2 | 2:C:239:ARG:CZ | 2.36 | 0.56 |
| 2:C:30:ASP:O | 2:C:31:ASP:HB3 | 2.05 | 0.56 |
| 2:C:70:ILE:H | 2:C:70:ILE:CD1 | 2.19 | 0.56 |
| 4:D:34:LEU:HA | 4:D:150:GLY:HA3 | 1.88 | 0.56 |
| 1:I:509:LEU:O | 1:I:548:GLY:HA3 | 2.05 | 0.56 |
| 3:J:1071:ASP:C | 3:J:1073:ASN:H | 2.09 | 0.56 |
| 3:J:365:LEU:O | 3:J:369:LEU:HB2 | 2.06 | 0.56 |
| 3:J:687:ARG:NH1 | 3:J:687:ARG:HG3 | 2.11 | 0.56 |
| 2:C:386:VAL:HG11 | 9:K:31:GLU:HA | 1.88 | 0.56 |
| 2:M:159:ASP:HB3 | 2:M:163:MET:CB | 2.35 | 0.56 |
| 1:A:155:LYS:CB | 1:A:156:ILE:HA | 2.35 | 0.56 |
| 3:B:12:ARG:HH11 | 3:B:596:LYS:HG2 | 1.70 | 0.56 |
| 2:C:286:ILE:O | 2:C:289:ALA:HB3 | 2.05 | 0.56 |
| 1:I:155:LYS:CB | 1:I:156:ILE:HA | 2.35 | 0.56 |
| 1:I:345:LYS:HG2 | 1:I:410:HIS:CD2 | 2.41 | 0.56 |
| 1:I:491:TYR:HD1 | 1:I:607:GLN:HE22 | 1.53 | 0.56 |
| 1:I:610:SER:O | 1:I:613:HIS:HB3 | 2.06 | 0.56 |
| 1:I:831:ARG:NH2 | 2:M:385:MET:HG3 | 2.20 | 0.56 |
| 1:I:317:ARG:HB2 | 3:J:1016:PRO:HB2 | 1.87 | 0.56 |
| 3:J:683:ASN:C | 3:J:685:GLN:H | 2.09 | 0.56 |
| 3:J:82:PRO:HG3 | 3:J:130:ILE:HD11 | 1.88 | 0.56 |
| 4:D:129:PRO:HG2 | 11:N:15:ALA:HB1 | 1.88 | 0.56 |
| 13:Y:63:GLU:O | 13:Y:67:LEU:HD13 | 2.06 | 0.56 |
| 1:A:742:GLN:CB | 3:B:919:MET:HE3 | 2.35 | 0.55 |
| 1:A:742:GLN:HB3 | 3:B:919:MET:HE1 | 1.88 | 0.55 |
| 3:B:1100:LEU:O | 3:B:1101:ILE:C | 2.44 | 0.55 |
| 3:B:325:LEU:HD13 | 3:B:330:ARG:H | 1.70 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:146:TYR:CE1 | 2:C:237:ILE:HG12 | 2.41 | 0.55 |
| 1:I:156:ILE:HD11 | 1:I:270:GLN:HG2 | 1.88 | 0.55 |
| 1:I:215:PRO:HB2 | 1:I:219:ILE:HD11 | 1.88 | 0.55 |
| 1:I:563:HIS:HB2 | 1:I:872:PHE:HE2 | 1.71 | 0.55 |
| 1:I:98:CYS:O | 1:I:99:ARG:HB2 | 2.06 | 0.55 |
| 3:J:24:VAL:HG21 | 3:J:426:LEU:HD13 | 1.87 | 0.55 |
| 2:M:53:ASP:C | 2:M:55:ALA:N | 2.59 | 0.55 |
| 3:J:934:ALA:HB2 | 11:W:47:ARG:HD3 | 1.87 | 0.55 |
| 1:A:249:LEU:HD13 | 1:A:266:TRP:CE3 | 2.41 | 0.55 |
| 3:B:197:ARG:HH22 | 3:B:359:LYS:HG2 | 1.71 | 0.55 |
| 3:B:318:ALA:O | 3:B:321:LYS:HB2 | 2.06 | 0.55 |
| 3:B:210:PHE:CZ | 3:B:323:ILE:HG22 | 2.38 | 0.55 |
| 3:B:760:THR:OG1 | 3:B:813:LYS:HD2 | 2.06 | 0.55 |
| 3:B:848:ASP:OD1 | 3:B:865:ARG:CZ | 2.54 | 0.55 |
| 5:E:39:LEU:HD22 | 5:E:41:ASP:H | 1.69 | 0.55 |
| 1:I:94:LEU:HD11 | 1:I:180:ILE:HG23 | 1.88 | 0.55 |
| 1:I:81:VAL:HG12 | 1:I:270:GLN:HG3 | 1.87 | 0.55 |
| 3:J:727:MET:HE3 | 3:J:898:PRO:HG3 | 1.87 | 0.55 |
| 3:J:922:GLY:O | 3:J:926:GLU:N | 2.34 | 0.55 |
| 3:J:902:LYS:CB | 11:W:42:ARG:NH1 | 2.69 | 0.55 |
| 1:A:610:SER:O | 1:A:613:HIS:HB3 | 2.05 | 0.55 |
| 1:A:650:ASP:HB3 | 1:A:723:ASN:ND2 | 2.21 | 0.55 |
| 3:B:762:GLU:O | 3:B:764:LYS:HG3 | 2.06 | 0.55 |
| 3:J:552:GLU:HA | 3:J:576:ARG:HH22 | 1.71 | 0.55 |
| 2:M:285:GLY:HA2 | 8:T:49:ASP:OD2 | 2.06 | 0.55 |
| 2:M:384:GLY:HA2 | 5:Q:61:PHE:CZ | 2.41 | 0.55 |
| 6:R:14:TYR:N | 6:R:14:TYR:CD1 | 2.74 | 0.55 |
| 4:O:137:GLN:HE21 | 11:W:63:THR:HG22 | 1.71 | 0.55 |
| 3:B:390:VAL:O | 3:B:394:ILE:HB | 2.06 | 0.55 |
| 1:I:25:THR:HG22 | 1:I:27:ILE:H | 1.71 | 0.55 |
| 1:I:293:ARG:HD3 | 1:I:296:ARG:HH22 | 1.71 | 0.55 |
| 1:I:305:LYS:HA | 1:I:310:ARG:HD2 | 1.88 | 0.55 |
| 1:I:752:VAL:C | 1:I:754:GLY:H | 2.10 | 0.55 |
| 1:I:849:ALA:HB2 | 9:U:15:PHE:CG | 2.40 | 0.55 |
| 3:J:1009:VAL:HB | 3:J:1014:ARG:O | 2.06 | 0.55 |
| 3:J:1074:LYS:HE2 | 3:J:1074:LYS:HA | 1.88 | 0.55 |
| 3:J:730:THR:HB | 3:J:732:TYR:CD1 | 2.38 | 0.55 |
| 3:J:727:MET:HE3 | 3:J:898:PRO:CG | 2.37 | 0.55 |
| 2:M:28:ILE:HG13 | 9:U:18:VAL:HG21 | 1.89 | 0.55 |
| 4:O:34:LEU:HD22 | 4:O:151:LYS:HB2 | 1.87 | 0.55 |
| 1:A:113:LYS:HA | 1:A:116:ARG:HB3 | 1.88 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:426:HIS:HD2 | 1:A:490:ARG:HH12 | 1.51 | 0.55 |
| 1:A:81:VAL:HG23 | 1:A:209:LEU:HB2 | 1.86 | 0.55 |
| 3:B:1031:MET:O | 3:B:1034:ASP:HB2 | 2.07 | 0.55 |
| 3:B:950:ILE:O | 3:B:952:GLN:N | 2.39 | 0.55 |
| 2:C:366:PHE:O | 2:C:368:GLY:N | 2.39 | 0.55 |
| 4:D:239:GLU:HA | 4:D:242:LEU:HD12 | 1.89 | 0.55 |
| 1:A:549:LYS:HB2 | 7:G:88:ASN:O | 2.06 | 0.55 |
| 1:I:26:ALA:HA | 1:I:74:HIS:CE1 | 2.41 | 0.55 |
| 3:J:106:ASN:O | 3:J:108:GLU:HG3 | 2.07 | 0.55 |
| 3:J:582:VAL:HG13 | 3:J:586:ASN:N | 2.21 | 0.55 |
| 3:J:745:VAL:HG21 | 3:J:891:LEU:HD11 | 1.88 | 0.55 |
| 3:J:910:LEU:HD22 | 3:J:911:ASN:H | 1.70 | 0.55 |
| 10:V:59:THR:HG21 | 10:V:65:PRO:CD | 2.35 | 0.55 |
| 1:A:58:CYS:HB2 | 1:A:59:PRO:CD | 2.36 | 0.55 |
| 2:C:318:ASP:O | 2:C:322:ARG:CZ | 2.54 | 0.55 |
| 7:G:79:THR:HG22 | 7:G:80:GLU:N | 2.20 | 0.55 |
| 1:I:337:VAL:HG21 | 1:I:419:PHE:CD1 | 2.41 | 0.55 |
| 1:I:604:GLY:C | 1:I:606:GLN:N | 2.58 | 0.55 |
| 1:I:704:LEU:HD13 | 1:I:781:PHE:HD1 | 1.72 | 0.55 |
| 1:A:532:ILE:HG23 | 10:L:40:PHE:CG | 2.41 | 0.55 |
| 4:D:253:ILE:HD11 | 10:L:76:ILE:HD12 | 1.88 | 0.55 |
| 2:M:390:MET:O | 2:M:391:ARG:HB3 | 2.04 | 0.55 |
| 7:S:6:ALA:HB1 | 7:S:62:ASN:OD1 | 2.07 | 0.55 |
| 8:T:46:ARG:HD2 | 8:T:48:SER:HB2 | 1.87 | 0.55 |
| 1:A:25:THR:HG22 | 1:A:27:ILE:H | 1.71 | 0.55 |
| 3:B:560:THR:HG22 | 3:B:562:PHE:N | 2.17 | 0.55 |
| 2:C:213:ILE:O | 2:C:213:ILE:HG22 | 2.07 | 0.55 |
| 2:C:146:TYR:HD1 | 2:C:238:LYS:H | 1.55 | 0.55 |
| 7:G:86:LEU:HD12 | 7:G:91:LYS:HG3 | 1.88 | 0.55 |
| 3:J:43:ILE:O | 3:J:43:ILE:HG22 | 2.06 | 0.55 |
| 5:Q:46:LEU:HD11 | 5:Q:77:TYR:HB2 | 1.88 | 0.55 |
| 5:Q:97:ILE:CD1 | 5:Q:113:ILE:HD11 | 2.34 | 0.55 |
| 3:B:1113:LEU:CD1 | 3:B:1113:LEU:H | 2.07 | 0.55 |
| 3:B:726:VAL:HG12 | 3:B:912:PRO:HG3 | 1.88 | 0.55 |
| 1:I:84:VAL:CG1 | 1:I:274:ALA:HB1 | 2.36 | 0.55 |
| 1:I:742:GLN:CB | 3:J:919:MET:CE | 2.85 | 0.55 |
| 3:J:657:TYR:O | 3:J:660:HIS:HB2 | 2.06 | 0.55 |
| 3:J:764:LYS:NZ | 3:J:772:LYS:O | 2.40 | 0.55 |
| 3:J:963:LEU:HD21 | 4:O:206:CYS:SG | 2.47 | 0.55 |
| 2:M:369:VAL:HG21 | 3:J:1037:ILE:HG21 | 1.87 | 0.55 |
| 11:N:42:ARG:CG | 11:N:43:TYR:H | 2.19 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:595:GLU:HB3 | 7:S:86:LEU:HD13 | 1.89 | 0.55 |
| 10:V:38:VAL:HG13 | 10:V:58:LEU:O | 2.06 | 0.55 |
| 11:W:3:ILE:HG22 | 11:W:4:PRO:HD2 | 1.88 | 0.55 |
| 13:Z:76:GLU:O | 13:Z:77:LYS:HB3 | 2.07 | 0.55 |
| 1:A:763:THR:CG2 | 1:A:772:TYR:HA | 2.37 | 0.55 |
| 3:B:765:TYR:CG | 3:B:766:PRO:HD2 | 2.42 | 0.55 |
| 3:B:946:TYR:HD2 | 3:B:947:LYS:H | 1.55 | 0.55 |
| 2:C:257:ASN:OD1 | 2:C:259:SER:HB2 | 2.07 | 0.55 |
| 1:A:595:GLU:N | 7:G:86:LEU:HD22 | 2.22 | 0.55 |
| 11:N:7:CYS:CB | 11:N:45:CYS:SG | 2.95 | 0.55 |
| 4:O:106:PRO:HA | 4:O:134:GLY:HA2 | 1.87 | 0.55 |
| 4:O:21:PRO:HG3 | 10:V:79:MET:SD | 2.47 | 0.55 |
| 1:A:249:LEU:HD22 | 1:A:266:TRP:CE2 | 2.42 | 0.55 |
| 1:A:387:ASP:OD2 | 1:A:388:LEU:N | 2.35 | 0.55 |
| 1:A:828:SER:C | 1:A:830:LEU:N | 2.61 | 0.55 |
| 1:A:501:ASP:OD2 | 3:B:913:HIS:CD2 | 2.60 | 0.55 |
| 1:I:589:LYS:O | 1:I:592:ILE:CG1 | 2.54 | 0.55 |
| 10:L:59:THR:CG2 | 10:L:65:PRO:HD3 | 2.35 | 0.55 |
| 2:M:124:ILE:HG21 | 2:M:267:VAL:HG13 | 1.89 | 0.55 |
| 3:B:139:ILE:HD13 | 11:N:61:HIS:CD2 | 2.42 | 0.55 |
| 3:B:147:ASP:OD2 | 3:B:148:PRO:HD2 | 2.07 | 0.54 |
| 3:B:346:ALA:O | 3:B:350:PHE:N | 2.36 | 0.54 |
| 5:E:27:LEU:HB2 | 5:E:51:VAL:HG11 | 1.89 | 0.54 |
| 1:A:540:LEU:HB3 | 7:G:66:TYR:OH | 2.06 | 0.54 |
| 1:I:203:ARG:HG3 | 1:I:205:GLU:HB2 | 1.88 | 0.54 |
| 1:I:608:PRO:C | 1:I:609:GLU:HG2 | 2.27 | 0.54 |
| 1:I:555:PHE:CD2 | 1:I:631:LEU:HD13 | 2.42 | 0.54 |
| 3:J:616:LEU:HD11 | 3:J:639:HIS:CE1 | 2.41 | 0.54 |
| 3:J:672:MET:HA | 3:J:675:GLN:HB2 | 1.88 | 0.54 |
| 3:J:799:SER:O | 3:J:800:PRO:O | 2.25 | 0.54 |
| 2:M:311:ARG:H | 2:M:311:ARG:HD3 | 1.72 | 0.54 |
| 11:N:35:LEU:CD2 | 11:N:40:VAL:HG21 | 2.37 | 0.54 |
| 4:O:134:GLY:N | 4:O:137:GLN:OE1 | 2.23 | 0.54 |
| 3:B:1010:GLN:HA | 3:B:1010:GLN:OE1 | 2.07 | 0.54 |
| 3:B:70:VAL:HG11 | 3:B:90:LEU:HD23 | 1.90 | 0.54 |
| 3:B:729:PHE:C | 3:B:731:GLY:H | 2.11 | 0.54 |
| 3:B:727:MET:CE | 3:B:898:PRO:CG | 2.85 | 0.54 |
| 3:J:157:SER:O | 3:J:158:GLU:HB2 | 2.07 | 0.54 |
| 3:J:365:LEU:HG | 3:J:369:LEU:HD12 | 1.90 | 0.54 |
| 3:J:159:ARG:HD3 | 3:J:399:ALA:HA | 1.89 | 0.54 |
| 3:J:98:LEU:C | 3:J:98:LEU:HD13 | 2.27 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:O:254:GLU:CG | 10:V:77:ARG:HH12 | 2.20 | 0.54 |
| 3:B:800:PRO:HB2 | 12:P:38:ARG:HA | 1.87 | 0.54 |
| 9:U:82:LEU:HD11 | 9:U:88:ILE:HD11 | 1.88 | 0.54 |
| 1:A:742:GLN:CB | 3:B:919:MET:CE | 2.86 | 0.54 |
| 3:B:365:LEU:O | 3:B:369:LEU:HB2 | 2.07 | 0.54 |
| 1:I:249:LEU:HD13 | 1:I:266:TRP:CE3 | 2.42 | 0.54 |
| 1:I:868:VAL:O | 1:I:871:ILE:HG22 | 2.06 | 0.54 |
| 3:J:172:VAL:HG22 | 3:J:189:ILE:HD11 | 1.89 | 0.54 |
| 5:Q:29:GLU:O | 5:Q:33:GLN:HG3 | 2.07 | 0.54 |
| 11:W:35:LEU:CD2 | 11:W:40:VAL:HG21 | 2.37 | 0.54 |
| 1:A:116:ARG:HE | 1:A:117:ILE:HG12 | 1.73 | 0.54 |
| 1:A:448:LEU:HD23 | 1:A:498:ALA:HA | 1.88 | 0.54 |
| 3:B:588:LEU:CD1 | 3:B:612:LYS:HB3 | 2.37 | 0.54 |
| 6:F:55:VAL:O | 6:F:59:LEU:HB2 | 2.08 | 0.54 |
| 3:J:582:VAL:HG13 | 3:J:586:ASN:H | 1.73 | 0.54 |
| 2:M:146:TYR:HB2 | 2:M:238:LYS:HD3 | 1.90 | 0.54 |
| 2:M:291:GLU:HA | 2:M:294:ILE:HD12 | 1.90 | 0.54 |
| 5:Q:66:THR:HG22 | 5:Q:68:HIS:NE2 | 2.21 | 0.54 |
| 1:A:84:VAL:CG1 | 1:A:274:ALA:HB1 | 2.37 | 0.54 |
| 1:A:84:VAL:HG11 | 1:A:274:ALA:HB1 | 1.88 | 0.54 |
| 1:A:507:TYR:O | 1:A:508:LEU:CB | 2.56 | 0.54 |
| 3:B:904:VAL:HG21 | 11:N:42:ARG:HE | 1.72 | 0.54 |
| 3:B:910:LEU:HD22 | 3:B:911:ASN:H | 1.68 | 0.54 |
| 2:C:107:LEU:O | 2:C:111:VAL:HG23 | 2.07 | 0.54 |
| 1:I:446:ASN:HD22 | 1:I:447:LEU:N | 2.05 | 0.54 |
| 3:J:457:GLU:OE1 | 3:J:652:ALA:HB2 | 2.08 | 0.54 |
| 3:J:518:SER:HB3 | 3:J:564:ASN:ND2 | 2.22 | 0.54 |
| 3:J:812:GLY:HA2 | 3:J:836:SER:CB | 2.36 | 0.54 |
| 1:A:470:GLU:HB2 | 9:K:41:LEU:HD12 | 1.89 | 0.54 |
| 2:M:52:PHE:O | 2:M:56:ILE:HG12 | 2.08 | 0.54 |
| 2:M:63:LEU:HD21 | 9:U:23:TRP:HZ3 | 1.72 | 0.54 |
| 1:A:102:GLY:H | 1:A:103:ARG:HE | 1.54 | 0.54 |
| 1:A:345:LYS:NZ | 1:A:370:ASP:O | 2.35 | 0.54 |
| 1:A:508:LEU:O | 1:A:514:THR:HG23 | 2.08 | 0.54 |
| 3:B:200:VAL:O | 3:B:200:VAL:HG13 | 2.08 | 0.54 |
| 3:B:463:ASN:HB3 | 3:B:467:VAL:CG1 | 2.38 | 0.54 |
| 3:B:707:ALA:C | 3:B:709:ASP:H | 2.10 | 0.54 |
| 6:F:65:ARG:O | 6:F:69:ARG:HG3 | 2.07 | 0.54 |
| 1:I:764:ARG:NH1 | 1:I:769:PHE:O | 2.40 | 0.54 |
| 3:J:368:GLN:O | 3:J:372:SER:HB3 | 2.07 | 0.54 |
| 9:K:31:GLU:O | 9:K:35:VAL:HG13 | 2.07 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:L:46:PRO:HD2 | 10:L:53:ILE:HA | 1.90 | 0.54 |
| 2:M:11:PRO:C | 2:M:13:LEU:H | 2.10 | 0.54 |
| 4:O:96:ILE:HG13 | 4:O:143:ALA:HB3 | 1.89 | 0.54 |
| 1:A:239:LEU:CD2 | 1:A:276:TYR:HE1 | 2.20 | 0.54 |
| 1:A:563:HIS:HB2 | 1:A:872:PHE:CE2 | 2.42 | 0.54 |
| 4:D:175:ASN:HA | 4:D:195:LEU:CD1 | 2.26 | 0.54 |
| 2:M:309:ASP:OD2 | 2:M:311:ARG:HD3 | 2.08 | 0.54 |
| 3:B:139:ILE:HG21 | 11:N:61:HIS:HD2 | 1.72 | 0.54 |
| 7:S:86:LEU:HD12 | 7:S:91:LYS:HG3 | 1.90 | 0.54 |
| 10:V:1:MET:HB3 | 10:V:20:GLU:OE1 | 2.08 | 0.54 |
| 1:A:352:ARG:HA | 1:A:406:ILE:HA | 1.90 | 0.54 |
| 1:A:608:PRO:C | 1:A:609:GLU:HG2 | 2.27 | 0.54 |
| 3:B:1071:ASP:C | 3:B:1073:ASN:H | 2.11 | 0.54 |
| 2:C:134:ARG:O | 2:C:138:LEU:HG | 2.08 | 0.54 |
| 2:C:322:ARG:HD2 | 2:C:322:ARG:H | 1.73 | 0.54 |
| 6:F:56:ILE:HD11 | 6:F:70:ALA:HA | 1.90 | 0.54 |
| 3:J:560:THR:HG22 | 3:J:562:PHE:N | 2.16 | 0.54 |
| 3:J:803:GLU:HB3 | 3:J:805:LYS:HZ1 | 1.72 | 0.54 |
| 4:O:209:CYS:SG | 16:O:1001:F3S:S2 | 3.06 | 0.54 |
| 7:S:56:LYS:O | 7:S:115:THR:HA | 2.06 | 0.54 |
| 3:B:926:GLU:HB3 | 3:B:988:VAL:HG22 | 1.89 | 0.54 |
| 1:A:12:GLY:HA2 | 2:C:358:ALA:O | 2.08 | 0.54 |
| 1:I:15:SER:HA | 1:I:203:ARG:NH2 | 2.21 | 0.54 |
| 1:I:448:LEU:HD23 | 1:I:498:ALA:HA | 1.89 | 0.54 |
| 3:J:800:PRO:HD3 | 3:J:850:VAL:HG23 | 1.88 | 0.54 |
| 3:J:803:GLU:HB3 | 3:J:805:LYS:HZ2 | 1.68 | 0.54 |
| 3:B:381:LEU:C | 3:B:383:ALA:H | 2.11 | 0.54 |
| 4:D:205:LEU:O | 4:D:207:GLU:N | 2.40 | 0.54 |
| 8:H:24:ASN:O | 8:H:26:ASP:N | 2.41 | 0.54 |
| 3:J:228:ARG:NH2 | 3:J:233:LEU:O | 2.41 | 0.54 |
| 3:J:680:TYR:HE1 | 3:J:687:ARG:HH12 | 1.56 | 0.54 |
| 3:J:699:GLN:HB2 | 3:J:720:ASN:HA | 1.90 | 0.54 |
| 2:M:337:GLU:OE1 | 2:M:337:GLU:N | 2.41 | 0.54 |
| 2:M:388:LEU:HD21 | 9:U:35:VAL:HG12 | 1.90 | 0.54 |
| 4:O:176:CYS:H | 4:O:195:LEU:HD21 | 1.73 | 0.54 |
| 6:R:56:ILE:HG23 | 6:R:69:ARG:HD2 | 1.90 | 0.54 |
| 3:B:582:VAL:HG13 | 3:B:586:ASN:N | 2.23 | 0.53 |
| 4:D:116:SER:OG | 4:D:121:VAL:O | 2.20 | 0.53 |
| 1:I:133:THR:HB | 1:I:137:LYS:NZ | 2.23 | 0.53 |
| 1:I:828:SER:C | 1:I:830:LEU:N | 2.61 | 0.53 |
| 3:J:356:VAL:HG11 | 3:J:404:VAL:HG12 | 1.91 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:290:ARG:HB2 | 2:M:321:THR:HG21 | 1.90 | 0.53 |
| 11:W:42:ARG:CG | 11:W:43:TYR:H | 2.21 | 0.53 |
| 1:A:95:LYS:NZ | 1:A:152:LYS:HB3 | 2.23 | 0.53 |
| 1:A:644:PHE:HA | 1:A:724:PHE:HE2 | 1.73 | 0.53 |
| 1:A:827:LEU:HG | 2:C:75:ALA:HB2 | 1.89 | 0.53 |
| 3:B:669:GLN:NE2 | 3:B:881:ARG:HA | 2.23 | 0.53 |
| 1:A:637:ARG:NH1 | 3:B:974:ARG:HH22 | 2.06 | 0.53 |
| 1:I:91:TYR:OH | 1:I:153:GLN:O | 2.18 | 0.53 |
| 1:A:558:LYS:CG | 3:J:104:GLU:HB2 | 2.28 | 0.53 |
| 3:J:367:TYR:HD2 | 3:J:367:TYR:C | 2.10 | 0.53 |
| 3:J:356:VAL:CG1 | 3:J:404:VAL:HG12 | 2.38 | 0.53 |
| 3:J:932:TYR:O | 3:J:932:TYR:CD2 | 2.61 | 0.53 |
| 2:M:301:LEU:O | 2:M:304:GLN:HB2 | 2.09 | 0.53 |
| 2:M:373:ILE:HD12 | 3:J:1049:LEU:HD22 | 1.90 | 0.53 |
| 4:O:180:VAL:CG2 | 4:O:190:LEU:HG | 2.38 | 0.53 |
| 4:O:190:LEU:HD22 | 4:O:195:LEU:HA | 1.89 | 0.53 |
| 1:A:337:VAL:HG23 | 1:A:433:HIS:ND1 | 2.23 | 0.53 |
| 1:A:350:PRO:HG3 | 1:A:468:GLN:NE2 | 2.23 | 0.53 |
| 3:B:103:VAL:HG12 | 3:B:103:VAL:O | 2.08 | 0.53 |
| 3:B:922:GLY:HA2 | 3:B:925:MET:CB | 2.26 | 0.53 |
| 5:E:88:GLU:H | 5:E:99:VAL:CG1 | 2.22 | 0.53 |
| 1:I:369:PRO:HG3 | 1:I:389:ARG:HA | 1.89 | 0.53 |
| 3:J:346:ALA:O | 3:J:350:PHE:N | 2.42 | 0.53 |
| 3:J:895:VAL:HG21 | 4:O:34:LEU:HD21 | 1.90 | 0.53 |
| 1:A:595:GLU:HB2 | 7:G:91:LYS:CE | 2.31 | 0.53 |
| 1:A:647:ARG:HB2 | 1:A:650:ASP:CG | 2.29 | 0.53 |
| 1:A:750:GLN:HG3 | 1:A:782:ILE:HD11 | 1.89 | 0.53 |
| 3:B:321:LYS:HA | 3:B:324:GLU:HB3 | 1.90 | 0.53 |
| 3:B:946:TYR:HD2 | 3:B:947:LYS:N | 2.06 | 0.53 |
| 2:C:145:GLU:HA | 2:C:239:ARG:H | 1.73 | 0.53 |
| 1:I:637:ARG:HH11 | 3:J:974:ARG:HH22 | 1.56 | 0.53 |
| 1:I:743:MET:HG3 | 3:J:919:MET:HE2 | 1.90 | 0.53 |
| 3:J:321:LYS:HA | 3:J:324:GLU:HB3 | 1.90 | 0.53 |
| 3:J:490:TYR:HE1 | 3:J:527:ILE:CG2 | 2.21 | 0.53 |
| 3:J:727:MET:CE | 3:J:898:PRO:HG3 | 2.39 | 0.53 |
| 7:S:85:SER:HB3 | 7:S:92:TYR:HB2 | 1.90 | 0.53 |
| 11:W:44:CYS:SG | 11:W:45:CYS:N | 2.81 | 0.53 |
| 1:A:764:ARG:NH1 | 1:A:769:PHE:O | 2.42 | 0.53 |
| 3:B:1069:TRP:HE1 | 3:B:1088:LEU:HB3 | 1.73 | 0.53 |
| 3:B:1077:TYR:HD1 | 3:B:1077:TYR:O | 1.91 | 0.53 |
| 3:B:87:LEU:HD23 | 3:B:688:THR:HG21 | 1.91 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:B:94:ALA:O | 3:B:119:LEU:N | 2.39 | 0.53 |
| 2:C:299:LYS:CA | 2:C:302:ALA:HB3 | 2.38 | 0.53 |
| 6:F:48:ASP:H | 6:F:51:SER:HG | 1.56 | 0.53 |
| 7:G:40:PHE:CE2 | 7:G:113:LEU:HD21 | 2.44 | 0.53 |
| 3:J:1069:TRP:CD1 | 3:J:1088:LEU:HD22 | 2.43 | 0.53 |
| 3:J:27:HIS:HD2 | 3:J:346:ALA:HB2 | 1.74 | 0.53 |
| 3:J:663:SER:HB3 | 3:J:664:PRO:HD3 | 1.89 | 0.53 |
| 3:J:946:TYR:HD2 | 3:J:947:LYS:N | 2.06 | 0.53 |
| 5:Q:109:HIS:HD2 | 5:Q:111:SER:H | 1.56 | 0.53 |
| 6:R:14:TYR:N | 6:R:14:TYR:HD1 | 2.06 | 0.53 |
| 3:B:578:PRO:HB3 | 3:B:615:TYR:CE1 | 2.44 | 0.53 |
| 3:B:943:THR:CG2 | 3:B:944:PRO:HD2 | 2.38 | 0.53 |
| 1:A:127:SER:HB2 | 2:C:360:ARG:NH1 | 2.23 | 0.53 |
| 1:I:584:SER:OG | 1:I:585:TYR:N | 2.40 | 0.53 |
| 1:I:607:GLN:O | 1:I:608:PRO:C | 2.47 | 0.53 |
| 3:J:760:THR:OG1 | 3:J:813:LYS:HD2 | 2.08 | 0.53 |
| 1:A:94:LEU:HD11 | 1:A:180:ILE:HG23 | 1.90 | 0.53 |
| 1:A:58:CYS:CB | 1:A:59:PRO:CD | 2.86 | 0.53 |
| 3:B:368:GLN:O | 3:B:372:SER:HB3 | 2.08 | 0.53 |
| 3:B:937:GLY:HA2 | 11:N:50:LEU:HD11 | 1.90 | 0.53 |
| 6:F:54:LYS:HA | 6:F:57:GLU:HB2 | 1.91 | 0.53 |
| 1:I:61:CYS:SG | 3:J:1070:TYR:HB3 | 2.48 | 0.53 |
| 3:J:390:VAL:O | 3:J:394:ILE:HB | 2.08 | 0.53 |
| 3:J:764:LYS:NZ | 3:J:814:VAL:O | 2.35 | 0.53 |
| 8:T:45:ILE:HG22 | 8:T:81:VAL:N | 2.24 | 0.53 |
| 1:A:199:PRO:O | 1:A:200:THR:OG1 | 2.23 | 0.53 |
| 1:A:26:ALA:HA | 1:A:74:HIS:CE1 | 2.44 | 0.53 |
| 3:B:474:ALA:HB2 | 3:B:578:PRO:HG3 | 1.91 | 0.53 |
| 2:C:190:ARG:CD | 2:C:191:LEU:H | 2.21 | 0.53 |
| 2:C:328:GLN:O | 2:C:333:GLY:HA3 | 2.09 | 0.53 |
| 2:C:76:GLN:O | 2:C:80:GLU:N | 2.37 | 0.53 |
| 5:E:17:GLU:OE2 | 5:E:20:LYS:NZ | 2.24 | 0.53 |
| 3:J:54:PRO:O | 3:J:56:LEU:N | 2.42 | 0.53 |
| 3:J:971:TYR:CE2 | 3:J:978:LYS:HB3 | 2.44 | 0.53 |
| 2:M:119:THR:N | 2:M:120:PRO:HD3 | 2.24 | 0.53 |
| 2:M:212:ASN:HD22 | 2:M:213:ILE:N | 2.07 | 0.53 |
| 2:M:329:ILE:HA | 2:M:334:VAL:CG1 | 2.35 | 0.53 |
| 1:I:874:ARG:HE | 2:M:53:ASP:CB | 2.21 | 0.53 |
| 7:S:21:GLY:HA3 | 7:S:26:LEU:HD12 | 1.90 | 0.53 |
| 9:U:82:LEU:HB2 | 9:U:84:ASN:HB2 | 1.91 | 0.53 |
| 1:A:113:LYS:HG2 | 1:A:116:ARG:CZ | 2.38 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:215:PRO:HB2 | 1:A:219:ILE:HD11 | 1.91 | 0.53 |
| 4:D:190:LEU:HD22 | 4:D:195:LEU:HA | 1.91 | 0.53 |
| 1:I:209:LEU:HD13 | 1:I:273:VAL:HG11 | 1.91 | 0.53 |
| 1:I:644:PHE:HA | 1:I:724:PHE:CE2 | 2.44 | 0.53 |
| 1:I:827:LEU:HD13 | 2:M:319:VAL:HG21 | 1.90 | 0.53 |
| 3:J:1069:TRP:HE1 | 3:J:1088:LEU:HB3 | 1.73 | 0.53 |
| 3:J:43:ILE:HG13 | 3:J:63:ILE:CD1 | 2.39 | 0.53 |
| 2:M:122:MET:HG2 | 2:M:274:THR:HG23 | 1.90 | 0.53 |
| 2:M:370:VAL:O | 2:M:373:ILE:HG22 | 2.09 | 0.53 |
| 2:M:391:ARG:H | 2:M:392:PRO:CD | 2.22 | 0.53 |
| 4:O:34:LEU:HA | 4:O:150:GLY:HA3 | 1.91 | 0.53 |
| 1:I:541:ALA:N | 7:S:72:CYS:O | 2.42 | 0.53 |
| 1:A:290:ARG:HD2 | 1:A:291:SER:N | 2.24 | 0.53 |
| 1:A:458:ASP:HA | 3:B:886:GLY:HA2 | 1.90 | 0.53 |
| 1:A:647:ARG:HB2 | 1:A:650:ASP:OD1 | 2.09 | 0.53 |
| 3:B:560:THR:HG22 | 3:B:561:ASP:N | 2.24 | 0.53 |
| 3:B:954:GLN:HA | 3:B:957:ILE:HD11 | 1.90 | 0.53 |
| 1:I:450:CYS:N | 1:I:451:PRO:CD | 2.72 | 0.53 |
| 1:I:458:ASP:HA | 3:J:886:GLY:HA2 | 1.91 | 0.53 |
| 3:J:1004:ARG:NH1 | 3:J:1025:GLY:H | 2.05 | 0.53 |
| 2:M:190:ARG:CZ | 2:M:191:LEU:HG | 2.39 | 0.53 |
| 2:M:212:ASN:C | 2:M:214:ASP:H | 2.12 | 0.53 |
| 2:M:289:ALA:O | 2:M:290:ARG:C | 2.48 | 0.53 |
| 3:B:367:TYR:HD2 | 3:B:367:TYR:C | 2.13 | 0.52 |
| 3:B:762:GLU:HG2 | 3:B:772:LYS:HA | 1.91 | 0.52 |
| 1:I:268:LEU:HD23 | 1:I:271:TYR:HD1 | 1.74 | 0.52 |
| 1:I:364:PHE:HD2 | 1:I:373:PRO:O | 1.93 | 0.52 |
| 1:I:378:VAL:HG23 | 1:I:407:ILE:HG22 | 1.91 | 0.52 |
| 1:I:336:GLU:OE1 | 1:I:436:ARG:NH1 | 2.43 | 0.52 |
| 1:I:775:SER:OG | 1:I:776:PRO:HD2 | 2.10 | 0.52 |
| 1:I:501:ASP:HB2 | 3:J:734:MET:SD | 2.49 | 0.52 |
| 3:J:83:MET:O | 3:J:87:LEU:HD12 | 2.09 | 0.52 |
| 2:M:13:LEU:HD23 | 2:M:16:LYS:NZ | 2.24 | 0.52 |
| 11:N:18:TRP:CD1 | 11:N:49:LEU:HD22 | 2.39 | 0.52 |
| 8:T:11:PRO:HD2 | 8:T:12:ARG:HD3 | 1.90 | 0.52 |
| 1:A:417:VAL:HG13 | 1:A:464:LEU:HD13 | 1.91 | 0.52 |
| 1:A:851:GLY:C | 1:A:853:ASP:H | 2.11 | 0.52 |
| 3:B:591:ILE:O | 3:B:594:ILE:HG12 | 2.09 | 0.52 |
| 3:B:602:ILE:HG22 | 3:B:603:THR:N | 2.24 | 0.52 |
| 5:E:130:GLU:HA | 5:E:133:LYS:HE2 | 1.90 | 0.52 |
| 1:I:679:TYR:OH | 1:I:693:GLU:HG2 | 2.08 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:253:ILE:CD1 | 10:L:76:ILE:HD12 | 2.39 | 0.52 |
| 3:B:702:LEU:HD13 | 11:N:47:ARG:HD2 | 1.91 | 0.52 |
| 3:B:1069:TRP:CH2 | 3:B:1077:TYR:HB2 | 2.44 | 0.52 |
| 3:B:425:HIS:HA | 3:B:428:ARG:HD3 | 1.91 | 0.52 |
| 3:B:461:GLY:O | 3:B:464:SER:HB3 | 2.09 | 0.52 |
| 3:B:48:GLU:HG2 | 3:B:58:VAL:HB | 1.91 | 0.52 |
| 3:B:895:VAL:HG21 | 4:D:34:LEU:HD21 | 1.92 | 0.52 |
| 5:E:66:THR:HG23 | 5:E:68:HIS:CE1 | 2.44 | 0.52 |
| 1:I:781:PHE:C | 1:I:781:PHE:CD2 | 2.83 | 0.52 |
| 3:J:533:GLY:O | 3:J:535:GLU:N | 2.41 | 0.52 |
| 3:J:834:ASP:O | 3:J:836:SER:N | 2.38 | 0.52 |
| 4:O:29:ARG:HG3 | 4:O:162:SER:O | 2.10 | 0.52 |
| 1:A:490:ARG:HA | 2:C:312:HIS:CE1 | 2.39 | 0.52 |
| 3:B:971:TYR:CE2 | 3:B:978:LYS:HB3 | 2.45 | 0.52 |
| 2:C:153:VAL:O | 2:C:153:VAL:HG13 | 2.09 | 0.52 |
| 2:C:237:ILE:CG1 | 2:C:238:LYS:N | 2.63 | 0.52 |
| 5:E:51:VAL:O | 5:E:53:THR:N | 2.41 | 0.52 |
| 1:I:349:VAL:HG21 | 1:I:409:ARG:NH2 | 2.24 | 0.52 |
| 1:I:742:GLN:HB3 | 3:J:919:MET:CE | 2.39 | 0.52 |
| 1:I:750:GLN:CG | 1:I:782:ILE:CD1 | 2.88 | 0.52 |
| 3:J:474:ALA:HB2 | 3:J:578:PRO:HG3 | 1.90 | 0.52 |
| 4:O:129:PRO:HG2 | 11:W:15:ALA:HB1 | 1.90 | 0.52 |
| 12:P:9:CYS:HB3 | 12:P:12:THR:O | 2.10 | 0.52 |
| 1:A:239:LEU:CD2 | 1:A:276:TYR:CE1 | 2.92 | 0.52 |
| 1:A:647:ARG:O | 1:A:650:ASP:HB2 | 2.08 | 0.52 |
| 3:B:82:PRO:CG | 3:B:143:GLU:OE1 | 2.48 | 0.52 |
| 3:B:435:ARG:HB3 | 3:B:437:GLN:HB2 | 1.90 | 0.52 |
| 3:B:677:LEU:HD12 | 3:B:992:LYS:HD3 | 1.90 | 0.52 |
| 2:C:124:ILE:O | 2:C:251:ILE:HG22 | 2.10 | 0.52 |
| 2:C:392:PRO:HG2 | 5:E:22:LEU:HD21 | 1.91 | 0.52 |
| 1:I:426:HIS:ND1 | 1:I:428:ILE:HG22 | 2.24 | 0.52 |
| 1:I:448:LEU:O | 1:I:496:ILE:HG23 | 2.10 | 0.52 |
| 1:I:563:HIS:HB2 | 1:I:872:PHE:CE2 | 2.44 | 0.52 |
| 3:J:21:LYS:HE2 | 3:J:475:GLN:OE1 | 2.09 | 0.52 |
| 2:M:112:ASP:O | 2:M:113:ALA:CB | 2.58 | 0.52 |
| 2:M:372:ASN:O | 2:M:375:ILE:HG22 | 2.09 | 0.52 |
| 9:U:38:ALA:HB1 | 9:U:42:GLN:HE22 | 1.75 | 0.52 |
| 11:W:4:PRO:HG2 | 11:W:48:MET:HE2 | 1.92 | 0.52 |
| 13:Y:71:ASN:HA | 13:Y:74:GLU:CD | 2.29 | 0.52 |
| 1:A:446:ASN:O | 1:A:448:LEU:N | 2.42 | 0.52 |
| 2:C:355:LEU:HD23 | 3:B:1109:ILE:HD11 | 1.91 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:B:162:VAL:HG11 | 3:B:412:GLN:NE2 | 2.25 | 0.52 |
| 1:I:457:PHE:HB2 | 3:J:737:SER:HB2 | 1.91 | 0.52 |
| 1:I:488:THR:HG23 | 1:I:490:ARG:H | 1.75 | 0.52 |
| 1:I:825:ASN:O | 1:I:827:LEU:N | 2.43 | 0.52 |
| 3:J:368:GLN:NE2 | 3:J:386:ARG:HE | 2.08 | 0.52 |
| 10:L:69:LEU:O | 10:L:73:ILE:N | 2.36 | 0.52 |
| 5:Q:18:PHE:CD2 | 9:U:47:ALA:HB1 | 2.45 | 0.52 |
| 11:W:43:TYR:HA | 11:W:46:ARG:HB2 | 1.91 | 0.52 |
| 1:A:215:PRO:HB3 | 3:B:1106:SER:HB3 | 1.90 | 0.52 |
| 1:A:369:PRO:HG3 | 1:A:389:ARG:HA | 1.91 | 0.52 |
| 1:A:743:MET:HG3 | 3:B:919:MET:HE2 | 1.91 | 0.52 |
| 1:A:868:VAL:HG22 | 2:C:39:LYS:HZ1 | 1.75 | 0.52 |
| 3:B:369:LEU:HG | 3:B:384:LEU:HD13 | 1.91 | 0.52 |
| 3:B:582:VAL:HG11 | 3:B:633:LEU:HD11 | 1.91 | 0.52 |
| 2:C:261:VAL:HG12 | 2:C:261:VAL:O | 2.10 | 0.52 |
| 2:C:70:ILE:O | 2:C:71:GLY:C | 2.48 | 0.52 |
| 4:D:131:VAL:HG22 | 4:D:132:LEU:H | 1.73 | 0.52 |
| 4:D:96:ILE:HG13 | 4:D:143:ALA:HB3 | 1.91 | 0.52 |
| 1:I:378:VAL:O | 1:I:378:VAL:CG2 | 2.55 | 0.52 |
| 1:I:664:GLU:OE1 | 1:I:707:LEU:HD22 | 2.09 | 0.52 |
| 3:J:130:ILE:HA | 3:J:133:TYR:CE1 | 2.45 | 0.52 |
| 3:J:215:PRO:O | 3:J:216:ALA:HB3 | 2.10 | 0.52 |
| 3:J:369:LEU:HG | 3:J:384:LEU:HD13 | 1.91 | 0.52 |
| 3:J:849:LEU:HB3 | 3:J:865:ARG:HB3 | 1.91 | 0.52 |
| 3:J:96:LEU:HB2 | 3:J:117:GLY:H | 1.75 | 0.52 |
| 2:M:153:VAL:HG23 | 2:M:168:GLN:O | 2.10 | 0.52 |
| 3:B:902:LYS:HE2 | 11:N:41:LYS:HB3 | 1.91 | 0.52 |
| 3:B:682:ALA:O | 11:N:59:VAL:HG13 | 2.10 | 0.52 |
| 4:O:101:GLU:O | 4:O:107:ARG:NH1 | 2.43 | 0.52 |
| 1:A:353:ILE:CG1 | 1:A:361:LEU:HD23 | 2.37 | 0.52 |
| 1:A:855:VAL:HG22 | 2:C:64:ILE:HB | 1.92 | 0.52 |
| 3:B:850:VAL:O | 12:P:35:PHE:CB | 2.57 | 0.52 |
| 4:D:180:VAL:HG21 | 4:D:190:LEU:HG | 1.92 | 0.52 |
| 5:E:81:VAL:O | 5:E:82:GLN:HB2 | 2.09 | 0.52 |
| 7:G:71:PHE:O | 7:G:114:ARG:HA | 2.10 | 0.52 |
| 3:J:1061:CYS:HA | 3:J:1088:LEU:HD23 | 1.92 | 0.52 |
| 3:J:193:THR:HG21 | 3:J:197:ARG:N | 2.25 | 0.52 |
| 1:I:761:TYR:OH | 3:J:621:GLU:OE1 | 2.20 | 0.52 |
| 3:J:848:ASP:OD1 | 3:J:865:ARG:CZ | 2.57 | 0.52 |
| 4:D:21:PRO:HG3 | 10:L:79:MET:SD | 2.49 | 0.52 |
| 2:M:103:GLY:HA2 | 2:M:106:ARG:HB3 | 1.90 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:902:LYS:HB2 | 11:W:42:ARG:HH11 | 1.75 | 0.52 |
| 1:A:155:LYS:HA | 1:A:156:ILE:O | 2.10 | 0.52 |
| 1:A:495:ILE:O | 1:A:495:ILE:HG13 | 2.10 | 0.52 |
| 1:A:632:PHE:HA | 1:A:635:PHE:CE1 | 2.45 | 0.52 |
| 3:B:367:TYR:HD2 | 3:B:367:TYR:O | 1.93 | 0.52 |
| 1:A:868:VAL:HG13 | 2:C:39:LYS:HE2 | 1.92 | 0.52 |
| 4:D:96:ILE:CG1 | 4:D:143:ALA:HB3 | 2.40 | 0.52 |
| 1:I:337:VAL:HG12 | 1:I:339:VAL:HG23 | 1.91 | 0.52 |
| 1:I:507:TYR:HB2 | 1:I:511:VAL:HG13 | 1.92 | 0.52 |
| 1:I:763:THR:CG2 | 1:I:772:TYR:HA | 2.40 | 0.52 |
| 3:J:911:ASN:HD21 | 3:J:913:HIS:HD2 | 1.57 | 0.52 |
| 9:K:69:PHE:HA | 9:K:74:LEU:HD11 | 1.92 | 0.52 |
| 9:K:86:LYS:N | 9:K:86:LYS:HD2 | 2.25 | 0.52 |
| 2:M:344:ARG:HB3 | 2:M:353:HIS:CD2 | 2.44 | 0.52 |
| 12:X:17:GLN:C | 12:X:19:LYS:H | 2.12 | 0.52 |
| 3:B:368:GLN:HE22 | 3:B:386:ARG:HH21 | 1.57 | 0.52 |
| 3:B:471:ALA:O | 3:B:473:MET:HG3 | 2.10 | 0.52 |
| 3:B:789:TYR:O | 3:B:791:LEU:N | 2.43 | 0.52 |
| 3:B:943:THR:HG22 | 3:B:944:PRO:HD2 | 1.91 | 0.52 |
| 4:D:176:CYS:H | 4:D:195:LEU:HD21 | 1.74 | 0.52 |
| 1:I:506:ALA:O | 1:I:510:THR:HG23 | 2.10 | 0.52 |
| 1:I:71:HIS:ND1 | 3:J:1070:TYR:HE2 | 2.07 | 0.52 |
| 3:J:560:THR:HG22 | 3:J:561:ASP:N | 2.25 | 0.52 |
| 1:I:441:LEU:HD12 | 3:J:873:THR:HG21 | 1.92 | 0.52 |
| 10:L:32:LEU:HD11 | 10:L:69:LEU:HD12 | 1.92 | 0.52 |
| 2:M:145:GLU:O | 2:M:147:THR:N | 2.43 | 0.52 |
| 7:S:42:ILE:HD12 | 7:S:46:ILE:HG21 | 1.91 | 0.52 |
| 9:U:43:LEU:C | 9:U:45:MET:H | 2.13 | 0.52 |
| 1:A:557:PRO:HD3 | 1:A:623:TYR:OH | 2.10 | 0.51 |
| 1:A:507:TYR:OH | 1:A:727:VAL:HG13 | 2.09 | 0.51 |
| 1:A:83:HIS:HB3 | 1:A:86:LEU:HB2 | 1.92 | 0.51 |
| 3:B:27:HIS:HD2 | 3:B:346:ALA:HB2 | 1.75 | 0.51 |
| 3:B:579:LEU:O | 3:B:613:ILE:HG23 | 2.09 | 0.51 |
| 3:B:685:GLN:HE22 | 3:B:867:ARG:HH22 | 1.58 | 0.51 |
| 3:B:727:MET:HE1 | 3:B:898:PRO:HG3 | 1.92 | 0.51 |
| 4:D:204:THR:O | 4:D:206:CYS:N | 2.43 | 0.51 |
| 7:G:29:VAL:HB | 7:G:40:PHE:HD1 | 1.75 | 0.51 |
| 8:H:63:ILE:HG22 | 8:H:64:ARG:N | 2.25 | 0.51 |
| 1:I:728:MET:CE | 3:J:913:HIS:HA | 2.40 | 0.51 |
| 1:I:837:THR:HG22 | 1:I:838:VAL:H | 1.75 | 0.51 |
| 1:I:95:LYS:HB3 | 1:I:138:LYS:HG3 | 1.92 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:602:ILE:HG22 | 3:J:603:THR:N | 2.25 | 0.51 |
| 3:J:94:ALA:O | 3:J:119:LEU:N | 2.37 | 0.51 |
| 3:J:800:PRO:HB2 | 12:X:38:ARG:HA | 1.92 | 0.51 |
| 1:A:541:ALA:CA | 7:G:72:CYS:H | 2.23 | 0.51 |
| 3:B:855:THR:O | 3:B:856:ALA:C | 2.48 | 0.51 |
| 7:G:86:LEU:HD12 | 7:G:91:LYS:CG | 2.39 | 0.51 |
| 1:I:737:VAL:HG23 | 1:I:738:LEU:HD22 | 1.93 | 0.51 |
| 3:J:624:ALA:HB1 | 3:J:639:HIS:CD2 | 2.45 | 0.51 |
| 3:J:419:TRP:CZ3 | 3:J:712:GLY:HA3 | 2.45 | 0.51 |
| 4:D:250:ILE:CD1 | 10:L:84:ILE:CD1 | 2.83 | 0.51 |
| 4:O:134:GLY:O | 4:O:135:THR:O | 2.28 | 0.51 |
| 5:Q:31:ARG:O | 5:Q:33:GLN:N | 2.42 | 0.51 |
| 1:A:446:ASN:HD22 | 1:A:447:LEU:N | 2.08 | 0.51 |
| 3:B:745:VAL:HG21 | 3:B:891:LEU:HD11 | 1.91 | 0.51 |
| 3:B:738:ILE:CD1 | 3:B:908:ILE:HG23 | 2.39 | 0.51 |
| 2:C:391:ARG:H | 2:C:392:PRO:CD | 2.22 | 0.51 |
| 1:A:541:ALA:CB | 7:G:71:PHE:HA | 2.40 | 0.51 |
| 1:I:486:ILE:HG12 | 1:I:496:ILE:HB | 1.93 | 0.51 |
| 1:I:594:LEU:O | 1:I:595:GLU:HG2 | 2.10 | 0.51 |
| 3:J:116:ILE:HD12 | 3:J:361:PHE:CZ | 2.46 | 0.51 |
| 5:Q:79:PRO:HG2 | 5:Q:149:VAL:HG21 | 1.92 | 0.51 |
| 9:U:12:ASP:O | 9:U:13:LEU:C | 2.47 | 0.51 |
| 2:M:388:LEU:HD21 | 9:U:35:VAL:CG1 | 2.39 | 0.51 |
| 11:W:42:ARG:HG3 | 11:W:43:TYR:H | 1.74 | 0.51 |
| 1:A:558:LYS:H | 1:A:558:LYS:CD | 2.23 | 0.51 |
| 1:A:612:LEU:C | 1:A:612:LEU:HD23 | 2.31 | 0.51 |
| 3:B:921:LEU:C | 3:B:923:GLN:H | 2.13 | 0.51 |
| 2:C:392:PRO:HB2 | 5:E:22:LEU:HD11 | 1.93 | 0.51 |
| 7:G:46:ILE:O | 7:G:46:ILE:CG2 | 2.58 | 0.51 |
| 1:I:105:LYS:NZ | 1:I:108:GLU:HB2 | 2.25 | 0.51 |
| 3:J:367:TYR:HD2 | 3:J:367:TYR:O | 1.93 | 0.51 |
| 3:J:569:ASN:HB3 | 3:J:574:ARG:HH12 | 1.76 | 0.51 |
| 3:J:735:GLU:O | 3:J:736:ASP:C | 2.49 | 0.51 |
| 3:J:92:TYR:O | 3:J:92:TYR:CD2 | 2.63 | 0.51 |
| 3:J:963:LEU:HD22 | 3:J:982:ARG:NH2 | 2.26 | 0.51 |
| 5:E:64:GLY:O | 9:K:42:GLN:OE1 | 2.28 | 0.51 |
| 2:M:146:TYR:CZ | 2:M:235:LYS:HB2 | 2.45 | 0.51 |
| 2:M:376:GLY:HA2 | 3:J:1049:LEU:HD21 | 1.91 | 0.51 |
| 2:M:55:ALA:CB | 2:M:58:GLU:OE2 | 2.58 | 0.51 |
| 2:M:55:ALA:O | 2:M:58:GLU:HB2 | 2.10 | 0.51 |
| 1:A:238:LYS:HE2 | 1:A:297:THR:HG22 | 1.92 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:170:ASN:HB3 | 3:B:300:HIS:HE1 | 1.76 | 0.51 |
| 3:B:517:TRP:HD1 | 3:B:531:GLN:H | 1.59 | 0.51 |
| 2:C:278:ARG:HD2 | 2:C:278:ARG:O | 2.11 | 0.51 |
| 7:G:17:SER:HB2 | 7:G:19:GLU:HG2 | 1.92 | 0.51 |
| 1:I:438:LEU:HD21 | 1:I:444:ARG:CZ | 2.40 | 0.51 |
| 1:I:7:LYS:HE2 | 2:M:365:GLU:OE2 | 2.11 | 0.51 |
| 3:J:644:SER:C | 3:J:646:ALA:H | 2.14 | 0.51 |
| 3:J:741:ASN:C | 3:J:741:ASN:OD1 | 2.49 | 0.51 |
| 3:J:970:VAL:HG22 | 3:J:979:ILE:HG12 | 1.92 | 0.51 |
| 3:J:978:LYS:HG2 | 4:O:166:TYR:CE2 | 2.46 | 0.51 |
| 1:A:317:ARG:NH1 | 3:B:1018:GLU:HG3 | 2.26 | 0.51 |
| 1:A:557:PRO:HA | 1:A:558:LYS:HZ2 | 1.75 | 0.51 |
| 3:B:1074:LYS:HE2 | 3:B:1074:LYS:HA | 1.93 | 0.51 |
| 3:B:356:VAL:HG22 | 3:B:393:ARG:NH1 | 2.25 | 0.51 |
| 3:B:665:ARG:HG3 | 3:B:920:THR:HG21 | 1.91 | 0.51 |
| 1:I:98:CYS:HB3 | 1:I:101:CYS:H | 1.76 | 0.51 |
| 3:J:469:ASN:N | 3:J:469:ASN:HD22 | 2.07 | 0.51 |
| 9:K:19:PHE:O | 9:K:20:ILE:C | 2.49 | 0.51 |
| 2:M:149:ILE:HB | 2:M:227:LEU:HA | 1.92 | 0.51 |
| 4:O:137:GLN:NE2 | 11:W:63:THR:HG22 | 2.26 | 0.51 |
| 1:A:209:LEU:HD13 | 1:A:273:VAL:HG11 | 1.92 | 0.51 |
| 1:A:290:ARG:NH1 | 1:A:291:SER:HB2 | 2.25 | 0.51 |
| 1:A:528:ALA:HB3 | 1:A:630:ASN:HD21 | 1.74 | 0.51 |
| 1:A:659:LYS:O | 1:A:663:ASN:HB2 | 2.09 | 0.51 |
| 3:B:1004:ARG:NH1 | 3:B:1024:GLY:HA2 | 2.25 | 0.51 |
| 3:B:1009:VAL:HB | 3:B:1014:ARG:O | 2.09 | 0.51 |
| 3:B:330:ARG:HA | 3:B:563:ILE:HD11 | 1.93 | 0.51 |
| 2:C:11:PRO:O | 2:C:14:GLU:HG3 | 2.11 | 0.51 |
| 5:E:87:GLY:O | 5:E:88:GLU:CB | 2.55 | 0.51 |
| 8:H:69:SER:HB2 | 8:H:75:VAL:HG22 | 1.93 | 0.51 |
| 1:I:290:ARG:NH1 | 1:I:291:SER:HB2 | 2.25 | 0.51 |
| 1:I:853:ASP:HB3 | 1:I:855:VAL:H | 1.76 | 0.51 |
| 3:J:435:ARG:HB3 | 3:J:437:GLN:HB2 | 1.93 | 0.51 |
| 2:M:369:VAL:O | 2:M:373:ILE:HB | 2.11 | 0.51 |
| 5:Q:120:TYR:CZ | 5:Q:122:ASN:HA | 2.46 | 0.51 |
| 5:Q:15:PRO:HB2 | 9:U:45:MET:O | 2.10 | 0.51 |
| 2:M:384:GLY:HA2 | 5:Q:61:PHE:HZ | 1.75 | 0.51 |
| 1:A:371:LYS:NZ | 1:A:373:PRO:HD3 | 2.26 | 0.51 |
| 1:A:539:ILE:HB | 1:A:545:TYR:HB2 | 1.93 | 0.51 |
| 3:B:931:LYS:HE2 | 3:B:985:PHE:O | 2.10 | 0.51 |
| 2:C:301:LEU:O | 2:C:304:GLN:N | 2.44 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:77:PRO:HG3 | 6:F:83:VAL:HG22 | 1.93 | 0.51 |
| 3:J:560:THR:CG2 | 3:J:561:ASP:N | 2.74 | 0.51 |
| 3:J:904:VAL:HG22 | 11:W:44:CYS:HB3 | 1.93 | 0.51 |
| 9:K:61:VAL:O | 9:K:62:ILE:HB | 2.11 | 0.51 |
| 9:K:91:SER:O | 9:K:92:LEU:HB3 | 2.11 | 0.51 |
| 2:M:121:MET:H | 2:M:275:ASN:ND2 | 2.09 | 0.51 |
| 2:M:286:ILE:HG13 | 8:T:49:ASP:OD2 | 2.11 | 0.51 |
| 1:I:859:TYR:HB2 | 2:M:64:ILE:HG23 | 1.93 | 0.51 |
| 6:R:13:PRO:HB3 | 6:R:73:ALA:HB3 | 1.92 | 0.51 |
| 1:I:532:ILE:HG23 | 10:V:40:PHE:CD2 | 2.46 | 0.51 |
| 1:A:604:GLY:C | 1:A:606:GLN:N | 2.62 | 0.51 |
| 3:B:497:VAL:HG12 | 3:B:498:GLU:N | 2.26 | 0.51 |
| 3:B:710:ILE:HD13 | 3:B:710:ILE:H | 1.76 | 0.51 |
| 3:B:834:ASP:O | 3:B:836:SER:N | 2.39 | 0.51 |
| 2:C:49:ASP:O | 2:C:51:ILE:N | 2.44 | 0.51 |
| 2:C:72:ILE:CG2 | 2:C:76:GLN:OE1 | 2.59 | 0.51 |
| 6:F:64:SER:H | 6:F:69:ARG:HH21 | 1.59 | 0.51 |
| 1:I:749:GLN:N | 1:I:781:PHE:HA | 2.25 | 0.51 |
| 1:I:465:HIS:CD2 | 3:J:1048:ARG:HD2 | 2.46 | 0.51 |
| 3:J:14:ILE:HG13 | 3:J:18:PHE:CE2 | 2.46 | 0.51 |
| 3:J:232:ILE:HG23 | 3:J:237:ASP:HB3 | 1.92 | 0.51 |
| 9:K:54:ASN:HD21 | 9:K:58:SER:CB | 2.24 | 0.51 |
| 5:Q:50:ASN:HB2 | 5:Q:73:ASP:OD2 | 2.11 | 0.51 |
| 1:A:293:ARG:HD3 | 1:A:296:ARG:HH22 | 1.76 | 0.51 |
| 1:A:305:LYS:HA | 1:A:310:ARG:HD2 | 1.91 | 0.51 |
| 1:A:324:THR:CG2 | 1:A:325:VAL:N | 2.73 | 0.51 |
| 3:B:67:LYS:HB3 | 3:B:68:PRO:HD2 | 1.93 | 0.51 |
| 3:B:699:GLN:HA | 11:N:51:SER:O | 2.11 | 0.51 |
| 3:B:875:GLY:HA2 | 3:B:887:VAL:HG13 | 1.93 | 0.51 |
| 3:B:932:TYR:CD2 | 3:B:932:TYR:O | 2.64 | 0.51 |
| 5:E:110:ILE:O | 5:E:113:ILE:HG22 | 2.11 | 0.51 |
| 1:I:290:ARG:HD2 | 1:I:291:SER:H | 1.76 | 0.51 |
| 3:J:729:PHE:O | 3:J:731:GLY:N | 2.43 | 0.51 |
| 3:J:950:ILE:O | 3:J:952:GLN:N | 2.45 | 0.51 |
| 3:J:975:THR:OG1 | 3:J:977:GLN:HG2 | 2.11 | 0.51 |
| 2:M:24:LEU:HD11 | 2:M:58:GLU:OE1 | 2.12 | 0.51 |
| 2:M:286:ILE:HG12 | 2:M:324:GLY:O | 2.10 | 0.51 |
| 10:V:82:HIS:O | 10:V:86:GLU:N | 2.43 | 0.51 |
| 1:A:525:LEU:HG | 10:L:40:PHE:HZ | 1.75 | 0.50 |
| 3:B:325:LEU:HD11 | 3:B:331:GLU:H | 1.76 | 0.50 |
| 3:B:582:VAL:HG13 | 3:B:586:ASN:H | 1.76 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:68:PRO:CD | 3:B:129:PRO:HG2 | 2.40 | 0.50 |
| 3:B:870:ARG:HH11 | 3:B:996:MET:HB2 | 1.74 | 0.50 |
| 4:D:131:VAL:CG2 | 4:D:132:LEU:H | 2.24 | 0.50 |
| 8:H:65:ILE:HD11 | 8:H:79:ARG:HG2 | 1.92 | 0.50 |
| 1:I:78:VAL:HG23 | 1:I:266:TRP:HZ3 | 1.75 | 0.50 |
| 3:J:291:GLN:O | 3:J:295:LYS:HG2 | 2.10 | 0.50 |
| 3:J:699:GLN:HA | 11:W:51:SER:O | 2.11 | 0.50 |
| 3:J:762:GLU:HG2 | 3:J:772:LYS:HA | 1.93 | 0.50 |
| 8:T:45:ILE:O | 8:T:81:VAL:HA | 2.12 | 0.50 |
| 1:A:549:LYS:HB2 | 1:A:549:LYS:HZ3 | 1.75 | 0.50 |
| 3:B:154:VAL:O | 3:B:155:ASN:C | 2.50 | 0.50 |
| 3:B:579:LEU:CD1 | 3:B:616:LEU:HD12 | 2.26 | 0.50 |
| 3:B:849:LEU:HB3 | 3:B:865:ARG:HB3 | 1.94 | 0.50 |
| 2:C:150:GLU:HB2 | 2:C:227:LEU:HB3 | 1.93 | 0.50 |
| 2:C:52:PHE:HA | 2:C:55:ALA:HB3 | 1.93 | 0.50 |
| 7:G:40:PHE:CZ | 7:G:115:THR:HG21 | 2.46 | 0.50 |
| 1:A:549:LYS:CB | 7:G:88:ASN:O | 2.60 | 0.50 |
| 7:G:37:ASN:O | 7:G:94:THR:HA | 2.10 | 0.50 |
| 1:I:320:PHE:HE2 | 1:I:348:THR:HG1 | 1.58 | 0.50 |
| 1:I:506:ALA:HA | 1:I:635:PHE:CE2 | 2.46 | 0.50 |
| 4:D:250:ILE:CD1 | 10:L:84:ILE:HD11 | 2.21 | 0.50 |
| 4:O:12:ARG:HA | 4:O:230:ILE:O | 2.11 | 0.50 |
| 8:T:42:LEU:CB | 8:T:43:PRO:HD2 | 2.31 | 0.50 |
| 1:A:353:ILE:HD11 | 1:A:407:ILE:HG23 | 1.92 | 0.50 |
| 1:A:450:CYS:N | 1:A:451:PRO:CD | 2.74 | 0.50 |
| 1:A:317:ARG:HB2 | 3:B:1016:PRO:HB2 | 1.93 | 0.50 |
| 3:B:325:LEU:HD22 | 3:B:330:ARG:HG3 | 1.93 | 0.50 |
| 3:B:729:PHE:O | 3:B:731:GLY:N | 2.44 | 0.50 |
| 3:B:763:VAL:HA | 3:B:770:GLU:CG | 2.41 | 0.50 |
| 6:F:15:SER:HA | 6:F:18:LYS:HZ1 | 1.76 | 0.50 |
| 1:I:239:LEU:CD2 | 1:I:276:TYR:CE1 | 2.94 | 0.50 |
| 1:I:238:LYS:HE2 | 1:I:297:THR:HG22 | 1.94 | 0.50 |
| 1:I:324:THR:CG2 | 1:I:325:VAL:H | 2.22 | 0.50 |
| 1:I:524:ILE:O | 1:I:525:LEU:HD22 | 2.11 | 0.50 |
| 1:I:644:PHE:HA | 1:I:724:PHE:HE2 | 1.77 | 0.50 |
| 3:J:103:VAL:O | 3:J:103:VAL:HG12 | 2.10 | 0.50 |
| 3:J:517:TRP:HD1 | 3:J:531:GLN:H | 1.59 | 0.50 |
| 3:J:921:LEU:C | 3:J:923:GLN:H | 2.13 | 0.50 |
| 10:L:40:PHE:HB3 | 10:L:58:LEU:HB3 | 1.93 | 0.50 |
| 1:I:859:TYR:HB3 | 2:M:64:ILE:HG12 | 1.93 | 0.50 |
| 7:S:57:VAL:HG13 | 7:S:115:THR:HG22 | 1.92 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:337:VAL:HG21 | 1:A:419:PHE:CD1 | 2.46 | 0.50 |
| 3:B:361:PHE:CE1 | 3:B:385:VAL:HG13 | 2.44 | 0.50 |
| 1:I:288:LYS:HG2 | 1:I:294:PRO:HA | 1.92 | 0.50 |
| 3:J:448:THR:HG22 | 3:J:452:ARG:HD2 | 1.93 | 0.50 |
| 9:U:41:LEU:O | 9:U:43:LEU:N | 2.44 | 0.50 |
| 13:Z:76:GLU:O | 13:Z:77:LYS:CB | 2.58 | 0.50 |
| 1:A:486:ILE:O | 1:A:486:ILE:HD13 | 2.11 | 0.50 |
| 1:A:728:MET:CE | 3:B:913:HIS:HA | 2.41 | 0.50 |
| 1:A:742:GLN:HB3 | 3:B:919:MET:CE | 2.41 | 0.50 |
| 1:A:653:LEU:HD11 | 1:A:745:ALA:HB2 | 1.94 | 0.50 |
| 3:B:533:GLY:O | 3:B:535:GLU:N | 2.45 | 0.50 |
| 3:B:900:THR:OG1 | 3:B:904:VAL:HB | 2.12 | 0.50 |
| 2:C:11:PRO:HB2 | 2:C:14:GLU:OE1 | 2.10 | 0.50 |
| 4:D:131:VAL:CG2 | 4:D:132:LEU:N | 2.74 | 0.50 |
| 8:H:58:LYS:HB2 | 8:H:61:ASP:HB2 | 1.93 | 0.50 |
| 1:I:446:ASN:HD22 | 1:I:448:LEU:H | 1.59 | 0.50 |
| 3:J:377:ARG:O | 3:J:378:LYS:HB2 | 2.12 | 0.50 |
| 3:J:453:MET:HG2 | 3:J:468:LYS:HD2 | 1.92 | 0.50 |
| 3:J:497:VAL:HG12 | 3:J:498:GLU:N | 2.25 | 0.50 |
| 3:J:330:ARG:NH2 | 3:J:565:GLU:OE1 | 2.44 | 0.50 |
| 2:M:339:ASN:N | 2:M:339:ASN:OD1 | 2.42 | 0.50 |
| 4:O:228:LEU:O | 4:O:229:GLU:HG3 | 2.11 | 0.50 |
| 7:S:80:GLU:HG3 | 7:S:81:LEU:H | 1.76 | 0.50 |
| 3:B:226:LEU:O | 3:B:230:LEU:HD12 | 2.12 | 0.50 |
| 3:B:813:LYS:O | 3:B:814:VAL:HG23 | 2.12 | 0.50 |
| 7:G:66:TYR:HB2 | 7:G:70:ASP:OD1 | 2.12 | 0.50 |
| 1:I:284:LEU:N | 1:I:285:PRO:HD2 | 2.27 | 0.50 |
| 1:I:465:HIS:NE2 | 3:J:1028:PHE:HD1 | 2.10 | 0.50 |
| 1:I:507:TYR:O | 1:I:508:LEU:CB | 2.57 | 0.50 |
| 1:I:653:LEU:HD11 | 1:I:745:ALA:HB2 | 1.94 | 0.50 |
| 3:J:1069:TRP:CH2 | 3:J:1077:TYR:HB2 | 2.46 | 0.50 |
| 3:J:34:PHE:HE1 | 3:J:351:ALA:HA | 1.75 | 0.50 |
| 3:J:557:HIS:CE1 | 3:J:566:VAL:HG13 | 2.47 | 0.50 |
| 2:M:238:LYS:HB2 | 2:M:239:ARG:NH1 | 2.27 | 0.50 |
| 2:M:349:VAL:CG2 | 2:M:352:LYS:HB2 | 2.42 | 0.50 |
| 3:B:934:ALA:HB2 | 11:N:47:ARG:HD3 | 1.92 | 0.50 |
| 10:V:15:LEU:HB3 | 10:V:55:VAL:CG2 | 2.41 | 0.50 |
| 1:A:468:GLN:HB2 | 3:B:1047:ASP:OD2 | 2.12 | 0.50 |
| 3:B:1067:ILE:CG2 | 3:B:1080:PRO:HG2 | 2.41 | 0.50 |
| 2:C:122:MET:SD | 2:C:256:SER:HA | 2.52 | 0.50 |
| 5:E:29:GLU:O | 5:E:33:GLN:HG3 | 2.11 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:40:PHE:HZ | 7:G:115:THR:HG21 | 1.77 | 0.50 |
| 1:I:369:PRO:HA | 1:I:410:HIS:HE1 | 1.77 | 0.50 |
| 1:I:640:GLU:OE1 | 3:J:974:ARG:NH1 | 2.45 | 0.50 |
| 3:J:239:VAL:HA | 3:J:253:PHE:CE2 | 2.46 | 0.50 |
| 3:J:473:MET:HA | 3:J:577:ARG:NH2 | 2.27 | 0.50 |
| 3:J:738:ILE:HG23 | 3:J:888:ILE:HA | 1.92 | 0.50 |
| 10:L:45:GLN:O | 10:L:46:PRO:O | 2.30 | 0.50 |
| 5:Q:168:TYR:O | 5:Q:175:ILE:HD13 | 2.11 | 0.50 |
| 1:I:547:THR:HG21 | 7:S:89:GLY:HA3 | 1.93 | 0.50 |
| 8:T:17:VAL:HG21 | 8:T:51:VAL:HG21 | 1.92 | 0.50 |
| 3:J:747:ARG:NH1 | 11:W:8:PHE:O | 2.44 | 0.50 |
| 1:A:372:TRP:O | 1:A:374:GLY:N | 2.45 | 0.50 |
| 3:B:125:SER:O | 3:B:131:SER:HB2 | 2.12 | 0.50 |
| 3:B:171:ARG:HB3 | 3:B:524:GLY:HA3 | 1.94 | 0.50 |
| 3:B:560:THR:CG2 | 3:B:561:ASP:N | 2.74 | 0.50 |
| 3:B:579:LEU:CD1 | 3:B:616:LEU:CD1 | 2.85 | 0.50 |
| 3:B:762:GLU:HG3 | 3:B:773:ILE:HG13 | 1.93 | 0.50 |
| 2:C:133:ASP:HB2 | 2:C:136:LYS:HG2 | 1.92 | 0.50 |
| 2:C:145:GLU:HG2 | 2:C:239:ARG:HA | 1.94 | 0.50 |
| 4:D:180:VAL:CG2 | 4:D:190:LEU:HG | 2.42 | 0.50 |
| 8:H:45:ILE:N | 8:H:79:ARG:HB3 | 2.27 | 0.50 |
| 1:I:532:ILE:HG22 | 10:V:58:LEU:HD22 | 1.93 | 0.50 |
| 3:J:855:THR:O | 3:J:856:ALA:C | 2.48 | 0.50 |
| 1:I:826:ALA:HB1 | 2:M:334:VAL:HG13 | 1.94 | 0.50 |
| 4:O:37:PRO:HA | 4:O:148:GLY:O | 2.12 | 0.50 |
| 1:I:532:ILE:HG13 | 10:V:12:TYR:OH | 2.12 | 0.50 |
| 10:V:46:PRO:O | 10:V:47:HIS:HB3 | 2.10 | 0.50 |
| 1:A:188:PRO:O | 1:A:192:VAL:HG23 | 2.12 | 0.50 |
| 1:A:4:LYS:HD2 | 3:B:1089:PHE:CB | 2.42 | 0.50 |
| 3:B:214:PHE:CD1 | 3:B:215:PRO:HD2 | 2.47 | 0.50 |
| 3:B:221:ILE:N | 3:B:221:ILE:HD13 | 2.26 | 0.50 |
| 3:B:345:LEU:N | 3:B:345:LEU:HD12 | 2.27 | 0.50 |
| 3:B:432:SER:HB3 | 3:B:435:ARG:HH21 | 1.77 | 0.50 |
| 3:B:624:ALA:HB1 | 3:B:639:HIS:CD2 | 2.47 | 0.50 |
| 2:C:393:ILE:HG22 | 2:C:394:LEU:H | 1.76 | 0.50 |
| 8:H:25:ILE:HA | 8:H:28:ALA:CB | 2.42 | 0.50 |
| 1:I:220:ARG:HH11 | 1:I:236:THR:CG2 | 2.22 | 0.50 |
| 1:I:259:GLN:HA | 1:I:262:ILE:HG22 | 1.94 | 0.50 |
| 1:I:58:CYS:CB | 1:I:59:PRO:CD | 2.89 | 0.50 |
| 3:J:348:ASP:N | 3:J:348:ASP:OD2 | 2.45 | 0.50 |
| 3:J:603:THR:O | 3:J:604:PHE:C | 2.49 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:769:GLN:O | 3:J:770:GLU:HB3 | 2.11 | 0.50 |
| 3:J:740:MET:O | 3:J:891:LEU:HA | 2.11 | 0.50 |
| 9:K:26:ARG:HB3 | 9:K:27:LEU:HD12 | 1.94 | 0.50 |
| 2:M:168:GLN:HG2 | 2:M:204:SER:CB | 2.42 | 0.50 |
| 2:M:276:ASN:O | 2:M:279:GLU:HB3 | 2.12 | 0.50 |
| 4:O:191:LYS:HB2 | 4:O:194:LYS:HD2 | 1.94 | 0.50 |
| 5:Q:113:ILE:HG23 | 5:Q:114:THR:N | 2.27 | 0.50 |
| 3:B:654:ILE:HG13 | 3:B:708:LEU:HD21 | 1.93 | 0.49 |
| 3:B:769:GLN:O | 3:B:770:GLU:HB3 | 2.10 | 0.49 |
| 3:B:803:GLU:HB3 | 3:B:805:LYS:HZ1 | 1.76 | 0.49 |
| 3:B:740:MET:O | 3:B:891:LEU:HA | 2.12 | 0.49 |
| 5:E:109:HIS:CD2 | 5:E:111:SER:H | 2.29 | 0.49 |
| 1:I:409:ARG:NH2 | 1:I:415:ASP:OD2 | 2.45 | 0.49 |
| 1:I:716:SER:CB | 1:I:726:TYR:OH | 2.60 | 0.49 |
| 3:J:128:ASP:OD1 | 3:J:130:ILE:HB | 2.12 | 0.49 |
| 3:J:544:ARG:NH1 | 3:J:544:ARG:HG3 | 2.17 | 0.49 |
| 4:O:125:SER:O | 4:O:127:ASP:N | 2.45 | 0.49 |
| 4:O:35:TYR:O | 4:O:149:TYR:HD2 | 1.95 | 0.49 |
| 2:M:386:VAL:HB | 9:U:31:GLU:HG2 | 1.94 | 0.49 |
| 1:A:425:LEU:O | 1:A:426:HIS:HB2 | 2.11 | 0.49 |
| 1:A:525:LEU:C | 1:A:527:VAL:H | 2.16 | 0.49 |
| 2:C:126:LEU:HG | 2:C:249:TYR:O | 2.12 | 0.49 |
| 1:A:831:ARG:NH2 | 2:C:385:MET:HG3 | 2.27 | 0.49 |
| 7:G:79:THR:CG2 | 7:G:80:GLU:H | 2.25 | 0.49 |
| 1:I:417:VAL:HG13 | 1:I:464:LEU:HD13 | 1.94 | 0.49 |
| 3:J:314:TYR:HE2 | 3:J:526:LEU:N | 2.02 | 0.49 |
| 3:J:475:GLN:HG2 | 3:J:476:ILE:H | 1.77 | 0.49 |
| 2:M:238:LYS:HB2 | 2:M:239:ARG:CZ | 2.42 | 0.49 |
| 1:A:325:VAL:O | 1:A:442:THR:HB | 2.11 | 0.49 |
| 3:B:655:ILE:HG12 | 3:B:669:GLN:HG2 | 1.94 | 0.49 |
| 2:C:122:MET:HG2 | 2:C:274:THR:HG23 | 1.95 | 0.49 |
| 1:I:353:ILE:CG1 | 1:I:361:LEU:HD23 | 2.39 | 0.49 |
| 3:J:759:SER:CB | 3:J:862:VAL:O | 2.42 | 0.49 |
| 2:M:357:ALA:O | 2:M:362:ASP:HB2 | 2.13 | 0.49 |
| 4:O:257:GLU:O | 4:O:260:LEU:HB3 | 2.12 | 0.49 |
| 10:V:21:ASP:OD1 | 10:V:22:HIS:N | 2.45 | 0.49 |
| 3:J:904:VAL:HG21 | 11:W:42:ARG:HG2 | 1.94 | 0.49 |
| 1:A:6:ILE:HD11 | 3:B:1091:VAL:HG11 | 1.93 | 0.49 |
| 1:A:23:SER:HA | 1:A:72:PHE:O | 2.11 | 0.49 |
| 3:B:338:TYR:CZ | 3:B:341:LYS:NZ | 2.81 | 0.49 |
| 3:B:430:ILE:HG22 | 3:B:431:SER:O | 2.12 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:B:753:THR:HG23 | 3:B:868:ASP:H | 1.77 | 0.49 |
| 3:B:764:LYS:NZ | 3:B:772:LYS:O | 2.45 | 0.49 |
| 1:A:501:ASP:OD2 | 3:B:913:HIS:HD2 | 1.95 | 0.49 |
| 2:C:179:VAL:HG23 | 2:C:182:ASP:H | 1.77 | 0.49 |
| 1:I:331:ASN:ND2 | 3:J:732:TYR:OH | 2.45 | 0.49 |
| 1:I:48:ARG:HB2 | 1:I:59:PRO:HB3 | 1.93 | 0.49 |
| 1:I:781:PHE:HD2 | 1:I:781:PHE:C | 2.14 | 0.49 |
| 3:J:477:ALA:HB3 | 3:J:574:ARG:CG | 2.42 | 0.49 |
| 3:J:729:PHE:C | 3:J:731:GLY:H | 2.15 | 0.49 |
| 2:M:349:VAL:HG21 | 2:M:352:LYS:HB2 | 1.93 | 0.49 |
| 7:S:31:MET:N | 7:S:38:VAL:O | 2.45 | 0.49 |
| 10:V:14:GLU:OE1 | 10:V:56:LYS:HG2 | 2.12 | 0.49 |
| 10:V:69:LEU:O | 10:V:72:ALA:N | 2.45 | 0.49 |
| 1:A:188:PRO:HD2 | 1:A:191:ASP:HB2 | 1.95 | 0.49 |
| 1:A:324:THR:CG2 | 1:A:325:VAL:H | 2.21 | 0.49 |
| 1:A:337:VAL:HG12 | 1:A:339:VAL:HG23 | 1.95 | 0.49 |
| 1:A:449:VAL:O | 1:A:449:VAL:HG12 | 2.12 | 0.49 |
| 3:B:551:ASP:OD2 | 3:B:551:ASP:N | 2.44 | 0.49 |
| 3:B:588:LEU:HD22 | 3:B:612:LYS:HG2 | 1.95 | 0.49 |
| 3:B:690:THR:O | 3:B:691:ARG:C | 2.50 | 0.49 |
| 3:B:965:ASP:O | 3:B:967:THR:N | 2.46 | 0.49 |
| 2:C:327:ARG:HH21 | 2:C:337:GLU:HG3 | 1.77 | 0.49 |
| 2:C:359:ALA:C | 2:C:361:GLY:N | 2.66 | 0.49 |
| 1:I:239:LEU:CD2 | 1:I:276:TYR:HE1 | 2.24 | 0.49 |
| 1:I:528:ALA:HB3 | 1:I:630:ASN:HD21 | 1.78 | 0.49 |
| 1:I:506:ALA:HA | 1:I:635:PHE:CD2 | 2.48 | 0.49 |
| 1:I:487:ILE:O | 1:I:858:MET:HG3 | 2.13 | 0.49 |
| 1:I:319:ASP:HB2 | 3:J:1052:ASN:HB3 | 1.93 | 0.49 |
| 3:J:325:LEU:HD12 | 3:J:328:GLY:HA2 | 1.95 | 0.49 |
| 3:J:677:LEU:HD21 | 3:J:994:HIS:HB3 | 1.94 | 0.49 |
| 3:J:927:GLY:HA2 | 3:J:987:VAL:O | 2.12 | 0.49 |
| 2:M:376:GLY:HA3 | 3:J:1050:LEU:HD13 | 1.94 | 0.49 |
| 2:M:390:MET:HB3 | 2:M:392:PRO:HD3 | 1.95 | 0.49 |
| 2:M:39:LYS:O | 2:M:43:VAL:HG23 | 2.12 | 0.49 |
| 2:M:75:ALA:O | 2:M:79:GLY:N | 2.29 | 0.49 |
| 11:N:38:LEU:HD23 | 11:N:39:GLY:N | 2.27 | 0.49 |
| 4:O:169:LYS:HG2 | 4:O:222:VAL:HG22 | 1.94 | 0.49 |
| 3:J:969:VAL:HG21 | 4:O:205:LEU:HB3 | 1.95 | 0.49 |
| 11:W:7:CYS:CB | 11:W:45:CYS:SG | 3.01 | 0.49 |
| 3:J:790:ARG:HH22 | 12:X:39:LYS:HE3 | 1.77 | 0.49 |
| 3:J:790:ARG:NH2 | 12:X:39:LYS:HE3 | 2.27 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:488:THR:HG23 | 1:A:490:ARG:H | 1.77 | 0.49 |
| 1:A:752:VAL:C | 1:A:754:GLY:N | 2.66 | 0.49 |
| 3:B:520:VAL:HG12 | 3:B:527:ILE:HB | 1.95 | 0.49 |
| 3:B:881:ARG:NH1 | 3:B:989:TYR:CB | 2.75 | 0.49 |
| 2:C:120:PRO:HA | 2:C:275:ASN:ND2 | 2.27 | 0.49 |
| 2:C:322:ARG:HD2 | 2:C:322:ARG:N | 2.27 | 0.49 |
| 1:A:826:ALA:HB1 | 2:C:334:VAL:HG13 | 1.94 | 0.49 |
| 4:D:228:LEU:O | 4:D:229:GLU:HG3 | 2.13 | 0.49 |
| 5:E:83:GLU:N | 5:E:145:ARG:HG3 | 2.25 | 0.49 |
| 7:G:86:LEU:CD1 | 7:G:91:LYS:HG3 | 2.42 | 0.49 |
| 1:I:353:ILE:HA | 1:I:357:ASN:HD21 | 1.77 | 0.49 |
| 1:I:372:TRP:O | 1:I:374:GLY:N | 2.45 | 0.49 |
| 3:J:789:TYR:O | 3:J:791:LEU:N | 2.45 | 0.49 |
| 9:K:27:LEU:HD21 | 9:K:78:ILE:HD13 | 1.95 | 0.49 |
| 7:S:87:ASN:C | 7:S:89:GLY:N | 2.65 | 0.49 |
| 1:A:203:ARG:HG3 | 1:A:205:GLU:HB2 | 1.94 | 0.49 |
| 1:A:575:CYS:CB | 1:A:580:CYS:SG | 3.01 | 0.49 |
| 1:A:607:GLN:HB2 | 1:A:608:PRO:CD | 2.43 | 0.49 |
| 1:A:853:ASP:HB3 | 1:A:855:VAL:H | 1.76 | 0.49 |
| 3:B:480:ILE:CG2 | 3:B:481:ASN:N | 2.75 | 0.49 |
| 2:C:61:GLU:C | 2:C:63:LEU:H | 2.16 | 0.49 |
| 5:E:92:VAL:HG13 | 5:E:97:ILE:HG23 | 1.94 | 0.49 |
| 6:F:18:LYS:HZ3 | 6:F:45:GLU:HG2 | 1.77 | 0.49 |
| 8:H:12:ARG:HH22 | 8:H:55:ILE:HD12 | 1.77 | 0.49 |
| 3:J:574:ARG:O | 3:J:574:ARG:HG3 | 2.12 | 0.49 |
| 2:M:72:ILE:H | 2:M:72:ILE:CD1 | 2.24 | 0.49 |
| 4:O:176:CYS:H | 4:O:195:LEU:CD2 | 2.26 | 0.49 |
| 1:A:308:ARG:HG3 | 1:A:312:ASN:HD22 | 1.78 | 0.49 |
| 2:C:237:ILE:CG1 | 2:C:238:LYS:H | 2.25 | 0.49 |
| 1:I:529:ASP:O | 1:I:529:ASP:CG | 2.51 | 0.49 |
| 3:J:578:PRO:HB3 | 3:J:615:TYR:CE1 | 2.47 | 0.49 |
| 3:J:910:LEU:CD2 | 3:J:911:ASN:N | 2.73 | 0.49 |
| 2:M:28:ILE:HG21 | 9:U:14:HIS:ND1 | 2.26 | 0.49 |
| 8:T:42:LEU:HB2 | 8:T:43:PRO:CD | 2.38 | 0.49 |
| 9:U:63:SER:HA | 9:U:66:GLU:HG3 | 1.95 | 0.49 |
| 1:A:55:GLY:O | 1:A:57:LYS:N | 2.46 | 0.49 |
| 3:B:193:THR:HG21 | 3:B:197:ARG:N | 2.28 | 0.49 |
| 2:C:321:THR:C | 2:C:322:ARG:NH1 | 2.66 | 0.49 |
| 4:D:169:LYS:HG2 | 4:D:222:VAL:HG22 | 1.94 | 0.49 |
| 5:E:82:GLN:H | 5:E:146:VAL:HB | 1.77 | 0.49 |
| 1:I:471:GLU:OE1 | 9:U:41:LEU:HD13 | 2.13 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:525:LEU:HA | 1:I:527:VAL:HG23 | 1.94 | 0.49 |
| 1:I:527:VAL:HB | 1:I:530:VAL:HB | 1.95 | 0.49 |
| 1:I:728:MET:HE3 | 3:J:913:HIS:HA | 1.94 | 0.49 |
| 3:J:972:ASP:O | 3:J:975:THR:HG23 | 2.13 | 0.49 |
| 3:J:975:THR:O | 4:O:26:ASN:ND2 | 2.46 | 0.49 |
| 3:J:853:THR:HG23 | 12:X:32:LYS:O | 2.12 | 0.49 |
| 1:A:374:GLY:C | 1:A:410:HIS:ND1 | 2.66 | 0.49 |
| 1:A:486:ILE:HG12 | 1:A:496:ILE:HB | 1.93 | 0.49 |
| 1:A:486:ILE:HG12 | 1:A:496:ILE:HD12 | 1.94 | 0.49 |
| 1:A:584:SER:OG | 1:A:585:TYR:N | 2.43 | 0.49 |
| 1:A:704:LEU:HD13 | 1:A:781:PHE:HD1 | 1.77 | 0.49 |
| 1:A:847:GLN:OE1 | 1:A:850:TYR:HA | 2.12 | 0.49 |
| 1:A:868:VAL:O | 1:A:871:ILE:HG22 | 2.12 | 0.49 |
| 1:A:4:LYS:NZ | 3:B:1115:LEU:HB3 | 2.27 | 0.49 |
| 7:G:8:GLU:O | 7:G:9:ILE:HG13 | 2.12 | 0.49 |
| 1:I:446:ASN:O | 1:I:448:LEU:N | 2.46 | 0.49 |
| 1:I:549:LYS:HB2 | 7:S:88:ASN:O | 2.13 | 0.49 |
| 1:I:847:GLN:HE22 | 2:M:314:LEU:HB3 | 1.78 | 0.49 |
| 3:J:419:TRP:HZ3 | 3:J:712:GLY:HA3 | 1.77 | 0.49 |
| 3:J:644:SER:N | 3:J:645:PRO:CD | 2.76 | 0.49 |
| 3:J:749:MET:CE | 3:J:907:ASP:HB3 | 2.43 | 0.49 |
| 1:I:501:ASP:OD2 | 3:J:913:HIS:HD2 | 1.94 | 0.49 |
| 2:M:342:LEU:CD2 | 2:M:374:ILE:HG21 | 2.43 | 0.49 |
| 6:R:72:LEU:HD23 | 6:R:86:ILE:HD12 | 1.90 | 0.49 |
| 1:A:16:PRO:HD3 | 1:A:206:TRP:CD1 | 2.48 | 0.48 |
| 1:A:353:ILE:HA | 1:A:357:ASN:HD21 | 1.77 | 0.48 |
| 1:A:402:ALA:O | 1:A:403:PRO:C | 2.50 | 0.48 |
| 3:B:1061:CYS:HA | 3:B:1088:LEU:HD23 | 1.95 | 0.48 |
| 3:B:958:LEU:HD21 | 4:D:181:ASN:O | 2.13 | 0.48 |
| 3:B:971:TYR:CZ | 4:D:165:ARG:HA | 2.48 | 0.48 |
| 2:C:312:HIS:O | 2:C:316:ILE:HG12 | 2.13 | 0.48 |
| 1:A:831:ARG:HH21 | 2:C:385:MET:HB2 | 1.77 | 0.48 |
| 2:C:390:MET:HG3 | 5:E:57:GLY:H | 1.78 | 0.48 |
| 7:G:60:SER:O | 7:G:112:PHE:HD1 | 1.96 | 0.48 |
| 1:I:8:GLY:HA2 | 2:M:365:GLU:HA | 1.94 | 0.48 |
| 2:M:392:PRO:HG3 | 5:Q:68:HIS:CE1 | 2.47 | 0.48 |
| 7:S:101:LEU:C | 7:S:103:VAL:N | 2.66 | 0.48 |
| 7:S:69:ASP:N | 7:S:69:ASP:OD2 | 2.45 | 0.48 |
| 1:A:422:GLN:NE2 | 1:A:463:ASN:HD21 | 2.10 | 0.48 |
| 1:A:78:VAL:HG23 | 1:A:266:TRP:HZ3 | 1.77 | 0.48 |
| 1:A:831:ARG:HH21 | 2:C:385:MET:CG | 2.26 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:1004:ARG:NH1 | 3:B:1025:GLY:H | 2.07 | 0.48 |
| 3:B:644:SER:C | 3:B:646:ALA:H | 2.17 | 0.48 |
| 3:B:699:GLN:NE2 | 11:N:48:MET:HE2 | 2.28 | 0.48 |
| 4:D:111:SER:O | 4:D:114:ILE:HD13 | 2.13 | 0.48 |
| 1:I:145:VAL:HG22 | 1:I:145:VAL:O | 2.12 | 0.48 |
| 1:I:337:VAL:HG23 | 1:I:433:HIS:ND1 | 2.28 | 0.48 |
| 1:I:543:ARG:HH11 | 1:I:545:TYR:HE1 | 1.61 | 0.48 |
| 3:J:617:ASP:O | 3:J:618:ALA:HB2 | 2.13 | 0.48 |
| 3:J:669:GLN:NE2 | 3:J:881:ARG:HA | 2.28 | 0.48 |
| 2:M:313:ILE:HA | 2:M:316:ILE:HG13 | 1.94 | 0.48 |
| 2:M:337:GLU:CD | 2:M:338:LYS:H | 2.16 | 0.48 |
| 2:M:35:LEU:O | 2:M:39:LYS:CG | 2.61 | 0.48 |
| 1:A:124:ARG:HH21 | 13:Y:81:ARG:NH1 | 1.98 | 0.48 |
| 1:A:620:SER:C | 1:A:622:GLU:H | 2.15 | 0.48 |
| 1:A:837:THR:HG22 | 1:A:838:VAL:N | 2.28 | 0.48 |
| 3:B:840:ARG:NH1 | 3:B:1021:ALA:HB2 | 2.28 | 0.48 |
| 3:B:1069:TRP:HE1 | 3:B:1088:LEU:CB | 2.25 | 0.48 |
| 2:C:146:TYR:HE1 | 2:C:237:ILE:HG12 | 1.76 | 0.48 |
| 2:C:390:MET:HB2 | 5:E:56:GLU:CG | 2.43 | 0.48 |
| 1:I:353:ILE:CD1 | 1:I:407:ILE:HG23 | 2.42 | 0.48 |
| 3:J:446:HIS:O | 3:J:447:GLY:C | 2.50 | 0.48 |
| 10:L:80:THR:O | 10:L:83:TYR:HB3 | 2.13 | 0.48 |
| 2:M:55:ALA:HA | 2:M:58:GLU:CG | 2.43 | 0.48 |
| 1:A:268:LEU:HD23 | 1:A:271:TYR:HD1 | 1.78 | 0.48 |
| 1:A:357:ASN:HD22 | 1:A:361:LEU:HD22 | 1.78 | 0.48 |
| 3:B:249:GLN:CG | 3:B:250:ASN:H | 2.23 | 0.48 |
| 3:B:34:PHE:HE1 | 3:B:351:ALA:HA | 1.78 | 0.48 |
| 3:B:475:GLN:HG2 | 3:B:476:ILE:H | 1.78 | 0.48 |
| 2:C:112:ASP:O | 2:C:113:ALA:CB | 2.60 | 0.48 |
| 6:F:69:ARG:HA | 6:F:72:LEU:HD12 | 1.94 | 0.48 |
| 1:I:575:CYS:CB | 1:I:580:CYS:SG | 3.02 | 0.48 |
| 3:J:191:SER:HB3 | 3:J:300:HIS:NE2 | 2.29 | 0.48 |
| 3:J:368:GLN:HE22 | 3:J:386:ARG:HH21 | 1.61 | 0.48 |
| 3:J:17:TYR:HH | 3:J:474:ALA:HA | 1.77 | 0.48 |
| 3:J:579:LEU:O | 3:J:613:ILE:HG23 | 2.13 | 0.48 |
| 3:J:67:LYS:HB3 | 3:J:68:PRO:HD2 | 1.94 | 0.48 |
| 3:J:75:ARG:N | 3:J:75:ARG:HE | 2.11 | 0.48 |
| 3:J:654:ILE:CG2 | 3:J:881:ARG:HG2 | 2.43 | 0.48 |
| 1:I:637:ARG:HH11 | 3:J:974:ARG:NH2 | 2.11 | 0.48 |
| 4:O:116:SER:OG | 4:O:121:VAL:O | 2.21 | 0.48 |
| 2:M:28:ILE:CG1 | 9:U:18:VAL:HG21 | 2.43 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:O:66:PRO:HG2 | 11:W:13:LEU:HD11 | 1.95 | 0.48 |
| 1:A:95:LYS:HB3 | 1:A:138:LYS:HG3 | 1.95 | 0.48 |
| 3:B:450:TRP:HZ3 | 3:B:621:GLU:OE2 | 1.97 | 0.48 |
| 3:B:680:TYR:HE1 | 3:B:687:ARG:HH12 | 1.60 | 0.48 |
| 2:C:144:LEU:O | 2:C:145:GLU:C | 2.51 | 0.48 |
| 2:C:27:LYS:O | 2:C:29:VAL:HG23 | 2.13 | 0.48 |
| 4:D:257:GLU:O | 4:D:260:LEU:HB3 | 2.13 | 0.48 |
| 1:I:645:THR:OG1 | 1:I:646:MET:N | 2.46 | 0.48 |
| 1:I:824:ILE:O | 1:I:828:SER:HB3 | 2.13 | 0.48 |
| 3:J:551:ASP:N | 3:J:551:ASP:OD2 | 2.47 | 0.48 |
| 3:J:555:VAL:HA | 3:J:567:HIS:O | 2.12 | 0.48 |
| 9:K:28:THR:OG1 | 9:K:31:GLU:CG | 2.58 | 0.48 |
| 11:N:33:LYS:HA | 11:N:36:ASP:HB2 | 1.96 | 0.48 |
| 4:O:205:LEU:O | 4:O:207:GLU:N | 2.46 | 0.48 |
| 5:Q:38:ILE:O | 5:Q:39:LEU:CB | 2.61 | 0.48 |
| 7:S:59:ILE:O | 7:S:59:ILE:HG22 | 2.13 | 0.48 |
| 8:T:18:PRO:HB2 | 8:T:67:ARG:HA | 1.95 | 0.48 |
| 11:W:20:SER:O | 11:W:24:ARG:HG3 | 2.14 | 0.48 |
| 3:J:702:LEU:HD13 | 11:W:47:ARG:HD2 | 1.96 | 0.48 |
| 1:A:512:LYS:N | 1:A:583:ASP:OD2 | 2.46 | 0.48 |
| 1:A:57:LYS:HB3 | 1:A:62:GLY:HA2 | 1.94 | 0.48 |
| 3:B:106:ASN:O | 3:B:108:GLU:HG3 | 2.12 | 0.48 |
| 3:B:644:SER:N | 3:B:645:PRO:CD | 2.76 | 0.48 |
| 3:B:657:TYR:HE2 | 3:B:946:TYR:CZ | 2.30 | 0.48 |
| 4:D:240:ARG:O | 4:D:244:GLU:HG2 | 2.13 | 0.48 |
| 5:E:163:THR:HG23 | 5:E:165:ARG:H | 1.77 | 0.48 |
| 7:G:66:TYR:HD1 | 7:G:114:ARG:HH11 | 1.62 | 0.48 |
| 1:I:102:GLY:H | 1:I:103:ARG:HE | 1.60 | 0.48 |
| 1:I:116:ARG:O | 1:I:130:ARG:NH2 | 2.46 | 0.48 |
| 1:I:428:ILE:HD11 | 1:I:485:ASN:HB3 | 1.95 | 0.48 |
| 3:J:227:MET:CE | 3:J:232:ILE:HG13 | 2.43 | 0.48 |
| 3:J:591:ILE:O | 3:J:594:ILE:HG12 | 2.13 | 0.48 |
| 9:K:61:VAL:HG12 | 9:K:62:ILE:H | 1.77 | 0.48 |
| 6:R:20:LEU:O | 6:R:23:ASP:HB2 | 2.13 | 0.48 |
| 2:M:270:ALA:HA | 8:T:14:HIS:ND1 | 2.28 | 0.48 |
| 8:T:44:TRP:O | 8:T:79:ARG:HD3 | 2.13 | 0.48 |
| 1:A:61:CYS:SG | 3:B:1070:TYR:CB | 3.00 | 0.48 |
| 3:B:181:SER:O | 3:B:182:ASN:HB2 | 2.13 | 0.48 |
| 3:B:473:MET:HA | 3:B:577:ARG:NH2 | 2.29 | 0.48 |
| 2:C:55:ALA:C | 2:C:58:GLU:HB2 | 2.33 | 0.48 |
| 4:D:178:LYS:O | 4:D:180:VAL:N | 2.46 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:F:46:LYS:HD3 | 6:F:76:CYS:HB2 | 1.96 | 0.48 |
| 3:J:102:PRO:HD2 | 3:J:109:ALA:HB3 | 1.95 | 0.48 |
| 4:O:131:VAL:HG22 | 4:O:132:LEU:H | 1.79 | 0.48 |
| 13:Z:59:ILE:HA | 13:Z:62:GLU:CD | 2.34 | 0.48 |
| 1:A:826:ALA:HB2 | 2:C:335:THR:HG23 | 1.95 | 0.48 |
| 3:B:240:TYR:HD2 | 3:B:244:LEU:HD23 | 1.79 | 0.48 |
| 3:B:191:SER:HB3 | 3:B:300:HIS:NE2 | 2.28 | 0.48 |
| 3:B:325:LEU:CD1 | 3:B:331:GLU:H | 2.25 | 0.48 |
| 3:B:336:ASP:HA | 3:B:341:LYS:HE3 | 1.94 | 0.48 |
| 3:B:448:THR:C | 3:B:450:TRP:N | 2.67 | 0.48 |
| 3:B:540:ILE:HG21 | 3:B:555:VAL:HG21 | 1.94 | 0.48 |
| 1:I:392:LYS:O | 1:I:393:ASP:C | 2.52 | 0.48 |
| 1:I:57:LYS:HB3 | 1:I:62:GLY:HA2 | 1.95 | 0.48 |
| 1:I:752:VAL:C | 1:I:754:GLY:N | 2.66 | 0.48 |
| 3:J:139:ILE:HG21 | 11:W:61:HIS:HD2 | 1.79 | 0.48 |
| 3:J:330:ARG:HA | 3:J:563:ILE:HD11 | 1.95 | 0.48 |
| 3:J:654:ILE:HG22 | 3:J:881:ARG:HG2 | 1.95 | 0.48 |
| 8:T:68:LYS:HA | 8:T:74:GLU:HA | 1.96 | 0.48 |
| 8:T:78:TYR:OH | 9:U:12:ASP:HB3 | 2.14 | 0.48 |
| 1:A:116:ARG:O | 1:A:130:ARG:NH2 | 2.47 | 0.48 |
| 1:A:99:ARG:HG2 | 1:A:183:ARG:NH1 | 2.29 | 0.48 |
| 3:B:294:ASP:O | 3:B:303:THR:HG23 | 2.13 | 0.48 |
| 3:B:550:SER:HB3 | 3:B:553:VAL:HG23 | 1.95 | 0.48 |
| 3:B:749:MET:CE | 3:B:907:ASP:HB3 | 2.43 | 0.48 |
| 2:C:322:ARG:HA | 8:H:43:PRO:O | 2.13 | 0.48 |
| 4:D:22:LEU:C | 4:D:24:PHE:H | 2.16 | 0.48 |
| 5:E:140:ASP:HB3 | 5:E:171:LYS:HG3 | 1.95 | 0.48 |
| 1:I:87:VAL:HG21 | 1:I:156:ILE:O | 2.14 | 0.48 |
| 1:I:203:ARG:CZ | 1:I:206:TRP:HB2 | 2.43 | 0.48 |
| 1:I:500:GLN:HB2 | 3:J:913:HIS:ND1 | 2.28 | 0.48 |
| 1:I:647:ARG:HB2 | 1:I:650:ASP:OD1 | 2.13 | 0.48 |
| 3:J:425:HIS:HA | 3:J:428:ARG:HD3 | 1.96 | 0.48 |
| 2:M:286:ILE:O | 2:M:289:ALA:HB3 | 2.13 | 0.48 |
| 5:Q:39:LEU:HD23 | 5:Q:41:ASP:H | 1.79 | 0.48 |
| 8:T:45:ILE:HB | 8:T:79:ARG:HB3 | 1.96 | 0.48 |
| 3:B:1036:LEU:HD22 | 3:B:1041:THR:CG2 | 2.43 | 0.48 |
| 3:B:480:ILE:HG22 | 3:B:481:ASN:H | 1.77 | 0.48 |
| 2:C:354:LEU:HD13 | 3:B:1104:LEU:CD2 | 2.43 | 0.48 |
| 1:A:831:ARG:HH21 | 2:C:385:MET:CB | 2.27 | 0.48 |
| 4:D:111:SER:C | 4:D:114:ILE:HD13 | 2.34 | 0.48 |
| 7:G:80:GLU:CG | 7:G:81:LEU:N | 2.77 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:354:THR:HB | 1:I:355:PRO:CD | 2.44 | 0.48 |
| 1:I:539:ILE:HB | 1:I:545:TYR:HB2 | 1.94 | 0.48 |
| 1:I:620:SER:C | 1:I:622:GLU:H | 2.18 | 0.48 |
| 1:I:93:PHE:HB3 | 1:I:184:LEU:CD2 | 2.44 | 0.48 |
| 3:J:1029:GLY:O | 3:J:1031:MET:N | 2.47 | 0.48 |
| 3:J:813:LYS:O | 3:J:814:VAL:HG23 | 2.13 | 0.48 |
| 3:J:900:THR:OG1 | 3:J:904:VAL:HB | 2.14 | 0.48 |
| 2:M:103:GLY:CA | 2:M:106:ARG:HB3 | 2.44 | 0.48 |
| 2:M:61:GLU:C | 2:M:63:LEU:N | 2.68 | 0.48 |
| 1:A:446:ASN:C | 1:A:446:ASN:ND2 | 2.65 | 0.47 |
| 3:B:683:ASN:C | 3:B:685:GLN:N | 2.64 | 0.47 |
| 8:H:80:TYR:CD1 | 8:H:81:VAL:O | 2.67 | 0.47 |
| 1:I:353:ILE:HD11 | 1:I:407:ILE:CG2 | 2.45 | 0.47 |
| 1:I:332:ILE:HA | 1:I:436:ARG:HH12 | 1.78 | 0.47 |
| 3:J:520:VAL:HG12 | 3:J:527:ILE:HB | 1.94 | 0.47 |
| 3:J:86:ARG:HG3 | 3:J:153:ILE:HD13 | 1.96 | 0.47 |
| 4:O:134:GLY:O | 4:O:135:THR:C | 2.52 | 0.47 |
| 4:D:55:ASP:HB3 | 12:P:45:VAL:HG21 | 1.96 | 0.47 |
| 9:U:28:THR:OG1 | 9:U:31:GLU:HG3 | 2.15 | 0.47 |
| 3:J:904:VAL:CG2 | 11:W:42:ARG:HG2 | 2.44 | 0.47 |
| 1:A:194:ILE:H | 1:A:194:ILE:HG13 | 1.34 | 0.47 |
| 1:A:420:ASN:HB2 | 1:A:430:MET:HG2 | 1.96 | 0.47 |
| 1:A:524:ILE:O | 1:A:525:LEU:HD22 | 2.14 | 0.47 |
| 3:B:634:THR:N | 3:B:635:PRO:HD3 | 2.29 | 0.47 |
| 5:E:96:GLY:HA2 | 5:E:110:ILE:HG12 | 1.96 | 0.47 |
| 1:I:23:SER:HA | 1:I:72:PHE:O | 2.14 | 0.47 |
| 1:I:830:LEU:HD22 | 1:I:846:VAL:HG21 | 1.96 | 0.47 |
| 3:J:1083:GLY:C | 3:J:1085:LYS:H | 2.16 | 0.47 |
| 3:J:325:LEU:HA | 3:J:329:ARG:H | 1.79 | 0.47 |
| 3:J:443:ARG:NH2 | 3:J:462:PRO:O | 2.47 | 0.47 |
| 3:J:727:MET:CE | 3:J:898:PRO:CG | 2.92 | 0.47 |
| 3:J:904:VAL:HG21 | 11:W:42:ARG:HE | 1.78 | 0.47 |
| 9:K:38:ALA:C | 9:K:42:GLN:NE2 | 2.67 | 0.47 |
| 10:L:45:GLN:HE22 | 10:L:48:PRO:HD3 | 1.78 | 0.47 |
| 2:M:289:ALA:O | 2:M:292:ILE:CG2 | 2.56 | 0.47 |
| 5:Q:12:ARG:HG3 | 5:Q:67:TYR:CZ | 2.49 | 0.47 |
| 5:Q:38:ILE:O | 5:Q:39:LEU:HB2 | 2.14 | 0.47 |
| 7:S:68:HIS:ND1 | 7:S:68:HIS:N | 2.46 | 0.47 |
| 10:V:12:TYR:CD1 | 10:V:57:ILE:O | 2.68 | 0.47 |
| 10:V:73:ILE:HG22 | 10:V:74:GLU:N | 2.29 | 0.47 |
| 1:A:457:PHE:HB2 | 3:B:737:SER:HB2 | 1.96 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:490:ARG:HD3 | 2:C:77:SER:HA | 1.97 | 0.47 |
| 1:A:691:THR:O | 1:A:695:SER:OG | 2.30 | 0.47 |
| 3:B:1113:LEU:N | 3:B:1113:LEU:HD12 | 2.11 | 0.47 |
| 3:B:1117:ASP:O | 3:B:1118:LYS:HB3 | 2.14 | 0.47 |
| 3:B:617:ASP:O | 3:B:618:ALA:HB2 | 2.14 | 0.47 |
| 2:C:15:GLU:O | 2:C:18:LYS:N | 2.47 | 0.47 |
| 2:C:376:GLY:HA3 | 3:B:1050:LEU:HD13 | 1.95 | 0.47 |
| 7:G:31:MET:HB2 | 7:G:38:VAL:O | 2.14 | 0.47 |
| 8:H:78:TYR:C | 8:H:79:ARG:HG2 | 2.35 | 0.47 |
| 1:I:104:VAL:HG12 | 1:I:137:LYS:HA | 1.97 | 0.47 |
| 1:I:524:ILE:O | 1:I:525:LEU:CD2 | 2.62 | 0.47 |
| 1:I:467:PRO:HA | 3:J:1048:ARG:NH2 | 2.29 | 0.47 |
| 3:J:294:ASP:O | 3:J:303:THR:HG23 | 2.14 | 0.47 |
| 3:J:48:GLU:HG3 | 3:J:365:LEU:HD23 | 1.95 | 0.47 |
| 3:J:813:LYS:N | 3:J:836:SER:HB3 | 2.20 | 0.47 |
| 1:I:742:GLN:HB2 | 3:J:919:MET:CE | 2.44 | 0.47 |
| 3:J:954:GLN:HA | 3:J:957:ILE:HD11 | 1.95 | 0.47 |
| 2:M:48:ILE:HG22 | 2:M:49:ASP:H | 1.78 | 0.47 |
| 11:N:42:ARG:HG3 | 11:N:43:TYR:H | 1.80 | 0.47 |
| 4:O:131:VAL:CG2 | 4:O:132:LEU:N | 2.78 | 0.47 |
| 4:O:240:ARG:O | 4:O:244:GLU:HG2 | 2.14 | 0.47 |
| 1:A:105:LYS:HZ3 | 1:A:108:GLU:HB2 | 1.79 | 0.47 |
| 1:A:99:ARG:HG2 | 1:A:183:ARG:HH12 | 1.79 | 0.47 |
| 1:A:559:ASP:OD2 | 3:J:109:ALA:HA | 2.15 | 0.47 |
| 1:A:750:GLN:CG | 1:A:782:ILE:CD1 | 2.92 | 0.47 |
| 1:A:833:GLU:CG | 1:A:839:ARG:HG3 | 2.44 | 0.47 |
| 3:B:603:THR:O | 3:B:604:PHE:C | 2.52 | 0.47 |
| 3:B:855:THR:CB | 3:B:857:GLU:HG2 | 2.31 | 0.47 |
| 5:E:72:PHE:HE1 | 5:E:74:MET:SD | 2.37 | 0.47 |
| 1:I:14:LEU:HB3 | 3:J:1108:ILE:HG23 | 1.96 | 0.47 |
| 3:J:200:VAL:HG13 | 3:J:200:VAL:O | 2.13 | 0.47 |
| 10:L:3:ILE:HG13 | 10:L:17:ILE:HD13 | 1.96 | 0.47 |
| 2:M:35:LEU:O | 2:M:39:LYS:HG2 | 2.15 | 0.47 |
| 11:N:3:ILE:HG22 | 11:N:4:PRO:CD | 2.43 | 0.47 |
| 1:I:541:ALA:CA | 7:S:72:CYS:H | 2.26 | 0.47 |
| 1:A:425:LEU:HD22 | 2:C:83:THR:HG21 | 1.96 | 0.47 |
| 1:A:98:CYS:HB3 | 1:A:101:CYS:H | 1.79 | 0.47 |
| 3:B:232:ILE:HG23 | 3:B:237:ASP:HB3 | 1.94 | 0.47 |
| 3:B:191:SER:HB3 | 3:B:300:HIS:CD2 | 2.49 | 0.47 |
| 3:B:377:ARG:O | 3:B:378:LYS:HB2 | 2.13 | 0.47 |
| 3:B:902:LYS:HB3 | 11:N:42:ARG:CD | 2.42 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:123:THR:HG22 | 2:C:252:LEU:HD23 | 1.96 | 0.47 |
| 1:I:113:LYS:HA | 1:I:116:ARG:HB3 | 1.95 | 0.47 |
| 1:I:490:ARG:NH1 | 2:M:80:GLU:HG3 | 2.29 | 0.47 |
| 3:J:1054:ASP:HB2 | 3:J:1094:SER:HA | 1.97 | 0.47 |
| 3:J:289:ALA:O | 3:J:293:ILE:CG1 | 2.62 | 0.47 |
| 3:J:320:SER:O | 3:J:320:SER:OG | 2.32 | 0.47 |
| 3:J:356:VAL:HG22 | 3:J:393:ARG:NH1 | 2.29 | 0.47 |
| 3:J:804:VAL:HG11 | 3:J:810:LEU:HD21 | 1.97 | 0.47 |
| 10:L:76:ILE:O | 10:L:77:ARG:C | 2.53 | 0.47 |
| 2:M:15:GLU:HA | 2:M:18:LYS:HE3 | 1.95 | 0.47 |
| 6:R:16:VAL:HG22 | 6:R:53:GLN:HE21 | 1.79 | 0.47 |
| 10:V:35:ILE:HD13 | 10:V:75:ASN:OD1 | 2.14 | 0.47 |
| 13:Z:69:GLU:O | 13:Z:73:LYS:NZ | 2.35 | 0.47 |
| 1:A:664:GLU:OE1 | 1:A:707:LEU:HD22 | 2.14 | 0.47 |
| 1:A:728:MET:HE3 | 3:B:913:HIS:HA | 1.95 | 0.47 |
| 3:B:324:GLU:O | 3:B:325:LEU:HB2 | 2.14 | 0.47 |
| 3:B:679:LEU:HD23 | 3:B:716:ARG:HG2 | 1.97 | 0.47 |
| 3:B:813:LYS:N | 3:B:836:SER:HB3 | 2.25 | 0.47 |
| 3:B:92:TYR:O | 3:B:92:TYR:CD2 | 2.68 | 0.47 |
| 3:B:881:ARG:NH1 | 3:B:989:TYR:HB3 | 2.22 | 0.47 |
| 4:D:176:CYS:H | 4:D:195:LEU:CD2 | 2.28 | 0.47 |
| 1:I:77:LEU:HD12 | 1:I:210:THR:C | 2.35 | 0.47 |
| 3:J:1069:TRP:HE1 | 3:J:1088:LEU:CB | 2.28 | 0.47 |
| 3:J:48:GLU:HG2 | 3:J:58:VAL:HB | 1.95 | 0.47 |
| 2:M:355:LEU:N | 2:M:355:LEU:HD23 | 2.29 | 0.47 |
| 2:M:28:ILE:CG2 | 9:U:14:HIS:HE1 | 2.18 | 0.47 |
| 11:W:33:LYS:HA | 11:W:36:ASP:HB2 | 1.96 | 0.47 |
| 1:A:99:ARG:HE | 1:A:183:ARG:NH2 | 2.12 | 0.47 |
| 1:A:319:ASP:O | 1:A:320:PHE:HB2 | 2.15 | 0.47 |
| 3:B:594:ILE:HB | 3:B:599:SER:HB2 | 1.97 | 0.47 |
| 3:B:663:SER:HB3 | 3:B:664:PRO:HD3 | 1.96 | 0.47 |
| 3:B:702:LEU:HD22 | 3:B:933:ALA:CB | 2.32 | 0.47 |
| 3:B:950:ILE:C | 3:B:952:GLN:N | 2.67 | 0.47 |
| 3:B:898:PRO:HA | 3:B:971:TYR:O | 2.14 | 0.47 |
| 3:B:930:GLY:HA3 | 3:B:987:VAL:HB | 1.97 | 0.47 |
| 1:I:433:HIS:HE2 | 1:I:453:TYR:HH | 1.57 | 0.47 |
| 1:I:763:THR:HG23 | 1:I:779:ARG:HH12 | 1.80 | 0.47 |
| 3:J:291:GLN:HB3 | 3:J:295:LYS:CE | 2.44 | 0.47 |
| 3:J:971:TYR:CE2 | 4:O:165:ARG:HA | 2.49 | 0.47 |
| 3:J:64:ARG:H | 3:J:97:TRP:HB2 | 1.80 | 0.47 |
| 5:Q:128:PHE:HE2 | 5:Q:133:LYS:HD3 | 1.80 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:557:HIS:N | 3:B:623:ASN:ND2 | 2.53 | 0.47 |
| 3:B:54:PRO:O | 3:B:56:LEU:N | 2.48 | 0.47 |
| 3:B:972:ASP:HB3 | 3:B:975:THR:HG23 | 1.97 | 0.47 |
| 2:C:393:ILE:HG13 | 2:C:393:ILE:H | 1.56 | 0.47 |
| 1:I:321:SER:O | 1:I:322:SER:HB2 | 2.14 | 0.47 |
| 3:J:368:GLN:HE22 | 3:J:386:ARG:HE | 1.62 | 0.47 |
| 3:J:463:ASN:HB3 | 3:J:467:VAL:CG1 | 2.44 | 0.47 |
| 9:K:70:ARG:C | 9:K:72:GLY:H | 2.16 | 0.47 |
| 9:K:82:LEU:HD23 | 9:K:86:LYS:O | 2.15 | 0.47 |
| 2:M:106:ARG:O | 2:M:107:LEU:C | 2.52 | 0.47 |
| 2:M:13:LEU:HD23 | 2:M:16:LYS:HZ2 | 1.78 | 0.47 |
| 8:T:25:ILE:HA | 8:T:28:ALA:HB3 | 1.97 | 0.47 |
| 8:T:42:LEU:HD13 | 8:T:79:ARG:O | 2.14 | 0.47 |
| 1:I:438:LEU:HD12 | 10:V:47:HIS:NE2 | 2.30 | 0.47 |
| 11:W:35:LEU:HD22 | 11:W:40:VAL:HG21 | 1.97 | 0.47 |
| 12:X:12:THR:O | 12:X:14:THR:N | 2.37 | 0.47 |
| 1:A:349:VAL:HG21 | 1:A:415:ASP:OD2 | 2.15 | 0.47 |
| 1:A:727:VAL:O | 1:A:729:ALA:O | 2.32 | 0.47 |
| 3:B:130:ILE:HA | 3:B:133:TYR:CE1 | 2.50 | 0.47 |
| 1:I:533:ASP:O | 1:I:534:LEU:C | 2.52 | 0.47 |
| 1:I:841:LEU:HB3 | 1:I:842:TYR:H | 1.54 | 0.47 |
| 1:A:590:ASN:CG | 3:J:377:ARG:HB2 | 2.34 | 0.47 |
| 3:J:412:GLN:HG3 | 3:J:425:HIS:NE2 | 2.30 | 0.47 |
| 3:J:972:ASP:OD2 | 3:J:974:ARG:CG | 2.59 | 0.47 |
| 4:O:94:THR:O | 4:O:95:LYS:HG3 | 2.15 | 0.47 |
| 5:Q:179:LYS:HD3 | 6:R:81:ASP:HB2 | 1.97 | 0.47 |
| 1:I:845:VAL:O | 8:T:43:PRO:HD3 | 2.15 | 0.47 |
| 4:O:256:LEU:HD13 | 10:V:3:ILE:HD12 | 1.97 | 0.47 |
| 10:V:46:PRO:HD2 | 10:V:52:LYS:O | 2.15 | 0.47 |
| 1:A:763:THR:HG21 | 1:A:772:TYR:HA | 1.97 | 0.47 |
| 3:B:239:VAL:HA | 3:B:253:PHE:CE2 | 2.48 | 0.47 |
| 3:B:946:TYR:CD2 | 3:B:947:LYS:N | 2.82 | 0.47 |
| 3:B:96:LEU:O | 3:B:115:TYR:HA | 2.15 | 0.47 |
| 2:C:390:MET:C | 2:C:391:ARG:CD | 2.83 | 0.47 |
| 1:I:568:VAL:HG21 | 1:I:597:VAL:HG11 | 1.96 | 0.47 |
| 3:J:401:GLY:O | 3:J:402:ASN:O | 2.32 | 0.47 |
| 3:J:926:GLU:HB3 | 3:J:988:VAL:CG2 | 2.43 | 0.47 |
| 9:K:42:GLN:O | 9:K:45:MET:HB2 | 2.15 | 0.47 |
| 9:K:82:LEU:CD2 | 9:K:82:LEU:N | 2.72 | 0.47 |
| 10:L:49:LEU:O | 10:L:50:SER:HB3 | 2.15 | 0.47 |
| 5:Q:110:ILE:CG2 | 5:Q:118:LEU:HB3 | 2.45 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:S:41:ASP:HB2 | 7:S:91:LYS:H | 1.80 | 0.47 |
| 3:J:902:LYS:CB | 11:W:42:ARG:HH11 | 2.27 | 0.47 |
| 1:A:524:ILE:O | 1:A:525:LEU:CD2 | 2.63 | 0.47 |
| 1:A:870:ARG:NH2 | 2:C:57:LYS:O | 2.48 | 0.47 |
| 3:B:298:LEU:O | 3:B:300:HIS:N | 2.48 | 0.47 |
| 3:B:391:THR:O | 3:B:394:ILE:HG22 | 2.15 | 0.47 |
| 3:B:437:GLN:OE1 | 3:B:438:PRO:HD2 | 2.15 | 0.47 |
| 3:B:574:ARG:O | 3:B:574:ARG:HG3 | 2.14 | 0.47 |
| 3:B:591:ILE:CG1 | 3:B:612:LYS:NZ | 2.71 | 0.47 |
| 3:B:677:LEU:HD21 | 3:B:994:HIS:HB3 | 1.97 | 0.47 |
| 3:B:781:ARG:HB2 | 3:B:831:ALA:N | 2.30 | 0.47 |
| 3:B:98:LEU:HD11 | 3:B:100:MET:CG | 2.38 | 0.47 |
| 2:C:189:GLY:O | 2:C:190:ARG:HB2 | 2.15 | 0.47 |
| 1:A:8:GLY:HA2 | 2:C:365:GLU:HA | 1.96 | 0.47 |
| 4:D:37:PRO:HA | 4:D:148:GLY:O | 2.14 | 0.47 |
| 5:E:18:PHE:CD2 | 9:K:47:ALA:HB2 | 2.50 | 0.47 |
| 5:E:13:ILE:HG23 | 5:E:25:ILE:HG21 | 1.97 | 0.47 |
| 7:G:15:ILE:HG22 | 7:G:51:GLN:O | 2.15 | 0.47 |
| 1:I:595:GLU:HB2 | 7:S:91:LYS:CE | 2.45 | 0.47 |
| 1:I:833:GLU:CG | 1:I:839:ARG:HG3 | 2.45 | 0.47 |
| 1:I:85:GLY:HA3 | 2:M:355:LEU:HD12 | 1.96 | 0.47 |
| 3:J:1012:LEU:O | 3:J:1095:TYR:CE2 | 2.64 | 0.47 |
| 3:J:1085:LYS:O | 3:J:1086:SER:OG | 2.30 | 0.47 |
| 3:J:683:ASN:C | 3:J:685:GLN:N | 2.68 | 0.47 |
| 9:K:67:GLU:CD | 9:K:70:ARG:HH21 | 2.17 | 0.47 |
| 2:M:55:ALA:C | 2:M:58:GLU:HB2 | 2.35 | 0.47 |
| 11:W:10:CYS:HB3 | 11:W:44:CYS:SG | 2.55 | 0.47 |
| 3:J:930:GLY:O | 11:W:47:ARG:NH1 | 2.48 | 0.47 |
| 1:A:16:PRO:HD3 | 1:A:206:TRP:HD1 | 1.80 | 0.46 |
| 1:A:594:LEU:O | 1:A:595:GLU:HG2 | 2.15 | 0.46 |
| 3:B:855:THR:C | 3:B:857:GLU:N | 2.66 | 0.46 |
| 3:B:921:LEU:O | 3:B:923:GLN:N | 2.46 | 0.46 |
| 3:B:963:LEU:HD22 | 3:B:982:ARG:NH2 | 2.30 | 0.46 |
| 4:D:45:TYR:HB2 | 4:D:142:GLU:O | 2.15 | 0.46 |
| 1:I:87:VAL:O | 1:I:91:TYR:HB2 | 2.15 | 0.46 |
| 3:J:840:ARG:NH1 | 3:J:1021:ALA:HB2 | 2.29 | 0.46 |
| 3:J:946:TYR:CD2 | 3:J:947:LYS:N | 2.83 | 0.46 |
| 1:I:874:ARG:HE | 2:M:53:ASP:HB3 | 1.79 | 0.46 |
| 11:N:38:LEU:HD23 | 11:N:39:GLY:H | 1.80 | 0.46 |
| 4:O:53:LEU:HD22 | 4:O:57:ILE:CG2 | 2.44 | 0.46 |
| 5:Q:31:ARG:C | 5:Q:33:GLN:N | 2.68 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:X:25:ARG:HD2 | 12:X:30:GLY:HA2 | 1.96 | 0.46 |
| 3:B:88:ARG:HG2 | 12:P:33:ILE:HD11 | 1.97 | 0.46 |
| 2:C:152:VAL:O | 2:C:152:VAL:HG22 | 2.14 | 0.46 |
| 2:C:163:MET:N | 2:C:164:SER:HA | 2.28 | 0.46 |
| 2:C:337:GLU:OE1 | 2:C:337:GLU:N | 2.47 | 0.46 |
| 4:D:134:GLY:O | 4:D:135:THR:O | 2.33 | 0.46 |
| 5:E:113:ILE:HG23 | 5:E:114:THR:N | 2.30 | 0.46 |
| 1:I:428:ILE:HG23 | 1:I:452:PRO:HB2 | 1.96 | 0.46 |
| 3:J:1067:ILE:CG2 | 3:J:1080:PRO:HG2 | 2.45 | 0.46 |
| 3:J:249:GLN:CG | 3:J:250:ASN:H | 2.24 | 0.46 |
| 3:J:582:VAL:HG11 | 3:J:633:LEU:HD11 | 1.95 | 0.46 |
| 3:J:881:ARG:CD | 3:J:989:TYR:HD2 | 2.27 | 0.46 |
| 2:M:140:VAL:O | 2:M:143:LYS:HB2 | 2.16 | 0.46 |
| 2:M:318:ASP:O | 2:M:322:ARG:HD2 | 2.15 | 0.46 |
| 1:I:537:PRO:O | 7:S:74:HIS:NE2 | 2.47 | 0.46 |
| 2:M:287:GLU:OE2 | 8:T:79:ARG:CZ | 2.63 | 0.46 |
| 1:A:759:ARG:NH2 | 1:A:763:THR:OG1 | 2.48 | 0.46 |
| 3:B:227:MET:CE | 3:B:232:ILE:HG13 | 2.46 | 0.46 |
| 3:B:953:LEU:O | 3:B:957:ILE:HG12 | 2.14 | 0.46 |
| 4:D:170:VAL:HG23 | 4:D:200:GLU:HG3 | 1.96 | 0.46 |
| 4:D:53:LEU:HD22 | 4:D:57:ILE:HG21 | 1.97 | 0.46 |
| 1:I:217:ILE:C | 1:I:219:ILE:H | 2.18 | 0.46 |
| 1:I:525:LEU:C | 1:I:527:VAL:H | 2.18 | 0.46 |
| 3:J:1010:GLN:HA | 3:J:1010:GLN:OE1 | 2.15 | 0.46 |
| 3:J:170:ASN:O | 3:J:171:ARG:O | 2.34 | 0.46 |
| 3:J:191:SER:HB3 | 3:J:300:HIS:CD2 | 2.51 | 0.46 |
| 3:J:873:THR:CG2 | 3:J:874:ILE:H | 2.26 | 0.46 |
| 4:D:254:GLU:HG2 | 10:L:77:ARG:NH1 | 2.31 | 0.46 |
| 2:M:295:ARG:O | 2:M:299:LYS:HB2 | 2.16 | 0.46 |
| 3:B:698:PRO:HG2 | 11:N:55:ILE:HD12 | 1.96 | 0.46 |
| 4:D:137:GLN:NE2 | 11:N:63:THR:HG22 | 2.30 | 0.46 |
| 4:O:206:CYS:O | 4:O:207:GLU:HB2 | 2.15 | 0.46 |
| 4:O:64:LEU:O | 11:W:6:ARG:HD2 | 2.15 | 0.46 |
| 9:U:70:ARG:HB3 | 9:U:70:ARG:CZ | 2.46 | 0.46 |
| 1:A:425:LEU:HD12 | 1:A:425:LEU:H | 1.80 | 0.46 |
| 1:A:672:VAL:HG11 | 1:A:776:PRO:HD3 | 1.98 | 0.46 |
| 3:B:1029:GLY:O | 3:B:1030:GLU:C | 2.53 | 0.46 |
| 2:C:277:ILE:C | 2:C:279:GLU:H | 2.19 | 0.46 |
| 2:C:321:THR:O | 2:C:321:THR:CG2 | 2.63 | 0.46 |
| 1:A:9:ILE:O | 2:C:363:VAL:O | 2.33 | 0.46 |
| 2:C:390:MET:O | 2:C:391:ARG:HD2 | 2.15 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:29:ARG:HG3 | 4:D:162:SER:O | 2.16 | 0.46 |
| 3:J:116:ILE:HG23 | 3:J:361:PHE:CZ | 2.50 | 0.46 |
| 3:J:170:ASN:HB3 | 3:J:300:HIS:HE1 | 1.80 | 0.46 |
| 3:J:248:VAL:HG21 | 3:J:329:ARG:HH22 | 1.80 | 0.46 |
| 3:J:569:ASN:HB3 | 3:J:574:ARG:CZ | 2.45 | 0.46 |
| 2:C:68:GLU:HB3 | 9:K:30:TYR:CZ | 2.50 | 0.46 |
| 2:M:268:ASP:OD1 | 2:M:270:ALA:HB3 | 2.15 | 0.46 |
| 2:M:341:VAL:HG11 | 2:M:357:ALA:HB1 | 1.97 | 0.46 |
| 4:O:208:GLU:N | 16:O:1001:F3S:S2 | 2.88 | 0.46 |
| 9:U:39:ARG:HE | 9:U:68:GLU:CD | 2.18 | 0.46 |
| 1:A:599:ASP:H | 1:A:602:ALA:HB3 | 1.80 | 0.46 |
| 1:A:830:LEU:HD23 | 1:A:840:SER:CB | 2.34 | 0.46 |
| 3:B:1077:TYR:O | 3:B:1077:TYR:CD1 | 2.69 | 0.46 |
| 3:B:721:ASN:HB3 | 11:N:47:ARG:HE | 1.80 | 0.46 |
| 3:B:870:ARG:NE | 3:B:996:MET:SD | 2.88 | 0.46 |
| 3:B:910:LEU:CD2 | 3:B:911:ASN:H | 2.25 | 0.46 |
| 3:B:937:GLY:HA3 | 11:N:32:GLY:CA | 2.46 | 0.46 |
| 2:C:72:ILE:HG23 | 2:C:76:GLN:OE1 | 2.15 | 0.46 |
| 1:I:433:HIS:NE2 | 1:I:453:TYR:OH | 2.43 | 0.46 |
| 1:I:486:ILE:HG12 | 1:I:496:ILE:HD12 | 1.97 | 0.46 |
| 1:I:58:CYS:HB2 | 1:I:59:PRO:CD | 2.39 | 0.46 |
| 1:I:631:LEU:O | 1:I:634:VAL:HB | 2.15 | 0.46 |
| 1:I:741:THR:O | 1:I:742:GLN:C | 2.54 | 0.46 |
| 3:J:162:VAL:HG11 | 3:J:412:GLN:HE21 | 1.80 | 0.46 |
| 3:J:343:LEU:HD22 | 3:J:575:VAL:HG22 | 1.98 | 0.46 |
| 3:J:723:ILE:HG12 | 3:J:907:ASP:OD2 | 2.16 | 0.46 |
| 3:J:848:ASP:HB2 | 3:J:867:ARG:HB2 | 1.98 | 0.46 |
| 2:M:231:ILE:H | 2:M:231:ILE:HD12 | 1.81 | 0.46 |
| 5:Q:79:PRO:HG3 | 5:Q:160:ILE:HG12 | 1.98 | 0.46 |
| 9:U:41:LEU:O | 9:U:42:GLN:C | 2.54 | 0.46 |
| 13:Y:57:GLY:HA2 | 13:Y:61:LEU:HD21 | 1.97 | 0.46 |
| 1:A:764:ARG:HB2 | 1:A:764:ARG:HH11 | 1.80 | 0.46 |
| 3:B:246:PRO:C | 3:B:248:VAL:N | 2.68 | 0.46 |
| 3:B:402:ASN:HB2 | 3:B:410:VAL:HB | 1.97 | 0.46 |
| 3:B:330:ARG:NH2 | 3:B:565:GLU:OE1 | 2.48 | 0.46 |
| 3:B:640:LEU:CD2 | 3:B:641:GLU:N | 2.67 | 0.46 |
| 3:B:992:LYS:HE3 | 3:B:996:MET:SD | 2.55 | 0.46 |
| 2:C:391:ARG:HB2 | 9:K:75:PRO:HB2 | 1.96 | 0.46 |
| 5:E:39:LEU:HD12 | 5:E:42:LEU:HG | 1.96 | 0.46 |
| 1:I:187:ILE:HA | 1:I:188:PRO:HD3 | 1.70 | 0.46 |
| 1:I:13:ILE:HG13 | 1:I:207:MET:HG2 | 1.97 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:316:LYS:HD2 | 3:J:1049:LEU:O | 2.15 | 0.46 |
| 3:J:11:TRP:O | 3:J:14:ILE:HG22 | 2.16 | 0.46 |
| 3:J:158:GLU:OE2 | 3:J:416:ARG:NH1 | 2.45 | 0.46 |
| 3:J:214:PHE:CD1 | 3:J:215:PRO:HD2 | 2.51 | 0.46 |
| 3:J:24:VAL:HG21 | 3:J:426:LEU:CD1 | 2.46 | 0.46 |
| 3:J:663:SER:CB | 3:J:664:PRO:HD3 | 2.46 | 0.46 |
| 3:J:781:ARG:CD | 3:J:782:GLY:H | 2.26 | 0.46 |
| 3:J:971:TYR:CZ | 3:J:978:LYS:HB3 | 2.50 | 0.46 |
| 9:K:86:LYS:H | 9:K:86:LYS:HD2 | 1.81 | 0.46 |
| 4:D:254:GLU:HG2 | 10:L:77:ARG:HH12 | 1.80 | 0.46 |
| 2:M:48:ILE:HG22 | 2:M:49:ASP:N | 2.31 | 0.46 |
| 2:M:86:THR:HA | 2:M:104:LEU:CD1 | 2.42 | 0.46 |
| 4:O:252:LYS:HD2 | 10:V:24:LEU:HD23 | 1.97 | 0.46 |
| 6:R:59:LEU:HD22 | 6:R:69:ARG:HD3 | 1.97 | 0.46 |
| 8:T:45:ILE:HG22 | 8:T:81:VAL:H | 1.79 | 0.46 |
| 3:B:133:TYR:HD2 | 3:B:137:LYS:HB3 | 1.80 | 0.46 |
| 3:B:260:SER:C | 3:B:262:ILE:H | 2.19 | 0.46 |
| 3:B:848:ASP:HB2 | 3:B:867:ARG:HB2 | 1.97 | 0.46 |
| 2:C:269:VAL:O | 8:H:14:HIS:HB3 | 2.15 | 0.46 |
| 2:C:51:ILE:HG13 | 2:C:51:ILE:H | 1.34 | 0.46 |
| 5:E:142:VAL:HA | 5:E:171:LYS:HA | 1.98 | 0.46 |
| 6:F:18:LYS:NZ | 6:F:45:GLU:HG2 | 2.29 | 0.46 |
| 1:I:723:ASN:O | 1:I:724:PHE:C | 2.51 | 0.46 |
| 3:J:586:ASN:HA | 3:J:587:PRO:HD3 | 1.82 | 0.46 |
| 3:J:691:ARG:NH1 | 3:J:756:ARG:NH2 | 2.64 | 0.46 |
| 3:J:797:VAL:HG12 | 3:J:798:VAL:N | 2.31 | 0.46 |
| 3:J:855:THR:CB | 3:J:857:GLU:HG2 | 2.34 | 0.46 |
| 8:T:46:ARG:HD3 | 8:T:48:SER:H | 1.80 | 0.46 |
| 9:U:39:ARG:O | 9:U:39:ARG:HG3 | 2.16 | 0.46 |
| 1:A:145:VAL:O | 1:A:145:VAL:HG22 | 2.16 | 0.46 |
| 3:B:289:ALA:O | 3:B:293:ILE:CG1 | 2.64 | 0.46 |
| 3:B:655:ILE:HG23 | 3:B:881:ARG:O | 2.16 | 0.46 |
| 2:C:179:VAL:CG2 | 2:C:232:LYS:HZ2 | 2.21 | 0.46 |
| 5:E:115:ASP:O | 5:E:116:ASP:HB2 | 2.16 | 0.46 |
| 1:I:371:LYS:HZ3 | 1:I:373:PRO:HD3 | 1.80 | 0.46 |
| 1:I:495:ILE:O | 1:I:495:ILE:HG13 | 2.16 | 0.46 |
| 3:J:448:THR:C | 3:J:450:TRP:N | 2.67 | 0.46 |
| 3:J:533:GLY:C | 3:J:535:GLU:H | 2.19 | 0.46 |
| 3:J:762:GLU:HG3 | 3:J:773:ILE:HG13 | 1.96 | 0.46 |
| 3:J:751:ARG:HG2 | 3:J:871:ILE:HG23 | 1.97 | 0.46 |
| 11:N:20:SER:O | 11:N:24:ARG:HG3 | 2.16 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:O:80:GLU:HA | 4:O:83:ILE:HD12 | 1.97 | 0.46 |
| 5:Q:43:GLY:CA | 5:Q:78:VAL:HG23 | 2.46 | 0.46 |
| 10:V:9:GLU:O | 10:V:11:ASN:N | 2.49 | 0.46 |
| 3:B:248:VAL:HG21 | 3:B:329:ARG:HH22 | 1.80 | 0.46 |
| 2:C:179:VAL:HG21 | 2:C:232:LYS:NZ | 2.25 | 0.46 |
| 2:C:281:GLU:OE1 | 2:C:326:VAL:HG12 | 2.15 | 0.46 |
| 5:E:124:ARG:HG3 | 5:E:126:ILE:CG1 | 2.46 | 0.46 |
| 7:G:84:SER:HA | 7:G:92:TYR:O | 2.16 | 0.46 |
| 7:G:9:ILE:HD13 | 7:G:104:LYS:HB2 | 1.98 | 0.46 |
| 1:I:445:LEU:HD21 | 1:I:450:CYS:HA | 1.97 | 0.46 |
| 1:I:851:GLY:C | 1:I:853:ASP:H | 2.19 | 0.46 |
| 3:J:325:LEU:HD21 | 3:J:332:PRO:HD3 | 1.97 | 0.46 |
| 3:J:402:ASN:HB2 | 3:J:410:VAL:HB | 1.98 | 0.46 |
| 3:J:950:ILE:C | 3:J:952:GLN:N | 2.70 | 0.46 |
| 10:L:47:HIS:O | 10:L:49:LEU:N | 2.49 | 0.46 |
| 4:O:131:VAL:CG2 | 4:O:132:LEU:H | 2.29 | 0.46 |
| 7:S:103:VAL:HG13 | 7:S:103:VAL:O | 2.16 | 0.46 |
| 8:T:80:TYR:O | 8:T:81:VAL:HG23 | 2.16 | 0.46 |
| 9:U:34:ARG:C | 9:U:37:SER:HB2 | 2.36 | 0.46 |
| 9:U:82:LEU:HB3 | 9:U:83:PRO:HD2 | 1.97 | 0.46 |
| 13:Y:71:ASN:O | 13:Y:74:GLU:HB2 | 2.15 | 0.46 |
| 1:A:329:ASP:CB | 1:A:332:ILE:HD12 | 2.45 | 0.46 |
| 1:A:532:ILE:HG23 | 10:L:40:PHE:CD2 | 2.51 | 0.46 |
| 1:A:487:ILE:O | 1:A:858:MET:HG3 | 2.15 | 0.46 |
| 3:B:170:ASN:O | 3:B:171:ARG:O | 2.34 | 0.46 |
| 3:B:174:VAL:HG12 | 3:B:175:ASP:N | 2.31 | 0.46 |
| 3:B:48:GLU:HG3 | 3:B:365:LEU:HD23 | 1.97 | 0.46 |
| 3:B:638:THR:HB | 3:B:639:HIS:HD2 | 1.68 | 0.46 |
| 3:B:895:VAL:HG11 | 4:D:34:LEU:CD2 | 2.46 | 0.46 |
| 4:D:133:LEU:HD22 | 4:D:137:GLN:HB3 | 1.98 | 0.46 |
| 4:D:134:GLY:O | 4:D:135:THR:C | 2.54 | 0.46 |
| 1:I:209:LEU:HD11 | 1:I:277:PHE:HE2 | 1.80 | 0.46 |
| 1:I:475:GLU:OE2 | 3:J:1043:MET:HB2 | 2.16 | 0.46 |
| 3:J:658:PRO:O | 3:J:660:HIS:N | 2.44 | 0.46 |
| 3:J:738:ILE:HD12 | 3:J:739:ILE:H | 1.81 | 0.46 |
| 3:J:81:SER:OG | 3:J:141:ILE:CG2 | 2.64 | 0.46 |
| 3:J:661:ASN:ND2 | 3:J:921:LEU:O | 2.48 | 0.46 |
| 2:M:297:ILE:O | 2:M:298:SER:C | 2.55 | 0.46 |
| 12:P:26:CYS:CB | 12:P:27:PRO:HD2 | 2.30 | 0.46 |
| 9:U:50:LEU:H | 9:U:50:LEU:HD12 | 1.79 | 0.46 |
| 12:X:9:CYS:HB3 | 12:X:12:THR:O | 2.16 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:45:MET:O | 1:A:47:PRO:HD3 | 2.15 | 0.45 |
| 1:A:553:SER:OG | 1:A:592:ILE:HA | 2.15 | 0.45 |
| 3:B:1054:ASP:HB2 | 3:B:1094:SER:HA | 1.98 | 0.45 |
| 3:B:200:VAL:O | 3:B:200:VAL:CG1 | 2.64 | 0.45 |
| 3:B:23:LEU:HB3 | 3:B:24:VAL:H | 1.52 | 0.45 |
| 3:B:557:HIS:CE1 | 3:B:566:VAL:HG13 | 2.52 | 0.45 |
| 3:B:96:LEU:HB2 | 3:B:117:GLY:H | 1.80 | 0.45 |
| 3:B:881:ARG:CD | 3:B:989:TYR:HD2 | 2.27 | 0.45 |
| 4:D:191:LYS:HB2 | 4:D:194:LYS:HD2 | 1.97 | 0.45 |
| 6:F:14:TYR:O | 6:F:18:LYS:HE3 | 2.16 | 0.45 |
| 7:G:94:THR:HG21 | 7:G:101:LEU:HD11 | 1.98 | 0.45 |
| 1:I:181:ARG:HG3 | 1:I:208:ILE:HB | 1.98 | 0.45 |
| 1:I:434:ARG:HB3 | 1:I:434:ARG:HE | 1.40 | 0.45 |
| 3:J:1004:ARG:NH1 | 3:J:1016:PRO:HB3 | 2.30 | 0.45 |
| 3:J:338:TYR:CZ | 3:J:341:LYS:NZ | 2.84 | 0.45 |
| 3:J:430:ILE:HG22 | 3:J:431:SER:O | 2.16 | 0.45 |
| 3:J:437:GLN:OE1 | 3:J:438:PRO:HD2 | 2.17 | 0.45 |
| 3:J:54:PRO:O | 3:J:55:GLY:C | 2.54 | 0.45 |
| 9:K:82:LEU:HD21 | 9:K:88:ILE:HG12 | 1.98 | 0.45 |
| 10:L:82:HIS:O | 10:L:86:GLU:N | 2.48 | 0.45 |
| 2:M:322:ARG:HD2 | 2:M:322:ARG:N | 2.32 | 0.45 |
| 11:N:6:ARG:HA | 11:N:12:SER:O | 2.15 | 0.45 |
| 1:I:722:PHE:CZ | 7:S:23:LEU:HG | 2.45 | 0.45 |
| 1:A:342:ILE:O | 1:A:345:LYS:N | 2.49 | 0.45 |
| 1:A:723:ASN:O | 1:A:724:PHE:C | 2.54 | 0.45 |
| 3:B:472:LEU:HD12 | 3:B:646:ALA:HA | 1.99 | 0.45 |
| 3:B:570:CYS:HB3 | 3:B:571:ASP:H | 1.59 | 0.45 |
| 3:B:633:LEU:HD13 | 3:B:640:LEU:HG | 1.99 | 0.45 |
| 2:C:339:ASN:N | 2:C:339:ASN:OD1 | 2.32 | 0.45 |
| 8:H:69:SER:HB2 | 8:H:75:VAL:CG2 | 2.46 | 0.45 |
| 1:I:518:LYS:H | 1:I:518:LYS:HG2 | 1.61 | 0.45 |
| 1:I:618:GLU:O | 1:I:619:TYR:CG | 2.69 | 0.45 |
| 1:I:708:ARG:O | 1:I:711:ALA:HB3 | 2.17 | 0.45 |
| 3:J:1036:LEU:HD22 | 3:J:1041:THR:HG21 | 1.98 | 0.45 |
| 3:J:110:GLU:HA | 3:J:111:PRO:HA | 1.51 | 0.45 |
| 3:J:246:PRO:O | 3:J:248:VAL:N | 2.44 | 0.45 |
| 3:J:983:ILE:HG22 | 3:J:984:TYR:O | 2.17 | 0.45 |
| 3:J:672:MET:CG | 3:J:993:LEU:HD21 | 2.27 | 0.45 |
| 9:K:50:LEU:CD2 | 9:K:74:LEU:HA | 2.36 | 0.45 |
| 2:M:290:ARG:HG3 | 2:M:321:THR:HG21 | 1.98 | 0.45 |
| 2:M:70:ILE:HA | 2:M:73:VAL:HG22 | 1.97 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:U:61:VAL:O | 9:U:63:SER:N | 2.42 | 0.45 |
| 11:W:35:LEU:HD22 | 11:W:46:ARG:HG3 | 1.99 | 0.45 |
| 13:Y:57:GLY:HA2 | 13:Y:61:LEU:CD2 | 2.46 | 0.45 |
| 1:A:234:ASP:C | 1:A:236:THR:H | 2.19 | 0.45 |
| 3:B:691:ARG:NH1 | 3:B:756:ARG:NH2 | 2.65 | 0.45 |
| 7:G:75:GLY:HA3 | 7:G:86:LEU:O | 2.16 | 0.45 |
| 3:J:123:LEU:O | 3:J:125:SER:N | 2.49 | 0.45 |
| 3:J:182:ASN:N | 3:J:182:ASN:HD22 | 2.14 | 0.45 |
| 3:J:264:ASN:H | 3:J:267:ASP:HB2 | 1.81 | 0.45 |
| 3:J:346:ALA:O | 3:J:350:PHE:HB2 | 2.16 | 0.45 |
| 3:J:921:LEU:O | 3:J:923:GLN:N | 2.48 | 0.45 |
| 10:L:7:LYS:HE3 | 10:L:12:TYR:CE2 | 2.48 | 0.45 |
| 5:Q:27:LEU:HD21 | 5:Q:31:ARG:NH2 | 2.31 | 0.45 |
| 7:S:66:TYR:N | 7:S:66:TYR:CD1 | 2.83 | 0.45 |
| 1:A:71:HIS:ND1 | 3:B:1070:TYR:CE2 | 2.82 | 0.45 |
| 1:I:346:THR:HG21 | 3:J:1003:ALA:HB1 | 1.97 | 0.45 |
| 1:I:371:LYS:HZ2 | 1:I:373:PRO:HD3 | 1.81 | 0.45 |
| 1:I:839:ARG:NH1 | 8:T:37:ILE:CG2 | 2.78 | 0.45 |
| 3:J:96:LEU:HD21 | 3:J:119:LEU:HB2 | 1.98 | 0.45 |
| 3:J:343:LEU:HB2 | 3:J:476:ILE:HG21 | 1.99 | 0.45 |
| 3:J:544:ARG:HB2 | 3:J:549:ILE:HG22 | 1.99 | 0.45 |
| 3:J:633:LEU:HD13 | 3:J:640:LEU:HG | 1.98 | 0.45 |
| 3:J:685:GLN:HE22 | 3:J:867:ARG:HH22 | 1.64 | 0.45 |
| 9:K:30:TYR:CD1 | 9:K:30:TYR:N | 2.85 | 0.45 |
| 12:P:37:VAL:HG22 | 12:P:38:ARG:N | 2.31 | 0.45 |
| 6:R:24:VAL:C | 6:R:26:ARG:H | 2.20 | 0.45 |
| 7:S:86:LEU:HG | 7:S:87:ASN:N | 2.31 | 0.45 |
| 9:U:31:GLU:CD | 9:U:78:ILE:HG21 | 2.37 | 0.45 |
| 1:A:392:LYS:O | 1:A:393:ASP:C | 2.54 | 0.45 |
| 1:A:525:LEU:HA | 1:A:527:VAL:HG23 | 1.97 | 0.45 |
| 1:A:93:PHE:HB3 | 1:A:184:LEU:CD2 | 2.46 | 0.45 |
| 3:B:215:PRO:O | 3:B:216:ALA:HB3 | 2.17 | 0.45 |
| 3:B:298:LEU:C | 3:B:300:HIS:N | 2.70 | 0.45 |
| 3:B:314:TYR:HE2 | 3:B:526:LEU:N | 2.02 | 0.45 |
| 3:B:544:ARG:NH2 | 3:B:620:GLU:OE2 | 2.50 | 0.45 |
| 3:B:591:ILE:HG12 | 3:B:612:LYS:HZ2 | 1.77 | 0.45 |
| 3:B:702:LEU:HB2 | 3:B:721:ASN:ND2 | 2.32 | 0.45 |
| 3:B:661:ASN:ND2 | 3:B:921:LEU:O | 2.48 | 0.45 |
| 2:C:359:ALA:O | 2:C:361:GLY:N | 2.49 | 0.45 |
| 4:D:53:LEU:HD11 | 11:N:2:LEU:HD12 | 1.98 | 0.45 |
| 1:I:155:LYS:HA | 1:I:156:ILE:O | 2.17 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:486:ILE:HA | 1:I:496:ILE:HD12 | 1.99 | 0.45 |
| 1:I:759:ARG:HE | 1:I:759:ARG:HB3 | 1.57 | 0.45 |
| 3:J:133:TYR:HD2 | 3:J:137:LYS:HB3 | 1.81 | 0.45 |
| 3:J:691:ARG:NH1 | 3:J:756:ARG:HH21 | 2.15 | 0.45 |
| 13:Z:61:LEU:O | 13:Z:65:LYS:HB2 | 2.16 | 0.45 |
| 1:A:446:ASN:O | 1:A:447:LEU:C | 2.55 | 0.45 |
| 1:A:527:VAL:HB | 1:A:530:VAL:HB | 1.98 | 0.45 |
| 3:B:98:LEU:CD1 | 3:B:100:MET:HG3 | 2.37 | 0.45 |
| 3:B:569:ASN:HB3 | 3:B:574:ARG:NH1 | 2.29 | 0.45 |
| 3:B:554:ASN:ND2 | 3:B:576:ARG:HH21 | 2.11 | 0.45 |
| 4:D:34:LEU:HD22 | 4:D:151:LYS:HB2 | 1.99 | 0.45 |
| 5:E:51:VAL:C | 5:E:53:THR:H | 2.19 | 0.45 |
| 8:H:13:ILE:HG23 | 8:H:14:HIS:CE1 | 2.51 | 0.45 |
| 1:I:16:PRO:HD3 | 1:I:206:TRP:CD1 | 2.52 | 0.45 |
| 1:I:279:ASN:ND2 | 1:I:295:LEU:O | 2.49 | 0.45 |
| 1:I:512:LYS:N | 1:I:583:ASP:OD2 | 2.50 | 0.45 |
| 3:J:768:GLY:O | 3:J:769:GLN:HB2 | 2.15 | 0.45 |
| 3:B:930:GLY:CA | 11:N:47:ARG:HH22 | 2.29 | 0.45 |
| 4:O:11:THR:HG22 | 4:O:232:SER:HB3 | 1.98 | 0.45 |
| 5:Q:101:LEU:HD21 | 5:Q:162:LEU:HD11 | 1.99 | 0.45 |
| 5:Q:15:PRO:HG3 | 5:Q:64:GLY:O | 2.15 | 0.45 |
| 10:V:84:ILE:O | 10:V:87:ILE:HG22 | 2.17 | 0.45 |
| 1:A:354:THR:HB | 1:A:355:PRO:CD | 2.46 | 0.45 |
| 1:A:5:ASN:O | 3:B:1116:GLU:N | 2.50 | 0.45 |
| 1:A:728:MET:HE1 | 3:B:912:PRO:O | 2.17 | 0.45 |
| 1:A:86:LEU:HD22 | 1:A:207:MET:HE3 | 1.99 | 0.45 |
| 3:B:1012:LEU:O | 3:B:1095:TYR:CE2 | 2.68 | 0.45 |
| 3:B:1069:TRP:NE1 | 3:B:1088:LEU:HD13 | 2.32 | 0.45 |
| 3:B:123:LEU:C | 3:B:125:SER:H | 2.20 | 0.45 |
| 3:B:555:VAL:HA | 3:B:567:HIS:O | 2.17 | 0.45 |
| 1:I:827:LEU:HD12 | 2:M:71:GLY:HA2 | 1.99 | 0.45 |
| 3:J:240:TYR:HD2 | 3:J:244:LEU:HD23 | 1.82 | 0.45 |
| 3:J:900:THR:HG21 | 3:J:968:GLU:OE2 | 2.16 | 0.45 |
| 2:M:210:PHE:HB3 | 2:M:211:ALA:H | 1.54 | 0.45 |
| 2:M:28:ILE:HG12 | 2:M:28:ILE:H | 1.60 | 0.45 |
| 11:N:35:LEU:HD23 | 11:N:40:VAL:HG21 | 1.98 | 0.45 |
| 11:N:4:PRO:HG2 | 11:N:48:MET:HE1 | 1.99 | 0.45 |
| 10:V:4:ARG:CG | 10:V:4:ARG:HH11 | 2.27 | 0.45 |
| 11:W:18:TRP:CZ2 | 11:W:22:ILE:HG13 | 2.52 | 0.45 |
| 13:Y:71:ASN:HA | 13:Y:74:GLU:OE1 | 2.16 | 0.45 |
| 1:A:634:VAL:HG12 | 1:A:635:PHE:N | 2.32 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:97:TRP:O | 3:B:98:LEU:HB3 | 2.17 | 0.45 |
| 2:C:171:ASN:HA | 2:C:174:LEU:HB3 | 1.98 | 0.45 |
| 1:I:430:MET:O | 1:I:431:MET:HG3 | 2.16 | 0.45 |
| 1:I:447:LEU:HD11 | 3:J:731:GLY:O | 2.16 | 0.45 |
| 1:I:556:LEU:HA | 1:I:557:PRO:HD3 | 1.90 | 0.45 |
| 3:J:34:PHE:HA | 3:J:38:LYS:HB3 | 1.98 | 0.45 |
| 3:J:555:VAL:HG22 | 3:J:568:VAL:HA | 1.99 | 0.45 |
| 3:J:454:CYS:HB2 | 3:J:649:GLY:N | 2.32 | 0.45 |
| 3:J:758:TYR:O | 3:J:759:SER:CB | 2.60 | 0.45 |
| 3:J:778:ALA:HA | 3:J:783:TYR:CE1 | 2.51 | 0.45 |
| 10:L:49:LEU:H | 10:L:49:LEU:HD22 | 1.82 | 0.45 |
| 10:L:87:ILE:HD13 | 10:L:87:ILE:HA | 1.79 | 0.45 |
| 2:M:226:ILE:HB | 2:M:227:LEU:HD12 | 1.97 | 0.45 |
| 2:M:55:ALA:HB2 | 2:M:58:GLU:OE2 | 2.17 | 0.45 |
| 11:N:35:LEU:HD22 | 11:N:40:VAL:HG21 | 1.98 | 0.45 |
| 3:J:930:GLY:CA | 11:W:47:ARG:HH22 | 2.27 | 0.45 |
| 1:A:206:TRP:C | 1:A:208:ILE:H | 2.20 | 0.45 |
| 1:A:456:ASP:OD1 | 1:A:460:ASP:OD2 | 2.35 | 0.45 |
| 3:B:148:PRO:HG3 | 3:B:422:MET:CE | 2.47 | 0.45 |
| 3:B:5:LEU:O | 3:B:5:LEU:HD22 | 2.17 | 0.45 |
| 3:B:657:TYR:HB3 | 3:B:660:HIS:CD2 | 2.52 | 0.45 |
| 4:D:125:SER:OG | 4:D:127:ASP:HB3 | 2.16 | 0.45 |
| 4:D:78:TRP:O | 4:D:80:GLU:N | 2.50 | 0.45 |
| 5:E:66:THR:CG2 | 5:E:68:HIS:CE1 | 2.99 | 0.45 |
| 1:I:327:SER:HB2 | 1:I:444:ARG:CD | 2.47 | 0.45 |
| 1:I:483:HIS:HD2 | 1:I:625:LYS:HG3 | 1.79 | 0.45 |
| 3:J:221:ILE:HD13 | 3:J:221:ILE:N | 2.31 | 0.45 |
| 3:J:226:LEU:O | 3:J:230:LEU:HD12 | 2.17 | 0.45 |
| 3:J:21:LYS:HA | 3:J:25:ARG:CZ | 2.47 | 0.45 |
| 3:J:260:SER:C | 3:J:262:ILE:H | 2.20 | 0.45 |
| 3:J:298:LEU:O | 3:J:300:HIS:N | 2.50 | 0.45 |
| 3:J:781:ARG:HB2 | 3:J:831:ALA:N | 2.32 | 0.45 |
| 3:J:956:GLU:O | 3:J:960:TYR:HD1 | 2.00 | 0.45 |
| 10:L:92:LYS:HE3 | 10:L:92:LYS:HA | 1.98 | 0.45 |
| 4:O:170:VAL:HG23 | 4:O:200:GLU:HG3 | 1.99 | 0.45 |
| 9:U:84:ASN:HB3 | 9:U:86:LYS:HB2 | 1.99 | 0.45 |
| 1:A:332:ILE:HA | 1:A:436:ARG:HH12 | 1.82 | 0.45 |
| 1:A:575:CYS:CB | 1:A:580:CYS:HG | 2.30 | 0.45 |
| 1:A:586:VAL:HA | 1:A:596:GLY:HA3 | 1.99 | 0.45 |
| 1:A:820:GLN:O | 1:A:823:LEU:HD12 | 2.17 | 0.45 |
| 3:B:291:GLN:HB3 | 3:B:295:LYS:CE | 2.44 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:353:LEU:CA | 3:B:404:VAL:HG11 | 2.16 | 0.45 |
| 3:B:687:ARG:NH1 | 3:B:689:ASP:OD1 | 2.49 | 0.45 |
| 3:B:792:LEU:HD21 | 3:B:809:VAL:HG12 | 1.98 | 0.45 |
| 2:C:170:ASP:OD1 | 2:C:171:ASN:N | 2.46 | 0.45 |
| 2:C:282:GLU:O | 8:H:50:PRO:HG3 | 2.17 | 0.45 |
| 1:I:181:ARG:O | 1:I:185:GLU:HG3 | 2.17 | 0.45 |
| 1:I:371:LYS:HZ2 | 1:I:373:PRO:CD | 2.30 | 0.45 |
| 1:I:564:GLY:O | 1:I:586:VAL:N | 2.47 | 0.45 |
| 1:I:607:GLN:HB2 | 1:I:608:PRO:CD | 2.47 | 0.45 |
| 1:I:508:LEU:HB3 | 1:I:638:PHE:HE2 | 1.81 | 0.45 |
| 3:J:554:ASN:O | 3:J:569:ASN:N | 2.48 | 0.45 |
| 3:J:569:ASN:HB3 | 3:J:574:ARG:NH1 | 2.32 | 0.45 |
| 2:M:106:ARG:O | 2:M:109:GLU:HB2 | 2.16 | 0.45 |
| 4:O:178:LYS:O | 4:O:180:VAL:N | 2.50 | 0.45 |
| 7:S:87:ASN:O | 7:S:89:GLY:N | 2.50 | 0.45 |
| 2:M:388:LEU:CD2 | 9:U:35:VAL:HG12 | 2.47 | 0.45 |
| 1:A:283:GLY:C | 1:A:285:PRO:HD2 | 2.37 | 0.44 |
| 3:B:108:GLU:O | 3:B:110:GLU:N | 2.51 | 0.44 |
| 3:B:239:VAL:HG22 | 3:B:253:PHE:HD2 | 1.82 | 0.44 |
| 3:B:936:SER:HA | 3:B:960:TYR:CE2 | 2.53 | 0.44 |
| 2:C:258:LEU:HD22 | 2:C:279:GLU:HG2 | 1.99 | 0.44 |
| 2:C:347:PHE:CE2 | 2:C:348:GLU:HG3 | 2.53 | 0.44 |
| 5:E:2:TYR:N | 5:E:2:TYR:CD1 | 2.85 | 0.44 |
| 1:I:528:ALA:O | 1:I:530:VAL:HG12 | 2.16 | 0.44 |
| 1:I:647:ARG:HB2 | 1:I:650:ASP:CG | 2.37 | 0.44 |
| 1:I:764:ARG:NH1 | 1:I:764:ARG:HB2 | 2.33 | 0.44 |
| 3:J:814:VAL:HG22 | 3:J:833:ARG:O | 2.17 | 0.44 |
| 1:I:641:LEU:O | 3:J:980:LYS:HB2 | 2.17 | 0.44 |
| 9:K:39:ARG:HD3 | 9:K:74:LEU:HD23 | 1.98 | 0.44 |
| 2:M:289:ALA:HA | 2:M:292:ILE:HG22 | 1.99 | 0.44 |
| 2:M:322:ARG:C | 2:M:324:GLY:H | 2.21 | 0.44 |
| 4:O:78:TRP:CD1 | 4:O:78:TRP:N | 2.85 | 0.44 |
| 3:B:243:SER:O | 3:B:249:GLN:OE1 | 2.35 | 0.44 |
| 3:B:325:LEU:HD12 | 3:B:328:GLY:HA2 | 1.98 | 0.44 |
| 3:B:490:TYR:HE1 | 3:B:527:ILE:CG2 | 2.30 | 0.44 |
| 3:B:86:ARG:HG3 | 3:B:153:ILE:HD13 | 1.98 | 0.44 |
| 1:A:648:LEU:HB2 | 3:B:924:ILE:HG21 | 1.99 | 0.44 |
| 2:C:318:ASP:OD2 | 2:C:322:ARG:NH2 | 2.51 | 0.44 |
| 6:F:23:ASP:HA | 6:F:26:ARG:HD2 | 2.00 | 0.44 |
| 7:G:64:PRO:O | 7:G:114:ARG:HD2 | 2.18 | 0.44 |
| 1:I:16:PRO:HD3 | 1:I:206:TRP:HD1 | 1.83 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:452:PRO:HG3 | 1:I:496:ILE:HG12 | 2.00 | 0.44 |
| 3:J:402:ASN:O | 3:J:403:TRP:HB2 | 2.18 | 0.44 |
| 3:J:634:THR:N | 3:J:635:PRO:HD3 | 2.33 | 0.44 |
| 3:J:855:THR:C | 3:J:857:GLU:N | 2.70 | 0.44 |
| 7:S:10:ILE:HD12 | 7:S:10:ILE:H | 1.81 | 0.44 |
| 1:A:500:GLN:HG3 | 1:A:501:ASP:H | 1.82 | 0.44 |
| 1:A:665:ILE:HG13 | 1:A:666:ASP:N | 2.32 | 0.44 |
| 1:A:346:THR:O | 3:B:1005:ALA:HB2 | 2.17 | 0.44 |
| 3:B:554:ASN:O | 3:B:569:ASN:N | 2.49 | 0.44 |
| 1:A:441:LEU:HD12 | 3:B:873:THR:HG21 | 2.00 | 0.44 |
| 4:D:34:LEU:O | 4:D:150:GLY:N | 2.49 | 0.44 |
| 7:G:75:GLY:HA3 | 7:G:87:ASN:HA | 1.98 | 0.44 |
| 1:I:347:LEU:HD13 | 1:I:466:VAL:CG2 | 2.47 | 0.44 |
| 1:I:561:ASN:HD22 | 1:I:590:ASN:H | 1.65 | 0.44 |
| 3:J:1104:LEU:HB3 | 3:J:1109:ILE:HB | 1.99 | 0.44 |
| 3:J:246:PRO:C | 3:J:248:VAL:N | 2.68 | 0.44 |
| 3:J:68:PRO:HA | 3:J:93:ALA:O | 2.16 | 0.44 |
| 3:J:657:TYR:HE2 | 3:J:946:TYR:CZ | 2.35 | 0.44 |
| 2:M:192:LYS:C | 2:M:194:GLY:N | 2.69 | 0.44 |
| 2:M:314:LEU:O | 2:M:315:LEU:C | 2.53 | 0.44 |
| 12:P:17:GLN:C | 12:P:19:LYS:H | 2.19 | 0.44 |
| 7:S:42:ILE:HD13 | 7:S:42:ILE:HA | 1.85 | 0.44 |
| 9:U:38:ALA:O | 9:U:41:LEU:N | 2.50 | 0.44 |
| 1:A:827:LEU:CD2 | 2:C:75:ALA:HB2 | 2.47 | 0.44 |
| 1:A:878:TRP:NE1 | 3:J:377:ARG:HD3 | 2.31 | 0.44 |
| 3:B:249:GLN:HB2 | 3:B:253:PHE:CZ | 2.52 | 0.44 |
| 3:B:368:GLN:NE2 | 3:B:386:ARG:HE | 2.16 | 0.44 |
| 3:B:419:TRP:HZ3 | 3:B:712:GLY:CA | 2.28 | 0.44 |
| 3:B:343:LEU:HB2 | 3:B:476:ILE:HG21 | 2.00 | 0.44 |
| 3:B:595:GLU:CA | 3:B:599:SER:HB3 | 2.39 | 0.44 |
| 3:B:82:PRO:HG3 | 3:B:130:ILE:CD1 | 2.47 | 0.44 |
| 1:A:647:ARG:HD3 | 3:B:965:ASP:HB3 | 1.99 | 0.44 |
| 3:B:971:TYR:CZ | 3:B:978:LYS:HB3 | 2.52 | 0.44 |
| 3:B:975:THR:OG1 | 3:B:977:GLN:HG2 | 2.17 | 0.44 |
| 2:C:310:ILE:O | 2:C:314:LEU:HD23 | 2.16 | 0.44 |
| 2:C:32:LEU:O | 2:C:36:ILE:HB | 2.17 | 0.44 |
| 4:D:35:TYR:O | 4:D:149:TYR:HD2 | 2.01 | 0.44 |
| 8:H:62:ILE:HG22 | 8:H:80:TYR:HA | 1.99 | 0.44 |
| 8:H:82:ILE:HA | 8:H:82:ILE:HD13 | 1.87 | 0.44 |
| 3:J:1069:TRP:HE3 | 3:J:1070:TYR:N | 2.14 | 0.44 |
| 3:J:753:THR:HG23 | 3:J:868:ASP:H | 1.82 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:655:ILE:HG23 | 3:J:881:ARG:O | 2.17 | 0.44 |
| 2:M:135:ASP:C | 2:M:137:ALA:H | 2.20 | 0.44 |
| 2:M:149:ILE:O | 2:M:153:VAL:HG12 | 2.18 | 0.44 |
| 2:M:70:ILE:HG12 | 2:M:315:LEU:HD11 | 2.00 | 0.44 |
| 7:S:72:CYS:HA | 7:S:114:ARG:HA | 1.99 | 0.44 |
| 8:T:80:TYR:CD1 | 8:T:81:VAL:O | 2.70 | 0.44 |
| 1:A:181:ARG:O | 1:A:185:GLU:HG3 | 2.17 | 0.44 |
| 1:A:209:LEU:HD11 | 1:A:277:PHE:HE2 | 1.82 | 0.44 |
| 1:A:275:THR:HA | 1:A:278:ASP:O | 2.18 | 0.44 |
| 3:B:12:ARG:HB2 | 3:B:592:GLU:OE2 | 2.17 | 0.44 |
| 3:B:804:VAL:HG11 | 3:B:810:LEU:HD21 | 1.99 | 0.44 |
| 3:B:911:ASN:HD21 | 3:B:913:HIS:HD2 | 1.65 | 0.44 |
| 2:C:188:ILE:HB | 2:C:189:GLY:H | 1.65 | 0.44 |
| 3:B:963:LEU:HD22 | 4:D:208:GLU:HG3 | 2.00 | 0.44 |
| 1:I:249:LEU:HD21 | 1:I:265:LEU:HB2 | 1.99 | 0.44 |
| 1:I:425:LEU:H | 1:I:425:LEU:HD12 | 1.81 | 0.44 |
| 1:I:747:LEU:HD22 | 1:I:786:PHE:CE1 | 2.53 | 0.44 |
| 3:J:108:GLU:HB2 | 3:J:109:ALA:H | 1.65 | 0.44 |
| 3:J:480:ILE:HG22 | 3:J:481:ASN:H | 1.83 | 0.44 |
| 3:J:484:ILE:H | 3:J:484:ILE:CD1 | 2.27 | 0.44 |
| 3:J:554:ASN:ND2 | 3:J:576:ARG:HH21 | 2.06 | 0.44 |
| 3:J:668:TYR:O | 3:J:671:ALA:HB3 | 2.17 | 0.44 |
| 2:M:141:ALA:HB2 | 2:M:251:ILE:HD11 | 1.99 | 0.44 |
| 1:A:409:ARG:NH2 | 1:A:415:ASP:OD2 | 2.49 | 0.44 |
| 1:A:448:LEU:O | 1:A:496:ILE:HG23 | 2.17 | 0.44 |
| 1:A:498:ALA:HB3 | 1:A:603:ILE:O | 2.18 | 0.44 |
| 1:A:506:ALA:O | 1:A:510:THR:HG23 | 2.18 | 0.44 |
| 1:A:526:GLY:HA2 | 10:L:44:TYR:CD1 | 2.53 | 0.44 |
| 1:A:723:ASN:ND2 | 1:A:725:ALA:H | 2.15 | 0.44 |
| 3:B:139:ILE:HD13 | 11:N:61:HIS:HD2 | 1.80 | 0.44 |
| 3:B:183:ILE:HG22 | 3:B:209:THR:N | 2.33 | 0.44 |
| 3:B:24:VAL:HG21 | 3:B:426:LEU:HD13 | 2.00 | 0.44 |
| 3:B:75:ARG:N | 3:B:75:ARG:HE | 2.15 | 0.44 |
| 1:A:874:ARG:HG3 | 2:C:54:LEU:HB2 | 1.99 | 0.44 |
| 7:G:101:LEU:HD12 | 7:G:104:LYS:HZ3 | 1.80 | 0.44 |
| 8:H:72:TYR:C | 8:H:74:GLU:H | 2.21 | 0.44 |
| 1:I:184:LEU:O | 1:I:186:LYS:N | 2.50 | 0.44 |
| 1:I:402:ALA:O | 1:I:403:PRO:C | 2.54 | 0.44 |
| 1:I:586:VAL:HA | 1:I:596:GLY:HA3 | 1.99 | 0.44 |
| 1:I:763:THR:HG21 | 1:I:772:TYR:HA | 1.99 | 0.44 |
| 1:I:864:LYS:NZ | 2:M:29:VAL:HA | 2.33 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:383:THR:HG22 | 3:J:1042:ALA:H | 1.82 | 0.44 |
| 3:J:111:PRO:O | 3:J:112:GLU:CB | 2.64 | 0.44 |
| 3:J:291:GLN:C | 3:J:293:ILE:N | 2.71 | 0.44 |
| 3:J:557:HIS:N | 3:J:623:ASN:ND2 | 2.57 | 0.44 |
| 3:J:658:PRO:HB2 | 3:J:666:ASN:ND2 | 2.33 | 0.44 |
| 1:I:728:MET:HE1 | 3:J:912:PRO:O | 2.17 | 0.44 |
| 2:M:109:GLU:OE2 | 2:M:117:PRO:HA | 2.16 | 0.44 |
| 2:M:125:TYR:HD2 | 2:M:250:ILE:HG23 | 1.82 | 0.44 |
| 1:I:870:ARG:CZ | 2:M:57:LYS:O | 2.66 | 0.44 |
| 11:W:38:LEU:HD23 | 11:W:39:GLY:N | 2.32 | 0.44 |
| 1:A:337:VAL:HG23 | 1:A:433:HIS:CG | 2.52 | 0.44 |
| 3:B:1001:LEU:O | 3:B:1020:ARG:HD3 | 2.17 | 0.44 |
| 3:B:244:LEU:C | 3:B:246:PRO:HD3 | 2.38 | 0.44 |
| 3:B:759:SER:CB | 3:B:862:VAL:O | 2.56 | 0.44 |
| 2:C:113:ALA:HB3 | 2:C:328:GLN:NE2 | 2.32 | 0.44 |
| 7:G:30:ASN:C | 7:G:31:MET:HG3 | 2.38 | 0.44 |
| 1:I:416:ILE:HD11 | 1:I:477:LYS:HG3 | 2.00 | 0.44 |
| 1:I:5:ASN:O | 3:J:1116:GLU:N | 2.51 | 0.44 |
| 3:J:325:LEU:O | 3:J:326:TYR:C | 2.56 | 0.44 |
| 3:J:910:LEU:CD2 | 3:J:911:ASN:H | 2.30 | 0.44 |
| 3:J:932:TYR:CD2 | 3:J:953:LEU:HD22 | 2.52 | 0.44 |
| 3:J:965:ASP:C | 3:J:967:THR:H | 2.21 | 0.44 |
| 2:M:352:LYS:O | 2:M:353:HIS:C | 2.56 | 0.44 |
| 8:T:46:ARG:CD | 8:T:48:SER:HB2 | 2.47 | 0.44 |
| 11:W:3:ILE:HG22 | 11:W:4:PRO:CD | 2.48 | 0.44 |
| 1:A:175:LEU:HD23 | 1:A:176:THR:H | 1.82 | 0.44 |
| 1:A:364:PHE:HD2 | 1:A:373:PRO:O | 2.00 | 0.44 |
| 1:A:524:ILE:CG2 | 1:A:634:VAL:HG13 | 2.48 | 0.44 |
| 1:A:679:TYR:OH | 1:A:693:GLU:HG2 | 2.17 | 0.44 |
| 1:A:829:ASP:HA | 2:C:369:VAL:HG13 | 1.99 | 0.44 |
| 3:B:812:GLY:HA2 | 3:B:836:SER:CB | 2.47 | 0.44 |
| 3:B:970:VAL:HG22 | 3:B:979:ILE:HG12 | 2.00 | 0.44 |
| 5:E:107:LEU:O | 5:E:162:LEU:N | 2.50 | 0.44 |
| 7:G:66:TYR:CD1 | 7:G:114:ARG:NH1 | 2.82 | 0.44 |
| 1:I:456:ASP:OD1 | 1:I:460:ASP:OD2 | 2.35 | 0.44 |
| 1:I:528:ALA:C | 1:I:530:VAL:H | 2.21 | 0.44 |
| 1:I:4:LYS:NZ | 3:J:1115:LEU:HB3 | 2.32 | 0.44 |
| 3:J:68:PRO:CD | 3:J:129:PRO:HG2 | 2.47 | 0.44 |
| 3:J:705:THR:HG22 | 3:J:706:ARG:H | 1.83 | 0.44 |
| 3:J:785:GLY:HA3 | 3:J:788:TYR:HE2 | 1.82 | 0.44 |
| 3:J:936:SER:HA | 3:J:960:TYR:CE2 | 2.53 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:115:LYS:HD3 | 2:M:278:ARG:HD2 | 2.00 | 0.44 |
| 11:N:22:ILE:HD12 | 11:N:22:ILE:H | 1.82 | 0.44 |
| 5:Q:56:GLU:HA | 5:Q:68:HIS:ND1 | 2.33 | 0.44 |
| 7:S:64:PRO:C | 7:S:114:ARG:HH11 | 2.21 | 0.44 |
| 8:T:44:TRP:HA | 8:T:80:TYR:HB3 | 2.00 | 0.44 |
| 13:Z:38:ILE:O | 13:Z:39:GLN:HB2 | 2.17 | 0.44 |
| 1:A:105:LYS:HZ2 | 1:A:108:GLU:HB2 | 1.81 | 0.44 |
| 1:A:500:GLN:HB2 | 3:B:913:HIS:CG | 2.53 | 0.44 |
| 1:A:588:ILE:HA | 1:A:592:ILE:O | 2.17 | 0.44 |
| 1:A:4:LYS:HG2 | 1:A:5:ASN:N | 2.32 | 0.44 |
| 1:A:637:ARG:HH11 | 3:B:974:ARG:HH22 | 1.66 | 0.44 |
| 1:A:747:LEU:HD23 | 1:A:747:LEU:N | 2.33 | 0.44 |
| 3:B:586:ASN:HA | 3:B:587:PRO:HD3 | 1.80 | 0.44 |
| 4:D:168:PRO:HG3 | 4:D:203:CYS:O | 2.18 | 0.44 |
| 4:D:64:LEU:O | 11:N:6:ARG:HD2 | 2.18 | 0.44 |
| 7:G:26:LEU:HD13 | 7:G:27:SER:N | 2.32 | 0.44 |
| 1:I:650:ASP:HB3 | 1:I:723:ASN:ND2 | 2.32 | 0.44 |
| 3:J:134:THR:O | 3:J:138:LEU:HD12 | 2.18 | 0.44 |
| 3:J:249:GLN:HB2 | 3:J:253:PHE:CZ | 2.53 | 0.44 |
| 3:J:720:ASN:N | 3:J:720:ASN:HD22 | 2.16 | 0.44 |
| 5:E:15:PRO:CG | 9:K:45:MET:HB3 | 2.41 | 0.44 |
| 5:Q:27:LEU:HD21 | 5:Q:31:ARG:CZ | 2.48 | 0.44 |
| 2:M:286:ILE:CD1 | 8:T:45:ILE:HG13 | 2.48 | 0.44 |
| 10:V:63:ILE:HG22 | 10:V:64:THR:H | 1.83 | 0.44 |
| 10:V:72:ALA:O | 10:V:75:ASN:HB2 | 2.18 | 0.44 |
| 13:Y:69:GLU:O | 13:Y:73:LYS:HG2 | 2.18 | 0.44 |
| 13:Y:67:LEU:HA | 13:Y:70:ASP:HB2 | 2.00 | 0.44 |
| 1:A:426:HIS:O | 1:A:429:SER:HB2 | 2.18 | 0.43 |
| 1:A:781:PHE:CD2 | 1:A:781:PHE:C | 2.91 | 0.43 |
| 3:B:253:PHE:N | 3:B:254:PRO:CD | 2.79 | 0.43 |
| 3:B:446:HIS:O | 3:B:447:GLY:C | 2.56 | 0.43 |
| 3:B:482:GLU:O | 3:B:483:ARG:C | 2.56 | 0.43 |
| 3:B:741:ASN:C | 3:B:741:ASN:OD1 | 2.56 | 0.43 |
| 3:B:814:VAL:HG22 | 3:B:833:ARG:O | 2.18 | 0.43 |
| 1:I:600:LYS:HB2 | 1:I:732:GLY:HA3 | 1.99 | 0.43 |
| 1:I:859:TYR:HB2 | 2:M:64:ILE:HG21 | 2.00 | 0.43 |
| 1:I:874:ARG:HD3 | 1:I:874:ARG:HA | 1.76 | 0.43 |
| 3:J:432:SER:HB3 | 3:J:435:ARG:HH21 | 1.81 | 0.43 |
| 3:J:50:PRO:C | 3:J:52:GLU:H | 2.21 | 0.43 |
| 10:L:47:HIS:O | 10:L:48:PRO:C | 2.56 | 0.43 |
| 4:O:59:ALA:O | 4:O:62:LEU:HB2 | 2.18 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:391:ARG:NH2 | 9:U:39:ARG:HD2 | 2.27 | 0.43 |
| 1:A:239:LEU:HD23 | 1:A:276:TYR:HE1 | 1.83 | 0.43 |
| 1:A:549:LYS:NZ | 7:G:89:GLY:HA2 | 2.33 | 0.43 |
| 1:A:672:VAL:O | 1:A:673:ASP:C | 2.56 | 0.43 |
| 1:A:723:ASN:C | 1:A:723:ASN:ND2 | 2.72 | 0.43 |
| 1:A:4:LYS:HZ2 | 3:B:1115:LEU:HB3 | 1.82 | 0.43 |
| 3:B:92:TYR:OH | 3:B:128:ASP:OD2 | 2.35 | 0.43 |
| 3:B:154:VAL:O | 3:B:156:GLY:N | 2.52 | 0.43 |
| 4:D:44:VAL:HG13 | 4:D:143:ALA:HB2 | 2.00 | 0.43 |
| 7:G:57:VAL:HG12 | 7:G:57:VAL:O | 2.18 | 0.43 |
| 1:I:665:ILE:HG13 | 1:I:666:ASP:N | 2.33 | 0.43 |
| 3:J:361:PHE:CE1 | 3:J:385:VAL:HG13 | 2.50 | 0.43 |
| 3:J:721:ASN:HB3 | 11:W:47:ARG:HE | 1.82 | 0.43 |
| 11:N:35:LEU:HD22 | 11:N:46:ARG:HG3 | 2.00 | 0.43 |
| 4:O:45:TYR:HB2 | 4:O:142:GLU:O | 2.18 | 0.43 |
| 3:J:895:VAL:HG11 | 4:O:34:LEU:HD21 | 2.00 | 0.43 |
| 5:Q:171:LYS:HE2 | 5:Q:173:GLU:HB2 | 1.99 | 0.43 |
| 5:Q:98:PHE:CE1 | 5:Q:107:LEU:HD13 | 2.53 | 0.43 |
| 6:R:7:VAL:HG12 | 6:R:8:GLU:N | 2.33 | 0.43 |
| 10:V:45:GLN:HG3 | 10:V:45:GLN:O | 2.19 | 0.43 |
| 3:J:139:ILE:HD13 | 11:W:61:HIS:CD2 | 2.53 | 0.43 |
| 1:A:828:SER:OG | 1:A:829:ASP:N | 2.51 | 0.43 |
| 3:B:123:LEU:C | 3:B:125:SER:N | 2.71 | 0.43 |
| 3:B:134:THR:O | 3:B:138:LEU:HD12 | 2.18 | 0.43 |
| 3:B:898:PRO:HB2 | 3:B:970:VAL:HG21 | 2.00 | 0.43 |
| 3:B:899:TYR:CE1 | 3:B:971:TYR:HB2 | 2.53 | 0.43 |
| 3:B:6:THR:HB | 3:B:9:GLU:CB | 2.48 | 0.43 |
| 2:C:286:ILE:HD12 | 8:H:45:ILE:HG13 | 1.99 | 0.43 |
| 5:E:27:LEU:HD21 | 5:E:31:ARG:NH1 | 2.33 | 0.43 |
| 2:C:287:GLU:OE2 | 8:H:79:ARG:CZ | 2.66 | 0.43 |
| 1:I:194:ILE:H | 1:I:194:ILE:HG13 | 1.42 | 0.43 |
| 1:I:272:HIS:HA | 1:I:275:THR:HB | 2.00 | 0.43 |
| 1:I:397:LEU:HA | 1:I:400:THR:OG1 | 2.18 | 0.43 |
| 1:I:475:GLU:OE1 | 3:J:1043:MET:N | 2.48 | 0.43 |
| 1:I:588:ILE:HA | 1:I:592:ILE:O | 2.18 | 0.43 |
| 3:J:183:ILE:HG22 | 3:J:209:THR:N | 2.33 | 0.43 |
| 9:K:71:ARG:HB2 | 9:K:71:ARG:HH11 | 1.83 | 0.43 |
| 10:L:15:LEU:HB3 | 10:L:55:VAL:HG23 | 2.01 | 0.43 |
| 2:M:391:ARG:NH2 | 9:U:39:ARG:NH1 | 2.58 | 0.43 |
| 3:J:971:TYR:CD2 | 4:O:164:VAL:O | 2.72 | 0.43 |
| 5:Q:11:VAL:HG12 | 5:Q:12:ARG:N | 2.31 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:R:15:SER:O | 6:R:19:LYS:HG2 | 2.18 | 0.43 |
| 8:T:40:GLU:OE1 | 13:Z:66:LYS:NZ | 2.46 | 0.43 |
| 10:V:48:PRO:C | 10:V:50:SER:H | 2.21 | 0.43 |
| 11:W:6:ARG:HA | 11:W:12:SER:O | 2.18 | 0.43 |
| 11:W:35:LEU:HD23 | 11:W:40:VAL:HG21 | 1.99 | 0.43 |
| 1:A:438:LEU:HD21 | 1:A:444:ARG:CZ | 2.47 | 0.43 |
| 1:A:541:ALA:HB3 | 1:A:542:PRO:CD | 2.44 | 0.43 |
| 3:B:1083:GLY:C | 3:B:1085:LYS:H | 2.22 | 0.43 |
| 3:B:43:ILE:HG13 | 3:B:63:ILE:HD12 | 2.00 | 0.43 |
| 3:B:55:GLY:O | 3:B:105:ASN:N | 2.51 | 0.43 |
| 3:B:580:ILE:HG13 | 3:B:642:ILE:HD13 | 2.00 | 0.43 |
| 3:B:629:GLU:HB3 | 3:B:630:PRO:HD2 | 2.00 | 0.43 |
| 3:B:672:MET:HA | 3:B:675:GLN:HB2 | 2.00 | 0.43 |
| 1:A:786:PHE:CD1 | 3:B:919:MET:HE1 | 2.53 | 0.43 |
| 2:C:111:VAL:HG12 | 2:C:329:ILE:HB | 1.99 | 0.43 |
| 5:E:42:LEU:HD13 | 5:E:74:MET:HE1 | 1.99 | 0.43 |
| 7:G:101:LEU:HD12 | 7:G:104:LYS:HZ1 | 1.80 | 0.43 |
| 1:I:90:ILE:CD1 | 1:I:207:MET:HB2 | 2.41 | 0.43 |
| 1:I:323:ARG:H | 3:J:1002:HIS:HB2 | 1.82 | 0.43 |
| 3:J:1100:LEU:O | 3:J:1101:ILE:C | 2.56 | 0.43 |
| 3:J:136:ASP:HA | 3:J:139:ILE:HD12 | 2.01 | 0.43 |
| 3:J:594:ILE:HB | 3:J:599:SER:HB2 | 2.00 | 0.43 |
| 3:J:803:GLU:HG2 | 3:J:846:ILE:HG13 | 1.99 | 0.43 |
| 2:M:246:GLY:O | 2:M:247:ASP:C | 2.57 | 0.43 |
| 11:N:43:TYR:HA | 11:N:46:ARG:HB2 | 1.99 | 0.43 |
| 1:A:112:GLU:O | 1:A:116:ARG:HB2 | 2.18 | 0.43 |
| 1:A:533:ASP:O | 1:A:534:LEU:C | 2.56 | 0.43 |
| 1:A:64:THR:HB | 1:A:65:LEU:H | 1.48 | 0.43 |
| 3:B:183:ILE:HG12 | 3:B:207:ASP:N | 2.33 | 0.43 |
| 3:B:296:TYR:CD1 | 3:B:296:TYR:N | 2.87 | 0.43 |
| 3:B:445:LEU:HD11 | 3:B:455:PRO:HB2 | 2.00 | 0.43 |
| 3:B:597:LEU:O | 3:B:598:GLU:HB2 | 2.19 | 0.43 |
| 3:B:757:LEU:HD21 | 3:B:863:LYS:HB3 | 2.01 | 0.43 |
| 5:E:175:ILE:HG22 | 5:E:175:ILE:O | 2.18 | 0.43 |
| 5:E:36:GLU:CG | 6:F:34:LEU:HD11 | 2.27 | 0.43 |
| 6:F:84:ARG:HG3 | 6:F:85:SER:N | 2.32 | 0.43 |
| 3:J:296:TYR:CD1 | 3:J:296:TYR:N | 2.87 | 0.43 |
| 3:J:148:PRO:HG3 | 3:J:422:MET:CE | 2.47 | 0.43 |
| 3:J:890:MET:HG3 | 3:J:891:LEU:N | 2.32 | 0.43 |
| 1:A:849:ALA:HB2 | 9:K:15:PHE:CD1 | 2.54 | 0.43 |
| 9:K:61:VAL:HG12 | 9:K:62:ILE:N | 2.33 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:274:THR:CG2 | 2:M:275:ASN:H | 2.07 | 0.43 |
| 5:Q:171:LYS:HB3 | 5:Q:174:TRP:CD1 | 2.54 | 0.43 |
| 6:R:64:SER:H | 6:R:69:ARG:HH21 | 1.66 | 0.43 |
| 10:V:78:GLY:O | 10:V:81:SER:HB2 | 2.18 | 0.43 |
| 1:A:353:ILE:CD1 | 1:A:407:ILE:HG23 | 2.47 | 0.43 |
| 1:A:457:PHE:C | 1:A:459:GLY:H | 2.21 | 0.43 |
| 3:B:191:SER:CB | 3:B:300:HIS:CD2 | 3.01 | 0.43 |
| 3:B:873:THR:HG23 | 3:B:874:ILE:HD12 | 2.00 | 0.43 |
| 3:B:875:GLY:HA2 | 3:B:887:VAL:CG1 | 2.48 | 0.43 |
| 2:C:238:LYS:O | 2:C:239:ARG:HB2 | 2.18 | 0.43 |
| 2:C:24:LEU:HD13 | 2:C:33:LYS:HA | 2.01 | 0.43 |
| 6:F:64:SER:N | 6:F:69:ARG:HH21 | 2.16 | 0.43 |
| 1:I:188:PRO:O | 1:I:192:VAL:HG23 | 2.19 | 0.43 |
| 1:I:347:LEU:HB2 | 1:I:411:LEU:HD22 | 2.01 | 0.43 |
| 3:J:1087:ASN:C | 3:J:1088:LEU:HG | 2.39 | 0.43 |
| 3:J:675:GLN:HG2 | 3:J:994:HIS:NE2 | 2.33 | 0.43 |
| 3:J:848:ASP:CG | 3:J:867:ARG:HH11 | 2.20 | 0.43 |
| 9:K:50:LEU:O | 9:K:51:ILE:C | 2.56 | 0.43 |
| 2:M:145:GLU:HG3 | 2:M:240:ALA:HB3 | 2.00 | 0.43 |
| 11:N:53:VAL:HG23 | 11:N:55:ILE:HG23 | 2.01 | 0.43 |
| 1:A:249:LEU:HD21 | 1:A:265:LEU:HB2 | 2.01 | 0.43 |
| 1:A:517:THR:HG22 | 1:A:519:GLU:H | 1.84 | 0.43 |
| 1:A:635:PHE:O | 1:A:639:VAL:HG23 | 2.19 | 0.43 |
| 3:B:1004:ARG:NH1 | 3:B:1016:PRO:HB3 | 2.34 | 0.43 |
| 3:B:81:SER:OG | 3:B:141:ILE:CG2 | 2.67 | 0.43 |
| 3:B:361:PHE:C | 3:B:361:PHE:CD2 | 2.92 | 0.43 |
| 3:B:654:ILE:HG22 | 3:B:881:ARG:HG2 | 2.01 | 0.43 |
| 3:B:687:ARG:HH11 | 3:B:687:ARG:CB | 2.31 | 0.43 |
| 3:B:685:GLN:NE2 | 3:B:867:ARG:HH22 | 2.17 | 0.43 |
| 2:C:146:TYR:HD1 | 2:C:238:LYS:N | 2.17 | 0.43 |
| 2:C:330:GLY:O | 2:C:331:ARG:C | 2.57 | 0.43 |
| 4:D:6:LEU:HB3 | 4:D:14:ASP:HB2 | 2.00 | 0.43 |
| 5:E:20:LYS:HA | 5:E:21:PRO:HD2 | 1.68 | 0.43 |
| 1:I:571:GLY:HA3 | 1:I:572:PRO:HD2 | 1.91 | 0.43 |
| 3:J:1077:TYR:HD1 | 3:J:1077:TYR:O | 2.02 | 0.43 |
| 3:J:1083:GLY:O | 3:J:1084:ASP:HB2 | 2.18 | 0.43 |
| 3:J:108:GLU:C | 3:J:108:GLU:OE2 | 2.56 | 0.43 |
| 3:J:217:VAL:HA | 3:J:218:PRO:HD3 | 1.90 | 0.43 |
| 3:J:5:LEU:O | 3:J:5:LEU:HD22 | 2.18 | 0.43 |
| 3:J:763:VAL:HA | 3:J:770:GLU:CG | 2.48 | 0.43 |
| 1:A:835:ASP:HA | 9:K:20:ILE:CD1 | 2.49 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:853:ASP:CB | 2:M:311:ARG:HH12 | 2.26 | 0.43 |
| 11:N:48:MET:HA | 11:N:48:MET:HE2 | 2.00 | 0.43 |
| 5:Q:146:VAL:HG12 | 5:Q:147:ILE:N | 2.34 | 0.43 |
| 3:J:698:PRO:HB2 | 11:W:53:VAL:CG2 | 2.47 | 0.43 |
| 1:A:631:LEU:O | 1:A:634:VAL:HB | 2.19 | 0.43 |
| 3:B:1074:LYS:HB3 | 3:B:1076:LYS:HE2 | 2.01 | 0.43 |
| 3:B:935:LEU:O | 11:N:46:ARG:NH1 | 2.51 | 0.43 |
| 4:D:94:THR:CG2 | 4:D:145:LEU:HB2 | 2.49 | 0.43 |
| 8:H:41:GLN:O | 8:H:42:LEU:HB3 | 2.19 | 0.43 |
| 1:I:365:VAL:HG11 | 1:I:401:LEU:HD11 | 2.01 | 0.43 |
| 3:J:1069:TRP:HB2 | 3:J:1078:VAL:O | 2.18 | 0.43 |
| 3:J:253:PHE:N | 3:J:254:PRO:CD | 2.80 | 0.43 |
| 3:J:402:ASN:O | 3:J:403:TRP:CB | 2.66 | 0.43 |
| 3:J:764:LYS:HZ2 | 3:J:772:LYS:C | 2.22 | 0.43 |
| 3:J:764:LYS:NZ | 3:J:814:VAL:H | 2.14 | 0.43 |
| 3:J:665:ARG:HH21 | 3:J:918:ARG:NE | 2.15 | 0.43 |
| 9:K:68:GLU:HG3 | 9:K:74:LEU:HG | 2.00 | 0.43 |
| 9:K:89:LEU:H | 9:K:89:LEU:HG | 1.77 | 0.43 |
| 1:I:812:ARG:NE | 2:M:86:THR:HG23 | 2.31 | 0.43 |
| 11:N:52:HIS:CE1 | 11:N:54:ASP:H | 2.36 | 0.43 |
| 4:O:133:LEU:HD22 | 4:O:137:GLN:HB3 | 2.01 | 0.43 |
| 7:S:90:ASN:N | 7:S:90:ASN:OD1 | 2.41 | 0.43 |
| 8:T:20:HIS:O | 8:T:21:GLU:HG3 | 2.19 | 0.43 |
| 1:A:98:CYS:CA | 1:A:146:CYS:SG | 3.05 | 0.43 |
| 1:A:349:VAL:HG21 | 1:A:409:ARG:NH2 | 2.33 | 0.43 |
| 1:A:415:ASP:H | 1:A:435:VAL:HG12 | 1.84 | 0.43 |
| 1:A:426:HIS:ND1 | 1:A:428:ILE:HG22 | 2.30 | 0.43 |
| 1:A:529:ASP:O | 1:A:529:ASP:CG | 2.57 | 0.43 |
| 3:B:549:ILE:HD13 | 3:B:549:ILE:HA | 1.75 | 0.43 |
| 3:B:848:ASP:CG | 3:B:867:ARG:HH11 | 2.22 | 0.43 |
| 3:B:88:ARG:CD | 3:B:853:THR:CG2 | 2.77 | 0.43 |
| 4:D:61:ARG:HG2 | 4:D:61:ARG:HH11 | 1.82 | 0.43 |
| 7:G:109:LYS:NZ | 3:J:378:LYS:CE | 2.78 | 0.43 |
| 1:I:259:GLN:HA | 1:I:262:ILE:CG2 | 2.49 | 0.43 |
| 3:J:14:ILE:O | 3:J:17:TYR:HB3 | 2.18 | 0.43 |
| 3:J:181:SER:O | 3:J:182:ASN:CB | 2.67 | 0.43 |
| 3:J:246:PRO:HD2 | 3:J:247:GLU:H | 1.84 | 0.43 |
| 3:J:480:ILE:CG2 | 3:J:481:ASN:N | 2.80 | 0.43 |
| 3:J:522:LEU:HD13 | 3:J:523:ASN:HB2 | 2.01 | 0.43 |
| 3:J:871:ILE:H | 3:J:871:ILE:HG13 | 1.62 | 0.43 |
| 10:L:35:ILE:O | 10:L:36:SER:C | 2.57 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:21:SER:O | 2:M:33:LYS:CE | 2.67 | 0.43 |
| 2:M:148:LYS:HE3 | 2:M:231:ILE:HG23 | 2.00 | 0.43 |
| 1:I:541:ALA:CB | 7:S:71:PHE:HA | 2.46 | 0.43 |
| 8:T:38:ARG:HB3 | 8:T:40:GLU:HG2 | 2.00 | 0.43 |
| 13:Y:77:LYS:HB3 | 13:Y:77:LYS:NZ | 2.34 | 0.43 |
| 13:Y:82:ARG:HA | 13:Y:82:ARG:HE | 1.83 | 0.43 |
| 1:A:353:ILE:O | 1:A:403:PRO:HA | 2.19 | 0.43 |
| 1:A:502:TYR:CD1 | 1:A:632:PHE:HB3 | 2.53 | 0.43 |
| 1:A:796:PHE:CZ | 3:B:445:LEU:HD13 | 2.54 | 0.43 |
| 3:B:1054:ASP:HB3 | 3:B:1095:TYR:N | 2.26 | 0.43 |
| 3:B:402:ASN:O | 3:B:403:TRP:CB | 2.67 | 0.43 |
| 3:B:600:GLY:C | 3:B:602:ILE:H | 2.22 | 0.43 |
| 3:B:735:GLU:OE2 | 3:B:735:GLU:HA | 2.18 | 0.43 |
| 2:C:11:PRO:O | 2:C:14:GLU:CG | 2.67 | 0.43 |
| 2:C:181:VAL:O | 2:C:184:VAL:HG12 | 2.19 | 0.43 |
| 6:F:13:PRO:HG2 | 6:F:16:VAL:CG2 | 2.48 | 0.43 |
| 1:I:234:ASP:C | 1:I:236:THR:H | 2.22 | 0.43 |
| 1:I:375:ALA:O | 1:I:377:TYR:N | 2.52 | 0.43 |
| 1:I:507:TYR:HA | 1:I:510:THR:H | 1.84 | 0.43 |
| 1:I:672:VAL:O | 1:I:675:LEU:N | 2.51 | 0.43 |
| 1:I:71:HIS:ND1 | 3:J:1070:TYR:CE2 | 2.86 | 0.43 |
| 2:M:373:ILE:CD1 | 3:J:1049:LEU:HD22 | 2.49 | 0.43 |
| 3:J:388:ASP:HB3 | 3:J:391:THR:HB | 2.01 | 0.43 |
| 3:J:445:LEU:HD11 | 3:J:455:PRO:HB3 | 2.01 | 0.43 |
| 3:J:461:GLY:HA3 | 3:J:462:PRO:HD3 | 1.91 | 0.43 |
| 3:J:55:GLY:O | 3:J:105:ASN:N | 2.51 | 0.43 |
| 3:J:416:ARG:NH1 | 3:J:687:ARG:HH21 | 2.17 | 0.43 |
| 2:M:237:ILE:C | 2:M:238:LYS:HG2 | 2.40 | 0.43 |
| 5:Q:38:ILE:HB | 5:Q:39:LEU:H | 1.43 | 0.43 |
| 7:S:33:CYS:HB2 | 7:S:36:PHE:O | 2.19 | 0.43 |
| 13:Z:59:ILE:HA | 13:Z:62:GLU:OE2 | 2.19 | 0.43 |
| 1:A:340:PRO:HB2 | 1:A:343:ILE:HG12 | 2.00 | 0.42 |
| 1:A:528:ALA:C | 1:A:530:VAL:H | 2.22 | 0.42 |
| 1:A:875:VAL:HB | 1:A:876:VAL:H | 1.71 | 0.42 |
| 1:A:87:VAL:O | 1:A:91:TYR:HB2 | 2.18 | 0.42 |
| 3:B:345:LEU:O | 3:B:346:ALA:C | 2.57 | 0.42 |
| 3:B:663:SER:CB | 3:B:664:PRO:HD3 | 2.48 | 0.42 |
| 3:B:690:THR:CG2 | 3:B:691:ARG:HG3 | 2.46 | 0.42 |
| 3:B:9:GLU:O | 3:B:10:ARG:C | 2.58 | 0.42 |
| 2:C:361:GLY:O | 2:C:362:ASP:O | 2.37 | 0.42 |
| 2:C:60:SER:O | 2:C:63:LEU:CB | 2.64 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:83:GLU:O | 5:E:145:ARG:HA | 2.19 | 0.42 |
| 7:G:86:LEU:HG | 7:G:87:ASN:N | 2.34 | 0.42 |
| 1:I:517:THR:HG22 | 1:I:518:LYS:N | 2.34 | 0.42 |
| 3:J:123:LEU:C | 3:J:125:SER:N | 2.72 | 0.42 |
| 3:J:132:GLN:HA | 3:J:132:GLN:OE1 | 2.19 | 0.42 |
| 3:J:174:VAL:HG12 | 3:J:175:ASP:N | 2.34 | 0.42 |
| 3:J:171:ARG:HB3 | 3:J:524:GLY:HA3 | 2.00 | 0.42 |
| 3:J:96:LEU:O | 3:J:115:TYR:HA | 2.19 | 0.42 |
| 3:J:970:VAL:O | 3:J:979:ILE:HG13 | 2.19 | 0.42 |
| 2:M:117:PRO:HD3 | 2:M:276:ASN:ND2 | 2.34 | 0.42 |
| 2:M:292:ILE:HG23 | 2:M:293:ILE:H | 1.83 | 0.42 |
| 4:O:178:LYS:HE2 | 4:O:178:LYS:HB2 | 1.89 | 0.42 |
| 12:P:12:THR:O | 12:P:14:THR:N | 2.39 | 0.42 |
| 11:W:52:HIS:NE2 | 11:W:54:ASP:HB2 | 2.34 | 0.42 |
| 12:X:37:VAL:HG22 | 12:X:38:ARG:N | 2.32 | 0.42 |
| 1:A:763:THR:HG23 | 1:A:779:ARG:HH12 | 1.85 | 0.42 |
| 1:A:84:VAL:O | 1:A:87:VAL:HG12 | 2.19 | 0.42 |
| 3:B:110:GLU:HA | 3:B:111:PRO:HA | 1.57 | 0.42 |
| 3:B:246:PRO:O | 3:B:248:VAL:N | 2.47 | 0.42 |
| 3:B:544:ARG:HB2 | 3:B:549:ILE:CG2 | 2.48 | 0.42 |
| 3:B:797:VAL:HG12 | 3:B:798:VAL:N | 2.33 | 0.42 |
| 2:C:271:LYS:O | 2:C:272:VAL:C | 2.57 | 0.42 |
| 2:C:31:ASP:C | 2:C:33:LYS:N | 2.71 | 0.42 |
| 1:I:349:VAL:HG21 | 1:I:415:ASP:OD2 | 2.18 | 0.42 |
| 1:I:357:ASN:HD22 | 1:I:361:LEU:HD22 | 1.83 | 0.42 |
| 1:I:555:PHE:HD2 | 1:I:631:LEU:HD13 | 1.81 | 0.42 |
| 1:I:558:LYS:HA | 1:I:590:ASN:O | 2.19 | 0.42 |
| 1:I:723:ASN:ND2 | 1:I:723:ASN:C | 2.72 | 0.42 |
| 1:I:826:ALA:H | 2:M:335:THR:HG23 | 1.83 | 0.42 |
| 1:I:879:LYS:NZ | 2:M:44:THR:HB | 2.34 | 0.42 |
| 3:J:191:SER:CB | 3:J:300:HIS:CD2 | 3.01 | 0.42 |
| 3:J:617:ASP:O | 3:J:618:ALA:CB | 2.66 | 0.42 |
| 3:J:750:TYR:OH | 3:J:990:TYR:O | 2.27 | 0.42 |
| 10:L:59:THR:HG22 | 10:L:65:PRO:HD3 | 1.99 | 0.42 |
| 2:M:174:LEU:HB2 | 2:M:179:VAL:HG13 | 2.00 | 0.42 |
| 4:D:64:LEU:HD22 | 11:N:6:ARG:HD3 | 2.01 | 0.42 |
| 9:U:46:GLY:O | 9:U:47:ALA:O | 2.38 | 0.42 |
| 12:X:33:ILE:HD13 | 12:X:33:ILE:HA | 1.90 | 0.42 |
| 3:B:446:HIS:HD2 | 3:B:448:THR:OG1 | 2.02 | 0.42 |
| 3:B:94:ALA:O | 3:B:118:ASP:HA | 2.19 | 0.42 |
| 7:G:42:ILE:HD13 | 7:G:46:ILE:HG21 | 2.00 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:418:ASN:HD21 | 3:J:421:SER:N | 2.00 | 0.42 |
| 3:J:597:LEU:O | 3:J:598:GLU:HB2 | 2.19 | 0.42 |
| 3:J:657:TYR:HB3 | 3:J:660:HIS:CD2 | 2.55 | 0.42 |
| 3:J:759:SER:CB | 3:J:863:LYS:HA | 2.47 | 0.42 |
| 2:C:391:ARG:HH22 | 9:K:42:GLN:HG2 | 1.82 | 0.42 |
| 2:M:146:TYR:O | 2:M:238:LYS:HD2 | 2.19 | 0.42 |
| 4:O:110:TYR:HA | 4:O:128:ILE:O | 2.19 | 0.42 |
| 4:O:68:MET:CE | 4:O:68:MET:HA | 2.49 | 0.42 |
| 4:O:128:ILE:CG1 | 11:W:16:ASP:HB3 | 2.49 | 0.42 |
| 1:A:17:ASP:O | 1:A:21:LYS:HG3 | 2.19 | 0.42 |
| 1:A:722:PHE:CD2 | 7:G:24:LYS:HG3 | 2.55 | 0.42 |
| 3:B:435:ARG:CB | 3:B:439:ASN:HD21 | 2.32 | 0.42 |
| 3:B:781:ARG:HD3 | 3:B:832:LYS:O | 2.20 | 0.42 |
| 1:A:637:ARG:HH11 | 3:B:974:ARG:HH12 | 1.68 | 0.42 |
| 4:D:115:LYS:O | 4:D:116:SER:HB3 | 2.18 | 0.42 |
| 5:E:31:ARG:O | 5:E:35:GLN:HB2 | 2.19 | 0.42 |
| 7:G:57:VAL:O | 7:G:59:ILE:HG13 | 2.19 | 0.42 |
| 7:G:83:ASP:HB3 | 7:G:94:THR:HB | 2.02 | 0.42 |
| 1:I:155:LYS:HB3 | 1:I:156:ILE:HA | 2.02 | 0.42 |
| 1:I:175:LEU:HD23 | 1:I:176:THR:H | 1.84 | 0.42 |
| 1:I:490:ARG:HG3 | 2:M:77:SER:HB3 | 2.01 | 0.42 |
| 1:I:716:SER:HB3 | 1:I:726:TYR:OH | 2.19 | 0.42 |
| 1:I:507:TYR:OH | 1:I:727:VAL:HG13 | 2.19 | 0.42 |
| 3:J:579:LEU:CD1 | 3:J:616:LEU:CD1 | 2.91 | 0.42 |
| 1:I:648:LEU:HB2 | 3:J:924:ILE:HG21 | 2.01 | 0.42 |
| 3:J:930:GLY:HA3 | 3:J:987:VAL:HB | 2.01 | 0.42 |
| 10:L:70:LEU:HA | 10:L:73:ILE:HB | 2.01 | 0.42 |
| 4:O:25:VAL:HG21 | 4:O:226:TYR:HD1 | 1.84 | 0.42 |
| 4:O:78:TRP:O | 4:O:80:GLU:N | 2.53 | 0.42 |
| 7:S:33:CYS:HB3 | 7:S:34:ASN:H | 1.62 | 0.42 |
| 10:V:45:GLN:HA | 10:V:46:PRO:HD2 | 1.73 | 0.42 |
| 13:Y:65:LYS:C | 13:Y:67:LEU:H | 2.23 | 0.42 |
| 1:A:452:PRO:HG3 | 1:A:496:ILE:HG12 | 2.01 | 0.42 |
| 1:A:57:LYS:HD2 | 1:A:60:THR:HA | 2.01 | 0.42 |
| 3:B:173:LEU:HA | 3:B:333:ASP:OD2 | 2.19 | 0.42 |
| 3:B:181:SER:HB3 | 3:B:183:ILE:CD1 | 2.50 | 0.42 |
| 3:B:196:TYR:CE1 | 3:B:303:THR:HB | 2.54 | 0.42 |
| 3:B:624:ALA:HB1 | 3:B:639:HIS:HD2 | 1.84 | 0.42 |
| 3:B:616:LEU:HD11 | 3:B:639:HIS:CE1 | 2.54 | 0.42 |
| 3:B:657:TYR:O | 3:B:658:PRO:C | 2.56 | 0.42 |
| 3:B:738:ILE:HD12 | 3:B:739:ILE:H | 1.84 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:B:741:ASN:OD1 | 3:B:744:SER:N | 2.44 | 0.42 |
| 2:C:11:PRO:HB2 | 2:C:14:GLU:CD | 2.40 | 0.42 |
| 2:C:70:ILE:HD13 | 2:C:71:GLY:H | 1.83 | 0.42 |
| 4:D:12:ARG:HA | 4:D:230:ILE:O | 2.19 | 0.42 |
| 4:D:259:LYS:O | 4:D:263:VAL:CG2 | 2.64 | 0.42 |
| 1:I:313:LEU:HA | 1:I:313:LEU:HD12 | 1.90 | 0.42 |
| 1:I:340:PRO:HB2 | 1:I:343:ILE:HG12 | 2.00 | 0.42 |
| 3:J:264:ASN:HB2 | 3:J:267:ASP:H | 1.84 | 0.42 |
| 3:J:501:ILE:N | 3:J:501:ILE:HD12 | 2.35 | 0.42 |
| 3:J:624:ALA:HB1 | 3:J:639:HIS:HD2 | 1.84 | 0.42 |
| 2:M:318:ASP:O | 2:M:322:ARG:NE | 2.53 | 0.42 |
| 7:S:15:ILE:HG13 | 7:S:31:MET:HE2 | 2.00 | 0.42 |
| 9:U:61:VAL:C | 9:U:63:SER:N | 2.69 | 0.42 |
| 1:A:499:ALA:HB3 | 3:B:734:MET:HE1 | 2.01 | 0.42 |
| 1:A:648:LEU:O | 1:A:651:VAL:HG12 | 2.19 | 0.42 |
| 3:B:1015:GLN:HE21 | 3:B:1096:ALA:HB2 | 1.80 | 0.42 |
| 3:B:644:SER:O | 3:B:647:ILE:HG13 | 2.20 | 0.42 |
| 3:B:6:THR:HB | 3:B:9:GLU:H | 1.85 | 0.42 |
| 3:B:958:LEU:C | 3:B:958:LEU:HD23 | 2.39 | 0.42 |
| 2:C:126:LEU:CD1 | 2:C:249:TYR:HB2 | 2.50 | 0.42 |
| 2:C:179:VAL:HG23 | 2:C:182:ASP:HB2 | 2.01 | 0.42 |
| 2:C:146:TYR:CE2 | 2:C:235:LYS:HB2 | 2.54 | 0.42 |
| 8:H:30:LYS:HA | 8:H:33:LYS:HE2 | 2.01 | 0.42 |
| 1:I:217:ILE:C | 1:I:219:ILE:N | 2.73 | 0.42 |
| 3:J:243:SER:O | 3:J:249:GLN:OE1 | 2.37 | 0.42 |
| 3:J:174:VAL:HG11 | 3:J:325:LEU:HD23 | 2.02 | 0.42 |
| 3:J:435:ARG:CB | 3:J:439:ASN:HD21 | 2.32 | 0.42 |
| 3:J:588:LEU:HD22 | 3:J:612:LYS:HG2 | 2.01 | 0.42 |
| 3:J:657:TYR:O | 3:J:658:PRO:C | 2.57 | 0.42 |
| 9:K:41:LEU:C | 9:K:43:LEU:N | 2.73 | 0.42 |
| 2:M:322:ARG:HG3 | 8:T:43:PRO:HA | 2.01 | 0.42 |
| 2:M:63:LEU:HD12 | 9:U:22:LEU:CD2 | 2.43 | 0.42 |
| 11:N:22:ILE:CD1 | 11:N:22:ILE:N | 2.83 | 0.42 |
| 4:O:111:SER:OG | 4:O:125:SER:O | 2.35 | 0.42 |
| 5:Q:128:PHE:CE2 | 5:Q:133:LYS:HD3 | 2.55 | 0.42 |
| 9:U:18:VAL:HG12 | 9:U:22:LEU:HD12 | 2.01 | 0.42 |
| 1:A:618:GLU:O | 1:A:619:TYR:CG | 2.72 | 0.42 |
| 3:B:365:LEU:HG | 3:B:369:LEU:HD12 | 2.02 | 0.42 |
| 3:B:338:TYR:HB2 | 3:B:448:THR:HG21 | 2.02 | 0.42 |
| 3:B:768:GLY:O | 3:B:769:GLN:HB2 | 2.19 | 0.42 |
| 3:B:778:ALA:HA | 3:B:783:TYR:CE1 | 2.55 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:21:SER:O | 2:C:25:PRO:HD3 | 2.19 | 0.42 |
| 7:G:79:THR:CG2 | 7:G:80:GLU:N | 2.82 | 0.42 |
| 1:I:220:ARG:NH1 | 1:I:236:THR:CG2 | 2.74 | 0.42 |
| 1:I:549:LYS:HZ3 | 1:I:549:LYS:HB2 | 1.84 | 0.42 |
| 1:I:612:LEU:C | 1:I:612:LEU:HD23 | 2.39 | 0.42 |
| 3:J:92:TYR:OH | 3:J:128:ASP:OD2 | 2.36 | 0.42 |
| 3:J:382:LYS:O | 3:J:382:LYS:HG2 | 2.19 | 0.42 |
| 3:J:793:GLU:HB3 | 3:J:794:ASP:H | 1.72 | 0.42 |
| 2:M:392:PRO:HG2 | 5:Q:22:LEU:HD21 | 2.01 | 0.42 |
| 1:I:871:ILE:HG13 | 2:M:54:LEU:HD11 | 2.01 | 0.42 |
| 4:O:178:LYS:HZ3 | 4:O:178:LYS:H | 1.67 | 0.42 |
| 7:S:42:ILE:HD11 | 7:S:71:PHE:CZ | 2.55 | 0.42 |
| 9:U:63:SER:C | 9:U:65:ALA:H | 2.22 | 0.42 |
| 10:V:3:ILE:HD13 | 10:V:17:ILE:HG23 | 2.01 | 0.42 |
| 1:A:104:VAL:HG12 | 1:A:137:LYS:HA | 2.02 | 0.42 |
| 1:A:380:ARG:HB3 | 1:A:381:PRO:HD2 | 2.01 | 0.42 |
| 1:A:394:ARG:O | 1:A:398:ALA:HB2 | 2.20 | 0.42 |
| 1:A:427:ARG:NH1 | 2:C:73:VAL:HG11 | 2.34 | 0.42 |
| 1:A:320:PHE:CE2 | 3:B:1005:ALA:HB1 | 2.55 | 0.42 |
| 3:B:1069:TRP:HE3 | 3:B:1070:TYR:N | 2.18 | 0.42 |
| 3:B:136:ASP:HA | 3:B:139:ILE:HD12 | 2.01 | 0.42 |
| 3:B:386:ARG:HB3 | 3:B:389:ILE:HD11 | 2.02 | 0.42 |
| 2:C:106:ARG:HH21 | 2:C:117:PRO:HB3 | 1.85 | 0.42 |
| 2:C:149:ILE:O | 2:C:153:VAL:HG12 | 2.19 | 0.42 |
| 2:C:389:THR:O | 2:C:390:MET:O | 2.37 | 0.42 |
| 1:A:827:LEU:CG | 2:C:75:ALA:HB2 | 2.49 | 0.42 |
| 4:D:107:ARG:N | 4:D:133:LEU:O | 2.51 | 0.42 |
| 4:D:206:CYS:O | 4:D:207:GLU:HB2 | 2.20 | 0.42 |
| 4:D:21:PRO:O | 4:D:24:PHE:HB3 | 2.20 | 0.42 |
| 7:G:18:ILE:HG22 | 7:G:18:ILE:O | 2.18 | 0.42 |
| 1:I:488:THR:HB | 1:I:495:ILE:HB | 2.02 | 0.42 |
| 3:J:537:ALA:HB2 | 3:J:557:HIS:CD2 | 2.55 | 0.42 |
| 4:O:128:ILE:HG12 | 11:W:16:ASP:HB3 | 2.01 | 0.42 |
| 12:X:28:TYR:O | 12:X:29:CYS:C | 2.57 | 0.42 |
| 1:A:548:GLY:O | 1:A:551:VAL:HG12 | 2.20 | 0.42 |
| 1:A:835:ASP:HA | 9:K:20:ILE:HD13 | 2.02 | 0.42 |
| 1:A:85:GLY:HA3 | 2:C:355:LEU:HD12 | 2.01 | 0.42 |
| 3:B:1029:GLY:O | 3:B:1031:MET:N | 2.52 | 0.42 |
| 3:B:111:PRO:O | 3:B:112:GLU:CB | 2.68 | 0.42 |
| 3:B:205:LEU:HD23 | 3:B:212:VAL:HG22 | 2.01 | 0.42 |
| 3:B:298:LEU:N | 3:B:299:PRO:HD3 | 2.35 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:B:388:ASP:HB3 | 3:B:391:THR:HB | 2.01 | 0.42 |
| 3:B:418:ASN:HD21 | 3:B:420:LEU:HB3 | 1.84 | 0.42 |
| 3:B:24:VAL:HG11 | 3:B:426:LEU:HD13 | 2.01 | 0.42 |
| 3:B:458:THR:CG2 | 3:B:464:SER:HA | 2.49 | 0.42 |
| 2:C:190:ARG:HD3 | 2:C:191:LEU:N | 2.31 | 0.42 |
| 2:C:202:GLU:O | 2:C:203:ASP:HB2 | 2.20 | 0.42 |
| 1:I:861:ALA:CB | 1:I:866:VAL:HG23 | 2.49 | 0.42 |
| 3:J:173:LEU:HA | 3:J:333:ASP:OD2 | 2.19 | 0.42 |
| 3:J:418:ASN:C | 3:J:418:ASN:ND2 | 2.73 | 0.42 |
| 3:J:435:ARG:HB3 | 3:J:439:ASN:HD21 | 1.84 | 0.42 |
| 3:J:752:SER:OG | 3:J:753:THR:N | 2.53 | 0.42 |
| 3:J:928:ILE:HD13 | 3:J:954:GLN:HE21 | 1.84 | 0.42 |
| 2:M:239:ARG:HE | 2:M:239:ARG:HB2 | 1.71 | 0.42 |
| 2:M:258:LEU:HB2 | 2:M:279:GLU:HG2 | 2.01 | 0.42 |
| 11:N:22:ILE:CD1 | 11:N:22:ILE:H | 2.33 | 0.42 |
| 11:N:24:ARG:HD2 | 11:N:34:VAL:HG13 | 2.02 | 0.42 |
| 7:S:42:ILE:HD11 | 7:S:71:PHE:CE1 | 2.55 | 0.42 |
| 10:V:60:ASP:C | 10:V:62:SER:H | 2.22 | 0.42 |
| 1:A:655:ASP:HB3 | 1:A:656:ASP:H | 1.61 | 0.42 |
| 1:A:672:VAL:O | 1:A:675:LEU:N | 2.52 | 0.42 |
| 3:B:1064:CYS:SG | 3:B:1081:ILE:HD12 | 2.60 | 0.42 |
| 3:B:1099:LEU:O | 3:B:1102:GLN:HB2 | 2.20 | 0.42 |
| 3:B:264:ASN:H | 3:B:267:ASP:HB2 | 1.85 | 0.42 |
| 3:B:469:ASN:ND2 | 3:B:469:ASN:N | 2.67 | 0.42 |
| 2:C:109:GLU:O | 2:C:113:ALA:CA | 2.51 | 0.42 |
| 1:A:823:LEU:HD13 | 2:C:75:ALA:O | 2.18 | 0.42 |
| 7:G:57:VAL:HG13 | 7:G:115:THR:HG22 | 2.02 | 0.42 |
| 1:I:188:PRO:HD2 | 1:I:191:ASP:HB2 | 2.00 | 0.42 |
| 1:I:212:LEU:CD2 | 1:I:242:ILE:HD13 | 2.49 | 0.42 |
| 1:I:553:SER:OG | 1:I:592:ILE:HA | 2.20 | 0.42 |
| 3:J:540:ILE:HG21 | 3:J:555:VAL:HG21 | 2.01 | 0.42 |
| 3:J:580:ILE:HA | 3:J:613:ILE:HD13 | 2.01 | 0.42 |
| 3:J:633:LEU:C | 3:J:635:PRO:CD | 2.88 | 0.42 |
| 3:J:669:GLN:C | 3:J:671:ALA:H | 2.23 | 0.42 |
| 3:J:87:LEU:HD22 | 3:J:851:LEU:HD13 | 2.02 | 0.42 |
| 10:L:29:ALA:HA | 10:L:32:LEU:HB2 | 2.02 | 0.42 |
| 10:L:3:ILE:H | 10:L:3:ILE:HD12 | 1.85 | 0.42 |
| 7:S:75:GLY:HA3 | 7:S:87:ASN:HA | 2.02 | 0.42 |
| 1:I:550:GLN:NE2 | 7:S:88:ASN:ND2 | 2.68 | 0.42 |
| 4:O:53:LEU:HD11 | 11:W:2:LEU:HD12 | 2.01 | 0.42 |
| 13:Y:65:LYS:C | 13:Y:67:LEU:N | 2.73 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:181:ARG:HG3 | 1:A:208:ILE:HB | 2.00 | 0.41 |
| 1:A:355:PRO:O | 1:A:357:ASN:OD1 | 2.37 | 0.41 |
| 1:A:439:LYS:H | 1:A:439:LYS:HG3 | 1.57 | 0.41 |
| 3:B:116:ILE:HD12 | 3:B:361:PHE:HZ | 1.83 | 0.41 |
| 3:B:388:ASP:OD1 | 3:B:391:THR:OG1 | 2.25 | 0.41 |
| 3:B:430:ILE:HG22 | 3:B:431:SER:N | 2.35 | 0.41 |
| 3:B:454:CYS:HB2 | 3:B:649:GLY:N | 2.35 | 0.41 |
| 3:B:785:GLY:HA3 | 3:B:788:TYR:HE2 | 1.84 | 0.41 |
| 3:B:874:ILE:H | 3:B:874:ILE:CD1 | 2.17 | 0.41 |
| 1:A:425:LEU:CD2 | 2:C:83:THR:HG21 | 2.50 | 0.41 |
| 4:D:144:ARG:C | 4:D:145:LEU:HD12 | 2.41 | 0.41 |
| 3:B:975:THR:O | 4:D:26:ASN:ND2 | 2.53 | 0.41 |
| 5:E:38:ILE:O | 5:E:39:LEU:HB2 | 2.20 | 0.41 |
| 8:H:64:ARG:HG3 | 8:H:78:TYR:HE2 | 1.84 | 0.41 |
| 1:I:349:VAL:HA | 1:I:350:PRO:HD2 | 1.80 | 0.41 |
| 1:I:364:PHE:CD2 | 1:I:373:PRO:O | 2.73 | 0.41 |
| 1:I:449:VAL:HG12 | 1:I:449:VAL:O | 2.20 | 0.41 |
| 1:I:548:GLY:HA2 | 1:I:551:VAL:HG12 | 2.02 | 0.41 |
| 1:I:644:PHE:HB3 | 3:J:728:SER:OG | 2.20 | 0.41 |
| 3:J:750:TYR:O | 3:J:992:LYS:NZ | 2.52 | 0.41 |
| 3:J:898:PRO:HB2 | 3:J:970:VAL:HG21 | 2.02 | 0.41 |
| 3:J:6:THR:HB | 3:J:9:GLU:CB | 2.50 | 0.41 |
| 9:K:74:LEU:HD22 | 9:K:76:ILE:HD12 | 2.01 | 0.41 |
| 4:O:204:THR:O | 4:O:206:CYS:N | 2.53 | 0.41 |
| 11:W:48:MET:HE3 | 11:W:48:MET:HA | 2.02 | 0.41 |
| 1:A:327:SER:HB2 | 1:A:444:ARG:CD | 2.47 | 0.41 |
| 1:A:445:LEU:HD21 | 1:A:450:CYS:HA | 2.02 | 0.41 |
| 1:A:609:GLU:HB3 | 1:A:614:TRP:CZ2 | 2.55 | 0.41 |
| 1:A:781:PHE:HD2 | 1:A:781:PHE:C | 2.23 | 0.41 |
| 3:B:148:PRO:HG3 | 3:B:422:MET:HE1 | 2.01 | 0.41 |
| 3:B:587:PRO:C | 3:B:588:LEU:HG | 2.40 | 0.41 |
| 3:B:723:ILE:HG12 | 3:B:907:ASP:OD2 | 2.19 | 0.41 |
| 4:D:125:SER:O | 4:D:127:ASP:N | 2.52 | 0.41 |
| 4:D:94:THR:O | 4:D:95:LYS:HG3 | 2.20 | 0.41 |
| 1:I:45:MET:O | 1:I:47:PRO:HD3 | 2.20 | 0.41 |
| 1:I:485:ASN:HD21 | 3:J:1039:PHE:HE2 | 1.67 | 0.41 |
| 1:I:486:ILE:HD12 | 1:I:616:ILE:HD13 | 2.02 | 0.41 |
| 1:I:708:ARG:HG3 | 1:I:709:SER:N | 2.35 | 0.41 |
| 1:I:839:ARG:NH2 | 9:U:83:PRO:HG3 | 2.35 | 0.41 |
| 3:J:1065:GLY:O | 3:J:1112:ARG:HA | 2.20 | 0.41 |
| 3:J:366:THR:O | 3:J:370:GLU:HG3 | 2.19 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:738:ILE:HD12 | 3:J:739:ILE:N | 2.34 | 0.41 |
| 3:J:764:LYS:HD3 | 3:J:815:SER:HB3 | 2.02 | 0.41 |
| 3:J:811:ILE:HB | 3:J:837:ILE:HB | 2.02 | 0.41 |
| 10:L:59:THR:HG21 | 10:L:65:PRO:HD3 | 2.02 | 0.41 |
| 10:L:87:ILE:C | 10:L:89:GLY:N | 2.74 | 0.41 |
| 2:M:234:ILE:HG13 | 2:M:234:ILE:H | 1.65 | 0.41 |
| 4:D:45:TYR:CD1 | 12:P:44:ILE:HG12 | 2.54 | 0.41 |
| 13:Z:55:LEU:HB3 | 13:Z:56:ASN:H | 1.63 | 0.41 |
| 1:A:95:LYS:HZ3 | 1:A:152:LYS:HB3 | 1.84 | 0.41 |
| 1:A:153:GLN:HG2 | 1:A:154:TYR:H | 1.85 | 0.41 |
| 3:B:157:SER:O | 3:B:158:GLU:CB | 2.67 | 0.41 |
| 3:B:256:LEU:C | 3:B:258:GLN:H | 2.24 | 0.41 |
| 3:B:54:PRO:O | 3:B:55:GLY:C | 2.58 | 0.41 |
| 3:B:633:LEU:C | 3:B:635:PRO:CD | 2.89 | 0.41 |
| 2:C:320:MET:HA | 2:C:327:ARG:HG2 | 2.02 | 0.41 |
| 2:C:57:LYS:HA | 2:C:57:LYS:HE3 | 2.02 | 0.41 |
| 1:I:153:GLN:HG2 | 1:I:154:TYR:H | 1.85 | 0.41 |
| 1:I:352:ARG:HD3 | 1:I:406:ILE:HG12 | 2.02 | 0.41 |
| 1:I:500:GLN:HG3 | 1:I:501:ASP:H | 1.85 | 0.41 |
| 1:I:742:GLN:HG2 | 1:I:747:LEU:HA | 2.02 | 0.41 |
| 1:I:874:ARG:HE | 2:M:53:ASP:HB2 | 1.85 | 0.41 |
| 3:J:138:LEU:HA | 3:J:141:ILE:CD1 | 2.43 | 0.41 |
| 3:J:549:ILE:HD13 | 3:J:549:ILE:HA | 1.80 | 0.41 |
| 3:J:603:THR:C | 3:J:605:ASP:N | 2.73 | 0.41 |
| 3:J:88:ARG:HG2 | 12:X:33:ILE:HD11 | 2.02 | 0.41 |
| 2:M:389:THR:HG21 | 9:U:79:ARG:NH1 | 2.34 | 0.41 |
| 2:M:80:GLU:CB | 2:M:81:PRO:HD3 | 2.50 | 0.41 |
| 12:P:26:CYS:CB | 12:P:27:PRO:CD | 2.87 | 0.41 |
| 5:Q:20:LYS:HA | 5:Q:21:PRO:HD2 | 1.80 | 0.41 |
| 7:S:104:LYS:O | 7:S:106:ILE:N | 2.54 | 0.41 |
| 9:U:60:ASP:O | 9:U:61:VAL:O | 2.38 | 0.41 |
| 4:O:256:LEU:CD1 | 10:V:3:ILE:HD12 | 2.50 | 0.41 |
| 10:V:45:GLN:HB3 | 10:V:53:ILE:HG22 | 2.01 | 0.41 |
| 1:A:212:LEU:CD2 | 1:A:242:ILE:HD13 | 2.50 | 0.41 |
| 1:A:290:ARG:HD2 | 1:A:291:SER:H | 1.84 | 0.41 |
| 1:A:778:ALA:O | 1:A:780:GLY:N | 2.53 | 0.41 |
| 3:B:402:ASN:O | 3:B:403:TRP:HB2 | 2.21 | 0.41 |
| 3:B:972:ASP:O | 3:B:975:THR:HG23 | 2.20 | 0.41 |
| 2:C:309:ASP:OD2 | 2:C:311:ARG:HD3 | 2.21 | 0.41 |
| 1:I:329:ASP:CB | 1:I:332:ILE:HD12 | 2.49 | 0.41 |
| 1:I:374:GLY:C | 1:I:410:HIS:ND1 | 2.74 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:I:541:ALA:CB | 1:I:542:PRO:HD2 | 2.46 | 0.41 |
| 1:I:600:LYS:HE3 | 1:I:732:GLY:HA2 | 2.00 | 0.41 |
| 1:I:879:LYS:HA | 1:I:879:LYS:HD3 | 1.90 | 0.41 |
| 3:J:1015:GLN:HE21 | 3:J:1096:ALA:HB2 | 1.81 | 0.41 |
| 3:J:133:TYR:CD2 | 3:J:141:ILE:HD11 | 2.56 | 0.41 |
| 3:J:154:VAL:O | 3:J:155:ASN:C | 2.59 | 0.41 |
| 3:J:659:GLU:O | 3:J:660:HIS:CD2 | 2.72 | 0.41 |
| 3:J:654:ILE:HG13 | 3:J:708:LEU:HD21 | 2.03 | 0.41 |
| 3:J:719:GLY:O | 3:J:989:TYR:CE1 | 2.74 | 0.41 |
| 3:J:64:ARG:CG | 3:J:97:TRP:CD1 | 3.01 | 0.41 |
| 3:J:97:TRP:O | 3:J:98:LEU:HB3 | 2.20 | 0.41 |
| 10:L:61:GLY:O | 10:L:62:SER:C | 2.58 | 0.41 |
| 7:S:36:PHE:CD2 | 7:S:96:ILE:HD11 | 2.54 | 0.41 |
| 9:U:61:VAL:C | 9:U:62:ILE:HG12 | 2.41 | 0.41 |
| 3:J:800:PRO:HG2 | 12:X:37:VAL:HA | 2.02 | 0.41 |
| 1:A:125:TRP:CZ3 | 8:H:82:ILE:HG21 | 2.56 | 0.41 |
| 1:A:155:LYS:HB3 | 1:A:156:ILE:HA | 2.01 | 0.41 |
| 1:A:87:VAL:HG21 | 1:A:156:ILE:O | 2.20 | 0.41 |
| 1:A:220:ARG:HH11 | 1:A:236:THR:CG2 | 2.27 | 0.41 |
| 1:A:465:HIS:NE2 | 3:B:1028:PHE:HD1 | 2.19 | 0.41 |
| 1:A:645:THR:OG1 | 1:A:646:MET:N | 2.54 | 0.41 |
| 3:B:291:GLN:C | 3:B:293:ILE:N | 2.74 | 0.41 |
| 3:B:589:VAL:O | 3:B:592:GLU:N | 2.54 | 0.41 |
| 3:B:617:ASP:O | 3:B:618:ALA:CB | 2.67 | 0.41 |
| 3:B:764:LYS:HZ1 | 3:B:772:LYS:C | 2.23 | 0.41 |
| 3:B:751:ARG:HG2 | 3:B:871:ILE:HG23 | 2.01 | 0.41 |
| 3:B:654:ILE:CG2 | 3:B:881:ARG:HG2 | 2.51 | 0.41 |
| 3:B:963:LEU:HD21 | 4:D:206:CYS:SG | 2.60 | 0.41 |
| 2:C:40:GLU:H | 2:C:40:GLU:HG2 | 1.62 | 0.41 |
| 4:D:178:LYS:O | 4:D:179:ALA:C | 2.59 | 0.41 |
| 4:D:65:ILE:HA | 4:D:66:PRO:HD3 | 1.95 | 0.41 |
| 5:E:102:GLY:HA3 | 5:E:103:PRO:HD3 | 1.95 | 0.41 |
| 1:I:239:LEU:HD23 | 1:I:276:TYR:HE1 | 1.85 | 0.41 |
| 1:I:422:GLN:NE2 | 1:I:463:ASN:HD21 | 2.19 | 0.41 |
| 1:I:768:HIS:NE2 | 3:J:450:TRP:CZ2 | 2.79 | 0.41 |
| 10:L:59:THR:HG21 | 10:L:63:ILE:O | 2.19 | 0.41 |
| 2:M:261:VAL:O | 2:M:261:VAL:CG1 | 2.67 | 0.41 |
| 1:I:870:ARG:HH21 | 2:M:61:GLU:H | 1.69 | 0.41 |
| 4:O:6:LEU:HB3 | 4:O:14:ASP:HB2 | 2.02 | 0.41 |
| 6:R:55:VAL:HG12 | 6:R:59:LEU:HD12 | 2.02 | 0.41 |
| 7:S:34:ASN:N | 7:S:34:ASN:OD1 | 2.53 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:V:47:HIS:O | 10:V:49:LEU:N | 2.53 | 0.41 |
| 1:A:568:VAL:HG21 | 1:A:597:VAL:HG11 | 2.01 | 0.41 |
| 1:A:708:ARG:HG3 | 1:A:709:SER:N | 2.34 | 0.41 |
| 1:A:805:GLY:C | 1:A:807:VAL:H | 2.24 | 0.41 |
| 3:B:440:PHE:C | 3:B:442:ALA:H | 2.23 | 0.41 |
| 3:B:987:VAL:HG11 | 11:N:47:ARG:NE | 2.36 | 0.41 |
| 2:C:28:ILE:HG23 | 2:C:30:ASP:CG | 2.41 | 0.41 |
| 1:A:831:ARG:NH2 | 2:C:385:MET:CG | 2.83 | 0.41 |
| 4:D:178:LYS:HB2 | 4:D:178:LYS:HE2 | 1.92 | 0.41 |
| 4:D:223:GLU:H | 4:D:223:GLU:HG3 | 1.69 | 0.41 |
| 4:D:11:THR:HG22 | 4:D:232:SER:HB3 | 2.03 | 0.41 |
| 1:I:198:ASP:HA | 1:I:199:PRO:HD2 | 1.99 | 0.41 |
| 1:I:820:GLN:O | 1:I:823:LEU:HD12 | 2.19 | 0.41 |
| 3:J:130:ILE:HA | 3:J:133:TYR:CD1 | 2.54 | 0.41 |
| 3:J:52:GLU:HB2 | 3:J:56:LEU:HB3 | 2.02 | 0.41 |
| 3:J:587:PRO:C | 3:J:588:LEU:HG | 2.40 | 0.41 |
| 3:J:918:ARG:O | 3:J:920:THR:HG23 | 2.21 | 0.41 |
| 9:K:39:ARG:HB3 | 9:K:65:ALA:HB1 | 2.03 | 0.41 |
| 2:M:258:LEU:HB2 | 2:M:279:GLU:CG | 2.49 | 0.41 |
| 2:M:312:HIS:O | 2:M:316:ILE:HG12 | 2.20 | 0.41 |
| 4:O:178:LYS:NZ | 4:O:178:LYS:H | 2.18 | 0.41 |
| 7:S:104:LYS:HZ2 | 7:S:104:LYS:HB3 | 1.84 | 0.41 |
| 7:S:76:TYR:CZ | 7:S:110:GLU:HG3 | 2.56 | 0.41 |
| 7:S:26:LEU:HD22 | 7:S:42:ILE:O | 2.21 | 0.41 |
| 9:U:43:LEU:C | 9:U:45:MET:N | 2.73 | 0.41 |
| 9:U:70:ARG:O | 9:U:72:GLY:N | 2.53 | 0.41 |
| 11:W:18:TRP:O | 11:W:20:SER:N | 2.50 | 0.41 |
| 13:Y:79:ASP:HB3 | 13:Y:80:SER:H | 1.72 | 0.41 |
| 1:A:313:LEU:HD12 | 1:A:313:LEU:HA | 1.93 | 0.41 |
| 1:A:326:ILE:HG21 | 1:A:462:MET:CG | 2.48 | 0.41 |
| 1:A:421:ARG:HB2 | 1:A:462:MET:CE | 2.49 | 0.41 |
| 1:A:741:THR:O | 1:A:742:GLN:C | 2.59 | 0.41 |
| 1:A:747:LEU:HD22 | 1:A:786:PHE:CE1 | 2.56 | 0.41 |
| 1:A:77:LEU:HD23 | 1:A:246:ASN:HD21 | 1.84 | 0.41 |
| 1:A:785:SER:C | 1:A:787:ARG:N | 2.73 | 0.41 |
| 3:B:1033:ARG:HG3 | 3:B:1033:ARG:HH11 | 1.85 | 0.41 |
| 3:B:1069:TRP:HB2 | 3:B:1078:VAL:O | 2.20 | 0.41 |
| 3:B:1085:LYS:HG2 | 3:B:1086:SER:N | 2.36 | 0.41 |
| 3:B:448:THR:HG22 | 3:B:452:ARG:HD2 | 2.03 | 0.41 |
| 3:B:867:ARG:NH2 | 4:D:54:TYR:CE2 | 2.89 | 0.41 |
| 2:C:158:ILE:HD11 | 2:C:165:ILE:HG23 | 2.02 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:34:LEU:O | 4:D:150:GLY:HA3 | 2.21 | 0.41 |
| 2:C:390:MET:HE2 | 5:E:66:THR:OG1 | 2.21 | 0.41 |
| 8:H:69:SER:HB3 | 8:H:72:TYR:H | 1.85 | 0.41 |
| 1:I:402:ALA:O | 1:I:405:TYR:HD1 | 2.03 | 0.41 |
| 1:I:425:LEU:O | 1:I:426:HIS:HB2 | 2.20 | 0.41 |
| 1:I:563:HIS:ND1 | 1:I:876:VAL:HG13 | 2.36 | 0.41 |
| 1:I:77:LEU:HD23 | 1:I:246:ASN:HD21 | 1.85 | 0.41 |
| 3:J:1109:ILE:O | 3:J:1111:PRO:HD3 | 2.21 | 0.41 |
| 3:J:81:SER:OG | 3:J:141:ILE:HG23 | 2.20 | 0.41 |
| 3:J:167:LEU:HB2 | 3:J:168:ALA:H | 1.74 | 0.41 |
| 3:J:490:TYR:CE1 | 3:J:527:ILE:CG2 | 3.03 | 0.41 |
| 3:J:919:MET:HE2 | 3:J:919:MET:HB3 | 1.88 | 0.41 |
| 3:J:92:TYR:O | 3:J:92:TYR:HD2 | 2.02 | 0.41 |
| 9:K:47:ALA:HA | 9:K:48:PRO:HD2 | 1.95 | 0.41 |
| 4:D:35:TYR:HE2 | 10:L:23:THR:HG21 | 1.86 | 0.41 |
| 2:M:125:TYR:HD1 | 2:M:271:LYS:HB2 | 1.85 | 0.41 |
| 2:M:12:TYR:C | 2:M:13:LEU:HG | 2.41 | 0.41 |
| 2:M:320:MET:O | 2:M:327:ARG:HG2 | 2.21 | 0.41 |
| 3:B:790:ARG:HH22 | 12:P:39:LYS:HE3 | 1.85 | 0.41 |
| 5:Q:66:THR:CG2 | 5:Q:68:HIS:NE2 | 2.84 | 0.41 |
| 5:Q:103:PRO:HD3 | 6:R:37:THR:HG23 | 2.03 | 0.41 |
| 1:A:125:TRP:HD1 | 1:A:128:ALA:HB3 | 1.85 | 0.41 |
| 1:A:199:PRO:C | 1:A:201:THR:H | 2.24 | 0.41 |
| 1:A:431:MET:CE | 1:A:482:VAL:HG13 | 2.50 | 0.41 |
| 1:A:430:MET:O | 1:A:431:MET:HG3 | 2.21 | 0.41 |
| 1:A:507:TYR:HB2 | 1:A:511:VAL:HG13 | 2.01 | 0.41 |
| 1:A:541:ALA:CB | 1:A:542:PRO:HD2 | 2.45 | 0.41 |
| 1:A:561:ASN:HA | 1:A:588:ILE:O | 2.20 | 0.41 |
| 1:A:763:THR:HG22 | 1:A:772:TYR:HA | 2.01 | 0.41 |
| 3:B:264:ASN:HB2 | 3:B:267:ASP:H | 1.85 | 0.41 |
| 3:B:533:GLY:C | 3:B:535:GLU:H | 2.23 | 0.41 |
| 3:B:661:ASN:HD22 | 3:B:920:THR:HA | 1.86 | 0.41 |
| 3:B:419:TRP:HZ3 | 3:B:712:GLY:C | 2.24 | 0.41 |
| 3:B:838:VAL:CG1 | 3:B:839:THR:N | 2.83 | 0.41 |
| 3:B:892:ILE:HA | 3:B:893:PRO:HD3 | 1.96 | 0.41 |
| 2:C:276:ASN:O | 2:C:279:GLU:HB3 | 2.20 | 0.41 |
| 2:C:323:THR:O | 2:C:325:ILE:N | 2.54 | 0.41 |
| 4:D:159:VAL:HG23 | 4:D:232:SER:HA | 2.03 | 0.41 |
| 5:E:171:LYS:HG2 | 5:E:172:LEU:H | 1.85 | 0.41 |
| 1:I:29:THR:HG1 | 1:I:45:MET:N | 2.19 | 0.41 |
| 3:J:1029:GLY:O | 3:J:1030:GLU:C | 2.59 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:123:LEU:C | 3:J:125:SER:H | 2.24 | 0.41 |
| 3:J:223:PHE:CD2 | 3:J:256:LEU:HD22 | 2.56 | 0.41 |
| 3:J:49:ILE:HG13 | 3:J:49:ILE:H | 1.65 | 0.41 |
| 3:J:816:PRO:HA | 3:J:817:PRO:HD3 | 1.85 | 0.41 |
| 3:J:997:VAL:O | 3:J:1000:LYS:O | 2.39 | 0.41 |
| 9:K:63:SER:HA | 9:K:66:GLU:HG3 | 2.03 | 0.41 |
| 2:M:31:ASP:C | 2:M:33:LYS:N | 2.72 | 0.41 |
| 4:O:111:SER:C | 4:O:114:ILE:HD13 | 2.41 | 0.41 |
| 4:O:21:PRO:HB3 | 10:V:34:ARG:HH21 | 1.84 | 0.41 |
| 4:O:35:TYR:HE2 | 10:V:23:THR:HG21 | 1.85 | 0.41 |
| 12:P:33:ILE:O | 12:P:34:ILE:C | 2.59 | 0.41 |
| 5:Q:5:ILE:O | 5:Q:74:MET:N | 2.53 | 0.41 |
| 11:W:22:ILE:HD12 | 11:W:22:ILE:H | 1.86 | 0.41 |
| 13:Y:69:GLU:HB3 | 13:Y:73:LYS:NZ | 2.36 | 0.41 |
| 1:A:371:LYS:HZ2 | 1:A:373:PRO:HD3 | 1.84 | 0.41 |
| 1:A:575:CYS:O | 1:A:577:ASN:N | 2.54 | 0.41 |
| 3:B:14:ILE:O | 3:B:17:TYR:HB3 | 2.21 | 0.41 |
| 3:B:34:PHE:CE1 | 3:B:351:ALA:HA | 2.56 | 0.41 |
| 3:B:580:ILE:HB | 3:B:640:LEU:HB3 | 2.03 | 0.41 |
| 2:C:125:TYR:HD1 | 2:C:271:LYS:CB | 2.30 | 0.41 |
| 2:C:126:LEU:HD11 | 2:C:249:TYR:HB2 | 2.03 | 0.41 |
| 2:C:245:LYS:HB2 | 2:C:250:ILE:HD11 | 2.03 | 0.41 |
| 7:G:15:ILE:HG13 | 7:G:31:MET:HE2 | 2.03 | 0.41 |
| 7:G:80:GLU:C | 7:G:81:LEU:HD12 | 2.41 | 0.41 |
| 1:I:329:ASP:HA | 1:I:330:PRO:HD3 | 1.74 | 0.41 |
| 1:I:537:PRO:HA | 1:I:546:TYR:CD2 | 2.55 | 0.41 |
| 1:I:86:LEU:HD13 | 1:I:207:MET:HG2 | 2.02 | 0.41 |
| 3:J:321:LYS:CA | 3:J:324:GLU:HB3 | 2.51 | 0.41 |
| 3:J:402:ASN:HB3 | 3:J:403:TRP:H | 1.46 | 0.41 |
| 3:J:580:ILE:HG13 | 3:J:642:ILE:HD13 | 2.03 | 0.41 |
| 3:J:589:VAL:O | 3:J:592:GLU:N | 2.54 | 0.41 |
| 3:J:99:THR:HG23 | 3:J:111:PRO:HB3 | 2.03 | 0.41 |
| 2:M:130:TYR:HD2 | 2:M:130:TYR:HA | 1.77 | 0.41 |
| 2:M:174:LEU:CB | 2:M:179:VAL:HG13 | 2.50 | 0.41 |
| 11:N:14:ILE:HD13 | 11:N:14:ILE:HA | 1.93 | 0.41 |
| 4:O:168:PRO:HG3 | 4:O:203:CYS:O | 2.21 | 0.41 |
| 4:O:61:ARG:HH11 | 4:O:61:ARG:HG2 | 1.86 | 0.41 |
| 3:B:78:ARG:HH22 | 12:P:30:GLY:HA3 | 1.85 | 0.41 |
| 5:Q:110:ILE:O | 5:Q:118:LEU:HD22 | 2.21 | 0.41 |
| 5:Q:163:THR:O | 5:Q:164:MET:HG3 | 2.21 | 0.41 |
| 7:S:83:ASP:N | 7:S:94:THR:O | 2.49 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:U:32:ILE:O | 9:U:36:ILE:HG12 | 2.20 | 0.41 |
| 1:A:378:VAL:CG2 | 1:A:378:VAL:O | 2.67 | 0.41 |
| 1:A:670:VAL:O | 1:A:674:ASN:ND2 | 2.54 | 0.41 |
| 3:B:102:PRO:HD2 | 3:B:109:ALA:HB3 | 2.01 | 0.41 |
| 3:B:228:ARG:NH2 | 3:B:233:LEU:O | 2.50 | 0.41 |
| 3:B:793:GLU:HB3 | 3:B:794:ASP:H | 1.72 | 0.41 |
| 3:B:82:PRO:HG3 | 3:B:130:ILE:HD11 | 2.02 | 0.41 |
| 3:B:950:ILE:C | 3:B:952:GLN:H | 2.24 | 0.41 |
| 7:G:102:LEU:HA | 7:G:106:ILE:HG21 | 2.03 | 0.41 |
| 7:G:107:SER:O | 7:G:109:LYS:N | 2.37 | 0.41 |
| 1:I:4:LYS:HG2 | 1:I:5:ASN:N | 2.36 | 0.41 |
| 3:J:419:TRP:HZ3 | 3:J:712:GLY:CA | 2.34 | 0.41 |
| 3:J:471:ALA:O | 3:J:473:MET:HG3 | 2.21 | 0.41 |
| 3:J:978:LYS:HZ3 | 4:O:205:LEU:HD22 | 1.85 | 0.41 |
| 2:M:146:TYR:O | 2:M:238:LYS:CD | 2.69 | 0.41 |
| 1:I:859:TYR:CB | 2:M:64:ILE:HG12 | 2.50 | 0.41 |
| 1:A:114:TYR:O | 1:A:118:TYR:HB2 | 2.20 | 0.41 |
| 1:A:184:LEU:O | 1:A:186:LYS:N | 2.54 | 0.41 |
| 1:A:371:LYS:HD3 | 1:A:372:TRP:N | 2.36 | 0.41 |
| 1:A:467:PRO:HA | 3:B:1048:ARG:NH2 | 2.36 | 0.41 |
| 3:B:304:SER:OG | 3:B:307:ASP:OD2 | 2.39 | 0.41 |
| 1:A:764:ARG:NH2 | 3:B:624:ALA:O | 2.54 | 0.41 |
| 3:B:978:LYS:HG2 | 4:D:166:TYR:CE2 | 2.56 | 0.41 |
| 4:D:78:TRP:CD1 | 4:D:78:TRP:N | 2.86 | 0.41 |
| 8:H:39:PRO:HB2 | 8:H:80:TYR:CE2 | 2.56 | 0.41 |
| 1:I:561:ASN:ND2 | 1:I:590:ASN:H | 2.18 | 0.41 |
| 1:I:716:SER:HB2 | 1:I:726:TYR:OH | 2.22 | 0.41 |
| 3:J:1113:LEU:HD12 | 3:J:1113:LEU:N | 2.08 | 0.41 |
| 3:J:88:ARG:CD | 3:J:853:THR:CG2 | 2.78 | 0.41 |
| 2:M:258:LEU:HA | 2:M:258:LEU:HD12 | 1.90 | 0.41 |
| 4:O:44:VAL:HG13 | 4:O:143:ALA:HB2 | 2.03 | 0.41 |
| 3:J:867:ARG:NH2 | 4:O:54:TYR:CE2 | 2.89 | 0.41 |
| 12:P:24:VAL:O | 12:P:24:VAL:CG1 | 2.67 | 0.41 |
| 5:Q:3:LYS:HE3 | 5:Q:3:LYS:HB2 | 1.60 | 0.41 |
| 9:U:18:VAL:HG12 | 9:U:22:LEU:CD1 | 2.50 | 0.41 |
| 9:U:42:GLN:HB2 | 9:U:42:GLN:HE21 | 1.78 | 0.41 |
| 9:U:61:VAL:CG1 | 9:U:62:ILE:N | 2.76 | 0.41 |
| 10:V:4:ARG:HG2 | 10:V:4:ARG:NH1 | 2.29 | 0.41 |
| 1:A:447:LEU:HD11 | 3:B:731:GLY:O | 2.20 | 0.40 |
| 1:A:53:GLU:O | 1:A:55:GLY:N | 2.54 | 0.40 |
| 1:A:8:GLY:O | 3:B:1114:VAL:HG22 | 2.21 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:138:LEU:HA | 3:B:141:ILE:CD1 | 2.41 | 0.40 |
| 3:B:221:ILE:HA | 3:B:222:PRO:HD3 | 1.95 | 0.40 |
| 3:B:446:HIS:H | 3:B:449:GLN:NE2 | 2.19 | 0.40 |
| 3:B:443:ARG:NH2 | 3:B:462:PRO:O | 2.54 | 0.40 |
| 3:B:489:LEU:HA | 3:B:489:LEU:HD23 | 1.87 | 0.40 |
| 3:B:691:ARG:NH1 | 3:B:756:ARG:HH21 | 2.18 | 0.40 |
| 3:B:81:SER:OG | 3:B:141:ILE:HG23 | 2.21 | 0.40 |
| 3:B:932:TYR:CD2 | 3:B:953:LEU:HD22 | 2.56 | 0.40 |
| 5:E:44:LEU:HD12 | 5:E:44:LEU:C | 2.41 | 0.40 |
| 1:I:114:TYR:O | 1:I:118:TYR:HB2 | 2.20 | 0.40 |
| 1:I:125:TRP:HD1 | 1:I:128:ALA:HB3 | 1.86 | 0.40 |
| 1:I:99:ARG:HG2 | 1:I:183:ARG:NH1 | 2.35 | 0.40 |
| 1:I:499:ALA:H | 1:I:502:TYR:HD2 | 1.69 | 0.40 |
| 1:I:608:PRO:HA | 1:I:862:HIS:CE1 | 2.56 | 0.40 |
| 1:I:651:VAL:HG21 | 1:I:743:MET:HB3 | 2.02 | 0.40 |
| 3:J:125:SER:O | 3:J:126:ALA:C | 2.59 | 0.40 |
| 3:J:157:SER:O | 3:J:158:GLU:CB | 2.68 | 0.40 |
| 3:J:256:LEU:C | 3:J:258:GLN:H | 2.24 | 0.40 |
| 2:C:49:ASP:CG | 3:J:382:LYS:HE2 | 2.41 | 0.40 |
| 3:J:644:SER:C | 3:J:646:ALA:N | 2.74 | 0.40 |
| 3:J:658:PRO:HB2 | 3:J:666:ASN:HD21 | 1.86 | 0.40 |
| 4:D:23:GLU:O | 10:L:27:LEU:HD13 | 2.21 | 0.40 |
| 2:M:103:GLY:HA2 | 2:M:106:ARG:HB2 | 2.02 | 0.40 |
| 2:M:344:ARG:HB3 | 2:M:353:HIS:NE2 | 2.36 | 0.40 |
| 4:O:183:CYS:HB2 | 16:O:1001:F3S:S1 | 2.61 | 0.40 |
| 4:O:131:VAL:HA | 11:W:2:LEU:CD1 | 2.49 | 0.40 |
| 9:U:23:TRP:HA | 9:U:23:TRP:CE3 | 2.56 | 0.40 |
| 11:W:3:ILE:HD11 | 11:W:18:TRP:CE3 | 2.56 | 0.40 |
| 12:X:33:ILE:O | 12:X:34:ILE:C | 2.60 | 0.40 |
| 1:A:203:ARG:CZ | 1:A:206:TRP:HB2 | 2.50 | 0.40 |
| 1:A:522:GLN:HG2 | 10:L:40:PHE:CE1 | 2.56 | 0.40 |
| 1:A:58:CYS:SG | 1:A:59:PRO:CD | 3.10 | 0.40 |
| 3:B:1083:GLY:O | 3:B:1084:ASP:HB2 | 2.21 | 0.40 |
| 3:B:174:VAL:HG11 | 3:B:325:LEU:HD23 | 2.03 | 0.40 |
| 3:B:752:SER:OG | 3:B:753:THR:N | 2.55 | 0.40 |
| 2:C:141:ALA:O | 2:C:145:GLU:HB2 | 2.21 | 0.40 |
| 5:E:90:LEU:HD12 | 5:E:100:ASN:HB2 | 2.01 | 0.40 |
| 6:F:31:SER:HB2 | 6:F:32:ASN:H | 1.70 | 0.40 |
| 1:I:500:GLN:HB2 | 3:J:913:HIS:CG | 2.56 | 0.40 |
| 1:I:575:CYS:O | 1:I:577:ASN:N | 2.52 | 0.40 |
| 3:J:1001:LEU:O | 3:J:1020:ARG:HD3 | 2.21 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:298:LEU:C | 3:J:300:HIS:N | 2.71 | 0.40 |
| 3:J:655:ILE:HG12 | 3:J:669:GLN:HG2 | 2.03 | 0.40 |
| 3:J:680:TYR:CE2 | 3:J:692:ALA:HB1 | 2.56 | 0.40 |
| 3:J:707:ALA:O | 3:J:709:ASP:N | 2.54 | 0.40 |
| 3:J:876:ASP:HB2 | 3:J:878:PHE:HE1 | 1.86 | 0.40 |
| 9:K:63:SER:O | 9:K:66:GLU:HB2 | 2.21 | 0.40 |
| 2:M:167:LEU:HD12 | 2:M:207:ASN:HD21 | 1.87 | 0.40 |
| 2:M:298:SER:O | 2:M:301:LEU:HD12 | 2.22 | 0.40 |
| 3:B:936:SER:O | 11:N:32:GLY:HA3 | 2.21 | 0.40 |
| 4:O:176:CYS:N | 4:O:195:LEU:HD21 | 2.37 | 0.40 |
| 5:Q:110:ILE:HD12 | 5:Q:118:LEU:HA | 2.04 | 0.40 |
| 7:S:36:PHE:CG | 7:S:96:ILE:HD11 | 2.56 | 0.40 |
| 8:T:17:VAL:HA | 8:T:18:PRO:HD3 | 1.83 | 0.40 |
| 1:I:471:GLU:OE1 | 9:U:41:LEU:CD1 | 2.70 | 0.40 |
| 11:W:21:PHE:O | 11:W:25:VAL:HG23 | 2.21 | 0.40 |
| 1:A:81:VAL:O | 1:A:209:LEU:N | 2.54 | 0.40 |
| 1:A:29:THR:HG1 | 1:A:45:MET:N | 2.19 | 0.40 |
| 1:A:480:MET:HG2 | 3:B:1039:PHE:CE1 | 2.56 | 0.40 |
| 1:A:634:VAL:O | 1:A:635:PHE:C | 2.60 | 0.40 |
| 3:B:245:ASP:N | 3:B:246:PRO:CD | 2.83 | 0.40 |
| 3:B:249:GLN:O | 3:B:253:PHE:CD1 | 2.74 | 0.40 |
| 3:B:353:LEU:HD12 | 3:B:404:VAL:HG13 | 2.03 | 0.40 |
| 3:B:669:GLN:C | 3:B:671:ALA:H | 2.25 | 0.40 |
| 3:B:902:LYS:HB2 | 11:N:42:ARG:NH1 | 2.37 | 0.40 |
| 2:C:391:ARG:HG3 | 2:C:391:ARG:NH1 | 2.33 | 0.40 |
| 5:E:151:SER:HB3 | 5:E:158:PRO:N | 2.36 | 0.40 |
| 1:I:105:LYS:HB3 | 1:I:109:ASP:OD1 | 2.21 | 0.40 |
| 1:I:326:ILE:HG21 | 1:I:462:MET:CG | 2.47 | 0.40 |
| 1:I:457:PHE:C | 1:I:459:GLY:H | 2.24 | 0.40 |
| 1:I:672:VAL:O | 1:I:673:ASP:C | 2.60 | 0.40 |
| 1:I:704:LEU:HD22 | 1:I:781:PHE:CD1 | 2.55 | 0.40 |
| 3:J:1015:GLN:HG2 | 3:J:1054:ASP:OD1 | 2.21 | 0.40 |
| 3:J:323:ILE:HG13 | 3:J:324:GLU:N | 2.35 | 0.40 |
| 3:J:361:PHE:CD2 | 3:J:361:PHE:C | 2.95 | 0.40 |
| 2:M:148:LYS:HG2 | 2:M:230:LYS:O | 2.21 | 0.40 |
| 1:I:818:TYR:OH | 2:M:348:GLU:OE2 | 2.25 | 0.40 |
| 2:M:53:ASP:O | 2:M:55:ALA:N | 2.54 | 0.40 |
| 5:Q:39:LEU:HD13 | 5:Q:42:LEU:HD21 | 2.02 | 0.40 |
| 5:Q:63:ASP:C | 5:Q:65:ALA:H | 2.24 | 0.40 |
| 6:R:63:VAL:HG12 | 6:R:63:VAL:O | 2.21 | 0.40 |
| 5:Q:64:GLY:O | 9:U:42:GLN:HG3 | 2.21 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:Y:69:GLU:O | 13:Y:70:ASP:C | 2.60 | 0.40 |
| 1:A:217:ILE:C | 1:A:219:ILE:H | 2.24 | 0.40 |
| 1:A:288:LYS:HG2 | 1:A:294:PRO:CA | 2.52 | 0.40 |
| 1:A:318:VAL:HG23 | 1:A:321:SER:HB2 | 2.03 | 0.40 |
| 1:A:732:GLY:O | 1:A:733:ALA:C | 2.60 | 0.40 |
| 1:A:866:VAL:O | 1:A:867:ASP:C | 2.60 | 0.40 |
| 3:B:234:THR:O | 3:B:237:ASP:HB2 | 2.22 | 0.40 |
| 3:B:320:SER:OG | 3:B:320:SER:O | 2.33 | 0.40 |
| 3:B:781:ARG:CD | 3:B:782:GLY:H | 2.33 | 0.40 |
| 3:B:811:ILE:O | 3:B:836:SER:HB2 | 2.21 | 0.40 |
| 4:D:151:LYS:O | 4:D:152:GLU:C | 2.60 | 0.40 |
| 4:D:178:LYS:C | 4:D:180:VAL:N | 2.75 | 0.40 |
| 1:I:217:ILE:O | 1:I:219:ILE:N | 2.54 | 0.40 |
| 1:I:312:ASN:HA | 1:I:315:GLY:O | 2.21 | 0.40 |
| 1:I:566:ALA:HB1 | 1:I:599:ASP:OD2 | 2.21 | 0.40 |
| 1:I:645:THR:HG22 | 1:I:724:PHE:CZ | 2.55 | 0.40 |
| 3:J:1066:TYR:CE1 | 3:J:1112:ARG:HD3 | 2.55 | 0.40 |
| 3:J:165:GLU:OE2 | 3:J:338:TYR:OH | 2.39 | 0.40 |
| 3:J:554:ASN:HD22 | 3:J:574:ARG:HH11 | 1.69 | 0.40 |
| 3:J:707:ALA:C | 3:J:709:ASP:N | 2.73 | 0.40 |
| 3:J:811:ILE:O | 3:J:836:SER:HB2 | 2.21 | 0.40 |
| 3:J:963:LEU:HA | 3:J:964:PRO:HD3 | 1.96 | 0.40 |
| 4:O:18:GLU:HB2 | 4:O:225:LYS:HE3 | 2.02 | 0.40 |
| 4:O:94:THR:CG2 | 4:O:145:LEU:HB2 | 2.52 | 0.40 |
| 6:R:72:LEU:C | 6:R:74:SER:H | 2.25 | 0.40 |
| 1:A:130:ARG:HB3 | 1:A:195:LEU:C | 2.42 | 0.40 |
| 1:A:600:LYS:HB2 | 1:A:732:GLY:HA3 | 2.03 | 0.40 |
| 3:B:1064:CYS:HG | 14:B:2001:ZN:ZN | 1.29 | 0.40 |
| 3:B:430:ILE:HD13 | 3:B:467:VAL:HB | 2.02 | 0.40 |
| 3:B:463:ASN:HB3 | 3:B:467:VAL:HG12 | 2.02 | 0.40 |
| 3:B:329:ARG:HD2 | 3:B:562:PHE:HB3 | 2.04 | 0.40 |
| 1:A:733:ALA:CB | 3:B:913:HIS:HE1 | 2.26 | 0.40 |
| 2:C:26:GLN:C | 2:C:28:ILE:N | 2.74 | 0.40 |
| 2:C:290:ARG:HG3 | 2:C:321:THR:HG21 | 2.04 | 0.40 |
| 2:C:370:VAL:O | 2:C:374:ILE:HD12 | 2.22 | 0.40 |
| 2:C:48:ILE:H | 2:C:50:LYS:HG3 | 1.87 | 0.40 |
| 4:D:22:LEU:C | 4:D:24:PHE:N | 2.74 | 0.40 |
| 5:E:147:ILE:HD11 | 5:E:163:THR:HG22 | 2.03 | 0.40 |
| 1:I:206:TRP:C | 1:I:208:ILE:H | 2.25 | 0.40 |
| 1:I:253:ILE:HG12 | 1:I:266:TRP:HZ2 | 1.87 | 0.40 |
| 1:I:353:ILE:HG21 | 1:I:358:ILE:HD12 | 2.04 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:415:ASP:H | 1:I:435:VAL:HG12 | 1.85 | 0.40 |
| 1:I:53:GLU:O | 1:I:55:GLY:N | 2.55 | 0.40 |
| 1:I:766:LEU:HD22 | 1:I:766:LEU:HA | 2.01 | 0.40 |
| 3:J:223:PHE:CE1 | 3:J:319:ILE:HG13 | 2.57 | 0.40 |
| 3:J:116:ILE:HD12 | 3:J:361:PHE:HZ | 1.86 | 0.40 |
| 3:J:600:GLY:C | 3:J:602:ILE:H | 2.24 | 0.40 |
| 3:J:676:ALA:O | 3:J:677:LEU:HD23 | 2.21 | 0.40 |
| 3:J:419:TRP:HZ3 | 3:J:712:GLY:C | 2.24 | 0.40 |
| 3:J:725:ALA:O | 3:J:909:ILE:HG23 | 2.21 | 0.40 |
| 3:J:853:THR:O | 3:J:861:LEU:N | 2.55 | 0.40 |
| 3:B:904:VAL:HG21 | 11:N:42:ARG:HG2 | 2.03 | 0.40 |
| 3:J:895:VAL:HG11 | 4:O:34:LEU:CG | 2.52 | 0.40 |
| 5:Q:92:VAL:HG12 | 5:Q:93:ASP:H | 1.85 | 0.40 |
| 1:I:539:ILE:HG21 | 7:S:46:ILE:HD11 | 2.04 | 0.40 |
| 10:V:29:ALA:O | 10:V:33:ARG:HG3 | 2.21 | 0.40 |
| 13:Y:57:GLY:CA | 13:Y:61:LEU:HD21 | 2.51 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|-----------|-----------|-----------|-------------|----|
| 1 | A | 828/880 (94%) | 597 (72%) | 154 (19%) | 77 (9%) | 1 | 8 |
| 1 | I | 828/880 (94%) | 594 (72%) | 157 (19%) | 77 (9%) | 1 | 8 |
| 2 | C | 366/395 (93%) | 225 (62%) | 92 (25%) | 49 (13%) | 0 | 3 |
| 2 | M | 366/395 (93%) | 232 (63%) | 84 (23%) | 50 (14%) | 0 | 3 |
| 3 | B | 1084/1124 (96%) | 752 (69%) | 215 (20%) | 117 (11%) | 0 | 6 |
| 3 | J | 1084/1124 (96%) | 752 (69%) | 217 (20%) | 115 (11%) | 0 | 6 |
| 4 | D | 262/265 (99%) | 199 (76%) | 50 (19%) | 13 (5%) | 2 | 22 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|------------|-----------|-------------|----|
| 4 | O | 262/265 (99%) | 198 (76%) | 53 (20%) | 11 (4%) | 3 | 26 |
| 5 | E | 172/180 (96%) | 125 (73%) | 35 (20%) | 12 (7%) | 1 | 13 |
| 5 | Q | 172/180 (96%) | 128 (74%) | 34 (20%) | 10 (6%) | 2 | 18 |
| 6 | F | 87/113 (77%) | 57 (66%) | 25 (29%) | 5 (6%) | 2 | 18 |
| 6 | R | 87/113 (77%) | 59 (68%) | 19 (22%) | 9 (10%) | 0 | 6 |
| 7 | G | 111/132 (84%) | 82 (74%) | 22 (20%) | 7 (6%) | 1 | 16 |
| 7 | S | 111/132 (84%) | 84 (76%) | 16 (14%) | 11 (10%) | 1 | 7 |
| 8 | H | 72/84 (86%) | 46 (64%) | 12 (17%) | 14 (19%) | 0 | 1 |
| 8 | T | 72/84 (86%) | 39 (54%) | 20 (28%) | 13 (18%) | 0 | 1 |
| 9 | K | 80/95 (84%) | 50 (62%) | 21 (26%) | 9 (11%) | 0 | 5 |
| 9 | U | 80/95 (84%) | 43 (54%) | 18 (22%) | 19 (24%) | 0 | 0 |
| 10 | L | 90/92 (98%) | 66 (73%) | 16 (18%) | 8 (9%) | 1 | 8 |
| 10 | V | 90/92 (98%) | 58 (64%) | 28 (31%) | 4 (4%) | 3 | 25 |
| 11 | N | 62/66 (94%) | 41 (66%) | 17 (27%) | 4 (6%) | 1 | 15 |
| 11 | W | 62/66 (94%) | 43 (69%) | 15 (24%) | 4 (6%) | 1 | 15 |
| 12 | P | 41/48 (85%) | 29 (71%) | 8 (20%) | 4 (10%) | 1 | 7 |
| 12 | X | 41/48 (85%) | 28 (68%) | 8 (20%) | 5 (12%) | 0 | 4 |
| 13 | Y | 43/104 (41%) | 26 (60%) | 13 (30%) | 4 (9%) | 1 | 8 |
| 13 | Z | 43/104 (41%) | 30 (70%) | 11 (26%) | 2 (5%) | 3 | 23 |
| All | All | 6596/7156 (92%) | 4583 (70%) | 1360 (21%) | 653 (10%) | 1 | 7 |

All (653) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 47 | PRO |
| 1 | A | 56 | GLN |
| 1 | A | 58 | CYS |
| 1 | A | 64 | THR |
| 1 | A | 145 | VAL |
| 1 | A | 207 | MET |
| 1 | A | 332 | ILE |
| 1 | A | 376 | ASN |
| 1 | A | 377 | TYR |
| 1 | A | 426 | HIS |
| 1 | A | 508 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 528 | ALA |
| 1 | A | 532 | ILE |
| 1 | A | 541 | ALA |
| 1 | A | 585 | TYR |
| 1 | A | 608 | PRO |
| 1 | A | 746 | MET |
| 1 | A | 829 | ASP |
| 1 | A | 842 | TYR |
| 1 | A | 865 | THR |
| 1 | A | 876 | VAL |
| 2 | C | 28 | ILE |
| 2 | C | 31 | ASP |
| 2 | C | 48 | ILE |
| 2 | C | 50 | LYS |
| 2 | C | 66 | PRO |
| 2 | C | 104 | LEU |
| 2 | C | 113 | ALA |
| 2 | C | 127 | THR |
| 2 | C | 188 | ILE |
| 2 | C | 191 | LEU |
| 2 | C | 193 | LEU |
| 2 | C | 211 | ALA |
| 2 | C | 275 | ASN |
| 2 | C | 306 | LEU |
| 2 | C | 324 | GLY |
| 2 | C | 362 | ASP |
| 2 | C | 364 | GLU |
| 2 | C | 365 | GLU |
| 2 | C | 390 | MET |
| 2 | C | 391 | ARG |
| 3 | B | 23 | LEU |
| 3 | B | 97 | TRP |
| 3 | B | 124 | LYS |
| 3 | B | 171 | ARG |
| 3 | B | 297 | PHE |
| 3 | B | 300 | HIS |
| 3 | B | 325 | LEU |
| 3 | B | 347 | GLY |
| 3 | B | 372 | SER |
| 3 | B | 378 | LYS |
| 3 | B | 382 | LYS |
| 3 | B | 402 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | B | 403 | TRP |
| 3 | B | 448 | THR |
| 3 | B | 473 | MET |
| 3 | B | 483 | ARG |
| 3 | B | 571 | ASP |
| 3 | B | 602 | ILE |
| 3 | B | 659 | GLU |
| 3 | B | 663 | SER |
| 3 | B | 730 | THR |
| 3 | B | 790 | ARG |
| 3 | B | 800 | PRO |
| 3 | B | 801 | GLU |
| 3 | B | 945 | PHE |
| 3 | B | 966 | ALA |
| 3 | B | 1030 | GLU |
| 3 | B | 1056 | THR |
| 3 | B | 1071 | ASP |
| 3 | B | 1114 | VAL |
| 3 | B | 1118 | LYS |
| 4 | D | 135 | THR |
| 4 | D | 152 | GLU |
| 4 | D | 205 | LEU |
| 5 | E | 39 | LEU |
| 5 | E | 88 | GLU |
| 5 | E | 116 | ASP |
| 6 | F | 3 | SER |
| 7 | G | 68 | HIS |
| 7 | G | 88 | ASN |
| 7 | G | 108 | ASN |
| 8 | H | 12 | ARG |
| 8 | H | 25 | ILE |
| 8 | H | 28 | ALA |
| 8 | H | 43 | PRO |
| 9 | K | 42 | GLN |
| 9 | K | 51 | ILE |
| 9 | K | 61 | VAL |
| 9 | K | 62 | ILE |
| 9 | K | 72 | GLY |
| 10 | L | 10 | SER |
| 10 | L | 36 | SER |
| 10 | L | 46 | PRO |
| 10 | L | 48 | PRO |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | N | 29 | GLU |
| 12 | P | 26 | CYS |
| 12 | P | 34 | ILE |
| 1 | I | 47 | PRO |
| 1 | I | 56 | GLN |
| 1 | I | 58 | CYS |
| 1 | I | 64 | THR |
| 1 | I | 145 | VAL |
| 1 | I | 207 | MET |
| 1 | I | 332 | ILE |
| 1 | I | 377 | TYR |
| 1 | I | 426 | HIS |
| 1 | I | 508 | LEU |
| 1 | I | 528 | ALA |
| 1 | I | 532 | ILE |
| 1 | I | 541 | ALA |
| 1 | I | 585 | TYR |
| 1 | I | 595 | GLU |
| 1 | I | 607 | GLN |
| 1 | I | 608 | PRO |
| 1 | I | 721 | PRO |
| 1 | I | 733 | ALA |
| 1 | I | 746 | MET |
| 1 | I | 825 | ASN |
| 1 | I | 826 | ALA |
| 1 | I | 829 | ASP |
| 1 | I | 842 | TYR |
| 1 | I | 865 | THR |
| 1 | I | 876 | VAL |
| 2 | M | 28 | ILE |
| 2 | M | 31 | ASP |
| 2 | M | 48 | ILE |
| 2 | M | 54 | LEU |
| 2 | M | 66 | PRO |
| 2 | M | 104 | LEU |
| 2 | M | 113 | ALA |
| 2 | M | 115 | LYS |
| 2 | M | 127 | THR |
| 2 | M | 146 | TYR |
| 2 | M | 213 | ILE |
| 2 | M | 306 | LEU |
| 2 | M | 365 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | M | 391 | ARG |
| 3 | J | 23 | LEU |
| 3 | J | 97 | TRP |
| 3 | J | 112 | GLU |
| 3 | J | 124 | LYS |
| 3 | J | 171 | ARG |
| 3 | J | 297 | PHE |
| 3 | J | 300 | HIS |
| 3 | J | 325 | LEU |
| 3 | J | 372 | SER |
| 3 | J | 378 | LYS |
| 3 | J | 402 | ASN |
| 3 | J | 403 | TRP |
| 3 | J | 448 | THR |
| 3 | J | 473 | MET |
| 3 | J | 483 | ARG |
| 3 | J | 530 | TYR |
| 3 | J | 571 | ASP |
| 3 | J | 602 | ILE |
| 3 | J | 659 | GLU |
| 3 | J | 663 | SER |
| 3 | J | 730 | THR |
| 3 | J | 790 | ARG |
| 3 | J | 800 | PRO |
| 3 | J | 801 | GLU |
| 3 | J | 945 | PHE |
| 3 | J | 966 | ALA |
| 3 | J | 1030 | GLU |
| 3 | J | 1056 | THR |
| 3 | J | 1071 | ASP |
| 3 | J | 1111 | PRO |
| 3 | J | 1114 | VAL |
| 3 | J | 1118 | LYS |
| 4 | O | 135 | THR |
| 4 | O | 152 | GLU |
| 4 | O | 205 | LEU |
| 5 | Q | 32 | GLN |
| 5 | Q | 39 | LEU |
| 5 | Q | 40 | LYS |
| 6 | R | 7 | VAL |
| 6 | R | 32 | ASN |
| 6 | R | 64 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | S | 65 | SER |
| 7 | S | 88 | ASN |
| 7 | S | 108 | ASN |
| 8 | T | 15 | TYR |
| 8 | T | 21 | GLU |
| 8 | T | 43 | PRO |
| 9 | U | 14 | HIS |
| 9 | U | 15 | PHE |
| 9 | U | 20 | ILE |
| 9 | U | 26 | ARG |
| 9 | U | 34 | ARG |
| 9 | U | 42 | GLN |
| 9 | U | 47 | ALA |
| 9 | U | 51 | ILE |
| 9 | U | 59 | THR |
| 9 | U | 61 | VAL |
| 11 | W | 29 | GLU |
| 12 | X | 26 | CYS |
| 12 | X | 34 | ILE |
| 13 | Z | 59 | ILE |
| 13 | Z | 77 | LYS |
| 1 | A | 27 | ILE |
| 1 | A | 150 | ASN |
| 1 | A | 155 | LYS |
| 1 | A | 185 | GLU |
| 1 | A | 307 | GLY |
| 1 | A | 355 | PRO |
| 1 | A | 378 | VAL |
| 1 | A | 392 | LYS |
| 1 | A | 393 | ASP |
| 1 | A | 447 | LEU |
| 1 | A | 529 | ASP |
| 1 | A | 534 | LEU |
| 1 | A | 576 | LYS |
| 1 | A | 595 | GLU |
| 1 | A | 607 | GLN |
| 1 | A | 621 | ASP |
| 1 | A | 682 | GLY |
| 1 | A | 721 | PRO |
| 1 | A | 733 | ALA |
| 1 | A | 749 | GLN |
| 1 | A | 763 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 764 | ARG |
| 1 | A | 825 | ASN |
| 1 | A | 826 | ALA |
| 1 | A | 841 | LEU |
| 2 | C | 115 | LYS |
| 2 | C | 190 | ARG |
| 2 | C | 210 | PHE |
| 2 | C | 264 | VAL |
| 2 | C | 299 | LYS |
| 2 | C | 331 | ARG |
| 2 | C | 360 | ARG |
| 2 | C | 367 | LYS |
| 3 | B | 30 | SER |
| 3 | B | 47 | GLY |
| 3 | B | 50 | PRO |
| 3 | B | 55 | GLY |
| 3 | B | 74 | ASP |
| 3 | B | 105 | ASN |
| 3 | B | 109 | ALA |
| 3 | B | 112 | GLU |
| 3 | B | 158 | GLU |
| 3 | B | 167 | LEU |
| 3 | B | 246 | PRO |
| 3 | B | 292 | ILE |
| 3 | B | 404 | VAL |
| 3 | B | 418 | ASN |
| 3 | B | 482 | GLU |
| 3 | B | 530 | TYR |
| 3 | B | 534 | GLY |
| 3 | B | 574 | ARG |
| 3 | B | 587 | PRO |
| 3 | B | 604 | PHE |
| 3 | B | 605 | ASP |
| 3 | B | 618 | ALA |
| 3 | B | 684 | TYR |
| 3 | B | 691 | ARG |
| 3 | B | 708 | LEU |
| 3 | B | 736 | ASP |
| 3 | B | 806 | GLY |
| 3 | B | 933 | ALA |
| 3 | B | 951 | GLU |
| 3 | B | 1001 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | B | 1065 | GLY |
| 3 | B | 1111 | PRO |
| 4 | D | 103 | PRO |
| 4 | D | 206 | CYS |
| 5 | E | 40 | LYS |
| 5 | E | 65 | ALA |
| 5 | E | 82 | GLN |
| 5 | E | 122 | ASN |
| 5 | E | 139 | GLY |
| 7 | G | 97 | SER |
| 8 | H | 56 | ASN |
| 8 | H | 74 | GLU |
| 8 | H | 80 | TYR |
| 8 | H | 81 | VAL |
| 9 | K | 47 | ALA |
| 10 | L | 50 | SER |
| 10 | L | 62 | SER |
| 11 | N | 63 | THR |
| 13 | Y | 66 | LYS |
| 1 | I | 27 | ILE |
| 1 | I | 80 | PRO |
| 1 | I | 150 | ASN |
| 1 | I | 155 | LYS |
| 1 | I | 185 | GLU |
| 1 | I | 307 | GLY |
| 1 | I | 372 | TRP |
| 1 | I | 376 | ASN |
| 1 | I | 378 | VAL |
| 1 | I | 392 | LYS |
| 1 | I | 393 | ASP |
| 1 | I | 447 | LEU |
| 1 | I | 454 | ASN |
| 1 | I | 482 | VAL |
| 1 | I | 529 | ASP |
| 1 | I | 534 | LEU |
| 1 | I | 576 | LYS |
| 1 | I | 621 | ASP |
| 1 | I | 682 | GLY |
| 1 | I | 741 | THR |
| 1 | I | 749 | GLN |
| 1 | I | 764 | ARG |
| 1 | I | 841 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | M | 44 | THR |
| 2 | M | 128 | ASP |
| 2 | M | 211 | ALA |
| 2 | M | 212 | ASN |
| 2 | M | 235 | LYS |
| 2 | M | 247 | ASP |
| 2 | M | 280 | ILE |
| 2 | M | 281 | GLU |
| 2 | M | 304 | GLN |
| 2 | M | 351 | VAL |
| 3 | J | 30 | SER |
| 3 | J | 50 | PRO |
| 3 | J | 51 | THR |
| 3 | J | 55 | GLY |
| 3 | J | 74 | ASP |
| 3 | J | 105 | ASN |
| 3 | J | 109 | ALA |
| 3 | J | 158 | GLU |
| 3 | J | 167 | LEU |
| 3 | J | 246 | PRO |
| 3 | J | 292 | ILE |
| 3 | J | 347 | GLY |
| 3 | J | 382 | LYS |
| 3 | J | 404 | VAL |
| 3 | J | 418 | ASN |
| 3 | J | 457 | GLU |
| 3 | J | 482 | GLU |
| 3 | J | 534 | GLY |
| 3 | J | 574 | ARG |
| 3 | J | 587 | PRO |
| 3 | J | 604 | PHE |
| 3 | J | 605 | ASP |
| 3 | J | 618 | ALA |
| 3 | J | 684 | TYR |
| 3 | J | 708 | LEU |
| 3 | J | 736 | ASP |
| 3 | J | 806 | GLY |
| 3 | J | 933 | ALA |
| 3 | J | 951 | GLU |
| 3 | J | 972 | ASP |
| 3 | J | 1001 | LEU |
| 3 | J | 1065 | GLY |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | O | 162 | SER |
| 4 | O | 179 | ALA |
| 6 | R | 49 | ALA |
| 7 | S | 80 | GLU |
| 7 | S | 97 | SER |
| 7 | S | 105 | ILE |
| 8 | T | 28 | ALA |
| 8 | T | 29 | TYR |
| 9 | U | 25 | ASN |
| 9 | U | 71 | ARG |
| 10 | V | 28 | ILE |
| 10 | V | 66 | LYS |
| 11 | W | 63 | THR |
| 1 | A | 80 | PRO |
| 1 | A | 106 | ILE |
| 1 | A | 121 | ILE |
| 1 | A | 286 | PRO |
| 1 | A | 356 | TRP |
| 1 | A | 372 | TRP |
| 1 | A | 454 | ASN |
| 1 | A | 514 | THR |
| 1 | A | 688 | PRO |
| 1 | A | 741 | THR |
| 1 | A | 852 | ASP |
| 2 | C | 58 | GLU |
| 2 | C | 145 | GLU |
| 2 | C | 192 | LYS |
| 2 | C | 196 | PHE |
| 2 | C | 235 | LYS |
| 2 | C | 272 | VAL |
| 2 | C | 290 | ARG |
| 2 | C | 302 | ALA |
| 3 | B | 51 | THR |
| 3 | B | 75 | ARG |
| 3 | B | 110 | GLU |
| 3 | B | 155 | ASN |
| 3 | B | 170 | ASN |
| 3 | B | 182 | ASN |
| 3 | B | 184 | THR |
| 3 | B | 247 | GLU |
| 3 | B | 276 | VAL |
| 3 | B | 449 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | B | 559 | VAL |
| 3 | B | 660 | HIS |
| 3 | B | 769 | GLN |
| 3 | B | 901 | VAL |
| 3 | B | 921 | LEU |
| 3 | B | 1080 | PRO |
| 4 | D | 23 | GLU |
| 4 | D | 70 | GLU |
| 4 | D | 179 | ALA |
| 5 | E | 52 | LYS |
| 6 | F | 43 | SER |
| 7 | G | 48 | ILE |
| 8 | H | 44 | TRP |
| 9 | K | 26 | ARG |
| 9 | K | 27 | LEU |
| 9 | K | 71 | ARG |
| 12 | P | 13 | PHE |
| 13 | Y | 56 | ASN |
| 13 | Y | 70 | ASP |
| 1 | I | 97 | THR |
| 1 | I | 106 | ILE |
| 1 | I | 235 | LEU |
| 1 | I | 356 | TRP |
| 1 | I | 514 | THR |
| 1 | I | 688 | PRO |
| 1 | I | 763 | THR |
| 1 | I | 864 | LYS |
| 2 | M | 50 | LYS |
| 2 | M | 71 | GLY |
| 2 | M | 114 | LYS |
| 2 | M | 278 | ARG |
| 2 | M | 279 | GLU |
| 2 | M | 337 | GLU |
| 2 | M | 367 | LYS |
| 3 | J | 47 | GLY |
| 3 | J | 75 | ARG |
| 3 | J | 110 | GLU |
| 3 | J | 170 | ASN |
| 3 | J | 182 | ASN |
| 3 | J | 184 | THR |
| 3 | J | 231 | GLY |
| 3 | J | 247 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | J | 276 | VAL |
| 3 | J | 332 | PRO |
| 3 | J | 449 | GLN |
| 3 | J | 559 | VAL |
| 3 | J | 657 | TYR |
| 3 | J | 660 | HIS |
| 3 | J | 691 | ARG |
| 3 | J | 759 | SER |
| 3 | J | 769 | GLN |
| 3 | J | 888 | ILE |
| 3 | J | 921 | LEU |
| 3 | J | 1080 | PRO |
| 4 | O | 103 | PRO |
| 4 | O | 206 | CYS |
| 5 | Q | 16 | ASN |
| 5 | Q | 56 | GLU |
| 5 | Q | 116 | ASP |
| 7 | S | 47 | ASN |
| 7 | S | 102 | LEU |
| 8 | T | 19 | LYS |
| 8 | T | 20 | HIS |
| 8 | T | 54 | SER |
| 8 | T | 81 | VAL |
| 9 | U | 13 | LEU |
| 9 | U | 16 | ASN |
| 9 | U | 44 | ALA |
| 12 | X | 13 | PHE |
| 12 | X | 28 | TYR |
| 1 | A | 54 | PRO |
| 1 | A | 97 | THR |
| 1 | A | 103 | ARG |
| 1 | A | 235 | LEU |
| 1 | A | 524 | ILE |
| 1 | A | 626 | TRP |
| 1 | A | 645 | THR |
| 1 | A | 686 | PRO |
| 2 | C | 45 | ARG |
| 2 | C | 67 | GLY |
| 2 | C | 238 | LYS |
| 3 | B | 111 | PRO |
| 3 | B | 210 | PHE |
| 3 | B | 223 | PHE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | B | 231 | GLY |
| 3 | B | 331 | GLU |
| 3 | B | 338 | TYR |
| 3 | B | 376 | GLY |
| 3 | B | 657 | TYR |
| 3 | B | 759 | SER |
| 3 | B | 860 | LYS |
| 3 | B | 1048 | ARG |
| 3 | B | 1087 | ASN |
| 4 | D | 162 | SER |
| 4 | D | 177 | GLU |
| 5 | E | 131 | LYS |
| 6 | F | 34 | LEU |
| 6 | F | 57 | GLU |
| 8 | H | 10 | ASP |
| 8 | H | 15 | TYR |
| 8 | H | 29 | TYR |
| 8 | H | 79 | ARG |
| 10 | L | 6 | LEU |
| 11 | N | 19 | GLN |
| 12 | P | 28 | TYR |
| 1 | I | 103 | ARG |
| 1 | I | 218 | THR |
| 1 | I | 286 | PRO |
| 1 | I | 355 | PRO |
| 1 | I | 537 | PRO |
| 1 | I | 686 | PRO |
| 1 | I | 852 | ASP |
| 2 | M | 12 | TYR |
| 2 | M | 144 | LEU |
| 2 | M | 193 | LEU |
| 2 | M | 210 | PHE |
| 2 | M | 218 | ALA |
| 3 | J | 98 | LEU |
| 3 | J | 111 | PRO |
| 3 | J | 113 | GLU |
| 3 | J | 331 | GLU |
| 3 | J | 338 | TYR |
| 3 | J | 486 | GLU |
| 3 | J | 901 | VAL |
| 4 | O | 7 | HIS |
| 4 | O | 70 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 5 | Q | 81 | VAL |
| 5 | Q | 139 | GLY |
| 6 | R | 25 | ILE |
| 6 | R | 43 | SER |
| 6 | R | 80 | SER |
| 7 | S | 48 | ILE |
| 7 | S | 99 | TYR |
| 8 | T | 12 | ARG |
| 9 | U | 19 | PHE |
| 11 | W | 6 | ARG |
| 11 | W | 19 | GLN |
| 1 | A | 391 | VAL |
| 1 | A | 403 | PRO |
| 1 | A | 482 | VAL |
| 1 | A | 537 | PRO |
| 1 | A | 543 | ARG |
| 1 | A | 779 | ARG |
| 2 | C | 144 | LEU |
| 2 | C | 161 | ALA |
| 2 | C | 213 | ILE |
| 2 | C | 239 | ARG |
| 2 | C | 348 | GLU |
| 3 | B | 98 | LEU |
| 3 | B | 103 | VAL |
| 3 | B | 194 | ALA |
| 3 | B | 441 | GLU |
| 3 | B | 635 | PRO |
| 3 | B | 915 | LEU |
| 3 | B | 1034 | ASP |
| 4 | D | 127 | ASP |
| 6 | F | 31 | SER |
| 11 | N | 6 | ARG |
| 1 | I | 54 | PRO |
| 1 | I | 143 | ALA |
| 1 | I | 524 | ILE |
| 1 | I | 543 | ARG |
| 1 | I | 645 | THR |
| 2 | M | 74 | ALA |
| 2 | M | 298 | SER |
| 3 | J | 103 | VAL |
| 3 | J | 194 | ALA |
| 3 | J | 210 | PHE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | J | 376 | GLY |
| 3 | J | 598 | GLU |
| 3 | J | 635 | PRO |
| 3 | J | 770 | GLU |
| 3 | J | 781 | ARG |
| 3 | J | 915 | LEU |
| 4 | O | 177 | GLU |
| 5 | Q | 38 | ILE |
| 8 | T | 80 | TYR |
| 1 | A | 143 | ALA |
| 2 | C | 114 | LYS |
| 2 | C | 128 | ASP |
| 3 | B | 332 | PRO |
| 3 | B | 377 | ARG |
| 3 | B | 438 | PRO |
| 3 | B | 598 | GLU |
| 3 | B | 703 | VAL |
| 3 | B | 770 | GLU |
| 3 | B | 779 | GLY |
| 3 | B | 972 | ASP |
| 4 | D | 79 | PRO |
| 4 | D | 94 | THR |
| 5 | E | 51 | VAL |
| 1 | I | 334 | ILE |
| 1 | I | 391 | VAL |
| 1 | I | 403 | PRO |
| 1 | I | 851 | GLY |
| 2 | M | 161 | ALA |
| 2 | M | 203 | ASP |
| 2 | M | 363 | VAL |
| 2 | M | 364 | GLU |
| 3 | J | 223 | PHE |
| 3 | J | 377 | ARG |
| 3 | J | 438 | PRO |
| 3 | J | 703 | VAL |
| 3 | J | 779 | GLY |
| 3 | J | 793 | GLU |
| 3 | J | 1048 | ARG |
| 3 | J | 1087 | ASN |
| 6 | R | 60 | SER |
| 8 | T | 11 | PRO |
| 9 | U | 70 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 12 | X | 18 | LEU |
| 1 | A | 530 | VAL |
| 1 | A | 851 | GLY |
| 2 | C | 71 | GLY |
| 3 | B | 299 | PRO |
| 3 | B | 328 | GLY |
| 3 | B | 591 | ILE |
| 3 | B | 814 | VAL |
| 3 | B | 944 | PRO |
| 3 | B | 950 | ILE |
| 8 | H | 59 | PRO |
| 1 | I | 121 | ILE |
| 2 | M | 24 | LEU |
| 2 | M | 67 | GLY |
| 2 | M | 119 | THR |
| 2 | M | 179 | VAL |
| 2 | M | 181 | VAL |
| 3 | J | 299 | PRO |
| 3 | J | 903 | GLY |
| 3 | J | 950 | ILE |
| 3 | J | 1108 | ILE |
| 3 | B | 767 | GLY |
| 3 | B | 1108 | ILE |
| 10 | L | 28 | ILE |
| 1 | I | 530 | VAL |
| 2 | M | 277 | ILE |
| 6 | R | 4 | VAL |
| 7 | S | 64 | PRO |
| 8 | T | 10 | ASP |
| 1 | A | 334 | ILE |
| 1 | A | 369 | PRO |
| 2 | C | 393 | ILE |
| 3 | B | 253 | PHE |
| 7 | G | 64 | PRO |
| 7 | G | 78 | VAL |
| 13 | Y | 57 | GLY |
| 2 | M | 260 | GLY |
| 2 | M | 261 | VAL |
| 3 | J | 645 | PRO |
| 3 | J | 944 | PRO |
| 5 | Q | 51 | VAL |
| 9 | U | 64 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | V | 48 | PRO |
| 2 | C | 181 | VAL |
| 3 | B | 645 | PRO |
| 3 | B | 888 | ILE |
| 5 | E | 25 | ILE |
| 1 | I | 330 | PRO |
| 1 | I | 369 | PRO |
| 3 | J | 591 | ILE |
| 9 | U | 62 | ILE |
| 10 | V | 46 | PRO |
| 1 | A | 760 | GLY |
| 4 | O | 79 | PRO |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|-----------|-------------|----|
| 1 | A | 729/766 (95%) | 601 (82%) | 128 (18%) | 2 | 11 |
| 1 | I | 729/766 (95%) | 604 (83%) | 125 (17%) | 2 | 13 |
| 2 | C | 318/340 (94%) | 241 (76%) | 77 (24%) | 1 | 4 |
| 2 | M | 318/340 (94%) | 226 (71%) | 92 (29%) | 0 | 2 |
| 3 | B | 937/965 (97%) | 772 (82%) | 165 (18%) | 2 | 11 |
| 3 | J | 937/965 (97%) | 771 (82%) | 166 (18%) | 2 | 11 |
| 4 | D | 241/242 (100%) | 220 (91%) | 21 (9%) | 12 | 43 |
| 4 | O | 241/242 (100%) | 221 (92%) | 20 (8%) | 13 | 46 |
| 5 | E | 156/159 (98%) | 128 (82%) | 28 (18%) | 2 | 10 |
| 5 | Q | 156/159 (98%) | 123 (79%) | 33 (21%) | 1 | 5 |
| 6 | F | 82/106 (77%) | 72 (88%) | 10 (12%) | 6 | 26 |
| 6 | R | 82/106 (77%) | 72 (88%) | 10 (12%) | 6 | 26 |
| 7 | G | 105/125 (84%) | 87 (83%) | 18 (17%) | 2 | 13 |
| 7 | S | 105/125 (84%) | 82 (78%) | 23 (22%) | 1 | 5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|------------|-------------|----|
| 8 | H | 67/75 (89%) | 49 (73%) | 18 (27%) | 0 | 3 |
| 8 | T | 67/75 (89%) | 54 (81%) | 13 (19%) | 1 | 8 |
| 9 | K | 72/84 (86%) | 48 (67%) | 24 (33%) | 0 | 1 |
| 9 | U | 72/84 (86%) | 50 (69%) | 22 (31%) | 0 | 2 |
| 10 | L | 81/81 (100%) | 66 (82%) | 15 (18%) | 2 | 9 |
| 10 | V | 81/81 (100%) | 63 (78%) | 18 (22%) | 1 | 5 |
| 11 | N | 58/60 (97%) | 48 (83%) | 10 (17%) | 2 | 12 |
| 11 | W | 58/60 (97%) | 48 (83%) | 10 (17%) | 2 | 12 |
| 12 | P | 39/43 (91%) | 32 (82%) | 7 (18%) | 2 | 10 |
| 12 | X | 39/43 (91%) | 32 (82%) | 7 (18%) | 2 | 10 |
| 13 | Y | 43/97 (44%) | 34 (79%) | 9 (21%) | 1 | 6 |
| 13 | Z | 43/97 (44%) | 34 (79%) | 9 (21%) | 1 | 6 |
| All | All | 5856/6286 (93%) | 4778 (82%) | 1078 (18%) | 2 | 9 |

All (1078) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 15 | SER |
| 1 | A | 29 | THR |
| 1 | A | 45 | MET |
| 1 | A | 48 | ARG |
| 1 | A | 56 | GLN |
| 1 | A | 58 | CYS |
| 1 | A | 60 | THR |
| 1 | A | 64 | THR |
| 1 | A | 65 | LEU |
| 1 | A | 82 | ILE |
| 1 | A | 84 | VAL |
| 1 | A | 100 | ARG |
| 1 | A | 101 | CYS |
| 1 | A | 103 | ARG |
| 1 | A | 105 | LYS |
| 1 | A | 107 | SER |
| 1 | A | 125 | TRP |
| 1 | A | 127 | SER |
| 1 | A | 130 | ARG |
| 1 | A | 133 | THR |
| 1 | A | 136 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 139 | THR |
| 1 | A | 141 | MET |
| 1 | A | 152 | LYS |
| 1 | A | 155 | LYS |
| 1 | A | 175 | LEU |
| 1 | A | 176 | THR |
| 1 | A | 178 | SER |
| 1 | A | 179 | ASP |
| 1 | A | 191 | ASP |
| 1 | A | 194 | ILE |
| 1 | A | 203 | ARG |
| 1 | A | 222 | SER |
| 1 | A | 232 | GLU |
| 1 | A | 238 | LYS |
| 1 | A | 239 | LEU |
| 1 | A | 243 | VAL |
| 1 | A | 248 | ARG |
| 1 | A | 261 | ILE |
| 1 | A | 264 | ASP |
| 1 | A | 278 | ASP |
| 1 | A | 289 | HIS |
| 1 | A | 290 | ARG |
| 1 | A | 301 | ARG |
| 1 | A | 306 | GLU |
| 1 | A | 308 | ARG |
| 1 | A | 313 | LEU |
| 1 | A | 314 | SER |
| 1 | A | 331 | ASN |
| 1 | A | 346 | THR |
| 1 | A | 349 | VAL |
| 1 | A | 356 | TRP |
| 1 | A | 366 | ILE |
| 1 | A | 376 | ASN |
| 1 | A | 377 | TYR |
| 1 | A | 386 | ILE |
| 1 | A | 388 | LEU |
| 1 | A | 394 | ARG |
| 1 | A | 421 | ARG |
| 1 | A | 425 | LEU |
| 1 | A | 427 | ARG |
| 1 | A | 428 | ILE |
| 1 | A | 429 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 434 | ARG |
| 1 | A | 436 | ARG |
| 1 | A | 438 | LEU |
| 1 | A | 441 | LEU |
| 1 | A | 442 | THR |
| 1 | A | 446 | ASN |
| 1 | A | 464 | LEU |
| 1 | A | 469 | SER |
| 1 | A | 471 | GLU |
| 1 | A | 479 | ILE |
| 1 | A | 481 | LEU |
| 1 | A | 486 | ILE |
| 1 | A | 487 | ILE |
| 1 | A | 488 | THR |
| 1 | A | 495 | ILE |
| 1 | A | 500 | GLN |
| 1 | A | 503 | ILE |
| 1 | A | 507 | TYR |
| 1 | A | 515 | LEU |
| 1 | A | 518 | LYS |
| 1 | A | 525 | LEU |
| 1 | A | 547 | THR |
| 1 | A | 550 | GLN |
| 1 | A | 558 | LYS |
| 1 | A | 559 | ASP |
| 1 | A | 561 | ASN |
| 1 | A | 573 | ARG |
| 1 | A | 574 | LEU |
| 1 | A | 593 | LEU |
| 1 | A | 597 | VAL |
| 1 | A | 605 | ASN |
| 1 | A | 609 | GLU |
| 1 | A | 616 | ILE |
| 1 | A | 618 | GLU |
| 1 | A | 633 | ARG |
| 1 | A | 637 | ARG |
| 1 | A | 644 | PHE |
| 1 | A | 667 | ARG |
| 1 | A | 675 | LEU |
| 1 | A | 684 | LEU |
| 1 | A | 687 | ILE |
| 1 | A | 691 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 692 | LEU |
| 1 | A | 693 | GLU |
| 1 | A | 702 | ASP |
| 1 | A | 708 | ARG |
| 1 | A | 716 | SER |
| 1 | A | 723 | ASN |
| 1 | A | 736 | SER |
| 1 | A | 737 | VAL |
| 1 | A | 739 | ASN |
| 1 | A | 752 | VAL |
| 1 | A | 755 | GLU |
| 1 | A | 759 | ARG |
| 1 | A | 764 | ARG |
| 1 | A | 766 | LEU |
| 1 | A | 779 | ARG |
| 1 | A | 781 | PHE |
| 1 | A | 787 | ARG |
| 1 | A | 823 | LEU |
| 1 | A | 828 | SER |
| 1 | A | 841 | LEU |
| 1 | A | 844 | GLU |
| 1 | A | 864 | LYS |
| 1 | A | 876 | VAL |
| 2 | C | 13 | LEU |
| 2 | C | 31 | ASP |
| 2 | C | 36 | ILE |
| 2 | C | 41 | ILE |
| 2 | C | 42 | ILE |
| 2 | C | 43 | VAL |
| 2 | C | 47 | GLU |
| 2 | C | 51 | ILE |
| 2 | C | 53 | ASP |
| 2 | C | 57 | LYS |
| 2 | C | 59 | TYR |
| 2 | C | 61 | GLU |
| 2 | C | 70 | ILE |
| 2 | C | 72 | ILE |
| 2 | C | 85 | MET |
| 2 | C | 107 | LEU |
| 2 | C | 116 | VAL |
| 2 | C | 118 | SER |
| 2 | C | 119 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 130 | TYR |
| 2 | C | 132 | ARG |
| 2 | C | 145 | GLU |
| 2 | C | 147 | THR |
| 2 | C | 163 | MET |
| 2 | C | 173 | MET |
| 2 | C | 174 | LEU |
| 2 | C | 176 | ASP |
| 2 | C | 188 | ILE |
| 2 | C | 190 | ARG |
| 2 | C | 193 | LEU |
| 2 | C | 201 | SER |
| 2 | C | 215 | SER |
| 2 | C | 229 | THR |
| 2 | C | 234 | ILE |
| 2 | C | 237 | ILE |
| 2 | C | 239 | ARG |
| 2 | C | 250 | ILE |
| 2 | C | 254 | ASP |
| 2 | C | 257 | ASN |
| 2 | C | 267 | VAL |
| 2 | C | 275 | ASN |
| 2 | C | 278 | ARG |
| 2 | C | 287 | GLU |
| 2 | C | 291 | GLU |
| 2 | C | 292 | ILE |
| 2 | C | 301 | LEU |
| 2 | C | 307 | ASP |
| 2 | C | 310 | ILE |
| 2 | C | 311 | ARG |
| 2 | C | 314 | LEU |
| 2 | C | 315 | LEU |
| 2 | C | 316 | ILE |
| 2 | C | 320 | MET |
| 2 | C | 322 | ARG |
| 2 | C | 326 | VAL |
| 2 | C | 329 | ILE |
| 2 | C | 331 | ARG |
| 2 | C | 335 | THR |
| 2 | C | 337 | GLU |
| 2 | C | 339 | ASN |
| 2 | C | 344 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 349 | VAL |
| 2 | C | 351 | VAL |
| 2 | C | 364 | GLU |
| 2 | C | 369 | VAL |
| 2 | C | 370 | VAL |
| 2 | C | 374 | ILE |
| 2 | C | 375 | ILE |
| 2 | C | 379 | ILE |
| 2 | C | 380 | LYS |
| 2 | C | 381 | LEU |
| 2 | C | 388 | LEU |
| 2 | C | 389 | THR |
| 2 | C | 390 | MET |
| 2 | C | 391 | ARG |
| 2 | C | 393 | ILE |
| 2 | C | 394 | LEU |
| 3 | B | 5 | LEU |
| 3 | B | 6 | THR |
| 3 | B | 8 | ASP |
| 3 | B | 20 | SER |
| 3 | B | 23 | LEU |
| 3 | B | 30 | SER |
| 3 | B | 33 | ASP |
| 3 | B | 34 | PHE |
| 3 | B | 51 | THR |
| 3 | B | 56 | LEU |
| 3 | B | 64 | ARG |
| 3 | B | 65 | ILE |
| 3 | B | 70 | VAL |
| 3 | B | 72 | GLU |
| 3 | B | 75 | ARG |
| 3 | B | 80 | ILE |
| 3 | B | 90 | LEU |
| 3 | B | 105 | ASN |
| 3 | B | 108 | GLU |
| 3 | B | 113 | GLU |
| 3 | B | 118 | ASP |
| 3 | B | 137 | LYS |
| 3 | B | 155 | ASN |
| 3 | B | 159 | ARG |
| 3 | B | 163 | THR |
| 3 | B | 182 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | B | 183 | ILE |
| 3 | B | 193 | THR |
| 3 | B | 203 | GLU |
| 3 | B | 207 | ASP |
| 3 | B | 221 | ILE |
| 3 | B | 227 | MET |
| 3 | B | 234 | THR |
| 3 | B | 245 | ASP |
| 3 | B | 282 | ARG |
| 3 | B | 296 | TYR |
| 3 | B | 322 | VAL |
| 3 | B | 327 | LEU |
| 3 | B | 335 | LYS |
| 3 | B | 348 | ASP |
| 3 | B | 361 | PHE |
| 3 | B | 367 | TYR |
| 3 | B | 369 | LEU |
| 3 | B | 371 | LYS |
| 3 | B | 374 | VAL |
| 3 | B | 378 | LYS |
| 3 | B | 391 | THR |
| 3 | B | 395 | ARG |
| 3 | B | 402 | ASN |
| 3 | B | 404 | VAL |
| 3 | B | 407 | ARG |
| 3 | B | 416 | ARG |
| 3 | B | 418 | ASN |
| 3 | B | 421 | SER |
| 3 | B | 432 | SER |
| 3 | B | 444 | ASP |
| 3 | B | 448 | THR |
| 3 | B | 453 | MET |
| 3 | B | 457 | GLU |
| 3 | B | 467 | VAL |
| 3 | B | 468 | LYS |
| 3 | B | 469 | ASN |
| 3 | B | 476 | ILE |
| 3 | B | 478 | VAL |
| 3 | B | 484 | ILE |
| 3 | B | 486 | GLU |
| 3 | B | 488 | THR |
| 3 | B | 497 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | B | 498 | GLU |
| 3 | B | 518 | SER |
| 3 | B | 530 | TYR |
| 3 | B | 531 | GLN |
| 3 | B | 544 | ARG |
| 3 | B | 549 | ILE |
| 3 | B | 551 | ASP |
| 3 | B | 564 | ASN |
| 3 | B | 570 | CYS |
| 3 | B | 572 | SER |
| 3 | B | 576 | ARG |
| 3 | B | 588 | LEU |
| 3 | B | 594 | ILE |
| 3 | B | 603 | THR |
| 3 | B | 606 | ASP |
| 3 | B | 607 | LEU |
| 3 | B | 608 | VAL |
| 3 | B | 626 | VAL |
| 3 | B | 628 | LEU |
| 3 | B | 634 | THR |
| 3 | B | 638 | THR |
| 3 | B | 640 | LEU |
| 3 | B | 643 | TRP |
| 3 | B | 650 | ILE |
| 3 | B | 655 | ILE |
| 3 | B | 659 | GLU |
| 3 | B | 669 | GLN |
| 3 | B | 685 | GLN |
| 3 | B | 686 | LEU |
| 3 | B | 687 | ARG |
| 3 | B | 688 | THR |
| 3 | B | 689 | ASP |
| 3 | B | 691 | ARG |
| 3 | B | 702 | LEU |
| 3 | B | 705 | THR |
| 3 | B | 708 | LEU |
| 3 | B | 710 | ILE |
| 3 | B | 714 | THR |
| 3 | B | 720 | ASN |
| 3 | B | 739 | ILE |
| 3 | B | 741 | ASN |
| 3 | B | 757 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | B | 765 | TYR |
| 3 | B | 770 | GLU |
| 3 | B | 780 | VAL |
| 3 | B | 781 | ARG |
| 3 | B | 787 | GLU |
| 3 | B | 789 | TYR |
| 3 | B | 794 | ASP |
| 3 | B | 800 | PRO |
| 3 | B | 814 | VAL |
| 3 | B | 843 | GLU |
| 3 | B | 846 | ILE |
| 3 | B | 850 | VAL |
| 3 | B | 855 | THR |
| 3 | B | 867 | ARG |
| 3 | B | 871 | ILE |
| 3 | B | 887 | VAL |
| 3 | B | 890 | MET |
| 3 | B | 895 | VAL |
| 3 | B | 910 | LEU |
| 3 | B | 911 | ASN |
| 3 | B | 915 | LEU |
| 3 | B | 919 | MET |
| 3 | B | 924 | ILE |
| 3 | B | 926 | GLU |
| 3 | B | 931 | LYS |
| 3 | B | 940 | VAL |
| 3 | B | 941 | ASP |
| 3 | B | 945 | PHE |
| 3 | B | 946 | TYR |
| 3 | B | 950 | ILE |
| 3 | B | 951 | GLU |
| 3 | B | 957 | ILE |
| 3 | B | 967 | THR |
| 3 | B | 975 | THR |
| 3 | B | 982 | ARG |
| 3 | B | 985 | PHE |
| 3 | B | 991 | GLN |
| 3 | B | 992 | LYS |
| 3 | B | 1004 | ARG |
| 3 | B | 1012 | LEU |
| 3 | B | 1016 | PRO |
| 3 | B | 1018 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | B | 1026 | LEU |
| 3 | B | 1030 | GLU |
| 3 | B | 1035 | CYS |
| 3 | B | 1045 | LEU |
| 3 | B | 1049 | LEU |
| 3 | B | 1050 | LEU |
| 3 | B | 1067 | ILE |
| 3 | B | 1078 | VAL |
| 3 | B | 1079 | CYS |
| 3 | B | 1108 | ILE |
| 3 | B | 1109 | ILE |
| 3 | B | 1113 | LEU |
| 3 | B | 1115 | LEU |
| 4 | D | 29 | ARG |
| 4 | D | 56 | GLU |
| 4 | D | 57 | ILE |
| 4 | D | 68 | MET |
| 4 | D | 82 | CYS |
| 4 | D | 89 | CYS |
| 4 | D | 113 | ASP |
| 4 | D | 132 | LEU |
| 4 | D | 135 | THR |
| 4 | D | 136 | ASN |
| 4 | D | 155 | LYS |
| 4 | D | 161 | LEU |
| 4 | D | 162 | SER |
| 4 | D | 165 | ARG |
| 4 | D | 170 | VAL |
| 4 | D | 180 | VAL |
| 4 | D | 195 | LEU |
| 4 | D | 201 | LEU |
| 4 | D | 204 | THR |
| 4 | D | 214 | ASN |
| 4 | D | 218 | ARG |
| 5 | E | 12 | ARG |
| 5 | E | 18 | PHE |
| 5 | E | 22 | LEU |
| 5 | E | 27 | LEU |
| 5 | E | 30 | LEU |
| 5 | E | 33 | GLN |
| 5 | E | 38 | ILE |
| 5 | E | 39 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 40 | LYS |
| 5 | E | 41 | ASP |
| 5 | E | 44 | LEU |
| 5 | E | 51 | VAL |
| 5 | E | 58 | ILE |
| 5 | E | 59 | LEU |
| 5 | E | 66 | THR |
| 5 | E | 67 | TYR |
| 5 | E | 69 | GLU |
| 5 | E | 76 | THR |
| 5 | E | 81 | VAL |
| 5 | E | 83 | GLU |
| 5 | E | 85 | VAL |
| 5 | E | 92 | VAL |
| 5 | E | 101 | LEU |
| 5 | E | 110 | ILE |
| 5 | E | 128 | PHE |
| 5 | E | 151 | SER |
| 5 | E | 163 | THR |
| 5 | E | 176 | THR |
| 6 | F | 14 | TYR |
| 6 | F | 15 | SER |
| 6 | F | 25 | ILE |
| 6 | F | 31 | SER |
| 6 | F | 33 | LEU |
| 6 | F | 34 | LEU |
| 6 | F | 47 | CYS |
| 6 | F | 59 | LEU |
| 6 | F | 64 | SER |
| 6 | F | 86 | ILE |
| 7 | G | 5 | VAL |
| 7 | G | 10 | ILE |
| 7 | G | 19 | GLU |
| 7 | G | 25 | ASN |
| 7 | G | 42 | ILE |
| 7 | G | 46 | ILE |
| 7 | G | 65 | SER |
| 7 | G | 77 | ILE |
| 7 | G | 78 | VAL |
| 7 | G | 86 | LEU |
| 7 | G | 92 | TYR |
| 7 | G | 95 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 97 | SER |
| 7 | G | 104 | LYS |
| 7 | G | 106 | ILE |
| 7 | G | 110 | GLU |
| 7 | G | 114 | ARG |
| 7 | G | 115 | THR |
| 8 | H | 12 | ARG |
| 8 | H | 13 | ILE |
| 8 | H | 19 | LYS |
| 8 | H | 22 | VAL |
| 8 | H | 31 | ILE |
| 8 | H | 37 | ILE |
| 8 | H | 38 | ARG |
| 8 | H | 43 | PRO |
| 8 | H | 44 | TRP |
| 8 | H | 45 | ILE |
| 8 | H | 46 | ARG |
| 8 | H | 48 | SER |
| 8 | H | 64 | ARG |
| 8 | H | 65 | ILE |
| 8 | H | 74 | GLU |
| 8 | H | 75 | VAL |
| 8 | H | 76 | VAL |
| 8 | H | 82 | ILE |
| 9 | K | 15 | PHE |
| 9 | K | 18 | VAL |
| 9 | K | 19 | PHE |
| 9 | K | 20 | ILE |
| 9 | K | 22 | LEU |
| 9 | K | 23 | TRP |
| 9 | K | 29 | ARG |
| 9 | K | 35 | VAL |
| 9 | K | 36 | ILE |
| 9 | K | 37 | SER |
| 9 | K | 41 | LEU |
| 9 | K | 42 | GLN |
| 9 | K | 45 | MET |
| 9 | K | 50 | LEU |
| 9 | K | 51 | ILE |
| 9 | K | 52 | ASP |
| 9 | K | 61 | VAL |
| 9 | K | 67 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | K | 71 | ARG |
| 9 | K | 74 | LEU |
| 9 | K | 81 | ARG |
| 9 | K | 82 | LEU |
| 9 | K | 89 | LEU |
| 9 | K | 90 | LEU |
| 10 | L | 9 | GLU |
| 10 | L | 24 | LEU |
| 10 | L | 43 | TYR |
| 10 | L | 44 | TYR |
| 10 | L | 45 | GLN |
| 10 | L | 47 | HIS |
| 10 | L | 49 | LEU |
| 10 | L | 55 | VAL |
| 10 | L | 57 | ILE |
| 10 | L | 69 | LEU |
| 10 | L | 70 | LEU |
| 10 | L | 73 | ILE |
| 10 | L | 79 | MET |
| 10 | L | 87 | ILE |
| 10 | L | 92 | LYS |
| 11 | N | 3 | ILE |
| 11 | N | 5 | ILE |
| 11 | N | 10 | CYS |
| 11 | N | 13 | LEU |
| 11 | N | 22 | ILE |
| 11 | N | 40 | VAL |
| 11 | N | 42 | ARG |
| 11 | N | 48 | MET |
| 11 | N | 55 | ILE |
| 11 | N | 64 | ARG |
| 12 | P | 10 | TRP |
| 12 | P | 21 | LEU |
| 12 | P | 24 | VAL |
| 12 | P | 31 | TYR |
| 12 | P | 34 | ILE |
| 12 | P | 35 | PHE |
| 12 | P | 46 | LYS |
| 13 | Y | 44 | LEU |
| 13 | Y | 60 | THR |
| 13 | Y | 69 | GLU |
| 13 | Y | 70 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | Y | 72 | TYR |
| 13 | Y | 77 | LYS |
| 13 | Y | 78 | ARG |
| 13 | Y | 79 | ASP |
| 13 | Y | 82 | ARG |
| 1 | I | 15 | SER |
| 1 | I | 29 | THR |
| 1 | I | 45 | MET |
| 1 | I | 48 | ARG |
| 1 | I | 56 | GLN |
| 1 | I | 58 | CYS |
| 1 | I | 60 | THR |
| 1 | I | 64 | THR |
| 1 | I | 82 | ILE |
| 1 | I | 84 | VAL |
| 1 | I | 100 | ARG |
| 1 | I | 101 | CYS |
| 1 | I | 103 | ARG |
| 1 | I | 105 | LYS |
| 1 | I | 107 | SER |
| 1 | I | 125 | TRP |
| 1 | I | 127 | SER |
| 1 | I | 130 | ARG |
| 1 | I | 133 | THR |
| 1 | I | 136 | VAL |
| 1 | I | 141 | MET |
| 1 | I | 152 | LYS |
| 1 | I | 155 | LYS |
| 1 | I | 175 | LEU |
| 1 | I | 176 | THR |
| 1 | I | 178 | SER |
| 1 | I | 179 | ASP |
| 1 | I | 194 | ILE |
| 1 | I | 203 | ARG |
| 1 | I | 209 | LEU |
| 1 | I | 217 | ILE |
| 1 | I | 222 | SER |
| 1 | I | 232 | GLU |
| 1 | I | 238 | LYS |
| 1 | I | 239 | LEU |
| 1 | I | 243 | VAL |
| 1 | I | 248 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 261 | ILE |
| 1 | I | 264 | ASP |
| 1 | I | 278 | ASP |
| 1 | I | 289 | HIS |
| 1 | I | 298 | LEU |
| 1 | I | 301 | ARG |
| 1 | I | 306 | GLU |
| 1 | I | 308 | ARG |
| 1 | I | 313 | LEU |
| 1 | I | 314 | SER |
| 1 | I | 331 | ASN |
| 1 | I | 346 | THR |
| 1 | I | 349 | VAL |
| 1 | I | 366 | ILE |
| 1 | I | 376 | ASN |
| 1 | I | 377 | TYR |
| 1 | I | 386 | ILE |
| 1 | I | 388 | LEU |
| 1 | I | 394 | ARG |
| 1 | I | 411 | LEU |
| 1 | I | 421 | ARG |
| 1 | I | 425 | LEU |
| 1 | I | 427 | ARG |
| 1 | I | 428 | ILE |
| 1 | I | 434 | ARG |
| 1 | I | 436 | ARG |
| 1 | I | 438 | LEU |
| 1 | I | 441 | LEU |
| 1 | I | 442 | THR |
| 1 | I | 446 | ASN |
| 1 | I | 464 | LEU |
| 1 | I | 469 | SER |
| 1 | I | 481 | LEU |
| 1 | I | 484 | LYS |
| 1 | I | 486 | ILE |
| 1 | I | 487 | ILE |
| 1 | I | 488 | THR |
| 1 | I | 495 | ILE |
| 1 | I | 500 | GLN |
| 1 | I | 503 | ILE |
| 1 | I | 507 | TYR |
| 1 | I | 515 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 518 | LYS |
| 1 | I | 525 | LEU |
| 1 | I | 547 | THR |
| 1 | I | 550 | GLN |
| 1 | I | 558 | LYS |
| 1 | I | 559 | ASP |
| 1 | I | 561 | ASN |
| 1 | I | 573 | ARG |
| 1 | I | 574 | LEU |
| 1 | I | 586 | VAL |
| 1 | I | 593 | LEU |
| 1 | I | 605 | ASN |
| 1 | I | 609 | GLU |
| 1 | I | 616 | ILE |
| 1 | I | 618 | GLU |
| 1 | I | 633 | ARG |
| 1 | I | 637 | ARG |
| 1 | I | 644 | PHE |
| 1 | I | 667 | ARG |
| 1 | I | 675 | LEU |
| 1 | I | 684 | LEU |
| 1 | I | 687 | ILE |
| 1 | I | 692 | LEU |
| 1 | I | 693 | GLU |
| 1 | I | 702 | ASP |
| 1 | I | 708 | ARG |
| 1 | I | 716 | SER |
| 1 | I | 723 | ASN |
| 1 | I | 736 | SER |
| 1 | I | 737 | VAL |
| 1 | I | 738 | LEU |
| 1 | I | 739 | ASN |
| 1 | I | 747 | LEU |
| 1 | I | 755 | GLU |
| 1 | I | 759 | ARG |
| 1 | I | 764 | ARG |
| 1 | I | 766 | LEU |
| 1 | I | 779 | ARG |
| 1 | I | 781 | PHE |
| 1 | I | 787 | ARG |
| 1 | I | 823 | LEU |
| 1 | I | 831 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 841 | LEU |
| 1 | I | 844 | GLU |
| 1 | I | 864 | LYS |
| 1 | I | 876 | VAL |
| 2 | M | 13 | LEU |
| 2 | M | 18 | LYS |
| 2 | M | 28 | ILE |
| 2 | M | 29 | VAL |
| 2 | M | 31 | ASP |
| 2 | M | 34 | ASN |
| 2 | M | 39 | LYS |
| 2 | M | 40 | GLU |
| 2 | M | 42 | ILE |
| 2 | M | 44 | THR |
| 2 | M | 45 | ARG |
| 2 | M | 46 | ASP |
| 2 | M | 53 | ASP |
| 2 | M | 57 | LYS |
| 2 | M | 61 | GLU |
| 2 | M | 70 | ILE |
| 2 | M | 73 | VAL |
| 2 | M | 78 | VAL |
| 2 | M | 83 | THR |
| 2 | M | 84 | GLN |
| 2 | M | 85 | MET |
| 2 | M | 102 | LEU |
| 2 | M | 104 | LEU |
| 2 | M | 106 | ARG |
| 2 | M | 107 | LEU |
| 2 | M | 116 | VAL |
| 2 | M | 127 | THR |
| 2 | M | 128 | ASP |
| 2 | M | 129 | GLU |
| 2 | M | 130 | TYR |
| 2 | M | 132 | ARG |
| 2 | M | 135 | ASP |
| 2 | M | 143 | LYS |
| 2 | M | 147 | THR |
| 2 | M | 156 | THR |
| 2 | M | 157 | SER |
| 2 | M | 159 | ASP |
| 2 | M | 160 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | M | 163 | MET |
| 2 | M | 165 | ILE |
| 2 | M | 171 | ASN |
| 2 | M | 173 | MET |
| 2 | M | 174 | LEU |
| 2 | M | 176 | ASP |
| 2 | M | 179 | VAL |
| 2 | M | 188 | ILE |
| 2 | M | 190 | ARG |
| 2 | M | 212 | ASN |
| 2 | M | 213 | ILE |
| 2 | M | 214 | ASP |
| 2 | M | 229 | THR |
| 2 | M | 231 | ILE |
| 2 | M | 235 | LYS |
| 2 | M | 239 | ARG |
| 2 | M | 247 | ASP |
| 2 | M | 250 | ILE |
| 2 | M | 251 | ILE |
| 2 | M | 254 | ASP |
| 2 | M | 267 | VAL |
| 2 | M | 275 | ASN |
| 2 | M | 276 | ASN |
| 2 | M | 277 | ILE |
| 2 | M | 278 | ARG |
| 2 | M | 280 | ILE |
| 2 | M | 303 | GLU |
| 2 | M | 306 | LEU |
| 2 | M | 308 | VAL |
| 2 | M | 309 | ASP |
| 2 | M | 311 | ARG |
| 2 | M | 313 | ILE |
| 2 | M | 315 | LEU |
| 2 | M | 316 | ILE |
| 2 | M | 322 | ARG |
| 2 | M | 325 | ILE |
| 2 | M | 327 | ARG |
| 2 | M | 329 | ILE |
| 2 | M | 335 | THR |
| 2 | M | 338 | LYS |
| 2 | M | 339 | ASN |
| 2 | M | 344 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | M | 351 | VAL |
| 2 | M | 355 | LEU |
| 2 | M | 369 | VAL |
| 2 | M | 370 | VAL |
| 2 | M | 375 | ILE |
| 2 | M | 379 | ILE |
| 2 | M | 380 | LYS |
| 2 | M | 381 | LEU |
| 2 | M | 386 | VAL |
| 2 | M | 387 | GLU |
| 2 | M | 389 | THR |
| 2 | M | 391 | ARG |
| 3 | J | 5 | LEU |
| 3 | J | 6 | THR |
| 3 | J | 8 | ASP |
| 3 | J | 20 | SER |
| 3 | J | 23 | LEU |
| 3 | J | 30 | SER |
| 3 | J | 33 | ASP |
| 3 | J | 51 | THR |
| 3 | J | 56 | LEU |
| 3 | J | 64 | ARG |
| 3 | J | 65 | ILE |
| 3 | J | 70 | VAL |
| 3 | J | 72 | GLU |
| 3 | J | 75 | ARG |
| 3 | J | 80 | ILE |
| 3 | J | 105 | ASN |
| 3 | J | 108 | GLU |
| 3 | J | 113 | GLU |
| 3 | J | 118 | ASP |
| 3 | J | 155 | ASN |
| 3 | J | 159 | ARG |
| 3 | J | 163 | THR |
| 3 | J | 179 | THR |
| 3 | J | 182 | ASN |
| 3 | J | 183 | ILE |
| 3 | J | 193 | THR |
| 3 | J | 196 | TYR |
| 3 | J | 203 | GLU |
| 3 | J | 207 | ASP |
| 3 | J | 221 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | J | 227 | MET |
| 3 | J | 234 | THR |
| 3 | J | 245 | ASP |
| 3 | J | 282 | ARG |
| 3 | J | 296 | TYR |
| 3 | J | 322 | VAL |
| 3 | J | 327 | LEU |
| 3 | J | 335 | LYS |
| 3 | J | 348 | ASP |
| 3 | J | 361 | PHE |
| 3 | J | 367 | TYR |
| 3 | J | 369 | LEU |
| 3 | J | 371 | LYS |
| 3 | J | 378 | LYS |
| 3 | J | 391 | THR |
| 3 | J | 394 | ILE |
| 3 | J | 395 | ARG |
| 3 | J | 402 | ASN |
| 3 | J | 404 | VAL |
| 3 | J | 407 | ARG |
| 3 | J | 416 | ARG |
| 3 | J | 418 | ASN |
| 3 | J | 421 | SER |
| 3 | J | 432 | SER |
| 3 | J | 444 | ASP |
| 3 | J | 448 | THR |
| 3 | J | 453 | MET |
| 3 | J | 457 | GLU |
| 3 | J | 467 | VAL |
| 3 | J | 468 | LYS |
| 3 | J | 469 | ASN |
| 3 | J | 476 | ILE |
| 3 | J | 478 | VAL |
| 3 | J | 484 | ILE |
| 3 | J | 486 | GLU |
| 3 | J | 488 | THR |
| 3 | J | 497 | VAL |
| 3 | J | 498 | GLU |
| 3 | J | 518 | SER |
| 3 | J | 530 | TYR |
| 3 | J | 531 | GLN |
| 3 | J | 544 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | J | 549 | ILE |
| 3 | J | 551 | ASP |
| 3 | J | 564 | ASN |
| 3 | J | 570 | CYS |
| 3 | J | 572 | SER |
| 3 | J | 576 | ARG |
| 3 | J | 588 | LEU |
| 3 | J | 594 | ILE |
| 3 | J | 603 | THR |
| 3 | J | 606 | ASP |
| 3 | J | 607 | LEU |
| 3 | J | 608 | VAL |
| 3 | J | 626 | VAL |
| 3 | J | 628 | LEU |
| 3 | J | 634 | THR |
| 3 | J | 638 | THR |
| 3 | J | 640 | LEU |
| 3 | J | 643 | TRP |
| 3 | J | 650 | ILE |
| 3 | J | 655 | ILE |
| 3 | J | 659 | GLU |
| 3 | J | 669 | GLN |
| 3 | J | 685 | GLN |
| 3 | J | 686 | LEU |
| 3 | J | 687 | ARG |
| 3 | J | 688 | THR |
| 3 | J | 689 | ASP |
| 3 | J | 691 | ARG |
| 3 | J | 702 | LEU |
| 3 | J | 705 | THR |
| 3 | J | 708 | LEU |
| 3 | J | 710 | ILE |
| 3 | J | 714 | THR |
| 3 | J | 720 | ASN |
| 3 | J | 727 | MET |
| 3 | J | 739 | ILE |
| 3 | J | 741 | ASN |
| 3 | J | 752 | SER |
| 3 | J | 757 | LEU |
| 3 | J | 765 | TYR |
| 3 | J | 770 | GLU |
| 3 | J | 780 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | J | 781 | ARG |
| 3 | J | 789 | TYR |
| 3 | J | 794 | ASP |
| 3 | J | 800 | PRO |
| 3 | J | 814 | VAL |
| 3 | J | 839 | THR |
| 3 | J | 843 | GLU |
| 3 | J | 846 | ILE |
| 3 | J | 855 | THR |
| 3 | J | 867 | ARG |
| 3 | J | 871 | ILE |
| 3 | J | 887 | VAL |
| 3 | J | 890 | MET |
| 3 | J | 891 | LEU |
| 3 | J | 895 | VAL |
| 3 | J | 910 | LEU |
| 3 | J | 911 | ASN |
| 3 | J | 915 | LEU |
| 3 | J | 919 | MET |
| 3 | J | 923 | GLN |
| 3 | J | 924 | ILE |
| 3 | J | 926 | GLU |
| 3 | J | 931 | LYS |
| 3 | J | 940 | VAL |
| 3 | J | 941 | ASP |
| 3 | J | 945 | PHE |
| 3 | J | 946 | TYR |
| 3 | J | 950 | ILE |
| 3 | J | 951 | GLU |
| 3 | J | 957 | ILE |
| 3 | J | 967 | THR |
| 3 | J | 975 | THR |
| 3 | J | 982 | ARG |
| 3 | J | 985 | PHE |
| 3 | J | 991 | GLN |
| 3 | J | 992 | LYS |
| 3 | J | 1004 | ARG |
| 3 | J | 1012 | LEU |
| 3 | J | 1018 | GLU |
| 3 | J | 1026 | LEU |
| 3 | J | 1030 | GLU |
| 3 | J | 1035 | CYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | J | 1045 | LEU |
| 3 | J | 1049 | LEU |
| 3 | J | 1050 | LEU |
| 3 | J | 1067 | ILE |
| 3 | J | 1078 | VAL |
| 3 | J | 1079 | CYS |
| 3 | J | 1108 | ILE |
| 3 | J | 1109 | ILE |
| 3 | J | 1113 | LEU |
| 3 | J | 1115 | LEU |
| 4 | O | 29 | ARG |
| 4 | O | 56 | GLU |
| 4 | O | 57 | ILE |
| 4 | O | 68 | MET |
| 4 | O | 89 | CYS |
| 4 | O | 113 | ASP |
| 4 | O | 132 | LEU |
| 4 | O | 135 | THR |
| 4 | O | 136 | ASN |
| 4 | O | 155 | LYS |
| 4 | O | 161 | LEU |
| 4 | O | 162 | SER |
| 4 | O | 165 | ARG |
| 4 | O | 170 | VAL |
| 4 | O | 180 | VAL |
| 4 | O | 195 | LEU |
| 4 | O | 201 | LEU |
| 4 | O | 204 | THR |
| 4 | O | 214 | ASN |
| 4 | O | 218 | ARG |
| 5 | Q | 4 | LEU |
| 5 | Q | 5 | ILE |
| 5 | Q | 17 | GLU |
| 5 | Q | 18 | PHE |
| 5 | Q | 22 | LEU |
| 5 | Q | 25 | ILE |
| 5 | Q | 27 | LEU |
| 5 | Q | 30 | LEU |
| 5 | Q | 32 | GLN |
| 5 | Q | 33 | GLN |
| 5 | Q | 38 | ILE |
| 5 | Q | 40 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | Q | 42 | LEU |
| 5 | Q | 48 | ILE |
| 5 | Q | 49 | LEU |
| 5 | Q | 51 | VAL |
| 5 | Q | 58 | ILE |
| 5 | Q | 60 | VAL |
| 5 | Q | 69 | GLU |
| 5 | Q | 76 | THR |
| 5 | Q | 85 | VAL |
| 5 | Q | 104 | MET |
| 5 | Q | 107 | LEU |
| 5 | Q | 110 | ILE |
| 5 | Q | 126 | ILE |
| 5 | Q | 127 | ILE |
| 5 | Q | 140 | ASP |
| 5 | Q | 149 | VAL |
| 5 | Q | 152 | THR |
| 5 | Q | 174 | TRP |
| 5 | Q | 175 | ILE |
| 5 | Q | 176 | THR |
| 5 | Q | 177 | GLN |
| 6 | R | 6 | ILE |
| 6 | R | 9 | GLU |
| 6 | R | 25 | ILE |
| 6 | R | 34 | LEU |
| 6 | R | 44 | VAL |
| 6 | R | 45 | GLU |
| 6 | R | 59 | LEU |
| 6 | R | 64 | SER |
| 6 | R | 67 | ASP |
| 6 | R | 87 | LEU |
| 7 | S | 10 | ILE |
| 7 | S | 23 | LEU |
| 7 | S | 25 | ASN |
| 7 | S | 27 | SER |
| 7 | S | 32 | SER |
| 7 | S | 33 | CYS |
| 7 | S | 34 | ASN |
| 7 | S | 39 | SER |
| 7 | S | 40 | PHE |
| 7 | S | 42 | ILE |
| 7 | S | 48 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | S | 62 | ASN |
| 7 | S | 68 | HIS |
| 7 | S | 69 | ASP |
| 7 | S | 77 | ILE |
| 7 | S | 79 | THR |
| 7 | S | 86 | LEU |
| 7 | S | 90 | ASN |
| 7 | S | 95 | ILE |
| 7 | S | 102 | LEU |
| 7 | S | 104 | LYS |
| 7 | S | 110 | GLU |
| 7 | S | 116 | SER |
| 8 | T | 12 | ARG |
| 8 | T | 19 | LYS |
| 8 | T | 25 | ILE |
| 8 | T | 30 | LYS |
| 8 | T | 37 | ILE |
| 8 | T | 38 | ARG |
| 8 | T | 42 | LEU |
| 8 | T | 44 | TRP |
| 8 | T | 46 | ARG |
| 8 | T | 62 | ILE |
| 8 | T | 70 | GLN |
| 8 | T | 72 | TYR |
| 8 | T | 81 | VAL |
| 9 | U | 14 | HIS |
| 9 | U | 15 | PHE |
| 9 | U | 23 | TRP |
| 9 | U | 26 | ARG |
| 9 | U | 29 | ARG |
| 9 | U | 37 | SER |
| 9 | U | 41 | LEU |
| 9 | U | 42 | GLN |
| 9 | U | 51 | ILE |
| 9 | U | 52 | ASP |
| 9 | U | 62 | ILE |
| 9 | U | 67 | GLU |
| 9 | U | 70 | ARG |
| 9 | U | 71 | ARG |
| 9 | U | 74 | LEU |
| 9 | U | 76 | ILE |
| 9 | U | 81 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | U | 88 | ILE |
| 9 | U | 89 | LEU |
| 9 | U | 90 | LEU |
| 9 | U | 91 | SER |
| 9 | U | 92 | LEU |
| 10 | V | 6 | LEU |
| 10 | V | 9 | GLU |
| 10 | V | 10 | SER |
| 10 | V | 14 | GLU |
| 10 | V | 16 | GLU |
| 10 | V | 24 | LEU |
| 10 | V | 38 | VAL |
| 10 | V | 43 | TYR |
| 10 | V | 47 | HIS |
| 10 | V | 49 | LEU |
| 10 | V | 54 | ILE |
| 10 | V | 63 | ILE |
| 10 | V | 64 | THR |
| 10 | V | 70 | LEU |
| 10 | V | 73 | ILE |
| 10 | V | 77 | ARG |
| 10 | V | 79 | MET |
| 10 | V | 92 | LYS |
| 11 | W | 3 | ILE |
| 11 | W | 5 | ILE |
| 11 | W | 10 | CYS |
| 11 | W | 13 | LEU |
| 11 | W | 22 | ILE |
| 11 | W | 40 | VAL |
| 11 | W | 42 | ARG |
| 11 | W | 48 | MET |
| 11 | W | 55 | ILE |
| 11 | W | 64 | ARG |
| 12 | X | 10 | TRP |
| 12 | X | 21 | LEU |
| 12 | X | 24 | VAL |
| 12 | X | 31 | TYR |
| 12 | X | 34 | ILE |
| 12 | X | 35 | PHE |
| 12 | X | 46 | LYS |
| 13 | Z | 41 | ILE |
| 13 | Z | 54 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | Z | 55 | LEU |
| 13 | Z | 56 | ASN |
| 13 | Z | 60 | THR |
| 13 | Z | 66 | LYS |
| 13 | Z | 69 | GLU |
| 13 | Z | 70 | ASP |
| 13 | Z | 82 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 56 | GLN |
| 1 | A | 63 | ASN |
| 1 | A | 119 | ASN |
| 1 | A | 259 | GLN |
| 1 | A | 312 | ASN |
| 1 | A | 331 | ASN |
| 1 | A | 367 | ASN |
| 1 | A | 420 | ASN |
| 1 | A | 422 | GLN |
| 1 | A | 446 | ASN |
| 1 | A | 465 | HIS |
| 1 | A | 483 | HIS |
| 1 | A | 485 | ASN |
| 1 | A | 561 | ASN |
| 1 | A | 567 | ASN |
| 1 | A | 590 | ASN |
| 1 | A | 677 | GLN |
| 1 | A | 723 | ASN |
| 2 | C | 38 | ASN |
| 2 | C | 207 | ASN |
| 2 | C | 209 | ASN |
| 2 | C | 275 | ASN |
| 2 | C | 276 | ASN |
| 2 | C | 328 | GLN |
| 3 | B | 27 | HIS |
| 3 | B | 40 | GLN |
| 3 | B | 164 | GLN |
| 3 | B | 182 | ASN |
| 3 | B | 300 | HIS |
| 3 | B | 368 | GLN |
| 3 | B | 412 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | B | 418 | ASN |
| 3 | B | 439 | ASN |
| 3 | B | 446 | HIS |
| 3 | B | 449 | GLN |
| 3 | B | 554 | ASN |
| 3 | B | 569 | ASN |
| 3 | B | 610 | GLN |
| 3 | B | 623 | ASN |
| 3 | B | 637 | HIS |
| 3 | B | 639 | HIS |
| 3 | B | 660 | HIS |
| 3 | B | 669 | GLN |
| 3 | B | 685 | GLN |
| 3 | B | 715 | ASN |
| 3 | B | 721 | ASN |
| 3 | B | 911 | ASN |
| 3 | B | 913 | HIS |
| 3 | B | 991 | GLN |
| 3 | B | 1015 | GLN |
| 3 | B | 1052 | ASN |
| 3 | B | 1087 | ASN |
| 5 | E | 16 | ASN |
| 5 | E | 33 | GLN |
| 5 | E | 109 | HIS |
| 5 | E | 112 | GLN |
| 6 | F | 61 | ASN |
| 7 | G | 88 | ASN |
| 8 | H | 20 | HIS |
| 9 | K | 42 | GLN |
| 9 | K | 54 | ASN |
| 10 | L | 22 | HIS |
| 11 | N | 19 | GLN |
| 11 | N | 57 | ASN |
| 1 | I | 5 | ASN |
| 1 | I | 56 | GLN |
| 1 | I | 63 | ASN |
| 1 | I | 119 | ASN |
| 1 | I | 259 | GLN |
| 1 | I | 312 | ASN |
| 1 | I | 331 | ASN |
| 1 | I | 367 | ASN |
| 1 | I | 420 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 422 | GLN |
| 1 | I | 426 | HIS |
| 1 | I | 446 | ASN |
| 1 | I | 483 | HIS |
| 1 | I | 485 | ASN |
| 1 | I | 522 | GLN |
| 1 | I | 561 | ASN |
| 1 | I | 567 | ASN |
| 1 | I | 677 | GLN |
| 1 | I | 723 | ASN |
| 2 | M | 38 | ASN |
| 2 | M | 207 | ASN |
| 2 | M | 209 | ASN |
| 2 | M | 212 | ASN |
| 2 | M | 276 | ASN |
| 2 | M | 328 | GLN |
| 3 | J | 27 | HIS |
| 3 | J | 40 | GLN |
| 3 | J | 106 | ASN |
| 3 | J | 182 | ASN |
| 3 | J | 300 | HIS |
| 3 | J | 368 | GLN |
| 3 | J | 412 | GLN |
| 3 | J | 418 | ASN |
| 3 | J | 439 | ASN |
| 3 | J | 446 | HIS |
| 3 | J | 449 | GLN |
| 3 | J | 531 | GLN |
| 3 | J | 554 | ASN |
| 3 | J | 567 | HIS |
| 3 | J | 569 | ASN |
| 3 | J | 610 | GLN |
| 3 | J | 623 | ASN |
| 3 | J | 637 | HIS |
| 3 | J | 639 | HIS |
| 3 | J | 660 | HIS |
| 3 | J | 669 | GLN |
| 3 | J | 685 | GLN |
| 3 | J | 715 | ASN |
| 3 | J | 720 | ASN |
| 3 | J | 721 | ASN |
| 3 | J | 911 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | J | 913 | HIS |
| 3 | J | 954 | GLN |
| 3 | J | 1015 | GLN |
| 3 | J | 1052 | ASN |
| 5 | Q | 33 | GLN |
| 5 | Q | 109 | HIS |
| 5 | Q | 112 | GLN |
| 5 | Q | 177 | GLN |
| 6 | R | 53 | GLN |
| 7 | S | 88 | ASN |
| 7 | S | 117 | GLN |
| 8 | T | 20 | HIS |
| 8 | T | 70 | GLN |
| 9 | U | 14 | HIS |
| 9 | U | 42 | GLN |
| 9 | U | 54 | ASN |
| 9 | U | 84 | ASN |
| 11 | W | 19 | GLN |
| 11 | W | 57 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 16 | F3S | D | 1001 | 4 | 0,9,9 | 0.00 | - | 0,15,15 | 0.00 | - |
| 16 | F3S | O | 1001 | - | 0,9,9 | 0.00 | - | 0,15,15 | 0.00 | - |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 16 | F3S | D | 1001 | 4 | - | 0/0/24/24 | 0/0/3/3 |
| 16 | F3S | O | 1001 | - | - | 0/0/24/24 | 0/0/3/3 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 16 | D | 1001 | F3S | 1 | 0 |
| 16 | O | 1001 | F3S | 6 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 836/880 (95%) | -0.16 | 10 (1%) 79 75 | 28, 71, 105, 133 | 0 |
| 1 | I | 836/880 (95%) | -0.17 | 15 (1%) 69 64 | 28, 71, 106, 133 | 0 |
| 2 | C | 370/395 (93%) | 0.18 | 23 (6%) 21 20 | 37, 78, 130, 138 | 0 |
| 2 | M | 370/395 (93%) | 0.07 | 16 (4%) 36 33 | 38, 79, 130, 138 | 0 |
| 3 | B | 1090/1124 (96%) | -0.14 | 18 (1%) 70 66 | 33, 66, 117, 149 | 0 |
| 3 | J | 1090/1124 (96%) | -0.13 | 24 (2%) 62 57 | 33, 67, 117, 149 | 0 |
| 4 | D | 264/265 (99%) | 0.08 | 10 (3%) 41 37 | 57, 86, 121, 139 | 0 |
| 4 | O | 264/265 (99%) | 0.19 | 15 (5%) 24 23 | 57, 86, 121, 139 | 0 |
| 5 | E | 176/180 (97%) | 0.17 | 7 (3%) 39 35 | 58, 98, 140, 143 | 0 |
| 5 | Q | 176/180 (97%) | 0.23 | 14 (7%) 13 13 | 58, 98, 139, 142 | 0 |
| 6 | F | 89/113 (78%) | 0.24 | 9 (10%) 8 8 | 100, 127, 132, 133 | 0 |
| 6 | R | 89/113 (78%) | 0.21 | 3 (3%) 46 41 | 100, 127, 132, 133 | 0 |
| 7 | G | 113/132 (85%) | 0.16 | 4 (3%) 44 40 | 65, 88, 108, 112 | 0 |
| 7 | S | 113/132 (85%) | 0.10 | 3 (2%) 55 51 | 66, 88, 108, 112 | 0 |
| 8 | H | 74/84 (88%) | -0.13 | 0 100 100 | 66, 81, 99, 102 | 0 |
| 8 | T | 74/84 (88%) | -0.18 | 1 (1%) 75 71 | 66, 81, 99, 102 | 0 |
| 9 | K | 82/95 (86%) | -0.40 | 1 (1%) 79 75 | 41, 57, 86, 94 | 0 |
| 9 | U | 82/95 (86%) | -0.33 | 1 (1%) 79 75 | 43, 58, 87, 93 | 0 |
| 10 | L | 92/92 (100%) | -0.12 | 1 (1%) 80 76 | 53, 73, 103, 107 | 0 |
| 10 | V | 92/92 (100%) | -0.02 | 1 (1%) 80 76 | 54, 73, 103, 107 | 0 |
| 11 | N | 64/66 (96%) | -0.12 | 1 (1%) 72 67 | 62, 80, 103, 124 | 0 |
| 11 | W | 64/66 (96%) | -0.06 | 1 (1%) 72 67 | 62, 80, 103, 124 | 0 |
| 12 | P | 43/48 (89%) | 0.07 | 1 (2%) 61 56 | 66, 89, 103, 110 | 0 |
| 12 | X | 43/48 (89%) | -0.10 | 2 (4%) 32 30 | 66, 89, 103, 110 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13 | Y | 45/104 (43%) | 0.59 | 6 (13%) 4 4 | 98, 108, 124, 125 | 0 |
| 13 | Z | 45/104 (43%) | 0.75 | 6 (13%) 4 4 | 98, 108, 124, 124 | 0 |
| All | All | 6676/7156 (93%) | -0.05 | 193 (2%) 52 48 | 28, 76, 127, 149 | 0 |

All (193) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | J | 278 | ILE | 7.3 |
| 6 | R | 89 | MET | 5.3 |
| 2 | C | 213 | ILE | 5.1 |
| 3 | B | 434 | ALA | 4.9 |
| 5 | E | 135 | VAL | 4.7 |
| 13 | Y | 82 | ARG | 4.7 |
| 1 | A | 60 | THR | 4.7 |
| 5 | E | 131 | LYS | 4.6 |
| 4 | O | 188 | PHE | 4.5 |
| 3 | B | 1069 | TRP | 4.4 |
| 5 | Q | 153 | VAL | 4.4 |
| 5 | E | 180 | LYS | 4.4 |
| 5 | E | 128 | PHE | 4.3 |
| 2 | C | 214 | ASP | 4.3 |
| 7 | G | 5 | VAL | 4.1 |
| 2 | M | 213 | ILE | 4.0 |
| 1 | I | 148 | HIS | 3.9 |
| 3 | J | 279 | GLY | 3.9 |
| 2 | C | 235 | LYS | 3.9 |
| 13 | Y | 81 | ARG | 3.8 |
| 3 | J | 244 | LEU | 3.8 |
| 4 | O | 217 | ILE | 3.8 |
| 2 | C | 180 | THR | 3.7 |
| 3 | B | 600 | GLY | 3.6 |
| 1 | A | 132 | LEU | 3.6 |
| 1 | I | 147 | PRO | 3.6 |
| 2 | M | 180 | THR | 3.6 |
| 2 | C | 234 | ILE | 3.6 |
| 4 | O | 171 | GLU | 3.5 |
| 3 | J | 194 | ALA | 3.5 |
| 4 | D | 217 | ILE | 3.5 |
| 3 | J | 831 | ALA | 3.5 |
| 5 | Q | 178 | THR | 3.4 |
| 3 | J | 277 | ALA | 3.4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | I | 294 | PRO | 3.4 |
| 13 | Z | 38 | ILE | 3.4 |
| 3 | J | 434 | ALA | 3.4 |
| 1 | I | 149 | CYS | 3.4 |
| 4 | O | 197 | VAL | 3.3 |
| 9 | K | 51 | ILE | 3.3 |
| 2 | M | 235 | LYS | 3.3 |
| 4 | O | 172 | ILE | 3.3 |
| 5 | Q | 175 | ILE | 3.3 |
| 4 | O | 175 | ASN | 3.3 |
| 4 | D | 190 | LEU | 3.3 |
| 5 | Q | 177 | GLN | 3.3 |
| 3 | B | 625 | TYR | 3.2 |
| 7 | S | 6 | ALA | 3.2 |
| 3 | J | 781 | ARG | 3.2 |
| 6 | F | 45 | GLU | 3.2 |
| 5 | Q | 152 | THR | 3.2 |
| 2 | C | 211 | ALA | 3.2 |
| 6 | R | 2 | SER | 3.1 |
| 3 | J | 1077 | TYR | 3.1 |
| 5 | Q | 179 | LYS | 3.1 |
| 5 | E | 132 | SER | 3.1 |
| 2 | M | 190 | ARG | 3.1 |
| 1 | A | 147 | PRO | 3.1 |
| 4 | O | 193 | GLY | 3.1 |
| 3 | J | 600 | GLY | 3.0 |
| 3 | J | 557 | HIS | 3.0 |
| 4 | O | 173 | LEU | 3.0 |
| 3 | J | 601 | ALA | 3.0 |
| 1 | A | 255 | ALA | 3.0 |
| 1 | I | 390 | TYR | 3.0 |
| 5 | Q | 135 | VAL | 3.0 |
| 4 | O | 170 | VAL | 3.0 |
| 4 | D | 175 | ASN | 2.9 |
| 3 | B | 557 | HIS | 2.9 |
| 3 | J | 271 | PHE | 2.9 |
| 3 | B | 264 | ASN | 2.9 |
| 2 | C | 262 | LEU | 2.9 |
| 2 | M | 160 | ILE | 2.9 |
| 2 | C | 220 | PHE | 2.9 |
| 5 | Q | 170 | GLY | 2.9 |
| 1 | I | 132 | LEU | 2.9 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | C | 212 | ASN | 2.9 |
| 3 | J | 1069 | TRP | 2.9 |
| 1 | A | 266 | TRP | 2.8 |
| 8 | T | 57 | ALA | 2.8 |
| 3 | J | 771 | ASP | 2.8 |
| 7 | S | 73 | GLY | 2.8 |
| 6 | F | 62 | ILE | 2.8 |
| 1 | I | 4 | LYS | 2.8 |
| 2 | M | 191 | LEU | 2.8 |
| 4 | O | 264 | VAL | 2.8 |
| 1 | I | 808 | ASP | 2.8 |
| 1 | I | 255 | ALA | 2.8 |
| 3 | B | 597 | LEU | 2.8 |
| 3 | J | 597 | LEU | 2.8 |
| 2 | M | 169 | LEU | 2.8 |
| 3 | B | 634 | THR | 2.8 |
| 4 | D | 188 | PHE | 2.8 |
| 1 | I | 60 | THR | 2.7 |
| 1 | I | 811 | VAL | 2.7 |
| 1 | A | 4 | LYS | 2.7 |
| 4 | D | 181 | ASN | 2.7 |
| 4 | D | 187 | VAL | 2.7 |
| 5 | E | 127 | ILE | 2.7 |
| 7 | S | 80 | GLU | 2.6 |
| 5 | Q | 58 | ILE | 2.6 |
| 2 | M | 168 | GLN | 2.6 |
| 6 | F | 1 | MET | 2.6 |
| 2 | C | 191 | LEU | 2.6 |
| 11 | W | 21 | PHE | 2.6 |
| 3 | J | 596 | LYS | 2.6 |
| 2 | M | 206 | LEU | 2.6 |
| 5 | Q | 180 | LYS | 2.5 |
| 3 | J | 602 | ILE | 2.5 |
| 2 | C | 151 | ASN | 2.5 |
| 2 | C | 237 | ILE | 2.5 |
| 13 | Y | 41 | ILE | 2.5 |
| 1 | I | 807 | VAL | 2.5 |
| 13 | Z | 41 | ILE | 2.5 |
| 11 | N | 27 | ALA | 2.5 |
| 6 | F | 2 | SER | 2.5 |
| 3 | B | 1078 | VAL | 2.5 |
| 1 | A | 808 | ASP | 2.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 13 | Z | 39 | GLN | 2.5 |
| 7 | G | 80 | GLU | 2.5 |
| 5 | Q | 129 | GLY | 2.5 |
| 3 | B | 279 | GLY | 2.4 |
| 2 | C | 201 | SER | 2.4 |
| 2 | C | 196 | PHE | 2.4 |
| 1 | A | 251 | GLU | 2.4 |
| 2 | C | 161 | ALA | 2.4 |
| 4 | O | 174 | ALA | 2.4 |
| 1 | I | 10 | LYS | 2.4 |
| 2 | C | 210 | PHE | 2.4 |
| 2 | C | 263 | SER | 2.4 |
| 2 | C | 217 | ALA | 2.4 |
| 12 | X | 34 | ILE | 2.3 |
| 4 | D | 189 | GLU | 2.3 |
| 13 | Y | 80 | SER | 2.3 |
| 5 | E | 178 | THR | 2.3 |
| 5 | Q | 117 | THR | 2.3 |
| 13 | Y | 48 | THR | 2.3 |
| 4 | O | 213 | CYS | 2.3 |
| 5 | Q | 171 | LYS | 2.3 |
| 12 | X | 30 | GLY | 2.3 |
| 10 | V | 3 | ILE | 2.3 |
| 2 | M | 167 | LEU | 2.3 |
| 7 | G | 6 | ALA | 2.3 |
| 7 | G | 114 | ARG | 2.2 |
| 3 | J | 792 | LEU | 2.2 |
| 4 | D | 88 | ASN | 2.2 |
| 3 | J | 280 | GLN | 2.2 |
| 5 | Q | 174 | TRP | 2.2 |
| 6 | F | 89 | MET | 2.2 |
| 3 | B | 766 | PRO | 2.2 |
| 3 | B | 182 | ASN | 2.2 |
| 3 | B | 948 | THR | 2.2 |
| 13 | Z | 56 | ASN | 2.2 |
| 1 | A | 807 | VAL | 2.2 |
| 4 | D | 186 | GLY | 2.2 |
| 2 | M | 161 | ALA | 2.2 |
| 13 | Y | 39 | GLN | 2.2 |
| 1 | I | 296 | ARG | 2.2 |
| 3 | B | 592 | GLU | 2.2 |
| 4 | O | 142 | GLU | 2.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 683 | GLU | 2.2 |
| 4 | O | 212 | TYR | 2.1 |
| 6 | F | 33 | LEU | 2.1 |
| 10 | L | 15 | LEU | 2.1 |
| 4 | O | 196 | SER | 2.1 |
| 2 | M | 232 | LYS | 2.1 |
| 3 | B | 54 | PRO | 2.1 |
| 12 | P | 33 | ILE | 2.1 |
| 1 | I | 292 | GLY | 2.1 |
| 3 | J | 207 | ASP | 2.1 |
| 3 | J | 224 | VAL | 2.1 |
| 3 | J | 1082 | HIS | 2.1 |
| 13 | Z | 42 | GLU | 2.1 |
| 2 | M | 214 | ASP | 2.1 |
| 2 | M | 241 | ILE | 2.1 |
| 2 | C | 184 | VAL | 2.1 |
| 2 | C | 226 | ILE | 2.1 |
| 3 | J | 245 | ASP | 2.1 |
| 6 | F | 77 | PRO | 2.1 |
| 2 | C | 183 | ASP | 2.1 |
| 6 | F | 76 | CYS | 2.1 |
| 2 | M | 155 | SER | 2.1 |
| 2 | M | 212 | ASN | 2.1 |
| 4 | D | 264 | VAL | 2.0 |
| 2 | C | 215 | SER | 2.0 |
| 3 | B | 1071 | ASP | 2.0 |
| 9 | U | 87 | ILE | 2.0 |
| 6 | R | 32 | ASN | 2.0 |
| 6 | F | 4 | VAL | 2.0 |
| 2 | C | 186 | LYS | 2.0 |
| 13 | Z | 40 | ASP | 2.0 |
| 3 | B | 49 | ILE | 2.0 |
| 3 | B | 193 | THR | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 14 | ZN | I | 1001 | 1/1 | 0.99 | 0.12 | -1.27 | 57,57,57,57 | 0 |
| 14 | ZN | A | 1002 | 1/1 | 0.98 | 0.06 | -1.37 | 69,69,69,69 | 0 |
| 16 | F3S | D | 1001 | 7/7 | 0.99 | 0.10 | -1.39 | 79,81,82,84 | 0 |
| 14 | ZN | X | 1001 | 1/1 | 0.98 | 0.09 | -1.40 | 54,54,54,54 | 0 |
| 16 | F3S | O | 1001 | 7/7 | 0.99 | 0.07 | -1.41 | 104,105,106,106 | 0 |
| 14 | ZN | A | 1001 | 1/1 | 0.98 | 0.04 | -1.81 | 46,46,46,46 | 0 |
| 14 | ZN | I | 1002 | 1/1 | 0.96 | 0.06 | -1.91 | 78,78,78,78 | 0 |
| 14 | ZN | N | 1001 | 1/1 | 0.99 | 0.07 | -1.95 | 56,56,56,56 | 0 |
| 14 | ZN | P | 1001 | 1/1 | 0.98 | 0.05 | -1.98 | 33,33,33,33 | 0 |
| 14 | ZN | B | 2001 | 1/1 | 0.98 | 0.03 | -2.19 | 66,66,66,66 | 0 |
| 14 | ZN | J | 2001 | 1/1 | 0.99 | 0.03 | -2.35 | 124,124,124,124 | 0 |
| 14 | ZN | W | 1001 | 1/1 | 0.99 | 0.11 | -4.74 | 63,63,63,63 | 0 |
| 15 | MG | A | 1003 | 1/1 | 0.98 | 0.05 | - | 2,2,2,2 | 0 |
| 15 | MG | I | 1003 | 1/1 | 0.99 | 0.03 | - | 2,2,2,2 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.