



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 2, 2019 – 10:27 PM EST

PDB ID : 4V8L  
EMDB ID: : EMD-2238  
Title : Cryo-EM Structure of the Mycobacterial Fatty Acid Synthase  
Authors : Boehringer, D.; Ban, N.; Leibundgut, M.  
Deposited on : 2012-12-06  
Resolution : 7.50 Å(reported)  
Based on PDB ID : 2UV8

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

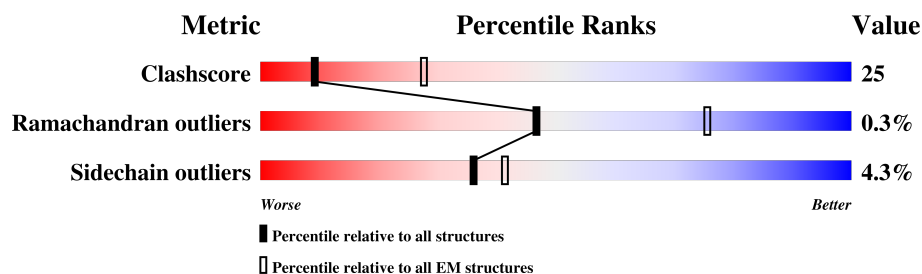
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.50 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<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 136327                      | 1886                        |
| Ramachandran outliers | 132723                      | 1663                        |
| Sidechain outliers    | 132532                      | 1531                        |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 3089   | 56% 33% • 9%     |
| 1   | B     | 3089   | 56% 33% • 9%     |
| 1   | C     | 3089   | 56% 33% • 9%     |
| 1   | D     | 3089   | 88% • 9%         |
| 1   | E     | 3089   | 88% • 9%         |
| 1   | F     | 3089   | 88% • 9%         |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 126306 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 FATTY ACID SYNTHASE.

| Mol | Chain | Residues | Atoms |       |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|----|---------|-------|
| 1   | D     | 2822     | Total | C     | N    | O    | S  | 0       | 0     |
|     |       |          | 21020 | 13294 | 3662 | 3998 | 66 |         |       |
| 1   | E     | 2822     | Total | C     | N    | O    | S  | 0       | 0     |
|     |       |          | 21020 | 13294 | 3662 | 3998 | 66 |         |       |
| 1   | F     | 2822     | Total | C     | N    | O    | S  | 0       | 0     |
|     |       |          | 21020 | 13294 | 3662 | 3998 | 66 |         |       |
| 1   | A     | 2822     | Total | C     | N    | O    | S  | 0       | 0     |
|     |       |          | 21020 | 13294 | 3662 | 3998 | 66 |         |       |
| 1   | B     | 2822     | Total | C     | N    | O    | S  | 0       | 0     |
|     |       |          | 21020 | 13294 | 3662 | 3998 | 66 |         |       |
| 1   | C     | 2822     | Total | C     | N    | O    | S  | 0       | 0     |
|     |       |          | 21020 | 13294 | 3662 | 3998 | 66 |         |       |

There are 1086 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| D     | 929     | UNK      | GLU    | conflict | UNP A0R1H7 |
| D     | 930     | UNK      | PRO    | conflict | UNP A0R1H7 |
| D     | 931     | UNK      | VAL    | conflict | UNP A0R1H7 |
| D     | 932     | UNK      | GLU    | conflict | UNP A0R1H7 |
| D     | 933     | UNK      | VAL    | conflict | UNP A0R1H7 |
| D     | 934     | UNK      | LEU    | conflict | UNP A0R1H7 |
| D     | 935     | UNK      | SER    | conflict | UNP A0R1H7 |
| D     | 936     | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 937     | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 938     | UNK      | GLN    | conflict | UNP A0R1H7 |
| D     | 939     | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 940     | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 941     | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 942     | UNK      | ASP    | conflict | UNP A0R1H7 |
| D     | 943     | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 944     | UNK      | SER    | conflict | UNP A0R1H7 |
| D     | 974     | UNK      | THR    | conflict | UNP A0R1H7 |
| D     | 975     | UNK      | GLU    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| D     | 976     | UNK      | TRP    | conflict | UNP A0R1H7 |
| D     | 977     | UNK      | GLN    | conflict | UNP A0R1H7 |
| D     | 978     | UNK      | VAL    | conflict | UNP A0R1H7 |
| D     | 979     | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 980     | UNK      | GLU    | conflict | UNP A0R1H7 |
| D     | 981     | UNK      | GLY    | conflict | UNP A0R1H7 |
| D     | 982     | UNK      | SER    | conflict | UNP A0R1H7 |
| D     | 983     | UNK      | ASP    | conflict | UNP A0R1H7 |
| D     | 984     | UNK      | ASN    | conflict | UNP A0R1H7 |
| D     | 985     | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 986     | UNK      | SER    | conflict | UNP A0R1H7 |
| D     | 987     | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 988     | UNK      | SER    | conflict | UNP A0R1H7 |
| D     | 989     | UNK      | HIS    | conflict | UNP A0R1H7 |
| D     | 990     | UNK      | PRO    | conflict | UNP A0R1H7 |
| D     | 991     | UNK      | SER    | conflict | UNP A0R1H7 |
| D     | 992     | UNK      | THR    | conflict | UNP A0R1H7 |
| D     | 993     | UNK      | GLY    | conflict | UNP A0R1H7 |
| D     | 994     | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 995     | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 996     | UNK      | LEU    | conflict | UNP A0R1H7 |
| D     | 997     | UNK      | GLU    | conflict | UNP A0R1H7 |
| D     | 998     | UNK      | VAL    | conflict | UNP A0R1H7 |
| D     | 999     | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 1000    | UNK      | ASP    | conflict | UNP A0R1H7 |
| D     | 1001    | UNK      | ASP    | conflict | UNP A0R1H7 |
| D     | 1002    | UNK      | GLN    | conflict | UNP A0R1H7 |
| D     | 1003    | UNK      | HIS    | conflict | UNP A0R1H7 |
| D     | 1004    | UNK      | VAL    | conflict | UNP A0R1H7 |
| D     | 1005    | UNK      | VAL    | conflict | UNP A0R1H7 |
| D     | 1006    | UNK      | LEU    | conflict | UNP A0R1H7 |
| D     | 1007    | UNK      | SER    | conflict | UNP A0R1H7 |
| D     | 1008    | UNK      | VAL    | conflict | UNP A0R1H7 |
| D     | 1009    | UNK      | PRO    | conflict | UNP A0R1H7 |
| D     | 1010    | UNK      | LEU    | conflict | UNP A0R1H7 |
| D     | 1011    | UNK      | SER    | conflict | UNP A0R1H7 |
| D     | 1012    | UNK      | GLY    | conflict | UNP A0R1H7 |
| D     | 1013    | UNK      | THR    | conflict | UNP A0R1H7 |
| D     | 1014    | UNK      | TRP    | conflict | UNP A0R1H7 |
| D     | 1196    | UNK      | GLY    | conflict | UNP A0R1H7 |
| D     | 1197    | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 1198    | UNK      | THR    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| D     | 1199    | UNK      | GLY    | conflict | UNP A0R1H7 |
| D     | 1200    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 1201    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 1202    | UNK      | GLU    | conflict | UNP A0R1H7 |
| D     | 1203    | UNK      | LEU    | conflict | UNP A0R1H7 |
| D     | 1204    | UNK      | THR    | conflict | UNP A0R1H7 |
| D     | 1205    | UNK      | ASP    | conflict | UNP A0R1H7 |
| D     | 1206    | UNK      | PRO    | conflict | UNP A0R1H7 |
| D     | 1207    | UNK      | VAL    | conflict | UNP A0R1H7 |
| D     | 1208    | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 1209    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 1210    | UNK      | GLY    | conflict | UNP A0R1H7 |
| D     | 1211    | UNK      | GLY    | conflict | UNP A0R1H7 |
| D     | 1212    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 1213    | UNK      | ILE    | conflict | UNP A0R1H7 |
| D     | 1214    | UNK      | SER    | conflict | UNP A0R1H7 |
| D     | 1215    | UNK      | ASP    | conflict | UNP A0R1H7 |
| D     | 1216    | UNK      | ASN    | conflict | UNP A0R1H7 |
| D     | 1217    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 1218    | UNK      | THR    | conflict | UNP A0R1H7 |
| D     | 1219    | UNK      | ASP    | conflict | UNP A0R1H7 |
| D     | 1220    | UNK      | THR    | conflict | UNP A0R1H7 |
| D     | 1221    | UNK      | PRO    | conflict | UNP A0R1H7 |
| D     | 1222    | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 1223    | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 1224    | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 1225    | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 1226    | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 1227    | UNK      | ASP    | conflict | UNP A0R1H7 |
| D     | 2076    | UNK      | GLY    | conflict | UNP A0R1H7 |
| D     | 2077    | UNK      | ASP    | conflict | UNP A0R1H7 |
| D     | 2078    | UNK      | ILE    | conflict | UNP A0R1H7 |
| D     | 2079    | UNK      | ASP    | conflict | UNP A0R1H7 |
| D     | 2080    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 2081    | UNK      | GLN    | conflict | UNP A0R1H7 |
| D     | 2082    | UNK      | TRP    | conflict | UNP A0R1H7 |
| D     | 2083    | UNK      | GLU    | conflict | UNP A0R1H7 |
| D     | 2084    | UNK      | GLN    | conflict | UNP A0R1H7 |
| D     | 2085    | UNK      | LEU    | conflict | UNP A0R1H7 |
| D     | 2086    | UNK      | SER    | conflict | UNP A0R1H7 |
| D     | 2087    | UNK      | GLN    | conflict | UNP A0R1H7 |
| D     | 2088    | UNK      | ARG    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| D     | 2089    | UNK      | PHE    | conflict | UNP A0R1H7 |
| D     | 2090    | UNK      | GLU    | conflict | UNP A0R1H7 |
| D     | 2091    | UNK      | GLY    | conflict | UNP A0R1H7 |
| D     | 2092    | UNK      | THR    | conflict | UNP A0R1H7 |
| D     | 2093    | UNK      | GLY    | conflict | UNP A0R1H7 |
| D     | 2094    | UNK      | HIS    | conflict | UNP A0R1H7 |
| D     | 2095    | UNK      | VAL    | conflict | UNP A0R1H7 |
| D     | 2096    | UNK      | VAL    | conflict | UNP A0R1H7 |
| D     | 2097    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 2098    | UNK      | THR    | conflict | UNP A0R1H7 |
| D     | 2099    | UNK      | GLN    | conflict | UNP A0R1H7 |
| D     | 2100    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 2101    | UNK      | ASN    | conflict | UNP A0R1H7 |
| D     | 2102    | UNK      | TRP    | conflict | UNP A0R1H7 |
| D     | 2103    | UNK      | TRP    | conflict | UNP A0R1H7 |
| D     | 2104    | UNK      | GLN    | conflict | UNP A0R1H7 |
| D     | 2105    | UNK      | GLY    | conflict | UNP A0R1H7 |
| D     | 2106    | UNK      | LYS    | conflict | UNP A0R1H7 |
| D     | 2107    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 2108    | UNK      | LEU    | conflict | UNP A0R1H7 |
| D     | 2109    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 2110    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 2111    | UNK      | GLY    | conflict | UNP A0R1H7 |
| D     | 2112    | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 2113    | UNK      | ASN    | conflict | UNP A0R1H7 |
| D     | 2114    | UNK      | VAL    | conflict | UNP A0R1H7 |
| D     | 2115    | UNK      | HIS    | conflict | UNP A0R1H7 |
| D     | 2116    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 2117    | UNK      | SER    | conflict | UNP A0R1H7 |
| D     | 2118    | UNK      | LEU    | conflict | UNP A0R1H7 |
| D     | 2119    | UNK      | PHE    | conflict | UNP A0R1H7 |
| D     | 2120    | UNK      | GLY    | conflict | UNP A0R1H7 |
| D     | 2121    | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 2122    | UNK      | ILE    | conflict | UNP A0R1H7 |
| D     | 2123    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 2124    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 2125    | UNK      | GLY    | conflict | UNP A0R1H7 |
| D     | 2126    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 2127    | UNK      | GLU    | conflict | UNP A0R1H7 |
| D     | 2128    | UNK      | ASN    | conflict | UNP A0R1H7 |
| D     | 2129    | UNK      | PRO    | conflict | UNP A0R1H7 |
| D     | 2130    | UNK      | GLY    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| D     | 2131    | UNK      | LYS    | conflict | UNP A0R1H7 |
| D     | 2132    | UNK      | GLY    | conflict | UNP A0R1H7 |
| D     | 2133    | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 2134    | UNK      | TYR    | conflict | UNP A0R1H7 |
| D     | 2135    | UNK      | SER    | conflict | UNP A0R1H7 |
| D     | 2422    | UNK      | GLU    | conflict | UNP A0R1H7 |
| D     | 2423    | UNK      | SER    | conflict | UNP A0R1H7 |
| D     | 2424    | UNK      | ASP    | conflict | UNP A0R1H7 |
| D     | 2425    | UNK      | ASP    | conflict | UNP A0R1H7 |
| D     | 2426    | UNK      | GLU    | conflict | UNP A0R1H7 |
| D     | 2427    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 2428    | UNK      | PRO    | conflict | UNP A0R1H7 |
| D     | 2429    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 2430    | UNK      | GLY    | conflict | UNP A0R1H7 |
| D     | 2431    | UNK      | THR    | conflict | UNP A0R1H7 |
| D     | 2432    | UNK      | ILE    | conflict | UNP A0R1H7 |
| D     | 2433    | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 2434    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 2435    | UNK      | LEU    | conflict | UNP A0R1H7 |
| D     | 2436    | UNK      | PRO    | conflict | UNP A0R1H7 |
| D     | 2437    | UNK      | SER    | conflict | UNP A0R1H7 |
| D     | 2438    | UNK      | PRO    | conflict | UNP A0R1H7 |
| D     | 2439    | UNK      | PRO    | conflict | UNP A0R1H7 |
| D     | 2440    | UNK      | ARG    | conflict | UNP A0R1H7 |
| D     | 2441    | UNK      | GLY    | conflict | UNP A0R1H7 |
| D     | 2442    | UNK      | TYR    | conflict | UNP A0R1H7 |
| D     | 2443    | UNK      | ASN    | conflict | UNP A0R1H7 |
| D     | 2444    | UNK      | PRO    | conflict | UNP A0R1H7 |
| D     | 2445    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 2446    | UNK      | PRO    | conflict | UNP A0R1H7 |
| D     | 2447    | UNK      | ALA    | conflict | UNP A0R1H7 |
| D     | 2448    | UNK      | PRO    | conflict | UNP A0R1H7 |
| D     | 2449    | UNK      | GLU    | conflict | UNP A0R1H7 |
| D     | 2450    | UNK      | TRP    | conflict | UNP A0R1H7 |
| D     | 2451    | UNK      | ASP    | conflict | UNP A0R1H7 |
| D     | 2452    | UNK      | ASP    | conflict | UNP A0R1H7 |
| D     | 2453    | UNK      | LEU    | conflict | UNP A0R1H7 |
| E     | 929     | UNK      | GLU    | conflict | UNP A0R1H7 |
| E     | 930     | UNK      | PRO    | conflict | UNP A0R1H7 |
| E     | 931     | UNK      | VAL    | conflict | UNP A0R1H7 |
| E     | 932     | UNK      | GLU    | conflict | UNP A0R1H7 |
| E     | 933     | UNK      | VAL    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| E     | 934     | UNK      | LEU    | conflict | UNP A0R1H7 |
| E     | 935     | UNK      | SER    | conflict | UNP A0R1H7 |
| E     | 936     | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 937     | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 938     | UNK      | GLN    | conflict | UNP A0R1H7 |
| E     | 939     | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 940     | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 941     | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 942     | UNK      | ASP    | conflict | UNP A0R1H7 |
| E     | 943     | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 944     | UNK      | SER    | conflict | UNP A0R1H7 |
| E     | 974     | UNK      | THR    | conflict | UNP A0R1H7 |
| E     | 975     | UNK      | GLU    | conflict | UNP A0R1H7 |
| E     | 976     | UNK      | TRP    | conflict | UNP A0R1H7 |
| E     | 977     | UNK      | GLN    | conflict | UNP A0R1H7 |
| E     | 978     | UNK      | VAL    | conflict | UNP A0R1H7 |
| E     | 979     | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 980     | UNK      | GLU    | conflict | UNP A0R1H7 |
| E     | 981     | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 982     | UNK      | SER    | conflict | UNP A0R1H7 |
| E     | 983     | UNK      | ASP    | conflict | UNP A0R1H7 |
| E     | 984     | UNK      | ASN    | conflict | UNP A0R1H7 |
| E     | 985     | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 986     | UNK      | SER    | conflict | UNP A0R1H7 |
| E     | 987     | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 988     | UNK      | SER    | conflict | UNP A0R1H7 |
| E     | 989     | UNK      | HIS    | conflict | UNP A0R1H7 |
| E     | 990     | UNK      | PRO    | conflict | UNP A0R1H7 |
| E     | 991     | UNK      | SER    | conflict | UNP A0R1H7 |
| E     | 992     | UNK      | THR    | conflict | UNP A0R1H7 |
| E     | 993     | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 994     | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 995     | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 996     | UNK      | LEU    | conflict | UNP A0R1H7 |
| E     | 997     | UNK      | GLU    | conflict | UNP A0R1H7 |
| E     | 998     | UNK      | VAL    | conflict | UNP A0R1H7 |
| E     | 999     | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 1000    | UNK      | ASP    | conflict | UNP A0R1H7 |
| E     | 1001    | UNK      | ASP    | conflict | UNP A0R1H7 |
| E     | 1002    | UNK      | GLN    | conflict | UNP A0R1H7 |
| E     | 1003    | UNK      | HIS    | conflict | UNP A0R1H7 |
| E     | 1004    | UNK      | VAL    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| E     | 1005    | UNK      | VAL    | conflict | UNP A0R1H7 |
| E     | 1006    | UNK      | LEU    | conflict | UNP A0R1H7 |
| E     | 1007    | UNK      | SER    | conflict | UNP A0R1H7 |
| E     | 1008    | UNK      | VAL    | conflict | UNP A0R1H7 |
| E     | 1009    | UNK      | PRO    | conflict | UNP A0R1H7 |
| E     | 1010    | UNK      | LEU    | conflict | UNP A0R1H7 |
| E     | 1011    | UNK      | SER    | conflict | UNP A0R1H7 |
| E     | 1012    | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 1013    | UNK      | THR    | conflict | UNP A0R1H7 |
| E     | 1014    | UNK      | TRP    | conflict | UNP A0R1H7 |
| E     | 1196    | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 1197    | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 1198    | UNK      | THR    | conflict | UNP A0R1H7 |
| E     | 1199    | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 1200    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 1201    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 1202    | UNK      | GLU    | conflict | UNP A0R1H7 |
| E     | 1203    | UNK      | LEU    | conflict | UNP A0R1H7 |
| E     | 1204    | UNK      | THR    | conflict | UNP A0R1H7 |
| E     | 1205    | UNK      | ASP    | conflict | UNP A0R1H7 |
| E     | 1206    | UNK      | PRO    | conflict | UNP A0R1H7 |
| E     | 1207    | UNK      | VAL    | conflict | UNP A0R1H7 |
| E     | 1208    | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 1209    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 1210    | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 1211    | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 1212    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 1213    | UNK      | ILE    | conflict | UNP A0R1H7 |
| E     | 1214    | UNK      | SER    | conflict | UNP A0R1H7 |
| E     | 1215    | UNK      | ASP    | conflict | UNP A0R1H7 |
| E     | 1216    | UNK      | ASN    | conflict | UNP A0R1H7 |
| E     | 1217    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 1218    | UNK      | THR    | conflict | UNP A0R1H7 |
| E     | 1219    | UNK      | ASP    | conflict | UNP A0R1H7 |
| E     | 1220    | UNK      | THR    | conflict | UNP A0R1H7 |
| E     | 1221    | UNK      | PRO    | conflict | UNP A0R1H7 |
| E     | 1222    | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 1223    | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 1224    | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 1225    | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 1226    | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 1227    | UNK      | ASP    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| E     | 2076    | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 2077    | UNK      | ASP    | conflict | UNP A0R1H7 |
| E     | 2078    | UNK      | ILE    | conflict | UNP A0R1H7 |
| E     | 2079    | UNK      | ASP    | conflict | UNP A0R1H7 |
| E     | 2080    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 2081    | UNK      | GLN    | conflict | UNP A0R1H7 |
| E     | 2082    | UNK      | TRP    | conflict | UNP A0R1H7 |
| E     | 2083    | UNK      | GLU    | conflict | UNP A0R1H7 |
| E     | 2084    | UNK      | GLN    | conflict | UNP A0R1H7 |
| E     | 2085    | UNK      | LEU    | conflict | UNP A0R1H7 |
| E     | 2086    | UNK      | SER    | conflict | UNP A0R1H7 |
| E     | 2087    | UNK      | GLN    | conflict | UNP A0R1H7 |
| E     | 2088    | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 2089    | UNK      | PHE    | conflict | UNP A0R1H7 |
| E     | 2090    | UNK      | GLU    | conflict | UNP A0R1H7 |
| E     | 2091    | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 2092    | UNK      | THR    | conflict | UNP A0R1H7 |
| E     | 2093    | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 2094    | UNK      | HIS    | conflict | UNP A0R1H7 |
| E     | 2095    | UNK      | VAL    | conflict | UNP A0R1H7 |
| E     | 2096    | UNK      | VAL    | conflict | UNP A0R1H7 |
| E     | 2097    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 2098    | UNK      | THR    | conflict | UNP A0R1H7 |
| E     | 2099    | UNK      | GLN    | conflict | UNP A0R1H7 |
| E     | 2100    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 2101    | UNK      | ASN    | conflict | UNP A0R1H7 |
| E     | 2102    | UNK      | TRP    | conflict | UNP A0R1H7 |
| E     | 2103    | UNK      | TRP    | conflict | UNP A0R1H7 |
| E     | 2104    | UNK      | GLN    | conflict | UNP A0R1H7 |
| E     | 2105    | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 2106    | UNK      | LYS    | conflict | UNP A0R1H7 |
| E     | 2107    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 2108    | UNK      | LEU    | conflict | UNP A0R1H7 |
| E     | 2109    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 2110    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 2111    | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 2112    | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 2113    | UNK      | ASN    | conflict | UNP A0R1H7 |
| E     | 2114    | UNK      | VAL    | conflict | UNP A0R1H7 |
| E     | 2115    | UNK      | HIS    | conflict | UNP A0R1H7 |
| E     | 2116    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 2117    | UNK      | SER    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| E     | 2118    | UNK      | LEU    | conflict | UNP A0R1H7 |
| E     | 2119    | UNK      | PHE    | conflict | UNP A0R1H7 |
| E     | 2120    | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 2121    | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 2122    | UNK      | ILE    | conflict | UNP A0R1H7 |
| E     | 2123    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 2124    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 2125    | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 2126    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 2127    | UNK      | GLU    | conflict | UNP A0R1H7 |
| E     | 2128    | UNK      | ASN    | conflict | UNP A0R1H7 |
| E     | 2129    | UNK      | PRO    | conflict | UNP A0R1H7 |
| E     | 2130    | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 2131    | UNK      | LYS    | conflict | UNP A0R1H7 |
| E     | 2132    | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 2133    | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 2134    | UNK      | TYR    | conflict | UNP A0R1H7 |
| E     | 2135    | UNK      | SER    | conflict | UNP A0R1H7 |
| E     | 2422    | UNK      | GLU    | conflict | UNP A0R1H7 |
| E     | 2423    | UNK      | SER    | conflict | UNP A0R1H7 |
| E     | 2424    | UNK      | ASP    | conflict | UNP A0R1H7 |
| E     | 2425    | UNK      | ASP    | conflict | UNP A0R1H7 |
| E     | 2426    | UNK      | GLU    | conflict | UNP A0R1H7 |
| E     | 2427    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 2428    | UNK      | PRO    | conflict | UNP A0R1H7 |
| E     | 2429    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 2430    | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 2431    | UNK      | THR    | conflict | UNP A0R1H7 |
| E     | 2432    | UNK      | ILE    | conflict | UNP A0R1H7 |
| E     | 2433    | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 2434    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 2435    | UNK      | LEU    | conflict | UNP A0R1H7 |
| E     | 2436    | UNK      | PRO    | conflict | UNP A0R1H7 |
| E     | 2437    | UNK      | SER    | conflict | UNP A0R1H7 |
| E     | 2438    | UNK      | PRO    | conflict | UNP A0R1H7 |
| E     | 2439    | UNK      | PRO    | conflict | UNP A0R1H7 |
| E     | 2440    | UNK      | ARG    | conflict | UNP A0R1H7 |
| E     | 2441    | UNK      | GLY    | conflict | UNP A0R1H7 |
| E     | 2442    | UNK      | TYR    | conflict | UNP A0R1H7 |
| E     | 2443    | UNK      | ASN    | conflict | UNP A0R1H7 |
| E     | 2444    | UNK      | PRO    | conflict | UNP A0R1H7 |
| E     | 2445    | UNK      | ALA    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| E     | 2446    | UNK      | PRO    | conflict | UNP A0R1H7 |
| E     | 2447    | UNK      | ALA    | conflict | UNP A0R1H7 |
| E     | 2448    | UNK      | PRO    | conflict | UNP A0R1H7 |
| E     | 2449    | UNK      | GLU    | conflict | UNP A0R1H7 |
| E     | 2450    | UNK      | TRP    | conflict | UNP A0R1H7 |
| E     | 2451    | UNK      | ASP    | conflict | UNP A0R1H7 |
| E     | 2452    | UNK      | ASP    | conflict | UNP A0R1H7 |
| E     | 2453    | UNK      | LEU    | conflict | UNP A0R1H7 |
| F     | 929     | UNK      | GLU    | conflict | UNP A0R1H7 |
| F     | 930     | UNK      | PRO    | conflict | UNP A0R1H7 |
| F     | 931     | UNK      | VAL    | conflict | UNP A0R1H7 |
| F     | 932     | UNK      | GLU    | conflict | UNP A0R1H7 |
| F     | 933     | UNK      | VAL    | conflict | UNP A0R1H7 |
| F     | 934     | UNK      | LEU    | conflict | UNP A0R1H7 |
| F     | 935     | UNK      | SER    | conflict | UNP A0R1H7 |
| F     | 936     | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 937     | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 938     | UNK      | GLN    | conflict | UNP A0R1H7 |
| F     | 939     | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 940     | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 941     | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 942     | UNK      | ASP    | conflict | UNP A0R1H7 |
| F     | 943     | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 944     | UNK      | SER    | conflict | UNP A0R1H7 |
| F     | 974     | UNK      | THR    | conflict | UNP A0R1H7 |
| F     | 975     | UNK      | GLU    | conflict | UNP A0R1H7 |
| F     | 976     | UNK      | TRP    | conflict | UNP A0R1H7 |
| F     | 977     | UNK      | GLN    | conflict | UNP A0R1H7 |
| F     | 978     | UNK      | VAL    | conflict | UNP A0R1H7 |
| F     | 979     | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 980     | UNK      | GLU    | conflict | UNP A0R1H7 |
| F     | 981     | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 982     | UNK      | SER    | conflict | UNP A0R1H7 |
| F     | 983     | UNK      | ASP    | conflict | UNP A0R1H7 |
| F     | 984     | UNK      | ASN    | conflict | UNP A0R1H7 |
| F     | 985     | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 986     | UNK      | SER    | conflict | UNP A0R1H7 |
| F     | 987     | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 988     | UNK      | SER    | conflict | UNP A0R1H7 |
| F     | 989     | UNK      | HIS    | conflict | UNP A0R1H7 |
| F     | 990     | UNK      | PRO    | conflict | UNP A0R1H7 |
| F     | 991     | UNK      | SER    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| F     | 992     | UNK      | THR    | conflict | UNP A0R1H7 |
| F     | 993     | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 994     | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 995     | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 996     | UNK      | LEU    | conflict | UNP A0R1H7 |
| F     | 997     | UNK      | GLU    | conflict | UNP A0R1H7 |
| F     | 998     | UNK      | VAL    | conflict | UNP A0R1H7 |
| F     | 999     | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 1000    | UNK      | ASP    | conflict | UNP A0R1H7 |
| F     | 1001    | UNK      | ASP    | conflict | UNP A0R1H7 |
| F     | 1002    | UNK      | GLN    | conflict | UNP A0R1H7 |
| F     | 1003    | UNK      | HIS    | conflict | UNP A0R1H7 |
| F     | 1004    | UNK      | VAL    | conflict | UNP A0R1H7 |
| F     | 1005    | UNK      | VAL    | conflict | UNP A0R1H7 |
| F     | 1006    | UNK      | LEU    | conflict | UNP A0R1H7 |
| F     | 1007    | UNK      | SER    | conflict | UNP A0R1H7 |
| F     | 1008    | UNK      | VAL    | conflict | UNP A0R1H7 |
| F     | 1009    | UNK      | PRO    | conflict | UNP A0R1H7 |
| F     | 1010    | UNK      | LEU    | conflict | UNP A0R1H7 |
| F     | 1011    | UNK      | SER    | conflict | UNP A0R1H7 |
| F     | 1012    | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 1013    | UNK      | THR    | conflict | UNP A0R1H7 |
| F     | 1014    | UNK      | TRP    | conflict | UNP A0R1H7 |
| F     | 1196    | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 1197    | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 1198    | UNK      | THR    | conflict | UNP A0R1H7 |
| F     | 1199    | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 1200    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 1201    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 1202    | UNK      | GLU    | conflict | UNP A0R1H7 |
| F     | 1203    | UNK      | LEU    | conflict | UNP A0R1H7 |
| F     | 1204    | UNK      | THR    | conflict | UNP A0R1H7 |
| F     | 1205    | UNK      | ASP    | conflict | UNP A0R1H7 |
| F     | 1206    | UNK      | PRO    | conflict | UNP A0R1H7 |
| F     | 1207    | UNK      | VAL    | conflict | UNP A0R1H7 |
| F     | 1208    | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 1209    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 1210    | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 1211    | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 1212    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 1213    | UNK      | ILE    | conflict | UNP A0R1H7 |
| F     | 1214    | UNK      | SER    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| F     | 1215    | UNK      | ASP    | conflict | UNP A0R1H7 |
| F     | 1216    | UNK      | ASN    | conflict | UNP A0R1H7 |
| F     | 1217    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 1218    | UNK      | THR    | conflict | UNP A0R1H7 |
| F     | 1219    | UNK      | ASP    | conflict | UNP A0R1H7 |
| F     | 1220    | UNK      | THR    | conflict | UNP A0R1H7 |
| F     | 1221    | UNK      | PRO    | conflict | UNP A0R1H7 |
| F     | 1222    | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 1223    | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 1224    | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 1225    | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 1226    | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 1227    | UNK      | ASP    | conflict | UNP A0R1H7 |
| F     | 2076    | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 2077    | UNK      | ASP    | conflict | UNP A0R1H7 |
| F     | 2078    | UNK      | ILE    | conflict | UNP A0R1H7 |
| F     | 2079    | UNK      | ASP    | conflict | UNP A0R1H7 |
| F     | 2080    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 2081    | UNK      | GLN    | conflict | UNP A0R1H7 |
| F     | 2082    | UNK      | TRP    | conflict | UNP A0R1H7 |
| F     | 2083    | UNK      | GLU    | conflict | UNP A0R1H7 |
| F     | 2084    | UNK      | GLN    | conflict | UNP A0R1H7 |
| F     | 2085    | UNK      | LEU    | conflict | UNP A0R1H7 |
| F     | 2086    | UNK      | SER    | conflict | UNP A0R1H7 |
| F     | 2087    | UNK      | GLN    | conflict | UNP A0R1H7 |
| F     | 2088    | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 2089    | UNK      | PHE    | conflict | UNP A0R1H7 |
| F     | 2090    | UNK      | GLU    | conflict | UNP A0R1H7 |
| F     | 2091    | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 2092    | UNK      | THR    | conflict | UNP A0R1H7 |
| F     | 2093    | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 2094    | UNK      | HIS    | conflict | UNP A0R1H7 |
| F     | 2095    | UNK      | VAL    | conflict | UNP A0R1H7 |
| F     | 2096    | UNK      | VAL    | conflict | UNP A0R1H7 |
| F     | 2097    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 2098    | UNK      | THR    | conflict | UNP A0R1H7 |
| F     | 2099    | UNK      | GLN    | conflict | UNP A0R1H7 |
| F     | 2100    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 2101    | UNK      | ASN    | conflict | UNP A0R1H7 |
| F     | 2102    | UNK      | TRP    | conflict | UNP A0R1H7 |
| F     | 2103    | UNK      | TRP    | conflict | UNP A0R1H7 |
| F     | 2104    | UNK      | GLN    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| F     | 2105    | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 2106    | UNK      | LYS    | conflict | UNP A0R1H7 |
| F     | 2107    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 2108    | UNK      | LEU    | conflict | UNP A0R1H7 |
| F     | 2109    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 2110    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 2111    | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 2112    | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 2113    | UNK      | ASN    | conflict | UNP A0R1H7 |
| F     | 2114    | UNK      | VAL    | conflict | UNP A0R1H7 |
| F     | 2115    | UNK      | HIS    | conflict | UNP A0R1H7 |
| F     | 2116    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 2117    | UNK      | SER    | conflict | UNP A0R1H7 |
| F     | 2118    | UNK      | LEU    | conflict | UNP A0R1H7 |
| F     | 2119    | UNK      | PHE    | conflict | UNP A0R1H7 |
| F     | 2120    | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 2121    | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 2122    | UNK      | ILE    | conflict | UNP A0R1H7 |
| F     | 2123    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 2124    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 2125    | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 2126    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 2127    | UNK      | GLU    | conflict | UNP A0R1H7 |
| F     | 2128    | UNK      | ASN    | conflict | UNP A0R1H7 |
| F     | 2129    | UNK      | PRO    | conflict | UNP A0R1H7 |
| F     | 2130    | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 2131    | UNK      | LYS    | conflict | UNP A0R1H7 |
| F     | 2132    | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 2133    | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 2134    | UNK      | TYR    | conflict | UNP A0R1H7 |
| F     | 2135    | UNK      | SER    | conflict | UNP A0R1H7 |
| F     | 2422    | UNK      | GLU    | conflict | UNP A0R1H7 |
| F     | 2423    | UNK      | SER    | conflict | UNP A0R1H7 |
| F     | 2424    | UNK      | ASP    | conflict | UNP A0R1H7 |
| F     | 2425    | UNK      | ASP    | conflict | UNP A0R1H7 |
| F     | 2426    | UNK      | GLU    | conflict | UNP A0R1H7 |
| F     | 2427    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 2428    | UNK      | PRO    | conflict | UNP A0R1H7 |
| F     | 2429    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 2430    | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 2431    | UNK      | THR    | conflict | UNP A0R1H7 |
| F     | 2432    | UNK      | ILE    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| F     | 2433    | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 2434    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 2435    | UNK      | LEU    | conflict | UNP A0R1H7 |
| F     | 2436    | UNK      | PRO    | conflict | UNP A0R1H7 |
| F     | 2437    | UNK      | SER    | conflict | UNP A0R1H7 |
| F     | 2438    | UNK      | PRO    | conflict | UNP A0R1H7 |
| F     | 2439    | UNK      | PRO    | conflict | UNP A0R1H7 |
| F     | 2440    | UNK      | ARG    | conflict | UNP A0R1H7 |
| F     | 2441    | UNK      | GLY    | conflict | UNP A0R1H7 |
| F     | 2442    | UNK      | TYR    | conflict | UNP A0R1H7 |
| F     | 2443    | UNK      | ASN    | conflict | UNP A0R1H7 |
| F     | 2444    | UNK      | PRO    | conflict | UNP A0R1H7 |
| F     | 2445    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 2446    | UNK      | PRO    | conflict | UNP A0R1H7 |
| F     | 2447    | UNK      | ALA    | conflict | UNP A0R1H7 |
| F     | 2448    | UNK      | PRO    | conflict | UNP A0R1H7 |
| F     | 2449    | UNK      | GLU    | conflict | UNP A0R1H7 |
| F     | 2450    | UNK      | TRP    | conflict | UNP A0R1H7 |
| F     | 2451    | UNK      | ASP    | conflict | UNP A0R1H7 |
| F     | 2452    | UNK      | ASP    | conflict | UNP A0R1H7 |
| F     | 2453    | UNK      | LEU    | conflict | UNP A0R1H7 |
| A     | 929     | UNK      | GLU    | conflict | UNP A0R1H7 |
| A     | 930     | UNK      | PRO    | conflict | UNP A0R1H7 |
| A     | 931     | UNK      | VAL    | conflict | UNP A0R1H7 |
| A     | 932     | UNK      | GLU    | conflict | UNP A0R1H7 |
| A     | 933     | UNK      | VAL    | conflict | UNP A0R1H7 |
| A     | 934     | UNK      | LEU    | conflict | UNP A0R1H7 |
| A     | 935     | UNK      | SER    | conflict | UNP A0R1H7 |
| A     | 936     | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 937     | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 938     | UNK      | GLN    | conflict | UNP A0R1H7 |
| A     | 939     | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 940     | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 941     | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 942     | UNK      | ASP    | conflict | UNP A0R1H7 |
| A     | 943     | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 944     | UNK      | SER    | conflict | UNP A0R1H7 |
| A     | 974     | UNK      | THR    | conflict | UNP A0R1H7 |
| A     | 975     | UNK      | GLU    | conflict | UNP A0R1H7 |
| A     | 976     | UNK      | TRP    | conflict | UNP A0R1H7 |
| A     | 977     | UNK      | GLN    | conflict | UNP A0R1H7 |
| A     | 978     | UNK      | VAL    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 979     | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 980     | UNK      | GLU    | conflict | UNP A0R1H7 |
| A     | 981     | UNK      | GLY    | conflict | UNP A0R1H7 |
| A     | 982     | UNK      | SER    | conflict | UNP A0R1H7 |
| A     | 983     | UNK      | ASP    | conflict | UNP A0R1H7 |
| A     | 984     | UNK      | ASN    | conflict | UNP A0R1H7 |
| A     | 985     | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 986     | UNK      | SER    | conflict | UNP A0R1H7 |
| A     | 987     | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 988     | UNK      | SER    | conflict | UNP A0R1H7 |
| A     | 989     | UNK      | HIS    | conflict | UNP A0R1H7 |
| A     | 990     | UNK      | PRO    | conflict | UNP A0R1H7 |
| A     | 991     | UNK      | SER    | conflict | UNP A0R1H7 |
| A     | 992     | UNK      | THR    | conflict | UNP A0R1H7 |
| A     | 993     | UNK      | GLY    | conflict | UNP A0R1H7 |
| A     | 994     | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 995     | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 996     | UNK      | LEU    | conflict | UNP A0R1H7 |
| A     | 997     | UNK      | GLU    | conflict | UNP A0R1H7 |
| A     | 998     | UNK      | VAL    | conflict | UNP A0R1H7 |
| A     | 999     | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 1000    | UNK      | ASP    | conflict | UNP A0R1H7 |
| A     | 1001    | UNK      | ASP    | conflict | UNP A0R1H7 |
| A     | 1002    | UNK      | GLN    | conflict | UNP A0R1H7 |
| A     | 1003    | UNK      | HIS    | conflict | UNP A0R1H7 |
| A     | 1004    | UNK      | VAL    | conflict | UNP A0R1H7 |
| A     | 1005    | UNK      | VAL    | conflict | UNP A0R1H7 |
| A     | 1006    | UNK      | LEU    | conflict | UNP A0R1H7 |
| A     | 1007    | UNK      | SER    | conflict | UNP A0R1H7 |
| A     | 1008    | UNK      | VAL    | conflict | UNP A0R1H7 |
| A     | 1009    | UNK      | PRO    | conflict | UNP A0R1H7 |
| A     | 1010    | UNK      | LEU    | conflict | UNP A0R1H7 |
| A     | 1011    | UNK      | SER    | conflict | UNP A0R1H7 |
| A     | 1012    | UNK      | GLY    | conflict | UNP A0R1H7 |
| A     | 1013    | UNK      | THR    | conflict | UNP A0R1H7 |
| A     | 1014    | UNK      | TRP    | conflict | UNP A0R1H7 |
| A     | 1196    | UNK      | GLY    | conflict | UNP A0R1H7 |
| A     | 1197    | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 1198    | UNK      | THR    | conflict | UNP A0R1H7 |
| A     | 1199    | UNK      | GLY    | conflict | UNP A0R1H7 |
| A     | 1200    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 1201    | UNK      | ALA    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 1202    | UNK      | GLU    | conflict | UNP A0R1H7 |
| A     | 1203    | UNK      | LEU    | conflict | UNP A0R1H7 |
| A     | 1204    | UNK      | THR    | conflict | UNP A0R1H7 |
| A     | 1205    | UNK      | ASP    | conflict | UNP A0R1H7 |
| A     | 1206    | UNK      | PRO    | conflict | UNP A0R1H7 |
| A     | 1207    | UNK      | VAL    | conflict | UNP A0R1H7 |
| A     | 1208    | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 1209    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 1210    | UNK      | GLY    | conflict | UNP A0R1H7 |
| A     | 1211    | UNK      | GLY    | conflict | UNP A0R1H7 |
| A     | 1212    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 1213    | UNK      | ILE    | conflict | UNP A0R1H7 |
| A     | 1214    | UNK      | SER    | conflict | UNP A0R1H7 |
| A     | 1215    | UNK      | ASP    | conflict | UNP A0R1H7 |
| A     | 1216    | UNK      | ASN    | conflict | UNP A0R1H7 |
| A     | 1217    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 1218    | UNK      | THR    | conflict | UNP A0R1H7 |
| A     | 1219    | UNK      | ASP    | conflict | UNP A0R1H7 |
| A     | 1220    | UNK      | THR    | conflict | UNP A0R1H7 |
| A     | 1221    | UNK      | PRO    | conflict | UNP A0R1H7 |
| A     | 1222    | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 1223    | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 1224    | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 1225    | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 1226    | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 1227    | UNK      | ASP    | conflict | UNP A0R1H7 |
| A     | 2076    | UNK      | GLY    | conflict | UNP A0R1H7 |
| A     | 2077    | UNK      | ASP    | conflict | UNP A0R1H7 |
| A     | 2078    | UNK      | ILE    | conflict | UNP A0R1H7 |
| A     | 2079    | UNK      | ASP    | conflict | UNP A0R1H7 |
| A     | 2080    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 2081    | UNK      | GLN    | conflict | UNP A0R1H7 |
| A     | 2082    | UNK      | TRP    | conflict | UNP A0R1H7 |
| A     | 2083    | UNK      | GLU    | conflict | UNP A0R1H7 |
| A     | 2084    | UNK      | GLN    | conflict | UNP A0R1H7 |
| A     | 2085    | UNK      | LEU    | conflict | UNP A0R1H7 |
| A     | 2086    | UNK      | SER    | conflict | UNP A0R1H7 |
| A     | 2087    | UNK      | GLN    | conflict | UNP A0R1H7 |
| A     | 2088    | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 2089    | UNK      | PHE    | conflict | UNP A0R1H7 |
| A     | 2090    | UNK      | GLU    | conflict | UNP A0R1H7 |
| A     | 2091    | UNK      | GLY    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 2092    | UNK      | THR    | conflict | UNP A0R1H7 |
| A     | 2093    | UNK      | GLY    | conflict | UNP A0R1H7 |
| A     | 2094    | UNK      | HIS    | conflict | UNP A0R1H7 |
| A     | 2095    | UNK      | VAL    | conflict | UNP A0R1H7 |
| A     | 2096    | UNK      | VAL    | conflict | UNP A0R1H7 |
| A     | 2097    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 2098    | UNK      | THR    | conflict | UNP A0R1H7 |
| A     | 2099    | UNK      | GLN    | conflict | UNP A0R1H7 |
| A     | 2100    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 2101    | UNK      | ASN    | conflict | UNP A0R1H7 |
| A     | 2102    | UNK      | TRP    | conflict | UNP A0R1H7 |
| A     | 2103    | UNK      | TRP    | conflict | UNP A0R1H7 |
| A     | 2104    | UNK      | GLN    | conflict | UNP A0R1H7 |
| A     | 2105    | UNK      | GLY    | conflict | UNP A0R1H7 |
| A     | 2106    | UNK      | LYS    | conflict | UNP A0R1H7 |
| A     | 2107    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 2108    | UNK      | LEU    | conflict | UNP A0R1H7 |
| A     | 2109    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 2110    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 2111    | UNK      | GLY    | conflict | UNP A0R1H7 |
| A     | 2112    | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 2113    | UNK      | ASN    | conflict | UNP A0R1H7 |
| A     | 2114    | UNK      | VAL    | conflict | UNP A0R1H7 |
| A     | 2115    | UNK      | HIS    | conflict | UNP A0R1H7 |
| A     | 2116    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 2117    | UNK      | SER    | conflict | UNP A0R1H7 |
| A     | 2118    | UNK      | LEU    | conflict | UNP A0R1H7 |
| A     | 2119    | UNK      | PHE    | conflict | UNP A0R1H7 |
| A     | 2120    | UNK      | GLY    | conflict | UNP A0R1H7 |
| A     | 2121    | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 2122    | UNK      | ILE    | conflict | UNP A0R1H7 |
| A     | 2123    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 2124    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 2125    | UNK      | GLY    | conflict | UNP A0R1H7 |
| A     | 2126    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 2127    | UNK      | GLU    | conflict | UNP A0R1H7 |
| A     | 2128    | UNK      | ASN    | conflict | UNP A0R1H7 |
| A     | 2129    | UNK      | PRO    | conflict | UNP A0R1H7 |
| A     | 2130    | UNK      | GLY    | conflict | UNP A0R1H7 |
| A     | 2131    | UNK      | LYS    | conflict | UNP A0R1H7 |
| A     | 2132    | UNK      | GLY    | conflict | UNP A0R1H7 |
| A     | 2133    | UNK      | ARG    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 2134    | UNK      | TYR    | conflict | UNP A0R1H7 |
| A     | 2135    | UNK      | SER    | conflict | UNP A0R1H7 |
| A     | 2422    | UNK      | GLU    | conflict | UNP A0R1H7 |
| A     | 2423    | UNK      | SER    | conflict | UNP A0R1H7 |
| A     | 2424    | UNK      | ASP    | conflict | UNP A0R1H7 |
| A     | 2425    | UNK      | ASP    | conflict | UNP A0R1H7 |
| A     | 2426    | UNK      | GLU    | conflict | UNP A0R1H7 |
| A     | 2427    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 2428    | UNK      | PRO    | conflict | UNP A0R1H7 |
| A     | 2429    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 2430    | UNK      | GLY    | conflict | UNP A0R1H7 |
| A     | 2431    | UNK      | THR    | conflict | UNP A0R1H7 |
| A     | 2432    | UNK      | ILE    | conflict | UNP A0R1H7 |
| A     | 2433    | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 2434    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 2435    | UNK      | LEU    | conflict | UNP A0R1H7 |
| A     | 2436    | UNK      | PRO    | conflict | UNP A0R1H7 |
| A     | 2437    | UNK      | SER    | conflict | UNP A0R1H7 |
| A     | 2438    | UNK      | PRO    | conflict | UNP A0R1H7 |
| A     | 2439    | UNK      | PRO    | conflict | UNP A0R1H7 |
| A     | 2440    | UNK      | ARG    | conflict | UNP A0R1H7 |
| A     | 2441    | UNK      | GLY    | conflict | UNP A0R1H7 |
| A     | 2442    | UNK      | TYR    | conflict | UNP A0R1H7 |
| A     | 2443    | UNK      | ASN    | conflict | UNP A0R1H7 |
| A     | 2444    | UNK      | PRO    | conflict | UNP A0R1H7 |
| A     | 2445    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 2446    | UNK      | PRO    | conflict | UNP A0R1H7 |
| A     | 2447    | UNK      | ALA    | conflict | UNP A0R1H7 |
| A     | 2448    | UNK      | PRO    | conflict | UNP A0R1H7 |
| A     | 2449    | UNK      | GLU    | conflict | UNP A0R1H7 |
| A     | 2450    | UNK      | TRP    | conflict | UNP A0R1H7 |
| A     | 2451    | UNK      | ASP    | conflict | UNP A0R1H7 |
| A     | 2452    | UNK      | ASP    | conflict | UNP A0R1H7 |
| A     | 2453    | UNK      | LEU    | conflict | UNP A0R1H7 |
| B     | 929     | UNK      | GLU    | conflict | UNP A0R1H7 |
| B     | 930     | UNK      | PRO    | conflict | UNP A0R1H7 |
| B     | 931     | UNK      | VAL    | conflict | UNP A0R1H7 |
| B     | 932     | UNK      | GLU    | conflict | UNP A0R1H7 |
| B     | 933     | UNK      | VAL    | conflict | UNP A0R1H7 |
| B     | 934     | UNK      | LEU    | conflict | UNP A0R1H7 |
| B     | 935     | UNK      | SER    | conflict | UNP A0R1H7 |
| B     | 936     | UNK      | ARG    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 937     | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 938     | UNK      | GLN    | conflict | UNP A0R1H7 |
| B     | 939     | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 940     | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 941     | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 942     | UNK      | ASP    | conflict | UNP A0R1H7 |
| B     | 943     | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 944     | UNK      | SER    | conflict | UNP A0R1H7 |
| B     | 974     | UNK      | THR    | conflict | UNP A0R1H7 |
| B     | 975     | UNK      | GLU    | conflict | UNP A0R1H7 |
| B     | 976     | UNK      | TRP    | conflict | UNP A0R1H7 |
| B     | 977     | UNK      | GLN    | conflict | UNP A0R1H7 |
| B     | 978     | UNK      | VAL    | conflict | UNP A0R1H7 |
| B     | 979     | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 980     | UNK      | GLU    | conflict | UNP A0R1H7 |
| B     | 981     | UNK      | GLY    | conflict | UNP A0R1H7 |
| B     | 982     | UNK      | SER    | conflict | UNP A0R1H7 |
| B     | 983     | UNK      | ASP    | conflict | UNP A0R1H7 |
| B     | 984     | UNK      | ASN    | conflict | UNP A0R1H7 |
| B     | 985     | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 986     | UNK      | SER    | conflict | UNP A0R1H7 |
| B     | 987     | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 988     | UNK      | SER    | conflict | UNP A0R1H7 |
| B     | 989     | UNK      | HIS    | conflict | UNP A0R1H7 |
| B     | 990     | UNK      | PRO    | conflict | UNP A0R1H7 |
| B     | 991     | UNK      | SER    | conflict | UNP A0R1H7 |
| B     | 992     | UNK      | THR    | conflict | UNP A0R1H7 |
| B     | 993     | UNK      | GLY    | conflict | UNP A0R1H7 |
| B     | 994     | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 995     | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 996     | UNK      | LEU    | conflict | UNP A0R1H7 |
| B     | 997     | UNK      | GLU    | conflict | UNP A0R1H7 |
| B     | 998     | UNK      | VAL    | conflict | UNP A0R1H7 |
| B     | 999     | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 1000    | UNK      | ASP    | conflict | UNP A0R1H7 |
| B     | 1001    | UNK      | ASP    | conflict | UNP A0R1H7 |
| B     | 1002    | UNK      | GLN    | conflict | UNP A0R1H7 |
| B     | 1003    | UNK      | HIS    | conflict | UNP A0R1H7 |
| B     | 1004    | UNK      | VAL    | conflict | UNP A0R1H7 |
| B     | 1005    | UNK      | VAL    | conflict | UNP A0R1H7 |
| B     | 1006    | UNK      | LEU    | conflict | UNP A0R1H7 |
| B     | 1007    | UNK      | SER    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 1008    | UNK      | VAL    | conflict | UNP A0R1H7 |
| B     | 1009    | UNK      | PRO    | conflict | UNP A0R1H7 |
| B     | 1010    | UNK      | LEU    | conflict | UNP A0R1H7 |
| B     | 1011    | UNK      | SER    | conflict | UNP A0R1H7 |
| B     | 1012    | UNK      | GLY    | conflict | UNP A0R1H7 |
| B     | 1013    | UNK      | THR    | conflict | UNP A0R1H7 |
| B     | 1014    | UNK      | TRP    | conflict | UNP A0R1H7 |
| B     | 1196    | UNK      | GLY    | conflict | UNP A0R1H7 |
| B     | 1197    | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 1198    | UNK      | THR    | conflict | UNP A0R1H7 |
| B     | 1199    | UNK      | GLY    | conflict | UNP A0R1H7 |
| B     | 1200    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 1201    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 1202    | UNK      | GLU    | conflict | UNP A0R1H7 |
| B     | 1203    | UNK      | LEU    | conflict | UNP A0R1H7 |
| B     | 1204    | UNK      | THR    | conflict | UNP A0R1H7 |
| B     | 1205    | UNK      | ASP    | conflict | UNP A0R1H7 |
| B     | 1206    | UNK      | PRO    | conflict | UNP A0R1H7 |
| B     | 1207    | UNK      | VAL    | conflict | UNP A0R1H7 |
| B     | 1208    | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 1209    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 1210    | UNK      | GLY    | conflict | UNP A0R1H7 |
| B     | 1211    | UNK      | GLY    | conflict | UNP A0R1H7 |
| B     | 1212    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 1213    | UNK      | ILE    | conflict | UNP A0R1H7 |
| B     | 1214    | UNK      | SER    | conflict | UNP A0R1H7 |
| B     | 1215    | UNK      | ASP    | conflict | UNP A0R1H7 |
| B     | 1216    | UNK      | ASN    | conflict | UNP A0R1H7 |
| B     | 1217    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 1218    | UNK      | THR    | conflict | UNP A0R1H7 |
| B     | 1219    | UNK      | ASP    | conflict | UNP A0R1H7 |
| B     | 1220    | UNK      | THR    | conflict | UNP A0R1H7 |
| B     | 1221    | UNK      | PRO    | conflict | UNP A0R1H7 |
| B     | 1222    | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 1223    | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 1224    | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 1225    | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 1226    | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 1227    | UNK      | ASP    | conflict | UNP A0R1H7 |
| B     | 2076    | UNK      | GLY    | conflict | UNP A0R1H7 |
| B     | 2077    | UNK      | ASP    | conflict | UNP A0R1H7 |
| B     | 2078    | UNK      | ILE    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 2079    | UNK      | ASP    | conflict | UNP A0R1H7 |
| B     | 2080    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 2081    | UNK      | GLN    | conflict | UNP A0R1H7 |
| B     | 2082    | UNK      | TRP    | conflict | UNP A0R1H7 |
| B     | 2083    | UNK      | GLU    | conflict | UNP A0R1H7 |
| B     | 2084    | UNK      | GLN    | conflict | UNP A0R1H7 |
| B     | 2085    | UNK      | LEU    | conflict | UNP A0R1H7 |
| B     | 2086    | UNK      | SER    | conflict | UNP A0R1H7 |
| B     | 2087    | UNK      | GLN    | conflict | UNP A0R1H7 |
| B     | 2088    | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 2089    | UNK      | PHE    | conflict | UNP A0R1H7 |
| B     | 2090    | UNK      | GLU    | conflict | UNP A0R1H7 |
| B     | 2091    | UNK      | GLY    | conflict | UNP A0R1H7 |
| B     | 2092    | UNK      | THR    | conflict | UNP A0R1H7 |
| B     | 2093    | UNK      | GLY    | conflict | UNP A0R1H7 |
| B     | 2094    | UNK      | HIS    | conflict | UNP A0R1H7 |
| B     | 2095    | UNK      | VAL    | conflict | UNP A0R1H7 |
| B     | 2096    | UNK      | VAL    | conflict | UNP A0R1H7 |
| B     | 2097    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 2098    | UNK      | THR    | conflict | UNP A0R1H7 |
| B     | 2099    | UNK      | GLN    | conflict | UNP A0R1H7 |
| B     | 2100    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 2101    | UNK      | ASN    | conflict | UNP A0R1H7 |
| B     | 2102    | UNK      | TRP    | conflict | UNP A0R1H7 |
| B     | 2103    | UNK      | TRP    | conflict | UNP A0R1H7 |
| B     | 2104    | UNK      | GLN    | conflict | UNP A0R1H7 |
| B     | 2105    | UNK      | GLY    | conflict | UNP A0R1H7 |
| B     | 2106    | UNK      | LYS    | conflict | UNP A0R1H7 |
| B     | 2107    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 2108    | UNK      | LEU    | conflict | UNP A0R1H7 |
| B     | 2109    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 2110    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 2111    | UNK      | GLY    | conflict | UNP A0R1H7 |
| B     | 2112    | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 2113    | UNK      | ASN    | conflict | UNP A0R1H7 |
| B     | 2114    | UNK      | VAL    | conflict | UNP A0R1H7 |
| B     | 2115    | UNK      | HIS    | conflict | UNP A0R1H7 |
| B     | 2116    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 2117    | UNK      | SER    | conflict | UNP A0R1H7 |
| B     | 2118    | UNK      | LEU    | conflict | UNP A0R1H7 |
| B     | 2119    | UNK      | PHE    | conflict | UNP A0R1H7 |
| B     | 2120    | UNK      | GLY    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 2121    | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 2122    | UNK      | ILE    | conflict | UNP A0R1H7 |
| B     | 2123    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 2124    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 2125    | UNK      | GLY    | conflict | UNP A0R1H7 |
| B     | 2126    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 2127    | UNK      | GLU    | conflict | UNP A0R1H7 |
| B     | 2128    | UNK      | ASN    | conflict | UNP A0R1H7 |
| B     | 2129    | UNK      | PRO    | conflict | UNP A0R1H7 |
| B     | 2130    | UNK      | GLY    | conflict | UNP A0R1H7 |
| B     | 2131    | UNK      | LYS    | conflict | UNP A0R1H7 |
| B     | 2132    | UNK      | GLY    | conflict | UNP A0R1H7 |
| B     | 2133    | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 2134    | UNK      | TYR    | conflict | UNP A0R1H7 |
| B     | 2135    | UNK      | SER    | conflict | UNP A0R1H7 |
| B     | 2422    | UNK      | GLU    | conflict | UNP A0R1H7 |
| B     | 2423    | UNK      | SER    | conflict | UNP A0R1H7 |
| B     | 2424    | UNK      | ASP    | conflict | UNP A0R1H7 |
| B     | 2425    | UNK      | ASP    | conflict | UNP A0R1H7 |
| B     | 2426    | UNK      | GLU    | conflict | UNP A0R1H7 |
| B     | 2427    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 2428    | UNK      | PRO    | conflict | UNP A0R1H7 |
| B     | 2429    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 2430    | UNK      | GLY    | conflict | UNP A0R1H7 |
| B     | 2431    | UNK      | THR    | conflict | UNP A0R1H7 |
| B     | 2432    | UNK      | ILE    | conflict | UNP A0R1H7 |
| B     | 2433    | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 2434    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 2435    | UNK      | LEU    | conflict | UNP A0R1H7 |
| B     | 2436    | UNK      | PRO    | conflict | UNP A0R1H7 |
| B     | 2437    | UNK      | SER    | conflict | UNP A0R1H7 |
| B     | 2438    | UNK      | PRO    | conflict | UNP A0R1H7 |
| B     | 2439    | UNK      | PRO    | conflict | UNP A0R1H7 |
| B     | 2440    | UNK      | ARG    | conflict | UNP A0R1H7 |
| B     | 2441    | UNK      | GLY    | conflict | UNP A0R1H7 |
| B     | 2442    | UNK      | TYR    | conflict | UNP A0R1H7 |
| B     | 2443    | UNK      | ASN    | conflict | UNP A0R1H7 |
| B     | 2444    | UNK      | PRO    | conflict | UNP A0R1H7 |
| B     | 2445    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 2446    | UNK      | PRO    | conflict | UNP A0R1H7 |
| B     | 2447    | UNK      | ALA    | conflict | UNP A0R1H7 |
| B     | 2448    | UNK      | PRO    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 2449    | UNK      | GLU    | conflict | UNP A0R1H7 |
| B     | 2450    | UNK      | TRP    | conflict | UNP A0R1H7 |
| B     | 2451    | UNK      | ASP    | conflict | UNP A0R1H7 |
| B     | 2452    | UNK      | ASP    | conflict | UNP A0R1H7 |
| B     | 2453    | UNK      | LEU    | conflict | UNP A0R1H7 |
| C     | 929     | UNK      | GLU    | conflict | UNP A0R1H7 |
| C     | 930     | UNK      | PRO    | conflict | UNP A0R1H7 |
| C     | 931     | UNK      | VAL    | conflict | UNP A0R1H7 |
| C     | 932     | UNK      | GLU    | conflict | UNP A0R1H7 |
| C     | 933     | UNK      | VAL    | conflict | UNP A0R1H7 |
| C     | 934     | UNK      | LEU    | conflict | UNP A0R1H7 |
| C     | 935     | UNK      | SER    | conflict | UNP A0R1H7 |
| C     | 936     | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 937     | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 938     | UNK      | GLN    | conflict | UNP A0R1H7 |
| C     | 939     | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 940     | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 941     | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 942     | UNK      | ASP    | conflict | UNP A0R1H7 |
| C     | 943     | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 944     | UNK      | SER    | conflict | UNP A0R1H7 |
| C     | 974     | UNK      | THR    | conflict | UNP A0R1H7 |
| C     | 975     | UNK      | GLU    | conflict | UNP A0R1H7 |
| C     | 976     | UNK      | TRP    | conflict | UNP A0R1H7 |
| C     | 977     | UNK      | GLN    | conflict | UNP A0R1H7 |
| C     | 978     | UNK      | VAL    | conflict | UNP A0R1H7 |
| C     | 979     | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 980     | UNK      | GLU    | conflict | UNP A0R1H7 |
| C     | 981     | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 982     | UNK      | SER    | conflict | UNP A0R1H7 |
| C     | 983     | UNK      | ASP    | conflict | UNP A0R1H7 |
| C     | 984     | UNK      | ASN    | conflict | UNP A0R1H7 |
| C     | 985     | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 986     | UNK      | SER    | conflict | UNP A0R1H7 |
| C     | 987     | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 988     | UNK      | SER    | conflict | UNP A0R1H7 |
| C     | 989     | UNK      | HIS    | conflict | UNP A0R1H7 |
| C     | 990     | UNK      | PRO    | conflict | UNP A0R1H7 |
| C     | 991     | UNK      | SER    | conflict | UNP A0R1H7 |
| C     | 992     | UNK      | THR    | conflict | UNP A0R1H7 |
| C     | 993     | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 994     | UNK      | ALA    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C     | 995     | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 996     | UNK      | LEU    | conflict | UNP A0R1H7 |
| C     | 997     | UNK      | GLU    | conflict | UNP A0R1H7 |
| C     | 998     | UNK      | VAL    | conflict | UNP A0R1H7 |
| C     | 999     | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 1000    | UNK      | ASP    | conflict | UNP A0R1H7 |
| C     | 1001    | UNK      | ASP    | conflict | UNP A0R1H7 |
| C     | 1002    | UNK      | GLN    | conflict | UNP A0R1H7 |
| C     | 1003    | UNK      | HIS    | conflict | UNP A0R1H7 |
| C     | 1004    | UNK      | VAL    | conflict | UNP A0R1H7 |
| C     | 1005    | UNK      | VAL    | conflict | UNP A0R1H7 |
| C     | 1006    | UNK      | LEU    | conflict | UNP A0R1H7 |
| C     | 1007    | UNK      | SER    | conflict | UNP A0R1H7 |
| C     | 1008    | UNK      | VAL    | conflict | UNP A0R1H7 |
| C     | 1009    | UNK      | PRO    | conflict | UNP A0R1H7 |
| C     | 1010    | UNK      | LEU    | conflict | UNP A0R1H7 |
| C     | 1011    | UNK      | SER    | conflict | UNP A0R1H7 |
| C     | 1012    | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 1013    | UNK      | THR    | conflict | UNP A0R1H7 |
| C     | 1014    | UNK      | TRP    | conflict | UNP A0R1H7 |
| C     | 1196    | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 1197    | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 1198    | UNK      | THR    | conflict | UNP A0R1H7 |
| C     | 1199    | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 1200    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 1201    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 1202    | UNK      | GLU    | conflict | UNP A0R1H7 |
| C     | 1203    | UNK      | LEU    | conflict | UNP A0R1H7 |
| C     | 1204    | UNK      | THR    | conflict | UNP A0R1H7 |
| C     | 1205    | UNK      | ASP    | conflict | UNP A0R1H7 |
| C     | 1206    | UNK      | PRO    | conflict | UNP A0R1H7 |
| C     | 1207    | UNK      | VAL    | conflict | UNP A0R1H7 |
| C     | 1208    | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 1209    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 1210    | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 1211    | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 1212    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 1213    | UNK      | ILE    | conflict | UNP A0R1H7 |
| C     | 1214    | UNK      | SER    | conflict | UNP A0R1H7 |
| C     | 1215    | UNK      | ASP    | conflict | UNP A0R1H7 |
| C     | 1216    | UNK      | ASN    | conflict | UNP A0R1H7 |
| C     | 1217    | UNK      | ALA    | conflict | UNP A0R1H7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C     | 1218    | UNK      | THR    | conflict | UNP A0R1H7 |
| C     | 1219    | UNK      | ASP    | conflict | UNP A0R1H7 |
| C     | 1220    | UNK      | THR    | conflict | UNP A0R1H7 |
| C     | 1221    | UNK      | PRO    | conflict | UNP A0R1H7 |
| C     | 1222    | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 1223    | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 1224    | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 1225    | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 1226    | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 1227    | UNK      | ASP    | conflict | UNP A0R1H7 |
| C     | 2076    | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 2077    | UNK      | ASP    | conflict | UNP A0R1H7 |
| C     | 2078    | UNK      | ILE    | conflict | UNP A0R1H7 |
| C     | 2079    | UNK      | ASP    | conflict | UNP A0R1H7 |
| C     | 2080    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 2081    | UNK      | GLN    | conflict | UNP A0R1H7 |
| C     | 2082    | UNK      | TRP    | conflict | UNP A0R1H7 |
| C     | 2083    | UNK      | GLU    | conflict | UNP A0R1H7 |
| C     | 2084    | UNK      | GLN    | conflict | UNP A0R1H7 |
| C     | 2085    | UNK      | LEU    | conflict | UNP A0R1H7 |
| C     | 2086    | UNK      | SER    | conflict | UNP A0R1H7 |
| C     | 2087    | UNK      | GLN    | conflict | UNP A0R1H7 |
| C     | 2088    | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 2089    | UNK      | PHE    | conflict | UNP A0R1H7 |
| C     | 2090    | UNK      | GLU    | conflict | UNP A0R1H7 |
| C     | 2091    | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 2092    | UNK      | THR    | conflict | UNP A0R1H7 |
| C     | 2093    | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 2094    | UNK      | HIS    | conflict | UNP A0R1H7 |
| C     | 2095    | UNK      | VAL    | conflict | UNP A0R1H7 |
| C     | 2096    | UNK      | VAL    | conflict | UNP A0R1H7 |
| C     | 2097    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 2098    | UNK      | THR    | conflict | UNP A0R1H7 |
| C     | 2099    | UNK      | GLN    | conflict | UNP A0R1H7 |
| C     | 2100    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 2101    | UNK      | ASN    | conflict | UNP A0R1H7 |
| C     | 2102    | UNK      | TRP    | conflict | UNP A0R1H7 |
| C     | 2103    | UNK      | TRP    | conflict | UNP A0R1H7 |
| C     | 2104    | UNK      | GLN    | conflict | UNP A0R1H7 |
| C     | 2105    | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 2106    | UNK      | LYS    | conflict | UNP A0R1H7 |
| C     | 2107    | UNK      | ALA    | conflict | UNP A0R1H7 |

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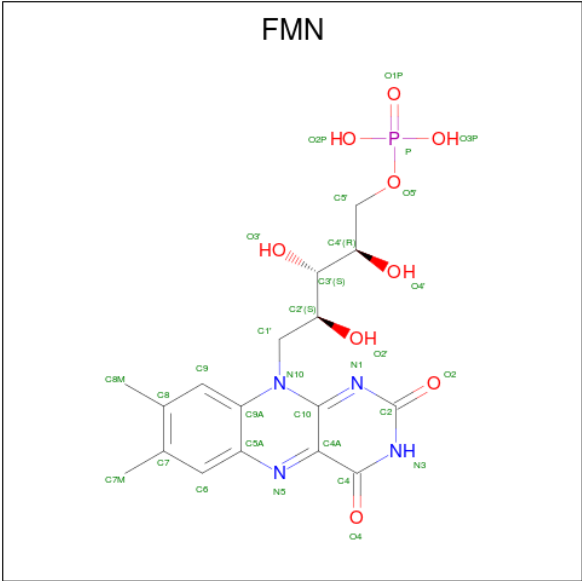
| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C     | 2108    | UNK      | LEU    | conflict | UNP A0R1H7 |
| C     | 2109    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 2110    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 2111    | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 2112    | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 2113    | UNK      | ASN    | conflict | UNP A0R1H7 |
| C     | 2114    | UNK      | VAL    | conflict | UNP A0R1H7 |
| C     | 2115    | UNK      | HIS    | conflict | UNP A0R1H7 |
| C     | 2116    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 2117    | UNK      | SER    | conflict | UNP A0R1H7 |
| C     | 2118    | UNK      | LEU    | conflict | UNP A0R1H7 |
| C     | 2119    | UNK      | PHE    | conflict | UNP A0R1H7 |
| C     | 2120    | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 2121    | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 2122    | UNK      | ILE    | conflict | UNP A0R1H7 |
| C     | 2123    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 2124    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 2125    | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 2126    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 2127    | UNK      | GLU    | conflict | UNP A0R1H7 |
| C     | 2128    | UNK      | ASN    | conflict | UNP A0R1H7 |
| C     | 2129    | UNK      | PRO    | conflict | UNP A0R1H7 |
| C     | 2130    | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 2131    | UNK      | LYS    | conflict | UNP A0R1H7 |
| C     | 2132    | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 2133    | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 2134    | UNK      | TYR    | conflict | UNP A0R1H7 |
| C     | 2135    | UNK      | SER    | conflict | UNP A0R1H7 |
| C     | 2422    | UNK      | GLU    | conflict | UNP A0R1H7 |
| C     | 2423    | UNK      | SER    | conflict | UNP A0R1H7 |
| C     | 2424    | UNK      | ASP    | conflict | UNP A0R1H7 |
| C     | 2425    | UNK      | ASP    | conflict | UNP A0R1H7 |
| C     | 2426    | UNK      | GLU    | conflict | UNP A0R1H7 |
| C     | 2427    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 2428    | UNK      | PRO    | conflict | UNP A0R1H7 |
| C     | 2429    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 2430    | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 2431    | UNK      | THR    | conflict | UNP A0R1H7 |
| C     | 2432    | UNK      | ILE    | conflict | UNP A0R1H7 |
| C     | 2433    | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 2434    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 2435    | UNK      | LEU    | conflict | UNP A0R1H7 |

*Continued on next page...*

Continued from previous page...

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C     | 2436    | UNK      | PRO    | conflict | UNP A0R1H7 |
| C     | 2437    | UNK      | SER    | conflict | UNP A0R1H7 |
| C     | 2438    | UNK      | PRO    | conflict | UNP A0R1H7 |
| C     | 2439    | UNK      | PRO    | conflict | UNP A0R1H7 |
| C     | 2440    | UNK      | ARG    | conflict | UNP A0R1H7 |
| C     | 2441    | UNK      | GLY    | conflict | UNP A0R1H7 |
| C     | 2442    | UNK      | TYR    | conflict | UNP A0R1H7 |
| C     | 2443    | UNK      | ASN    | conflict | UNP A0R1H7 |
| C     | 2444    | UNK      | PRO    | conflict | UNP A0R1H7 |
| C     | 2445    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 2446    | UNK      | PRO    | conflict | UNP A0R1H7 |
| C     | 2447    | UNK      | ALA    | conflict | UNP A0R1H7 |
| C     | 2448    | UNK      | PRO    | conflict | UNP A0R1H7 |
| C     | 2449    | UNK      | GLU    | conflict | UNP A0R1H7 |
| C     | 2450    | UNK      | TRP    | conflict | UNP A0R1H7 |
| C     | 2451    | UNK      | ASP    | conflict | UNP A0R1H7 |
| C     | 2452    | UNK      | ASP    | conflict | UNP A0R1H7 |
| C     | 2453    | UNK      | LEU    | conflict | UNP A0R1H7 |

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 2   | F     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |
| 2   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |
| 2   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |
| 2   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |



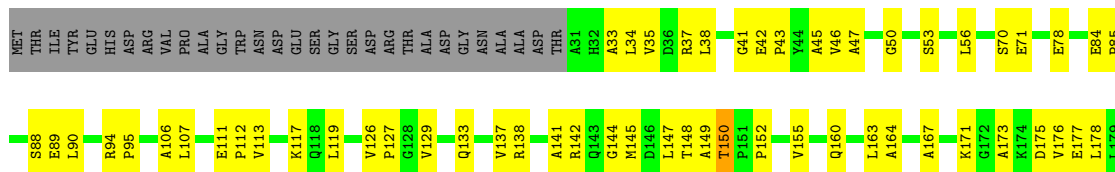




|       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |
|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|
| ALA   | K1706 | I1503 | H1412 | R1195 | P1099 | X994  | G900 | A792 | N882 | D589 | T485 | R381 | V292 | A182 |
| PRO   | T1710 | R1504 | D1307 | X1196 | D1100 | X995  | I901 | R793 | G883 | L590 | Q486 | R381 | V292 | Q183 |
| SER   | N1617 | Q1308 | Q1308 | X1197 |       | X996  | V904 | L794 | M684 | L590 | Q487 | R381 | E293 | L184 |
| GLY   | L1618 | Q1507 | D1414 | X1198 | V1103 | X997  | V904 | H795 | A885 | L593 | N488 | Q384 | V294 |      |
| A1712 | V1619 | I1508 | G1415 | X1199 | G1104 | X998  | F915 | F796 | S886 | L594 | T489 | Q384 |      | R195 |
| PRO   | G713  | I1508 | V1416 | X1199 | A1105 | X999  | F915 | Q797 | G887 | L595 | L490 | T389 | L301 |      |
| ARG   | L1714 | D1511 | L1417 | X1200 | C1106 | X1000 | L924 | D798 | R688 |      |      | V390 |      | I198 |
| PRO   | F1622 | F1623 | R1312 | X1204 | X1001 | X1001 |      | F799 |      | Y598 | Q500 | V390 | I305 |      |
| ASP   | F1623 | D1514 | X1314 | X1205 | V1110 | X1002 | L924 |      |      |      | V501 | V393 | I305 | G202 |
| ASP   | T1624 | R1314 | X1314 | X1206 | V1110 | X1003 | A928 | E803 | I695 | R602 | V501 | P394 | I307 | D203 |
| ILE   | L1625 | E1723 | R1315 | X1207 | F1111 | X1004 | X929 | E803 | H696 |      | K504 | P394 | I307 | R204 |
| THR   | F1629 | V1519 | V1316 | X1207 | F1111 | X1005 | X930 | A808 | E697 | M606 | R505 |      | W311 | P205 |
| PHE   |       |       | G1317 | X1212 | A1117 | X1006 | X931 |      | I698 |      |      | W400 |      | P206 |
| ASP   | I1633 | E1531 | I1318 | I1213 | A1118 | X1007 | X931 | D811 | G613 |      | Q508 | T314 | T314 | M207 |
| ALA   | R1634 | E1532 | D1319 | X1215 | T1119 | X1008 | X932 | D811 | N700 | G614 | V315 | P405 | V315 | V208 |
| N1732 | V1533 | V1533 | V1320 | X1216 | E1120 | X1009 | X934 | L816 | A701 |      | R511 | T406 | G316 | S209 |
| ASP   | V1637 | N1534 | E1323 | X1217 | F1123 | X1010 | X935 | E817 |      | P618 | P516 | V407 | L317 | V210 |
| ALA   | P1638 | F1535 | V1324 | X1218 | P1124 | X1011 | X936 |      | L709 |      |      | V408 |      | T211 |
| THR   | A1639 | V1536 | V1325 | X1219 | P1124 | X1012 | X937 | L826 |      |      |      | K409 | E327 |      |
| VAL   | R1736 | L1537 | E1326 | X1220 | T1126 | X1013 | X938 | L827 | A713 |      | D518 | P411 | S328 | L222 |
| D1737 | T1651 | R1538 | V1327 | X1221 | E1127 | X1014 | X939 | W836 |      | Y624 | V521 | P411 | I329 |      |
| LEU   | V1652 | G1539 | X1328 | X1222 | G1128 | X1015 | X940 | D832 | A716 | L625 | V521 | D412 | L330 | V232 |
| LEU   | L1741 | S1540 | A1329 | X1224 | L1129 | X1017 | X941 | A833 | V719 |      | V522 |      |      | L233 |
| ALA   | Q1541 | Q1541 | R1330 | X1225 | L1129 | X1018 | X942 | E834 |      | W629 | S523 | V415 | W336 |      |
| LEU   | P1657 | V1542 | I1331 | X1226 | L1132 | F1019 | X943 | E834 |      |      |      | K416 | E339 | V236 |
| SER   | K1658 | E1543 | I1331 | X1227 | V1133 | X1020 | X944 | W836 | K735 | L637 | V526 | L417 | I340 | L237 |
| ASP   | E1659 | I1544 | V1336 | V1228 | V1133 | L1021 | X944 | W837 | P736 | P637 |      | E418 | I341 | S238 |
| LYS   | L1660 | C1547 | M1337 | V1228 | P1146 | L1021 | L957 | W837 | Y737 | M638 | D534 | T419 | T341 |      |
| MET   | C1661 | L1551 | A1338 | R1237 | K1147 | V1025 | L957 |      |      |      |      | K420 | E342 | L248 |
| ARG   | R1662 | E1552 | A1339 | R1263 | R1149 | E1034 | R961 | G854 | T745 | D641 | E538 | L424 | L343 | T249 |
| ILE   | G1663 | I1553 | I1339 | R1263 | A1150 | V1035 | R962 | R855 | Y746 | G642 | L539 | L424 | R344 | G250 |
| ASP   | A1660 | L1554 | R1342 | R1263 | E1150 | D1036 | V964 | R857 | L747 | T643 | N540 |      |      | T251 |
| GLN   | L1666 | E1555 | L1343 | G1268 | E1151 | D1036 | V964 | W857 | Q748 | L644 | E541 | R427 | A348 |      |
| ILE   | E1667 | E1556 | L1344 | M1269 | E1151 | D1036 | V964 | N858 | W749 |      | V542 |      | R349 | L255 |
| ALA   | A1668 | E1557 | A1345 | V1270 | F1152 | D1037 | P965 | R859 | L750 | T647 | G543 | T436 | K350 | S256 |
| GLU   | L1668 | E1557 | A1345 | V1270 | F1152 | D1037 | P966 | R859 | L750 | T647 | G543 | T436 | K350 | S257 |
| ALA   |       |       | P1346 | L1271 | T1162 | V1045 | P967 | R860 | R751 |      | T544 | P437 | I351 |      |
| LEU   | W1671 | R1560 | V1467 | L1271 | D1163 | L1046 | P967 | R861 | R751 |      | T544 | P437 | I351 |      |
| ASP   | Q1672 | R1561 | V1467 | A1275 | T1164 | L1046 | P967 | R862 | L756 |      | S545 | T438 | L352 | L260 |
| SER   | F1673 | E1562 | V1468 | A1351 | A1275 | V1068 | A971 |      |      |      |      | V440 | L354 |      |
| ALA   | A1674 | Q1276 | F1352 | Q1276 | G1167 | T1069 | X974 | R868 | S763 |      | F549 | D441 | G355 | A266 |
| GLU   |       | Q1276 | F1352 | Q1276 | G1167 | T1069 | X974 | R868 | S763 |      | F549 | D441 | G355 | A267 |
| ALA   |       | L1470 | P1353 | P1353 | R1168 | V1070 | X974 | R872 | D766 |      | P551 | K443 | G357 | K268 |
| PRO   | W1679 | H1578 | I1357 | I1357 | P1171 | W1072 | X975 | R872 | D766 |      | P551 | K443 | G357 | K269 |
| ILE   | D1684 | V1579 | Q1358 | Q1358 | P1171 | W1072 | X975 | R872 | D766 |      | P551 | K443 | G357 | K270 |
| THR   | L1685 | P1580 | Q1358 | Q1358 | P1171 | W1072 | X975 | R872 | D766 |      | P551 | K443 | G357 | K271 |
| ASP   | L1686 | F1581 | M1362 | M1362 | P1171 | W1072 | X975 | R872 | D766 |      | P551 | K443 | G357 | K272 |
| GLY   | L1686 | H1582 | M1362 | M1362 | P1171 | W1072 | X975 | R872 | D766 |      | P551 | K443 | G357 | K273 |
| ALA   | F1687 | H1582 | M1362 | M1362 | P1171 | W1072 | X975 | R872 | D766 |      | P551 | K443 | G357 | K274 |
| PRO   |       |       | V1376 | V1376 | R1177 | T1084 | X981 | R877 | D776 |      | I563 | E456 | L363 |      |
| ALA   | K1483 |       | V1376 | V1376 | R1177 | T1084 | X981 | R877 | D776 |      | I563 | E456 | L363 |      |
| SER   | E1690 | L1586 | M1484 | K1285 | R1177 | F1087 | X982 | R880 | T778 |      | H575 | Q462 | L364 | K276 |
| ALA   |       | L1586 | M1484 | K1285 | R1177 | F1087 | X982 | R880 | T778 |      | H575 | Q462 | L364 | K277 |
| ARG   |       | L1586 | M1484 | K1285 | R1177 | F1087 | X982 | R880 | T778 |      | H575 | Q462 | L364 | K278 |
| ARG   | G1694 | V1590 | D1485 | P1287 | A1179 | G1088 | X983 | E885 | W779 | T688 | L576 | K462 | A365 |      |
| ALA   | L1695 | V1590 | D1485 | P1287 | A1179 | G1088 | X983 | E885 | W779 | T688 | L576 | K462 | A365 |      |
| ASN   | L1695 | V1590 | D1485 | P1287 | A1179 | G1088 | X983 | E885 | W779 | T688 | L576 | K462 | A365 |      |
| GLN   | L1695 | V1590 | D1485 | P1287 | A1179 | G1088 | X983 | E885 | W779 | T688 | L576 | K462 | A365 |      |
| ALA   | L1695 | V1590 | D1485 | P1287 | A1179 | G1088 | X983 | E885 | W779 | T688 | L576 | K462 | A365 |      |
| PRO   | L1695 | V1590 | D1485 | P1287 | A1179 | G1088 | X983 | E885 | W779 | T688 | L576 | K462 | A365 |      |
| PRO   | L1695 | V1590 | D1485 | P1287 | A1179 | G1088 | X983 | E885 | W779 | T688 | L576 | K462 | A365 |      |
| ALA   | L1695 | V1590 | D1485 | P1287 | A1179 | G1088 | X983 | E885 | W779 | T688 | L576 | K462 | A365 |      |
| LEU   | R1699 | E1598 | S1391 | P1289 | L1185 | L1091 | X986 | D887 | R781 | T671 | B580 | L475 | R369 | A281 |
| ALA   |       |       | S1391 | P1289 | L1185 | L1091 | X986 | D887 | R781 | T671 | B580 | L475 | R369 | A282 |
| PRO   | F1700 | D1604 | N1399 | N1399 | L1188 | P1093 | X988 | T892 | F783 |      | G583 | E476 | I373 |      |
| VAL   | I1701 | K1605 | P1400 | P1400 | L1291 | T1094 | X989 | T895 | W787 |      | H584 | L479 | I373 |      |
| ASP   | E1702 | V1701 | A1405 | A1405 | L1291 | T1094 | X989 | T895 | W787 |      | H584 | L479 | I373 |      |
| LEU   | I1611 | I1703 | A1405 | A1405 | L1291 | T1094 | X989 | T895 | W787 |      | H584 | L479 | I373 |      |
| ALA   | I1703 | I1703 | A1405 | A1405 | L1291 | T1094 | X989 | T895 | W787 |      | H584 | L479 | I373 |      |
| PRO   | G1704 | G1612 | S1496 | S1496 | L1291 | T1094 | X989 | T895 | W787 |      | H584 | L479 | I373 |      |
| GLY   | W1706 | R1612 | W1408 | W1408 | L1291 | T1094 | X989 | T895 | W787 |      | H584 | L479 | I373 |      |
| ALA   |       |       | W1408 | W1408 | L1291 | T1094 | X989 | T895 | W787 |      | H584 | L479 | I373 |      |





WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

 **EMDataBank**  
Unified Data Resource for 3DEM

|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| L2992 | L2993 | V2994 | T2995 | G2998 | H3001 | V3002 | L3005 | V3009 | F3014 | I3015 | A3016 | A3017 | L3018 | D3019 | E3022 | R3023 | A3044 | P3050 | M3051 | D3057 | R3058 | R3059 | H3062 | P3065 | E3066 | Q3069 | S3076 | T3077 | P2980 | L3081 | L3089 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| L2906 | A2911 | R2916 | G2919 | R2920 | P2921 | L2922 | F2923 | L2924 | V2925 | S2926 | Q2927 | L2930 | K2935 | G2936 | A2939 | V2940 | F2941 | Q2942 | M2943 | L2946 | G2947 | Q2948 | R2951 | V2954 | I2955 | P2956 | P2957 | N2958 | R2959 | S2960 | L2961 | D2962 | D2966 | W2976 | V2977 | R2978 | E2979 | P2980 | L2983 | R2984 | G2985 | K2986 | F2987 | P2988 | L2989 |       |       |       |       |       |       |       |       |       |       |
| R2808 | L2809 | G2810 | F2811 | L2812 | Q2815 | L2820 | L2821 | L2822 | A2823 | R2824 | L2827 | A2828 | K2829 | K2830 | M2831 | G2832 | L2833 | P2834 | V2835 | Q2843 | S2844 | F2845 | A2846 | L2847 | G2848 | G2859 | A2860 | L2861 | T2871 | L2876 | L2879 | G2880 | V2881 | G2882 | A2883 | D2884 | D2885 | I2886 | L2889 | S2890 | K2891 | H2892 | L2893 | D2894 | S2895 | T2896 | P2901 | N2902 | E2903 |       |       |       |       |       |       |
| Q2711 | E2712 | V2713 | V2717 | V2718 | V2722 | V2727 | V2727 | Y2730 | P2736 | C2740 | A2741 | A2743 | S2746 | V2751 | L2754 | L2763 | A2764 | G2765 | D2768 | D2769 | L2770 | E2773 | L2776 | G2779 | T2784 | A2785 | D2786 | T2787 | E2788 | M2789 | M2790 | R2791 | K2799 | D2800 | S2801 | R2802 | D2805 | R2806 | R2807 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| P2612 | R2613 | K2614 | L2617 | S2618 | R2619 | T2620 | G2622 | A2623 | Q2624 | L2625 | D2630 | P2631 | T2632 | V2633 | D2645 | R2646 | V2647 | A2648 | L2649 | L2649 | V2650 | N2651 | P2652 | P2653 | S2662 | P2666 | T2667 | W2672 | A2679 | S2680 | T2681 | M2686 | T2690 | S2691 | M2692 | Q2693 | G2694 | G2696 | M2696 | H2697 | G2698 | R2699 | L2700 | A2704 | K2705 | P2706 | I2709 | L2710 |       |       |       |       |       |       |       |
| M2481 | E2482 | V2483 | L2487 | V2492 | L2495 | K2503 | W2504 | E2505 | M2416 | S2417 | G2418 | D2421 | X2422 | X2425 | X2426 | X2427 | X2428 | X2429 | X2430 | X2431 | X2432 | X2433 | X2434 | X2435 | X2436 | X2437 | X2442 | X2443 | X2444 | X2445 | X2448 | X2449 | X2450 | X2451 | X2452 | X2453 | D2454 | A2458 | V2461 | V2462 | E2468 | L2469 | G2470 | P2471 | Y2472 | R2478 | V2811 |       |       |       |       |       |       |       |       |
| K2261 | E2137 | W2265 | V2140 | V2141 | T2163 | W2164 | L2165 | T2167 | R2170 | D2173 | D2174 | R2175 | L2176 | K2180 | R2188 | F2189 | T2192 | L2193 | W2194 | T2195 | V2196 | P2197 | A2198 | R2199 | M2200 | D2205 | L2209 | W2210 | E2211 | W2212 | V2213 | G2214 | T2215 | E2216 | K2229 | P2234 | T2235 | L2236 | L2237 | F2238 | R2244 | V2245 | A2246 | V2252 | R2255 |       |       |       |       |       |       |       |       |       |       |
| L2070 | E2074 | X2077 | X2078 | X2079 | X2080 | X2081 | X2082 | X2083 | X2084 | X2085 | X2086 | X2087 | X2088 | X2089 | X2090 | X2091 | X2092 | X2093 | X2094 | X2095 | X2096 | X2097 | X2098 | X2099 | X2100 | X2101 | X2102 | X2103 | X2104 | X2105 | X2106 | X2107 | X2108 | X2112 | X2113 | X2114 | X2115 | X2116 | X2117 | X2118 | X2119 | X2120 | X2121 | X2122 | X2123 | X2124 | X2125 | X2126 | X2127 | X2128 | X2129 | X2130 | X2131 | X2132 | X2135 |
| VAL   | ALA   | ALA   | ARG   | ARG   | GLY   | ILE   | SER   | VAL   | VAL   | SER   | PRO   | ALA   | PRO   | SER   | TRP   | ALA   | ALA   | GLY   | GLY   | HIS   | LYS   | ASP   | ALA   | VAL   | PHE   | GLY   | VAL   | THR   | THR   | GLY   | THR   | ASP   | VAL   | LEU   | LEU   | GLY   | GLY   | ASP   | ASP   | VAL   | ASP   | LYS   | VAL   | GLY   | ILE   | LYS   | ARG   | GLY   | ALA   | ALA   | TYR   | ILE   | THR   |       |       |
| SER   | GLU   | LEU   | ASN   | THR   | LEU   | GLY   | ALA   | ILE   | ASP   | GLY   | ALA   | GLY   | ALA   | ALA   | ASP   | LEU   | GLY   | GLY   | VAL   | GLN   | VAL   | THR   | LYS   | LEU   | ALA   | ARG   | PRO   | PHE   | GLY   | GLY   | ASP   | VAL   | LEU   | LEU   | GLY   | SER   | ASP   | VAL   | GLY   | PRO   | LYS   | VAL   | ILE   | LYS   | ARG   | GLY   | ALA   | ALA   | TYR   | ILE   | THR   |       |       |       |       |

## 4 Experimental information

| Property                             | Value                  | Source    |
|--------------------------------------|------------------------|-----------|
| Reconstruction method                | SINGLE PARTICLE        | Depositor |
| Imposed symmetry                     | POINT, D3              | Depositor |
| Number of particles used             | 106884                 | Depositor |
| Resolution determination method      | Not provided           | Depositor |
| CTF correction method                | EACH IMAGE             | Depositor |
| Microscope                           | FEI TITAN KRIOS        | Depositor |
| Voltage (kV)                         | 300                    | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 20                     | Depositor |
| Minimum defocus (nm)                 | 1500                   | Depositor |
| Maximum defocus (nm)                 | 5000                   | Depositor |
| Magnification                        | 100000                 | Depositor |
| Image detector                       | FEI FALCON I (4k x 4k) | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN

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         | $\# Z  > 2$ | RMSZ        | $\# Z  > 2$ |
| 1   | A     | 0.24         | 0/20319     | 0.48        | 0/27667     |
| 1   | B     | 0.24         | 0/20319     | 0.48        | 0/27667     |
| 1   | C     | 0.24         | 0/20319     | 0.48        | 0/27667     |
| 1   | D     | 0.24         | 0/20319     | 0.48        | 0/27667     |
| 1   | E     | 0.24         | 0/20319     | 0.48        | 0/27667     |
| 1   | F     | 0.24         | 0/20319     | 0.48        | 0/27667     |
| All | All   | 0.24         | 0/121914    | 0.48        | 0/166002    |

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 |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 5                   |
| 1   | B     | 0                   | 5                   |
| 1   | C     | 0                   | 5                   |
| 1   | D     | 0                   | 5                   |
| 1   | E     | 0                   | 5                   |
| 1   | F     | 0                   | 5                   |
| All | All   | 0                   | 30                  |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 1148 | GLU  | Peptide |

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| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 150  | THR  | Peptide |
| 1   | A     | 202  | GLY  | Peptide |
| 1   | A     | 2584 | ASP  | Peptide |
| 1   | A     | 357  | GLY  | Peptide |
| 1   | B     | 1148 | GLU  | Peptide |
| 1   | B     | 150  | THR  | Peptide |
| 1   | B     | 202  | GLY  | Peptide |
| 1   | B     | 2584 | ASP  | Peptide |
| 1   | B     | 357  | GLY  | Peptide |
| 1   | C     | 1148 | GLU  | Peptide |
| 1   | C     | 150  | THR  | Peptide |
| 1   | C     | 202  | GLY  | Peptide |
| 1   | C     | 2584 | ASP  | Peptide |
| 1   | C     | 357  | GLY  | Peptide |
| 1   | D     | 1148 | GLU  | Peptide |
| 1   | D     | 150  | THR  | Peptide |
| 1   | D     | 202  | GLY  | Peptide |
| 1   | D     | 2584 | ASP  | Peptide |
| 1   | D     | 357  | GLY  | Peptide |
| 1   | E     | 1148 | GLU  | Peptide |
| 1   | E     | 150  | THR  | Peptide |
| 1   | E     | 202  | GLY  | Peptide |
| 1   | E     | 2584 | ASP  | Peptide |
| 1   | E     | 357  | GLY  | Peptide |
| 1   | F     | 1148 | GLU  | Peptide |
| 1   | F     | 150  | THR  | Peptide |
| 1   | F     | 202  | GLY  | Peptide |
| 1   | F     | 2584 | ASP  | Peptide |
| 1   | F     | 357  | GLY  | 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     | 21020 | 0        | 20990    | 1056    | 0            |
| 1   | B     | 21020 | 0        | 20990    | 1067    | 0            |
| 1   | C     | 21020 | 0        | 20990    | 1051    | 0            |
| 1   | D     | 21020 | 0        | 20990    | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 1   | E     | 21020  | 0        | 20990    | 0       | 0            |
| 1   | F     | 21020  | 0        | 20990    | 0       | 0            |
| 2   | A     | 31     | 0        | 19       | 5       | 0            |
| 2   | B     | 31     | 0        | 19       | 5       | 0            |
| 2   | C     | 31     | 0        | 19       | 4       | 0            |
| 2   | D     | 31     | 0        | 19       | 0       | 0            |
| 2   | E     | 31     | 0        | 19       | 0       | 0            |
| 2   | F     | 31     | 0        | 19       | 0       | 0            |
| All | All   | 126306 | 0        | 126054   | 3117    | 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 25.

All (3117) 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) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:793:ARG:O    | 1:A:2435:UNK:HG2 | 1.31                     | 1.30              |
| 1:B:793:ARG:O    | 1:B:2435:UNK:HG2 | 1.31                     | 1.28              |
| 1:B:2100:UNK:O   | 1:B:2103:UNK:HG3 | 1.36                     | 1.26              |
| 1:A:2105:UNK:O   | 1:A:2108:UNK:HG3 | 1.34                     | 1.25              |
| 1:B:2105:UNK:O   | 1:B:2108:UNK:HG3 | 1.34                     | 1.25              |
| 1:C:2100:UNK:O   | 1:C:2103:UNK:HG3 | 1.36                     | 1.23              |
| 1:C:793:ARG:O    | 1:C:2435:UNK:HG2 | 1.31                     | 1.23              |
| 1:A:2093:UNK:HG1 | 1:A:2129:UNK:O   | 1.40                     | 1.22              |
| 1:A:2100:UNK:O   | 1:A:2103:UNK:HG3 | 1.36                     | 1.21              |
| 1:C:2105:UNK:O   | 1:C:2108:UNK:HG3 | 1.34                     | 1.21              |
| 1:C:2093:UNK:HG1 | 1:C:2129:UNK:O   | 1.39                     | 1.21              |
| 1:B:992:UNK:CG   | 1:B:996:UNK:HG3  | 1.72                     | 1.20              |
| 1:C:992:UNK:CG   | 1:C:996:UNK:HG3  | 1.72                     | 1.18              |
| 1:B:2093:UNK:HG1 | 1:B:2129:UNK:O   | 1.39                     | 1.18              |
| 1:A:992:UNK:CG   | 1:A:996:UNK:HG3  | 1.72                     | 1.18              |
| 1:B:2451:UNK:HG1 | 1:B:2454:ASP:OD2 | 1.44                     | 1.17              |
| 1:C:2451:UNK:HG1 | 1:C:2454:ASP:OD2 | 1.44                     | 1.16              |
| 1:A:2451:UNK:HG1 | 1:A:2454:ASP:OD2 | 1.44                     | 1.15              |
| 1:C:2094:UNK:HG2 | 1:C:2096:UNK:HG3 | 1.32                     | 1.12              |
| 1:C:2450:UNK:HG1 | 1:C:3016:ALA:HB1 | 1.23                     | 1.11              |
| 1:A:2450:UNK:HG1 | 1:A:3016:ALA:HB1 | 1.23                     | 1.11              |
| 1:B:2097:UNK:O   | 1:B:2100:UNK:HG3 | 1.51                     | 1.10              |
| 1:B:2450:UNK:HG1 | 1:B:3016:ALA:HB1 | 1.23                     | 1.09              |
| 1:A:2097:UNK:O   | 1:A:2100:UNK:HG3 | 1.51                     | 1.09              |
| 1:B:975:UNK:HG3  | 1:B:993:UNK:CG   | 1.83                     | 1.09              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:2097:UNK:O   | 1:C:2100:UNK:HG3 | 1.51                     | 1.09              |
| 1:A:975:UNK:HG3  | 1:A:993:UNK:CG   | 1.82                     | 1.08              |
| 1:A:2094:UNK:HG2 | 1:A:2096:UNK:HG3 | 1.32                     | 1.08              |
| 1:C:975:UNK:HG3  | 1:C:993:UNK:CG   | 1.83                     | 1.07              |
| 1:B:2094:UNK:HG2 | 1:B:2096:UNK:HG3 | 1.32                     | 1.07              |
| 1:A:981:UNK:HG1  | 1:A:987:UNK:HG2  | 1.37                     | 1.06              |
| 1:C:981:UNK:HG1  | 1:C:987:UNK:HG2  | 1.37                     | 1.04              |
| 1:C:934:UNK:O    | 1:C:937:UNK:HG3  | 1.57                     | 1.04              |
| 1:A:934:UNK:O    | 1:A:937:UNK:HG3  | 1.58                     | 1.03              |
| 1:B:981:UNK:HG1  | 1:B:987:UNK:HG2  | 1.37                     | 1.02              |
| 1:B:934:UNK:O    | 1:B:937:UNK:HG3  | 1.57                     | 1.02              |
| 1:B:2094:UNK:CG  | 1:B:2096:UNK:HG3 | 1.90                     | 1.02              |
| 1:C:975:UNK:CG   | 1:C:993:UNK:HG1  | 1.90                     | 1.01              |
| 1:C:992:UNK:CG   | 1:C:996:UNK:CG   | 2.39                     | 1.01              |
| 1:B:975:UNK:CG   | 1:B:993:UNK:HG1  | 1.90                     | 1.01              |
| 1:A:975:UNK:CG   | 1:A:993:UNK:HG1  | 1.89                     | 1.01              |
| 1:C:2094:UNK:CG  | 1:C:2096:UNK:HG3 | 1.90                     | 1.01              |
| 1:C:932:UNK:O    | 1:C:936:UNK:HG2  | 1.61                     | 1.00              |
| 1:A:2094:UNK:CG  | 1:A:2096:UNK:HG3 | 1.90                     | 1.00              |
| 1:B:2088:UNK:O   | 1:B:2091:UNK:HG3 | 1.61                     | 1.00              |
| 1:A:992:UNK:CG   | 1:A:996:UNK:CG   | 2.39                     | 1.00              |
| 1:A:2113:UNK:O   | 1:A:2116:UNK:HG3 | 1.62                     | 1.00              |
| 1:C:2113:UNK:O   | 1:C:2116:UNK:HG3 | 1.62                     | 1.00              |
| 1:B:992:UNK:CG   | 1:B:996:UNK:CG   | 2.39                     | 0.99              |
| 1:B:1220:UNK:HG3 | 1:B:1221:UNK:N   | 1.78                     | 0.99              |
| 1:B:2433:UNK:HA  | 1:B:2524:CYS:HB3 | 1.44                     | 0.99              |
| 1:A:2088:UNK:O   | 1:A:2091:UNK:HG3 | 1.61                     | 0.99              |
| 1:B:976:UNK:HG3  | 1:B:993:UNK:HB1  | 1.43                     | 0.99              |
| 1:B:932:UNK:O    | 1:B:936:UNK:HG2  | 1.61                     | 0.99              |
| 1:C:2088:UNK:O   | 1:C:2091:UNK:HG3 | 1.61                     | 0.99              |
| 1:A:992:UNK:HG1  | 1:A:996:UNK:HG3  | 1.41                     | 0.98              |
| 1:B:792:ALA:O    | 1:B:2433:UNK:CG  | 2.12                     | 0.98              |
| 1:A:932:UNK:O    | 1:A:936:UNK:HG2  | 1.61                     | 0.98              |
| 1:A:792:ALA:O    | 1:A:2433:UNK:CG  | 2.12                     | 0.98              |
| 1:B:2113:UNK:O   | 1:B:2116:UNK:HG3 | 1.62                     | 0.98              |
| 1:C:1220:UNK:HG3 | 1:C:1221:UNK:N   | 1.78                     | 0.98              |
| 1:C:792:ALA:O    | 1:C:2433:UNK:CG  | 2.12                     | 0.98              |
| 1:C:992:UNK:HG1  | 1:C:996:UNK:HG3  | 1.41                     | 0.98              |
| 1:A:976:UNK:HG3  | 1:A:993:UNK:HB1  | 1.43                     | 0.98              |
| 1:B:992:UNK:HG1  | 1:B:996:UNK:HG3  | 1.41                     | 0.97              |
| 1:C:975:UNK:HG3  | 1:C:993:UNK:HG1  | 0.99                     | 0.97              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:2096:UNK:O   | 1:B:2099:UNK:HG3  | 1.65                     | 0.97              |
| 1:A:2433:UNK:HA  | 1:A:2524:CYS:HB3  | 1.44                     | 0.97              |
| 1:C:1003:UNK:HG2 | 1:C:1004:UNK:N    | 1.78                     | 0.97              |
| 1:B:975:UNK:HG3  | 1:B:993:UNK:HG1   | 0.99                     | 0.97              |
| 1:C:407:VAL:HB   | 1:C:933:UNK:HG1   | 1.47                     | 0.96              |
| 1:A:3080:ARG:HG3 | 1:A:3080:ARG:HH11 | 1.29                     | 0.96              |
| 1:B:1003:UNK:HG2 | 1:B:1004:UNK:N    | 1.78                     | 0.96              |
| 1:C:2096:UNK:O   | 1:C:2099:UNK:HG3  | 1.65                     | 0.96              |
| 1:C:2433:UNK:HA  | 1:C:2524:CYS:HB3  | 1.44                     | 0.96              |
| 1:A:2096:UNK:O   | 1:A:2099:UNK:HG3  | 1.65                     | 0.96              |
| 1:B:407:VAL:HB   | 1:B:933:UNK:HG1   | 1.47                     | 0.96              |
| 1:C:3080:ARG:HG3 | 1:C:3080:ARG:HH11 | 1.29                     | 0.96              |
| 1:A:407:VAL:HB   | 1:A:933:UNK:HG1   | 1.47                     | 0.96              |
| 1:A:1220:UNK:HG3 | 1:A:1221:UNK:N    | 1.78                     | 0.95              |
| 1:A:793:ARG:HD3  | 1:A:2435:UNK:HG1  | 1.48                     | 0.95              |
| 1:C:976:UNK:HG3  | 1:C:993:UNK:HB1   | 1.43                     | 0.95              |
| 1:A:975:UNK:HG3  | 1:A:993:UNK:HG1   | 0.99                     | 0.95              |
| 1:B:3080:ARG:HG3 | 1:B:3080:ARG:HH11 | 1.29                     | 0.95              |
| 1:A:792:ALA:O    | 1:A:2433:UNK:HG1  | 1.67                     | 0.94              |
| 1:C:792:ALA:O    | 1:C:2433:UNK:HG1  | 1.67                     | 0.94              |
| 1:A:1003:UNK:HG2 | 1:A:1004:UNK:N    | 1.79                     | 0.94              |
| 1:B:792:ALA:O    | 1:B:2433:UNK:HG1  | 1.67                     | 0.94              |
| 1:B:793:ARG:HD3  | 1:B:2435:UNK:HG1  | 1.48                     | 0.94              |
| 1:B:992:UNK:HG1  | 1:B:996:UNK:CG    | 1.97                     | 0.93              |
| 1:C:793:ARG:HD3  | 1:C:2435:UNK:HG1  | 1.48                     | 0.93              |
| 1:A:793:ARG:O    | 1:A:2435:UNK:CG   | 2.16                     | 0.93              |
| 1:C:793:ARG:O    | 1:C:2435:UNK:CG   | 2.17                     | 0.93              |
| 1:A:992:UNK:HG1  | 1:A:996:UNK:CG    | 1.97                     | 0.93              |
| 1:B:793:ARG:O    | 1:B:2435:UNK:CG   | 2.17                     | 0.93              |
| 1:C:1212:UNK:HG2 | 1:C:1342:ARG:HH21 | 1.32                     | 0.93              |
| 1:A:929:UNK:O    | 1:A:930:UNK:HG3   | 1.69                     | 0.93              |
| 1:A:2127:UNK:O   | 1:A:2130:UNK:HG3  | 1.69                     | 0.93              |
| 1:B:2127:UNK:O   | 1:B:2130:UNK:HG3  | 1.70                     | 0.92              |
| 1:B:929:UNK:O    | 1:B:930:UNK:HG3   | 1.69                     | 0.92              |
| 1:B:1225:UNK:HG1 | 1:B:1283:ASP:OD1  | 1.70                     | 0.92              |
| 1:C:992:UNK:HG1  | 1:C:996:UNK:CG    | 1.97                     | 0.92              |
| 1:C:1225:UNK:HG1 | 1:C:1283:ASP:OD1  | 1.70                     | 0.92              |
| 1:A:1013:UNK:HG2 | 1:A:1014:UNK:N    | 1.84                     | 0.91              |
| 1:A:939:UNK:O    | 1:A:940:UNK:HG3   | 1.70                     | 0.91              |
| 1:C:1012:UNK:O   | 1:C:1013:UNK:HG3  | 1.69                     | 0.91              |
| 1:C:939:UNK:O    | 1:C:940:UNK:HG3   | 1.70                     | 0.91              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1212:UNK:HG2 | 1:A:1342:ARG:HH21 | 1.32                     | 0.91              |
| 1:B:1212:UNK:HG2 | 1:B:1342:ARG:HH21 | 1.32                     | 0.91              |
| 1:A:1225:UNK:HG1 | 1:A:1283:ASP:OD1  | 1.70                     | 0.91              |
| 1:C:2127:UNK:O   | 1:C:2130:UNK:HG3  | 1.69                     | 0.91              |
| 1:B:1012:UNK:O   | 1:B:1013:UNK:HG3  | 1.69                     | 0.91              |
| 1:A:2112:UNK:O   | 1:A:2115:UNK:HG3  | 1.70                     | 0.91              |
| 1:B:2112:UNK:O   | 1:B:2115:UNK:HG3  | 1.70                     | 0.91              |
| 1:A:943:UNK:O    | 1:A:944:UNK:HG3   | 1.71                     | 0.91              |
| 1:C:929:UNK:O    | 1:C:930:UNK:HG3   | 1.69                     | 0.91              |
| 1:C:1013:UNK:HG2 | 1:C:1014:UNK:N    | 1.84                     | 0.90              |
| 1:C:943:UNK:O    | 1:C:944:UNK:HG3   | 1.71                     | 0.90              |
| 1:C:2112:UNK:O   | 1:C:2115:UNK:HG3  | 1.70                     | 0.90              |
| 1:A:1012:UNK:O   | 1:A:1013:UNK:HG3  | 1.69                     | 0.90              |
| 1:B:939:UNK:O    | 1:B:940:UNK:HG3   | 1.70                     | 0.90              |
| 1:B:943:UNK:O    | 1:B:944:UNK:HG3   | 1.71                     | 0.90              |
| 1:B:1013:UNK:HG2 | 1:B:1014:UNK:N    | 1.84                     | 0.90              |
| 1:C:2093:UNK:HA  | 1:C:2097:UNK:HG1  | 1.52                     | 0.90              |
| 1:C:981:UNK:CG   | 1:C:987:UNK:HG2   | 2.02                     | 0.89              |
| 1:B:2093:UNK:HA  | 1:B:2097:UNK:HG1  | 1.52                     | 0.89              |
| 1:A:2093:UNK:HA  | 1:A:2097:UNK:HG1  | 1.52                     | 0.89              |
| 1:A:981:UNK:CG   | 1:A:987:UNK:HG2   | 2.02                     | 0.89              |
| 1:C:1002:UNK:O   | 1:C:1003:UNK:HG3  | 1.73                     | 0.89              |
| 1:C:2434:UNK:HG3 | 1:C:2524:CYS:HA   | 1.54                     | 0.89              |
| 1:B:1002:UNK:O   | 1:B:1003:UNK:HG3  | 1.73                     | 0.89              |
| 1:B:2103:UNK:HG2 | 1:B:2104:UNK:N    | 1.89                     | 0.88              |
| 1:B:981:UNK:CG   | 1:B:987:UNK:HG2   | 2.02                     | 0.88              |
| 1:B:2100:UNK:O   | 1:B:2103:UNK:CG   | 2.22                     | 0.88              |
| 1:C:2100:UNK:O   | 1:C:2103:UNK:CG   | 2.22                     | 0.88              |
| 1:C:928:ALA:HB1  | 1:C:931:UNK:HB1   | 1.55                     | 0.88              |
| 1:A:1002:UNK:O   | 1:A:1003:UNK:HG3  | 1.73                     | 0.88              |
| 1:B:2112:UNK:H   | 1:B:2115:UNK:CG   | 1.87                     | 0.88              |
| 1:A:2103:UNK:HG2 | 1:A:2104:UNK:N    | 1.89                     | 0.87              |
| 1:A:2451:UNK:CG  | 1:A:2454:ASP:OD2  | 2.22                     | 0.87              |
| 1:B:2112:UNK:H   | 1:B:2115:UNK:HG1  | 1.40                     | 0.87              |
| 1:A:2434:UNK:HG3 | 1:A:2524:CYS:HA   | 1.54                     | 0.87              |
| 1:B:2434:UNK:HG3 | 1:B:2524:CYS:HA   | 1.54                     | 0.87              |
| 1:B:928:ALA:HB1  | 1:B:931:UNK:HB1   | 1.55                     | 0.87              |
| 1:C:2112:UNK:H   | 1:C:2115:UNK:HG1  | 1.40                     | 0.87              |
| 1:B:2086:UNK:O   | 1:B:2089:UNK:HG3  | 1.74                     | 0.87              |
| 1:A:928:ALA:HB1  | 1:A:931:UNK:HB1   | 1.55                     | 0.87              |
| 1:B:2126:UNK:O   | 1:B:2129:UNK:HG3  | 1.75                     | 0.87              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:2086:UNK:O    | 1:A:2089:UNK:HG3 | 1.74                     | 0.86              |
| 1:A:2112:UNK:H    | 1:A:2115:UNK:CG  | 1.87                     | 0.86              |
| 1:C:992:UNK:CG    | 1:C:994:UNK:HG3  | 2.05                     | 0.86              |
| 1:A:2112:UNK:H    | 1:A:2115:UNK:HG1 | 1.40                     | 0.86              |
| 1:C:2112:UNK:H    | 1:C:2115:UNK:CG  | 1.87                     | 0.86              |
| 1:C:2451:UNK:CG   | 1:C:2454:ASP:OD2 | 2.22                     | 0.86              |
| 1:A:2126:UNK:O    | 1:A:2129:UNK:HG3 | 1.75                     | 0.86              |
| 1:A:992:UNK:CG    | 1:A:994:UNK:HG3  | 2.05                     | 0.86              |
| 1:C:2086:UNK:O    | 1:C:2089:UNK:HG3 | 1.74                     | 0.86              |
| 1:B:992:UNK:CG    | 1:B:994:UNK:CG   | 2.53                     | 0.86              |
| 1:A:2100:UNK:O    | 1:A:2103:UNK:CG  | 2.22                     | 0.86              |
| 1:B:2451:UNK:CG   | 1:B:2454:ASP:OD2 | 2.22                     | 0.86              |
| 1:A:931:UNK:HG1   | 1:A:933:UNK:CG   | 2.06                     | 0.86              |
| 1:A:992:UNK:CG    | 1:A:994:UNK:CG   | 2.53                     | 0.86              |
| 1:C:2126:UNK:O    | 1:C:2129:UNK:HG3 | 1.75                     | 0.86              |
| 1:C:992:UNK:CG    | 1:C:994:UNK:CG   | 2.53                     | 0.85              |
| 1:A:2085:UNK:O    | 1:A:2088:UNK:HG3 | 1.76                     | 0.85              |
| 1:B:2081:UNK:O    | 1:B:2084:UNK:HG3 | 1.76                     | 0.85              |
| 1:B:992:UNK:CG    | 1:B:994:UNK:HG3  | 2.05                     | 0.85              |
| 1:C:2103:UNK:HG2  | 1:C:2104:UNK:N   | 1.89                     | 0.85              |
| 1:B:1218:UNK:HG2  | 1:B:1441:GLN:OE1 | 1.77                     | 0.85              |
| 1:B:2085:UNK:O    | 1:B:2088:UNK:HG3 | 1.76                     | 0.85              |
| 1:B:935:UNK:O     | 1:B:939:UNK:HG3  | 1.77                     | 0.85              |
| 1:C:2081:UNK:O    | 1:C:2084:UNK:HG3 | 1.76                     | 0.85              |
| 1:C:1218:UNK:HG2  | 1:C:1441:GLN:OE1 | 1.77                     | 0.85              |
| 1:C:2085:UNK:O    | 1:C:2088:UNK:HG3 | 1.76                     | 0.85              |
| 1:A:1218:UNK:HG2  | 1:A:1441:GLN:OE1 | 1.77                     | 0.85              |
| 1:A:935:UNK:O     | 1:A:939:UNK:HG3  | 1.77                     | 0.85              |
| 1:A:2118:UNK:O    | 1:A:2122:UNK:HG3 | 1.76                     | 0.85              |
| 1:B:2118:UNK:O    | 1:B:2122:UNK:HG3 | 1.76                     | 0.84              |
| 1:A:2081:UNK:O    | 1:A:2084:UNK:HG3 | 1.76                     | 0.84              |
| 1:A:992:UNK:HG3   | 1:A:996:UNK:CG   | 2.07                     | 0.84              |
| 1:B:931:UNK:HG1   | 1:B:933:UNK:CG   | 2.06                     | 0.84              |
| 1:A:999:UNK:HG2   | 1:A:1007:UNK:CG  | 2.07                     | 0.84              |
| 1:C:2118:UNK:O    | 1:C:2122:UNK:HG3 | 1.76                     | 0.84              |
| 1:B:1538:ARG:HH11 | 1:B:1722:PRO:HB3 | 1.43                     | 0.84              |
| 1:C:935:UNK:O     | 1:C:939:UNK:HG3  | 1.77                     | 0.84              |
| 1:B:999:UNK:HG2   | 1:B:1007:UNK:CG  | 2.07                     | 0.84              |
| 1:C:931:UNK:HG1   | 1:C:933:UNK:CG   | 2.06                     | 0.83              |
| 1:A:43:PRO:HG2    | 1:A:348:ALA:HA   | 1.60                     | 0.83              |
| 1:C:992:UNK:HG3   | 1:C:996:UNK:CG   | 2.07                     | 0.83              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:2105:UNK:O    | 1:B:2108:UNK:CG  | 2.24                     | 0.83              |
| 1:A:992:UNK:HG1   | 1:A:994:UNK:CG   | 2.09                     | 0.83              |
| 1:C:999:UNK:O     | 1:C:1007:UNK:HG3 | 1.80                     | 0.82              |
| 1:C:1538:ARG:HH11 | 1:C:1722:PRO:HB3 | 1.43                     | 0.82              |
| 1:C:2097:UNK:O    | 1:C:2100:UNK:CG  | 2.27                     | 0.82              |
| 1:B:992:UNK:HG3   | 1:B:996:UNK:CG   | 2.07                     | 0.82              |
| 1:B:992:UNK:HG1   | 1:B:994:UNK:CG   | 2.09                     | 0.82              |
| 1:C:999:UNK:HG2   | 1:C:1007:UNK:CG  | 2.07                     | 0.82              |
| 1:A:2097:UNK:O    | 1:A:2100:UNK:CG  | 2.27                     | 0.82              |
| 1:C:992:UNK:HG1   | 1:C:994:UNK:CG   | 2.09                     | 0.82              |
| 1:A:2016:VAL:HG13 | 1:A:2020:PRO:HG3 | 1.62                     | 0.82              |
| 1:B:2097:UNK:O    | 1:B:2100:UNK:CG  | 2.27                     | 0.82              |
| 1:C:2016:VAL:HG13 | 1:C:2020:PRO:HG3 | 1.62                     | 0.82              |
| 1:B:999:UNK:O     | 1:B:1007:UNK:HG3 | 1.80                     | 0.81              |
| 1:A:2105:UNK:O    | 1:A:2108:UNK:CG  | 2.25                     | 0.81              |
| 1:A:2093:UNK:CG   | 1:A:2129:UNK:O   | 2.27                     | 0.81              |
| 1:B:2730:TYR:OH   | 1:B:3059:ARG:NH1 | 2.14                     | 0.81              |
| 1:B:43:PRO:HG2    | 1:B:348:ALA:HA   | 1.60                     | 0.81              |
| 1:B:2016:VAL:HG13 | 1:B:2020:PRO:HG3 | 1.62                     | 0.81              |
| 1:A:967:VAL:HA    | 1:A:970:ILE:HB   | 1.63                     | 0.81              |
| 1:C:2091:UNK:O    | 1:C:2132:UNK:HG1 | 1.80                     | 0.81              |
| 1:C:43:PRO:HG2    | 1:C:348:ALA:HA   | 1.60                     | 0.81              |
| 1:C:138:ARG:NH2   | 1:C:175:ASP:OD2  | 2.14                     | 0.81              |
| 1:A:2091:UNK:O    | 1:A:2132:UNK:HG1 | 1.80                     | 0.81              |
| 1:A:2730:TYR:OH   | 1:A:3059:ARG:NH1 | 2.14                     | 0.81              |
| 1:B:2091:UNK:O    | 1:B:2132:UNK:HG1 | 1.80                     | 0.81              |
| 1:A:138:ARG:NH2   | 1:A:175:ASP:OD2  | 2.14                     | 0.80              |
| 1:B:2093:UNK:CG   | 1:B:2129:UNK:O   | 2.27                     | 0.80              |
| 1:C:46:VAL:HB     | 1:C:155:VAL:HG13 | 1.63                     | 0.80              |
| 1:A:995:UNK:HB1   | 1:A:1011:UNK:HG3 | 1.63                     | 0.80              |
| 1:A:1538:ARG:HH11 | 1:A:1722:PRO:HB3 | 1.43                     | 0.80              |
| 1:C:2093:UNK:CG   | 1:C:2129:UNK:O   | 2.27                     | 0.80              |
| 1:B:995:UNK:HB1   | 1:B:1011:UNK:HG3 | 1.63                     | 0.80              |
| 1:C:2730:TYR:OH   | 1:C:3059:ARG:NH1 | 2.14                     | 0.80              |
| 1:A:931:UNK:CG    | 1:A:933:UNK:CG   | 2.60                     | 0.80              |
| 1:C:2123:UNK:O    | 1:C:2126:UNK:HG3 | 1.82                     | 0.80              |
| 1:B:138:ARG:NH2   | 1:B:175:ASP:OD2  | 2.14                     | 0.80              |
| 1:C:967:VAL:HA    | 1:C:970:ILE:HB   | 1.63                     | 0.80              |
| 1:A:1001:UNK:HG1  | 1:A:1018:ARG:NH2 | 1.97                     | 0.80              |
| 1:B:46:VAL:HB     | 1:B:155:VAL:HG13 | 1.63                     | 0.80              |
| 1:A:999:UNK:O     | 1:A:1007:UNK:HG3 | 1.80                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:273:ARG:HB2   | 1:C:282:VAL:H     | 1.47                     | 0.80              |
| 1:C:1001:UNK:HG1  | 1:C:1018:ARG:NH2  | 1.97                     | 0.79              |
| 1:A:46:VAL:HB     | 1:A:155:VAL:HG13  | 1.63                     | 0.79              |
| 1:B:931:UNK:CG    | 1:B:933:UNK:CG    | 2.60                     | 0.79              |
| 1:C:2105:UNK:O    | 1:C:2108:UNK:CG   | 2.24                     | 0.79              |
| 1:C:1220:UNK:CG   | 1:C:1221:UNK:N    | 2.46                     | 0.79              |
| 1:A:2098:UNK:O    | 1:A:2102:UNK:HG3  | 1.82                     | 0.79              |
| 1:B:1001:UNK:HG1  | 1:B:1018:ARG:NH2  | 1.97                     | 0.79              |
| 1:B:2610:ARG:HH12 | 1:B:2700:LEU:HD11 | 1.47                     | 0.79              |
| 1:C:931:UNK:CG    | 1:C:933:UNK:CG    | 2.60                     | 0.79              |
| 1:A:273:ARG:HB2   | 1:A:282:VAL:H     | 1.47                     | 0.79              |
| 1:B:2084:UNK:O    | 1:B:2087:UNK:HG3  | 1.82                     | 0.79              |
| 1:B:2098:UNK:O    | 1:B:2102:UNK:HG3  | 1.82                     | 0.78              |
| 1:C:2077:UNK:HG2  | 1:C:2079:UNK:HG3  | 1.65                     | 0.78              |
| 1:B:2077:UNK:HG2  | 1:B:2079:UNK:HG3  | 1.65                     | 0.78              |
| 1:B:2123:UNK:O    | 1:B:2126:UNK:HG3  | 1.82                     | 0.78              |
| 1:A:931:UNK:HG1   | 1:A:933:UNK:HG2   | 1.65                     | 0.78              |
| 1:C:2610:ARG:HH12 | 1:C:2700:LEU:HD11 | 1.47                     | 0.78              |
| 1:C:995:UNK:HB1   | 1:C:1011:UNK:HG3  | 1.63                     | 0.78              |
| 1:A:2084:UNK:O    | 1:A:2087:UNK:HG3  | 1.82                     | 0.78              |
| 1:B:930:UNK:O     | 1:B:930:UNK:HG2   | 1.83                     | 0.78              |
| 1:B:967:VAL:HA    | 1:B:970:ILE:HB    | 1.63                     | 0.78              |
| 1:B:273:ARG:HB2   | 1:B:282:VAL:H     | 1.47                     | 0.78              |
| 1:C:2098:UNK:O    | 1:C:2102:UNK:HG3  | 1.82                     | 0.78              |
| 1:C:930:UNK:HG2   | 1:C:930:UNK:O     | 1.83                     | 0.78              |
| 1:A:2077:UNK:HG2  | 1:A:2079:UNK:HG3  | 1.65                     | 0.78              |
| 1:A:2123:UNK:O    | 1:A:2126:UNK:HG3  | 1.82                     | 0.78              |
| 1:A:971:ALA:O     | 1:A:974:UNK:HG3   | 1.84                     | 0.78              |
| 1:C:2084:UNK:O    | 1:C:2087:UNK:HG3  | 1.82                     | 0.78              |
| 1:B:2135:UNK:HG3  | 1:B:2136:ASP:N    | 1.99                     | 0.77              |
| 1:C:971:ALA:O     | 1:C:974:UNK:HG3   | 1.84                     | 0.77              |
| 1:B:1220:UNK:CG   | 1:B:1221:UNK:N    | 2.46                     | 0.77              |
| 1:A:1329:ALA:HB3  | 1:A:1337:MET:H    | 1.48                     | 0.77              |
| 1:A:2135:UNK:HG3  | 1:A:2136:ASP:N    | 1.99                     | 0.77              |
| 1:A:930:UNK:O     | 1:A:930:UNK:HG2   | 1.83                     | 0.77              |
| 1:B:1329:ALA:HB3  | 1:B:1337:MET:H    | 1.49                     | 0.77              |
| 1:C:2135:UNK:HG3  | 1:C:2136:ASP:N    | 1.99                     | 0.77              |
| 1:C:2100:UNK:HG2  | 1:C:2101:UNK:N    | 2.00                     | 0.77              |
| 1:C:1329:ALA:HB3  | 1:C:1337:MET:H    | 1.49                     | 0.77              |
| 1:C:931:UNK:HG1   | 1:C:933:UNK:HG2   | 1.65                     | 0.77              |
| 1:B:971:ALA:O     | 1:B:974:UNK:HG3   | 1.84                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:931:UNK:CG    | 1:C:933:UNK:HG2   | 2.15                     | 0.77              |
| 1:B:931:UNK:CG    | 1:B:933:UNK:HG2   | 2.15                     | 0.77              |
| 1:A:257:ARG:HH12  | 1:C:1695:LEU:HD23 | 1.51                     | 0.76              |
| 1:A:2610:ARG:HH12 | 1:A:2700:LEU:HD11 | 1.47                     | 0.76              |
| 1:A:931:UNK:CG    | 1:A:933:UNK:HG2   | 2.15                     | 0.76              |
| 1:B:1695:LEU:HD23 | 1:C:257:ARG:HH12  | 1.50                     | 0.76              |
| 1:A:1695:LEU:HD23 | 1:B:257:ARG:HH12  | 1.51                     | 0.76              |
| 1:A:2557:LEU:O    | 1:A:2613:ARG:N    | 2.18                     | 0.76              |
| 1:A:944:UNK:HG2   | 1:A:944:UNK:O     | 1.85                     | 0.76              |
| 1:B:931:UNK:HG1   | 1:B:933:UNK:HG2   | 1.65                     | 0.76              |
| 1:C:934:UNK:O     | 1:C:937:UNK:CG    | 2.34                     | 0.76              |
| 1:A:1097:VAL:HB   | 1:A:1146:PRO:HB2  | 1.68                     | 0.76              |
| 1:B:1097:VAL:HB   | 1:B:1146:PRO:HB2  | 1.68                     | 0.76              |
| 1:A:1220:UNK:CG   | 1:A:1221:UNK:N    | 2.46                     | 0.76              |
| 1:A:2100:UNK:HG2  | 1:A:2101:UNK:N    | 2.00                     | 0.76              |
| 1:B:2557:LEU:O    | 1:B:2613:ARG:N    | 2.18                     | 0.76              |
| 1:A:995:UNK:HB1   | 1:A:1011:UNK:CG   | 2.17                     | 0.75              |
| 1:B:2124:UNK:O    | 1:B:2127:UNK:HG3  | 1.86                     | 0.75              |
| 1:C:2452:UNK:HG2  | 1:C:2453:UNK:N    | 2.01                     | 0.75              |
| 1:A:940:UNK:O     | 1:A:940:UNK:HG2   | 1.86                     | 0.75              |
| 1:B:2126:UNK:C    | 1:B:2129:UNK:HG3  | 2.16                     | 0.75              |
| 1:B:2452:UNK:HG2  | 1:B:2453:UNK:N    | 2.00                     | 0.75              |
| 1:B:2418:GLY:O    | 1:B:2422:UNK:HG3  | 1.87                     | 0.75              |
| 1:B:944:UNK:O     | 1:B:944:UNK:HG2   | 1.85                     | 0.75              |
| 1:C:2124:UNK:O    | 1:C:2127:UNK:HG3  | 1.87                     | 0.75              |
| 1:A:2452:UNK:HG2  | 1:A:2453:UNK:N    | 2.00                     | 0.75              |
| 1:A:2418:GLY:O    | 1:A:2422:UNK:HG3  | 1.87                     | 0.75              |
| 1:B:2645:ASP:OD2  | 1:B:2691:SER:N    | 2.19                     | 0.75              |
| 1:A:1212:UNK:HG2  | 1:A:1342:ARG:NH2  | 2.02                     | 0.75              |
| 1:B:2088:UNK:O    | 1:B:2091:UNK:CG   | 2.35                     | 0.75              |
| 1:B:2100:UNK:HG2  | 1:B:2101:UNK:N    | 2.00                     | 0.75              |
| 1:B:995:UNK:HB1   | 1:B:1011:UNK:CG   | 2.17                     | 0.75              |
| 1:C:2122:UNK:O    | 1:C:2125:UNK:HG3  | 1.87                     | 0.75              |
| 1:A:2122:UNK:O    | 1:A:2125:UNK:HG3  | 1.87                     | 0.74              |
| 1:C:2418:GLY:O    | 1:C:2422:UNK:HG3  | 1.87                     | 0.74              |
| 1:C:445:VAL:HG13  | 1:C:475:LEU:HD21  | 1.69                     | 0.74              |
| 1:C:944:UNK:HG2   | 1:C:944:UNK:O     | 1.85                     | 0.74              |
| 1:C:995:UNK:HB1   | 1:C:1011:UNK:CG   | 2.17                     | 0.74              |
| 1:C:1097:VAL:HB   | 1:C:1146:PRO:HB2  | 1.68                     | 0.74              |
| 1:C:2088:UNK:O    | 1:C:2091:UNK:CG   | 2.35                     | 0.74              |
| 1:B:1212:UNK:HG2  | 1:B:1342:ARG:NH2  | 2.02                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:445:VAL:HG13  | 1:B:475:LEU:HD21  | 1.69                     | 0.74              |
| 1:A:2124:UNK:O    | 1:A:2127:UNK:HG3  | 1.86                     | 0.74              |
| 1:C:33:ALA:HB2    | 1:C:390:VAL:HA    | 1.70                     | 0.74              |
| 1:A:1556:GLU:OE2  | 1:A:1560:ARG:NH2  | 2.20                     | 0.74              |
| 1:A:33:ALA:HB2    | 1:A:390:VAL:HA    | 1.70                     | 0.74              |
| 1:B:940:UNK:HG2   | 1:B:940:UNK:O     | 1.86                     | 0.74              |
| 1:A:934:UNK:O     | 1:A:937:UNK:CG    | 2.34                     | 0.74              |
| 1:C:940:UNK:HG2   | 1:C:940:UNK:O     | 1.86                     | 0.74              |
| 1:A:2087:UNK:HA   | 1:A:2090:UNK:HG3  | 1.70                     | 0.74              |
| 1:A:2126:UNK:C    | 1:A:2129:UNK:HG3  | 2.17                     | 0.74              |
| 1:A:2645:ASP:OD2  | 1:A:2691:SER:N    | 2.19                     | 0.74              |
| 1:A:994:UNK:HG2   | 1:A:996:UNK:HG3   | 1.70                     | 0.74              |
| 1:B:2122:UNK:O    | 1:B:2125:UNK:HG3  | 1.87                     | 0.74              |
| 1:C:1212:UNK:CG   | 1:C:1342:ARG:HE   | 2.01                     | 0.74              |
| 1:C:2557:LEU:O    | 1:C:2613:ARG:N    | 2.18                     | 0.74              |
| 1:B:1212:UNK:CG   | 1:B:1342:ARG:HE   | 2.01                     | 0.74              |
| 1:B:33:ALA:HB2    | 1:B:390:VAL:HA    | 1.69                     | 0.74              |
| 1:C:1212:UNK:HG2  | 1:C:1342:ARG:NH2  | 2.02                     | 0.74              |
| 1:A:799:PHE:CZ    | 1:A:2433:UNK:HG3  | 2.23                     | 0.74              |
| 1:A:992:UNK:HG3   | 1:A:996:UNK:HG3   | 1.66                     | 0.74              |
| 1:B:1001:UNK:O    | 1:B:1002:UNK:HG3  | 1.88                     | 0.74              |
| 1:B:1556:GLU:OE2  | 1:B:1560:ARG:NH2  | 2.20                     | 0.74              |
| 1:C:1168:ARG:N    | 1:C:1194:ILE:O    | 2.21                     | 0.74              |
| 1:C:1556:GLU:OE2  | 1:C:1560:ARG:NH2  | 2.20                     | 0.74              |
| 1:A:1212:UNK:CG   | 1:A:1342:ARG:HE   | 2.01                     | 0.73              |
| 1:B:1226:UNK:HG3  | 1:B:1313:VAL:HG12 | 1.70                     | 0.73              |
| 1:B:2087:UNK:HA   | 1:B:2090:UNK:HG3  | 1.70                     | 0.73              |
| 1:B:934:UNK:O     | 1:B:937:UNK:CG    | 2.34                     | 0.73              |
| 1:C:2126:UNK:C    | 1:C:2129:UNK:HG3  | 2.17                     | 0.73              |
| 1:A:992:UNK:HG2   | 1:A:994:UNK:CG    | 2.17                     | 0.73              |
| 1:A:1168:ARG:N    | 1:A:1194:ILE:O    | 2.21                     | 0.73              |
| 1:B:992:UNK:HG2   | 1:B:994:UNK:CG    | 2.17                     | 0.73              |
| 1:C:994:UNK:HG2   | 1:C:996:UNK:HG3   | 1.70                     | 0.73              |
| 1:B:3015:ILE:HG12 | 1:B:3023:ARG:HG3  | 1.69                     | 0.73              |
| 1:C:2096:UNK:O    | 1:C:2099:UNK:CG   | 2.37                     | 0.73              |
| 1:B:799:PHE:CZ    | 1:B:2433:UNK:HG3  | 2.23                     | 0.73              |
| 1:C:799:PHE:CZ    | 1:C:2433:UNK:HG3  | 2.23                     | 0.73              |
| 1:B:994:UNK:HG2   | 1:B:996:UNK:HG3   | 1.70                     | 0.73              |
| 1:C:3015:ILE:HG12 | 1:C:3023:ARG:HG3  | 1.69                     | 0.73              |
| 1:A:2883:ALA:O    | 1:A:2916:ARG:NH1  | 2.22                     | 0.73              |
| 1:B:2053:ALA:O    | 1:B:2807:ARG:NH2  | 2.21                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2096:UNK:O    | 1:B:2099:UNK:CG   | 2.36                     | 0.73              |
| 1:C:2053:ALA:O    | 1:C:2807:ARG:NH2  | 2.21                     | 0.73              |
| 1:C:437:PRO:HG3   | 1:C:876:LEU:HB3   | 1.70                     | 0.73              |
| 1:C:980:UNK:O     | 1:C:981:UNK:HG3   | 1.89                     | 0.73              |
| 1:B:2093:UNK:HA   | 1:B:2097:UNK:CG   | 2.19                     | 0.73              |
| 1:C:1001:UNK:O    | 1:C:1002:UNK:HG3  | 1.88                     | 0.73              |
| 1:C:992:UNK:HG2   | 1:C:994:UNK:CG    | 2.17                     | 0.73              |
| 1:A:2053:ALA:O    | 1:A:2807:ARG:NH2  | 2.21                     | 0.72              |
| 1:B:437:PRO:HG3   | 1:B:876:LEU:HB3   | 1.70                     | 0.72              |
| 1:C:976:UNK:HG3   | 1:C:993:UNK:CB    | 2.19                     | 0.72              |
| 1:B:1168:ARG:N    | 1:B:1194:ILE:O    | 2.21                     | 0.72              |
| 1:C:2883:ALA:O    | 1:C:2916:ARG:NH1  | 2.22                     | 0.72              |
| 1:C:936:UNK:HB1   | 1:C:941:UNK:HB1   | 1.71                     | 0.72              |
| 1:A:1226:UNK:HG3  | 1:A:1313:VAL:HG12 | 1.70                     | 0.72              |
| 1:B:1253:ARG:HH11 | 1:B:1253:ARG:HG3  | 1.55                     | 0.72              |
| 1:C:1253:ARG:HH11 | 1:C:1253:ARG:HG3  | 1.54                     | 0.72              |
| 1:C:1226:UNK:HG3  | 1:C:1313:VAL:HG12 | 1.70                     | 0.72              |
| 1:C:1400:PRO:HD2  | 1:C:1416:VAL:HG22 | 1.72                     | 0.72              |
| 1:A:2093:UNK:HA   | 1:A:2097:UNK:CG   | 2.19                     | 0.72              |
| 1:B:1400:PRO:HD2  | 1:B:1416:VAL:HG22 | 1.72                     | 0.72              |
| 1:A:1001:UNK:O    | 1:A:1002:UNK:HG3  | 1.88                     | 0.72              |
| 1:C:70:SER:OG     | 1:C:142:ARG:NH2   | 2.23                     | 0.72              |
| 1:C:2645:ASP:OD2  | 1:C:2691:SER:N    | 2.19                     | 0.72              |
| 1:A:2088:UNK:O    | 1:A:2091:UNK:CG   | 2.35                     | 0.72              |
| 1:A:95:PRO:HB2    | 1:C:1237:ARG:NH1  | 2.05                     | 0.72              |
| 1:A:980:UNK:O     | 1:A:981:UNK:HG3   | 1.89                     | 0.72              |
| 1:B:2121:UNK:O    | 1:B:2124:UNK:HG3  | 1.90                     | 0.72              |
| 1:B:936:UNK:HB1   | 1:B:941:UNK:HB1   | 1.71                     | 0.72              |
| 1:A:70:SER:OG     | 1:A:142:ARG:NH2   | 2.23                     | 0.72              |
| 1:A:2113:UNK:O    | 1:A:2116:UNK:CG   | 2.38                     | 0.72              |
| 1:A:3015:ILE:HG12 | 1:A:3023:ARG:HG3  | 1.69                     | 0.72              |
| 1:A:445:VAL:HG13  | 1:A:475:LEU:HD21  | 1.69                     | 0.72              |
| 1:B:1218:UNK:CG   | 1:B:1441:GLN:OE1  | 2.38                     | 0.72              |
| 1:C:2093:UNK:HA   | 1:C:2097:UNK:CG   | 2.19                     | 0.72              |
| 1:A:992:UNK:HG2   | 1:A:994:UNK:HG3   | 1.72                     | 0.72              |
| 1:B:980:UNK:O     | 1:B:981:UNK:HG3   | 1.89                     | 0.72              |
| 1:A:1253:ARG:HG3  | 1:A:1253:ARG:HH11 | 1.55                     | 0.72              |
| 1:A:1400:PRO:HD2  | 1:A:1416:VAL:HG22 | 1.72                     | 0.72              |
| 1:B:2883:ALA:O    | 1:B:2916:ARG:NH1  | 2.22                     | 0.72              |
| 1:C:992:UNK:HG2   | 1:C:994:UNK:HG3   | 1.72                     | 0.72              |
| 1:C:2087:UNK:HA   | 1:C:2090:UNK:HG3  | 1.70                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2268:GLN:OE1  | 1:C:2319:ARG:NH1  | 2.23                     | 0.71              |
| 1:A:2121:UNK:O    | 1:A:2124:UNK:HG3  | 1.90                     | 0.71              |
| 1:B:1237:ARG:NH1  | 1:C:95:PRO:HB2    | 2.05                     | 0.71              |
| 1:B:70:SER:OG     | 1:B:142:ARG:NH2   | 2.23                     | 0.71              |
| 1:B:2268:GLN:OE1  | 1:B:2319:ARG:NH1  | 2.23                     | 0.71              |
| 1:A:1237:ARG:NH1  | 1:B:95:PRO:HB2    | 2.05                     | 0.71              |
| 1:A:981:UNK:HG1   | 1:A:987:UNK:CG    | 2.19                     | 0.71              |
| 1:C:1218:UNK:CG   | 1:C:1441:GLN:OE1  | 2.38                     | 0.71              |
| 1:C:2113:UNK:O    | 1:C:2116:UNK:CG   | 2.38                     | 0.71              |
| 1:A:976:UNK:HG3   | 1:A:993:UNK:CB    | 2.19                     | 0.71              |
| 1:A:982:UNK:HG2   | 1:A:983:UNK:N     | 2.05                     | 0.71              |
| 1:B:2998:GLY:N    | 1:B:3002:VAL:O    | 2.23                     | 0.71              |
| 1:B:976:UNK:HG3   | 1:B:993:UNK:CB    | 2.19                     | 0.71              |
| 1:B:982:UNK:HG2   | 1:B:983:UNK:N     | 2.05                     | 0.71              |
| 1:A:981:UNK:HB2   | 1:A:984:UNK:CG    | 2.21                     | 0.71              |
| 1:A:936:UNK:HB1   | 1:A:941:UNK:HB1   | 1.71                     | 0.71              |
| 1:C:1634:ARG:HH11 | 1:C:1639:ALA:H    | 1.39                     | 0.71              |
| 1:C:2121:UNK:O    | 1:C:2124:UNK:HG3  | 1.90                     | 0.71              |
| 1:A:2096:UNK:O    | 1:A:2099:UNK:CG   | 2.37                     | 0.70              |
| 1:C:1507:GLN:O    | 1:C:1562:ARG:NH1  | 2.24                     | 0.70              |
| 1:C:982:UNK:HG2   | 1:C:983:UNK:N     | 2.05                     | 0.70              |
| 1:A:437:PRO:HG3   | 1:A:876:LEU:HB3   | 1.70                     | 0.70              |
| 1:C:2112:UNK:O    | 1:C:2115:UNK:CG   | 2.38                     | 0.70              |
| 1:A:1218:UNK:CG   | 1:A:1441:GLN:OE1  | 2.38                     | 0.70              |
| 1:A:2268:GLN:OE1  | 1:A:2319:ARG:NH1  | 2.23                     | 0.70              |
| 1:A:2558:LEU:HG   | 1:A:2612:PRO:HA   | 1.73                     | 0.70              |
| 1:A:1507:GLN:O    | 1:A:1562:ARG:NH1  | 2.24                     | 0.70              |
| 1:B:981:UNK:HB2   | 1:B:984:UNK:CG    | 2.21                     | 0.70              |
| 1:C:981:UNK:HG1   | 1:C:987:UNK:CG    | 2.19                     | 0.70              |
| 1:B:137:VAL:HG22  | 1:B:354:LEU:HD13  | 1.74                     | 0.70              |
| 1:B:1634:ARG:HH11 | 1:B:1639:ALA:H    | 1.39                     | 0.70              |
| 1:A:2743:ALA:HB1  | 1:A:2940:VAL:HG23 | 1.73                     | 0.70              |
| 1:A:2998:GLY:N    | 1:A:3002:VAL:O    | 2.23                     | 0.70              |
| 1:C:981:UNK:HB2   | 1:C:984:UNK:CG    | 2.21                     | 0.70              |
| 1:C:2558:LEU:HG   | 1:C:2612:PRO:HA   | 1.73                     | 0.70              |
| 1:B:580:ARG:HD2   | 1:B:614:GLY:HA3   | 1.73                     | 0.70              |
| 1:C:974:UNK:HG1   | 1:C:977:UNK:HB1   | 1.74                     | 0.70              |
| 1:B:2112:UNK:O    | 1:B:2115:UNK:CG   | 2.38                     | 0.70              |
| 1:B:2743:ALA:HB1  | 1:B:2940:VAL:HG23 | 1.73                     | 0.70              |
| 1:B:992:UNK:HG2   | 1:B:994:UNK:HG3   | 1.72                     | 0.70              |
| 1:A:1634:ARG:HH11 | 1:A:1639:ALA:H    | 1.39                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2112:UNK:O    | 1:A:2115:UNK:CG   | 2.38                     | 0.69              |
| 1:C:1035:VAL:HG12 | 1:C:1037:ASP:H    | 1.57                     | 0.69              |
| 1:C:580:ARG:HD2   | 1:C:614:GLY:HA3   | 1.72                     | 0.69              |
| 1:A:1035:VAL:HG12 | 1:A:1037:ASP:H    | 1.57                     | 0.69              |
| 1:A:2860:ALA:HB3  | 1:A:2906:LEU:HD21 | 1.73                     | 0.69              |
| 1:A:580:ARG:HD2   | 1:A:614:GLY:HA3   | 1.73                     | 0.69              |
| 1:B:2860:ALA:HB3  | 1:B:2906:LEU:HD21 | 1.73                     | 0.69              |
| 1:C:2860:ALA:HB3  | 1:C:2906:LEU:HD21 | 1.73                     | 0.69              |
| 1:B:2215:THR:HB   | 1:B:2229:LYS:HB2  | 1.74                     | 0.69              |
| 1:C:2085:UNK:O    | 1:C:2088:UNK:CG   | 2.41                     | 0.69              |
| 1:A:1012:UNK:O    | 1:A:1013:UNK:CG   | 2.41                     | 0.69              |
| 1:B:1177:ARG:HB2  | 1:B:1184:LEU:HD23 | 1.74                     | 0.69              |
| 1:A:137:VAL:HG22  | 1:A:354:LEU:HD13  | 1.74                     | 0.69              |
| 1:B:1164:THR:N    | 1:B:1167:GLY:O    | 2.25                     | 0.69              |
| 1:B:2558:LEU:HG   | 1:B:2612:PRO:HA   | 1.74                     | 0.69              |
| 1:C:2122:UNK:HA   | 1:C:2125:UNK:HG3  | 1.75                     | 0.69              |
| 1:A:2215:THR:HB   | 1:A:2229:LYS:HB2  | 1.74                     | 0.69              |
| 1:B:2122:UNK:HA   | 1:B:2125:UNK:HG3  | 1.75                     | 0.69              |
| 1:C:2647:VAL:HG22 | 1:C:2769:ASP:HB2  | 1.75                     | 0.69              |
| 1:B:1046:LEU:HD13 | 1:B:1129:LEU:HD22 | 1.75                     | 0.69              |
| 1:B:1507:GLN:O    | 1:B:1562:ARG:NH1  | 2.24                     | 0.69              |
| 1:C:1046:LEU:HD13 | 1:C:1129:LEU:HD22 | 1.75                     | 0.69              |
| 1:C:2743:ALA:HB1  | 1:C:2940:VAL:HG23 | 1.73                     | 0.69              |
| 1:C:2998:GLY:N    | 1:C:3002:VAL:O    | 2.23                     | 0.69              |
| 1:A:1046:LEU:HD13 | 1:A:1129:LEU:HD22 | 1.75                     | 0.69              |
| 1:C:2445:UNK:HG2  | 1:C:2985:GLY:O    | 1.93                     | 0.69              |
| 1:C:2112:UNK:C    | 1:C:2115:UNK:HG3  | 2.22                     | 0.69              |
| 1:B:2085:UNK:O    | 1:B:2088:UNK:CG   | 2.40                     | 0.69              |
| 1:B:2946:LEU:HD11 | 1:B:2992:GLY:HA3  | 1.75                     | 0.69              |
| 1:A:2445:UNK:HG2  | 1:A:2985:GLY:O    | 1.93                     | 0.68              |
| 1:C:992:UNK:HG3   | 1:C:996:UNK:HG3   | 1.66                     | 0.68              |
| 1:B:2113:UNK:C    | 1:B:2116:UNK:HG3  | 2.23                     | 0.68              |
| 1:A:1177:ARG:HB2  | 1:A:1184:LEU:HD23 | 1.74                     | 0.68              |
| 1:A:511:ARG:HD3   | 1:A:543:GLY:HA3   | 1.76                     | 0.68              |
| 1:B:2112:UNK:C    | 1:B:2115:UNK:HG3  | 2.22                     | 0.68              |
| 1:B:2113:UNK:O    | 1:B:2116:UNK:CG   | 2.37                     | 0.68              |
| 1:C:2093:UNK:CG   | 1:C:2132:UNK:HB1  | 2.24                     | 0.68              |
| 1:B:1035:VAL:HG12 | 1:B:1037:ASP:H    | 1.57                     | 0.68              |
| 1:B:340:ILE:HD13  | 1:B:364:THR:HG21  | 1.75                     | 0.68              |
| 1:C:1164:THR:N    | 1:C:1167:GLY:O    | 2.25                     | 0.68              |
| 1:C:1177:ARG:HB2  | 1:C:1184:LEU:HD23 | 1.74                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2112:UNK:C    | 1:A:2115:UNK:HG3  | 2.22                     | 0.68              |
| 1:A:340:ILE:HD13  | 1:A:364:THR:HG21  | 1.75                     | 0.68              |
| 1:C:2113:UNK:C    | 1:C:2116:UNK:HG3  | 2.23                     | 0.68              |
| 1:C:511:ARG:HD3   | 1:C:543:GLY:HA3   | 1.76                     | 0.68              |
| 1:A:2093:UNK:CG   | 1:A:2132:UNK:HB1  | 2.24                     | 0.68              |
| 1:B:2093:UNK:CG   | 1:B:2132:UNK:HB1  | 2.24                     | 0.68              |
| 1:B:2647:VAL:HG22 | 1:B:2769:ASP:HB2  | 1.75                     | 0.68              |
| 1:C:137:VAL:HG22  | 1:C:354:LEU:HD13  | 1.74                     | 0.68              |
| 1:C:2215:THR:HB   | 1:C:2229:LYS:HB2  | 1.74                     | 0.68              |
| 1:A:2080:UNK:HB2  | 1:A:2082:UNK:HG3  | 1.75                     | 0.68              |
| 1:A:2946:LEU:HD11 | 1:A:2992:GLY:HA3  | 1.75                     | 0.68              |
| 1:C:269:GLU:HB3   | 1:C:282:VAL:HA    | 1.75                     | 0.68              |
| 1:A:2085:UNK:O    | 1:A:2088:UNK:CG   | 2.40                     | 0.68              |
| 1:B:2445:UNK:HG2  | 1:B:2985:GLY:O    | 1.93                     | 0.68              |
| 1:C:1488:VAL:HG21 | 1:C:1580:PRO:HD2  | 1.76                     | 0.68              |
| 1:C:2097:UNK:C    | 1:C:2100:UNK:HG3  | 2.24                     | 0.68              |
| 1:A:992:UNK:HG3   | 1:A:996:UNK:HG2   | 1.76                     | 0.68              |
| 1:A:1724:TYR:OH   | 1:B:267:GLU:OE2   | 2.08                     | 0.68              |
| 1:B:511:ARG:HD3   | 1:B:543:GLY:HA3   | 1.76                     | 0.68              |
| 1:C:2080:UNK:HB2  | 1:C:2082:UNK:HG3  | 1.75                     | 0.68              |
| 1:A:2112:UNK:HG2  | 1:A:2114:UNK:HG3  | 1.77                     | 0.67              |
| 1:A:2122:UNK:HA   | 1:A:2125:UNK:HG3  | 1.75                     | 0.67              |
| 1:A:974:UNK:HG1   | 1:A:977:UNK:HB1   | 1.74                     | 0.67              |
| 1:C:2946:LEU:HD11 | 1:C:2992:GLY:HA3  | 1.75                     | 0.67              |
| 1:C:3080:ARG:HH11 | 1:C:3080:ARG:CG   | 2.07                     | 0.67              |
| 1:A:2113:UNK:C    | 1:A:2116:UNK:HG3  | 2.23                     | 0.67              |
| 1:B:1163:ASP:HB3  | 1:B:1199:UNK:HG3  | 1.76                     | 0.67              |
| 1:B:974:UNK:HG1   | 1:B:977:UNK:HB1   | 1.74                     | 0.67              |
| 1:A:1164:THR:N    | 1:A:1167:GLY:O    | 2.25                     | 0.67              |
| 1:B:2103:UNK:CG   | 1:B:2104:UNK:N    | 2.58                     | 0.67              |
| 1:C:2112:UNK:HG2  | 1:C:2114:UNK:HG3  | 1.77                     | 0.67              |
| 1:B:2086:UNK:C    | 1:B:2089:UNK:HG3  | 2.25                     | 0.67              |
| 1:B:2093:UNK:HG3  | 1:B:2132:UNK:HB1  | 1.77                     | 0.67              |
| 1:B:3080:ARG:CG   | 1:B:3080:ARG:HH11 | 2.07                     | 0.67              |
| 1:B:792:ALA:HA    | 1:B:799:PHE:HE2   | 1.60                     | 0.67              |
| 1:C:2103:UNK:CG   | 1:C:2104:UNK:N    | 2.58                     | 0.67              |
| 1:C:2093:UNK:HG3  | 1:C:2132:UNK:HB1  | 1.77                     | 0.67              |
| 1:C:340:ILE:HD13  | 1:C:364:THR:HG21  | 1.75                     | 0.67              |
| 1:A:2112:UNK:N    | 1:A:2115:UNK:CG   | 2.57                     | 0.67              |
| 1:A:2126:UNK:O    | 1:A:2129:UNK:CG   | 2.43                     | 0.67              |
| 1:B:2080:UNK:HB2  | 1:B:2082:UNK:HG3  | 1.75                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:269:GLU:HB3   | 1:B:282:VAL:HA    | 1.75                     | 0.67              |
| 1:A:2081:UNK:O    | 1:A:2084:UNK:CG   | 2.43                     | 0.67              |
| 1:A:2097:UNK:C    | 1:A:2100:UNK:HG3  | 2.24                     | 0.67              |
| 1:B:2080:UNK:O    | 1:B:2083:UNK:HG3  | 1.94                     | 0.67              |
| 1:B:931:UNK:CG    | 1:B:933:UNK:HG3   | 2.25                     | 0.67              |
| 1:A:1008:UNK:HG3  | 1:A:1019:PHE:HB3  | 1.76                     | 0.67              |
| 1:A:2103:UNK:CG   | 1:A:2104:UNK:N    | 2.58                     | 0.67              |
| 1:B:1488:VAL:HG12 | 1:B:1490:ARG:NH1  | 2.10                     | 0.67              |
| 1:A:1488:VAL:HG21 | 1:A:1580:PRO:HD2  | 1.76                     | 0.66              |
| 1:A:2084:UNK:C    | 1:A:2087:UNK:HG3  | 2.25                     | 0.66              |
| 1:A:2647:VAL:HG22 | 1:A:2769:ASP:HB2  | 1.75                     | 0.66              |
| 1:A:269:GLU:HB3   | 1:A:282:VAL:HA    | 1.75                     | 0.66              |
| 1:C:1008:UNK:HG3  | 1:C:1019:PHE:HB3  | 1.76                     | 0.66              |
| 1:C:970:ILE:HG12  | 1:C:996:UNK:HG1   | 1.76                     | 0.66              |
| 1:A:2080:UNK:O    | 1:A:2083:UNK:HG3  | 1.95                     | 0.66              |
| 1:A:2093:UNK:HG3  | 1:A:2132:UNK:HB1  | 1.77                     | 0.66              |
| 1:A:511:ARG:HB2   | 1:A:540:ASN:HB2   | 1.77                     | 0.66              |
| 1:A:792:ALA:HA    | 1:A:799:PHE:HE2   | 1.60                     | 0.66              |
| 1:B:1012:UNK:O    | 1:B:1013:UNK:CG   | 2.41                     | 0.66              |
| 1:B:1168:ARG:HB2  | 1:B:1197:UNK:HB2  | 1.77                     | 0.66              |
| 1:B:2084:UNK:C    | 1:B:2087:UNK:HG3  | 2.25                     | 0.66              |
| 1:C:1163:ASP:HB3  | 1:C:1199:UNK:HG3  | 1.76                     | 0.66              |
| 1:C:981:UNK:O     | 1:C:981:UNK:HG2   | 1.95                     | 0.66              |
| 1:C:992:UNK:HG3   | 1:C:996:UNK:HG2   | 1.76                     | 0.66              |
| 1:B:2097:UNK:C    | 1:B:2100:UNK:HG3  | 2.24                     | 0.66              |
| 1:B:992:UNK:HG3   | 1:B:996:UNK:HG2   | 1.76                     | 0.66              |
| 1:C:1358:GLN:HG2  | 1:C:1423:THR:HG23 | 1.78                     | 0.66              |
| 1:B:2081:UNK:O    | 1:B:2084:UNK:CG   | 2.43                     | 0.66              |
| 1:B:2126:UNK:O    | 1:B:2129:UNK:CG   | 2.43                     | 0.66              |
| 1:C:2080:UNK:O    | 1:C:2083:UNK:HG3  | 1.94                     | 0.66              |
| 1:C:511:ARG:HB2   | 1:C:540:ASN:HB2   | 1.78                     | 0.66              |
| 1:A:1412:HIS:HD2  | 1:A:1413:PRO:HD2  | 1.61                     | 0.66              |
| 1:B:511:ARG:HB2   | 1:B:540:ASN:HB2   | 1.77                     | 0.66              |
| 1:B:981:UNK:HG1   | 1:B:987:UNK:CG    | 2.19                     | 0.66              |
| 1:C:2126:UNK:O    | 1:C:2129:UNK:CG   | 2.43                     | 0.66              |
| 1:C:683:GLY:HA2   | 1:C:700:ASN:HB2   | 1.78                     | 0.66              |
| 1:A:1163:ASP:HB3  | 1:A:1199:UNK:HG3  | 1.76                     | 0.66              |
| 1:B:1167:GLY:HA3  | 1:B:1195:ARG:HA   | 1.77                     | 0.66              |
| 1:B:1412:HIS:HD2  | 1:B:1413:PRO:HD2  | 1.61                     | 0.66              |
| 1:C:1168:ARG:HB2  | 1:C:1197:UNK:HB2  | 1.77                     | 0.66              |
| 1:A:2591:ARG:HH12 | 1:C:2012:GLY:C    | 1.99                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1008:UNK:HG3  | 1:B:1019:PHE:HB3  | 1.76                     | 0.66              |
| 1:C:792:ALA:HA    | 1:C:799:PHE:HE2   | 1.60                     | 0.66              |
| 1:A:1084:THR:HG21 | 1:A:1274:ALA:HA   | 1.78                     | 0.66              |
| 1:A:1358:GLN:HG2  | 1:A:1423:THR:HG23 | 1.78                     | 0.66              |
| 1:B:2112:UNK:HG2  | 1:B:2114:UNK:HG3  | 1.77                     | 0.66              |
| 1:B:35:VAL:HG11   | 1:B:147:LEU:HB3   | 1.78                     | 0.66              |
| 1:C:1132:LEU:HD11 | 1:C:1192:PHE:HB3  | 1.78                     | 0.66              |
| 1:C:931:UNK:CG    | 1:C:933:UNK:HG3   | 2.24                     | 0.66              |
| 1:A:931:UNK:CG    | 1:A:933:UNK:HG3   | 2.25                     | 0.66              |
| 1:C:1084:THR:HG21 | 1:C:1274:ALA:HA   | 1.78                     | 0.66              |
| 1:C:2081:UNK:O    | 1:C:2084:UNK:CG   | 2.43                     | 0.66              |
| 1:C:2112:UNK:N    | 1:C:2115:UNK:CG   | 2.57                     | 0.66              |
| 1:B:2012:GLY:C    | 1:C:2591:ARG:HH12 | 1.99                     | 0.66              |
| 1:A:2086:UNK:C    | 1:A:2089:UNK:HG3  | 2.25                     | 0.66              |
| 1:B:1358:GLN:HG2  | 1:B:1423:THR:HG23 | 1.78                     | 0.66              |
| 1:B:2112:UNK:N    | 1:B:2115:UNK:CG   | 2.57                     | 0.66              |
| 1:B:666:VAL:HG21  | 1:B:904:VAL:HB    | 1.78                     | 0.66              |
| 1:C:997:UNK:O     | 1:C:1009:UNK:N    | 2.29                     | 0.66              |
| 1:A:997:UNK:O     | 1:A:1009:UNK:N    | 2.29                     | 0.65              |
| 1:A:1167:GLY:HA3  | 1:A:1195:ARG:HA   | 1.78                     | 0.65              |
| 1:A:2112:UNK:N    | 1:A:2115:UNK:HG1  | 2.11                     | 0.65              |
| 1:A:2679:ALA:HB3  | 1:A:2762:VAL:HG12 | 1.78                     | 0.65              |
| 1:B:1534:ASN:HB2  | 1:B:1543:ALA:HB3  | 1.78                     | 0.65              |
| 1:B:1488:VAL:HG21 | 1:B:1580:PRO:HD2  | 1.77                     | 0.65              |
| 1:B:2123:UNK:C    | 1:B:2126:UNK:HG3  | 2.26                     | 0.65              |
| 1:B:970:ILE:HG12  | 1:B:996:UNK:HG1   | 1.76                     | 0.65              |
| 1:A:1488:VAL:HG12 | 1:A:1490:ARG:NH1  | 2.10                     | 0.65              |
| 1:A:970:ILE:HG12  | 1:A:996:UNK:HG1   | 1.76                     | 0.65              |
| 1:B:2706:PRO:HG2  | 1:B:2709:ILE:HG23 | 1.79                     | 0.65              |
| 1:C:2123:UNK:C    | 1:C:2126:UNK:HG3  | 2.26                     | 0.65              |
| 1:A:2123:UNK:C    | 1:A:2126:UNK:HG3  | 2.26                     | 0.65              |
| 1:A:2012:GLY:C    | 1:B:2591:ARG:HH12 | 1.99                     | 0.65              |
| 1:B:683:GLY:HA2   | 1:B:700:ASN:HB2   | 1.78                     | 0.65              |
| 1:C:1534:ASN:HB2  | 1:C:1543:ALA:HB3  | 1.79                     | 0.65              |
| 1:C:2084:UNK:C    | 1:C:2087:UNK:HG3  | 2.25                     | 0.65              |
| 1:B:1417:LEU:O    | 1:B:1423:THR:OG1  | 2.14                     | 0.65              |
| 1:C:203:ASP:OD1   | 1:C:204:ARG:N     | 2.29                     | 0.65              |
| 1:C:2876:LEU:HD11 | 1:C:2886:ILE:HD11 | 1.79                     | 0.65              |
| 1:C:924:LEU:O     | 1:C:929:UNK:N     | 2.30                     | 0.65              |
| 1:A:981:UNK:HG2   | 1:A:981:UNK:O     | 1.95                     | 0.65              |
| 1:B:2112:UNK:N    | 1:B:2115:UNK:HG1  | 2.11                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2679:ALA:HB3  | 1:B:2762:VAL:HG12 | 1.78                     | 0.65              |
| 1:C:1488:VAL:HG12 | 1:C:1490:ARG:NH1  | 2.10                     | 0.65              |
| 1:C:2086:UNK:C    | 1:C:2089:UNK:HG3  | 2.25                     | 0.65              |
| 1:A:35:VAL:HG11   | 1:A:147:LEU:HB3   | 1.78                     | 0.65              |
| 1:A:450:ASN:HA    | 1:A:483:ARG:HH11  | 1.62                     | 0.65              |
| 1:B:3080:ARG:NH1  | 1:B:3080:ARG:HG3  | 2.09                     | 0.65              |
| 1:C:1012:UNK:O    | 1:C:1013:UNK:CG   | 2.41                     | 0.65              |
| 1:A:2876:LEU:HD11 | 1:A:2886:ILE:HD11 | 1.79                     | 0.65              |
| 1:B:1132:LEU:HD11 | 1:B:1192:PHE:HB3  | 1.78                     | 0.65              |
| 1:C:1412:HIS:HD2  | 1:C:1413:PRO:HD2  | 1.61                     | 0.65              |
| 1:C:1417:LEU:O    | 1:C:1423:THR:OG1  | 2.14                     | 0.65              |
| 1:C:666:VAL:HG21  | 1:C:904:VAL:HB    | 1.78                     | 0.65              |
| 1:A:1168:ARG:HB2  | 1:A:1197:UNK:HB2  | 1.77                     | 0.65              |
| 1:A:666:VAL:HG21  | 1:A:904:VAL:HB    | 1.78                     | 0.65              |
| 1:B:1084:THR:HG21 | 1:B:1274:ALA:HA   | 1.78                     | 0.65              |
| 1:B:2876:LEU:HD11 | 1:B:2886:ILE:HD11 | 1.79                     | 0.65              |
| 1:B:500:GLN:O     | 1:B:504:LYS:N     | 2.24                     | 0.65              |
| 1:A:1536:ASN:HA   | 1:A:1679:TRP:HB3  | 1.79                     | 0.65              |
| 1:A:3080:ARG:HH11 | 1:A:3080:ARG:CG   | 2.07                     | 0.65              |
| 1:A:943:UNK:O     | 1:A:944:UNK:CG    | 2.44                     | 0.65              |
| 1:A:999:UNK:CG    | 1:A:1007:UNK:CG   | 2.75                     | 0.65              |
| 1:B:997:UNK:O     | 1:B:1009:UNK:N    | 2.29                     | 0.65              |
| 1:B:203:ASP:OD1   | 1:B:204:ARG:N     | 2.29                     | 0.65              |
| 1:C:999:UNK:CG    | 1:C:1007:UNK:CG   | 2.75                     | 0.65              |
| 1:C:1167:GLY:HA3  | 1:C:1195:ARG:HA   | 1.78                     | 0.65              |
| 1:A:2652:ILE:HG12 | 1:A:2722:VAL:HG22 | 1.79                     | 0.65              |
| 1:B:943:UNK:O     | 1:B:944:UNK:CG    | 2.44                     | 0.65              |
| 1:C:2652:ILE:HG12 | 1:C:2722:VAL:HG22 | 1.79                     | 0.65              |
| 1:C:2706:PRO:HG2  | 1:C:2709:ILE:HG23 | 1.79                     | 0.65              |
| 1:C:35:VAL:HG11   | 1:C:147:LEU:HB3   | 1.77                     | 0.64              |
| 1:C:1536:ASN:HA   | 1:C:1679:TRP:HB3  | 1.78                     | 0.64              |
| 1:A:56:LEU:HD22   | 1:A:119:LEU:HD13  | 1.79                     | 0.64              |
| 1:A:1417:LEU:O    | 1:A:1423:THR:OG1  | 2.14                     | 0.64              |
| 1:A:408:VAL:HG13  | 1:A:943:UNK:HG1   | 1.80                     | 0.64              |
| 1:B:238:SER:HG    | 1:B:249:THR:HG1   | 1.42                     | 0.64              |
| 1:B:981:UNK:O     | 1:B:981:UNK:HG2   | 1.95                     | 0.64              |
| 1:A:2120:UNK:O    | 1:A:2123:UNK:HG3  | 1.97                     | 0.64              |
| 1:A:2706:PRO:HG2  | 1:A:2709:ILE:HG23 | 1.78                     | 0.64              |
| 1:A:924:LEU:O     | 1:A:929:UNK:N     | 2.30                     | 0.64              |
| 1:A:1534:ASN:HB2  | 1:A:1543:ALA:HB3  | 1.78                     | 0.64              |
| 1:B:924:LEU:O     | 1:B:929:UNK:N     | 2.30                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:450:ASN:HA    | 1:C:483:ARG:HH11  | 1.62                     | 0.64              |
| 1:C:943:UNK:O     | 1:C:944:UNK:CG    | 2.44                     | 0.64              |
| 1:A:34:LEU:O      | 1:A:38:LEU:N      | 2.25                     | 0.64              |
| 1:A:643:ILE:HD12  | 1:A:915:PHE:HZ    | 1.62                     | 0.64              |
| 1:B:999:UNK:CG    | 1:B:1007:UNK:CG   | 2.75                     | 0.64              |
| 1:B:2120:UNK:O    | 1:B:2123:UNK:HG3  | 1.97                     | 0.64              |
| 1:B:2428:UNK:O    | 1:B:2428:UNK:HG2  | 1.98                     | 0.64              |
| 1:B:42:GLU:HB3    | 1:B:349:ARG:HG3   | 1.79                     | 0.64              |
| 1:C:2449:UNK:O    | 1:C:2449:UNK:HG2  | 1.98                     | 0.64              |
| 1:C:2679:ALA:HB3  | 1:C:2762:VAL:HG12 | 1.78                     | 0.64              |
| 1:C:408:VAL:HG13  | 1:C:943:UNK:HG1   | 1.79                     | 0.64              |
| 1:A:1132:LEU:HD11 | 1:A:1192:PHE:HB3  | 1.78                     | 0.64              |
| 1:A:1214:UNK:HB1  | 1:A:1320:VAL:HB   | 1.80                     | 0.64              |
| 1:A:683:GLY:HA2   | 1:A:700:ASN:HB2   | 1.78                     | 0.64              |
| 1:A:792:ALA:O     | 1:A:2433:UNK:HG2  | 1.96                     | 0.64              |
| 1:B:2080:UNK:HG2  | 1:B:2083:UNK:HG3  | 1.79                     | 0.64              |
| 1:C:2120:UNK:O    | 1:C:2123:UNK:HG3  | 1.97                     | 0.64              |
| 1:B:56:LEU:HD22   | 1:B:119:LEU:HD13  | 1.79                     | 0.64              |
| 1:A:203:ASP:OD1   | 1:A:204:ARG:N     | 2.30                     | 0.64              |
| 1:A:2252:VAL:HA   | 1:A:2255:ARG:HE   | 1.62                     | 0.64              |
| 1:B:1536:ASN:HA   | 1:B:1679:TRP:HB3  | 1.78                     | 0.64              |
| 1:B:2252:VAL:HA   | 1:B:2255:ARG:HE   | 1.62                     | 0.64              |
| 1:C:803:GLU:OE1   | 1:C:2431:UNK:HG3  | 1.98                     | 0.64              |
| 1:B:2449:UNK:HG2  | 1:B:2449:UNK:O    | 1.98                     | 0.64              |
| 1:A:42:GLU:HB3    | 1:A:349:ARG:HG3   | 1.79                     | 0.63              |
| 1:C:2080:UNK:HG2  | 1:C:2083:UNK:HG3  | 1.79                     | 0.63              |
| 1:C:42:GLU:HB3    | 1:C:349:ARG:HG3   | 1.79                     | 0.63              |
| 1:A:974:UNK:CG    | 1:A:977:UNK:HB1   | 2.29                     | 0.63              |
| 1:C:643:ILE:HD12  | 1:C:915:PHE:HZ    | 1.62                     | 0.63              |
| 1:A:2428:UNK:O    | 1:A:2428:UNK:HG2  | 1.98                     | 0.63              |
| 1:A:892:ILE:HG22  | 2:A:4000:FMN:HM82 | 1.80                     | 0.63              |
| 1:B:2176:LEU:HG   | 1:B:2180:LYS:HE3  | 1.80                     | 0.63              |
| 1:B:450:ASN:HA    | 1:B:483:ARG:HH11  | 1.62                     | 0.63              |
| 1:B:643:ILE:HD12  | 1:B:915:PHE:HZ    | 1.62                     | 0.63              |
| 1:B:974:UNK:CG    | 1:B:977:UNK:HB1   | 2.29                     | 0.63              |
| 1:C:360:LEU:HD12  | 1:C:363:LEU:HD23  | 1.80                     | 0.63              |
| 1:A:2080:UNK:HG2  | 1:A:2083:UNK:HG3  | 1.79                     | 0.63              |
| 1:A:2422:UNK:HG2  | 1:A:2422:UNK:O    | 1.98                     | 0.63              |
| 1:C:1214:UNK:HB1  | 1:C:1320:VAL:HB   | 1.80                     | 0.63              |
| 1:C:2252:VAL:HA   | 1:C:2255:ARG:HE   | 1.62                     | 0.63              |
| 1:C:2428:UNK:HG2  | 1:C:2428:UNK:O    | 1.98                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1072:TRP:NE1  | 1:A:1077:VAL:HG22 | 2.14                     | 0.63              |
| 1:A:2092:UNK:HA   | 1:A:2189:PHE:HB2  | 1.81                     | 0.63              |
| 1:B:2297:ARG:H    | 1:B:2297:ARG:HD3  | 1.64                     | 0.63              |
| 1:C:1072:TRP:NE1  | 1:C:1077:VAL:HG22 | 2.14                     | 0.63              |
| 1:C:2094:UNK:CG   | 1:C:2096:UNK:CG   | 2.75                     | 0.63              |
| 1:A:2135:UNK:HG3  | 1:A:2136:ASP:H    | 1.64                     | 0.63              |
| 1:B:1072:TRP:NE1  | 1:B:1077:VAL:HG22 | 2.14                     | 0.63              |
| 1:B:1212:UNK:HG2  | 1:B:1212:UNK:O    | 1.99                     | 0.63              |
| 1:B:2125:UNK:HA   | 1:B:2128:UNK:HG3  | 1.81                     | 0.63              |
| 1:B:2652:ILE:HG12 | 1:B:2722:VAL:HG22 | 1.79                     | 0.63              |
| 1:B:585:HIS:CD2   | 1:B:586:SER:H     | 2.17                     | 0.63              |
| 1:B:408:VAL:HG13  | 1:B:943:UNK:HG1   | 1.79                     | 0.63              |
| 1:A:2948:GLN:HG2  | 1:A:2951:ARG:HH21 | 1.64                     | 0.63              |
| 1:B:1215:UNK:HG2  | 1:B:1216:UNK:N    | 2.14                     | 0.63              |
| 1:C:1212:UNK:O    | 1:C:1212:UNK:HG2  | 1.99                     | 0.63              |
| 1:C:2092:UNK:O    | 1:C:2092:UNK:HG2  | 1.99                     | 0.63              |
| 1:A:1212:UNK:HG2  | 1:A:1212:UNK:O    | 1.99                     | 0.63              |
| 1:A:2117:UNK:O    | 1:A:2121:UNK:HG3  | 1.98                     | 0.63              |
| 1:A:2047:THR:OG1  | 1:A:2205:ASP:OD2  | 2.17                     | 0.63              |
| 1:A:980:UNK:C     | 1:A:981:UNK:HG3   | 2.29                     | 0.63              |
| 1:B:2117:UNK:O    | 1:B:2121:UNK:HG3  | 1.98                     | 0.63              |
| 1:B:360:LEU:HD12  | 1:B:363:LEU:HD23  | 1.80                     | 0.63              |
| 1:A:2173:ASP:OD2  | 1:A:2799:LYS:NZ   | 2.32                     | 0.63              |
| 1:A:2297:ARG:HD3  | 1:A:2297:ARG:H    | 1.64                     | 0.63              |
| 1:A:360:LEU:HD12  | 1:A:363:LEU:HD23  | 1.80                     | 0.63              |
| 1:A:803:GLU:OE1   | 1:A:2431:UNK:HG3  | 1.98                     | 0.63              |
| 1:B:1212:UNK:HG2  | 1:B:1342:ARG:HE   | 1.64                     | 0.63              |
| 1:B:2047:THR:OG1  | 1:B:2205:ASP:OD2  | 2.17                     | 0.63              |
| 1:B:803:GLU:OE1   | 1:B:2431:UNK:HG3  | 1.98                     | 0.63              |
| 1:B:750:LEU:HD12  | 1:B:827:LEU:HD11  | 1.81                     | 0.63              |
| 1:A:1215:UNK:HG2  | 1:A:1216:UNK:N    | 2.14                     | 0.62              |
| 1:A:1315:ARG:HH21 | 1:A:1323:GLU:HG2  | 1.64                     | 0.62              |
| 1:A:1412:HIS:ND1  | 1:A:1415:GLY:O    | 2.26                     | 0.62              |
| 1:A:2125:UNK:HA   | 1:A:2128:UNK:HG3  | 1.81                     | 0.62              |
| 1:A:750:LEU:HD12  | 1:A:827:LEU:HD11  | 1.81                     | 0.62              |
| 1:C:1126:ILE:HG22 | 1:C:1196:UNK:HG1  | 1.81                     | 0.62              |
| 1:C:1412:HIS:ND1  | 1:C:1415:GLY:O    | 2.26                     | 0.62              |
| 1:C:2422:UNK:HG2  | 1:C:2422:UNK:O    | 1.98                     | 0.62              |
| 1:C:974:UNK:CG    | 1:C:977:UNK:HB1   | 2.29                     | 0.62              |
| 1:A:664:LEU:HD13  | 1:A:701:ALA:HB1   | 1.81                     | 0.62              |
| 1:B:1126:ILE:HG22 | 1:B:1196:UNK:HG1  | 1.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2422:UNK:HG2  | 1:B:2422:UNK:O    | 1.98                     | 0.62              |
| 1:B:34:LEU:O      | 1:B:38:LEU:N      | 2.25                     | 0.62              |
| 1:B:980:UNK:C     | 1:B:981:UNK:HG3   | 2.29                     | 0.62              |
| 1:C:1376:VAL:HA   | 1:C:1470:LEU:HD13 | 1.81                     | 0.62              |
| 1:C:2117:UNK:O    | 1:C:2121:UNK:HG3  | 1.98                     | 0.62              |
| 1:A:2092:UNK:O    | 1:A:2092:UNK:HG2  | 1.99                     | 0.62              |
| 1:B:1002:UNK:O    | 1:B:1003:UNK:CG   | 2.47                     | 0.62              |
| 1:B:1214:UNK:HB1  | 1:B:1320:VAL:HB   | 1.80                     | 0.62              |
| 1:B:664:LEU:HD13  | 1:B:701:ALA:HB1   | 1.81                     | 0.62              |
| 1:C:56:LEU:HD22   | 1:C:119:LEU:HD13  | 1.79                     | 0.62              |
| 1:C:2176:LEU:HG   | 1:C:2180:LYS:HE3  | 1.80                     | 0.62              |
| 1:A:2449:UNK:O    | 1:A:2449:UNK:HG2  | 1.98                     | 0.62              |
| 1:B:892:ILE:HG22  | 2:B:4000:FMN:HM82 | 1.80                     | 0.62              |
| 1:B:1376:VAL:HA   | 1:B:1470:LEU:HD13 | 1.81                     | 0.62              |
| 1:C:1095:LEU:HD12 | 1:C:1096:THR:H    | 1.64                     | 0.62              |
| 1:C:1212:UNK:HG2  | 1:C:1342:ARG:HE   | 1.64                     | 0.62              |
| 1:C:585:HIS:CD2   | 1:C:586:SER:H     | 2.17                     | 0.62              |
| 1:A:1376:VAL:HA   | 1:A:1470:LEU:HD13 | 1.81                     | 0.62              |
| 1:A:500:GLN:O     | 1:A:504:LYS:N     | 2.24                     | 0.62              |
| 1:C:992:UNK:CG    | 1:C:994:UNK:HG2   | 2.29                     | 0.62              |
| 1:A:1622:PRO:HD3  | 1:A:1685:LEU:HD11 | 1.81                     | 0.62              |
| 1:A:1702:GLU:OE2  | 1:A:1711:VAL:HG13 | 1.99                     | 0.62              |
| 1:A:585:HIS:CD2   | 1:A:586:SER:H     | 2.17                     | 0.62              |
| 1:B:1702:GLU:OE2  | 1:B:1711:VAL:HG13 | 1.99                     | 0.62              |
| 1:B:2173:ASP:OD2  | 1:B:2799:LYS:NZ   | 2.32                     | 0.62              |
| 1:B:2765:GLY:HA2  | 1:B:2940:VAL:HG21 | 1.82                     | 0.62              |
| 1:C:2765:GLY:HA2  | 1:C:2940:VAL:HG21 | 1.82                     | 0.62              |
| 1:C:792:ALA:O     | 1:C:2433:UNK:HG2  | 1.96                     | 0.62              |
| 1:A:992:UNK:CG    | 1:A:994:UNK:HG2   | 2.29                     | 0.62              |
| 1:B:1353:PRO:HG3  | 1:B:1702:GLU:OE2  | 2.00                     | 0.62              |
| 1:B:1725:SER:HB3  | 1:C:260:LEU:HD13  | 1.82                     | 0.62              |
| 1:B:2237:LEU:HB2  | 1:B:2287:LEU:HD11 | 1.82                     | 0.62              |
| 1:B:792:ALA:O     | 1:B:2433:UNK:HG2  | 1.96                     | 0.62              |
| 1:B:415:VAL:HG22  | 1:B:937:UNK:HG1   | 1.81                     | 0.62              |
| 1:B:975:UNK:HG3   | 1:B:993:UNK:CB    | 2.29                     | 0.62              |
| 1:C:1215:UNK:HG2  | 1:C:1216:UNK:N    | 2.14                     | 0.62              |
| 1:A:1002:UNK:O    | 1:A:1003:UNK:CG   | 2.47                     | 0.62              |
| 1:A:1095:LEU:HD12 | 1:A:1096:THR:H    | 1.64                     | 0.62              |
| 1:B:2092:UNK:HA   | 1:B:2189:PHE:HB2  | 1.81                     | 0.62              |
| 1:C:164:ALA:HA    | 1:C:178:LEU:HD13  | 1.82                     | 0.62              |
| 1:C:2096:UNK:HG2  | 1:C:2097:UNK:N    | 2.14                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:980:UNK:C    | 1:C:981:UNK:HG3   | 2.29                     | 0.62              |
| 1:A:1002:UNK:HG2 | 1:A:1002:UNK:O    | 1.99                     | 0.62              |
| 1:A:238:SER:OG   | 1:A:249:THR:OG1   | 2.16                     | 0.62              |
| 1:B:2096:UNK:HG2 | 1:B:2097:UNK:N    | 2.14                     | 0.62              |
| 1:B:992:UNK:HG3  | 1:B:996:UNK:HG3   | 1.66                     | 0.62              |
| 1:C:415:VAL:HG22 | 1:C:937:UNK:HG1   | 1.81                     | 0.62              |
| 1:B:2948:GLN:HG2 | 1:B:2951:ARG:HH21 | 1.64                     | 0.61              |
| 1:C:1431:ALA:HB3 | 1:C:1459:THR:HG21 | 1.82                     | 0.61              |
| 1:C:1702:GLU:OE2 | 1:C:1711:VAL:HG13 | 1.99                     | 0.61              |
| 1:C:203:ASP:O    | 1:C:205:PRO:HD3   | 2.00                     | 0.61              |
| 1:C:2092:UNK:HA  | 1:C:2189:PHE:HB2  | 1.81                     | 0.61              |
| 1:C:2047:THR:OG1 | 1:C:2205:ASP:OD2  | 2.17                     | 0.61              |
| 1:C:2297:ARG:HD3 | 1:C:2297:ARG:H    | 1.64                     | 0.61              |
| 1:C:2948:GLN:HG2 | 1:C:2951:ARG:HH21 | 1.64                     | 0.61              |
| 1:C:664:LEU:HD13 | 1:C:701:ALA:HB1   | 1.81                     | 0.61              |
| 1:C:975:UNK:HG3  | 1:C:993:UNK:CB    | 2.29                     | 0.61              |
| 1:A:2122:UNK:C   | 1:A:2125:UNK:HG3  | 2.30                     | 0.61              |
| 1:A:3080:ARG:HG3 | 1:A:3080:ARG:NH1  | 2.09                     | 0.61              |
| 1:A:511:ARG:HH11 | 1:A:543:GLY:HA3   | 1.65                     | 0.61              |
| 1:A:793:ARG:HD3  | 1:A:2435:UNK:CG   | 2.27                     | 0.61              |
| 1:B:575:HIS:HD2  | 1:B:644:LEU:HD22  | 1.66                     | 0.61              |
| 1:B:409:LYS:HD2  | 1:B:933:UNK:HA    | 1.82                     | 0.61              |
| 1:B:939:UNK:O    | 1:B:940:UNK:CG    | 2.47                     | 0.61              |
| 1:B:971:ALA:O    | 1:B:974:UNK:CG    | 2.48                     | 0.61              |
| 1:C:1622:PRO:HD3 | 1:C:1685:LEU:HD11 | 1.81                     | 0.61              |
| 1:C:2125:UNK:HA  | 1:C:2128:UNK:HG3  | 1.81                     | 0.61              |
| 1:C:575:HIS:HD2  | 1:C:644:LEU:HD22  | 1.66                     | 0.61              |
| 1:A:939:UNK:O    | 1:A:940:UNK:CG    | 2.47                     | 0.61              |
| 1:B:2092:UNK:HG2 | 1:B:2092:UNK:O    | 1.99                     | 0.61              |
| 1:B:511:ARG:HH11 | 1:B:543:GLY:HA3   | 1.66                     | 0.61              |
| 1:B:984:UNK:CG   | 1:B:987:UNK:CG    | 2.79                     | 0.61              |
| 1:C:2103:UNK:HG1 | 1:C:2919:GLY:O    | 2.00                     | 0.61              |
| 1:C:34:LEU:H     | 1:C:393:VAL:HG21  | 1.65                     | 0.61              |
| 1:C:970:ILE:CG1  | 1:C:996:UNK:HG1   | 2.31                     | 0.61              |
| 1:A:1725:SER:HB3 | 1:B:260:LEU:HD13  | 1.82                     | 0.61              |
| 1:A:415:VAL:CG2  | 1:A:937:UNK:HG1   | 2.31                     | 0.61              |
| 1:A:976:UNK:O    | 1:A:976:UNK:HG2   | 2.01                     | 0.61              |
| 1:B:415:VAL:CG2  | 1:B:937:UNK:HG1   | 2.31                     | 0.61              |
| 1:C:1002:UNK:O   | 1:C:1003:UNK:CG   | 2.47                     | 0.61              |
| 1:C:2112:UNK:N   | 1:C:2115:UNK:HG1  | 2.11                     | 0.61              |
| 1:C:2434:UNK:CG  | 1:C:2523:GLU:O    | 2.48                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:892:ILE:HG22  | 2:C:4000:FMN:HM82 | 1.80                     | 0.61              |
| 1:A:164:ALA:HA    | 1:A:178:LEU:HD13  | 1.82                     | 0.61              |
| 1:B:106:ALA:HB1   | 1:B:112:PRO:HB2   | 1.82                     | 0.61              |
| 1:B:1622:PRO:HD3  | 1:B:1685:LEU:HD11 | 1.81                     | 0.61              |
| 1:B:34:LEU:H      | 1:B:393:VAL:HG21  | 1.65                     | 0.61              |
| 1:B:929:UNK:O     | 1:B:930:UNK:CG    | 2.45                     | 0.61              |
| 1:A:1431:ALA:HB3  | 1:A:1459:THR:HG21 | 1.82                     | 0.61              |
| 1:A:2176:LEU:HG   | 1:A:2180:LYS:HE3  | 1.80                     | 0.61              |
| 1:A:2469:LEU:HD11 | 1:A:2653:VAL:HB   | 1.82                     | 0.61              |
| 1:A:409:LYS:HD2   | 1:A:933:UNK:HA    | 1.82                     | 0.61              |
| 1:A:415:VAL:HG22  | 1:A:937:UNK:HG1   | 1.81                     | 0.61              |
| 1:A:575:HIS:HD2   | 1:A:644:LEU:HD22  | 1.66                     | 0.61              |
| 1:A:984:UNK:HG2   | 1:A:987:UNK:CG    | 2.31                     | 0.61              |
| 1:B:2469:LEU:HD11 | 1:B:2653:VAL:HB   | 1.82                     | 0.61              |
| 1:C:1227:UNK:O    | 1:C:1227:UNK:HG2  | 2.00                     | 0.61              |
| 1:A:260:LEU:HD13  | 1:C:1725:SER:HB3  | 1.82                     | 0.61              |
| 1:C:409:LYS:HD2   | 1:C:933:UNK:HA    | 1.82                     | 0.61              |
| 1:C:971:ALA:O     | 1:C:974:UNK:CG    | 2.48                     | 0.61              |
| 1:C:984:UNK:HG2   | 1:C:987:UNK:CG    | 2.31                     | 0.61              |
| 1:A:1126:ILE:HG22 | 1:A:1196:UNK:HG1  | 1.81                     | 0.61              |
| 1:A:1353:PRO:HG3  | 1:A:1702:GLU:OE2  | 2.00                     | 0.61              |
| 1:A:929:UNK:O     | 1:A:930:UNK:CG    | 2.45                     | 0.61              |
| 1:B:2122:UNK:C    | 1:B:2125:UNK:HG3  | 2.30                     | 0.61              |
| 1:B:2135:UNK:HG3  | 1:B:2136:ASP:H    | 1.64                     | 0.61              |
| 1:C:2469:LEU:HD11 | 1:C:2653:VAL:HB   | 1.82                     | 0.61              |
| 1:C:3058:ARG:HB2  | 1:C:3089:LEU:HB2  | 1.82                     | 0.61              |
| 1:C:34:LEU:O      | 1:C:38:LEU:N      | 2.25                     | 0.61              |
| 1:C:511:ARG:HH11  | 1:C:543:GLY:HA3   | 1.66                     | 0.61              |
| 1:A:106:ALA:HB1   | 1:A:112:PRO:HB2   | 1.82                     | 0.61              |
| 1:A:1212:UNK:HG2  | 1:A:1342:ARG:HE   | 1.64                     | 0.61              |
| 1:A:2103:UNK:HG1  | 1:A:2919:GLY:O    | 2.00                     | 0.61              |
| 1:A:580:ARG:HG2   | 1:A:590:LEU:HD21  | 1.83                     | 0.61              |
| 1:B:1007:UNK:HB2  | 1:B:1018:ARG:HE   | 1.66                     | 0.61              |
| 1:B:1227:UNK:O    | 1:B:1227:UNK:HG2  | 2.00                     | 0.61              |
| 1:B:1431:ALA:HB3  | 1:B:1459:THR:HG21 | 1.82                     | 0.61              |
| 1:B:126:VAL:HG12  | 1:B:182:ALA:HB1   | 1.83                     | 0.61              |
| 1:B:70:SER:HG     | 1:B:142:ARG:HH22  | 1.49                     | 0.61              |
| 1:C:1353:PRO:HG3  | 1:C:1702:GLU:OE2  | 2.00                     | 0.61              |
| 1:C:415:VAL:CG2   | 1:C:937:UNK:HG1   | 2.31                     | 0.61              |
| 1:C:750:LEU:HD12  | 1:C:827:LEU:HD11  | 1.81                     | 0.61              |
| 1:B:2334:HIS:HD2  | 1:B:2391:LYS:HG3  | 1.66                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2434:UNK:CG   | 1:B:2523:GLU:O    | 2.48                     | 0.61              |
| 1:B:979:UNK:HG2   | 1:B:979:UNK:O     | 2.01                     | 0.61              |
| 1:B:984:UNK:HG2   | 1:B:987:UNK:CG    | 2.31                     | 0.61              |
| 1:C:1007:UNK:HG2  | 1:C:1007:UNK:O    | 2.01                     | 0.61              |
| 1:C:488:ASN:HA    | 1:C:521:VAL:HB    | 1.83                     | 0.61              |
| 1:A:1007:UNK:O    | 1:A:1007:UNK:HG2  | 2.01                     | 0.61              |
| 1:A:1227:UNK:HG2  | 1:A:1227:UNK:O    | 2.00                     | 0.61              |
| 1:A:680:ALA:HA    | 1:A:685:ALA:HB2   | 1.83                     | 0.61              |
| 1:A:984:UNK:CG    | 1:A:987:UNK:CG    | 2.79                     | 0.61              |
| 1:B:3058:ARG:HB2  | 1:B:3089:LEU:HB2  | 1.82                     | 0.61              |
| 1:B:970:ILE:CG1   | 1:B:996:UNK:HG1   | 2.31                     | 0.61              |
| 1:C:1315:ARG:HH21 | 1:C:1323:GLU:HG2  | 1.64                     | 0.61              |
| 1:A:2765:GLY:HA2  | 1:A:2940:VAL:HG21 | 1.82                     | 0.60              |
| 1:A:34:LEU:H      | 1:A:393:VAL:HG21  | 1.65                     | 0.60              |
| 1:A:970:ILE:CG1   | 1:A:996:UNK:HG1   | 2.31                     | 0.60              |
| 1:A:980:UNK:HB2   | 1:A:989:UNK:HB2   | 1.83                     | 0.60              |
| 1:B:1095:LEU:HD12 | 1:B:1096:THR:H    | 1.64                     | 0.60              |
| 1:B:438:THR:HA    | 1:B:880:HIS:HE1   | 1.66                     | 0.60              |
| 1:C:2173:ASP:OD2  | 1:C:2799:LYS:NZ   | 2.32                     | 0.60              |
| 1:C:984:UNK:CG    | 1:C:987:UNK:CG    | 2.79                     | 0.60              |
| 1:A:1007:UNK:HB2  | 1:A:1018:ARG:HE   | 1.66                     | 0.60              |
| 1:A:2096:UNK:HG2  | 1:A:2097:UNK:N    | 2.14                     | 0.60              |
| 1:A:2647:VAL:HA   | 1:A:2650:TRP:HD1  | 1.66                     | 0.60              |
| 1:B:1315:ARG:HH21 | 1:B:1323:GLU:HG2  | 1.64                     | 0.60              |
| 1:B:488:ASN:HA    | 1:B:521:VAL:HB    | 1.83                     | 0.60              |
| 1:C:1532:ILE:HA   | 1:C:1544:ILE:HG12 | 1.83                     | 0.60              |
| 1:A:257:ARG:HH12  | 1:C:1695:LEU:CD2  | 2.13                     | 0.60              |
| 1:C:2237:LEU:HB2  | 1:C:2287:LEU:HD11 | 1.82                     | 0.60              |
| 1:C:238:SER:OG    | 1:C:249:THR:OG1   | 2.15                     | 0.60              |
| 1:C:580:ARG:HG2   | 1:C:590:LEU:HD21  | 1.83                     | 0.60              |
| 1:C:980:UNK:HB2   | 1:C:989:UNK:HB2   | 1.83                     | 0.60              |
| 1:A:1989:PHE:HD1  | 1:A:1992:LYS:HZ3  | 1.49                     | 0.60              |
| 1:A:203:ASP:O     | 1:A:205:PRO:HD3   | 2.01                     | 0.60              |
| 1:A:2112:UNK:CG   | 1:A:2114:UNK:HG3  | 2.31                     | 0.60              |
| 1:A:2237:LEU:HB2  | 1:A:2287:LEU:HD11 | 1.82                     | 0.60              |
| 1:A:2372:MET:HB3  | 1:A:2394:LEU:HD22 | 1.83                     | 0.60              |
| 1:A:2434:UNK:CG   | 1:A:2523:GLU:O    | 2.48                     | 0.60              |
| 1:B:1098:VAL:HG12 | 1:B:1100:ASP:H    | 1.66                     | 0.60              |
| 1:C:2800:PHE:HE1  | 1:C:2812:LEU:HD22 | 1.67                     | 0.60              |
| 1:A:1537:LEU:HB2  | 1:A:1541:GLN:H    | 1.67                     | 0.60              |
| 1:A:2121:UNK:C    | 1:A:2124:UNK:HG3  | 2.31                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:438:THR:HA    | 1:A:880:HIS:HE1   | 1.66                     | 0.60              |
| 1:A:971:ALA:O     | 1:A:974:UNK:CG    | 2.48                     | 0.60              |
| 1:A:979:UNK:O     | 1:A:979:UNK:HG2   | 2.01                     | 0.60              |
| 1:B:1002:UNK:O    | 1:B:1002:UNK:HG2  | 2.00                     | 0.60              |
| 1:B:164:ALA:HA    | 1:B:178:LEU:HD13  | 1.82                     | 0.60              |
| 1:B:203:ASP:O     | 1:B:205:PRO:HD3   | 2.01                     | 0.60              |
| 1:B:2121:UNK:C    | 1:B:2124:UNK:HG3  | 2.31                     | 0.60              |
| 1:B:680:ALA:HA    | 1:B:685:ALA:HB2   | 1.83                     | 0.60              |
| 1:C:1537:LEU:HB2  | 1:C:1541:GLN:H    | 1.67                     | 0.60              |
| 1:C:2112:UNK:CG   | 1:C:2114:UNK:HG3  | 2.31                     | 0.60              |
| 1:C:2686:MET:HE1  | 1:C:2935:LYS:HG3  | 1.83                     | 0.60              |
| 1:A:2121:UNK:O    | 1:A:2124:UNK:CG   | 2.49                     | 0.60              |
| 1:B:2212:TRP:HA   | 1:B:2229:LYS:HD3  | 1.83                     | 0.60              |
| 1:B:2103:UNK:HG1  | 1:B:2919:GLY:O    | 2.00                     | 0.60              |
| 1:C:126:VAL:HG12  | 1:C:182:ALA:HB1   | 1.83                     | 0.60              |
| 1:C:2212:TRP:HA   | 1:C:2229:LYS:HD3  | 1.83                     | 0.60              |
| 1:B:1695:LEU:CD2  | 1:C:257:ARG:HH12  | 2.13                     | 0.60              |
| 1:C:2962:ASP:N    | 1:C:2962:ASP:OD1  | 2.34                     | 0.60              |
| 1:C:929:UNK:O     | 1:C:930:UNK:CG    | 2.45                     | 0.60              |
| 1:A:2651:ASN:HD22 | 1:A:2718:VAL:HG12 | 1.67                     | 0.60              |
| 1:A:3058:ARG:HB2  | 1:A:3089:LEU:HB2  | 1.82                     | 0.60              |
| 1:A:488:ASN:HA    | 1:A:521:VAL:HB    | 1.83                     | 0.60              |
| 1:B:1012:UNK:C    | 1:B:1013:UNK:HG3  | 2.32                     | 0.60              |
| 1:A:1309:VAL:HG22 | 1:A:1331:ILE:HG12 | 1.84                     | 0.60              |
| 1:A:1695:LEU:CD2  | 1:B:257:ARG:HH12  | 2.13                     | 0.60              |
| 1:A:2334:HIS:HD2  | 1:A:2391:LYS:HG3  | 1.66                     | 0.60              |
| 1:B:2651:ASN:HD22 | 1:B:2718:VAL:HG12 | 1.67                     | 0.60              |
| 1:B:670:GLY:O     | 1:B:682:ASN:ND2   | 2.35                     | 0.60              |
| 1:B:687:GLY:O     | 1:B:695:ILE:N     | 2.34                     | 0.60              |
| 1:B:688:ARG:O     | 1:B:872:ARG:NE    | 2.34                     | 0.60              |
| 1:C:2135:UNK:HG3  | 1:C:2136:ASP:H    | 1.64                     | 0.60              |
| 1:C:976:UNK:HG2   | 1:C:976:UNK:O     | 2.01                     | 0.60              |
| 1:A:670:GLY:O     | 1:A:682:ASN:ND2   | 2.35                     | 0.60              |
| 1:A:931:UNK:O     | 1:A:934:UNK:HG3   | 2.02                     | 0.60              |
| 1:A:975:UNK:HG3   | 1:A:993:UNK:CB    | 2.29                     | 0.60              |
| 1:B:1435:VAL:HG11 | 1:B:1463:CYS:HB3  | 1.84                     | 0.60              |
| 1:B:2112:UNK:CG   | 1:B:2114:UNK:HG3  | 2.31                     | 0.60              |
| 1:B:2647:VAL:HA   | 1:B:2650:TRP:HD1  | 1.66                     | 0.60              |
| 1:B:580:ARG:HG2   | 1:B:590:LEU:HD21  | 1.83                     | 0.60              |
| 1:C:1002:UNK:O    | 1:C:1002:UNK:HG2  | 1.99                     | 0.60              |
| 1:C:1098:VAL:HG12 | 1:C:1100:ASP:H    | 1.66                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2081:UNK:O    | 1:C:2085:UNK:HG2  | 2.02                     | 0.60              |
| 1:C:2651:ASN:HD22 | 1:C:2718:VAL:HG12 | 1.67                     | 0.60              |
| 1:C:2461:VAL:HG11 | 1:C:2751:VAL:HG22 | 1.84                     | 0.60              |
| 1:A:1532:ILE:HA   | 1:A:1544:ILE:HG12 | 1.83                     | 0.60              |
| 1:A:126:VAL:HG12  | 1:A:182:ALA:HB1   | 1.83                     | 0.60              |
| 1:A:2081:UNK:O    | 1:A:2085:UNK:HG2  | 2.02                     | 0.60              |
| 1:B:1537:LEU:HB2  | 1:B:1541:GLN:H    | 1.67                     | 0.60              |
| 1:B:931:UNK:O     | 1:B:934:UNK:HG3   | 2.02                     | 0.60              |
| 1:C:1007:UNK:HB2  | 1:C:1018:ARG:HE   | 1.66                     | 0.60              |
| 1:C:2121:UNK:O    | 1:C:2124:UNK:CG   | 2.49                     | 0.60              |
| 1:C:2122:UNK:C    | 1:C:2125:UNK:HG3  | 2.30                     | 0.60              |
| 1:C:2334:HIS:HD2  | 1:C:2391:LYS:HG3  | 1.66                     | 0.60              |
| 1:C:670:GLY:O     | 1:C:682:ASN:ND2   | 2.35                     | 0.60              |
| 1:C:688:ARG:O     | 1:C:872:ARG:NE    | 2.34                     | 0.60              |
| 1:C:939:UNK:O     | 1:C:940:UNK:CG    | 2.47                     | 0.60              |
| 1:A:1012:UNK:C    | 1:A:1013:UNK:HG3  | 2.32                     | 0.59              |
| 1:B:1532:ILE:HA   | 1:B:1544:ILE:HG12 | 1.83                     | 0.59              |
| 1:C:410:LEU:HB3   | 1:C:1025:VAL:HG21 | 1.84                     | 0.59              |
| 1:C:1435:VAL:HG11 | 1:C:1463:CYS:HB3  | 1.84                     | 0.59              |
| 1:C:2121:UNK:C    | 1:C:2124:UNK:HG3  | 2.31                     | 0.59              |
| 1:A:410:LEU:HB3   | 1:A:1025:VAL:HG21 | 1.84                     | 0.59              |
| 1:B:1656:LYS:HG2  | 1:B:1660:LEU:HG   | 1.85                     | 0.59              |
| 1:B:1989:PHE:HD1  | 1:B:1992:LYS:HZ3  | 1.50                     | 0.59              |
| 1:B:2081:UNK:O    | 1:B:2085:UNK:HG2  | 2.02                     | 0.59              |
| 1:B:2121:UNK:O    | 1:B:2124:UNK:CG   | 2.49                     | 0.59              |
| 1:B:2372:MET:HB3  | 1:B:2394:LEU:HD22 | 1.83                     | 0.59              |
| 1:C:2056:PHE:HZ   | 1:C:2180:LYS:HE2  | 1.67                     | 0.59              |
| 1:C:2429:UNK:O    | 1:C:2429:UNK:HG2  | 2.02                     | 0.59              |
| 1:C:680:ALA:HA    | 1:C:685:ALA:HB2   | 1.83                     | 0.59              |
| 1:A:2431:UNK:HG2  | 1:A:2431:UNK:O    | 2.01                     | 0.59              |
| 1:B:795:HIS:HB3   | 1:B:799:PHE:CZ    | 2.37                     | 0.59              |
| 1:C:106:ALA:HB1   | 1:C:112:PRO:HB2   | 1.82                     | 0.59              |
| 1:C:2431:UNK:O    | 1:C:2431:UNK:HG2  | 2.01                     | 0.59              |
| 1:C:2712:GLU:HA   | 1:C:2717:VAL:HG11 | 1.83                     | 0.59              |
| 1:A:1098:VAL:HG12 | 1:A:1100:ASP:H    | 1.66                     | 0.59              |
| 1:A:2800:PHE:HE1  | 1:A:2812:LEU:HD22 | 1.67                     | 0.59              |
| 1:A:2820:ILE:HD13 | 1:A:2943:MET:HG2  | 1.84                     | 0.59              |
| 1:A:795:HIS:HB3   | 1:A:799:PHE:CZ    | 2.37                     | 0.59              |
| 1:B:1002:UNK:C    | 1:B:1003:UNK:HG3  | 2.33                     | 0.59              |
| 1:A:2056:PHE:HZ   | 1:A:2180:LYS:HE2  | 1.67                     | 0.59              |
| 1:A:688:ARG:O     | 1:A:872:ARG:NE    | 2.34                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2667:THR:HG21 | 1:B:3058:ARG:NH1  | 2.17                     | 0.59              |
| 1:C:1336:VAL:HG12 | 1:C:1337:MET:HG3  | 1.85                     | 0.59              |
| 1:C:2372:MET:HB3  | 1:C:2394:LEU:HD22 | 1.83                     | 0.59              |
| 1:A:2212:TRP:HA   | 1:A:2229:LYS:HD3  | 1.83                     | 0.59              |
| 1:B:793:ARG:HD3   | 1:B:2435:UNK:CG   | 2.27                     | 0.59              |
| 1:B:976:UNK:O     | 1:B:976:UNK:HG2   | 2.01                     | 0.59              |
| 1:B:980:UNK:HB2   | 1:B:989:UNK:HB2   | 1.83                     | 0.59              |
| 1:C:2889:ILE:HG12 | 1:C:2922:LEU:HB3  | 1.84                     | 0.59              |
| 1:C:931:UNK:O     | 1:C:934:UNK:HG3   | 2.02                     | 0.59              |
| 1:B:2431:UNK:HG2  | 1:B:2431:UNK:O    | 2.01                     | 0.59              |
| 1:A:1656:LYS:HG2  | 1:A:1660:LEU:HG   | 1.85                     | 0.59              |
| 1:A:2667:THR:HG21 | 1:A:3058:ARG:NH1  | 2.17                     | 0.59              |
| 1:A:2693:GLN:O    | 1:A:2697:HIS:ND1  | 2.33                     | 0.59              |
| 1:A:2712:GLU:HA   | 1:A:2717:VAL:HG11 | 1.83                     | 0.59              |
| 1:A:2686:MET:HE1  | 1:A:2935:LYS:HG3  | 1.83                     | 0.59              |
| 1:B:1007:UNK:HG2  | 1:B:1007:UNK:O    | 2.01                     | 0.59              |
| 1:B:992:UNK:CG    | 1:B:994:UNK:HG2   | 2.30                     | 0.59              |
| 1:C:1701:VAL:HG22 | 1:C:1732:LEU:HB2  | 1.84                     | 0.59              |
| 1:A:2094:UNK:CG   | 1:A:2096:UNK:CG   | 2.75                     | 0.59              |
| 1:B:1336:VAL:HG12 | 1:B:1337:MET:HG3  | 1.85                     | 0.59              |
| 1:B:2056:PHE:HZ   | 1:B:2180:LYS:HE2  | 1.67                     | 0.59              |
| 1:B:2403:ILE:HG23 | 1:B:2408:LEU:HD12 | 1.85                     | 0.59              |
| 1:B:2461:VAL:HG11 | 1:B:2751:VAL:HG22 | 1.84                     | 0.59              |
| 1:C:1616:PRO:HG3  | 1:C:1668:LEU:HD13 | 1.85                     | 0.59              |
| 1:C:2135:UNK:CG   | 1:C:2136:ASP:N    | 2.66                     | 0.59              |
| 1:C:2647:VAL:HA   | 1:C:2650:TRP:HD1  | 1.66                     | 0.59              |
| 1:A:150:THR:O     | 1:A:152:PRO:HD3   | 2.03                     | 0.59              |
| 1:A:943:UNK:C     | 1:A:944:UNK:HG3   | 2.32                     | 0.59              |
| 1:B:2800:PHE:HE1  | 1:B:2812:LEU:HD22 | 1.67                     | 0.59              |
| 1:B:934:UNK:C     | 1:B:937:UNK:HG3   | 2.32                     | 0.59              |
| 1:C:1309:VAL:HG22 | 1:C:1331:ILE:HG12 | 1.84                     | 0.59              |
| 1:B:2686:MET:HE1  | 1:B:2935:LYS:HG3  | 1.83                     | 0.58              |
| 1:B:462:GLN:HG3   | 1:B:468:PHE:HD1   | 1.68                     | 0.58              |
| 1:C:2124:UNK:O    | 1:C:2127:UNK:CG   | 2.51                     | 0.58              |
| 1:C:836:VAL:HG12  | 1:C:837:VAL:H     | 1.67                     | 0.58              |
| 1:C:979:UNK:O     | 1:C:979:UNK:HG2   | 2.01                     | 0.58              |
| 1:A:1001:UNK:C    | 1:A:1002:UNK:HG3  | 2.33                     | 0.58              |
| 1:A:1336:VAL:HG12 | 1:A:1337:MET:HG3  | 1.85                     | 0.58              |
| 1:A:1616:PRO:HG3  | 1:A:1668:LEU:HD13 | 1.85                     | 0.58              |
| 1:C:1012:UNK:C    | 1:C:1013:UNK:HG3  | 2.32                     | 0.58              |
| 1:C:438:THR:HA    | 1:C:880:HIS:HE1   | 1.66                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:943:UNK:C     | 1:C:944:UNK:HG3   | 2.32                     | 0.58              |
| 1:A:2429:UNK:HG2  | 1:A:2429:UNK:O    | 2.02                     | 0.58              |
| 1:A:2889:ILE:HG12 | 1:A:2922:LEU:HB3  | 1.84                     | 0.58              |
| 1:B:1001:UNK:C    | 1:B:1002:UNK:HG3  | 2.33                     | 0.58              |
| 1:B:1008:UNK:CG   | 1:B:1019:PHE:HB3  | 2.33                     | 0.58              |
| 1:B:1327:VAL:HB   | 1:B:1339:ALA:HB3  | 1.86                     | 0.58              |
| 1:B:1701:VAL:HG22 | 1:B:1732:LEU:HB2  | 1.84                     | 0.58              |
| 1:C:1001:UNK:C    | 1:C:1002:UNK:HG3  | 2.33                     | 0.58              |
| 1:C:150:THR:O     | 1:C:152:PRO:HD3   | 2.03                     | 0.58              |
| 1:C:621:SER:OG    | 1:C:643:ILE:HD13  | 2.04                     | 0.58              |
| 1:A:1008:UNK:O    | 1:A:1008:UNK:HG2  | 2.03                     | 0.58              |
| 1:A:735:LYS:HD2   | 1:A:860:VAL:HG23  | 1.86                     | 0.58              |
| 1:B:1253:ARG:NH1  | 1:B:1253:ARG:HG3  | 2.18                     | 0.58              |
| 1:B:2712:GLU:HA   | 1:B:2717:VAL:HG11 | 1.84                     | 0.58              |
| 1:C:795:HIS:HB3   | 1:C:799:PHE:CZ    | 2.37                     | 0.58              |
| 1:C:990:UNK:CG    | 1:C:998:UNK:HB2   | 2.34                     | 0.58              |
| 1:A:1008:UNK:CG   | 1:A:1019:PHE:HB3  | 2.33                     | 0.58              |
| 1:A:1327:VAL:HB   | 1:A:1339:ALA:HB3  | 1.86                     | 0.58              |
| 1:A:2461:VAL:HG11 | 1:A:2751:VAL:HG22 | 1.84                     | 0.58              |
| 1:C:1253:ARG:HG3  | 1:C:1253:ARG:NH1  | 2.18                     | 0.58              |
| 1:C:2667:THR:HG21 | 1:C:3058:ARG:NH1  | 2.17                     | 0.58              |
| 1:A:1701:VAL:HG22 | 1:A:1732:LEU:HB2  | 1.84                     | 0.58              |
| 1:A:2124:UNK:C    | 1:A:2127:UNK:HG3  | 2.34                     | 0.58              |
| 1:B:836:VAL:HG12  | 1:B:837:VAL:H     | 1.67                     | 0.58              |
| 1:C:2521:VAL:HG13 | 1:C:2529:ARG:HH11 | 1.68                     | 0.58              |
| 1:A:117:LYS:NZ    | 1:C:1087:PHE:HB3  | 2.18                     | 0.58              |
| 1:A:836:VAL:HG12  | 1:A:837:VAL:H     | 1.67                     | 0.58              |
| 1:B:1008:UNK:O    | 1:B:1008:UNK:HG2  | 2.03                     | 0.58              |
| 1:B:1616:PRO:HG3  | 1:B:1668:LEU:HD13 | 1.85                     | 0.58              |
| 1:B:2487:LEU:HD11 | 1:B:2495:LEU:HD12 | 1.86                     | 0.58              |
| 1:B:2787:THR:HA   | 1:B:2790:MET:HG3  | 1.86                     | 0.58              |
| 1:B:2876:LEU:HB3  | 1:B:2881:VAL:HG12 | 1.86                     | 0.58              |
| 1:C:1989:PHE:HD1  | 1:C:1992:LYS:HZ3  | 1.51                     | 0.58              |
| 1:C:687:GLY:O     | 1:C:695:ILE:N     | 2.34                     | 0.58              |
| 1:A:2101:UNK:O    | 1:A:2105:UNK:HG3  | 2.04                     | 0.58              |
| 1:A:441:ASP:OD2   | 1:A:443:LYS:HB3   | 2.04                     | 0.58              |
| 1:A:511:ARG:HD2   | 1:A:517:ILE:O     | 2.04                     | 0.58              |
| 1:A:784:GLU:OE2   | 1:A:787:LEU:HD12  | 2.04                     | 0.58              |
| 1:B:410:LEU:HB3   | 1:B:1025:VAL:HG21 | 1.84                     | 0.58              |
| 1:B:970:ILE:CD1   | 1:B:996:UNK:HG1   | 2.34                     | 0.58              |
| 1:C:1656:LYS:HG2  | 1:C:1660:LEU:HG   | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:970:ILE:CD1   | 1:C:996:UNK:HG1   | 2.34                     | 0.58              |
| 1:A:2487:LEU:HD11 | 1:A:2495:LEU:HD12 | 1.86                     | 0.58              |
| 1:B:2339:TRP:HB2  | 1:B:2398:LEU:HD11 | 1.86                     | 0.58              |
| 1:B:2820:ILE:HD13 | 1:B:2943:MET:HG2  | 1.84                     | 0.58              |
| 1:B:776:ASP:O     | 1:B:779:TRP:N     | 2.31                     | 0.58              |
| 1:B:990:UNK:CG    | 1:B:998:UNK:HB2   | 2.34                     | 0.58              |
| 1:A:2521:VAL:HG13 | 1:A:2529:ARG:HH11 | 1.68                     | 0.58              |
| 1:A:2554:ALA:HB1  | 1:A:2614:LYS:NZ   | 2.19                     | 0.58              |
| 1:A:2787:THR:HA   | 1:A:2790:MET:HG3  | 1.86                     | 0.58              |
| 1:B:1309:VAL:HG22 | 1:B:1331:ILE:HG12 | 1.84                     | 0.58              |
| 1:B:784:GLU:OE2   | 1:B:787:LEU:HD12  | 2.03                     | 0.58              |
| 1:B:943:UNK:C     | 1:B:944:UNK:HG3   | 2.32                     | 0.58              |
| 1:A:1091:LEU:HD13 | 1:A:1281:ALA:HB3  | 1.86                     | 0.57              |
| 1:A:1435:VAL:HG11 | 1:A:1463:CYS:HB3  | 1.84                     | 0.57              |
| 1:A:462:GLN:HG3   | 1:A:468:PHE:HD1   | 1.68                     | 0.57              |
| 1:B:1412:HIS:ND1  | 1:B:1415:GLY:O    | 2.26                     | 0.57              |
| 1:C:1008:UNK:HG2  | 1:C:1008:UNK:O    | 2.03                     | 0.57              |
| 1:C:2403:ILE:HG23 | 1:C:2408:LEU:HD12 | 1.85                     | 0.57              |
| 1:C:441:ASP:OD2   | 1:C:443:LYS:HB3   | 2.04                     | 0.57              |
| 1:A:1002:UNK:C    | 1:A:1003:UNK:HG3  | 2.33                     | 0.57              |
| 1:A:1087:PHE:HB3  | 1:B:117:LYS:NZ    | 2.18                     | 0.57              |
| 1:A:476:GLU:HA    | 1:A:479:LEU:HB2   | 1.86                     | 0.57              |
| 1:A:924:LEU:HA    | 1:A:928:ALA:HB3   | 1.87                     | 0.57              |
| 1:A:999:UNK:CG    | 1:A:1007:UNK:HG2  | 2.34                     | 0.57              |
| 1:B:1009:UNK:HG2  | 1:B:1009:UNK:O    | 2.04                     | 0.57              |
| 1:B:1095:LEU:HD22 | 1:B:1289:PRO:HA   | 1.85                     | 0.57              |
| 1:B:1226:UNK:HG3  | 1:B:1313:VAL:CG1  | 2.35                     | 0.57              |
| 1:B:2124:UNK:C    | 1:B:2127:UNK:HG3  | 2.34                     | 0.57              |
| 1:C:1002:UNK:C    | 1:C:1003:UNK:HG3  | 2.33                     | 0.57              |
| 1:C:2101:UNK:O    | 1:C:2105:UNK:HG3  | 2.04                     | 0.57              |
| 1:C:2487:LEU:HD11 | 1:C:2495:LEU:HD12 | 1.86                     | 0.57              |
| 1:A:1095:LEU:HD22 | 1:A:1289:PRO:HA   | 1.85                     | 0.57              |
| 1:A:2339:TRP:HB2  | 1:A:2398:LEU:HD11 | 1.86                     | 0.57              |
| 1:B:2101:UNK:O    | 1:B:2105:UNK:HG3  | 2.04                     | 0.57              |
| 1:B:621:SER:OG    | 1:B:643:ILE:HD13  | 2.04                     | 0.57              |
| 1:C:2339:TRP:HB2  | 1:C:2398:LEU:HD11 | 1.86                     | 0.57              |
| 1:C:2554:ALA:HB1  | 1:C:2614:LYS:NZ   | 2.19                     | 0.57              |
| 1:C:934:UNK:C     | 1:C:937:UNK:HG3   | 2.32                     | 0.57              |
| 1:A:1405:ALA:HB3  | 1:A:1408:VAL:HG23 | 1.86                     | 0.57              |
| 1:A:621:SER:OG    | 1:A:643:ILE:HD13  | 2.04                     | 0.57              |
| 1:A:939:UNK:C     | 1:A:940:UNK:HG3   | 2.33                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:990:UNK:CG    | 1:A:998:UNK:HB2   | 2.34                     | 0.57              |
| 1:C:1017:ILE:HG23 | 1:C:1045:VAL:HG21 | 1.87                     | 0.57              |
| 1:B:1087:PHE:HB3  | 1:C:117:LYS:NZ    | 2.19                     | 0.57              |
| 1:C:129:VAL:HG13  | 1:C:356:PRO:HG2   | 1.85                     | 0.57              |
| 1:C:511:ARG:HD2   | 1:C:517:ILE:O     | 2.04                     | 0.57              |
| 1:A:2124:UNK:O    | 1:A:2127:UNK:CG   | 2.51                     | 0.57              |
| 1:A:970:ILE:CD1   | 1:A:996:UNK:HG1   | 2.34                     | 0.57              |
| 1:B:2521:VAL:HG13 | 1:B:2529:ARG:HH11 | 1.68                     | 0.57              |
| 1:B:2889:ILE:HG12 | 1:B:2922:LEU:HB3  | 1.84                     | 0.57              |
| 1:B:2983:LEU:HB3  | 1:B:2987:PHE:O    | 2.05                     | 0.57              |
| 1:B:129:VAL:HG13  | 1:B:356:PRO:HG2   | 1.85                     | 0.57              |
| 1:B:924:LEU:HA    | 1:B:928:ALA:HB3   | 1.86                     | 0.57              |
| 1:C:1445:VAL:HG23 | 1:C:1448:ALA:HB2  | 1.87                     | 0.57              |
| 1:C:2086:UNK:HA   | 1:C:2089:UNK:HG3  | 1.86                     | 0.57              |
| 1:C:2124:UNK:C    | 1:C:2127:UNK:HG3  | 2.34                     | 0.57              |
| 1:C:2820:ILE:HD13 | 1:C:2943:MET:HG2  | 1.84                     | 0.57              |
| 1:C:2846:ALA:HA   | 1:C:3001:HIS:O    | 2.05                     | 0.57              |
| 1:C:476:GLU:HA    | 1:C:479:LEU:HB2   | 1.86                     | 0.57              |
| 1:C:490:LEU:HD23  | 1:C:523:SER:HB2   | 1.87                     | 0.57              |
| 1:C:924:LEU:HA    | 1:C:928:ALA:HB3   | 1.87                     | 0.57              |
| 1:C:999:UNK:CG    | 1:C:1007:UNK:HG2  | 2.34                     | 0.57              |
| 1:A:1009:UNK:HG2  | 1:A:1009:UNK:O    | 2.03                     | 0.57              |
| 1:A:2709:ILE:O    | 1:A:2713:VAL:HG13 | 2.05                     | 0.57              |
| 1:B:2429:UNK:O    | 1:B:2429:UNK:HG2  | 2.02                     | 0.57              |
| 1:B:975:UNK:HG2   | 1:B:976:UNK:N     | 2.20                     | 0.57              |
| 1:C:1009:UNK:O    | 1:C:1009:UNK:HG2  | 2.04                     | 0.57              |
| 1:C:1008:UNK:CG   | 1:C:1019:PHE:HB3  | 2.33                     | 0.57              |
| 1:C:1095:LEU:HD22 | 1:C:1289:PRO:HA   | 1.85                     | 0.57              |
| 1:C:2622:GLY:HA2  | 1:C:2812:LEU:HD11 | 1.87                     | 0.57              |
| 1:C:939:UNK:C     | 1:C:940:UNK:HG3   | 2.33                     | 0.57              |
| 1:A:2403:ILE:HG23 | 1:A:2408:LEU:HD12 | 1.85                     | 0.57              |
| 1:A:2846:ALA:HA   | 1:A:3001:HIS:O    | 2.05                     | 0.57              |
| 1:B:1445:VAL:HG23 | 1:B:1448:ALA:HB2  | 1.87                     | 0.57              |
| 1:B:2846:ALA:HA   | 1:B:3001:HIS:O    | 2.05                     | 0.57              |
| 1:C:2876:LEU:HB3  | 1:C:2881:VAL:HG12 | 1.86                     | 0.57              |
| 1:C:784:GLU:OE2   | 1:C:787:LEU:HD12  | 2.03                     | 0.57              |
| 1:A:1537:LEU:HD11 | 1:A:1714:LEU:HB3  | 1.87                     | 0.57              |
| 1:A:2876:LEU:HB3  | 1:A:2881:VAL:HG12 | 1.86                     | 0.57              |
| 1:A:980:UNK:O     | 1:A:981:UNK:CG    | 2.53                     | 0.57              |
| 1:B:2084:UNK:O    | 1:B:2087:UNK:CG   | 2.52                     | 0.57              |
| 1:B:441:ASP:OD2   | 1:B:443:LYS:HB3   | 2.04                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:735:LYS:HD2   | 1:B:860:VAL:HG23  | 1.85                     | 0.57              |
| 1:B:978:UNK:HB2   | 1:B:991:UNK:HG2   | 1.87                     | 0.57              |
| 1:C:1091:LEU:HD13 | 1:C:1281:ALA:HB3  | 1.86                     | 0.57              |
| 1:C:127:PRO:HG3   | 1:C:183:GLN:HA    | 1.86                     | 0.57              |
| 1:C:929:UNK:C     | 1:C:930:UNK:HG3   | 2.35                     | 0.57              |
| 1:B:127:PRO:HG3   | 1:B:183:GLN:HA    | 1.86                     | 0.57              |
| 1:B:2100:UNK:CG   | 1:B:2101:UNK:N    | 2.68                     | 0.57              |
| 1:B:511:ARG:NH1   | 1:B:543:GLY:HA3   | 2.19                     | 0.57              |
| 1:C:462:GLN:HG3   | 1:C:468:PHE:HD1   | 1.68                     | 0.57              |
| 1:B:2124:UNK:O    | 1:B:2127:UNK:CG   | 2.51                     | 0.57              |
| 1:B:868:ARG:HB3   | 1:B:872:ARG:HH11  | 1.70                     | 0.57              |
| 1:C:2521:VAL:HG13 | 1:C:2529:ARG:NH1  | 2.20                     | 0.57              |
| 1:C:2787:THR:HA   | 1:C:2790:MET:HG3  | 1.86                     | 0.57              |
| 1:C:980:UNK:O     | 1:C:981:UNK:CG    | 2.53                     | 0.57              |
| 1:A:127:PRO:HG3   | 1:A:183:GLN:HA    | 1.85                     | 0.56              |
| 1:A:129:VAL:HG13  | 1:A:356:PRO:HG2   | 1.85                     | 0.56              |
| 1:A:511:ARG:NH1   | 1:A:543:GLY:HA3   | 2.19                     | 0.56              |
| 1:A:868:ARG:HB3   | 1:A:872:ARG:HH11  | 1.70                     | 0.56              |
| 1:B:1126:ILE:O    | 1:B:1197:UNK:CG   | 2.53                     | 0.56              |
| 1:B:2961:LEU:HD23 | 1:B:2978:ARG:HB3  | 1.87                     | 0.56              |
| 1:C:868:ARG:HB3   | 1:C:872:ARG:HH11  | 1.70                     | 0.56              |
| 1:A:490:LEU:HD23  | 1:A:523:SER:HB2   | 1.87                     | 0.56              |
| 1:C:735:LYS:HD2   | 1:C:860:VAL:HG23  | 1.85                     | 0.56              |
| 1:C:793:ARG:HD3   | 1:C:2435:UNK:CG   | 2.27                     | 0.56              |
| 1:A:2086:UNK:HA   | 1:A:2089:UNK:HG3  | 1.86                     | 0.56              |
| 1:A:745:THR:OG1   | 1:A:834:GLU:O     | 2.19                     | 0.56              |
| 1:B:999:UNK:CG    | 1:B:1007:UNK:HG2  | 2.34                     | 0.56              |
| 1:B:1637:VAL:HG21 | 1:B:1671:TRP:CG   | 2.40                     | 0.56              |
| 1:B:511:ARG:HD2   | 1:B:517:ILE:O     | 2.04                     | 0.56              |
| 1:C:1420:THR:OG1  | 1:C:1485:HIS:NE2  | 2.38                     | 0.56              |
| 1:C:1537:LEU:HD11 | 1:C:1714:LEU:HB3  | 1.86                     | 0.56              |
| 1:A:37:ARG:O      | 1:A:41:GLY:N      | 2.38                     | 0.56              |
| 1:A:976:UNK:CG    | 1:A:993:UNK:HB1   | 2.29                     | 0.56              |
| 1:B:1001:UNK:O    | 1:B:1002:UNK:CG   | 2.53                     | 0.56              |
| 1:B:150:THR:O     | 1:B:152:PRO:HD3   | 2.03                     | 0.56              |
| 1:B:2521:VAL:HG13 | 1:B:2529:ARG:NH1  | 2.20                     | 0.56              |
| 1:B:2554:ALA:HB1  | 1:B:2614:LYS:NZ   | 2.19                     | 0.56              |
| 1:B:2709:ILE:O    | 1:B:2713:VAL:HG13 | 2.05                     | 0.56              |
| 1:B:2481:MET:O    | 1:B:2959:ARG:NH2  | 2.39                     | 0.56              |
| 1:B:476:GLU:HA    | 1:B:479:LEU:HB2   | 1.86                     | 0.56              |
| 1:B:939:UNK:C     | 1:B:940:UNK:HG3   | 2.33                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:177:GLU:HB3   | 1:C:317:LEU:HD13  | 1.87                     | 0.56              |
| 1:A:1017:ILE:HG23 | 1:A:1045:VAL:HG21 | 1.87                     | 0.56              |
| 1:A:1253:ARG:NH1  | 1:A:1253:ARG:HG3  | 2.18                     | 0.56              |
| 1:A:2521:VAL:HG13 | 1:A:2529:ARG:NH1  | 2.20                     | 0.56              |
| 1:A:2881:VAL:HG13 | 1:A:2885:ASP:HB2  | 1.88                     | 0.56              |
| 1:A:776:ASP:O     | 1:A:779:TRP:N     | 2.31                     | 0.56              |
| 1:A:978:UNK:HB2   | 1:A:991:UNK:HG2   | 1.87                     | 0.56              |
| 1:B:1091:LEU:HD13 | 1:B:1281:ALA:HB3  | 1.86                     | 0.56              |
| 1:B:177:GLU:HB3   | 1:B:317:LEU:HD13  | 1.87                     | 0.56              |
| 1:C:1126:ILE:O    | 1:C:1197:UNK:CG   | 2.53                     | 0.56              |
| 1:C:2957:PRO:HD3  | 1:C:2980:PRO:HB3  | 1.88                     | 0.56              |
| 1:C:511:ARG:NH1   | 1:C:543:GLY:HA3   | 2.19                     | 0.56              |
| 1:A:975:UNK:HG2   | 1:A:976:UNK:N     | 2.20                     | 0.56              |
| 1:A:990:UNK:HG2   | 1:A:990:UNK:O     | 2.05                     | 0.56              |
| 1:B:2622:GLY:HA2  | 1:B:2812:LEU:HD11 | 1.87                     | 0.56              |
| 1:C:2693:GLN:O    | 1:C:2697:HIS:ND1  | 2.33                     | 0.56              |
| 1:A:2983:LEU:HB3  | 1:A:2987:PHE:O    | 2.05                     | 0.56              |
| 1:B:1511:ASP:H    | 1:B:1514:ASP:HB2  | 1.71                     | 0.56              |
| 1:B:2962:ASP:OD1  | 1:B:2962:ASP:N    | 2.34                     | 0.56              |
| 1:C:1327:VAL:HB   | 1:C:1339:ALA:HB3  | 1.86                     | 0.56              |
| 1:C:1511:ASP:H    | 1:C:1514:ASP:HB2  | 1.71                     | 0.56              |
| 1:C:475:LEU:O     | 1:C:479:LEU:N     | 2.37                     | 0.56              |
| 1:A:1637:VAL:HG21 | 1:A:1671:TRP:CG   | 2.40                     | 0.56              |
| 1:B:2478:ARG:NH1  | 1:B:2482:GLU:OE1  | 2.39                     | 0.56              |
| 1:C:1226:UNK:HG3  | 1:C:1313:VAL:CG1  | 2.35                     | 0.56              |
| 1:C:1637:VAL:HG21 | 1:C:1671:TRP:CG   | 2.40                     | 0.56              |
| 1:C:2478:ARG:NH1  | 1:C:2482:GLU:OE1  | 2.39                     | 0.56              |
| 1:A:1126:ILE:O    | 1:A:1197:UNK:CG   | 2.53                     | 0.56              |
| 1:A:1226:UNK:HG3  | 1:A:1313:VAL:CG1  | 2.35                     | 0.56              |
| 1:A:1511:ASP:H    | 1:A:1514:ASP:HB2  | 1.71                     | 0.56              |
| 1:A:2478:ARG:NH1  | 1:A:2482:GLU:OE1  | 2.39                     | 0.56              |
| 1:A:2961:LEU:HD23 | 1:A:2978:ARG:HB3  | 1.87                     | 0.56              |
| 1:B:1537:LEU:HD11 | 1:B:1714:LEU:HB3  | 1.87                     | 0.56              |
| 1:B:2086:UNK:HA   | 1:B:2089:UNK:HG3  | 1.86                     | 0.56              |
| 1:B:2094:UNK:CG   | 1:B:2096:UNK:CG   | 2.75                     | 0.56              |
| 1:C:2084:UNK:O    | 1:C:2087:UNK:CG   | 2.52                     | 0.56              |
| 1:C:2709:ILE:O    | 1:C:2713:VAL:HG13 | 2.05                     | 0.56              |
| 1:C:2961:LEU:HD23 | 1:C:2978:ARG:HB3  | 1.87                     | 0.56              |
| 1:C:2983:LEU:HB3  | 1:C:2987:PHE:O    | 2.05                     | 0.56              |
| 1:C:978:UNK:HB2   | 1:C:991:UNK:HG2   | 1.87                     | 0.56              |
| 1:C:992:UNK:CG    | 1:C:996:UNK:HG2   | 2.32                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2102:UNK:C    | 1:A:2105:UNK:HG3  | 2.36                     | 0.56              |
| 1:A:687:GLY:O     | 1:A:695:ILE:N     | 2.34                     | 0.56              |
| 1:B:1017:ILE:HG23 | 1:B:1045:VAL:HG21 | 1.87                     | 0.56              |
| 1:B:1618:LEU:HG   | 1:B:1619:VAL:HG23 | 1.88                     | 0.56              |
| 1:B:490:LEU:HD23  | 1:B:523:SER:HB2   | 1.87                     | 0.56              |
| 1:C:1618:LEU:HG   | 1:C:1619:VAL:HG23 | 1.88                     | 0.56              |
| 1:C:2102:UNK:C    | 1:C:2105:UNK:HG3  | 2.36                     | 0.56              |
| 1:A:1445:VAL:HG23 | 1:A:1448:ALA:HB2  | 1.87                     | 0.56              |
| 1:A:2084:UNK:O    | 1:A:2087:UNK:CG   | 2.52                     | 0.56              |
| 1:B:1420:THR:OG1  | 1:B:1485:HIS:NE2  | 2.38                     | 0.56              |
| 1:B:2303:ASP:N    | 1:B:2303:ASP:OD1  | 2.39                     | 0.56              |
| 1:B:990:UNK:HG2   | 1:B:990:UNK:O     | 2.05                     | 0.56              |
| 1:C:1405:ALA:HB3  | 1:C:1408:VAL:HG23 | 1.86                     | 0.56              |
| 1:C:37:ARG:O      | 1:C:41:GLY:N      | 2.39                     | 0.56              |
| 1:C:975:UNK:HG2   | 1:C:976:UNK:N     | 2.20                     | 0.56              |
| 1:C:990:UNK:HG2   | 1:C:990:UNK:O     | 2.05                     | 0.56              |
| 1:A:934:UNK:C     | 1:A:937:UNK:HG3   | 2.32                     | 0.55              |
| 1:B:2743:ALA:HB3  | 1:B:2939:ALA:HB3  | 1.88                     | 0.55              |
| 1:B:540:ASN:HD21  | 1:B:544:ILE:HG13  | 1.71                     | 0.55              |
| 1:B:929:UNK:C     | 1:B:930:UNK:HG3   | 2.35                     | 0.55              |
| 1:A:2743:ALA:HB3  | 1:A:2939:ALA:HB3  | 1.88                     | 0.55              |
| 1:A:2481:MET:O    | 1:A:2959:ARG:NH2  | 2.39                     | 0.55              |
| 1:B:1405:ALA:HB3  | 1:B:1408:VAL:HG23 | 1.87                     | 0.55              |
| 1:A:1618:LEU:HG   | 1:A:1619:VAL:HG23 | 1.88                     | 0.55              |
| 1:A:929:UNK:C     | 1:A:930:UNK:HG3   | 2.35                     | 0.55              |
| 1:B:2102:UNK:C    | 1:B:2105:UNK:HG3  | 2.36                     | 0.55              |
| 1:B:475:LEU:O     | 1:B:479:LEU:N     | 2.37                     | 0.55              |
| 1:B:737:TYR:HE1   | 1:B:862:VAL:HA    | 1.72                     | 0.55              |
| 1:B:931:UNK:HG2   | 1:B:934:UNK:N     | 2.21                     | 0.55              |
| 1:A:2135:UNK:CG   | 1:A:2136:ASP:N    | 2.66                     | 0.55              |
| 1:A:2622:GLY:HA2  | 1:A:2812:LEU:HD11 | 1.87                     | 0.55              |
| 1:B:975:UNK:CG    | 1:B:976:UNK:N     | 2.70                     | 0.55              |
| 1:B:980:UNK:O     | 1:B:981:UNK:CG    | 2.53                     | 0.55              |
| 1:C:1496:SER:HB3  | 1:C:1578:ASP:HB3  | 1.89                     | 0.55              |
| 1:C:2442:UNK:HG2  | 1:C:2442:UNK:O    | 2.07                     | 0.55              |
| 1:C:2481:MET:O    | 1:C:2959:ARG:NH2  | 2.39                     | 0.55              |
| 1:A:540:ASN:HD21  | 1:A:544:ILE:HG13  | 1.71                     | 0.55              |
| 1:B:1010:UNK:O    | 1:B:1017:ILE:N    | 2.29                     | 0.55              |
| 1:B:551:PRO:HG3   | 1:B:560:VAL:HG21  | 1.89                     | 0.55              |
| 1:C:1010:UNK:O    | 1:C:1017:ILE:N    | 2.29                     | 0.55              |
| 1:C:2881:VAL:HG13 | 1:C:2885:ASP:HB2  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:177:GLU:HB3  | 1:A:317:LEU:HD13  | 1.87                     | 0.55              |
| 1:B:2704:ALA:O   | 1:B:2705:LYS:HD3  | 2.07                     | 0.55              |
| 1:A:1690:GLU:O   | 1:A:1694:GLY:N    | 2.40                     | 0.55              |
| 1:A:1734:SER:HA  | 1:A:1741:LEU:HD11 | 1.89                     | 0.55              |
| 1:A:931:UNK:HG2  | 1:A:933:UNK:CG    | 2.37                     | 0.55              |
| 1:B:2458:ALA:HA  | 1:B:2824:ARG:HD2  | 1.89                     | 0.55              |
| 1:C:2810:GLY:HA2 | 1:C:2896:THR:HA   | 1.89                     | 0.55              |
| 1:A:737:TYR:HE1  | 1:A:862:VAL:HA    | 1.72                     | 0.55              |
| 1:A:931:UNK:HG2  | 1:A:934:UNK:N     | 2.21                     | 0.55              |
| 1:B:1496:SER:HB3 | 1:B:1578:ASP:HB3  | 1.88                     | 0.55              |
| 1:B:2135:UNK:CG  | 1:B:2136:ASP:N    | 2.66                     | 0.55              |
| 1:B:238:SER:OG   | 1:B:249:THR:OG1   | 2.15                     | 0.55              |
| 1:B:2957:PRO:HD3 | 1:B:2980:PRO:HB3  | 1.88                     | 0.55              |
| 1:C:1690:GLU:O   | 1:C:1694:GLY:N    | 2.40                     | 0.55              |
| 1:C:737:TYR:HE1  | 1:C:862:VAL:HA    | 1.72                     | 0.55              |
| 1:A:2087:UNK:CA  | 1:A:2090:UNK:HG3  | 2.37                     | 0.55              |
| 1:A:2704:ALA:O   | 1:A:2705:LYS:HD3  | 2.07                     | 0.55              |
| 1:A:2458:ALA:HA  | 1:A:2824:ARG:HD2  | 1.89                     | 0.55              |
| 1:B:2418:GLY:O   | 1:B:2422:UNK:N    | 2.40                     | 0.55              |
| 1:C:1001:UNK:O   | 1:C:1002:UNK:CG   | 2.53                     | 0.55              |
| 1:C:144:GLY:O    | 1:C:148:THR:N     | 2.34                     | 0.55              |
| 1:B:1724:TYR:OH  | 1:C:267:GLU:OE2   | 2.07                     | 0.55              |
| 1:C:994:UNK:CG   | 1:C:996:UNK:HG3   | 2.37                     | 0.55              |
| 1:A:1001:UNK:O   | 1:A:1002:UNK:CG   | 2.53                     | 0.55              |
| 1:A:2418:GLY:O   | 1:A:2422:UNK:N    | 2.40                     | 0.54              |
| 1:B:1163:ASP:CB  | 1:B:1199:UNK:HG3  | 2.37                     | 0.54              |
| 1:B:1690:GLU:O   | 1:B:1694:GLY:N    | 2.40                     | 0.54              |
| 1:B:2442:UNK:HG2 | 1:B:2442:UNK:O    | 2.07                     | 0.54              |
| 1:B:763:SER:O    | 1:B:766:ASP:N     | 2.41                     | 0.54              |
| 1:A:2303:ASP:N   | 1:A:2303:ASP:OD1  | 2.39                     | 0.54              |
| 1:A:2810:GLY:HA2 | 1:A:2896:THR:HA   | 1.89                     | 0.54              |
| 1:A:33:ALA:O     | 1:A:37:ARG:N      | 2.35                     | 0.54              |
| 1:A:975:UNK:CG   | 1:A:976:UNK:N     | 2.70                     | 0.54              |
| 1:B:2810:GLY:HA2 | 1:B:2896:THR:HA   | 1.89                     | 0.54              |
| 1:C:540:ASN:HD21 | 1:C:544:ILE:HG13  | 1.71                     | 0.54              |
| 1:C:975:UNK:CG   | 1:C:976:UNK:N     | 2.70                     | 0.54              |
| 1:C:978:UNK:HB2  | 1:C:991:UNK:CG    | 2.37                     | 0.54              |
| 1:A:2957:PRO:HD3 | 1:A:2980:PRO:HB3  | 1.88                     | 0.54              |
| 1:C:2704:ALA:O   | 1:C:2705:LYS:HD3  | 2.07                     | 0.54              |
| 1:C:931:UNK:HG2  | 1:C:934:UNK:N     | 2.21                     | 0.54              |
| 1:A:1010:UNK:O   | 1:A:1017:ILE:N    | 2.29                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2417:SER:O    | 1:A:2421:ASP:N    | 2.40                     | 0.54              |
| 1:B:2115:UNK:HA   | 1:B:2118:UNK:HG3  | 1.90                     | 0.54              |
| 1:B:2881:VAL:HG13 | 1:B:2885:ASP:HB2  | 1.88                     | 0.54              |
| 1:C:2743:ALA:HB3  | 1:C:2939:ALA:HB3  | 1.88                     | 0.54              |
| 1:C:763:SER:O     | 1:C:766:ASP:N     | 2.41                     | 0.54              |
| 1:C:931:UNK:HG2   | 1:C:933:UNK:CG    | 2.37                     | 0.54              |
| 1:A:3018:LEU:O    | 1:A:3022:GLU:HB2  | 2.08                     | 0.54              |
| 1:A:668:THR:OG1   | 1:A:698:ILE:HD11  | 2.08                     | 0.54              |
| 1:B:2693:GLN:O    | 1:B:2697:HIS:ND1  | 2.33                     | 0.54              |
| 1:C:2103:UNK:O    | 1:C:2106:UNK:HG3  | 2.08                     | 0.54              |
| 1:C:2458:ALA:HA   | 1:C:2824:ARG:HD2  | 1.89                     | 0.54              |
| 1:C:2860:ALA:HB1  | 1:C:3005:LEU:HD13 | 1.90                     | 0.54              |
| 1:A:1496:SER:HB3  | 1:A:1578:ASP:HB3  | 1.89                     | 0.54              |
| 1:B:580:ARG:HH11  | 1:B:614:GLY:HA3   | 1.72                     | 0.54              |
| 1:C:273:ARG:HD2   | 1:C:282:VAL:HG12  | 1.90                     | 0.54              |
| 1:C:580:ARG:HH11  | 1:C:614:GLY:HA3   | 1.73                     | 0.54              |
| 1:C:716:ALA:HA    | 1:C:719:VAL:HG23  | 1.90                     | 0.54              |
| 1:A:2122:UNK:CA   | 1:A:2125:UNK:HG3  | 2.38                     | 0.54              |
| 1:A:2246:ALA:C    | 1:A:2255:ARG:HH12 | 2.11                     | 0.54              |
| 1:A:456:GLU:HG2   | 1:A:486:GLN:HE21  | 1.73                     | 0.54              |
| 1:A:763:SER:O     | 1:A:766:ASP:N     | 2.41                     | 0.54              |
| 1:B:2768:ASP:OD2  | 1:B:2936:GLY:N    | 2.41                     | 0.54              |
| 1:B:37:ARG:O      | 1:B:41:GLY:N      | 2.39                     | 0.54              |
| 1:C:1003:UNK:CG   | 1:C:1004:UNK:N    | 2.53                     | 0.54              |
| 1:C:1163:ASP:CB   | 1:C:1199:UNK:HG3  | 2.38                     | 0.54              |
| 1:C:1357:ILE:HG13 | 1:C:1710:THR:HG21 | 1.89                     | 0.54              |
| 1:C:2100:UNK:CG   | 1:C:2101:UNK:N    | 2.68                     | 0.54              |
| 1:C:2115:UNK:HA   | 1:C:2118:UNK:HG3  | 1.90                     | 0.54              |
| 1:C:2127:UNK:O    | 1:C:2130:UNK:CG   | 2.52                     | 0.54              |
| 1:C:2418:GLY:O    | 1:C:2422:UNK:N    | 2.40                     | 0.54              |
| 1:A:1357:ILE:HG13 | 1:A:1710:THR:HG21 | 1.89                     | 0.54              |
| 1:A:2112:UNK:N    | 1:A:2115:UNK:HG3  | 2.23                     | 0.54              |
| 1:A:2492:VAL:HG21 | 1:A:2527:VAL:HG22 | 1.90                     | 0.54              |
| 1:A:978:UNK:HB2   | 1:A:991:UNK:CG    | 2.37                     | 0.54              |
| 1:B:273:ARG:HD2   | 1:B:282:VAL:HG12  | 1.90                     | 0.54              |
| 1:B:668:THR:OG1   | 1:B:698:ILE:HD11  | 2.08                     | 0.54              |
| 1:B:978:UNK:HB2   | 1:B:991:UNK:CG    | 2.37                     | 0.54              |
| 1:C:456:GLU:HG2   | 1:C:486:GLN:HE21  | 1.73                     | 0.54              |
| 1:B:2104:UNK:HA   | 1:B:2107:UNK:HG3  | 1.90                     | 0.54              |
| 1:C:3018:LEU:O    | 1:C:3022:GLU:HB2  | 2.08                     | 0.54              |
| 1:C:33:ALA:O      | 1:C:37:ARG:N      | 2.35                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2012:GLY:C    | 1:B:2591:ARG:NH1  | 2.61                     | 0.54              |
| 1:A:980:UNK:N     | 1:A:989:UNK:O     | 2.41                     | 0.54              |
| 1:A:994:UNK:CG    | 1:A:996:UNK:HG3   | 2.37                     | 0.54              |
| 1:B:1734:SER:HA   | 1:B:1741:LEU:HD11 | 1.89                     | 0.54              |
| 1:B:2100:UNK:C    | 1:B:2103:UNK:HG3  | 2.31                     | 0.54              |
| 1:B:2860:ALA:HB1  | 1:B:3005:LEU:HD13 | 1.90                     | 0.54              |
| 1:B:624:TYR:HA    | 1:B:629:TRP:CD1   | 2.43                     | 0.54              |
| 1:C:2087:UNK:CA   | 1:C:2090:UNK:HG3  | 2.37                     | 0.54              |
| 1:C:624:TYR:HA    | 1:C:629:TRP:CD1   | 2.43                     | 0.54              |
| 1:A:2100:UNK:CG   | 1:A:2101:UNK:N    | 2.68                     | 0.53              |
| 1:A:2442:UNK:HG2  | 1:A:2442:UNK:O    | 2.07                     | 0.53              |
| 1:A:267:GLU:OE2   | 1:C:1724:TYR:OH   | 2.07                     | 0.53              |
| 1:A:368:ILE:HG21  | 1:A:373:ILE:HG13  | 1.90                     | 0.53              |
| 1:A:475:LEU:O     | 1:A:479:LEU:N     | 2.37                     | 0.53              |
| 1:B:1089:ALA:O    | 1:B:1091:LEU:N    | 2.41                     | 0.53              |
| 1:B:2417:SER:O    | 1:B:2421:ASP:N    | 2.40                     | 0.53              |
| 1:B:456:GLU:HG2   | 1:B:486:GLN:HE21  | 1.73                     | 0.53              |
| 1:C:1323:GLU:N    | 1:C:1343:LEU:O    | 2.41                     | 0.53              |
| 1:C:2551:PRO:O    | 1:C:2617:LEU:HB2  | 2.08                     | 0.53              |
| 1:C:2653:VAL:HA   | 1:C:3051:MET:HE3  | 1.90                     | 0.53              |
| 1:A:1089:ALA:O    | 1:A:1091:LEU:N    | 2.42                     | 0.53              |
| 1:A:624:TYR:HA    | 1:A:629:TRP:CD1   | 2.43                     | 0.53              |
| 1:B:2103:UNK:O    | 1:B:2106:UNK:HG3  | 2.08                     | 0.53              |
| 1:B:2425:UNK:O    | 1:B:2425:UNK:HG2  | 2.09                     | 0.53              |
| 1:B:2492:VAL:HG21 | 1:B:2527:VAL:HG22 | 1.90                     | 0.53              |
| 1:C:1734:SER:HA   | 1:C:1741:LEU:HD11 | 1.89                     | 0.53              |
| 1:C:2104:UNK:HA   | 1:C:2107:UNK:HG3  | 1.90                     | 0.53              |
| 1:C:2303:ASP:OD1  | 1:C:2303:ASP:N    | 2.39                     | 0.53              |
| 1:C:33:ALA:O      | 1:C:37:ARG:HG2    | 2.08                     | 0.53              |
| 1:C:551:PRO:HG3   | 1:C:560:VAL:HG21  | 1.89                     | 0.53              |
| 1:C:992:UNK:HG2   | 1:C:994:UNK:HG2   | 1.87                     | 0.53              |
| 1:C:999:UNK:HG3   | 1:C:1007:UNK:HG2  | 1.90                     | 0.53              |
| 1:A:1163:ASP:CB   | 1:A:1199:UNK:HG3  | 2.38                     | 0.53              |
| 1:A:580:ARG:HH11  | 1:A:614:GLY:HA3   | 1.72                     | 0.53              |
| 1:B:2088:UNK:HG2  | 1:B:2188:ARG:HH12 | 1.73                     | 0.53              |
| 1:B:992:UNK:HG2   | 1:B:994:UNK:HG2   | 1.87                     | 0.53              |
| 1:B:994:UNK:CG    | 1:B:996:UNK:HG3   | 2.37                     | 0.53              |
| 1:C:2768:ASP:OD2  | 1:C:2936:GLY:N    | 2.41                     | 0.53              |
| 1:A:1323:GLU:N    | 1:A:1343:LEU:O    | 2.41                     | 0.53              |
| 1:A:2088:UNK:HG2  | 1:A:2188:ARG:HH12 | 1.74                     | 0.53              |
| 1:A:2425:UNK:O    | 1:A:2425:UNK:HG2  | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2768:ASP:OD2  | 1:A:2936:GLY:N    | 2.41                     | 0.53              |
| 1:A:526:ILE:HD12  | 1:A:549:PHE:HB3   | 1.90                     | 0.53              |
| 1:C:2122:UNK:CA   | 1:C:2125:UNK:HG3  | 2.38                     | 0.53              |
| 1:C:668:THR:OG1   | 1:C:698:ILE:HD11  | 2.08                     | 0.53              |
| 1:C:836:VAL:HG21  | 1:C:2437:UNK:HB2  | 1.90                     | 0.53              |
| 1:C:970:ILE:HD13  | 1:C:996:UNK:HG1   | 1.91                     | 0.53              |
| 1:A:1425:VAL:HG13 | 1:A:1474:LEU:HD13 | 1.91                     | 0.53              |
| 1:A:2085:UNK:C    | 1:A:2088:UNK:HG3  | 2.38                     | 0.53              |
| 1:A:2104:UNK:HA   | 1:A:2107:UNK:HG3  | 1.90                     | 0.53              |
| 1:A:792:ALA:HA    | 1:A:799:PHE:CE2   | 2.43                     | 0.53              |
| 1:A:992:UNK:CG    | 1:A:996:UNK:HG2   | 2.32                     | 0.53              |
| 1:B:2551:PRO:O    | 1:B:2617:LEU:HB2  | 2.08                     | 0.53              |
| 1:B:3018:LEU:O    | 1:B:3022:GLU:HB2  | 2.08                     | 0.53              |
| 1:C:1089:ALA:O    | 1:C:1091:LEU:N    | 2.42                     | 0.53              |
| 1:C:2492:VAL:HG21 | 1:C:2527:VAL:HG22 | 1.90                     | 0.53              |
| 1:C:500:GLN:O     | 1:C:504:LYS:N     | 2.24                     | 0.53              |
| 1:C:980:UNK:N     | 1:C:989:UNK:O     | 2.41                     | 0.53              |
| 1:A:2081:UNK:C    | 1:A:2084:UNK:HG3  | 2.39                     | 0.53              |
| 1:A:2591:ARG:NH1  | 1:C:2012:GLY:C    | 2.61                     | 0.53              |
| 1:A:551:PRO:HG3   | 1:A:560:VAL:HG21  | 1.89                     | 0.53              |
| 1:A:716:ALA:HA    | 1:A:719:VAL:HG23  | 1.90                     | 0.53              |
| 1:B:1148:GLU:O    | 1:B:1150:ALA:N    | 2.42                     | 0.53              |
| 1:B:1538:ARG:NH1  | 1:B:1722:PRO:HB3  | 2.18                     | 0.53              |
| 1:B:2086:UNK:O    | 1:B:2089:UNK:CG   | 2.52                     | 0.53              |
| 1:B:411:PRO:HD2   | 1:B:1025:VAL:HG11 | 1.91                     | 0.53              |
| 1:B:980:UNK:N     | 1:B:989:UNK:O     | 2.41                     | 0.53              |
| 1:C:1425:VAL:HG13 | 1:C:1474:LEU:HD13 | 1.91                     | 0.53              |
| 1:C:2123:UNK:O    | 1:C:2126:UNK:CG   | 2.55                     | 0.53              |
| 1:C:2631:PRO:HG3  | 1:C:2649:LEU:HD13 | 1.90                     | 0.53              |
| 1:C:745:THR:HG23  | 1:C:834:GLU:HA    | 1.90                     | 0.53              |
| 1:A:1087:PHE:HB3  | 1:B:117:LYS:HZ1   | 1.74                     | 0.53              |
| 1:A:836:VAL:HG21  | 1:A:2437:UNK:HB2  | 1.90                     | 0.53              |
| 1:A:970:ILE:HD13  | 1:A:996:UNK:HG1   | 1.91                     | 0.53              |
| 1:A:999:UNK:HG3   | 1:A:1007:UNK:HG2  | 1.90                     | 0.53              |
| 1:B:33:ALA:O      | 1:B:37:ARG:HG2    | 2.08                     | 0.53              |
| 1:B:526:ILE:HD12  | 1:B:549:PHE:HB3   | 1.90                     | 0.53              |
| 1:B:992:UNK:HG1   | 1:B:994:UNK:HG3   | 1.81                     | 0.53              |
| 1:C:1226:UNK:HB1  | 1:C:1282:THR:HG21 | 1.90                     | 0.53              |
| 1:C:2082:UNK:O    | 1:C:2086:UNK:HG3  | 2.09                     | 0.53              |
| 1:A:1420:THR:OG1  | 1:A:1485:HIS:NE2  | 2.38                     | 0.53              |
| 1:A:2088:UNK:C    | 1:A:2188:ARG:NH1  | 2.72                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2135:UNK:CG   | 1:A:2136:ASP:H    | 2.22                     | 0.53              |
| 1:A:588:GLU:HB3   | 1:A:593:LEU:HD11  | 1.91                     | 0.53              |
| 1:A:961:ARG:NH2   | 1:A:1196:UNK:O    | 2.42                     | 0.53              |
| 1:B:1151:GLU:HB2  | 1:B:1179:ALA:HB3  | 1.90                     | 0.53              |
| 1:B:1488:VAL:HG12 | 1:B:1490:ARG:HH11 | 1.73                     | 0.53              |
| 1:B:2012:GLY:C    | 1:C:2591:ARG:NH1  | 2.61                     | 0.53              |
| 1:B:2135:UNK:CG   | 1:B:2136:ASP:H    | 2.22                     | 0.53              |
| 1:B:2246:ALA:C    | 1:B:2255:ARG:HH12 | 2.11                     | 0.53              |
| 1:B:836:VAL:HG21  | 1:B:2437:UNK:HB2  | 1.90                     | 0.53              |
| 1:B:931:UNK:HG2   | 1:B:933:UNK:CG    | 2.37                     | 0.53              |
| 1:C:1174:VAL:HB   | 1:C:1188:LEU:HB3  | 1.91                     | 0.53              |
| 1:C:1634:ARG:HD2  | 1:C:1638:PRO:HA   | 1.91                     | 0.53              |
| 1:A:1148:GLU:O    | 1:A:1150:ALA:N    | 2.42                     | 0.53              |
| 1:A:1151:GLU:HB2  | 1:A:1179:ALA:HB3  | 1.90                     | 0.53              |
| 1:B:2631:PRO:HG3  | 1:B:2649:LEU:HD13 | 1.90                     | 0.53              |
| 1:B:2740:CYS:HB2  | 1:B:2998:GLY:HA2  | 1.91                     | 0.53              |
| 1:B:970:ILE:HD13  | 1:B:996:UNK:HG1   | 1.91                     | 0.53              |
| 1:C:2246:ALA:C    | 1:C:2255:ARG:HH12 | 2.11                     | 0.53              |
| 1:C:2425:UNK:HG2  | 1:C:2425:UNK:O    | 2.09                     | 0.53              |
| 1:A:2860:ALA:HB1  | 1:A:3005:LEU:HD13 | 1.90                     | 0.53              |
| 1:A:33:ALA:O      | 1:A:37:ARG:HG2    | 2.08                     | 0.53              |
| 1:A:992:UNK:HG2   | 1:A:994:UNK:HG2   | 1.87                     | 0.53              |
| 1:B:1323:GLU:N    | 1:B:1343:LEU:O    | 2.42                     | 0.53              |
| 1:B:2087:UNK:CA   | 1:B:2090:UNK:HG3  | 2.37                     | 0.53              |
| 1:B:33:ALA:O      | 1:B:37:ARG:N      | 2.35                     | 0.53              |
| 1:C:2088:UNK:C    | 1:C:2188:ARG:NH1  | 2.72                     | 0.53              |
| 1:C:2094:UNK:H    | 1:C:2097:UNK:HG3  | 1.74                     | 0.53              |
| 1:C:2112:UNK:N    | 1:C:2115:UNK:HG3  | 2.23                     | 0.53              |
| 1:A:1634:ARG:HD2  | 1:A:1638:PRO:HA   | 1.91                     | 0.52              |
| 1:A:2103:UNK:O    | 1:A:2106:UNK:HG3  | 2.08                     | 0.52              |
| 1:A:2115:UNK:HA   | 1:A:2118:UNK:HG3  | 1.90                     | 0.52              |
| 1:A:2551:PRO:O    | 1:A:2617:LEU:HB2  | 2.08                     | 0.52              |
| 1:B:961:ARG:NH2   | 1:B:1196:UNK:O    | 2.42                     | 0.52              |
| 1:B:2081:UNK:C    | 1:B:2084:UNK:HG3  | 2.39                     | 0.52              |
| 1:C:1530:LEU:HD21 | 1:C:1554:LEU:HD22 | 1.91                     | 0.52              |
| 1:C:2215:THR:HG22 | 1:C:2216:GLU:HG3  | 1.91                     | 0.52              |
| 1:C:2740:CYS:HB2  | 1:C:2998:GLY:HA2  | 1.92                     | 0.52              |
| 1:C:368:ILE:HG21  | 1:C:373:ILE:HG13  | 1.90                     | 0.52              |
| 1:A:208:VAL:HG12  | 1:A:248:ILE:HG12  | 1.92                     | 0.52              |
| 1:B:2085:UNK:C    | 1:B:2088:UNK:HG3  | 2.38                     | 0.52              |
| 1:B:2112:UNK:N    | 1:B:2115:UNK:HG3  | 2.23                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2085:UNK:C    | 1:C:2088:UNK:HG3  | 2.38                     | 0.52              |
| 1:C:2554:ALA:HB1  | 1:C:2614:LYS:HZ2  | 1.74                     | 0.52              |
| 1:C:411:PRO:HD2   | 1:C:1025:VAL:HG11 | 1.91                     | 0.52              |
| 1:A:1174:VAL:HB   | 1:A:1188:LEU:HB3  | 1.91                     | 0.52              |
| 1:B:1001:UNK:HG1  | 1:B:1018:ARG:HH22 | 1.74                     | 0.52              |
| 1:B:716:ALA:HA    | 1:B:719:VAL:HG23  | 1.90                     | 0.52              |
| 1:C:71:GLU:HG2    | 1:C:142:ARG:NH2   | 2.24                     | 0.52              |
| 1:A:1530:LEU:HD21 | 1:A:1554:LEU:HD22 | 1.91                     | 0.52              |
| 1:A:1733:ASN:HD22 | 1:A:1736:ARG:HD2  | 1.74                     | 0.52              |
| 1:A:2089:UNK:HA   | 1:A:2188:ARG:HH11 | 1.74                     | 0.52              |
| 1:A:2808:ARG:HB2  | 1:A:2895:SER:O    | 2.10                     | 0.52              |
| 1:A:71:GLU:HG2    | 1:A:142:ARG:NH2   | 2.24                     | 0.52              |
| 1:A:745:THR:HG23  | 1:A:834:GLU:HA    | 1.90                     | 0.52              |
| 1:A:931:UNK:HG2   | 1:A:933:UNK:HG2   | 1.91                     | 0.52              |
| 1:B:2094:UNK:HG2  | 1:B:2096:UNK:CG   | 2.23                     | 0.52              |
| 1:B:71:GLU:HG2    | 1:B:142:ARG:NH2   | 2.24                     | 0.52              |
| 1:C:1151:GLU:HB2  | 1:C:1179:ALA:HB3  | 1.90                     | 0.52              |
| 1:C:1538:ARG:NH1  | 1:C:1722:PRO:HB3  | 2.18                     | 0.52              |
| 1:A:400:TRP:CZ3   | 1:A:636:PRO:HB2   | 2.45                     | 0.52              |
| 1:B:1287:VAL:O    | 1:B:1291:LYS:HG3  | 2.10                     | 0.52              |
| 1:B:1357:ILE:HG13 | 1:B:1710:THR:HG21 | 1.89                     | 0.52              |
| 1:B:2089:UNK:HA   | 1:B:2188:ARG:HH11 | 1.74                     | 0.52              |
| 1:B:2094:UNK:H    | 1:B:2097:UNK:HG3  | 1.75                     | 0.52              |
| 1:B:2236:LEU:HD23 | 1:B:2288:HIS:HB2  | 1.92                     | 0.52              |
| 1:B:368:ILE:HG21  | 1:B:373:ILE:HG13  | 1.90                     | 0.52              |
| 1:C:1148:GLU:O    | 1:C:1150:ALA:N    | 2.42                     | 0.52              |
| 1:C:2135:UNK:CG   | 1:C:2136:ASP:H    | 2.22                     | 0.52              |
| 1:A:411:PRO:HD2   | 1:A:1025:VAL:HG11 | 1.91                     | 0.52              |
| 1:A:1110:VAL:HG13 | 1:A:1172:VAL:HG11 | 1.92                     | 0.52              |
| 1:A:1287:VAL:O    | 1:A:1291:LYS:HG3  | 2.10                     | 0.52              |
| 1:A:2631:PRO:HG3  | 1:A:2649:LEU:HD13 | 1.90                     | 0.52              |
| 1:B:999:UNK:HG3   | 1:B:1007:UNK:HG2  | 1.90                     | 0.52              |
| 1:B:1093:PRO:HB3  | 1:B:1277:HIS:HE1  | 1.75                     | 0.52              |
| 1:B:2087:UNK:HA   | 1:B:2090:UNK:CG   | 2.39                     | 0.52              |
| 1:B:2808:ARG:HB2  | 1:B:2895:SER:O    | 2.10                     | 0.52              |
| 1:B:745:THR:HG23  | 1:B:834:GLU:HA    | 1.90                     | 0.52              |
| 1:C:2081:UNK:C    | 1:C:2084:UNK:HG3  | 2.39                     | 0.52              |
| 1:C:526:ILE:HD12  | 1:C:549:PHE:HB3   | 1.90                     | 0.52              |
| 1:A:1093:PRO:HB3  | 1:A:1277:HIS:HE1  | 1.75                     | 0.52              |
| 1:A:1164:THR:HA   | 1:A:1204:UNK:O    | 2.10                     | 0.52              |
| 1:A:2094:UNK:H    | 1:A:2097:UNK:HG3  | 1.75                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:273:ARG:HD2   | 1:A:282:VAL:HG12  | 1.90                     | 0.52              |
| 1:B:1110:VAL:HG13 | 1:B:1172:VAL:HG11 | 1.92                     | 0.52              |
| 1:B:1226:UNK:HB1  | 1:B:1282:THR:HG21 | 1.90                     | 0.52              |
| 1:C:1110:VAL:HG13 | 1:C:1172:VAL:HG11 | 1.92                     | 0.52              |
| 1:C:961:ARG:NH2   | 1:C:1196:UNK:O    | 2.42                     | 0.52              |
| 1:C:1287:VAL:O    | 1:C:1291:LYS:HG3  | 2.10                     | 0.52              |
| 1:C:208:VAL:HB    | 1:C:255:LEU:HD13  | 1.92                     | 0.52              |
| 1:C:2122:UNK:HA   | 1:C:2125:UNK:CG   | 2.40                     | 0.52              |
| 1:B:2122:UNK:CA   | 1:B:2125:UNK:HG3  | 2.38                     | 0.52              |
| 1:C:577:GLU:OE2   | 2:C:4000:FMN:O3'  | 2.28                     | 0.52              |
| 1:A:2215:THR:HG22 | 1:A:2216:GLU:HG3  | 1.92                     | 0.52              |
| 1:A:2740:CYS:HB2  | 1:A:2998:GLY:HA2  | 1.92                     | 0.52              |
| 1:A:577:GLU:OE2   | 2:A:4000:FMN:O3'  | 2.28                     | 0.52              |
| 1:B:1425:VAL:HG13 | 1:B:1474:LEU:HD13 | 1.91                     | 0.52              |
| 1:B:1622:PRO:HD3  | 1:B:1685:LEU:HD21 | 1.92                     | 0.52              |
| 1:C:2087:UNK:C    | 1:C:2090:UNK:HG3  | 2.40                     | 0.52              |
| 1:C:2088:UNK:HG2  | 1:C:2188:ARG:HH12 | 1.73                     | 0.52              |
| 1:C:208:VAL:HG12  | 1:C:248:ILE:HG12  | 1.92                     | 0.52              |
| 1:C:400:TRP:CZ3   | 1:C:636:PRO:HB2   | 2.45                     | 0.52              |
| 1:A:542:VAL:HG11  | 1:A:964:VAL:HB    | 1.92                     | 0.52              |
| 1:B:106:ALA:O     | 1:B:112:PRO:HD2   | 2.10                     | 0.52              |
| 1:B:1174:VAL:HB   | 1:B:1188:LEU:HB3  | 1.91                     | 0.52              |
| 1:B:144:GLY:O     | 1:B:148:THR:N     | 2.34                     | 0.52              |
| 1:B:2087:UNK:C    | 1:B:2090:UNK:HG3  | 2.40                     | 0.52              |
| 1:B:2122:UNK:HA   | 1:B:2125:UNK:CG   | 2.40                     | 0.52              |
| 1:B:2698:GLY:HA3  | 1:B:2705:LYS:HG3  | 1.92                     | 0.52              |
| 1:B:588:GLU:HB3   | 1:B:593:LEU:HD11  | 1.91                     | 0.52              |
| 1:C:106:ALA:O     | 1:C:112:PRO:HD2   | 2.10                     | 0.52              |
| 1:C:1119:THR:O    | 1:C:1123:PHE:HB2  | 2.10                     | 0.52              |
| 1:C:2094:UNK:HG2  | 1:C:2096:UNK:CG   | 2.23                     | 0.52              |
| 1:C:2236:LEU:HD23 | 1:C:2288:HIS:HB2  | 1.92                     | 0.52              |
| 1:A:2094:UNK:HG2  | 1:A:2096:UNK:CG   | 2.23                     | 0.51              |
| 1:A:2552:ASP:OD1  | 1:A:2552:ASP:N    | 2.43                     | 0.51              |
| 1:A:336:TRP:CE2   | 1:A:360:LEU:HD11  | 2.45                     | 0.51              |
| 1:B:1530:LEU:HD21 | 1:B:1554:LEU:HD22 | 1.91                     | 0.51              |
| 1:B:176:VAL:O     | 1:B:180:ALA:N     | 2.36                     | 0.51              |
| 1:B:2088:UNK:C    | 1:B:2188:ARG:NH1  | 2.72                     | 0.51              |
| 1:B:336:TRP:CE2   | 1:B:360:LEU:HD11  | 2.45                     | 0.51              |
| 1:B:405:PRO:HG3   | 1:B:625:LEU:HG    | 1.92                     | 0.51              |
| 1:C:420:LYS:HB3   | 1:C:641:ASP:OD2   | 2.10                     | 0.51              |
| 1:C:932:UNK:O     | 1:C:936:UNK:CG    | 2.48                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:984:UNK:HG2   | 1:C:987:UNK:HG2   | 1.92                     | 0.51              |
| 1:A:1226:UNK:HB1  | 1:A:1282:THR:HG21 | 1.90                     | 0.51              |
| 1:A:1488:VAL:HG12 | 1:A:1490:ARG:HH11 | 1.73                     | 0.51              |
| 1:B:1598:GLU:HG2  | 1:B:1666:ILE:HD13 | 1.93                     | 0.51              |
| 1:B:2082:UNK:O    | 1:B:2086:UNK:HG3  | 2.09                     | 0.51              |
| 1:C:1164:THR:HA   | 1:C:1204:UNK:O    | 2.10                     | 0.51              |
| 1:A:2082:UNK:O    | 1:A:2086:UNK:HG3  | 2.09                     | 0.51              |
| 1:A:2087:UNK:HA   | 1:A:2090:UNK:CG   | 2.39                     | 0.51              |
| 1:B:2215:THR:HG22 | 1:B:2216:GLU:HG3  | 1.91                     | 0.51              |
| 1:C:2790:MET:HG2  | 1:C:2809:LEU:HD11 | 1.93                     | 0.51              |
| 1:C:588:GLU:HB3   | 1:C:593:LEU:HD11  | 1.91                     | 0.51              |
| 1:A:1119:THR:O    | 1:A:1123:PHE:HB2  | 2.10                     | 0.51              |
| 1:A:2086:UNK:O    | 1:A:2089:UNK:CG   | 2.52                     | 0.51              |
| 1:A:2087:UNK:C    | 1:A:2090:UNK:HG3  | 2.40                     | 0.51              |
| 1:A:2401:ILE:HG23 | 1:A:2403:ILE:H    | 1.75                     | 0.51              |
| 1:A:2690:THR:O    | 1:A:2693:GLN:HG2  | 2.11                     | 0.51              |
| 1:B:1733:ASN:HD22 | 1:B:1736:ARG:HD2  | 1.74                     | 0.51              |
| 1:B:2123:UNK:O    | 1:B:2126:UNK:CG   | 2.56                     | 0.51              |
| 1:B:2434:UNK:O    | 1:B:2434:UNK:HG2  | 2.11                     | 0.51              |
| 1:B:542:VAL:HG11  | 1:B:964:VAL:HB    | 1.92                     | 0.51              |
| 1:B:400:TRP:CZ3   | 1:B:636:PRO:HB2   | 2.45                     | 0.51              |
| 1:B:420:LYS:HB3   | 1:B:641:ASP:OD2   | 2.10                     | 0.51              |
| 1:C:508:GLN:HA    | 1:C:540:ASN:HB3   | 1.92                     | 0.51              |
| 1:A:1622:PRO:HD3  | 1:A:1685:LEU:HD21 | 1.92                     | 0.51              |
| 1:A:206:PRO:HG2   | 1:A:294:VAL:HA    | 1.92                     | 0.51              |
| 1:B:1634:ARG:HD2  | 1:B:1638:PRO:HA   | 1.91                     | 0.51              |
| 1:B:745:THR:OG1   | 1:B:834:GLU:O     | 2.19                     | 0.51              |
| 1:C:2417:SER:O    | 1:C:2421:ASP:N    | 2.40                     | 0.51              |
| 1:A:2122:UNK:HA   | 1:A:2125:UNK:CG   | 2.40                     | 0.51              |
| 1:B:2690:THR:O    | 1:B:2693:GLN:HG2  | 2.11                     | 0.51              |
| 1:B:984:UNK:HG2   | 1:B:987:UNK:HG2   | 1.93                     | 0.51              |
| 1:A:2790:MET:HG2  | 1:A:2809:LEU:HD11 | 1.93                     | 0.51              |
| 1:A:420:LYS:HB3   | 1:A:641:ASP:OD2   | 2.10                     | 0.51              |
| 1:A:937:UNK:HG2   | 1:A:938:UNK:N     | 2.26                     | 0.51              |
| 1:B:206:PRO:HG2   | 1:B:294:VAL:HA    | 1.92                     | 0.51              |
| 1:C:2089:UNK:HA   | 1:C:2188:ARG:HH11 | 1.74                     | 0.51              |
| 1:C:2401:ILE:HG23 | 1:C:2403:ILE:H    | 1.76                     | 0.51              |
| 1:C:746:TYR:HA    | 1:C:749:TRP:HD1   | 1.76                     | 0.51              |
| 1:A:2434:UNK:HG2  | 1:A:2434:UNK:O    | 2.11                     | 0.51              |
| 1:B:1164:THR:HA   | 1:B:1204:UNK:O    | 2.10                     | 0.51              |
| 1:B:2401:ILE:HG23 | 1:B:2403:ILE:H    | 1.76                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:208:VAL:HB    | 1:B:255:LEU:HD13  | 1.92                     | 0.51              |
| 1:C:1488:VAL:HG12 | 1:C:1490:ARG:HH11 | 1.73                     | 0.51              |
| 1:C:1598:GLU:HG2  | 1:C:1666:ILE:HD13 | 1.92                     | 0.51              |
| 1:C:1733:ASN:HD22 | 1:C:1736:ARG:HD2  | 1.74                     | 0.51              |
| 1:C:792:ALA:HA    | 1:C:799:PHE:CE2   | 2.43                     | 0.51              |
| 1:A:106:ALA:O     | 1:A:112:PRO:HD2   | 2.10                     | 0.51              |
| 1:A:2105:UNK:HG2  | 1:A:2106:UNK:N    | 2.26                     | 0.51              |
| 1:A:2123:UNK:O    | 1:A:2126:UNK:CG   | 2.56                     | 0.51              |
| 1:A:2653:VAL:HA   | 1:A:3051:MET:HE3  | 1.92                     | 0.51              |
| 1:A:2667:THR:HG21 | 1:A:3058:ARG:HH11 | 1.76                     | 0.51              |
| 1:B:1119:THR:O    | 1:B:1123:PHE:HB2  | 2.10                     | 0.51              |
| 1:B:937:UNK:HG2   | 1:B:938:UNK:N     | 2.25                     | 0.51              |
| 1:B:981:UNK:HG1   | 1:B:987:UNK:C     | 2.41                     | 0.51              |
| 1:C:2754:ILE:HA   | 1:C:2759:ALA:O    | 2.11                     | 0.51              |
| 1:C:1001:UNK:HG1  | 1:C:1018:ARG:HH22 | 1.74                     | 0.51              |
| 1:C:2086:UNK:O    | 1:C:2089:UNK:CG   | 2.52                     | 0.51              |
| 1:C:2698:GLY:HA3  | 1:C:2705:LYS:HG3  | 1.92                     | 0.51              |
| 1:C:937:UNK:HG2   | 1:C:938:UNK:N     | 2.25                     | 0.51              |
| 1:C:936:UNK:O     | 1:C:941:UNK:N     | 2.44                     | 0.51              |
| 1:A:2236:LEU:HD23 | 1:A:2288:HIS:HB2  | 1.92                     | 0.50              |
| 1:A:2554:ALA:HB1  | 1:A:2614:LYS:HZ2  | 1.74                     | 0.50              |
| 1:A:272:GLU:HB3   | 1:A:280:GLY:O     | 2.11                     | 0.50              |
| 1:A:42:GLU:H      | 1:A:42:GLU:CD     | 2.14                     | 0.50              |
| 1:B:1317:GLY:H    | 1:B:1324:VAL:HG12 | 1.76                     | 0.50              |
| 1:B:42:GLU:CD     | 1:B:42:GLU:H      | 2.14                     | 0.50              |
| 1:C:1986:LEU:HA   | 1:C:1989:PHE:HD2  | 1.76                     | 0.50              |
| 1:C:2056:PHE:CZ   | 1:C:2180:LYS:HE2  | 2.47                     | 0.50              |
| 1:C:2452:UNK:CG   | 1:C:2453:UNK:N    | 2.73                     | 0.50              |
| 1:A:1331:ILE:HG13 | 1:A:1336:VAL:HG21 | 1.94                     | 0.50              |
| 1:A:1634:ARG:HH11 | 1:A:1639:ALA:N    | 2.08                     | 0.50              |
| 1:B:746:TYR:HA    | 1:B:749:TRP:HD1   | 1.76                     | 0.50              |
| 1:C:1622:PRO:HD3  | 1:C:1685:LEU:HD21 | 1.92                     | 0.50              |
| 1:C:2104:UNK:C    | 1:C:2107:UNK:HG3  | 2.42                     | 0.50              |
| 1:C:2361:VAL:HG11 | 1:C:2398:LEU:HD23 | 1.93                     | 0.50              |
| 1:C:2434:UNK:HG2  | 1:C:2434:UNK:O    | 2.11                     | 0.50              |
| 1:C:336:TRP:CE2   | 1:C:360:LEU:HD11  | 2.45                     | 0.50              |
| 1:C:42:GLU:H      | 1:C:42:GLU:CD     | 2.14                     | 0.50              |
| 1:A:1598:GLU:HG2  | 1:A:1666:ILE:HD13 | 1.93                     | 0.50              |
| 1:A:2245:VAL:HG13 | 1:A:2255:ARG:CZ   | 2.42                     | 0.50              |
| 1:A:2662:SER:HB2  | 1:A:2833:LEU:HD22 | 1.93                     | 0.50              |
| 1:A:2180:LYS:HZ1  | 1:A:2962:ASP:HB3  | 1.75                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:780:ARG:HD2   | 1:A:816:LEU:HB3   | 1.93                     | 0.50              |
| 1:B:1590:VAL:HG11 | 1:B:1671:TRP:CD2  | 2.47                     | 0.50              |
| 1:B:2104:UNK:C    | 1:B:2107:UNK:HG3  | 2.42                     | 0.50              |
| 1:B:2653:VAL:HA   | 1:B:3051:MET:HE3  | 1.93                     | 0.50              |
| 1:C:1093:PRO:HB3  | 1:C:1277:HIS:HE1  | 1.75                     | 0.50              |
| 1:C:1212:UNK:HG1  | 1:C:1342:ARG:HE   | 1.76                     | 0.50              |
| 1:C:2245:VAL:HG13 | 1:C:2255:ARG:CZ   | 2.41                     | 0.50              |
| 1:C:2808:ARG:HB2  | 1:C:2895:SER:O    | 2.10                     | 0.50              |
| 1:A:1317:GLY:H    | 1:A:1324:VAL:HG12 | 1.76                     | 0.50              |
| 1:A:1380:ALA:HB1  | 1:A:1474:LEU:HD12 | 1.93                     | 0.50              |
| 1:A:2261:LYS:HA   | 1:A:2265:TRP:HB2  | 1.94                     | 0.50              |
| 1:C:1590:VAL:HG11 | 1:C:1671:TRP:CD2  | 2.47                     | 0.50              |
| 1:A:257:ARG:NH1   | 1:C:1695:LEU:HD23 | 2.23                     | 0.50              |
| 1:C:272:GLU:HB3   | 1:C:280:GLY:O     | 2.11                     | 0.50              |
| 1:C:780:ARG:HD2   | 1:C:816:LEU:HB3   | 1.93                     | 0.50              |
| 1:A:1538:ARG:NH1  | 1:A:1722:PRO:HB3  | 2.18                     | 0.50              |
| 1:A:2698:GLY:HA3  | 1:A:2705:LYS:HG3  | 1.92                     | 0.50              |
| 1:B:2127:UNK:O    | 1:B:2130:UNK:CG   | 2.52                     | 0.50              |
| 1:C:2140:VAL:HG22 | 1:C:2165:ILE:HD12 | 1.93                     | 0.50              |
| 1:A:1590:VAL:HG11 | 1:A:1671:TRP:CD2  | 2.47                     | 0.50              |
| 1:B:1331:ILE:HG13 | 1:B:1336:VAL:HG21 | 1.94                     | 0.50              |
| 1:C:1010:UNK:CG   | 1:C:1017:ILE:HB   | 2.42                     | 0.50              |
| 1:A:208:VAL:HB    | 1:A:255:LEU:HD13  | 1.92                     | 0.50              |
| 1:A:2754:ILE:HA   | 1:A:2759:ALA:O    | 2.11                     | 0.50              |
| 1:A:932:UNK:O     | 1:A:936:UNK:CG    | 2.48                     | 0.50              |
| 1:A:936:UNK:O     | 1:A:941:UNK:N     | 2.45                     | 0.50              |
| 1:B:1711:VAL:HA   | 1:B:1714:LEU:HG   | 1.93                     | 0.50              |
| 1:B:208:VAL:HG12  | 1:B:248:ILE:HG12  | 1.92                     | 0.50              |
| 1:B:207:MET:HA    | 1:B:249:THR:HG22  | 1.94                     | 0.50              |
| 1:B:272:GLU:HB3   | 1:B:280:GLY:O     | 2.11                     | 0.50              |
| 1:B:133:GLN:HG2   | 1:B:355:GLY:HA2   | 1.94                     | 0.50              |
| 1:B:936:UNK:O     | 1:B:941:UNK:N     | 2.44                     | 0.50              |
| 1:C:1207:UNK:HG2  | 1:C:1207:UNK:O    | 2.12                     | 0.50              |
| 1:C:2552:ASP:N    | 1:C:2552:ASP:OD1  | 2.43                     | 0.50              |
| 1:C:405:PRO:HG3   | 1:C:625:LEU:HG    | 1.93                     | 0.50              |
| 1:A:1212:UNK:O    | 1:A:1342:ARG:NH2  | 2.45                     | 0.50              |
| 1:A:1212:UNK:HG1  | 1:A:1342:ARG:HE   | 1.75                     | 0.50              |
| 1:A:1986:LEU:HA   | 1:A:1989:PHE:HD2  | 1.76                     | 0.50              |
| 1:A:2623:ALA:HB2  | 1:A:2812:LEU:HD21 | 1.94                     | 0.50              |
| 1:A:2811:PHE:HB3  | 1:A:2894:THR:HG22 | 1.94                     | 0.50              |
| 1:A:405:PRO:HG3   | 1:A:625:LEU:HG    | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:505:ARG:HA    | 1:A:508:GLN:HB2   | 1.94                     | 0.50              |
| 1:A:981:UNK:HG1   | 1:A:987:UNK:C     | 2.41                     | 0.50              |
| 1:C:206:PRO:HG2   | 1:C:294:VAL:HA    | 1.92                     | 0.50              |
| 1:C:2274:LEU:HD23 | 1:C:2277:ILE:HD12 | 1.94                     | 0.50              |
| 1:C:2690:THR:O    | 1:C:2693:GLN:HG2  | 2.11                     | 0.50              |
| 1:C:542:VAL:HG11  | 1:C:964:VAL:HB    | 1.92                     | 0.50              |
| 1:C:981:UNK:HG1   | 1:C:987:UNK:C     | 2.41                     | 0.50              |
| 1:A:1212:UNK:HG2  | 1:A:1342:ARG:NE   | 2.26                     | 0.50              |
| 1:A:133:GLN:HG2   | 1:A:355:GLY:HA2   | 1.94                     | 0.50              |
| 1:B:2334:HIS:HB3  | 1:B:2391:LYS:HA   | 1.94                     | 0.50              |
| 1:C:981:UNK:CG    | 1:C:987:UNK:O     | 2.60                     | 0.50              |
| 1:C:981:UNK:HG1   | 1:C:987:UNK:O     | 2.12                     | 0.50              |
| 1:A:2334:HIS:HB3  | 1:A:2391:LYS:HA   | 1.94                     | 0.49              |
| 1:A:990:UNK:HG3   | 1:A:998:UNK:HB2   | 1.94                     | 0.49              |
| 1:B:2557:LEU:HD22 | 1:B:2613:ARG:HB2  | 1.94                     | 0.49              |
| 1:B:2829:LEU:HD21 | 1:B:3014:PHE:HE2  | 1.76                     | 0.49              |
| 1:B:2667:THR:HG21 | 1:B:3058:ARG:HH11 | 1.76                     | 0.49              |
| 1:B:990:UNK:HG3   | 1:B:998:UNK:HB2   | 1.94                     | 0.49              |
| 1:C:1331:ILE:HG13 | 1:C:1336:VAL:HG21 | 1.94                     | 0.49              |
| 1:C:1711:VAL:HA   | 1:C:1714:LEU:HG   | 1.94                     | 0.49              |
| 1:C:2261:LYS:HA   | 1:C:2265:TRP:HB2  | 1.94                     | 0.49              |
| 1:C:2557:LEU:HD22 | 1:C:2613:ARG:HB2  | 1.94                     | 0.49              |
| 1:A:1001:UNK:HG1  | 1:A:1018:ARG:HH22 | 1.74                     | 0.49              |
| 1:A:2104:UNK:C    | 1:A:2107:UNK:HG3  | 2.42                     | 0.49              |
| 1:A:2127:UNK:O    | 1:A:2130:UNK:CG   | 2.52                     | 0.49              |
| 1:A:984:UNK:HG2   | 1:A:987:UNK:HG2   | 1.93                     | 0.49              |
| 1:B:1986:LEU:HA   | 1:B:1989:PHE:HD2  | 1.76                     | 0.49              |
| 1:B:2056:PHE:CZ   | 1:B:2180:LYS:HE2  | 2.47                     | 0.49              |
| 1:B:2140:VAL:HG22 | 1:B:2165:ILE:HD12 | 1.93                     | 0.49              |
| 1:B:2361:VAL:HG11 | 1:B:2398:LEU:HD23 | 1.93                     | 0.49              |
| 1:B:2754:ILE:HA   | 1:B:2759:ALA:O    | 2.11                     | 0.49              |
| 1:C:1317:GLY:H    | 1:C:1324:VAL:HG12 | 1.76                     | 0.49              |
| 1:C:2811:PHE:HB3  | 1:C:2894:THR:HG22 | 1.94                     | 0.49              |
| 1:A:1207:UNK:HG2  | 1:A:1207:UNK:O    | 2.12                     | 0.49              |
| 1:A:2140:VAL:HG22 | 1:A:2165:ILE:HD12 | 1.93                     | 0.49              |
| 1:A:2056:PHE:CZ   | 1:A:2180:LYS:HE2  | 2.47                     | 0.49              |
| 1:A:647:THR:OG1   | 2:A:4000:FMN:O3P  | 2.27                     | 0.49              |
| 1:A:508:GLN:HA    | 1:A:540:ASN:HB3   | 1.92                     | 0.49              |
| 1:A:981:UNK:CG    | 1:A:987:UNK:O     | 2.60                     | 0.49              |
| 1:B:1212:UNK:HG1  | 1:B:1342:ARG:HE   | 1.75                     | 0.49              |
| 1:B:1212:UNK:O    | 1:B:1342:ARG:NH2  | 2.45                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1178:ASN:HB2  | 1:C:1185:LEU:HD11 | 1.94                     | 0.49              |
| 1:C:1212:UNK:O    | 1:C:1342:ARG:NH2  | 2.45                     | 0.49              |
| 1:A:2361:VAL:HG11 | 1:A:2398:LEU:HD23 | 1.93                     | 0.49              |
| 1:B:1119:THR:HA   | 1:B:1123:PHE:CD1  | 2.47                     | 0.49              |
| 1:B:577:GLU:OE2   | 2:B:4000:FMN:O3'  | 2.28                     | 0.49              |
| 1:C:1119:THR:HA   | 1:C:1123:PHE:CD1  | 2.48                     | 0.49              |
| 1:C:1637:VAL:HG21 | 1:C:1671:TRP:CD2  | 2.48                     | 0.49              |
| 1:C:2662:SER:HB2  | 1:C:2833:LEU:HD22 | 1.93                     | 0.49              |
| 1:C:776:ASP:O     | 1:C:779:TRP:N     | 2.31                     | 0.49              |
| 1:A:2274:LEU:HD23 | 1:A:2277:ILE:HD12 | 1.94                     | 0.49              |
| 1:A:2557:LEU:HD22 | 1:A:2613:ARG:HB2  | 1.94                     | 0.49              |
| 1:A:3080:ARG:NH1  | 1:A:3080:ARG:CG   | 2.72                     | 0.49              |
| 1:B:1637:VAL:HG21 | 1:B:1671:TRP:CD2  | 2.48                     | 0.49              |
| 1:B:2105:UNK:HG2  | 1:B:2106:UNK:N    | 2.26                     | 0.49              |
| 1:B:2245:VAL:HG13 | 1:B:2255:ARG:CZ   | 2.41                     | 0.49              |
| 1:B:981:UNK:HG1   | 1:B:987:UNK:O     | 2.12                     | 0.49              |
| 1:C:1380:ALA:HB1  | 1:C:1474:LEU:HD12 | 1.94                     | 0.49              |
| 1:C:184:LEU:HB3   | 1:C:311:TRP:HE3   | 1.78                     | 0.49              |
| 1:A:981:UNK:HG1   | 1:A:987:UNK:O     | 2.12                     | 0.49              |
| 1:B:1212:UNK:HG2  | 1:B:1342:ARG:NE   | 2.26                     | 0.49              |
| 1:B:2662:SER:HB2  | 1:B:2833:LEU:HD22 | 1.94                     | 0.49              |
| 1:B:505:ARG:HA    | 1:B:508:GLN:HB2   | 1.94                     | 0.49              |
| 1:B:508:GLN:HA    | 1:B:540:ASN:HB3   | 1.92                     | 0.49              |
| 1:B:976:UNK:CG    | 1:B:993:UNK:HB1   | 2.29                     | 0.49              |
| 1:C:207:MET:HA    | 1:C:249:THR:HG22  | 1.94                     | 0.49              |
| 1:A:1119:THR:HA   | 1:A:1123:PHE:CD1  | 2.47                     | 0.49              |
| 1:A:184:LEU:HB3   | 1:A:311:TRP:HE3   | 1.78                     | 0.49              |
| 1:A:2503:LYS:HE3  | 1:A:2505:GLU:OE2  | 2.13                     | 0.49              |
| 1:B:2790:MET:HG2  | 1:B:2809:LEU:HD11 | 1.93                     | 0.49              |
| 1:B:932:UNK:HA    | 1:B:935:UNK:HG3   | 1.94                     | 0.49              |
| 1:C:2087:UNK:HA   | 1:C:2090:UNK:CG   | 2.39                     | 0.49              |
| 1:C:2105:UNK:HG2  | 1:C:2106:UNK:N    | 2.26                     | 0.49              |
| 1:C:3080:ARG:NH1  | 1:C:3080:ARG:HG3  | 2.09                     | 0.49              |
| 1:A:1010:UNK:CG   | 1:A:1017:ILE:HB   | 2.42                     | 0.49              |
| 1:A:207:MET:HA    | 1:A:249:THR:HG22  | 1.94                     | 0.49              |
| 1:A:2829:LEU:HD21 | 1:A:3014:PHE:HE2  | 1.77                     | 0.49              |
| 1:B:1010:UNK:CG   | 1:B:1017:ILE:HB   | 2.42                     | 0.49              |
| 1:B:1291:LYS:HA   | 1:B:1344:ALA:HB3  | 1.95                     | 0.49              |
| 1:B:2261:LYS:HA   | 1:B:2265:TRP:HB2  | 1.93                     | 0.49              |
| 1:B:981:UNK:CG    | 1:B:987:UNK:O     | 2.60                     | 0.49              |
| 1:A:117:LYS:HZ1   | 1:C:1087:PHE:HB3  | 1.78                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1362:MET:HG3  | 1:C:1430:VAL:HG21 | 1.95                     | 0.49              |
| 1:C:305:ILE:HD13  | 1:C:327:GLU:HG2   | 1.95                     | 0.49              |
| 1:A:1695:LEU:HD23 | 1:B:257:ARG:NH1   | 2.23                     | 0.49              |
| 1:A:2291:LEU:HD21 | 1:A:2332:LEU:HD22 | 1.95                     | 0.49              |
| 1:A:2962:ASP:N    | 1:A:2962:ASP:OD1  | 2.34                     | 0.49              |
| 1:A:444:ILE:HD12  | 1:A:655:ALA:HA    | 1.95                     | 0.49              |
| 1:A:790:ALA:HB3   | 1:A:826:LEU:HD21  | 1.95                     | 0.49              |
| 1:B:1380:ALA:HB1  | 1:B:1474:LEU:HD12 | 1.93                     | 0.49              |
| 1:B:184:LEU:HB3   | 1:B:311:TRP:HE3   | 1.78                     | 0.49              |
| 1:B:2087:UNK:O    | 1:B:2090:UNK:HG3  | 2.13                     | 0.49              |
| 1:B:2274:LEU:HD23 | 1:B:2277:ILE:HD12 | 1.94                     | 0.49              |
| 1:B:780:ARG:HD2   | 1:B:816:LEU:HB3   | 1.93                     | 0.49              |
| 1:B:792:ALA:HA    | 1:B:799:PHE:CE2   | 2.43                     | 0.49              |
| 1:C:999:UNK:O     | 1:C:1007:UNK:N    | 2.46                     | 0.49              |
| 1:C:2094:UNK:O    | 1:C:2098:UNK:HG3  | 2.13                     | 0.49              |
| 1:C:932:UNK:HA    | 1:C:935:UNK:HG3   | 1.94                     | 0.49              |
| 1:C:992:UNK:HG1   | 1:C:994:UNK:HG3   | 1.81                     | 0.49              |
| 1:A:746:TYR:HA    | 1:A:749:TRP:HD1   | 1.76                     | 0.49              |
| 1:B:999:UNK:O     | 1:B:1007:UNK:N    | 2.46                     | 0.49              |
| 1:C:2334:HIS:HB3  | 1:C:2391:LYS:HA   | 1.94                     | 0.49              |
| 1:C:997:UNK:HB1   | 1:C:1009:UNK:HG2  | 1.95                     | 0.49              |
| 1:A:1012:UNK:HG2  | 1:A:1012:UNK:O    | 2.13                     | 0.48              |
| 1:A:1111:PHE:HE1  | 1:A:1129:LEU:HD11 | 1.78                     | 0.48              |
| 1:A:1637:VAL:HG21 | 1:A:1671:TRP:CD2  | 2.48                     | 0.48              |
| 1:A:2087:UNK:O    | 1:A:2090:UNK:HG3  | 2.13                     | 0.48              |
| 1:A:868:ARG:HB3   | 1:A:872:ARG:NH1   | 2.28                     | 0.48              |
| 1:B:1207:UNK:HG2  | 1:B:1207:UNK:O    | 2.12                     | 0.48              |
| 1:B:2094:UNK:O    | 1:B:2098:UNK:HG3  | 2.13                     | 0.48              |
| 1:B:2120:UNK:HG2  | 1:B:2121:UNK:N    | 2.28                     | 0.48              |
| 1:B:361:THR:HG21  | 1:B:377:PRO:HG3   | 1.95                     | 0.48              |
| 1:B:444:ILE:HD12  | 1:B:655:ALA:HA    | 1.95                     | 0.48              |
| 1:C:2100:UNK:C    | 1:C:2103:UNK:HG3  | 2.31                     | 0.48              |
| 1:C:2118:UNK:HG2  | 1:C:2119:UNK:N    | 2.28                     | 0.48              |
| 1:C:2667:THR:HG21 | 1:C:3058:ARG:HH11 | 1.76                     | 0.48              |
| 1:C:2829:LEU:HD21 | 1:C:3014:PHE:HE2  | 1.76                     | 0.48              |
| 1:A:999:UNK:O     | 1:A:1007:UNK:N    | 2.46                     | 0.48              |
| 1:A:1225:UNK:HG1  | 1:A:1283:ASP:CG   | 2.34                     | 0.48              |
| 1:A:1651:THR:HB   | 1:A:1656:LYS:HD2  | 1.95                     | 0.48              |
| 1:A:2926:SER:HB3  | 1:A:2976:TRP:HH2  | 1.79                     | 0.48              |
| 1:B:2086:UNK:CA   | 1:B:2089:UNK:HG3  | 2.43                     | 0.48              |
| 1:C:1533:VAL:HG13 | 1:C:1582:HIS:HB2  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2086:UNK:CA   | 1:A:2089:UNK:HG3  | 2.43                     | 0.48              |
| 1:A:932:UNK:HA    | 1:A:935:UNK:HG3   | 1.94                     | 0.48              |
| 1:B:1003:UNK:CG   | 1:B:1004:UNK:N    | 2.53                     | 0.48              |
| 1:B:1533:VAL:HG13 | 1:B:1582:HIS:HB2  | 1.95                     | 0.48              |
| 1:B:2115:UNK:O    | 1:B:2119:UNK:HG3  | 2.13                     | 0.48              |
| 1:B:2291:LEU:HD21 | 1:B:2332:LEU:HD22 | 1.95                     | 0.48              |
| 1:B:2820:ILE:HD12 | 1:B:2822:LEU:HD21 | 1.95                     | 0.48              |
| 1:B:501:VAL:HA    | 1:B:504:LYS:HE2   | 1.96                     | 0.48              |
| 1:B:790:ALA:HB3   | 1:B:826:LEU:HD21  | 1.95                     | 0.48              |
| 1:C:133:GLN:HG2   | 1:C:355:GLY:HA2   | 1.94                     | 0.48              |
| 1:C:2503:LYS:HE3  | 1:C:2505:GLU:OE2  | 2.13                     | 0.48              |
| 1:C:2623:ALA:HB2  | 1:C:2812:LEU:HD21 | 1.94                     | 0.48              |
| 1:C:361:THR:HG21  | 1:C:377:PRO:HG3   | 1.95                     | 0.48              |
| 1:C:996:UNK:O     | 1:C:996:UNK:HG2   | 2.13                     | 0.48              |
| 1:A:1435:VAL:HG22 | 1:A:1703:ILE:HD12 | 1.95                     | 0.48              |
| 1:A:2167:THR:HB   | 1:A:2198:ALA:HB3  | 1.96                     | 0.48              |
| 1:A:2103:UNK:CG   | 1:A:2919:GLY:O    | 2.62                     | 0.48              |
| 1:B:2623:ALA:HB2  | 1:B:2812:LEU:HD21 | 1.94                     | 0.48              |
| 1:C:2667:THR:HB   | 1:C:3081:LEU:HD11 | 1.95                     | 0.48              |
| 1:C:2848:GLY:H    | 1:C:3001:HIS:CD2  | 2.31                     | 0.48              |
| 1:A:1711:VAL:HA   | 1:A:1714:LEU:HG   | 1.93                     | 0.48              |
| 1:A:1996:PRO:O    | 1:A:2000:LEU:N    | 2.41                     | 0.48              |
| 1:A:2060:TRP:HZ2  | 1:A:2966:ASP:HA   | 1.79                     | 0.48              |
| 1:A:2170:ARG:HB2  | 1:A:2175:ARG:HG3  | 1.95                     | 0.48              |
| 1:B:1103:VAL:HG21 | 1:B:1269:MET:SD   | 2.54                     | 0.48              |
| 1:B:1435:VAL:HG22 | 1:B:1703:ILE:HD12 | 1.95                     | 0.48              |
| 1:B:2167:THR:HB   | 1:B:2198:ALA:HB3  | 1.96                     | 0.48              |
| 1:B:2667:THR:HB   | 1:B:3081:LEU:HD11 | 1.96                     | 0.48              |
| 1:B:1087:PHE:HB3  | 1:C:117:LYS:HZ3   | 1.77                     | 0.48              |
| 1:C:1381:ASP:OD1  | 1:C:1391:SER:OG   | 2.22                     | 0.48              |
| 1:C:2736:PRO:HG2  | 1:C:2746:SER:HA   | 1.96                     | 0.48              |
| 1:C:505:ARG:HA    | 1:C:508:GLN:HB2   | 1.94                     | 0.48              |
| 1:C:976:UNK:CG    | 1:C:993:UNK:HB1   | 2.29                     | 0.48              |
| 1:A:2848:GLY:H    | 1:A:3001:HIS:CD2  | 2.31                     | 0.48              |
| 1:A:184:LEU:HD13  | 1:A:311:TRP:HB3   | 1.96                     | 0.48              |
| 1:B:1133:VAL:O    | 1:B:1193:ALA:N    | 2.42                     | 0.48              |
| 1:B:1695:LEU:HD23 | 1:C:257:ARG:NH1   | 2.23                     | 0.48              |
| 1:B:2060:TRP:HZ2  | 1:B:2966:ASP:HA   | 1.79                     | 0.48              |
| 1:B:2645:ASP:OD1  | 1:B:2647:VAL:HG23 | 2.14                     | 0.48              |
| 1:B:2811:PHE:HB3  | 1:B:2894:THR:HG22 | 1.94                     | 0.48              |
| 1:B:982:UNK:CG    | 1:B:983:UNK:N     | 2.76                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1012:UNK:HG2  | 1:C:1012:UNK:O    | 2.13                     | 0.48              |
| 1:C:1103:VAL:HG21 | 1:C:1269:MET:SD   | 2.54                     | 0.48              |
| 1:C:1291:LYS:HA   | 1:C:1344:ALA:HB3  | 1.95                     | 0.48              |
| 1:C:2087:UNK:O    | 1:C:2090:UNK:HG3  | 2.13                     | 0.48              |
| 1:C:2088:UNK:O    | 1:C:2188:ARG:NH1  | 2.47                     | 0.48              |
| 1:C:2645:ASP:OD1  | 1:C:2647:VAL:HG23 | 2.13                     | 0.48              |
| 1:C:2648:ALA:HA   | 1:C:2718:VAL:HG13 | 1.96                     | 0.48              |
| 1:C:2820:ILE:HD12 | 1:C:2822:LEU:HD21 | 1.95                     | 0.48              |
| 1:C:444:ILE:HD12  | 1:C:655:ALA:HA    | 1.95                     | 0.48              |
| 1:A:1178:ASN:HB2  | 1:A:1185:LEU:HD11 | 1.94                     | 0.48              |
| 1:A:2115:UNK:O    | 1:A:2119:UNK:HG3  | 2.13                     | 0.48              |
| 1:B:1362:MET:HG3  | 1:B:1430:VAL:HG21 | 1.95                     | 0.48              |
| 1:B:1508:ILE:HB   | 1:B:1562:ARG:HD3  | 1.96                     | 0.48              |
| 1:B:2103:UNK:CG   | 1:B:2919:GLY:O    | 2.62                     | 0.48              |
| 1:B:803:GLU:OE1   | 1:B:2431:UNK:CG   | 2.62                     | 0.48              |
| 1:B:931:UNK:CG    | 1:B:934:UNK:HG3   | 2.44                     | 0.48              |
| 1:C:1634:ARG:HH11 | 1:C:1639:ALA:N    | 2.08                     | 0.48              |
| 1:C:2060:TRP:HZ2  | 1:C:2966:ASP:HA   | 1.79                     | 0.48              |
| 1:A:1103:VAL:HG21 | 1:A:1269:MET:SD   | 2.54                     | 0.48              |
| 1:A:1163:ASP:CG   | 1:A:1199:UNK:HG3  | 2.34                     | 0.48              |
| 1:A:1291:LYS:HA   | 1:A:1344:ALA:HB3  | 1.95                     | 0.48              |
| 1:A:1362:MET:HG3  | 1:A:1430:VAL:HG21 | 1.95                     | 0.48              |
| 1:A:144:GLY:O     | 1:A:148:THR:N     | 2.34                     | 0.48              |
| 1:A:2180:LYS:NZ   | 1:A:2962:ASP:HB3  | 2.29                     | 0.48              |
| 1:A:2088:UNK:O    | 1:A:2188:ARG:NH1  | 2.47                     | 0.48              |
| 1:A:2592:PRO:HA   | 1:A:2599:TRP:CD1  | 2.49                     | 0.48              |
| 1:A:2666:PRO:CB   | 1:A:2727:VAL:HA   | 2.44                     | 0.48              |
| 1:A:931:UNK:CG    | 1:A:934:UNK:HG3   | 2.44                     | 0.48              |
| 1:A:985:UNK:HG2   | 1:A:986:UNK:N     | 2.29                     | 0.48              |
| 1:B:305:ILE:HD13  | 1:B:327:GLU:HG2   | 1.95                     | 0.48              |
| 1:C:1212:UNK:HG2  | 1:C:1342:ARG:NE   | 2.26                     | 0.48              |
| 1:C:2094:UNK:HG1  | 1:C:2096:UNK:HG3  | 1.90                     | 0.48              |
| 1:C:2115:UNK:O    | 1:C:2119:UNK:HG3  | 2.13                     | 0.48              |
| 1:C:2167:THR:HB   | 1:C:2198:ALA:HB3  | 1.96                     | 0.48              |
| 1:C:2666:PRO:CB   | 1:C:2727:VAL:HA   | 2.44                     | 0.48              |
| 1:C:868:ARG:HB3   | 1:C:872:ARG:NH1   | 2.28                     | 0.48              |
| 1:C:990:UNK:HG3   | 1:C:998:UNK:HB2   | 1.94                     | 0.48              |
| 1:A:2094:UNK:O    | 1:A:2098:UNK:HG3  | 2.13                     | 0.48              |
| 1:A:2120:UNK:HG2  | 1:A:2121:UNK:N    | 2.28                     | 0.48              |
| 1:A:2645:ASP:OD1  | 1:A:2647:VAL:HG23 | 2.14                     | 0.48              |
| 1:A:2667:THR:HB   | 1:A:3081:LEU:HD11 | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:305:ILE:HD13  | 1:A:327:GLU:HG2   | 1.95                     | 0.48              |
| 1:A:997:UNK:N     | 1:A:1009:UNK:O    | 2.47                     | 0.48              |
| 1:B:171:LYS:HE3   | 1:B:173:ALA:HB3   | 1.96                     | 0.48              |
| 1:B:2088:UNK:O    | 1:B:2188:ARG:NH1  | 2.47                     | 0.48              |
| 1:B:647:THR:HG22  | 1:B:901:ILE:HD11  | 1.96                     | 0.48              |
| 1:C:1467:VAL:HA   | 1:C:1605:LYS:HD2  | 1.96                     | 0.48              |
| 1:C:2592:PRO:HA   | 1:C:2599:TRP:CD1  | 2.49                     | 0.48              |
| 1:C:2926:SER:HB3  | 1:C:2976:TRP:HH2  | 1.78                     | 0.48              |
| 1:C:997:UNK:N     | 1:C:1009:UNK:O    | 2.47                     | 0.48              |
| 1:A:2820:ILE:HD12 | 1:A:2822:LEU:HD21 | 1.95                     | 0.48              |
| 1:A:2762:VAL:HG22 | 1:A:2822:LEU:HB2  | 1.96                     | 0.48              |
| 1:B:2352:ILE:HG12 | 1:B:2412:ALA:HB1  | 1.96                     | 0.48              |
| 1:B:575:HIS:CD2   | 1:B:644:LEU:HD22  | 2.49                     | 0.48              |
| 1:B:808:ALA:HB3   | 1:B:811:ASP:HB2   | 1.96                     | 0.48              |
| 1:B:997:UNK:N     | 1:B:1009:UNK:O    | 2.47                     | 0.48              |
| 1:C:1651:THR:HB   | 1:C:1656:LYS:HD2  | 1.95                     | 0.48              |
| 1:C:171:LYS:HE3   | 1:C:173:ALA:HB3   | 1.96                     | 0.48              |
| 1:C:2448:UNK:HG2  | 1:C:2448:UNK:O    | 2.13                     | 0.48              |
| 1:C:301:LEU:HD13  | 1:C:330:LEU:HD22  | 1.96                     | 0.48              |
| 1:C:641:ASP:OD1   | 1:C:641:ASP:N     | 2.47                     | 0.48              |
| 1:C:575:HIS:CD2   | 1:C:644:LEU:HD22  | 2.48                     | 0.48              |
| 1:A:176:VAL:O     | 1:A:180:ALA:N     | 2.36                     | 0.47              |
| 1:A:2736:PRO:HG2  | 1:A:2746:SER:HA   | 1.96                     | 0.47              |
| 1:A:996:UNK:O     | 1:A:996:UNK:HG2   | 2.13                     | 0.47              |
| 1:B:2180:LYS:NZ   | 1:B:2962:ASP:HB3  | 2.29                     | 0.47              |
| 1:B:2448:UNK:O    | 1:B:2448:UNK:HG2  | 2.13                     | 0.47              |
| 1:B:2666:PRO:CB   | 1:B:2727:VAL:HA   | 2.44                     | 0.47              |
| 1:B:670:GLY:HA3   | 1:B:899:ALA:HB2   | 1.96                     | 0.47              |
| 1:B:674:TRP:CD1   | 1:B:895:THR:HG21  | 2.49                     | 0.47              |
| 1:C:1013:UNK:CG   | 1:C:1014:UNK:N    | 2.58                     | 0.47              |
| 1:C:1435:VAL:HG22 | 1:C:1703:ILE:HD12 | 1.95                     | 0.47              |
| 1:C:2843:GLN:HG2  | 1:C:2845:PHE:CZ   | 2.49                     | 0.47              |
| 1:A:2348:GLN:O    | 1:A:2416:MET:HG3  | 2.15                     | 0.47              |
| 1:A:2554:ALA:HB1  | 1:A:2614:LYS:HD2  | 1.95                     | 0.47              |
| 1:B:1012:UNK:HG2  | 1:B:1012:UNK:O    | 2.14                     | 0.47              |
| 1:B:1111:PHE:HE1  | 1:B:1129:LEU:HD11 | 1.78                     | 0.47              |
| 1:B:1651:THR:HB   | 1:B:1656:LYS:HD2  | 1.95                     | 0.47              |
| 1:B:2101:UNK:HG2  | 1:B:2102:UNK:N    | 2.29                     | 0.47              |
| 1:B:2434:UNK:HG3  | 1:B:2523:GLU:O    | 2.14                     | 0.47              |
| 1:B:2503:LYS:HE3  | 1:B:2505:GLU:OE2  | 2.13                     | 0.47              |
| 1:B:2592:PRO:HA   | 1:B:2599:TRP:CD1  | 2.49                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2848:GLY:H    | 1:B:3001:HIS:CD2  | 2.31                     | 0.47              |
| 1:B:2884:ASP:HA   | 1:B:2916:ARG:NH1  | 2.30                     | 0.47              |
| 1:C:1010:UNK:HG2  | 1:C:1017:ILE:HB   | 1.96                     | 0.47              |
| 1:C:2180:LYS:NZ   | 1:C:2962:ASP:HB3  | 2.29                     | 0.47              |
| 1:C:2554:ALA:HB1  | 1:C:2614:LYS:HD2  | 1.95                     | 0.47              |
| 1:C:184:LEU:HD13  | 1:C:311:TRP:HB3   | 1.96                     | 0.47              |
| 1:C:606:ASN:HD22  | 1:C:606:ASN:H     | 1.62                     | 0.47              |
| 1:C:647:THR:HG22  | 1:C:901:ILE:HD11  | 1.96                     | 0.47              |
| 1:A:1533:VAL:HG13 | 1:A:1582:HIS:HB2  | 1.95                     | 0.47              |
| 1:A:2434:UNK:HG3  | 1:A:2523:GLU:O    | 2.14                     | 0.47              |
| 1:B:1072:TRP:HE1  | 1:B:1077:VAL:HG22 | 1.80                     | 0.47              |
| 1:B:1178:ASN:HB2  | 1:B:1185:LEU:HD11 | 1.94                     | 0.47              |
| 1:B:1625:LEU:HD11 | 1:B:1660:LEU:HB3  | 1.95                     | 0.47              |
| 1:B:2927:GLN:HE22 | 1:B:2941:PHE:C    | 2.17                     | 0.47              |
| 1:B:365:ALA:O     | 1:B:369:ARG:N     | 2.42                     | 0.47              |
| 1:C:1163:ASP:CG   | 1:C:1199:UNK:HG3  | 2.34                     | 0.47              |
| 1:C:1225:UNK:HG1  | 1:C:1283:ASP:CG   | 2.34                     | 0.47              |
| 1:C:1450:ALA:N    | 1:C:1613:ARG:O    | 2.48                     | 0.47              |
| 1:C:176:VAL:O     | 1:C:180:ALA:N     | 2.36                     | 0.47              |
| 1:C:790:ALA:HB3   | 1:C:826:LEU:HD21  | 1.95                     | 0.47              |
| 1:A:365:ALA:HB3   | 1:A:366:PRO:HD3   | 1.96                     | 0.47              |
| 1:A:674:TRP:CD1   | 1:A:895:THR:HG21  | 2.50                     | 0.47              |
| 1:B:2123:UNK:HA   | 1:B:2126:UNK:HG3  | 1.97                     | 0.47              |
| 1:B:2093:UNK:HG1  | 1:B:2132:UNK:HB1  | 1.95                     | 0.47              |
| 1:B:2252:VAL:HG22 | 1:B:2255:ARG:NH2  | 2.30                     | 0.47              |
| 1:B:2648:ALA:HA   | 1:B:2718:VAL:HG13 | 1.96                     | 0.47              |
| 1:B:2461:VAL:HG21 | 1:B:2751:VAL:HG13 | 1.96                     | 0.47              |
| 1:C:2170:ARG:HB2  | 1:C:2175:ARG:HG3  | 1.95                     | 0.47              |
| 1:C:365:ALA:HB3   | 1:C:366:PRO:HD3   | 1.96                     | 0.47              |
| 1:C:808:ALA:HB3   | 1:C:811:ASP:HB2   | 1.96                     | 0.47              |
| 1:C:674:TRP:CD1   | 1:C:895:THR:HG21  | 2.49                     | 0.47              |
| 1:C:985:UNK:HG2   | 1:C:986:UNK:N     | 2.29                     | 0.47              |
| 1:A:1508:ILE:HB   | 1:A:1562:ARG:HD3  | 1.97                     | 0.47              |
| 1:A:2118:UNK:HG2  | 1:A:2119:UNK:N    | 2.28                     | 0.47              |
| 1:A:2648:ALA:HA   | 1:A:2718:VAL:HG13 | 1.96                     | 0.47              |
| 1:A:2843:GLN:HG2  | 1:A:2845:PHE:CZ   | 2.49                     | 0.47              |
| 1:A:2927:GLN:HE22 | 1:A:2941:PHE:C    | 2.17                     | 0.47              |
| 1:A:997:UNK:HB1   | 1:A:1009:UNK:CG   | 2.44                     | 0.47              |
| 1:B:2170:ARG:HB2  | 1:B:2175:ARG:HG3  | 1.96                     | 0.47              |
| 1:B:832:ASP:O     | 1:B:836:VAL:HG23  | 2.14                     | 0.47              |
| 1:B:985:UNK:HG2   | 1:B:986:UNK:N     | 2.29                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:997:UNK:HB1   | 1:B:1009:UNK:HG2  | 1.95                     | 0.47              |
| 1:C:1455:VAL:HB   | 1:C:1480:ARG:HH12 | 1.80                     | 0.47              |
| 1:C:2103:UNK:CG   | 1:C:2919:GLY:O    | 2.62                     | 0.47              |
| 1:C:2123:UNK:HA   | 1:C:2126:UNK:HG3  | 1.97                     | 0.47              |
| 1:C:2461:VAL:HG21 | 1:C:2751:VAL:HG13 | 1.96                     | 0.47              |
| 1:A:2093:UNK:HG1  | 1:A:2132:UNK:HB1  | 1.95                     | 0.47              |
| 1:A:2448:UNK:HG2  | 1:A:2448:UNK:O    | 2.13                     | 0.47              |
| 1:A:606:ASN:HD22  | 1:A:606:ASN:H     | 1.63                     | 0.47              |
| 1:A:997:UNK:HB1   | 1:A:1009:UNK:HG2  | 1.95                     | 0.47              |
| 1:B:1590:VAL:HG11 | 1:B:1671:TRP:CE2  | 2.50                     | 0.47              |
| 1:B:2376:LEU:HD22 | 1:B:2392:VAL:HG21 | 1.97                     | 0.47              |
| 1:B:2681:THR:O    | 1:B:2764:ALA:HA   | 2.15                     | 0.47              |
| 1:B:641:ASP:OD1   | 1:B:641:ASP:N     | 2.47                     | 0.47              |
| 1:B:683:GLY:CA    | 1:B:700:ASN:HB2   | 2.44                     | 0.47              |
| 1:B:932:UNK:O     | 1:B:936:UNK:CG    | 2.47                     | 0.47              |
| 1:B:996:UNK:HG2   | 1:B:996:UNK:O     | 2.13                     | 0.47              |
| 1:C:1723:GLU:C    | 1:C:1725:SER:H    | 2.18                     | 0.47              |
| 1:C:2927:GLN:HE22 | 1:C:2941:PHE:C    | 2.17                     | 0.47              |
| 1:C:966:PRO:O     | 1:C:970:ILE:N     | 2.48                     | 0.47              |
| 1:C:997:UNK:HB1   | 1:C:1009:UNK:CG   | 2.45                     | 0.47              |
| 1:A:1672:GLN:HE21 | 1:A:1672:GLN:HB3  | 1.58                     | 0.47              |
| 1:A:1723:GLU:C    | 1:A:1725:SER:H    | 2.18                     | 0.47              |
| 1:A:2800:PHE:CE1  | 1:A:2812:LEU:HD22 | 2.50                     | 0.47              |
| 1:A:2884:ASP:HA   | 1:A:2916:ARG:NH1  | 2.29                     | 0.47              |
| 1:B:1163:ASP:CG   | 1:B:1199:UNK:HG3  | 2.34                     | 0.47              |
| 1:B:1455:VAL:HB   | 1:B:1480:ARG:HH12 | 1.80                     | 0.47              |
| 1:B:184:LEU:HD13  | 1:B:311:TRP:HB3   | 1.96                     | 0.47              |
| 1:B:365:ALA:HB3   | 1:B:366:PRO:HD3   | 1.96                     | 0.47              |
| 1:B:745:THR:HG22  | 1:B:747:LEU:H     | 1.80                     | 0.47              |
| 1:C:2120:UNK:HG2  | 1:C:2121:UNK:N    | 2.28                     | 0.47              |
| 1:C:2773:GLU:HA   | 1:C:2776:ILE:HG22 | 1.97                     | 0.47              |
| 1:C:2762:VAL:HG22 | 1:C:2822:LEU:HB2  | 1.96                     | 0.47              |
| 1:A:1381:ASP:OD1  | 1:A:1391:SER:OG   | 2.22                     | 0.47              |
| 1:A:1625:LEU:HD11 | 1:A:1660:LEU:HB3  | 1.96                     | 0.47              |
| 1:A:2101:UNK:HG2  | 1:A:2102:UNK:N    | 2.29                     | 0.47              |
| 1:A:782:ARG:HD3   | 1:A:853:LEU:HD22  | 1.97                     | 0.47              |
| 1:A:713:ALA:O     | 1:A:868:ARG:NH2   | 2.48                     | 0.47              |
| 1:B:1672:GLN:HB3  | 1:B:1672:GLN:HE21 | 1.58                     | 0.47              |
| 1:B:2630:ASP:HB3  | 1:B:2633:VAL:HG23 | 1.97                     | 0.47              |
| 1:B:2926:SER:HB3  | 1:B:2976:TRP:HH2  | 1.79                     | 0.47              |
| 1:C:1625:LEU:HD11 | 1:C:1660:LEU:HB3  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:210:VAL:HG22  | 1:C:287:PHE:CD1   | 2.50                     | 0.47              |
| 1:C:832:ASP:O     | 1:C:836:VAL:HG23  | 2.14                     | 0.47              |
| 1:C:670:GLY:HA3   | 1:C:899:ALA:HB2   | 1.96                     | 0.47              |
| 1:C:941:UNK:HG3   | 1:C:942:UNK:N     | 2.30                     | 0.47              |
| 1:A:1010:UNK:HG2  | 1:A:1017:ILE:HB   | 1.96                     | 0.47              |
| 1:A:1467:VAL:HA   | 1:A:1605:LYS:HD2  | 1.96                     | 0.47              |
| 1:A:2210:VAL:HB   | 1:A:2277:ILE:HD11 | 1.96                     | 0.47              |
| 1:A:301:LEU:HD13  | 1:A:330:LEU:HD22  | 1.96                     | 0.47              |
| 1:A:966:PRO:O     | 1:A:970:ILE:N     | 2.48                     | 0.47              |
| 1:B:2125:UNK:HA   | 1:B:2128:UNK:CG   | 2.45                     | 0.47              |
| 1:B:2450:UNK:HG1  | 1:B:3016:ALA:CB   | 2.17                     | 0.47              |
| 1:B:2762:VAL:HG22 | 1:B:2822:LEU:HB2  | 1.96                     | 0.47              |
| 1:B:778:THR:HG21  | 1:B:854:GLY:HA3   | 1.97                     | 0.47              |
| 1:B:868:ARG:HB3   | 1:B:872:ARG:NH1   | 2.28                     | 0.47              |
| 1:B:931:UNK:HG2   | 1:B:933:UNK:HG2   | 1.92                     | 0.47              |
| 1:C:1276:GLN:HE21 | 1:C:1292:LEU:HD13 | 1.79                     | 0.47              |
| 1:C:2086:UNK:CA   | 1:C:2089:UNK:HG3  | 2.43                     | 0.47              |
| 1:C:2376:LEU:HD22 | 1:C:2392:VAL:HG21 | 1.97                     | 0.47              |
| 1:C:803:GLU:OE1   | 1:C:2431:UNK:CG   | 2.62                     | 0.47              |
| 1:C:2681:THR:O    | 1:C:2764:ALA:HA   | 2.15                     | 0.47              |
| 1:C:931:UNK:CG    | 1:C:934:UNK:HG3   | 2.44                     | 0.47              |
| 1:A:198:ILE:HG12  | 1:C:1087:PHE:CE1  | 2.50                     | 0.47              |
| 1:A:803:GLU:OE1   | 1:A:2431:UNK:CG   | 2.62                     | 0.47              |
| 1:A:2785:ALA:HB1  | 1:A:2809:LEU:HG   | 1.97                     | 0.47              |
| 1:A:808:ALA:HB3   | 1:A:811:ASP:HB2   | 1.96                     | 0.47              |
| 1:A:832:ASP:O     | 1:A:836:VAL:HG23  | 2.14                     | 0.47              |
| 1:B:1010:UNK:HG2  | 1:B:1017:ILE:HB   | 1.96                     | 0.47              |
| 1:B:1457:GLU:OE2  | 1:B:1614:TYR:OH   | 2.30                     | 0.47              |
| 1:B:2554:ALA:HB1  | 1:B:2614:LYS:HD2  | 1.96                     | 0.47              |
| 1:B:210:VAL:HG22  | 1:B:287:PHE:CD1   | 2.50                     | 0.47              |
| 1:B:585:HIS:HD2   | 1:B:586:SER:H     | 1.62                     | 0.47              |
| 1:B:713:ALA:O     | 1:B:868:ARG:NH2   | 2.48                     | 0.47              |
| 1:B:782:ARG:HD3   | 1:B:853:LEU:HD22  | 1.97                     | 0.47              |
| 1:B:941:UNK:HG3   | 1:B:942:UNK:N     | 2.30                     | 0.47              |
| 1:C:2291:LEU:HD21 | 1:C:2332:LEU:HD22 | 1.95                     | 0.47              |
| 1:A:141:ALA:O     | 1:A:145:MET:HB2   | 2.15                     | 0.47              |
| 1:A:2482:GLU:HG2  | 1:A:2956:PRO:HB3  | 1.97                     | 0.47              |
| 1:B:1723:GLU:C    | 1:B:1725:SER:H    | 2.18                     | 0.47              |
| 1:B:2843:GLN:HG2  | 1:B:2845:PHE:CZ   | 2.49                     | 0.47              |
| 1:B:301:LEU:HD13  | 1:B:330:LEU:HD22  | 1.96                     | 0.47              |
| 1:B:992:UNK:CG    | 1:B:996:UNK:HG2   | 2.32                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1111:PHE:HE1  | 1:C:1129:LEU:HD11 | 1.78                     | 0.47              |
| 1:C:2101:UNK:HG2  | 1:C:2102:UNK:N    | 2.29                     | 0.47              |
| 1:C:2125:UNK:HA   | 1:C:2128:UNK:CG   | 2.44                     | 0.47              |
| 1:C:2427:UNK:HG2  | 1:C:2427:UNK:O    | 2.15                     | 0.47              |
| 1:C:3080:ARG:NH1  | 1:C:3080:ARG:CG   | 2.72                     | 0.47              |
| 1:C:836:VAL:HG12  | 1:C:837:VAL:N     | 2.29                     | 0.47              |
| 1:A:2058:ASP:N    | 1:A:2058:ASP:OD1  | 2.46                     | 0.46              |
| 1:A:836:VAL:HG12  | 1:A:837:VAL:N     | 2.29                     | 0.46              |
| 1:B:997:UNK:HB1   | 1:B:1009:UNK:CG   | 2.44                     | 0.46              |
| 1:B:1467:VAL:HA   | 1:B:1605:LYS:HD2  | 1.96                     | 0.46              |
| 1:B:836:VAL:HG12  | 1:B:837:VAL:N     | 2.29                     | 0.46              |
| 1:B:94:ARG:HG3    | 1:B:95:PRO:HD3    | 1.98                     | 0.46              |
| 1:A:1237:ARG:CZ   | 1:B:95:PRO:HB2    | 2.46                     | 0.46              |
| 1:B:966:PRO:O     | 1:B:970:ILE:N     | 2.48                     | 0.46              |
| 1:C:1590:VAL:HG11 | 1:C:1671:TRP:CE2  | 2.50                     | 0.46              |
| 1:C:2104:UNK:HA   | 1:C:2107:UNK:CG   | 2.46                     | 0.46              |
| 1:C:2210:VAL:HB   | 1:C:2277:ILE:HD11 | 1.97                     | 0.46              |
| 1:C:2252:VAL:HG13 | 1:C:2255:ARG:HH21 | 1.81                     | 0.46              |
| 1:C:222:LEU:HD21  | 1:C:236:VAL:HA    | 1.97                     | 0.46              |
| 1:A:2077:UNK:CG   | 1:A:2079:UNK:HG3  | 2.41                     | 0.46              |
| 1:A:2096:UNK:C    | 1:A:2099:UNK:HG3  | 2.43                     | 0.46              |
| 1:A:670:GLY:HA3   | 1:A:899:ALA:HB2   | 1.96                     | 0.46              |
| 1:A:778:THR:HG21  | 1:A:854:GLY:HA3   | 1.97                     | 0.46              |
| 1:A:941:UNK:HG3   | 1:A:942:UNK:N     | 2.30                     | 0.46              |
| 1:B:2961:LEU:HD22 | 1:B:2976:TRP:CD1  | 2.51                     | 0.46              |
| 1:B:518:ASP:HA    | 1:B:543:GLY:O     | 2.15                     | 0.46              |
| 1:C:1508:ILE:HB   | 1:C:1562:ARG:HD3  | 1.97                     | 0.46              |
| 1:C:2096:UNK:C    | 1:C:2099:UNK:HG3  | 2.43                     | 0.46              |
| 1:C:2352:ILE:HG12 | 1:C:2412:ALA:HB1  | 1.96                     | 0.46              |
| 1:C:501:VAL:HA    | 1:C:504:LYS:HE2   | 1.96                     | 0.46              |
| 1:C:656:THR:HG1   | 1:C:880:HIS:CE1   | 2.30                     | 0.46              |
| 1:C:84:GLU:HB2    | 1:C:85:PRO:HD3    | 1.97                     | 0.46              |
| 1:C:713:ALA:O     | 1:C:868:ARG:NH2   | 2.48                     | 0.46              |
| 1:C:931:UNK:HG2   | 1:C:933:UNK:HG2   | 1.92                     | 0.46              |
| 1:A:171:LYS:HE3   | 1:A:173:ALA:HB3   | 1.96                     | 0.46              |
| 1:A:210:VAL:HG22  | 1:A:287:PHE:CD1   | 2.50                     | 0.46              |
| 1:A:2252:VAL:HG13 | 1:A:2255:ARG:HH21 | 1.80                     | 0.46              |
| 1:A:2352:ILE:HG12 | 1:A:2412:ALA:HB1  | 1.96                     | 0.46              |
| 1:A:2681:THR:O    | 1:A:2764:ALA:HA   | 2.15                     | 0.46              |
| 1:A:2978:ARG:NH1  | 1:A:2979:GLU:OE2  | 2.49                     | 0.46              |
| 1:A:361:THR:HG21  | 1:A:377:PRO:HG3   | 1.95                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:365:ALA:O     | 1:A:369:ARG:N     | 2.42                     | 0.46              |
| 1:B:1001:UNK:O    | 1:B:1005:UNK:HB2  | 2.16                     | 0.46              |
| 1:B:1319:ASP:HB2  | 1:B:1342:ARG:NH1  | 2.31                     | 0.46              |
| 1:B:2118:UNK:HG2  | 1:B:2119:UNK:N    | 2.28                     | 0.46              |
| 1:B:205:PRO:CD    | 1:B:289:PRO:HB3   | 2.46                     | 0.46              |
| 1:B:996:UNK:HA    | 1:B:1010:UNK:HA   | 1.97                     | 0.46              |
| 1:C:2434:UNK:HG3  | 1:C:2523:GLU:O    | 2.14                     | 0.46              |
| 1:C:2884:ASP:HA   | 1:C:2916:ARG:NH1  | 2.29                     | 0.46              |
| 1:C:982:UNK:CG    | 1:C:983:UNK:N     | 2.76                     | 0.46              |
| 1:A:1612:GLY:N    | 1:A:1623:PHE:O    | 2.48                     | 0.46              |
| 1:A:1699:ARG:HG3  | 1:A:1730:GLU:HB3  | 1.97                     | 0.46              |
| 1:A:2461:VAL:HG21 | 1:A:2751:VAL:HG13 | 1.96                     | 0.46              |
| 1:A:518:ASP:HA    | 1:A:543:GLY:O     | 2.15                     | 0.46              |
| 1:A:683:GLY:CA    | 1:A:700:ASN:HB2   | 2.44                     | 0.46              |
| 1:A:84:GLU:HB2    | 1:A:85:PRO:HD3    | 1.98                     | 0.46              |
| 1:B:1634:ARG:HH11 | 1:B:1639:ALA:N    | 2.08                     | 0.46              |
| 1:B:2252:VAL:HG13 | 1:B:2255:ARG:HH21 | 1.81                     | 0.46              |
| 1:B:2736:PRO:HG2  | 1:B:2746:SER:HA   | 1.95                     | 0.46              |
| 1:C:2348:GLN:O    | 1:C:2416:MET:HG3  | 2.15                     | 0.46              |
| 1:C:518:ASP:HA    | 1:C:543:GLY:O     | 2.15                     | 0.46              |
| 1:A:1325:LEU:HD11 | 1:A:1343:LEU:HD22 | 1.98                     | 0.46              |
| 1:A:1346:PRO:HG2  | 1:A:1699:ARG:HD3  | 1.98                     | 0.46              |
| 1:A:2961:LEU:HD22 | 1:A:2976:TRP:CD1  | 2.51                     | 0.46              |
| 1:B:1237:ARG:CZ   | 1:C:95:PRO:HB2    | 2.46                     | 0.46              |
| 1:B:1276:GLN:HE21 | 1:B:1292:LEU:HD13 | 1.79                     | 0.46              |
| 1:B:1699:ARG:HG3  | 1:B:1730:GLU:HB3  | 1.97                     | 0.46              |
| 1:B:2543:PHE:HA   | 1:B:2624:GLN:HE22 | 1.81                     | 0.46              |
| 1:B:2554:ALA:HB1  | 1:B:2614:LYS:HZ2  | 1.78                     | 0.46              |
| 1:B:768:LYS:HA    | 1:B:775:LEU:HD11  | 1.97                     | 0.46              |
| 1:C:2252:VAL:HG22 | 1:C:2255:ARG:NH2  | 2.30                     | 0.46              |
| 1:C:745:THR:HG22  | 1:C:747:LEU:H     | 1.80                     | 0.46              |
| 1:C:782:ARG:HD3   | 1:C:853:LEU:HD22  | 1.97                     | 0.46              |
| 1:B:2104:UNK:HA   | 1:B:2107:UNK:CG   | 2.46                     | 0.46              |
| 1:C:1325:LEU:HD11 | 1:C:1343:LEU:HD22 | 1.98                     | 0.46              |
| 1:C:141:ALA:O     | 1:C:145:MET:HB2   | 2.15                     | 0.46              |
| 1:C:1699:ARG:HG3  | 1:C:1730:GLU:HB3  | 1.97                     | 0.46              |
| 1:C:2361:VAL:HG21 | 1:C:2401:ILE:HD11 | 1.98                     | 0.46              |
| 1:C:406:THR:OG1   | 1:C:418:GLU:OE1   | 2.34                     | 0.46              |
| 1:C:534:ASP:O     | 1:C:538:GLU:HG3   | 2.16                     | 0.46              |
| 1:C:778:THR:HG21  | 1:C:854:GLY:HA3   | 1.97                     | 0.46              |
| 1:A:1072:TRP:CD1  | 1:A:1097:VAL:HG22 | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1590:VAL:HG11 | 1:A:1671:TRP:CE2  | 2.50                     | 0.46              |
| 1:A:3065:PRO:O    | 1:A:3069:GLN:N    | 2.42                     | 0.46              |
| 1:A:575:HIS:CD2   | 1:A:644:LEU:HD22  | 2.49                     | 0.46              |
| 1:B:1072:TRP:CD1  | 1:B:1097:VAL:HG22 | 2.51                     | 0.46              |
| 1:B:141:ALA:O     | 1:B:145:MET:HB2   | 2.15                     | 0.46              |
| 1:B:2210:VAL:HB   | 1:B:2277:ILE:HD11 | 1.96                     | 0.46              |
| 1:B:2348:GLN:O    | 1:B:2416:MET:HG3  | 2.15                     | 0.46              |
| 1:B:406:THR:OG1   | 1:B:418:GLU:OE1   | 2.34                     | 0.46              |
| 1:B:540:ASN:ND2   | 1:B:544:ILE:HG13  | 2.30                     | 0.46              |
| 1:B:606:ASN:H     | 1:B:606:ASN:HD22  | 1.62                     | 0.46              |
| 1:B:84:GLU:HB2    | 1:B:85:PRO:HD3    | 1.97                     | 0.46              |
| 1:C:1001:UNK:O    | 1:C:1005:UNK:HB2  | 2.16                     | 0.46              |
| 1:C:1094:THR:O    | 1:C:1288:PRO:HG2  | 2.15                     | 0.46              |
| 1:C:1319:ASP:HB2  | 1:C:1342:ARG:NH1  | 2.31                     | 0.46              |
| 1:C:1346:PRO:HG2  | 1:C:1699:ARG:HD3  | 1.98                     | 0.46              |
| 1:C:2482:GLU:HG2  | 1:C:2956:PRO:HB3  | 1.97                     | 0.46              |
| 1:C:2957:PRO:HB3  | 1:C:2979:GLU:C    | 2.36                     | 0.46              |
| 1:A:1205:UNK:HG2  | 1:A:1206:UNK:N    | 2.30                     | 0.46              |
| 1:A:1276:GLN:HE21 | 1:A:1292:LEU:HD13 | 1.79                     | 0.46              |
| 1:A:1212:UNK:CG   | 1:A:1342:ARG:HH21 | 2.17                     | 0.46              |
| 1:A:167:ALA:HB3   | 1:A:178:LEU:HD21  | 1.98                     | 0.46              |
| 1:A:2104:UNK:HA   | 1:A:2107:UNK:CG   | 2.46                     | 0.46              |
| 1:A:2376:LEU:HD22 | 1:A:2392:VAL:HG21 | 1.97                     | 0.46              |
| 1:A:2630:ASP:HB3  | 1:A:2633:VAL:HG23 | 1.97                     | 0.46              |
| 1:A:2957:PRO:HB3  | 1:A:2979:GLU:C    | 2.36                     | 0.46              |
| 1:A:501:VAL:HA    | 1:A:504:LYS:HE2   | 1.96                     | 0.46              |
| 1:A:277:LEU:HD22  | 1:A:676:GLY:O     | 2.16                     | 0.46              |
| 1:B:2957:PRO:HB3  | 1:B:2979:GLU:C    | 2.36                     | 0.46              |
| 1:B:2978:ARG:NH1  | 1:B:2979:GLU:OE2  | 2.49                     | 0.46              |
| 1:C:94:ARG:HG3    | 1:C:95:PRO:HD3    | 1.98                     | 0.46              |
| 1:C:996:UNK:HA    | 1:C:1010:UNK:HA   | 1.97                     | 0.46              |
| 1:A:1455:VAL:HB   | 1:A:1480:ARG:HH12 | 1.80                     | 0.46              |
| 1:A:2212:TRP:HA   | 1:A:2229:LYS:HB3  | 1.98                     | 0.46              |
| 1:A:2252:VAL:HG22 | 1:A:2255:ARG:NH2  | 2.30                     | 0.46              |
| 1:A:2610:ARG:NH1  | 1:A:2700:LEU:HD21 | 2.31                     | 0.46              |
| 1:A:2773:GLU:HA   | 1:A:2776:ILE:HG22 | 1.97                     | 0.46              |
| 1:A:2790:MET:SD   | 1:A:2800:PHE:HB2  | 2.56                     | 0.46              |
| 1:A:647:THR:HG22  | 1:A:901:ILE:HD11  | 1.96                     | 0.46              |
| 1:A:95:PRO:HB2    | 1:C:1237:ARG:CZ   | 2.45                     | 0.46              |
| 1:B:111:GLU:HB2   | 1:B:112:PRO:HD3   | 1.98                     | 0.46              |
| 1:B:1205:UNK:HG2  | 1:B:1206:UNK:N    | 2.31                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1304:LYS:O    | 1:B:1307:ASP:HB2  | 2.16                     | 0.46              |
| 1:B:2619:ARG:NH1  | 1:B:2779:GLY:HA2  | 2.31                     | 0.46              |
| 1:B:984:UNK:HG1   | 1:B:987:UNK:CG    | 2.46                     | 0.46              |
| 1:C:111:GLU:HB2   | 1:C:112:PRO:HD3   | 1.98                     | 0.46              |
| 1:C:1205:UNK:HG2  | 1:C:1206:UNK:N    | 2.30                     | 0.46              |
| 1:C:2619:ARG:NH1  | 1:C:2779:GLY:HA2  | 2.31                     | 0.46              |
| 1:C:2946:LEU:HD22 | 1:C:2994:VAL:HG23 | 1.98                     | 0.46              |
| 1:A:1087:PHE:CE1  | 1:B:198:ILE:HG12  | 2.51                     | 0.46              |
| 1:A:205:PRO:CD    | 1:A:289:PRO:HB3   | 2.46                     | 0.46              |
| 1:A:2123:UNK:HA   | 1:A:2126:UNK:HG3  | 1.97                     | 0.46              |
| 1:A:2125:UNK:HA   | 1:A:2128:UNK:CG   | 2.45                     | 0.46              |
| 1:A:2879:LEU:HD13 | 1:A:3009:VAL:HG11 | 1.98                     | 0.46              |
| 1:A:745:THR:HG22  | 1:A:747:LEU:H     | 1.80                     | 0.46              |
| 1:A:868:ARG:HD3   | 1:A:872:ARG:HH12  | 1.81                     | 0.46              |
| 1:B:2770:LEU:HB3  | 1:B:2815:GLN:HB3  | 1.97                     | 0.46              |
| 1:C:1072:TRP:CD1  | 1:C:1097:VAL:HG22 | 2.51                     | 0.46              |
| 1:C:1304:LYS:O    | 1:C:1307:ASP:HB2  | 2.16                     | 0.46              |
| 1:B:1087:PHE:CE1  | 1:C:198:ILE:HG12  | 2.51                     | 0.46              |
| 1:C:2234:PRO:HB2  | 1:C:2287:LEU:HD13 | 1.98                     | 0.46              |
| 1:C:2879:LEU:HD13 | 1:C:3009:VAL:HG11 | 1.98                     | 0.46              |
| 1:C:408:VAL:CG1   | 1:C:943:UNK:HG1   | 2.46                     | 0.46              |
| 1:A:111:GLU:HB2   | 1:A:112:PRO:HD3   | 1.98                     | 0.45              |
| 1:A:2100:UNK:C    | 1:A:2103:UNK:HG3  | 2.31                     | 0.45              |
| 1:A:2137:GLU:O    | 1:A:2163:THR:N    | 2.30                     | 0.45              |
| 1:A:2891:LYS:HG3  | 1:A:2924:ILE:HD13 | 1.98                     | 0.45              |
| 1:B:1094:THR:O    | 1:B:1288:PRO:HG2  | 2.15                     | 0.45              |
| 1:B:1325:LEU:HD11 | 1:B:1343:LEU:HD22 | 1.98                     | 0.45              |
| 1:B:2094:UNK:HG1  | 1:B:2096:UNK:HG3  | 1.90                     | 0.45              |
| 1:B:793:ARG:HA    | 1:B:2435:UNK:HG1  | 1.97                     | 0.45              |
| 1:B:2672:TRP:CD1  | 1:B:2831:MET:HG2  | 2.52                     | 0.45              |
| 1:B:2773:GLU:HA   | 1:B:2776:ILE:HG22 | 1.97                     | 0.45              |
| 1:B:2889:ILE:HD11 | 1:B:2922:LEU:HD22 | 1.98                     | 0.45              |
| 1:A:1003:UNK:CG   | 1:A:1004:UNK:N    | 2.53                     | 0.45              |
| 1:A:1094:THR:O    | 1:A:1288:PRO:HG2  | 2.15                     | 0.45              |
| 1:A:1319:ASP:HB2  | 1:A:1342:ARG:NH1  | 2.31                     | 0.45              |
| 1:A:1450:ALA:N    | 1:A:1613:ARG:O    | 2.48                     | 0.45              |
| 1:A:2543:PHE:HA   | 1:A:2624:GLN:HE22 | 1.81                     | 0.45              |
| 1:A:793:ARG:HA    | 1:A:2435:UNK:HG1  | 1.98                     | 0.45              |
| 1:A:996:UNK:HA    | 1:A:1010:UNK:HA   | 1.97                     | 0.45              |
| 1:B:1702:GLU:OE1  | 1:B:1712:ALA:N    | 2.49                     | 0.45              |
| 1:B:2234:PRO:HB2  | 1:B:2287:LEU:HD13 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2482:GLU:HG2  | 1:B:2956:PRO:HB3  | 1.97                     | 0.45              |
| 1:B:2946:LEU:HD22 | 1:B:2994:VAL:HG23 | 1.98                     | 0.45              |
| 1:C:1462:ALA:HB2  | 1:C:1468:TYR:HE1  | 1.81                     | 0.45              |
| 1:C:2212:TRP:HA   | 1:C:2229:LYS:HB3  | 1.98                     | 0.45              |
| 1:C:2961:LEU:HD22 | 1:C:2976:TRP:CD1  | 2.51                     | 0.45              |
| 1:C:47:ALA:O      | 1:C:353:ASP:HA    | 2.17                     | 0.45              |
| 1:C:540:ASN:ND2   | 1:C:544:ILE:HG13  | 2.30                     | 0.45              |
| 1:C:277:LEU:HD22  | 1:C:676:GLY:O     | 2.16                     | 0.45              |
| 1:C:683:GLY:CA    | 1:C:700:ASN:HB2   | 2.44                     | 0.45              |
| 1:A:1133:VAL:O    | 1:A:1193:ALA:N    | 2.42                     | 0.45              |
| 1:A:1462:ALA:HB2  | 1:A:1468:TYR:HE1  | 1.81                     | 0.45              |
| 1:A:1483:LYS:O    | 1:A:1487:ILE:HG23 | 2.17                     | 0.45              |
| 1:A:2619:ARG:NH1  | 1:A:2779:GLY:HA2  | 2.31                     | 0.45              |
| 1:A:944:UNK:O     | 1:A:944:UNK:CG    | 2.59                     | 0.45              |
| 1:A:94:ARG:HG3    | 1:A:95:PRO:HD3    | 1.98                     | 0.45              |
| 1:B:1352:PHE:HA   | 1:B:1353:PRO:HD3  | 1.72                     | 0.45              |
| 1:B:1462:ALA:HB2  | 1:B:1468:TYR:HE1  | 1.81                     | 0.45              |
| 1:B:2891:LYS:HG3  | 1:B:2924:ILE:HD13 | 1.99                     | 0.45              |
| 1:B:351:ILE:HB    | 1:B:375:ILE:HG12  | 1.99                     | 0.45              |
| 1:C:2070:LEU:O    | 1:C:2074:GLU:HG3  | 2.16                     | 0.45              |
| 1:C:205:PRO:CD    | 1:C:289:PRO:HB3   | 2.46                     | 0.45              |
| 1:C:2472:TYR:CZ   | 1:C:2930:LEU:HD22 | 2.52                     | 0.45              |
| 1:C:381:ARG:O     | 1:C:384:GLN:HG2   | 2.17                     | 0.45              |
| 1:C:746:TYR:HB2   | 1:C:833:ALA:HB1   | 1.99                     | 0.45              |
| 1:C:984:UNK:HG1   | 1:C:987:UNK:CG    | 2.46                     | 0.45              |
| 1:A:222:LEU:HD21  | 1:A:236:VAL:HA    | 1.97                     | 0.45              |
| 1:A:2246:ALA:N    | 1:A:2255:ARG:NH1  | 2.64                     | 0.45              |
| 1:A:2672:TRP:CD1  | 1:A:2831:MET:HG2  | 2.52                     | 0.45              |
| 1:A:2845:PHE:HD2  | 1:A:2860:ALA:HA   | 1.82                     | 0.45              |
| 1:A:2889:ILE:HD11 | 1:A:2922:LEU:HD22 | 1.98                     | 0.45              |
| 1:A:747:LEU:HD22  | 1:A:751:ARG:CZ    | 2.47                     | 0.45              |
| 1:A:784:GLU:OE2   | 1:A:816:LEU:HD21  | 2.16                     | 0.45              |
| 1:B:1001:UNK:HG1  | 1:B:1018:ARG:HH21 | 1.80                     | 0.45              |
| 1:B:1346:PRO:HG2  | 1:B:1699:ARG:HD3  | 1.98                     | 0.45              |
| 1:B:2096:UNK:C    | 1:B:2099:UNK:HG3  | 2.43                     | 0.45              |
| 1:B:2769:ASP:OD1  | 1:B:2770:LEU:N    | 2.49                     | 0.45              |
| 1:B:2785:ALA:HB1  | 1:B:2809:LEU:HG   | 1.97                     | 0.45              |
| 1:B:2879:LEU:HD13 | 1:B:3009:VAL:HG11 | 1.98                     | 0.45              |
| 1:B:47:ALA:O      | 1:B:353:ASP:HA    | 2.17                     | 0.45              |
| 1:C:1212:UNK:HG2  | 1:C:1342:ARG:CZ   | 2.47                     | 0.45              |
| 1:C:1483:LYS:O    | 1:C:1487:ILE:HG23 | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:585:HIS:CB    | 1:C:694:ASP:HB2   | 2.47                     | 0.45              |
| 1:C:684:MET:HG3   | 1:C:895:THR:HA    | 1.98                     | 0.45              |
| 1:A:2427:UNK:HG2  | 1:A:2427:UNK:O    | 2.15                     | 0.45              |
| 1:A:222:LEU:HD13  | 1:A:248:ILE:HD12  | 1.99                     | 0.45              |
| 1:A:2770:LEU:HB3  | 1:A:2815:GLN:HB3  | 1.97                     | 0.45              |
| 1:A:381:ARG:O     | 1:A:384:GLN:HG2   | 2.17                     | 0.45              |
| 1:A:544:ILE:O     | 1:A:546:HIS:N     | 2.41                     | 0.45              |
| 1:A:684:MET:HG3   | 1:A:895:THR:HA    | 1.98                     | 0.45              |
| 1:B:2246:ALA:N    | 1:B:2255:ARG:NH1  | 2.64                     | 0.45              |
| 1:B:207:MET:HG3   | 1:B:292:VAL:HB    | 1.98                     | 0.45              |
| 1:B:746:TYR:HB2   | 1:B:833:ALA:HB1   | 1.99                     | 0.45              |
| 1:B:868:ARG:HD3   | 1:B:872:ARG:HH12  | 1.81                     | 0.45              |
| 1:C:2785:ALA:HB1  | 1:C:2809:LEU:HG   | 1.97                     | 0.45              |
| 1:C:2790:MET:SD   | 1:C:2800:PHE:HB2  | 2.56                     | 0.45              |
| 1:C:351:ILE:HB    | 1:C:375:ILE:HG12  | 1.99                     | 0.45              |
| 1:C:511:ARG:CB    | 1:C:540:ASN:HB2   | 2.46                     | 0.45              |
| 1:C:768:LYS:HA    | 1:C:775:LEU:HD11  | 1.97                     | 0.45              |
| 1:A:1001:UNK:O    | 1:A:1005:UNK:HB2  | 2.15                     | 0.45              |
| 1:A:1702:GLU:OE1  | 1:A:1712:ALA:N    | 2.49                     | 0.45              |
| 1:A:2070:LEU:O    | 1:A:2074:GLU:HG3  | 2.16                     | 0.45              |
| 1:A:534:ASP:O     | 1:A:538:GLU:HG3   | 2.16                     | 0.45              |
| 1:A:540:ASN:ND2   | 1:A:544:ILE:HG13  | 2.30                     | 0.45              |
| 1:A:408:VAL:CG1   | 1:A:943:UNK:HG1   | 2.46                     | 0.45              |
| 1:B:1519:VAL:HG13 | 1:B:1530:LEU:HD23 | 1.98                     | 0.45              |
| 1:B:1450:ALA:N    | 1:B:1613:ARG:O    | 2.48                     | 0.45              |
| 1:B:195:ARG:NH1   | 1:B:198:ILE:HD12  | 2.31                     | 0.45              |
| 1:B:585:HIS:CB    | 1:B:694:ASP:HB2   | 2.47                     | 0.45              |
| 1:C:1488:VAL:HB   | 1:C:1579:VAL:HG22 | 1.99                     | 0.45              |
| 1:C:1553:ALA:O    | 1:C:1557:GLU:HG2  | 2.17                     | 0.45              |
| 1:C:167:ALA:HB3   | 1:C:178:LEU:HD21  | 1.98                     | 0.45              |
| 1:C:2630:ASP:HB3  | 1:C:2633:VAL:HG23 | 1.97                     | 0.45              |
| 1:A:1072:TRP:HE1  | 1:A:1077:VAL:HG22 | 1.80                     | 0.45              |
| 1:A:2080:UNK:HG2  | 1:A:2083:UNK:CG   | 2.45                     | 0.45              |
| 1:A:2361:VAL:HG21 | 1:A:2401:ILE:HD11 | 1.98                     | 0.45              |
| 1:A:406:THR:OG1   | 1:A:418:GLU:OE1   | 2.34                     | 0.45              |
| 1:A:768:LYS:HA    | 1:A:775:LEU:HD11  | 1.98                     | 0.45              |
| 1:B:1488:VAL:HB   | 1:B:1579:VAL:HG22 | 1.99                     | 0.45              |
| 1:B:1605:LYS:H    | 1:B:1658:LYS:HE2  | 1.82                     | 0.45              |
| 1:B:1996:PRO:O    | 1:B:2000:LEU:N    | 2.41                     | 0.45              |
| 1:B:2137:GLU:O    | 1:B:2163:THR:N    | 2.30                     | 0.45              |
| 1:B:2212:TRP:HA   | 1:B:2229:LYS:HB3  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2452:UNK:CG   | 1:B:2453:UNK:N    | 2.73                     | 0.45              |
| 1:B:2790:MET:SD   | 1:B:2800:PHE:HB2  | 2.56                     | 0.45              |
| 1:B:2452:UNK:HA   | 1:B:3017:ALA:HA   | 1.99                     | 0.45              |
| 1:B:3080:ARG:CG   | 1:B:3080:ARG:NH1  | 2.72                     | 0.45              |
| 1:B:534:ASP:O     | 1:B:538:GLU:HG3   | 2.16                     | 0.45              |
| 1:C:1684:ASP:HA   | 1:C:1687:PHE:HD2  | 1.82                     | 0.45              |
| 1:C:747:LEU:HD22  | 1:C:751:ARG:CZ    | 2.47                     | 0.45              |
| 1:C:763:SER:HB3   | 1:C:766:ASP:HB2   | 1.99                     | 0.45              |
| 1:A:195:ARG:NH1   | 1:A:198:ILE:HD12  | 2.31                     | 0.45              |
| 1:B:1212:UNK:HG2  | 1:B:1342:ARG:CZ   | 2.47                     | 0.45              |
| 1:B:2361:VAL:HG21 | 1:B:2401:ILE:HD11 | 1.98                     | 0.45              |
| 1:B:2845:PHE:HD2  | 1:B:2860:ALA:HA   | 1.81                     | 0.45              |
| 1:B:763:SER:HB3   | 1:B:766:ASP:HB2   | 1.99                     | 0.45              |
| 1:C:195:ARG:NH1   | 1:C:198:ILE:HD12  | 2.31                     | 0.45              |
| 1:C:1996:PRO:O    | 1:C:2000:LEU:N    | 2.41                     | 0.45              |
| 1:C:2114:UNK:HA   | 1:C:2117:UNK:HG3  | 1.99                     | 0.45              |
| 1:C:2093:UNK:HG1  | 1:C:2132:UNK:HB1  | 1.95                     | 0.45              |
| 1:C:222:LEU:HD13  | 1:C:248:ILE:HD12  | 1.99                     | 0.45              |
| 1:C:2610:ARG:NH1  | 1:C:2700:LEU:HD21 | 2.31                     | 0.45              |
| 1:C:2769:ASP:OD1  | 1:C:2770:LEU:N    | 2.49                     | 0.45              |
| 1:C:2770:LEU:HB3  | 1:C:2815:GLN:HB3  | 1.97                     | 0.45              |
| 1:C:2845:PHE:HD2  | 1:C:2860:ALA:HA   | 1.81                     | 0.45              |
| 1:C:784:GLU:OE2   | 1:C:816:LEU:HD21  | 2.16                     | 0.45              |
| 1:A:1605:LYS:H    | 1:A:1658:LYS:HE2  | 1.82                     | 0.45              |
| 1:A:351:ILE:HB    | 1:A:375:ILE:HG12  | 1.99                     | 0.45              |
| 1:B:1171:PRO:HA   | 1:B:1191:ARG:HG2  | 1.99                     | 0.45              |
| 1:B:1284:GLY:HA2  | 1:B:1343:LEU:HD11 | 1.99                     | 0.45              |
| 1:B:167:ALA:HB3   | 1:B:178:LEU:HD21  | 1.98                     | 0.45              |
| 1:B:222:LEU:HD21  | 1:B:236:VAL:HA    | 1.97                     | 0.45              |
| 1:B:2610:ARG:NH1  | 1:B:2700:LEU:HD21 | 2.31                     | 0.45              |
| 1:B:336:TRP:CH2   | 1:B:360:LEU:HD21  | 2.52                     | 0.45              |
| 1:B:784:GLU:OE2   | 1:B:816:LEU:HD21  | 2.16                     | 0.45              |
| 1:B:997:UNK:O     | 1:B:1009:UNK:HG3  | 2.17                     | 0.45              |
| 1:C:1072:TRP:HE1  | 1:C:1077:VAL:HG22 | 1.80                     | 0.45              |
| 1:C:1634:ARG:NH1  | 1:C:1639:ALA:N    | 2.65                     | 0.45              |
| 1:A:2591:ARG:HH12 | 1:C:2014:SER:H    | 1.65                     | 0.45              |
| 1:C:2296:ASN:HB3  | 1:C:2299:MET:SD   | 2.57                     | 0.45              |
| 1:C:2672:TRP:CD1  | 1:C:2831:MET:HG2  | 2.52                     | 0.45              |
| 1:C:2845:PHE:CD2  | 1:C:2860:ALA:HA   | 2.52                     | 0.45              |
| 1:C:544:ILE:O     | 1:C:546:HIS:N     | 2.40                     | 0.45              |
| 1:A:1488:VAL:HB   | 1:A:1579:VAL:HG22 | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2014:SER:H    | 1:B:2591:ARG:HH12 | 1.65                     | 0.45              |
| 1:A:2946:LEU:HD22 | 1:A:2994:VAL:HG23 | 1.98                     | 0.45              |
| 1:A:746:TYR:HB2   | 1:A:833:ALA:HB1   | 1.99                     | 0.45              |
| 1:A:799:PHE:CZ    | 1:A:2433:UNK:CG   | 2.99                     | 0.45              |
| 1:A:997:UNK:O     | 1:A:1009:UNK:HG3  | 2.17                     | 0.45              |
| 1:B:2619:ARG:HH12 | 1:B:2779:GLY:HA2  | 1.81                     | 0.45              |
| 1:B:381:ARG:O     | 1:B:384:GLN:HG2   | 2.17                     | 0.45              |
| 1:B:544:ILE:O     | 1:B:546:HIS:N     | 2.41                     | 0.45              |
| 1:C:1001:UNK:HG1  | 1:C:1018:ARG:HH21 | 1.80                     | 0.45              |
| 1:C:1581:PHE:HB2  | 1:C:1586:LEU:HD22 | 1.99                     | 0.45              |
| 1:C:2246:ALA:N    | 1:C:2255:ARG:HH12 | 2.15                     | 0.45              |
| 1:C:2246:ALA:N    | 1:C:2255:ARG:NH1  | 2.64                     | 0.45              |
| 1:C:2800:PHE:CE1  | 1:C:2812:LEU:HD22 | 2.50                     | 0.45              |
| 1:C:2978:ARG:NH1  | 1:C:2979:GLU:OE2  | 2.49                     | 0.45              |
| 1:C:868:ARG:HD3   | 1:C:872:ARG:HH12  | 1.81                     | 0.45              |
| 1:A:999:UNK:C     | 1:A:1007:UNK:HG3  | 2.46                     | 0.44              |
| 1:A:1212:UNK:HG2  | 1:A:1342:ARG:CZ   | 2.47                     | 0.44              |
| 1:A:2845:PHE:CD2  | 1:A:2860:ALA:HA   | 2.52                     | 0.44              |
| 1:A:210:VAL:HG22  | 1:A:287:PHE:HD1   | 1.83                     | 0.44              |
| 1:A:984:UNK:HG1   | 1:A:987:UNK:CG    | 2.46                     | 0.44              |
| 1:B:1285:LYS:HB3  | 1:B:1286:PRO:HD2  | 1.99                     | 0.44              |
| 1:B:2300:PHE:CZ   | 1:B:2398:LEU:HB3  | 2.52                     | 0.44              |
| 1:B:2427:UNK:O    | 1:B:2427:UNK:HG2  | 2.15                     | 0.44              |
| 1:B:2891:LYS:HZ2  | 1:B:2903:GLU:HG2  | 1.82                     | 0.44              |
| 1:B:664:LEU:HB3   | 1:B:701:ALA:HB1   | 1.99                     | 0.44              |
| 1:B:799:PHE:CZ    | 1:B:2433:UNK:CG   | 2.99                     | 0.44              |
| 1:C:997:UNK:O     | 1:C:1009:UNK:HG3  | 2.18                     | 0.44              |
| 1:C:1702:GLU:OE1  | 1:C:1712:ALA:N    | 2.49                     | 0.44              |
| 1:C:2891:LYS:HG3  | 1:C:2924:ILE:HD13 | 1.98                     | 0.44              |
| 1:C:365:ALA:O     | 1:C:369:ARG:N     | 2.42                     | 0.44              |
| 1:C:664:LEU:HB3   | 1:C:701:ALA:HB1   | 1.99                     | 0.44              |
| 1:A:1304:LYS:O    | 1:A:1307:ASP:HB2  | 2.16                     | 0.44              |
| 1:A:1634:ARG:NH1  | 1:A:1639:ALA:N    | 2.65                     | 0.44              |
| 1:A:207:MET:HG3   | 1:A:292:VAL:HB    | 1.98                     | 0.44              |
| 1:B:1612:GLY:N    | 1:B:1623:PHE:O    | 2.48                     | 0.44              |
| 1:B:2299:MET:H    | 1:B:2299:MET:HG2  | 1.68                     | 0.44              |
| 1:B:277:LEU:HD22  | 1:B:676:GLY:O     | 2.16                     | 0.44              |
| 1:B:210:VAL:HG22  | 1:B:287:PHE:HD1   | 1.82                     | 0.44              |
| 1:B:550:LYS:HD3   | 1:B:577:GLU:OE2   | 2.17                     | 0.44              |
| 1:B:999:UNK:HG2   | 1:B:1007:UNK:HG1  | 1.96                     | 0.44              |
| 1:C:207:MET:HG3   | 1:C:292:VAL:HB    | 1.98                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:210:VAL:HG22  | 1:C:287:PHE:HD1   | 1.83                     | 0.44              |
| 1:C:2300:PHE:CZ   | 1:C:2398:LEU:HB3  | 2.52                     | 0.44              |
| 1:C:2452:UNK:HA   | 1:C:3017:ALA:HA   | 1.98                     | 0.44              |
| 1:C:2543:PHE:HA   | 1:C:2624:GLN:HE22 | 1.81                     | 0.44              |
| 1:C:2619:ARG:HH12 | 1:C:2779:GLY:HA2  | 1.81                     | 0.44              |
| 1:C:2831:MET:HB3  | 1:C:2831:MET:HE2  | 1.88                     | 0.44              |
| 1:C:671:THR:HB    | 1:C:682:ASN:CG    | 2.38                     | 0.44              |
| 1:A:2120:UNK:O    | 1:A:2123:UNK:CG   | 2.66                     | 0.44              |
| 1:A:2246:ALA:N    | 1:A:2255:ARG:HH12 | 2.15                     | 0.44              |
| 1:A:2300:PHE:CZ   | 1:A:2398:LEU:HB3  | 2.52                     | 0.44              |
| 1:A:2452:UNK:CG   | 1:A:2453:UNK:N    | 2.73                     | 0.44              |
| 1:A:2555:SER:HA   | 1:A:2556:PRO:HD2  | 1.84                     | 0.44              |
| 1:A:47:ALA:O      | 1:A:353:ASP:HA    | 2.17                     | 0.44              |
| 1:A:511:ARG:CB    | 1:A:540:ASN:HB2   | 2.46                     | 0.44              |
| 1:A:664:LEU:HB3   | 1:A:701:ALA:HB1   | 1.99                     | 0.44              |
| 1:B:1350:TYR:CD1  | 1:B:1703:ILE:HD11 | 2.53                     | 0.44              |
| 1:B:2080:UNK:HG2  | 1:B:2083:UNK:CG   | 2.45                     | 0.44              |
| 1:B:2472:TYR:CZ   | 1:B:2930:LEU:HD22 | 2.52                     | 0.44              |
| 1:B:684:MET:HG3   | 1:B:895:THR:HA    | 1.98                     | 0.44              |
| 1:B:747:LEU:HD22  | 1:B:751:ARG:CZ    | 2.47                     | 0.44              |
| 1:C:1171:PRO:HA   | 1:C:1191:ARG:HG2  | 1.99                     | 0.44              |
| 1:C:2209:LEU:O    | 1:C:2213:VAL:HG23 | 2.18                     | 0.44              |
| 1:C:2891:LYS:HZ2  | 1:C:2903:GLU:HG2  | 1.83                     | 0.44              |
| 1:C:336:TRP:CH2   | 1:C:360:LEU:HD21  | 2.52                     | 0.44              |
| 1:A:1519:VAL:HG13 | 1:A:1530:LEU:HD23 | 1.99                     | 0.44              |
| 1:A:583:GLY:HA2   | 1:A:892:ILE:HD13  | 2.00                     | 0.44              |
| 1:B:999:UNK:C     | 1:B:1007:UNK:HG3  | 2.47                     | 0.44              |
| 1:B:1553:ALA:O    | 1:B:1557:GLU:HG2  | 2.17                     | 0.44              |
| 1:B:2083:UNK:HA   | 1:B:2086:UNK:HG3  | 2.00                     | 0.44              |
| 1:B:222:LEU:HD13  | 1:B:248:ILE:HD12  | 1.99                     | 0.44              |
| 1:B:44:TYR:O      | 1:B:153:VAL:N     | 2.44                     | 0.44              |
| 1:C:1605:LYS:H    | 1:C:1658:LYS:HE2  | 1.82                     | 0.44              |
| 1:C:2080:UNK:HG2  | 1:C:2083:UNK:CG   | 2.45                     | 0.44              |
| 1:C:2889:ILE:HD11 | 1:C:2922:LEU:HD22 | 1.98                     | 0.44              |
| 1:C:583:GLY:HA2   | 1:C:892:ILE:HD13  | 2.00                     | 0.44              |
| 1:A:1284:GLY:HA2  | 1:A:1343:LEU:HD11 | 1.99                     | 0.44              |
| 1:A:1350:TYR:CD1  | 1:A:1703:ILE:HD11 | 2.53                     | 0.44              |
| 1:A:2452:UNK:HA   | 1:A:3017:ALA:HA   | 1.98                     | 0.44              |
| 1:A:2591:ARG:NH1  | 1:C:2014:SER:N    | 2.66                     | 0.44              |
| 1:A:2619:ARG:HH12 | 1:A:2779:GLY:HA2  | 1.81                     | 0.44              |
| 1:A:2472:TYR:CZ   | 1:A:2930:LEU:HD22 | 2.52                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:475:LEU:HD23  | 1:A:475:LEU:HA    | 1.79                     | 0.44              |
| 1:A:671:THR:HB    | 1:A:682:ASN:CG    | 2.38                     | 0.44              |
| 1:B:1225:UNK:HG1  | 1:B:1283:ASP:CG   | 2.34                     | 0.44              |
| 1:B:1503:ILE:HB   | 1:B:1542:TYR:HB2  | 2.00                     | 0.44              |
| 1:B:2296:ASN:HB3  | 1:B:2299:MET:SD   | 2.57                     | 0.44              |
| 1:B:2334:HIS:CD2  | 1:B:2391:LYS:HG3  | 2.50                     | 0.44              |
| 1:A:2014:SER:N    | 1:B:2591:ARG:NH1  | 2.66                     | 0.44              |
| 1:B:515:ALA:HA    | 1:B:516:PRO:HD3   | 1.84                     | 0.44              |
| 1:C:1093:PRO:HB3  | 1:C:1277:HIS:CE1  | 2.52                     | 0.44              |
| 1:C:970:ILE:HG23  | 1:C:992:UNK:HG1   | 2.00                     | 0.44              |
| 1:A:2234:PRO:HB2  | 1:A:2287:LEU:HD13 | 1.98                     | 0.44              |
| 1:A:2769:ASP:OD1  | 1:A:2770:LEU:N    | 2.49                     | 0.44              |
| 1:B:1634:ARG:NH1  | 1:B:1639:ALA:N    | 2.65                     | 0.44              |
| 1:B:1684:ASP:HA   | 1:B:1687:PHE:HD2  | 1.82                     | 0.44              |
| 1:B:1723:GLU:O    | 1:B:1725:SER:N    | 2.51                     | 0.44              |
| 1:B:2114:UNK:HA   | 1:B:2117:UNK:HG3  | 1.99                     | 0.44              |
| 1:B:2246:ALA:N    | 1:B:2255:ARG:HH12 | 2.15                     | 0.44              |
| 1:C:1350:TYR:CD1  | 1:C:1703:ILE:HD11 | 2.53                     | 0.44              |
| 1:C:1723:GLU:O    | 1:C:1725:SER:N    | 2.51                     | 0.44              |
| 1:C:2119:UNK:HG2  | 1:C:2120:UNK:N    | 2.33                     | 0.44              |
| 1:C:793:ARG:HA    | 1:C:2435:UNK:HG1  | 1.97                     | 0.44              |
| 1:C:2580:PHE:HE1  | 1:C:2603:ARG:HH21 | 1.66                     | 0.44              |
| 1:C:2471:PRO:HA   | 1:C:2625:ILE:HA   | 2.00                     | 0.44              |
| 1:A:412:ASP:H     | 1:A:1025:VAL:CG2  | 2.31                     | 0.44              |
| 1:A:1705:VAL:O    | 1:A:1735:GLU:HB2  | 2.18                     | 0.44              |
| 1:A:2296:ASN:HB3  | 1:A:2299:MET:SD   | 2.57                     | 0.44              |
| 1:A:88:SER:HB3    | 1:A:314:THR:OG1   | 2.18                     | 0.44              |
| 1:A:550:LYS:HD3   | 1:A:577:GLU:OE2   | 2.17                     | 0.44              |
| 1:A:585:HIS:CB    | 1:A:694:ASP:HB2   | 2.47                     | 0.44              |
| 1:A:657:THR:HB    | 1:A:662:LYS:HE3   | 2.00                     | 0.44              |
| 1:B:1537:LEU:HD13 | 1:B:1541:GLN:HB2  | 2.00                     | 0.44              |
| 1:B:2014:SER:H    | 1:C:2591:ARG:HH12 | 1.65                     | 0.44              |
| 1:B:2209:LEU:O    | 1:B:2213:VAL:HG23 | 2.18                     | 0.44              |
| 1:B:2297:ARG:HH22 | 1:B:2391:LYS:HZ3  | 1.65                     | 0.44              |
| 1:B:671:THR:HB    | 1:B:682:ASN:CG    | 2.38                     | 0.44              |
| 1:B:782:ARG:NH1   | 1:B:857:VAL:HG22  | 2.33                     | 0.44              |
| 1:B:944:UNK:CG    | 1:B:944:UNK:O     | 2.59                     | 0.44              |
| 1:C:1284:GLY:HA2  | 1:C:1343:LEU:HD11 | 1.99                     | 0.44              |
| 1:C:1537:LEU:HD13 | 1:C:1541:GLN:HB2  | 2.00                     | 0.44              |
| 1:C:1582:HIS:HA   | 1:C:1674:ALA:O    | 2.18                     | 0.44              |
| 1:C:782:ARG:NH1   | 1:C:857:VAL:HG22  | 2.33                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:745:THR:OG1   | 1:C:834:GLU:O     | 2.19                     | 0.44              |
| 1:A:1171:PRO:HA   | 1:A:1191:ARG:HG2  | 1.99                     | 0.44              |
| 1:A:1581:PHE:HB2  | 1:A:1586:LEU:HD22 | 1.99                     | 0.44              |
| 1:A:163:LEU:HD13  | 1:A:181:LEU:HD23  | 2.00                     | 0.44              |
| 1:A:2013:LEU:HA   | 1:A:2013:LEU:HD23 | 1.87                     | 0.44              |
| 1:A:2252:VAL:HG22 | 1:A:2255:ARG:HH21 | 1.82                     | 0.44              |
| 1:A:763:SER:HB3   | 1:A:766:ASP:HB2   | 1.99                     | 0.44              |
| 1:B:2845:PHE:CD2  | 1:B:2860:ALA:HA   | 2.52                     | 0.44              |
| 1:B:408:VAL:CG1   | 1:B:943:UNK:HG1   | 2.46                     | 0.44              |
| 1:C:2122:UNK:O    | 1:C:2125:UNK:CG   | 2.63                     | 0.44              |
| 1:C:2334:HIS:CD2  | 1:C:2391:LYS:HG3  | 2.50                     | 0.44              |
| 1:C:2958:ASN:HD22 | 1:C:2976:TRP:HE1  | 1.65                     | 0.44              |
| 1:C:393:VAL:HG12  | 1:C:394:PRO:N     | 2.32                     | 0.44              |
| 1:A:1553:ALA:O    | 1:A:1557:GLU:HG2  | 2.17                     | 0.44              |
| 1:A:1684:ASP:HA   | 1:A:1687:PHE:HD2  | 1.82                     | 0.44              |
| 1:A:2094:UNK:HG1  | 1:A:2096:UNK:HG3  | 1.90                     | 0.44              |
| 1:B:1483:LYS:O    | 1:B:1487:ILE:HG23 | 2.17                     | 0.44              |
| 1:B:2119:UNK:HG2  | 1:B:2120:UNK:N    | 2.33                     | 0.44              |
| 1:B:2462:VAL:HG13 | 1:B:2835:VAL:HG13 | 2.00                     | 0.44              |
| 1:B:2753:LYS:HA   | 1:B:2753:LYS:HD3  | 1.83                     | 0.44              |
| 1:B:2958:ASN:HD22 | 1:B:2976:TRP:HE1  | 1.65                     | 0.44              |
| 1:B:647:THR:OG1   | 2:B:4000:FMN:O3P  | 2.27                     | 0.44              |
| 1:B:995:UNK:HB1   | 1:B:1011:UNK:HG2  | 1.99                     | 0.44              |
| 1:C:1285:LYS:HB3  | 1:C:1286:PRO:HD2  | 1.99                     | 0.44              |
| 1:C:1733:ASN:H    | 1:C:1737:ASP:HB2  | 1.83                     | 0.44              |
| 1:C:550:LYS:HD3   | 1:C:577:GLU:OE2   | 2.17                     | 0.44              |
| 1:C:857:VAL:HG13  | 1:C:859:PHE:H     | 1.83                     | 0.44              |
| 1:A:1093:PRO:HB3  | 1:A:1277:HIS:CE1  | 2.52                     | 0.43              |
| 1:A:1133:VAL:N    | 1:A:1193:ALA:O    | 2.48                     | 0.43              |
| 1:A:1268:GLY:HA2  | 1:A:1271:LEU:HD12 | 1.99                     | 0.43              |
| 1:A:1285:LYS:HB3  | 1:A:1286:PRO:HD2  | 1.99                     | 0.43              |
| 1:A:1733:ASN:H    | 1:A:1737:ASP:HB2  | 1.83                     | 0.43              |
| 1:A:2083:UNK:HA   | 1:A:2086:UNK:HG3  | 2.00                     | 0.43              |
| 1:A:2297:ARG:HH22 | 1:A:2391:LYS:HZ3  | 1.66                     | 0.43              |
| 1:A:2989:LEU:HA   | 1:A:2989:LEU:HD12 | 1.77                     | 0.43              |
| 1:A:782:ARG:NH1   | 1:A:857:VAL:HG22  | 2.33                     | 0.43              |
| 1:A:981:UNK:CG    | 1:A:987:UNK:C     | 2.96                     | 0.43              |
| 1:B:1093:PRO:HB3  | 1:B:1277:HIS:CE1  | 2.52                     | 0.43              |
| 1:B:2903:GLU:OE2  | 1:B:2995:THR:OG1  | 2.36                     | 0.43              |
| 1:B:344:HIS:CD2   | 1:B:373:ILE:HG13  | 2.53                     | 0.43              |
| 1:B:583:GLY:HA2   | 1:B:892:ILE:HD13  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:602:ARG:NH2   | 1:B:641:ASP:OD1   | 2.27                     | 0.43              |
| 1:B:657:THR:HB    | 1:B:662:LYS:HE3   | 2.00                     | 0.43              |
| 1:C:2120:UNK:O    | 1:C:2123:UNK:CG   | 2.65                     | 0.43              |
| 1:C:2710:LEU:O    | 1:C:2713:VAL:HG22 | 2.18                     | 0.43              |
| 1:C:931:UNK:HG3   | 1:C:934:UNK:HG3   | 2.00                     | 0.43              |
| 1:A:3044:ALA:HB1  | 1:A:3050:PRO:HB3  | 2.00                     | 0.43              |
| 1:A:336:TRP:CH2   | 1:A:360:LEU:HD21  | 2.52                     | 0.43              |
| 1:A:602:ARG:NH2   | 1:A:641:ASP:OD1   | 2.27                     | 0.43              |
| 1:A:695:ILE:HG22  | 1:A:697:GLU:HG3   | 2.01                     | 0.43              |
| 1:A:982:UNK:CG    | 1:A:983:UNK:N     | 2.76                     | 0.43              |
| 1:A:999:UNK:HG2   | 1:A:1007:UNK:HG1  | 1.96                     | 0.43              |
| 1:B:2070:LEU:O    | 1:B:2074:GLU:HG3  | 2.16                     | 0.43              |
| 1:B:2120:UNK:O    | 1:B:2123:UNK:CG   | 2.66                     | 0.43              |
| 1:B:340:ILE:HD11  | 1:B:351:ILE:HD13  | 2.01                     | 0.43              |
| 1:C:1133:VAL:O    | 1:C:1193:ALA:N    | 2.42                     | 0.43              |
| 1:C:1163:ASP:HA   | 1:C:1168:ARG:HA   | 2.01                     | 0.43              |
| 1:C:34:LEU:O      | 1:C:38:LEU:HG     | 2.18                     | 0.43              |
| 1:C:874:ASP:OD2   | 1:C:877:TRP:CD1   | 2.72                     | 0.43              |
| 1:A:2114:UNK:HA   | 1:A:2117:UNK:HG3  | 1.99                     | 0.43              |
| 1:A:393:VAL:HG12  | 1:A:394:PRO:N     | 2.32                     | 0.43              |
| 1:A:641:ASP:N     | 1:A:641:ASP:OD1   | 2.48                     | 0.43              |
| 1:B:1705:VAL:O    | 1:B:1735:GLU:HB2  | 2.18                     | 0.43              |
| 1:B:970:ILE:HG23  | 1:B:992:UNK:HG1   | 2.00                     | 0.43              |
| 1:C:1268:GLY:HA2  | 1:C:1271:LEU:HD12 | 2.00                     | 0.43              |
| 1:C:1612:GLY:N    | 1:C:1623:PHE:O    | 2.48                     | 0.43              |
| 1:C:2180:LYS:HZ1  | 1:C:2962:ASP:HB3  | 1.82                     | 0.43              |
| 1:C:2462:VAL:HG13 | 1:C:2835:VAL:HG13 | 2.00                     | 0.43              |
| 1:C:981:UNK:HG2   | 1:C:988:UNK:HA    | 2.01                     | 0.43              |
| 1:A:1582:HIS:HA   | 1:A:1674:ALA:O    | 2.18                     | 0.43              |
| 1:A:2541:ARG:O    | 1:A:2621:VAL:HG13 | 2.18                     | 0.43              |
| 1:A:341:THR:HG23  | 1:A:344:HIS:ND1   | 2.34                     | 0.43              |
| 1:A:580:ARG:HD3   | 1:A:896:ALA:HB3   | 2.01                     | 0.43              |
| 1:B:2541:ARG:O    | 1:B:2621:VAL:HG13 | 2.18                     | 0.43              |
| 1:B:2580:PHE:HE1  | 1:B:2603:ARG:HH21 | 1.66                     | 0.43              |
| 1:B:2710:LEU:O    | 1:B:2713:VAL:HG22 | 2.18                     | 0.43              |
| 1:B:393:VAL:HG12  | 1:B:394:PRO:N     | 2.32                     | 0.43              |
| 1:B:857:VAL:HG13  | 1:B:859:PHE:H     | 1.83                     | 0.43              |
| 1:B:981:UNK:CG    | 1:B:987:UNK:C     | 2.96                     | 0.43              |
| 1:C:2115:UNK:HA   | 1:C:2118:UNK:CG   | 2.49                     | 0.43              |
| 1:C:657:THR:HB    | 1:C:662:LYS:HE3   | 2.00                     | 0.43              |
| 1:A:1163:ASP:HA   | 1:A:1168:ARG:HA   | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1723:GLU:O    | 1:A:1725:SER:N    | 2.51                     | 0.43              |
| 1:A:2209:LEU:O    | 1:A:2213:VAL:HG23 | 2.18                     | 0.43              |
| 1:A:344:HIS:CD2   | 1:A:373:ILE:HG13  | 2.53                     | 0.43              |
| 1:B:1268:GLY:HA2  | 1:B:1271:LEU:HD12 | 1.99                     | 0.43              |
| 1:B:2092:UNK:CG   | 1:B:2092:UNK:O    | 2.64                     | 0.43              |
| 1:B:2512:TRP:O    | 1:B:2520:LEU:HD12 | 2.19                     | 0.43              |
| 1:B:2471:PRO:HA   | 1:B:2625:ILE:HA   | 2.00                     | 0.43              |
| 1:B:516:PRO:HA    | 1:B:962:MET:SD    | 2.58                     | 0.43              |
| 1:C:1519:VAL:HG13 | 1:C:1530:LEU:HD23 | 1.99                     | 0.43              |
| 1:C:2095:UNK:C    | 1:C:2098:UNK:HG3  | 2.49                     | 0.43              |
| 1:C:2706:PRO:O    | 1:C:2709:ILE:HG12 | 2.19                     | 0.43              |
| 1:C:276:LYS:HB3   | 1:C:587:TRP:CH2   | 2.53                     | 0.43              |
| 1:C:3044:ALA:HB1  | 1:C:3050:PRO:HB3  | 2.00                     | 0.43              |
| 1:C:647:THR:N     | 2:C:4000:FMN:O3P  | 2.51                     | 0.43              |
| 1:A:2297:ARG:HH12 | 1:A:2391:LYS:NZ   | 2.17                     | 0.43              |
| 1:A:2591:ARG:HH12 | 1:C:2014:SER:N    | 2.16                     | 0.43              |
| 1:A:2462:VAL:HG13 | 1:A:2835:VAL:HG13 | 2.00                     | 0.43              |
| 1:A:315:VAL:C     | 1:A:317:LEU:H     | 2.22                     | 0.43              |
| 1:A:874:ASP:OD2   | 1:A:877:TRP:CD1   | 2.71                     | 0.43              |
| 1:B:1581:PHE:HB2  | 1:B:1586:LEU:HD22 | 1.99                     | 0.43              |
| 1:B:2426:UNK:HG2  | 1:B:2426:UNK:O    | 2.18                     | 0.43              |
| 1:B:2610:ARG:NH1  | 1:B:2700:LEU:HD11 | 2.25                     | 0.43              |
| 1:B:276:LYS:HB3   | 1:B:587:TRP:CH2   | 2.53                     | 0.43              |
| 1:B:315:VAL:C     | 1:B:317:LEU:H     | 2.22                     | 0.43              |
| 1:B:412:ASP:H     | 1:B:1025:VAL:CG2  | 2.31                     | 0.43              |
| 1:C:999:UNK:C     | 1:C:1007:UNK:HG3  | 2.47                     | 0.43              |
| 1:C:163:LEU:HD13  | 1:C:181:LEU:HD23  | 2.00                     | 0.43              |
| 1:C:2083:UNK:HA   | 1:C:2086:UNK:HG3  | 2.00                     | 0.43              |
| 1:C:344:HIS:CD2   | 1:C:373:ILE:HG13  | 2.53                     | 0.43              |
| 1:C:340:ILE:HD11  | 1:C:351:ILE:HD13  | 2.01                     | 0.43              |
| 1:C:580:ARG:HD3   | 1:C:896:ALA:HB3   | 2.01                     | 0.43              |
| 1:C:695:ILE:HG22  | 1:C:697:GLU:HG3   | 2.00                     | 0.43              |
| 1:C:782:ARG:HH11  | 1:C:857:VAL:HG22  | 1.83                     | 0.43              |
| 1:A:2471:PRO:HA   | 1:A:2625:ILE:HA   | 2.00                     | 0.43              |
| 1:A:2891:LYS:HZ2  | 1:A:2903:GLU:HG2  | 1.83                     | 0.43              |
| 1:A:857:VAL:HG13  | 1:A:859:PHE:H     | 1.83                     | 0.43              |
| 1:A:931:UNK:HG3   | 1:A:934:UNK:HG3   | 2.01                     | 0.43              |
| 1:B:1582:HIS:HA   | 1:B:1674:ALA:O    | 2.18                     | 0.43              |
| 1:B:2786:ASP:OD2  | 1:B:2789:MET:HG2  | 2.19                     | 0.43              |
| 1:B:658:SER:HB2   | 1:B:661:VAL:HG23  | 2.01                     | 0.43              |
| 1:B:940:UNK:O     | 1:B:940:UNK:CG    | 2.60                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1705:VAL:O    | 1:C:1735:GLU:HB2  | 2.18                     | 0.43              |
| 1:C:2903:GLU:OE2  | 1:C:2995:THR:OG1  | 2.36                     | 0.43              |
| 1:C:88:SER:HB3    | 1:C:314:THR:OG1   | 2.18                     | 0.43              |
| 1:A:1070:VAL:N    | 1:A:1152:PHE:O    | 2.52                     | 0.43              |
| 1:A:2710:LEU:O    | 1:A:2713:VAL:HG22 | 2.18                     | 0.43              |
| 1:A:2903:GLU:OE2  | 1:A:2995:THR:OG1  | 2.36                     | 0.43              |
| 1:A:2958:ASN:HD22 | 1:A:2976:TRP:HE1  | 1.65                     | 0.43              |
| 1:A:408:VAL:HG13  | 1:A:943:UNK:CG    | 2.48                     | 0.43              |
| 1:A:276:LYS:HB3   | 1:A:587:TRP:CH2   | 2.53                     | 0.43              |
| 1:B:1021:LEU:HB3  | 1:B:1034:GLU:HG2  | 2.01                     | 0.43              |
| 1:B:1619:VAL:HA   | 1:B:1620:PRO:HD2  | 1.80                     | 0.43              |
| 1:B:88:SER:HB3    | 1:B:314:THR:OG1   | 2.18                     | 0.43              |
| 1:B:34:LEU:O      | 1:B:38:LEU:HG     | 2.18                     | 0.43              |
| 1:B:488:ASN:OD1   | 1:B:523:SER:OG    | 2.34                     | 0.43              |
| 1:B:647:THR:N     | 2:B:4000:FMN:O3P  | 2.51                     | 0.43              |
| 1:B:856:PRO:HG2   | 1:B:874:ASP:HB2   | 2.00                     | 0.43              |
| 1:B:931:UNK:HG3   | 1:B:934:UNK:HG3   | 2.01                     | 0.43              |
| 1:B:981:UNK:HG2   | 1:B:988:UNK:HA    | 2.00                     | 0.43              |
| 1:C:2064:ARG:HG2  | 1:C:2100:UNK:HG1  | 2.01                     | 0.43              |
| 1:B:2014:SER:N    | 1:C:2591:ARG:NH1  | 2.66                     | 0.43              |
| 1:C:2810:GLY:HA2  | 1:C:2896:THR:HG22 | 2.01                     | 0.43              |
| 1:C:613:GLY:HA2   | 2:C:4000:FMN:O5'  | 2.19                     | 0.43              |
| 1:A:1352:PHE:HA   | 1:A:1353:PRO:HD3  | 1.72                     | 0.43              |
| 1:A:1503:ILE:HB   | 1:A:1542:TYR:HB2  | 2.00                     | 0.43              |
| 1:A:2119:UNK:HG2  | 1:A:2120:UNK:N    | 2.34                     | 0.43              |
| 1:A:2122:UNK:O    | 1:A:2125:UNK:CG   | 2.63                     | 0.43              |
| 1:A:2299:MET:HG2  | 1:A:2299:MET:H    | 1.68                     | 0.43              |
| 1:A:2530:TYR:O    | 1:A:2533:ALA:N    | 2.52                     | 0.43              |
| 1:A:2706:PRO:O    | 1:A:2709:ILE:HG12 | 2.19                     | 0.43              |
| 1:A:2786:ASP:OD2  | 1:A:2789:MET:HG2  | 2.19                     | 0.43              |
| 1:A:34:LEU:O      | 1:A:38:LEU:HG     | 2.19                     | 0.43              |
| 1:A:340:ILE:HD11  | 1:A:351:ILE:HD13  | 2.01                     | 0.43              |
| 1:A:709:LEU:HD21  | 1:A:872:ARG:NE    | 2.34                     | 0.43              |
| 1:A:981:UNK:HG2   | 1:A:988:UNK:HA    | 2.01                     | 0.43              |
| 1:B:1133:VAL:N    | 1:B:1193:ALA:O    | 2.48                     | 0.43              |
| 1:B:1317:GLY:O    | 1:B:1324:VAL:HG12 | 2.19                     | 0.43              |
| 1:B:163:LEU:HD13  | 1:B:181:LEU:HD23  | 2.00                     | 0.43              |
| 1:B:2665:THR:HA   | 1:B:2666:PRO:HD3  | 1.86                     | 0.43              |
| 1:B:3044:ALA:HB1  | 1:B:3050:PRO:HB3  | 2.00                     | 0.43              |
| 1:B:307:ILE:HG22  | 1:B:311:TRP:CE2   | 2.54                     | 0.43              |
| 1:B:511:ARG:CB    | 1:B:540:ASN:HB2   | 2.46                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:782:ARG:HH11 | 1:B:857:VAL:HG22  | 1.83                     | 0.43              |
| 1:B:780:ARG:NH1  | 1:B:817:GLU:OE2   | 2.52                     | 0.43              |
| 1:C:2530:TYR:O   | 1:C:2533:ALA:N    | 2.52                     | 0.43              |
| 1:C:475:LEU:HA   | 1:C:475:LEU:HD23  | 1.79                     | 0.43              |
| 1:C:856:PRO:HG2  | 1:C:874:ASP:HB2   | 2.00                     | 0.43              |
| 1:A:1084:THR:CG2 | 1:A:1274:ALA:HA   | 2.48                     | 0.43              |
| 1:A:2092:UNK:O   | 1:A:2092:UNK:CG   | 2.64                     | 0.43              |
| 1:A:2244:ARG:HG2 | 1:A:2245:VAL:N    | 2.34                     | 0.43              |
| 1:A:2580:PHE:HE1 | 1:A:2603:ARG:HH21 | 1.66                     | 0.43              |
| 1:A:2695:MET:HG3 | 1:A:2696:TYR:N    | 2.34                     | 0.43              |
| 1:A:780:ARG:NH1  | 1:A:817:GLU:OE2   | 2.52                     | 0.43              |
| 1:A:885:GLU:HG2  | 1:A:887:ASP:H     | 1.84                     | 0.43              |
| 1:A:999:UNK:HG2  | 1:A:1007:UNK:HG3  | 1.96                     | 0.43              |
| 1:B:2810:GLY:HA2 | 1:B:2896:THR:HG22 | 2.01                     | 0.43              |
| 1:B:393:VAL:O    | 1:B:395:GLU:N     | 2.52                     | 0.43              |
| 1:B:695:ILE:HG22 | 1:B:697:GLU:HG3   | 2.00                     | 0.43              |
| 1:C:1117:ALA:HA  | 1:C:1120:GLU:HB2  | 2.01                     | 0.43              |
| 1:C:2058:ASP:N   | 1:C:2058:ASP:OD1  | 2.46                     | 0.43              |
| 1:C:2096:UNK:CG  | 1:C:2097:UNK:N    | 2.82                     | 0.43              |
| 1:C:2137:GLU:O   | 1:C:2163:THR:N    | 2.30                     | 0.43              |
| 1:C:2557:LEU:HB3 | 1:C:2613:ARG:HB2  | 2.01                     | 0.43              |
| 1:A:2426:UNK:O   | 1:A:2426:UNK:HG2  | 2.18                     | 0.42              |
| 1:A:782:ARG:HH11 | 1:A:857:VAL:HG22  | 1.83                     | 0.42              |
| 1:A:1087:PHE:HD2 | 1:B:117:LYS:HZ1   | 1.67                     | 0.42              |
| 1:B:1733:ASN:H   | 1:B:1737:ASP:HB2  | 1.83                     | 0.42              |
| 1:B:2244:ARG:HG2 | 1:B:2245:VAL:N    | 2.34                     | 0.42              |
| 1:B:2957:PRO:HB3 | 1:B:2980:PRO:N    | 2.34                     | 0.42              |
| 1:B:874:ASP:OD2  | 1:B:877:TRP:CD1   | 2.72                     | 0.42              |
| 1:C:1084:THR:CG2 | 1:C:1274:ALA:HA   | 2.49                     | 0.42              |
| 1:C:1317:GLY:O   | 1:C:1324:VAL:HG12 | 2.19                     | 0.42              |
| 1:C:1660:LEU:HA  | 1:C:1660:LEU:HD23 | 1.86                     | 0.42              |
| 1:C:78:GLU:HB2   | 1:C:176:VAL:HG21  | 2.01                     | 0.42              |
| 1:B:1087:PHE:CZ  | 1:C:203:ASP:OD2   | 2.72                     | 0.42              |
| 1:C:2426:UNK:HG2 | 1:C:2426:UNK:O    | 2.18                     | 0.42              |
| 1:B:2014:SER:N   | 1:C:2591:ARG:HH12 | 2.16                     | 0.42              |
| 1:C:2541:ARG:O   | 1:C:2621:VAL:HG13 | 2.18                     | 0.42              |
| 1:C:2889:ILE:HB  | 1:C:2924:ILE:HG12 | 2.01                     | 0.42              |
| 1:A:1662:ARG:HG3 | 1:A:1663:LYS:N    | 2.34                     | 0.42              |
| 1:A:2810:GLY:HA2 | 1:A:2896:THR:HG22 | 2.01                     | 0.42              |
| 1:B:1117:ALA:HA  | 1:B:1120:GLU:HB2  | 2.01                     | 0.42              |
| 1:B:1551:LEU:HA  | 1:B:1551:LEU:HD13 | 1.80                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2115:UNK:HA   | 1:B:2118:UNK:CG   | 2.48                     | 0.42              |
| 1:B:2180:LYS:HZ1  | 1:B:2962:ASP:HB3  | 1.82                     | 0.42              |
| 1:B:2296:ASN:ND2  | 1:B:2395:THR:HG21 | 2.34                     | 0.42              |
| 1:B:2706:PRO:O    | 1:B:2709:ILE:HG12 | 2.19                     | 0.42              |
| 1:B:2800:PHE:CE1  | 1:B:2812:LEU:HD22 | 2.50                     | 0.42              |
| 1:B:2891:LYS:HZ1  | 1:B:2904:THR:N    | 2.17                     | 0.42              |
| 1:B:355:GLY:HA2   | 1:B:356:PRO:HD3   | 1.86                     | 0.42              |
| 1:C:1533:VAL:N    | 1:C:1543:ALA:O    | 2.52                     | 0.42              |
| 1:C:1662:ARG:HG3  | 1:C:1663:LYS:N    | 2.34                     | 0.42              |
| 1:C:2077:UNK:CG   | 1:C:2079:UNK:HG3  | 2.41                     | 0.42              |
| 1:C:2141:VAL:HG22 | 1:C:2238:PHE:HD2  | 1.85                     | 0.42              |
| 1:C:341:THR:HG23  | 1:C:344:HIS:ND1   | 2.34                     | 0.42              |
| 1:C:709:LEU:HD21  | 1:C:872:ARG:NE    | 2.34                     | 0.42              |
| 1:C:516:PRO:HA    | 1:C:962:MET:SD    | 2.58                     | 0.42              |
| 1:A:1504:ARG:HA   | 1:A:1540:SER:O    | 2.19                     | 0.42              |
| 1:A:2095:UNK:C    | 1:A:2098:UNK:HG3  | 2.49                     | 0.42              |
| 1:A:211:THR:HB    | 1:A:286:VAL:HB    | 2.02                     | 0.42              |
| 1:A:2141:VAL:HG22 | 1:A:2238:PHE:HD2  | 1.85                     | 0.42              |
| 1:A:2808:ARG:HH21 | 1:A:2901:PRO:HD3  | 1.85                     | 0.42              |
| 1:A:2957:PRO:HB3  | 1:A:2980:PRO:N    | 2.34                     | 0.42              |
| 1:A:613:GLY:HA2   | 2:A:4000:FMN:O5'  | 2.19                     | 0.42              |
| 1:B:2122:UNK:O    | 1:B:2125:UNK:CG   | 2.63                     | 0.42              |
| 1:B:2252:VAL:HG22 | 1:B:2255:ARG:HH21 | 1.82                     | 0.42              |
| 1:B:2911:ALA:O    | 1:B:2916:ARG:HB2  | 2.19                     | 0.42              |
| 1:B:45:ALA:O      | 1:B:351:ILE:HA    | 2.20                     | 0.42              |
| 1:C:1275:ALA:HB2  | 1:C:1311:PHE:CE2  | 2.55                     | 0.42              |
| 1:C:307:ILE:HG22  | 1:C:311:TRP:CE2   | 2.54                     | 0.42              |
| 1:C:438:THR:HA    | 1:C:880:HIS:CE1   | 2.51                     | 0.42              |
| 1:C:999:UNK:HG2   | 1:C:1007:UNK:HG1  | 1.96                     | 0.42              |
| 1:A:1106:CYS:SG   | 1:A:1174:VAL:HG11 | 2.60                     | 0.42              |
| 1:A:1317:GLY:O    | 1:A:1324:VAL:HG12 | 2.19                     | 0.42              |
| 1:A:2105:UNK:C    | 1:A:2108:UNK:HG3  | 2.34                     | 0.42              |
| 1:A:516:PRO:HA    | 1:A:962:MET:SD    | 2.58                     | 0.42              |
| 1:A:970:ILE:HG23  | 1:A:992:UNK:HG1   | 2.00                     | 0.42              |
| 1:B:1163:ASP:HA   | 1:B:1168:ARG:HA   | 2.01                     | 0.42              |
| 1:B:2095:UNK:C    | 1:B:2098:UNK:HG3  | 2.49                     | 0.42              |
| 1:B:53:SER:HA     | 1:B:359:ILE:HG13  | 2.01                     | 0.42              |
| 1:C:2252:VAL:HG22 | 1:C:2255:ARG:HH21 | 1.82                     | 0.42              |
| 1:C:2584:ASP:O    | 1:C:2586:GLU:N    | 2.53                     | 0.42              |
| 1:A:1021:LEU:HB3  | 1:A:1034:GLU:HG2  | 2.01                     | 0.42              |
| 1:A:107:LEU:HD13  | 1:A:113:VAL:HB    | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1087:PHE:CZ   | 1:B:203:ASP:OD2   | 2.72                     | 0.42              |
| 1:A:1280:THR:O    | 1:A:1288:PRO:HB3  | 2.20                     | 0.42              |
| 1:A:1399:ASN:HA   | 1:A:1400:PRO:HD3  | 1.86                     | 0.42              |
| 1:A:1537:LEU:HD13 | 1:A:1541:GLN:HB2  | 2.00                     | 0.42              |
| 1:A:2512:TRP:O    | 1:A:2520:LEU:HD12 | 2.19                     | 0.42              |
| 1:B:1280:THR:O    | 1:B:1288:PRO:HB3  | 2.20                     | 0.42              |
| 1:B:1660:LEU:HD23 | 1:B:1660:LEU:HA   | 1.85                     | 0.42              |
| 1:B:211:THR:HB    | 1:B:286:VAL:HB    | 2.01                     | 0.42              |
| 1:B:2695:MET:HG3  | 1:B:2696:TYR:N    | 2.34                     | 0.42              |
| 1:B:2836:LEU:HA   | 1:B:2836:LEU:HD23 | 1.87                     | 0.42              |
| 1:B:2444:UNK:HB2  | 1:B:2988:PRO:HB3  | 2.01                     | 0.42              |
| 1:B:341:THR:HG23  | 1:B:344:HIS:ND1   | 2.34                     | 0.42              |
| 1:C:1106:CYS:SG   | 1:C:1174:VAL:HG11 | 2.60                     | 0.42              |
| 1:C:2244:ARG:HG2  | 1:C:2245:VAL:N    | 2.34                     | 0.42              |
| 1:C:2444:UNK:HB2  | 1:C:2988:PRO:HB3  | 2.01                     | 0.42              |
| 1:C:2512:TRP:O    | 1:C:2520:LEU:HD12 | 2.19                     | 0.42              |
| 1:C:2620:THR:OG1  | 1:C:2791:ARG:NH2  | 2.53                     | 0.42              |
| 1:C:2911:ALA:O    | 1:C:2916:ARG:HB2  | 2.19                     | 0.42              |
| 1:C:2961:LEU:HD22 | 1:C:2976:TRP:HD1  | 1.85                     | 0.42              |
| 1:C:981:UNK:CG    | 1:C:987:UNK:C     | 2.96                     | 0.42              |
| 1:C:999:UNK:HG2   | 1:C:1007:UNK:HG3  | 1.96                     | 0.42              |
| 1:A:2610:ARG:NH1  | 1:A:2700:LEU:HD11 | 2.25                     | 0.42              |
| 1:A:2805:ASP:OD2  | 1:A:2807:ARG:HB2  | 2.20                     | 0.42              |
| 1:B:107:LEU:HD13  | 1:B:113:VAL:HB    | 2.01                     | 0.42              |
| 1:B:2294:SER:HB3  | 1:B:2310:LYS:HB2  | 2.02                     | 0.42              |
| 1:B:2297:ARG:HH12 | 1:B:2391:LYS:NZ   | 2.17                     | 0.42              |
| 1:B:2889:ILE:HB   | 1:B:2924:ILE:HG12 | 2.01                     | 0.42              |
| 1:B:42:GLU:HA     | 1:B:43:PRO:HD3    | 1.91                     | 0.42              |
| 1:B:613:GLY:HA2   | 2:B:4000:FMN:O5'  | 2.19                     | 0.42              |
| 1:C:1504:ARG:HA   | 1:C:1540:SER:O    | 2.19                     | 0.42              |
| 1:C:1637:VAL:HA   | 1:C:1638:PRO:HD2  | 1.91                     | 0.42              |
| 1:C:2297:ARG:HH12 | 1:C:2391:LYS:NZ   | 2.17                     | 0.42              |
| 1:C:2846:ALA:O    | 1:C:2859:GLY:HA3  | 2.19                     | 0.42              |
| 1:C:3065:PRO:O    | 1:C:3069:GLN:N    | 2.42                     | 0.42              |
| 1:C:45:ALA:O      | 1:C:351:ILE:HA    | 2.20                     | 0.42              |
| 1:C:970:ILE:O     | 1:C:974:UNK:HG3   | 2.20                     | 0.42              |
| 1:A:1275:ALA:O    | 1:A:1279:VAL:HG23 | 2.20                     | 0.42              |
| 1:A:2115:UNK:HA   | 1:A:2118:UNK:CG   | 2.49                     | 0.42              |
| 1:A:2911:ALA:O    | 1:A:2916:ARG:HB2  | 2.19                     | 0.42              |
| 1:A:2889:ILE:HG13 | 1:A:2922:LEU:HD13 | 2.02                     | 0.42              |
| 1:A:307:ILE:HG22  | 1:A:311:TRP:CE2   | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:647:THR:N     | 2:A:4000:FMN:O3P  | 2.51                     | 0.42              |
| 1:A:856:PRO:HG2   | 1:A:874:ASP:HB2   | 2.00                     | 0.42              |
| 1:B:1275:ALA:HB2  | 1:B:1311:PHE:CE2  | 2.55                     | 0.42              |
| 1:B:1504:ARG:HA   | 1:B:1540:SER:O    | 2.19                     | 0.42              |
| 1:B:1656:LYS:N    | 1:B:1657:PRO:HD2  | 2.35                     | 0.42              |
| 1:B:1703:ILE:HG22 | 1:B:1704:GLY:H    | 1.85                     | 0.42              |
| 1:B:479:LEU:HD21  | 1:B:485:ILE:HD11  | 2.02                     | 0.42              |
| 1:B:668:THR:HG23  | 1:B:683:GLY:HA3   | 2.02                     | 0.42              |
| 1:B:885:GLU:HG2   | 1:B:887:ASP:H     | 1.84                     | 0.42              |
| 1:C:1120:GLU:HA   | 1:C:1125:VAL:CG2  | 2.50                     | 0.42              |
| 1:C:2120:UNK:C    | 1:C:2123:UNK:HG3  | 2.50                     | 0.42              |
| 1:C:2125:UNK:CA   | 1:C:2128:UNK:HG3  | 2.49                     | 0.42              |
| 1:C:2297:ARG:HH22 | 1:C:2391:LYS:HZ3  | 1.67                     | 0.42              |
| 1:C:2891:LYS:NZ   | 1:C:2903:GLU:HB3  | 2.35                     | 0.42              |
| 1:C:50:GLY:O      | 1:C:53:SER:OG     | 2.36                     | 0.42              |
| 1:C:658:SER:HB2   | 1:C:661:VAL:HG23  | 2.01                     | 0.42              |
| 1:C:795:HIS:NE2   | 1:C:797:GLN:HB2   | 2.35                     | 0.42              |
| 1:C:780:ARG:NH1   | 1:C:817:GLU:OE2   | 2.52                     | 0.42              |
| 1:A:1687:PHE:CE1  | 1:A:1723:GLU:HG2  | 2.55                     | 0.42              |
| 1:A:2296:ASN:ND2  | 1:A:2395:THR:HG21 | 2.34                     | 0.42              |
| 1:A:336:TRP:HE3   | 1:A:339:GLU:OE2   | 2.03                     | 0.42              |
| 1:A:488:ASN:OD1   | 1:A:523:SER:OG    | 2.34                     | 0.42              |
| 1:B:2300:PHE:HZ   | 1:B:2398:LEU:HB3  | 1.85                     | 0.42              |
| 1:B:2620:THR:OG1  | 1:B:2791:ARG:NH2  | 2.53                     | 0.42              |
| 1:B:2846:ALA:O    | 1:B:2859:GLY:HA3  | 2.19                     | 0.42              |
| 1:B:2961:LEU:HD22 | 1:B:2976:TRP:HD1  | 1.85                     | 0.42              |
| 1:B:436:THR:OG1   | 1:B:437:PRO:HD3   | 2.19                     | 0.42              |
| 1:B:999:UNK:O     | 1:B:1007:UNK:CG   | 2.61                     | 0.42              |
| 1:C:1021:LEU:HB3  | 1:C:1034:GLU:HG2  | 2.01                     | 0.42              |
| 1:C:412:ASP:H     | 1:C:1025:VAL:CG2  | 2.31                     | 0.42              |
| 1:C:1503:ILE:HB   | 1:C:1542:TYR:HB2  | 2.00                     | 0.42              |
| 1:C:1656:LYS:N    | 1:C:1657:PRO:HD2  | 2.35                     | 0.42              |
| 1:C:2113:UNK:HG2  | 1:C:2114:UNK:N    | 2.35                     | 0.42              |
| 1:C:315:VAL:C     | 1:C:317:LEU:H     | 2.22                     | 0.42              |
| 1:C:336:TRP:HE3   | 1:C:339:GLU:OE2   | 2.03                     | 0.42              |
| 1:C:479:LEU:HD21  | 1:C:485:ILE:HD11  | 2.02                     | 0.42              |
| 1:C:957:LEU:O     | 1:C:1034:GLU:HB2  | 2.20                     | 0.42              |
| 1:A:1228:VAL:HB   | 1:A:1311:PHE:HB2  | 2.02                     | 0.42              |
| 1:A:1380:ALA:HB1  | 1:A:1474:LEU:CD1  | 2.50                     | 0.42              |
| 1:A:2064:ARG:HG2  | 1:A:2100:UNK:HG1  | 2.01                     | 0.42              |
| 1:A:2055:VAL:HG22 | 1:A:2194:TRP:CD1  | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2584:ASP:O    | 1:A:2586:GLU:N    | 2.53                     | 0.42              |
| 1:A:2620:THR:OG1  | 1:A:2791:ARG:NH2  | 2.53                     | 0.42              |
| 1:A:2753:LYS:HA   | 1:A:2753:LYS:HD3  | 1.83                     | 0.42              |
| 1:A:2846:ALA:O    | 1:A:2859:GLY:HA3  | 2.20                     | 0.42              |
| 1:A:658:SER:HB2   | 1:A:661:VAL:HG23  | 2.01                     | 0.42              |
| 1:A:78:GLU:HB2    | 1:A:176:VAL:HG21  | 2.01                     | 0.42              |
| 1:B:2530:TYR:O    | 1:B:2533:ALA:N    | 2.52                     | 0.42              |
| 1:B:2557:LEU:HB3  | 1:B:2613:ARG:HB2  | 2.01                     | 0.42              |
| 1:B:2800:PHE:CZ   | 1:B:2812:LEU:HD13 | 2.55                     | 0.42              |
| 1:B:408:VAL:HG13  | 1:B:943:UNK:CG    | 2.48                     | 0.42              |
| 1:C:1275:ALA:O    | 1:C:1279:VAL:HG23 | 2.20                     | 0.42              |
| 1:C:1280:THR:O    | 1:C:1288:PRO:HB3  | 2.20                     | 0.42              |
| 1:C:2294:SER:HB3  | 1:C:2310:LYS:HB2  | 2.02                     | 0.42              |
| 1:C:436:THR:OG1   | 1:C:437:PRO:HD3   | 2.19                     | 0.42              |
| 1:C:53:SER:HA     | 1:C:359:ILE:HG13  | 2.01                     | 0.42              |
| 1:A:1008:UNK:CG   | 1:A:1008:UNK:O    | 2.67                     | 0.42              |
| 1:A:1275:ALA:HB2  | 1:A:1311:PHE:CE2  | 2.55                     | 0.42              |
| 1:A:1460:ALA:O    | 1:A:1464:VAL:HG22 | 2.20                     | 0.42              |
| 1:A:2123:UNK:CA   | 1:A:2126:UNK:HG3  | 2.50                     | 0.42              |
| 1:A:2125:UNK:CA   | 1:A:2128:UNK:HG3  | 2.49                     | 0.42              |
| 1:A:2800:PHE:CZ   | 1:A:2812:LEU:HD13 | 2.55                     | 0.42              |
| 1:A:436:THR:OG1   | 1:A:437:PRO:HD3   | 2.19                     | 0.42              |
| 1:A:668:THR:HG23  | 1:A:683:GLY:HA3   | 2.02                     | 0.42              |
| 1:B:2055:VAL:HG22 | 1:B:2194:TRP:CD1  | 2.55                     | 0.42              |
| 1:B:2584:ASP:O    | 1:B:2586:GLU:N    | 2.53                     | 0.42              |
| 1:B:2892:HIS:HA   | 1:B:2942:GLN:HE22 | 1.85                     | 0.42              |
| 1:B:970:ILE:O     | 1:B:974:UNK:HG3   | 2.20                     | 0.42              |
| 1:C:1228:VAL:HB   | 1:C:1311:PHE:HB2  | 2.02                     | 0.42              |
| 1:C:2354:SER:O    | 1:C:2358:GLU:HG3  | 2.20                     | 0.42              |
| 1:C:2957:PRO:HB3  | 1:C:2980:PRO:N    | 2.34                     | 0.42              |
| 1:C:668:THR:HG23  | 1:C:683:GLY:HA3   | 2.02                     | 0.42              |
| 1:A:1117:ALA:HA   | 1:A:1120:GLU:HB2  | 2.01                     | 0.41              |
| 1:A:1656:LYS:N    | 1:A:1657:PRO:HD2  | 2.35                     | 0.41              |
| 1:A:203:ASP:OD2   | 1:C:1087:PHE:CZ   | 2.72                     | 0.41              |
| 1:A:2096:UNK:CG   | 1:A:2097:UNK:N    | 2.82                     | 0.41              |
| 1:A:2300:PHE:HZ   | 1:A:2398:LEU:HB3  | 1.85                     | 0.41              |
| 1:A:2891:LYS:NZ   | 1:A:2903:GLU:HB3  | 2.35                     | 0.41              |
| 1:A:53:SER:HA     | 1:A:359:ILE:HG13  | 2.01                     | 0.41              |
| 1:A:976:UNK:CG    | 1:A:976:UNK:O     | 2.68                     | 0.41              |
| 1:B:1120:GLU:HA   | 1:B:1125:VAL:CG2  | 2.50                     | 0.41              |
| 1:B:1611:ILE:HG23 | 1:B:1624:THR:HA   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2077:UNK:CG   | 1:B:2079:UNK:HG3  | 2.41                     | 0.41              |
| 1:B:2125:UNK:CA   | 1:B:2128:UNK:HG3  | 2.49                     | 0.41              |
| 1:B:2141:VAL:HG22 | 1:B:2238:PHE:HD2  | 1.85                     | 0.41              |
| 1:B:2354:SER:O    | 1:B:2358:GLU:HG3  | 2.20                     | 0.41              |
| 1:B:2405:MET:HA   | 1:B:2405:MET:HE2  | 2.02                     | 0.41              |
| 1:A:2014:SER:N    | 1:B:2591:ARG:HH12 | 2.16                     | 0.41              |
| 1:B:2808:ARG:HH21 | 1:B:2901:PRO:HD3  | 1.85                     | 0.41              |
| 1:B:2889:ILE:HG13 | 1:B:2922:LEU:HD13 | 2.02                     | 0.41              |
| 1:B:709:LEU:HD21  | 1:B:872:ARG:NE    | 2.34                     | 0.41              |
| 1:C:1352:PHE:HA   | 1:C:1353:PRO:HD3  | 1.72                     | 0.41              |
| 1:C:1703:ILE:HG22 | 1:C:1704:GLY:H    | 1.85                     | 0.41              |
| 1:C:2299:MET:HG2  | 1:C:2299:MET:H    | 1.68                     | 0.41              |
| 1:C:2450:UNK:HG1  | 1:C:3016:ALA:CB   | 2.17                     | 0.41              |
| 1:C:160:GLN:HA    | 1:C:329:ILE:HD13  | 2.02                     | 0.41              |
| 1:A:2294:SER:HB3  | 1:A:2310:LYS:HB2  | 2.02                     | 0.41              |
| 1:A:266:ALA:O     | 1:A:270:GLU:HG3   | 2.20                     | 0.41              |
| 1:A:438:THR:HA    | 1:A:880:HIS:CE1   | 2.51                     | 0.41              |
| 1:A:669:LYS:O     | 1:A:682:ASN:HB3   | 2.20                     | 0.41              |
| 1:A:970:ILE:O     | 1:A:974:UNK:HG3   | 2.20                     | 0.41              |
| 1:A:984:UNK:HG2   | 1:A:984:UNK:O     | 2.20                     | 0.41              |
| 1:B:78:GLU:HB2    | 1:B:176:VAL:HG21  | 2.01                     | 0.41              |
| 1:B:266:ALA:O     | 1:B:270:GLU:HG3   | 2.20                     | 0.41              |
| 1:B:50:GLY:O      | 1:B:53:SER:OG     | 2.36                     | 0.41              |
| 1:C:1611:ILE:HG23 | 1:C:1624:THR:HA   | 2.02                     | 0.41              |
| 1:A:2591:ARG:NH1  | 1:C:2014:SER:H    | 2.19                     | 0.41              |
| 1:C:2200:MET:HE3  | 1:C:2200:MET:HB3  | 1.95                     | 0.41              |
| 1:C:2503:LYS:HG3  | 1:C:2513:TYR:HB2  | 2.02                     | 0.41              |
| 1:C:2786:ASP:OD2  | 1:C:2789:MET:HG2  | 2.19                     | 0.41              |
| 1:C:2800:PHE:CZ   | 1:C:2812:LEU:HD13 | 2.55                     | 0.41              |
| 1:C:2808:ARG:HH21 | 1:C:2901:PRO:HD3  | 1.85                     | 0.41              |
| 1:C:360:LEU:HA    | 1:C:363:LEU:HB3   | 2.02                     | 0.41              |
| 1:C:559:SER:O     | 1:C:563:ILE:HG12  | 2.20                     | 0.41              |
| 1:C:618:PRO:HB3   | 1:C:915:PHE:HA    | 2.02                     | 0.41              |
| 1:C:756:LEU:HD13  | 1:C:859:PHE:CD2   | 2.55                     | 0.41              |
| 1:A:70:SER:HG     | 1:A:142:ARG:HH22  | 1.65                     | 0.41              |
| 1:A:1611:ILE:HG23 | 1:A:1624:THR:HA   | 2.02                     | 0.41              |
| 1:A:2444:UNK:HB2  | 1:A:2988:PRO:HB3  | 2.01                     | 0.41              |
| 1:A:2563:LEU:HD21 | 1:A:2567:PHE:HB2  | 2.02                     | 0.41              |
| 1:A:2919:GLY:O    | 1:A:2921:PRO:HD3  | 2.21                     | 0.41              |
| 1:A:360:LEU:HA    | 1:A:363:LEU:HB3   | 2.02                     | 0.41              |
| 1:A:559:SER:O     | 1:A:563:ILE:HG12  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:795:HIS:NE2   | 1:A:797:GLN:HB2   | 2.35                     | 0.41              |
| 1:B:1228:VAL:HB   | 1:B:1311:PHE:HB2  | 2.02                     | 0.41              |
| 1:B:1706:LYS:HA   | 1:B:1735:GLU:HG3  | 2.02                     | 0.41              |
| 1:B:2064:ARG:HG2  | 1:B:2100:UNK:HG1  | 2.01                     | 0.41              |
| 1:B:2805:ASP:OD2  | 1:B:2807:ARG:HB2  | 2.20                     | 0.41              |
| 1:B:336:TRP:HE3   | 1:B:339:GLU:OE2   | 2.03                     | 0.41              |
| 1:B:487:PHE:O     | 1:B:521:VAL:N     | 2.51                     | 0.41              |
| 1:C:1095:LEU:HD23 | 1:C:1098:VAL:HA   | 2.03                     | 0.41              |
| 1:C:2123:UNK:CA   | 1:C:2126:UNK:HG3  | 2.50                     | 0.41              |
| 1:C:2695:MET:HG3  | 1:C:2696:TYR:N    | 2.34                     | 0.41              |
| 1:C:211:THR:HB    | 1:C:286:VAL:HB    | 2.01                     | 0.41              |
| 1:C:369:ARG:HD2   | 1:C:369:ARG:HA    | 1.85                     | 0.41              |
| 1:A:2557:LEU:HB3  | 1:A:2613:ARG:HB2  | 2.01                     | 0.41              |
| 1:A:2892:HIS:HA   | 1:A:2942:GLN:HE22 | 1.85                     | 0.41              |
| 1:B:1095:LEU:HD23 | 1:B:1098:VAL:HA   | 2.02                     | 0.41              |
| 1:B:1106:CYS:SG   | 1:B:1174:VAL:HG11 | 2.60                     | 0.41              |
| 1:B:1224:UNK:HG2  | 1:B:1224:UNK:O    | 2.20                     | 0.41              |
| 1:B:1662:ARG:HG3  | 1:B:1663:LYS:N    | 2.34                     | 0.41              |
| 1:B:2891:LYS:NZ   | 1:B:2903:GLU:HB3  | 2.35                     | 0.41              |
| 1:B:436:THR:HG22  | 1:B:460:GLY:HA3   | 2.03                     | 0.41              |
| 1:B:580:ARG:HD3   | 1:B:896:ALA:HB3   | 2.01                     | 0.41              |
| 1:B:980:UNK:C     | 1:B:981:UNK:CG    | 2.96                     | 0.41              |
| 1:C:2055:VAL:HG22 | 1:C:2194:TRP:CD1  | 2.55                     | 0.41              |
| 1:C:2296:ASN:ND2  | 1:C:2395:THR:HG21 | 2.34                     | 0.41              |
| 1:C:266:ALA:O     | 1:C:270:GLU:HG3   | 2.20                     | 0.41              |
| 1:C:669:LYS:O     | 1:C:682:ASN:HB3   | 2.20                     | 0.41              |
| 1:A:1703:ILE:HG22 | 1:A:1704:GLY:H    | 1.85                     | 0.41              |
| 1:A:2134:UNK:HB1  | 1:A:2189:PHE:HD2  | 1.85                     | 0.41              |
| 1:A:2354:SER:O    | 1:A:2358:GLU:HG3  | 2.20                     | 0.41              |
| 1:A:2492:VAL:HG12 | 1:A:2526:ILE:HG22 | 2.02                     | 0.41              |
| 1:A:233:LEU:HB3   | 1:A:251:THR:OG1   | 2.21                     | 0.41              |
| 1:A:2889:ILE:HB   | 1:A:2924:ILE:HG12 | 2.01                     | 0.41              |
| 1:B:1460:ALA:O    | 1:B:1464:VAL:HG22 | 2.20                     | 0.41              |
| 1:B:2096:UNK:CG   | 1:B:2097:UNK:N    | 2.82                     | 0.41              |
| 1:B:2123:UNK:CA   | 1:B:2126:UNK:HG3  | 2.50                     | 0.41              |
| 1:B:2205:ASP:O    | 1:B:2209:LEU:HB2  | 2.21                     | 0.41              |
| 1:B:2503:LYS:HG3  | 1:B:2513:TYR:HB2  | 2.02                     | 0.41              |
| 1:B:793:ARG:HH12  | 1:B:2523:GLU:CD   | 2.24                     | 0.41              |
| 1:B:2563:LEU:HD21 | 1:B:2567:PHE:HB2  | 2.02                     | 0.41              |
| 1:B:669:LYS:O     | 1:B:682:ASN:HB3   | 2.20                     | 0.41              |
| 1:A:117:LYS:HZ1   | 1:C:1087:PHE:HD2  | 1.68                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1399:ASN:HA   | 1:C:1400:PRO:HD3  | 1.86                     | 0.41              |
| 1:C:1672:GLN:HE21 | 1:C:1672:GLN:HB3  | 1.58                     | 0.41              |
| 1:C:1687:PHE:CE1  | 1:C:1723:GLU:HG2  | 2.55                     | 0.41              |
| 1:C:2092:UNK:O    | 1:C:2092:UNK:CG   | 2.64                     | 0.41              |
| 1:C:2104:UNK:CA   | 1:C:2107:UNK:HG3  | 2.50                     | 0.41              |
| 1:C:2889:ILE:HG13 | 1:C:2922:LEU:HD13 | 2.02                     | 0.41              |
| 1:C:374:GLY:C     | 1:C:375:ILE:HG13  | 2.41                     | 0.41              |
| 1:C:417:LEU:HD21  | 1:C:625:LEU:HD21  | 2.02                     | 0.41              |
| 1:C:885:GLU:HG2   | 1:C:887:ASP:H     | 1.84                     | 0.41              |
| 1:A:1491:ASP:HB2  | 1:A:1495:ARG:HB2  | 2.02                     | 0.41              |
| 1:A:2014:SER:H    | 1:B:2591:ARG:NH1  | 2.18                     | 0.41              |
| 1:A:202:GLY:O     | 1:A:289:PRO:HD2   | 2.21                     | 0.41              |
| 1:A:2113:UNK:HA   | 1:A:2116:UNK:HG3  | 2.03                     | 0.41              |
| 1:A:2113:UNK:HG2  | 1:A:2114:UNK:N    | 2.35                     | 0.41              |
| 1:A:587:TRP:CZ2   | 1:A:694:ASP:OD2   | 2.74                     | 0.41              |
| 1:A:756:LEU:HD13  | 1:A:859:PHE:CD2   | 2.55                     | 0.41              |
| 1:B:2058:ASP:N    | 1:B:2058:ASP:OD1  | 2.46                     | 0.41              |
| 1:B:2483:VAL:HG13 | 1:B:2954:VAL:HG11 | 2.03                     | 0.41              |
| 1:B:936:UNK:HA    | 1:B:939:UNK:CG    | 2.51                     | 0.41              |
| 1:C:1634:ARG:NH1  | 1:C:1639:ALA:H    | 2.11                     | 0.41              |
| 1:C:1706:LYS:HA   | 1:C:1735:GLU:HG3  | 2.03                     | 0.41              |
| 1:C:2113:UNK:HA   | 1:C:2116:UNK:HG3  | 2.03                     | 0.41              |
| 1:C:2468:GLU:OE2  | 1:C:2478:ARG:NH2  | 2.48                     | 0.41              |
| 1:C:585:HIS:HB3   | 1:C:694:ASP:HB2   | 2.03                     | 0.41              |
| 1:A:957:LEU:O     | 1:A:1034:GLU:HB2  | 2.20                     | 0.41              |
| 1:A:1400:PRO:O    | 1:A:1415:GLY:HA2  | 2.21                     | 0.41              |
| 1:A:1535:PHE:O    | 1:A:1679:TRP:N    | 2.48                     | 0.41              |
| 1:A:2141:VAL:HG22 | 1:A:2238:PHE:CD2  | 2.56                     | 0.41              |
| 1:A:2770:LEU:CB   | 1:A:2815:GLN:HB3  | 2.51                     | 0.41              |
| 1:A:160:GLN:HA    | 1:A:329:ILE:HD13  | 2.02                     | 0.41              |
| 1:A:393:VAL:O     | 1:A:395:GLU:N     | 2.52                     | 0.41              |
| 1:B:1275:ALA:O    | 1:B:1279:VAL:HG23 | 2.20                     | 0.41              |
| 1:B:1400:PRO:O    | 1:B:1415:GLY:HA2  | 2.21                     | 0.41              |
| 1:B:1491:ASP:HB2  | 1:B:1495:ARG:HB2  | 2.02                     | 0.41              |
| 1:B:2120:UNK:C    | 1:B:2123:UNK:HG3  | 2.50                     | 0.41              |
| 1:B:2286:ARG:HD3  | 1:B:2331:SER:OG   | 2.20                     | 0.41              |
| 1:B:233:LEU:HB3   | 1:B:251:THR:OG1   | 2.21                     | 0.41              |
| 1:B:2770:LEU:CB   | 1:B:2815:GLN:HB3  | 2.51                     | 0.41              |
| 1:B:202:GLY:O     | 1:B:289:PRO:HD2   | 2.21                     | 0.41              |
| 1:B:709:LEU:HD11  | 1:B:872:ARG:CZ    | 2.51                     | 0.41              |
| 1:C:1460:ALA:O    | 1:C:1464:VAL:HG22 | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2286:ARG:HD3  | 1:C:2331:SER:OG   | 2.20                     | 0.41              |
| 1:C:2710:LEU:HD12 | 1:C:2713:VAL:HG21 | 2.03                     | 0.41              |
| 1:C:2805:ASP:OD2  | 1:C:2807:ARG:HB2  | 2.20                     | 0.41              |
| 1:C:2919:GLY:O    | 1:C:2921:PRO:HD3  | 2.21                     | 0.41              |
| 1:C:515:ALA:HA    | 1:C:516:PRO:HD3   | 1.84                     | 0.41              |
| 1:A:1099:PRO:HB2  | 1:A:1295:TRP:HE1  | 1.86                     | 0.41              |
| 1:A:2831:MET:HB3  | 1:A:2831:MET:HE2  | 1.87                     | 0.41              |
| 1:A:479:LEU:HD21  | 1:A:485:ILE:HD11  | 2.02                     | 0.41              |
| 1:B:1164:THR:HG22 | 1:B:1204:UNK:HB2  | 2.03                     | 0.41              |
| 1:B:1695:LEU:HD12 | 1:B:1695:LEU:HA   | 1.71                     | 0.41              |
| 1:B:2113:UNK:HA   | 1:B:2116:UNK:HG3  | 2.03                     | 0.41              |
| 1:B:2891:LYS:HZ2  | 1:B:2903:GLU:CG   | 2.34                     | 0.41              |
| 1:B:3065:PRO:O    | 1:B:3069:GLN:N    | 2.42                     | 0.41              |
| 1:B:160:GLN:HA    | 1:B:329:ILE:HD13  | 2.02                     | 0.41              |
| 1:B:374:GLY:C     | 1:B:375:ILE:HG13  | 2.41                     | 0.41              |
| 1:B:559:SER:O     | 1:B:563:ILE:HG12  | 2.20                     | 0.41              |
| 1:B:957:LEU:O     | 1:B:1034:GLU:HB2  | 2.20                     | 0.41              |
| 1:C:107:LEU:HD13  | 1:C:113:VAL:HB    | 2.01                     | 0.41              |
| 1:C:2114:UNK:O    | 1:C:2118:UNK:HG3  | 2.21                     | 0.41              |
| 1:C:2428:UNK:O    | 1:C:2428:UNK:CG   | 2.67                     | 0.41              |
| 1:C:3062:HIS:H    | 1:C:3066:GLU:HG3  | 1.86                     | 0.41              |
| 1:A:133:GLN:O     | 1:A:137:VAL:HG23  | 2.21                     | 0.41              |
| 1:A:1634:ARG:NH1  | 1:A:1639:ALA:H    | 2.11                     | 0.41              |
| 1:A:2104:UNK:CA   | 1:A:2107:UNK:HG3  | 2.50                     | 0.41              |
| 1:A:2961:LEU:HD22 | 1:A:2976:TRP:HD1  | 1.85                     | 0.41              |
| 1:A:45:ALA:O      | 1:A:351:ILE:HA    | 2.20                     | 0.41              |
| 1:A:594:LEU:O     | 1:A:598:TYR:HB2   | 2.21                     | 0.41              |
| 1:A:585:HIS:HB3   | 1:A:694:ASP:HB2   | 2.03                     | 0.41              |
| 1:A:936:UNK:HA    | 1:A:939:UNK:CG    | 2.51                     | 0.41              |
| 1:B:1017:ILE:HG12 | 1:B:1045:VAL:HG11 | 2.03                     | 0.41              |
| 1:B:1687:PHE:CE1  | 1:B:1723:GLU:HG2  | 2.55                     | 0.41              |
| 1:B:2104:UNK:CA   | 1:B:2107:UNK:HG3  | 2.50                     | 0.41              |
| 1:B:2989:LEU:HD12 | 1:B:2989:LEU:HA   | 1.77                     | 0.41              |
| 1:B:360:LEU:HA    | 1:B:363:LEU:HB3   | 2.03                     | 0.41              |
| 1:B:618:PRO:HB3   | 1:B:915:PHE:HA    | 2.02                     | 0.41              |
| 1:B:795:HIS:NE2   | 1:B:797:GLN:HB2   | 2.35                     | 0.41              |
| 1:C:1002:UNK:CG   | 1:C:1005:UNK:HB2  | 2.51                     | 0.41              |
| 1:C:1491:ASP:HB2  | 1:C:1495:ARG:HB2  | 2.02                     | 0.41              |
| 1:C:2492:VAL:HG12 | 1:C:2526:ILE:HG22 | 2.02                     | 0.41              |
| 1:C:3057:ASP:N    | 1:C:3057:ASP:OD1  | 2.54                     | 0.41              |
| 1:A:1224:UNK:HG2  | 1:A:1224:UNK:O    | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2114:UNK:O    | 1:A:2118:UNK:HG3  | 2.21                     | 0.41              |
| 1:A:3057:ASP:N    | 1:A:3057:ASP:OD1  | 2.54                     | 0.41              |
| 1:A:278:ARG:HD2   | 1:A:674:TRP:CE3   | 2.56                     | 0.41              |
| 1:A:795:HIS:HE2   | 1:A:797:GLN:HB2   | 1.86                     | 0.41              |
| 1:A:985:UNK:O     | 1:A:988:UNK:HG3   | 2.21                     | 0.41              |
| 1:B:1637:VAL:HA   | 1:B:1638:PRO:HD2  | 1.90                     | 0.41              |
| 1:B:2212:TRP:O    | 1:B:2229:LYS:HB3  | 2.21                     | 0.41              |
| 1:B:2405:MET:O    | 1:B:2409:ALA:HB3  | 2.21                     | 0.41              |
| 1:B:3057:ASP:N    | 1:B:3057:ASP:OD1  | 2.54                     | 0.41              |
| 1:B:3062:HIS:H    | 1:B:3066:GLU:HG3  | 1.86                     | 0.41              |
| 1:B:369:ARG:HA    | 1:B:369:ARG:HD2   | 1.85                     | 0.41              |
| 1:C:1099:PRO:HB2  | 1:C:1295:TRP:HE1  | 1.86                     | 0.41              |
| 1:C:1986:LEU:HA   | 1:C:1989:PHE:CD2  | 2.56                     | 0.41              |
| 1:C:2010:GLN:OE1  | 1:C:2013:LEU:HD11 | 2.21                     | 0.41              |
| 1:C:233:LEU:HB3   | 1:C:251:THR:OG1   | 2.21                     | 0.41              |
| 1:C:2889:ILE:HD12 | 1:C:2993:LEU:HD23 | 2.03                     | 0.41              |
| 1:C:2978:ARG:HG3  | 1:C:2979:GLU:HG3  | 2.03                     | 0.41              |
| 1:C:436:THR:HG22  | 1:C:460:GLY:HA3   | 2.03                     | 0.41              |
| 1:C:936:UNK:HA    | 1:C:939:UNK:CG    | 2.51                     | 0.41              |
| 1:A:2098:UNK:HG2  | 1:A:2099:UNK:N    | 2.36                     | 0.41              |
| 1:A:2212:TRP:O    | 1:A:2229:LYS:HB3  | 2.21                     | 0.41              |
| 1:A:2334:HIS:CD2  | 1:A:2391:LYS:HG3  | 2.50                     | 0.41              |
| 1:A:793:ARG:HH12  | 1:A:2523:GLU:CD   | 2.24                     | 0.41              |
| 1:B:1462:ALA:HB2  | 1:B:1468:TYR:CE1  | 2.56                     | 0.41              |
| 1:B:2919:GLY:O    | 1:B:2921:PRO:HD3  | 2.21                     | 0.41              |
| 1:B:2927:GLN:HE21 | 1:B:2927:GLN:HB3  | 1.70                     | 0.41              |
| 1:B:594:LEU:O     | 1:B:598:TYR:HB2   | 2.21                     | 0.41              |
| 1:C:2483:VAL:HG13 | 1:C:2954:VAL:HG11 | 2.03                     | 0.41              |
| 1:C:278:ARG:HD2   | 1:C:674:TRP:CE3   | 2.56                     | 0.41              |
| 1:C:2989:LEU:HD12 | 1:C:2989:LEU:HA   | 1.77                     | 0.41              |
| 1:C:594:LEU:O     | 1:C:598:TYR:HB2   | 2.21                     | 0.41              |
| 1:C:709:LEU:HD11  | 1:C:872:ARG:CZ    | 2.51                     | 0.41              |
| 1:A:1087:PHE:CD1  | 1:B:198:ILE:HG23  | 2.56                     | 0.40              |
| 1:A:1095:LEU:HD13 | 1:A:1289:PRO:CB   | 2.52                     | 0.40              |
| 1:A:1120:GLU:HA   | 1:A:1125:VAL:CG2  | 2.50                     | 0.40              |
| 1:A:2086:UNK:HA   | 1:A:2089:UNK:CG   | 2.51                     | 0.40              |
| 1:A:2093:UNK:HB2  | 1:A:2129:UNK:HB2  | 2.03                     | 0.40              |
| 1:B:358:ASP:OD2   | 1:B:361:THR:HB    | 2.21                     | 0.40              |
| 1:C:1133:VAL:N    | 1:C:1193:ALA:O    | 2.48                     | 0.40              |
| 1:C:1224:UNK:O    | 1:C:1224:UNK:HG2  | 2.20                     | 0.40              |
| 1:C:180:ALA:O     | 1:C:184:LEU:HG    | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2300:PHE:HZ   | 1:C:2398:LEU:HB3  | 1.85                     | 0.40              |
| 1:C:273:ARG:HD2   | 1:C:282:VAL:CG1   | 2.51                     | 0.40              |
| 1:C:602:ARG:NH2   | 1:C:641:ASP:OD1   | 2.27                     | 0.40              |
| 1:C:984:UNK:HG2   | 1:C:984:UNK:O     | 2.20                     | 0.40              |
| 1:A:1462:ALA:HB2  | 1:A:1468:TYR:CE1  | 2.56                     | 0.40              |
| 1:A:1604:ASP:N    | 1:A:1604:ASP:OD1  | 2.55                     | 0.40              |
| 1:A:1695:LEU:HA   | 1:A:1695:LEU:HD12 | 1.71                     | 0.40              |
| 1:A:1702:GLU:OE1  | 1:A:1711:VAL:HG22 | 2.22                     | 0.40              |
| 1:A:2010:GLN:OE1  | 1:A:2013:LEU:HD11 | 2.21                     | 0.40              |
| 1:A:2120:UNK:C    | 1:A:2123:UNK:HG3  | 2.50                     | 0.40              |
| 1:A:2405:MET:HA   | 1:A:2405:MET:HE2  | 2.03                     | 0.40              |
| 1:A:2710:LEU:HD12 | 1:A:2713:VAL:HG21 | 2.03                     | 0.40              |
| 1:A:278:ARG:HD2   | 1:A:674:TRP:HE3   | 1.87                     | 0.40              |
| 1:A:709:LEU:HD11  | 1:A:872:ARG:CZ    | 2.51                     | 0.40              |
| 1:B:1237:ARG:HG2  | 1:B:1237:ARG:HH11 | 1.86                     | 0.40              |
| 1:B:133:GLN:O     | 1:B:137:VAL:HG23  | 2.21                     | 0.40              |
| 1:B:1381:ASP:OD1  | 1:B:1391:SER:OG   | 2.22                     | 0.40              |
| 1:B:1533:VAL:N    | 1:B:1543:ALA:O    | 2.52                     | 0.40              |
| 1:B:1604:ASP:OD1  | 1:B:1604:ASP:N    | 2.55                     | 0.40              |
| 1:B:2400:ASP:N    | 1:B:2400:ASP:OD1  | 2.45                     | 0.40              |
| 1:B:2978:ARG:HG3  | 1:B:2979:GLU:HG3  | 2.03                     | 0.40              |
| 1:B:417:LEU:HD21  | 1:B:625:LEU:HD21  | 2.02                     | 0.40              |
| 1:B:756:LEU:HD13  | 1:B:859:PHE:CD2   | 2.55                     | 0.40              |
| 1:B:999:UNK:HG2   | 1:B:1007:UNK:HG3  | 1.96                     | 0.40              |
| 1:C:1215:UNK:CG   | 1:C:1216:UNK:N    | 2.84                     | 0.40              |
| 1:C:133:GLN:O     | 1:C:137:VAL:HG23  | 2.21                     | 0.40              |
| 1:C:1400:PRO:O    | 1:C:1415:GLY:HA2  | 2.21                     | 0.40              |
| 1:B:1087:PHE:CD1  | 1:C:198:ILE:HG23  | 2.56                     | 0.40              |
| 1:C:2114:UNK:O    | 1:C:2117:UNK:HG3  | 2.21                     | 0.40              |
| 1:C:2449:UNK:O    | 1:C:2449:UNK:CG   | 2.68                     | 0.40              |
| 1:C:2892:HIS:HA   | 1:C:2942:GLN:HE22 | 1.85                     | 0.40              |
| 1:C:393:VAL:O     | 1:C:395:GLU:N     | 2.52                     | 0.40              |
| 1:C:544:ILE:C     | 1:C:546:HIS:H     | 2.22                     | 0.40              |
| 1:A:2286:ARG:HD3  | 1:A:2331:SER:OG   | 2.20                     | 0.40              |
| 1:A:2346:MET:O    | 1:A:2349:ASN:N    | 2.55                     | 0.40              |
| 1:A:487:PHE:O     | 1:A:521:VAL:N     | 2.51                     | 0.40              |
| 1:A:618:PRO:HB3   | 1:A:915:PHE:HA    | 2.02                     | 0.40              |
| 1:B:1095:LEU:HD13 | 1:B:1289:PRO:CB   | 2.52                     | 0.40              |
| 1:B:1616:PRO:HG2  | 1:B:1619:VAL:HB   | 2.04                     | 0.40              |
| 1:B:2014:SER:H    | 1:C:2591:ARG:NH1  | 2.19                     | 0.40              |
| 1:B:2114:UNK:O    | 1:B:2117:UNK:HG3  | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2093:UNK:HB2  | 1:B:2129:UNK:HB2  | 2.03                     | 0.40              |
| 1:B:2672:TRP:CZ3  | 1:B:2830:LYS:HG2  | 2.56                     | 0.40              |
| 1:B:984:UNK:HG2   | 1:B:984:UNK:O     | 2.20                     | 0.40              |
| 1:A:198:ILE:HG23  | 1:C:1087:PHE:CD1  | 2.56                     | 0.40              |
| 1:C:1237:ARG:HH11 | 1:C:1237:ARG:HG2  | 1.86                     | 0.40              |
| 1:C:2141:VAL:HG22 | 1:C:2238:PHE:CD2  | 2.56                     | 0.40              |
| 1:C:2405:MET:O    | 1:C:2409:ALA:HB3  | 2.21                     | 0.40              |
| 1:C:793:ARG:HH12  | 1:C:2523:GLU:CD   | 2.24                     | 0.40              |
| 1:C:2574:GLU:HG3  | 1:C:2599:TRP:CE2  | 2.57                     | 0.40              |
| 1:C:2672:TRP:CZ3  | 1:C:2830:LYS:HG2  | 2.56                     | 0.40              |
| 1:C:2770:LEU:CB   | 1:C:2815:GLN:HB3  | 2.51                     | 0.40              |
| 1:C:745:THR:HG22  | 1:C:747:LEU:N     | 2.37                     | 0.40              |
| 1:C:799:PHE:CZ    | 1:C:2433:UNK:CG   | 2.99                     | 0.40              |
| 1:C:794:LEU:HD12  | 1:C:830:TYR:HB3   | 2.04                     | 0.40              |
| 1:C:976:UNK:O     | 1:C:976:UNK:CG    | 2.68                     | 0.40              |
| 1:C:995:UNK:HB1   | 1:C:1011:UNK:HG2  | 1.99                     | 0.40              |
| 1:A:1706:LYS:HA   | 1:A:1735:GLU:HG3  | 2.03                     | 0.40              |
| 1:A:180:ALA:O     | 1:A:184:LEU:HG    | 2.21                     | 0.40              |
| 1:A:2611:VAL:HA   | 1:A:2612:PRO:HD3  | 1.86                     | 0.40              |
| 1:A:2618:SER:HB3  | 1:A:2786:ASP:OD1  | 2.21                     | 0.40              |
| 1:A:2672:TRP:CZ3  | 1:A:2830:LYS:HG2  | 2.56                     | 0.40              |
| 1:A:417:LEU:HD21  | 1:A:625:LEU:HD21  | 2.02                     | 0.40              |
| 1:A:745:THR:HG22  | 1:A:747:LEU:N     | 2.37                     | 0.40              |
| 1:B:1002:UNK:CG   | 1:B:1005:UNK:HB2  | 2.51                     | 0.40              |
| 1:B:1087:PHE:HZ   | 1:C:203:ASP:OD2   | 2.05                     | 0.40              |
| 1:B:142:ARG:HD3   | 1:B:142:ARG:HA    | 1.91                     | 0.40              |
| 1:B:1380:ALA:HB1  | 1:B:1474:LEU:CD1  | 2.50                     | 0.40              |
| 1:B:1353:PRO:HB2  | 1:B:1707:SER:HB2  | 2.04                     | 0.40              |
| 1:B:2907:HIS:HA   | 1:B:2910:ILE:HG12 | 2.04                     | 0.40              |
| 1:B:336:TRP:HE1   | 1:B:364:THR:HG22  | 1.86                     | 0.40              |
| 1:B:544:ILE:C     | 1:B:546:HIS:H     | 2.22                     | 0.40              |
| 1:B:587:TRP:CZ2   | 1:B:694:ASP:OD2   | 2.74                     | 0.40              |
| 1:C:1095:LEU:HD12 | 1:C:1096:THR:N    | 2.35                     | 0.40              |
| 1:C:1535:PHE:O    | 1:C:1679:TRP:N    | 2.48                     | 0.40              |
| 1:C:1616:PRO:HG2  | 1:C:1619:VAL:HB   | 2.04                     | 0.40              |
| 1:C:1619:VAL:HA   | 1:C:1620:PRO:HD2  | 1.80                     | 0.40              |
| 1:C:2093:UNK:HB2  | 1:C:2129:UNK:HB2  | 2.03                     | 0.40              |
| 1:A:1013:UNK:CG   | 1:A:1014:UNK:N    | 2.58                     | 0.40              |
| 1:A:1629:PHE:O    | 1:A:1633:ILE:HG13 | 2.22                     | 0.40              |
| 1:A:2114:UNK:O    | 1:A:2117:UNK:HG3  | 2.22                     | 0.40              |
| 1:A:2205:ASP:O    | 1:A:2209:LEU:HB2  | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2405:MET:O    | 1:A:2409:ALA:HB3  | 2.21                     | 0.40              |
| 1:A:2503:LYS:HG3  | 1:A:2513:TYR:HB2  | 2.02                     | 0.40              |
| 1:A:2836:LEU:HD23 | 1:A:2836:LEU:HA   | 1.87                     | 0.40              |
| 1:A:358:ASP:OD2   | 1:A:361:THR:HB    | 2.21                     | 0.40              |
| 1:A:374:GLY:C     | 1:A:375:ILE:HG13  | 2.41                     | 0.40              |
| 1:A:544:ILE:C     | 1:A:546:HIS:H     | 2.22                     | 0.40              |
| 1:B:1099:PRO:HB2  | 1:B:1295:TRP:HE1  | 1.86                     | 0.40              |
| 1:B:2346:MET:O    | 1:B:2349:ASN:N    | 2.55                     | 0.40              |
| 1:B:2492:VAL:HG12 | 1:B:2526:ILE:HG22 | 2.02                     | 0.40              |
| 1:B:2557:LEU:HD23 | 1:B:2558:LEU:N    | 2.37                     | 0.40              |
| 1:B:2611:VAL:HA   | 1:B:2612:PRO:HD3  | 1.86                     | 0.40              |
| 1:B:273:ARG:HD2   | 1:B:282:VAL:CG1   | 2.51                     | 0.40              |
| 1:B:541:GLU:HG3   | 1:B:542:VAL:N     | 2.37                     | 0.40              |
| 1:B:585:HIS:HB3   | 1:B:694:ASP:HB2   | 2.03                     | 0.40              |
| 1:B:985:UNK:O     | 1:B:988:UNK:HG3   | 2.21                     | 0.40              |
| 1:C:2930:LEU:HD23 | 1:C:2930:LEU:HA   | 1.93                     | 0.40              |
| 1:C:408:VAL:HG23  | 1:C:418:GLU:HB2   | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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     | 2637/3089 (85%)   | 2489 (94%)  | 140 (5%) | 8 (0%)   | 43          | 81 |
| 1   | B     | 2637/3089 (85%)   | 2489 (94%)  | 140 (5%) | 8 (0%)   | 43          | 81 |
| 1   | C     | 2637/3089 (85%)   | 2489 (94%)  | 139 (5%) | 9 (0%)   | 43          | 81 |
| 1   | D     | 2637/3089 (85%)   | 2488 (94%)  | 140 (5%) | 9 (0%)   | 43          | 81 |
| 1   | E     | 2637/3089 (85%)   | 2488 (94%)  | 141 (5%) | 8 (0%)   | 43          | 81 |
| 1   | F     | 2637/3089 (85%)   | 2488 (94%)  | 140 (5%) | 9 (0%)   | 43          | 81 |
| All | All   | 15822/18534 (85%) | 14931 (94%) | 840 (5%) | 51 (0%)  | 47          | 81 |

All (51) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 1148 | GLU  |
| 1   | E     | 1148 | GLU  |
| 1   | F     | 1148 | GLU  |
| 1   | A     | 1148 | GLU  |
| 1   | B     | 1148 | GLU  |
| 1   | C     | 1148 | GLU  |
| 1   | D     | 1724 | TYR  |
| 1   | E     | 1724 | TYR  |
| 1   | F     | 1724 | TYR  |
| 1   | A     | 1724 | TYR  |
| 1   | B     | 1724 | TYR  |
| 1   | C     | 1724 | TYR  |
| 1   | D     | 149  | ALA  |
| 1   | D     | 1652 | TRP  |
| 1   | D     | 1705 | VAL  |
| 1   | E     | 149  | ALA  |
| 1   | E     | 1652 | TRP  |
| 1   | E     | 1705 | VAL  |
| 1   | F     | 149  | ALA  |
| 1   | F     | 1652 | TRP  |
| 1   | F     | 1705 | VAL  |
| 1   | A     | 149  | ALA  |
| 1   | A     | 1652 | TRP  |
| 1   | A     | 1705 | VAL  |
| 1   | B     | 149  | ALA  |
| 1   | B     | 1652 | TRP  |
| 1   | B     | 1705 | VAL  |
| 1   | C     | 149  | ALA  |
| 1   | C     | 1652 | TRP  |
| 1   | C     | 1705 | VAL  |
| 1   | D     | 89   | GLU  |
| 1   | E     | 89   | GLU  |
| 1   | F     | 89   | GLU  |
| 1   | A     | 89   | GLU  |
| 1   | B     | 89   | GLU  |
| 1   | C     | 89   | GLU  |
| 1   | D     | 1068 | VAL  |
| 1   | D     | 1285 | LYS  |
| 1   | E     | 1068 | VAL  |
| 1   | E     | 1285 | LYS  |
| 1   | F     | 1068 | VAL  |
| 1   | F     | 1285 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1068 | VAL  |
| 1   | A     | 1285 | LYS  |
| 1   | B     | 1068 | VAL  |
| 1   | B     | 1285 | LYS  |
| 1   | C     | 1068 | VAL  |
| 1   | C     | 1285 | LYS  |
| 1   | D     | 2585 | PRO  |
| 1   | F     | 2585 | PRO  |
| 1   | C     | 2585 | 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 PDB entries followed by that with respect to all EM entries.

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     | 2076/2264 (92%)   | 1987 (96%)  | 89 (4%)  | 32          | 61 |
| 1   | B     | 2076/2264 (92%)   | 1986 (96%)  | 90 (4%)  | 32          | 61 |
| 1   | C     | 2076/2264 (92%)   | 1987 (96%)  | 89 (4%)  | 32          | 61 |
| 1   | D     | 2076/2264 (92%)   | 1987 (96%)  | 89 (4%)  | 32          | 61 |
| 1   | E     | 2076/2264 (92%)   | 1987 (96%)  | 89 (4%)  | 32          | 61 |
| 1   | F     | 2076/2264 (92%)   | 1987 (96%)  | 89 (4%)  | 32          | 61 |
| All | All   | 12456/13584 (92%) | 11921 (96%) | 535 (4%) | 36          | 61 |

All (535) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 90  | LEU  |
| 1   | D     | 208 | VAL  |
| 1   | D     | 209 | SER  |
| 1   | D     | 232 | VAL  |
| 1   | D     | 233 | LEU  |
| 1   | D     | 248 | ILE  |
| 1   | D     | 251 | THR  |
| 1   | D     | 342 | GLU  |
| 1   | D     | 344 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 358  | ASP  |
| 1   | D     | 361  | THR  |
| 1   | D     | 389  | THR  |
| 1   | D     | 390  | VAL  |
| 1   | D     | 400  | TRP  |
| 1   | D     | 409  | LYS  |
| 1   | D     | 424  | LEU  |
| 1   | D     | 427  | ARG  |
| 1   | D     | 439  | THR  |
| 1   | D     | 456  | GLU  |
| 1   | D     | 517  | ILE  |
| 1   | D     | 544  | ILE  |
| 1   | D     | 580  | ARG  |
| 1   | D     | 584  | HIS  |
| 1   | D     | 595  | LEU  |
| 1   | D     | 606  | ASN  |
| 1   | D     | 621  | SER  |
| 1   | D     | 638  | MET  |
| 1   | D     | 644  | LEU  |
| 1   | D     | 654  | GLU  |
| 1   | D     | 694  | ASP  |
| 1   | D     | 696  | HIS  |
| 1   | D     | 699  | ASP  |
| 1   | D     | 791  | GLU  |
| 1   | D     | 857  | VAL  |
| 1   | D     | 1021 | LEU  |
| 1   | D     | 1096 | THR  |
| 1   | D     | 1105 | ARG  |
| 1   | D     | 1127 | GLU  |
| 1   | D     | 1162 | THR  |
| 1   | D     | 1253 | ARG  |
| 1   | D     | 1358 | GLN  |
| 1   | D     | 1421 | GLN  |
| 1   | D     | 1468 | TYR  |
| 1   | D     | 1471 | GLU  |
| 1   | D     | 1488 | VAL  |
| 1   | D     | 1508 | ILE  |
| 1   | D     | 1544 | ILE  |
| 1   | D     | 1551 | LEU  |
| 1   | D     | 1564 | ILE  |
| 1   | D     | 1618 | LEU  |
| 1   | D     | 1651 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 1662 | ARG  |
| 1   | D     | 1672 | GLN  |
| 1   | D     | 1673 | PHE  |
| 1   | D     | 1745 | ASP  |
| 1   | D     | 2059 | ARG  |
| 1   | D     | 2067 | LEU  |
| 1   | D     | 2070 | LEU  |
| 1   | D     | 2192 | THR  |
| 1   | D     | 2196 | VAL  |
| 1   | D     | 2209 | LEU  |
| 1   | D     | 2294 | SER  |
| 1   | D     | 2297 | ARG  |
| 1   | D     | 2299 | MET  |
| 1   | D     | 2303 | ASP  |
| 1   | D     | 2306 | TYR  |
| 1   | D     | 2395 | THR  |
| 1   | D     | 2401 | ILE  |
| 1   | D     | 2620 | THR  |
| 1   | D     | 2692 | MET  |
| 1   | D     | 2742 | THR  |
| 1   | D     | 2784 | THR  |
| 1   | D     | 2800 | PHE  |
| 1   | D     | 2802 | ARG  |
| 1   | D     | 2809 | LEU  |
| 1   | D     | 2827 | LEU  |
| 1   | D     | 2861 | LEU  |
| 1   | D     | 2871 | THR  |
| 1   | D     | 2879 | LEU  |
| 1   | D     | 2894 | THR  |
| 1   | D     | 2916 | ARG  |
| 1   | D     | 2930 | LEU  |
| 1   | D     | 2935 | LYS  |
| 1   | D     | 2962 | ASP  |
| 1   | D     | 3001 | HIS  |
| 1   | D     | 3019 | ASP  |
| 1   | D     | 3076 | SER  |
| 1   | D     | 3077 | THR  |
| 1   | D     | 3080 | ARG  |
| 1   | E     | 90   | LEU  |
| 1   | E     | 208  | VAL  |
| 1   | E     | 209  | SER  |
| 1   | E     | 232  | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 233  | LEU  |
| 1   | E     | 248  | ILE  |
| 1   | E     | 251  | THR  |
| 1   | E     | 342  | GLU  |
| 1   | E     | 344  | HIS  |
| 1   | E     | 358  | ASP  |
| 1   | E     | 361  | THR  |
| 1   | E     | 389  | THR  |
| 1   | E     | 390  | VAL  |
| 1   | E     | 400  | TRP  |
| 1   | E     | 409  | LYS  |
| 1   | E     | 424  | LEU  |
| 1   | E     | 427  | ARG  |
| 1   | E     | 439  | THR  |
| 1   | E     | 456  | GLU  |
| 1   | E     | 517  | ILE  |
| 1   | E     | 544  | ILE  |
| 1   | E     | 580  | ARG  |
| 1   | E     | 584  | HIS  |
| 1   | E     | 595  | LEU  |
| 1   | E     | 606  | ASN  |
| 1   | E     | 621  | SER  |
| 1   | E     | 638  | MET  |
| 1   | E     | 644  | LEU  |
| 1   | E     | 654  | GLU  |
| 1   | E     | 694  | ASP  |
| 1   | E     | 696  | HIS  |
| 1   | E     | 699  | ASP  |
| 1   | E     | 791  | GLU  |
| 1   | E     | 857  | VAL  |
| 1   | E     | 1021 | LEU  |
| 1   | E     | 1096 | THR  |
| 1   | E     | 1105 | ARG  |
| 1   | E     | 1127 | GLU  |
| 1   | E     | 1162 | THR  |
| 1   | E     | 1253 | ARG  |
| 1   | E     | 1358 | GLN  |
| 1   | E     | 1421 | GLN  |
| 1   | E     | 1468 | TYR  |
| 1   | E     | 1471 | GLU  |
| 1   | E     | 1488 | VAL  |
| 1   | E     | 1508 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 1544 | ILE  |
| 1   | E     | 1551 | LEU  |
| 1   | E     | 1564 | ILE  |
| 1   | E     | 1618 | LEU  |
| 1   | E     | 1651 | THR  |
| 1   | E     | 1662 | ARG  |
| 1   | E     | 1672 | GLN  |
| 1   | E     | 1673 | PHE  |
| 1   | E     | 1745 | ASP  |
| 1   | E     | 2059 | ARG  |
| 1   | E     | 2067 | LEU  |
| 1   | E     | 2070 | LEU  |
| 1   | E     | 2192 | THR  |
| 1   | E     | 2196 | VAL  |
| 1   | E     | 2209 | LEU  |
| 1   | E     | 2294 | SER  |
| 1   | E     | 2297 | ARG  |
| 1   | E     | 2299 | MET  |
| 1   | E     | 2303 | ASP  |
| 1   | E     | 2306 | TYR  |
| 1   | E     | 2395 | THR  |
| 1   | E     | 2401 | ILE  |
| 1   | E     | 2620 | THR  |
| 1   | E     | 2692 | MET  |
| 1   | E     | 2742 | THR  |
| 1   | E     | 2784 | THR  |
| 1   | E     | 2800 | PHE  |
| 1   | E     | 2802 | ARG  |
| 1   | E     | 2809 | LEU  |
| 1   | E     | 2827 | LEU  |
| 1   | E     | 2861 | LEU  |
| 1   | E     | 2871 | THR  |
| 1   | E     | 2879 | LEU  |
| 1   | E     | 2894 | THR  |
| 1   | E     | 2916 | ARG  |
| 1   | E     | 2930 | LEU  |
| 1   | E     | 2935 | LYS  |
| 1   | E     | 2962 | ASP  |
| 1   | E     | 3001 | HIS  |
| 1   | E     | 3019 | ASP  |
| 1   | E     | 3076 | SER  |
| 1   | E     | 3077 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 3080 | ARG  |
| 1   | F     | 90   | LEU  |
| 1   | F     | 208  | VAL  |
| 1   | F     | 209  | SER  |
| 1   | F     | 232  | VAL  |
| 1   | F     | 233  | LEU  |
| 1   | F     | 248  | ILE  |
| 1   | F     | 251  | THR  |
| 1   | F     | 342  | GLU  |
| 1   | F     | 344  | HIS  |
| 1   | F     | 358  | ASP  |
| 1   | F     | 361  | THR  |
| 1   | F     | 389  | THR  |
| 1   | F     | 390  | VAL  |
| 1   | F     | 400  | TRP  |
| 1   | F     | 409  | LYS  |
| 1   | F     | 424  | LEU  |
| 1   | F     | 427  | ARG  |
| 1   | F     | 439  | THR  |
| 1   | F     | 456  | GLU  |
| 1   | F     | 517  | ILE  |
| 1   | F     | 544  | ILE  |
| 1   | F     | 580  | ARG  |
| 1   | F     | 584  | HIS  |
| 1   | F     | 595  | LEU  |
| 1   | F     | 606  | ASN  |
| 1   | F     | 621  | SER  |
| 1   | F     | 638  | MET  |
| 1   | F     | 644  | LEU  |
| 1   | F     | 654  | GLU  |
| 1   | F     | 694  | ASP  |
| 1   | F     | 696  | HIS  |
| 1   | F     | 699  | ASP  |
| 1   | F     | 791  | GLU  |
| 1   | F     | 857  | VAL  |
| 1   | F     | 1021 | LEU  |
| 1   | F     | 1096 | THR  |
| 1   | F     | 1105 | ARG  |
| 1   | F     | 1127 | GLU  |
| 1   | F     | 1162 | THR  |
| 1   | F     | 1253 | ARG  |
| 1   | F     | 1358 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 1421 | GLN  |
| 1   | F     | 1468 | TYR  |
| 1   | F     | 1471 | GLU  |
| 1   | F     | 1488 | VAL  |
| 1   | F     | 1508 | ILE  |
| 1   | F     | 1544 | ILE  |
| 1   | F     | 1551 | LEU  |
| 1   | F     | 1564 | ILE  |
| 1   | F     | 1618 | LEU  |
| 1   | F     | 1651 | THR  |
| 1   | F     | 1662 | ARG  |
| 1   | F     | 1672 | GLN  |
| 1   | F     | 1673 | PHE  |
| 1   | F     | 1745 | ASP  |
| 1   | F     | 2059 | ARG  |
| 1   | F     | 2067 | LEU  |
| 1   | F     | 2070 | LEU  |
| 1   | F     | 2192 | THR  |
| 1   | F     | 2196 | VAL  |
| 1   | F     | 2209 | LEU  |
| 1   | F     | 2294 | SER  |
| 1   | F     | 2297 | ARG  |
| 1   | F     | 2299 | MET  |
| 1   | F     | 2303 | ASP  |
| 1   | F     | 2306 | TYR  |
| 1   | F     | 2395 | THR  |
| 1   | F     | 2401 | ILE  |
| 1   | F     | 2620 | THR  |
| 1   | F     | 2692 | MET  |
| 1   | F     | 2742 | THR  |
| 1   | F     | 2784 | THR  |
| 1   | F     | 2800 | PHE  |
| 1   | F     | 2802 | ARG  |
| 1   | F     | 2809 | LEU  |
| 1   | F     | 2827 | LEU  |
| 1   | F     | 2861 | LEU  |
| 1   | F     | 2871 | THR  |
| 1   | F     | 2879 | LEU  |
| 1   | F     | 2894 | THR  |
| 1   | F     | 2916 | ARG  |
| 1   | F     | 2930 | LEU  |
| 1   | F     | 2935 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 2962 | ASP  |
| 1   | F     | 3001 | HIS  |
| 1   | F     | 3019 | ASP  |
| 1   | F     | 3076 | SER  |
| 1   | F     | 3077 | THR  |
| 1   | F     | 3080 | ARG  |
| 1   | A     | 90   | LEU  |
| 1   | A     | 208  | VAL  |
| 1   | A     | 209  | SER  |
| 1   | A     | 232  | VAL  |
| 1   | A     | 233  | LEU  |
| 1   | A     | 248  | ILE  |
| 1   | A     | 251  | THR  |
| 1   | A     | 342  | GLU  |
| 1   | A     | 344  | HIS  |
| 1   | A     | 358  | ASP  |
| 1   | A     | 361  | THR  |
| 1   | A     | 389  | THR  |
| 1   | A     | 390  | VAL  |
| 1   | A     | 400  | TRP  |
| 1   | A     | 409  | LYS  |
| 1   | A     | 424  | LEU  |
| 1   | A     | 427  | ARG  |
| 1   | A     | 439  | THR  |
| 1   | A     | 456  | GLU  |
| 1   | A     | 517  | ILE  |
| 1   | A     | 544  | ILE  |
| 1   | A     | 580  | ARG  |
| 1   | A     | 584  | HIS  |
| 1   | A     | 595  | LEU  |
| 1   | A     | 606  | ASN  |
| 1   | A     | 621  | SER  |
| 1   | A     | 638  | MET  |
| 1   | A     | 644  | LEU  |
| 1   | A     | 654  | GLU  |
| 1   | A     | 694  | ASP  |
| 1   | A     | 696  | HIS  |
| 1   | A     | 699  | ASP  |
| 1   | A     | 791  | GLU  |
| 1   | A     | 857  | VAL  |
| 1   | A     | 1021 | LEU  |
| 1   | A     | 1096 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1105 | ARG  |
| 1   | A     | 1127 | GLU  |
| 1   | A     | 1162 | THR  |
| 1   | A     | 1253 | ARG  |
| 1   | A     | 1358 | GLN  |
| 1   | A     | 1421 | GLN  |
| 1   | A     | 1468 | TYR  |
| 1   | A     | 1471 | GLU  |
| 1   | A     | 1488 | VAL  |
| 1   | A     | 1508 | ILE  |
| 1   | A     | 1544 | ILE  |
| 1   | A     | 1551 | LEU  |
| 1   | A     | 1564 | ILE  |
| 1   | A     | 1618 | LEU  |
| 1   | A     | 1651 | THR  |
| 1   | A     | 1662 | ARG  |
| 1   | A     | 1672 | GLN  |
| 1   | A     | 1673 | PHE  |
| 1   | A     | 1745 | ASP  |
| 1   | A     | 2059 | ARG  |
| 1   | A     | 2067 | LEU  |
| 1   | A     | 2070 | LEU  |
| 1   | A     | 2192 | THR  |
| 1   | A     | 2196 | VAL  |
| 1   | A     | 2209 | LEU  |
| 1   | A     | 2294 | SER  |
| 1   | A     | 2297 | ARG  |
| 1   | A     | 2299 | MET  |
| 1   | A     | 2303 | ASP  |
| 1   | A     | 2306 | TYR  |
| 1   | A     | 2395 | THR  |
| 1   | A     | 2401 | ILE  |
| 1   | A     | 2620 | THR  |
| 1   | A     | 2692 | MET  |
| 1   | A     | 2742 | THR  |
| 1   | A     | 2784 | THR  |
| 1   | A     | 2800 | PHE  |
| 1   | A     | 2802 | ARG  |
| 1   | A     | 2809 | LEU  |
| 1   | A     | 2827 | LEU  |
| 1   | A     | 2861 | LEU  |
| 1   | A     | 2871 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2879 | LEU  |
| 1   | A     | 2894 | THR  |
| 1   | A     | 2916 | ARG  |
| 1   | A     | 2930 | LEU  |
| 1   | A     | 2935 | LYS  |
| 1   | A     | 2962 | ASP  |
| 1   | A     | 3001 | HIS  |
| 1   | A     | 3019 | ASP  |
| 1   | A     | 3076 | SER  |
| 1   | A     | 3077 | THR  |
| 1   | A     | 3080 | ARG  |
| 1   | B     | 90   | LEU  |
| 1   | B     | 208  | VAL  |
| 1   | B     | 209  | SER  |
| 1   | B     | 232  | VAL  |
| 1   | B     | 233  | LEU  |
| 1   | B     | 248  | ILE  |
| 1   | B     | 251  | THR  |
| 1   | B     | 342  | GLU  |
| 1   | B     | 344  | HIS  |
| 1   | B     | 358  | ASP  |
| 1   | B     | 361  | THR  |
| 1   | B     | 389  | THR  |
| 1   | B     | 390  | VAL  |
| 1   | B     | 400  | TRP  |
| 1   | B     | 409  | LYS  |
| 1   | B     | 424  | LEU  |
| 1   | B     | 427  | ARG  |
| 1   | B     | 439  | THR  |
| 1   | B     | 456  | GLU  |
| 1   | B     | 517  | ILE  |
| 1   | B     | 544  | ILE  |
| 1   | B     | 580  | ARG  |
| 1   | B     | 584  | HIS  |
| 1   | B     | 595  | LEU  |
| 1   | B     | 606  | ASN  |
| 1   | B     | 621  | SER  |
| 1   | B     | 638  | MET  |
| 1   | B     | 644  | LEU  |
| 1   | B     | 654  | GLU  |
| 1   | B     | 694  | ASP  |
| 1   | B     | 696  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 699  | ASP  |
| 1   | B     | 791  | GLU  |
| 1   | B     | 857  | VAL  |
| 1   | B     | 1021 | LEU  |
| 1   | B     | 1096 | THR  |
| 1   | B     | 1105 | ARG  |
| 1   | B     | 1127 | GLU  |
| 1   | B     | 1162 | THR  |
| 1   | B     | 1253 | ARG  |
| 1   | B     | 1358 | GLN  |
| 1   | B     | 1401 | THR  |
| 1   | B     | 1421 | GLN  |
| 1   | B     | 1468 | TYR  |
| 1   | B     | 1471 | GLU  |
| 1   | B     | 1488 | VAL  |
| 1   | B     | 1508 | ILE  |
| 1   | B     | 1544 | ILE  |
| 1   | B     | 1551 | LEU  |
| 1   | B     | 1564 | ILE  |
| 1   | B     | 1618 | LEU  |
| 1   | B     | 1651 | THR  |
| 1   | B     | 1662 | ARG  |
| 1   | B     | 1672 | GLN  |
| 1   | B     | 1673 | PHE  |
| 1   | B     | 1745 | ASP  |
| 1   | B     | 2059 | ARG  |
| 1   | B     | 2067 | LEU  |
| 1   | B     | 2070 | LEU  |
| 1   | B     | 2192 | THR  |
| 1   | B     | 2196 | VAL  |
| 1   | B     | 2209 | LEU  |
| 1   | B     | 2294 | SER  |
| 1   | B     | 2297 | ARG  |
| 1   | B     | 2299 | MET  |
| 1   | B     | 2303 | ASP  |
| 1   | B     | 2306 | TYR  |
| 1   | B     | 2395 | THR  |
| 1   | B     | 2401 | ILE  |
| 1   | B     | 2620 | THR  |
| 1   | B     | 2692 | MET  |
| 1   | B     | 2742 | THR  |
| 1   | B     | 2784 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 2800 | PHE  |
| 1   | B     | 2802 | ARG  |
| 1   | B     | 2809 | LEU  |
| 1   | B     | 2827 | LEU  |
| 1   | B     | 2861 | LEU  |
| 1   | B     | 2871 | THR  |
| 1   | B     | 2879 | LEU  |
| 1   | B     | 2894 | THR  |
| 1   | B     | 2916 | ARG  |
| 1   | B     | 2930 | LEU  |
| 1   | B     | 2935 | LYS  |
| 1   | B     | 2962 | ASP  |
| 1   | B     | 3001 | HIS  |
| 1   | B     | 3019 | ASP  |
| 1   | B     | 3076 | SER  |
| 1   | B     | 3077 | THR  |
| 1   | B     | 3080 | ARG  |
| 1   | C     | 90   | LEU  |
| 1   | C     | 208  | VAL  |
| 1   | C     | 209  | SER  |
| 1   | C     | 232  | VAL  |
| 1   | C     | 233  | LEU  |
| 1   | C     | 248  | ILE  |
| 1   | C     | 251  | THR  |
| 1   | C     | 342  | GLU  |
| 1   | C     | 344  | HIS  |
| 1   | C     | 358  | ASP  |
| 1   | C     | 361  | THR  |
| 1   | C     | 389  | THR  |
| 1   | C     | 390  | VAL  |
| 1   | C     | 400  | TRP  |
| 1   | C     | 409  | LYS  |
| 1   | C     | 424  | LEU  |
| 1   | C     | 427  | ARG  |
| 1   | C     | 439  | THR  |
| 1   | C     | 456  | GLU  |
| 1   | C     | 517  | ILE  |
| 1   | C     | 544  | ILE  |
| 1   | C     | 580  | ARG  |
| 1   | C     | 584  | HIS  |
| 1   | C     | 595  | LEU  |
| 1   | C     | 606  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 621  | SER  |
| 1   | C     | 638  | MET  |
| 1   | C     | 644  | LEU  |
| 1   | C     | 654  | GLU  |
| 1   | C     | 694  | ASP  |
| 1   | C     | 696  | HIS  |
| 1   | C     | 699  | ASP  |
| 1   | C     | 791  | GLU  |
| 1   | C     | 857  | VAL  |
| 1   | C     | 1021 | LEU  |
| 1   | C     | 1096 | THR  |
| 1   | C     | 1105 | ARG  |
| 1   | C     | 1127 | GLU  |
| 1   | C     | 1162 | THR  |
| 1   | C     | 1253 | ARG  |
| 1   | C     | 1358 | GLN  |
| 1   | C     | 1421 | GLN  |
| 1   | C     | 1468 | TYR  |
| 1   | C     | 1471 | GLU  |
| 1   | C     | 1488 | VAL  |
| 1   | C     | 1508 | ILE  |
| 1   | C     | 1544 | ILE  |
| 1   | C     | 1551 | LEU  |
| 1   | C     | 1564 | ILE  |
| 1   | C     | 1618 | LEU  |
| 1   | C     | 1651 | THR  |
| 1   | C     | 1662 | ARG  |
| 1   | C     | 1672 | GLN  |
| 1   | C     | 1673 | PHE  |
| 1   | C     | 1745 | ASP  |
| 1   | C     | 2059 | ARG  |
| 1   | C     | 2067 | LEU  |
| 1   | C     | 2070 | LEU  |
| 1   | C     | 2192 | THR  |
| 1   | C     | 2196 | VAL  |
| 1   | C     | 2209 | LEU  |
| 1   | C     | 2294 | SER  |
| 1   | C     | 2297 | ARG  |
| 1   | C     | 2299 | MET  |
| 1   | C     | 2303 | ASP  |
| 1   | C     | 2306 | TYR  |
| 1   | C     | 2395 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 2401 | ILE  |
| 1   | C     | 2620 | THR  |
| 1   | C     | 2692 | MET  |
| 1   | C     | 2742 | THR  |
| 1   | C     | 2784 | THR  |
| 1   | C     | 2800 | PHE  |
| 1   | C     | 2802 | ARG  |
| 1   | C     | 2809 | LEU  |
| 1   | C     | 2827 | LEU  |
| 1   | C     | 2861 | LEU  |
| 1   | C     | 2871 | THR  |
| 1   | C     | 2879 | LEU  |
| 1   | C     | 2894 | THR  |
| 1   | C     | 2916 | ARG  |
| 1   | C     | 2930 | LEU  |
| 1   | C     | 2935 | LYS  |
| 1   | C     | 2962 | ASP  |
| 1   | C     | 3001 | HIS  |
| 1   | C     | 3019 | ASP  |
| 1   | C     | 3076 | SER  |
| 1   | C     | 3077 | THR  |
| 1   | C     | 3080 | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 386  | ASN  |
| 1   | A     | 486  | GLN  |
| 1   | A     | 540  | ASN  |
| 1   | A     | 585  | HIS  |
| 1   | A     | 606  | ASN  |
| 1   | A     | 1057 | ASN  |
| 1   | A     | 1134 | HIS  |
| 1   | A     | 1276 | GLN  |
| 1   | A     | 1277 | HIS  |
| 1   | A     | 1355 | GLN  |
| 1   | A     | 1582 | HIS  |
| 1   | A     | 1617 | ASN  |
| 1   | A     | 1672 | GLN  |
| 1   | A     | 2288 | HIS  |
| 1   | A     | 2334 | HIS  |
| 1   | A     | 2349 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2651 | ASN  |
| 1   | A     | 2699 | ASN  |
| 1   | A     | 2815 | GLN  |
| 1   | A     | 2850 | HIS  |
| 1   | A     | 2927 | GLN  |
| 1   | A     | 2942 | GLN  |
| 1   | A     | 2973 | HIS  |
| 1   | B     | 386  | ASN  |
| 1   | B     | 486  | GLN  |
| 1   | B     | 540  | ASN  |
| 1   | B     | 575  | HIS  |
| 1   | B     | 585  | HIS  |
| 1   | B     | 1057 | ASN  |
| 1   | B     | 1134 | HIS  |
| 1   | B     | 1276 | GLN  |
| 1   | B     | 1277 | HIS  |
| 1   | B     | 1355 | GLN  |
| 1   | B     | 1582 | HIS  |
| 1   | B     | 1617 | ASN  |
| 1   | B     | 1672 | GLN  |
| 1   | B     | 2288 | HIS  |
| 1   | B     | 2296 | ASN  |
| 1   | B     | 2334 | HIS  |
| 1   | B     | 2349 | ASN  |
| 1   | B     | 2651 | ASN  |
| 1   | B     | 2699 | ASN  |
| 1   | B     | 2815 | GLN  |
| 1   | B     | 2850 | HIS  |
| 1   | B     | 2927 | GLN  |
| 1   | B     | 2942 | GLN  |
| 1   | B     | 2973 | HIS  |
| 1   | C     | 386  | ASN  |
| 1   | C     | 486  | GLN  |
| 1   | C     | 540  | ASN  |
| 1   | C     | 575  | HIS  |
| 1   | C     | 585  | HIS  |
| 1   | C     | 1057 | ASN  |
| 1   | C     | 1134 | HIS  |
| 1   | C     | 1276 | GLN  |
| 1   | C     | 1277 | HIS  |
| 1   | C     | 1355 | GLN  |
| 1   | C     | 1582 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1617 | ASN  |
| 1   | C     | 1672 | GLN  |
| 1   | C     | 2288 | HIS  |
| 1   | C     | 2296 | ASN  |
| 1   | C     | 2334 | HIS  |
| 1   | C     | 2349 | ASN  |
| 1   | C     | 2651 | ASN  |
| 1   | C     | 2699 | ASN  |
| 1   | C     | 2815 | GLN  |
| 1   | C     | 2850 | HIS  |
| 1   | C     | 2927 | GLN  |
| 1   | C     | 2942 | GLN  |
| 1   | C     | 2973 | HIS  |

### 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](#)

6 ligands are modelled in this entry.

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 | $\# Z  > 2$ |
| 2   | FMN  | A     | 4000 | -    | 31,33,33     | 1.35 | 4 (12%)     | 40,50,50    | 1.58 | 7 (17%)     |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | FMN  | B     | 4000 | -    | 31,33,33     | 1.36 | 4 (12%)  | 40,50,50    | 1.57 | 7 (17%)  |
| 2   | FMN  | C     | 4000 | -    | 31,33,33     | 1.36 | 4 (12%)  | 40,50,50    | 1.56 | 7 (17%)  |
| 2   | FMN  | D     | 4000 | -    | 31,33,33     | 1.36 | 4 (12%)  | 40,50,50    | 1.57 | 7 (17%)  |
| 2   | FMN  | E     | 4000 | -    | 31,33,33     | 1.36 | 4 (12%)  | 40,50,50    | 1.57 | 7 (17%)  |
| 2   | FMN  | F     | 4000 | -    | 31,33,33     | 1.35 | 4 (12%)  | 40,50,50    | 1.56 | 7 (17%)  |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | FMN  | A     | 4000 | -    | -       | 5/18/18/18 | 0/3/3/3 |
| 2   | FMN  | B     | 4000 | -    | -       | 5/18/18/18 | 0/3/3/3 |
| 2   | FMN  | C     | 4000 | -    | -       | 5/18/18/18 | 0/3/3/3 |
| 2   | FMN  | D     | 4000 | -    | -       | 5/18/18/18 | 0/3/3/3 |
| 2   | FMN  | E     | 4000 | -    | -       | 5/18/18/18 | 0/3/3/3 |
| 2   | FMN  | F     | 4000 | -    | -       | 5/18/18/18 | 0/3/3/3 |

All (24) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 2   | B     | 4000 | FMN  | C4A-N5 | 3.76 | 1.38        | 1.33     |
| 2   | E     | 4000 | FMN  | C4A-N5 | 3.73 | 1.38        | 1.33     |
| 2   | C     | 4000 | FMN  | C4A-N5 | 3.69 | 1.38        | 1.33     |
| 2   | F     | 4000 | FMN  | C4A-N5 | 3.69 | 1.38        | 1.33     |
| 2   | A     | 4000 | FMN  | C4A-N5 | 3.69 | 1.38        | 1.33     |
| 2   | D     | 4000 | FMN  | C4A-N5 | 3.69 | 1.38        | 1.33     |
| 2   | C     | 4000 | FMN  | C10-N1 | 3.44 | 1.37        | 1.33     |
| 2   | E     | 4000 | FMN  | C10-N1 | 3.40 | 1.37        | 1.33     |
| 2   | D     | 4000 | FMN  | C10-N1 | 3.39 | 1.37        | 1.33     |
| 2   | B     | 4000 | FMN  | C10-N1 | 3.39 | 1.37        | 1.33     |
| 2   | F     | 4000 | FMN  | C10-N1 | 3.36 | 1.37        | 1.33     |
| 2   | A     | 4000 | FMN  | C10-N1 | 3.36 | 1.37        | 1.33     |
| 2   | C     | 4000 | FMN  | C4-N3  | 3.33 | 1.38        | 1.33     |
| 2   | E     | 4000 | FMN  | C4-N3  | 3.28 | 1.38        | 1.33     |
| 2   | A     | 4000 | FMN  | C4-N3  | 3.27 | 1.38        | 1.33     |
| 2   | F     | 4000 | FMN  | C4-N3  | 3.27 | 1.38        | 1.33     |
| 2   | D     | 4000 | FMN  | C4-N3  | 3.27 | 1.38        | 1.33     |
| 2   | B     | 4000 | FMN  | C4-N3  | 3.26 | 1.38        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 2   | C     | 4000 | FMN  | C5A-N5 | 2.21 | 1.38        | 1.35     |
| 2   | F     | 4000 | FMN  | C5A-N5 | 2.21 | 1.38        | 1.35     |
| 2   | D     | 4000 | FMN  | C5A-N5 | 2.20 | 1.38        | 1.35     |
| 2   | B     | 4000 | FMN  | C5A-N5 | 2.15 | 1.38        | 1.35     |
| 2   | A     | 4000 | FMN  | C5A-N5 | 2.15 | 1.38        | 1.35     |
| 2   | E     | 4000 | FMN  | C5A-N5 | 2.13 | 1.38        | 1.35     |

All (42) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 4000 | FMN  | C4-N3-C2    | 5.93  | 120.15      | 115.14   |
| 2   | D     | 4000 | FMN  | C4-N3-C2    | 5.93  | 120.15      | 115.14   |
| 2   | B     | 4000 | FMN  | C4-N3-C2    | 5.91  | 120.13      | 115.14   |
| 2   | E     | 4000 | FMN  | C4-N3-C2    | 5.88  | 120.11      | 115.14   |
| 2   | F     | 4000 | FMN  | C4-N3-C2    | 5.86  | 120.09      | 115.14   |
| 2   | C     | 4000 | FMN  | C4-N3-C2    | 5.85  | 120.08      | 115.14   |
| 2   | A     | 4000 | FMN  | C1'-N10-C9A | 3.36  | 121.24      | 118.31   |
| 2   | C     | 4000 | FMN  | C1'-N10-C9A | 3.35  | 121.23      | 118.31   |
| 2   | D     | 4000 | FMN  | C1'-N10-C9A | 3.34  | 121.22      | 118.31   |
| 2   | E     | 4000 | FMN  | C1'-N10-C9A | 3.34  | 121.22      | 118.31   |
| 2   | B     | 4000 | FMN  | C1'-N10-C9A | 3.34  | 121.22      | 118.31   |
| 2   | F     | 4000 | FMN  | C1'-N10-C9A | 3.29  | 121.18      | 118.31   |
| 2   | E     | 4000 | FMN  | C4A-N5-C5A  | 3.10  | 119.95      | 116.77   |
| 2   | A     | 4000 | FMN  | C4A-N5-C5A  | 3.08  | 119.94      | 116.77   |
| 2   | D     | 4000 | FMN  | C4A-N5-C5A  | 3.07  | 119.93      | 116.77   |
| 2   | B     | 4000 | FMN  | C4A-N5-C5A  | 3.05  | 119.90      | 116.77   |
| 2   | C     | 4000 | FMN  | C4A-N5-C5A  | 3.05  | 119.90      | 116.77   |
| 2   | F     | 4000 | FMN  | C4A-N5-C5A  | 3.05  | 119.90      | 116.77   |
| 2   | B     | 4000 | FMN  | C5A-C9A-N10 | 2.75  | 119.81      | 117.71   |
| 2   | C     | 4000 | FMN  | C5A-C9A-N10 | 2.73  | 119.80      | 117.71   |
| 2   | D     | 4000 | FMN  | C5A-C9A-N10 | 2.73  | 119.80      | 117.71   |
| 2   | A     | 4000 | FMN  | C5A-C9A-N10 | 2.72  | 119.79      | 117.71   |
| 2   | F     | 4000 | FMN  | C5A-C9A-N10 | 2.71  | 119.78      | 117.71   |
| 2   | E     | 4000 | FMN  | C5A-C9A-N10 | 2.65  | 119.74      | 117.71   |
| 2   | A     | 4000 | FMN  | C4A-C4-N3   | -2.64 | 119.80      | 123.47   |
| 2   | D     | 4000 | FMN  | C4A-C4-N3   | -2.64 | 119.80      | 123.47   |
| 2   | F     | 4000 | FMN  | C4A-C4-N3   | -2.63 | 119.81      | 123.47   |
| 2   | C     | 4000 | FMN  | C4A-C4-N3   | -2.63 | 119.81      | 123.47   |
| 2   | E     | 4000 | FMN  | C4A-C4-N3   | -2.63 | 119.82      | 123.47   |
| 2   | E     | 4000 | FMN  | C4-C4A-N5   | 2.61  | 121.47      | 118.59   |
| 2   | B     | 4000 | FMN  | C4A-C4-N3   | -2.61 | 119.84      | 123.47   |
| 2   | B     | 4000 | FMN  | C4-C4A-N5   | 2.59  | 121.45      | 118.59   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2   | A     | 4000 | FMN  | C4-C4A-N5  | 2.59  | 121.45      | 118.59   |
| 2   | D     | 4000 | FMN  | C4-C4A-N5  | 2.59  | 121.45      | 118.59   |
| 2   | E     | 4000 | FMN  | C10-C4A-N5 | -2.57 | 119.36      | 121.25   |
| 2   | F     | 4000 | FMN  | C4-C4A-N5  | 2.54  | 121.39      | 118.59   |
| 2   | C     | 4000 | FMN  | C4-C4A-N5  | 2.53  | 121.39      | 118.59   |
| 2   | B     | 4000 | FMN  | C10-C4A-N5 | -2.49 | 119.42      | 121.25   |
| 2   | A     | 4000 | FMN  | C10-C4A-N5 | -2.48 | 119.43      | 121.25   |
| 2   | D     | 4000 | FMN  | C10-C4A-N5 | -2.48 | 119.43      | 121.25   |
| 2   | C     | 4000 | FMN  | C10-C4A-N5 | -2.43 | 119.46      | 121.25   |
| 2   | F     | 4000 | FMN  | C10-C4A-N5 | -2.41 | 119.48      | 121.25   |

There are no chirality outliers.

All (30) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | B     | 4000 | FMN  | O3'-C3'-C4'-C5' |
| 2   | C     | 4000 | FMN  | O3'-C3'-C4'-C5' |
| 2   | A     | 4000 | FMN  | O3'-C3'-C4'-C5' |
| 2   | F     | 4000 | FMN  | O3'-C3'-C4'-C5' |
| 2   | D     | 4000 | FMN  | O3'-C3'-C4'-C5' |
| 2   | E     | 4000 | FMN  | O3'-C3'-C4'-C5' |
| 2   | B     | 4000 | FMN  | C2'-C3'-C4'-C5' |
| 2   | C     | 4000 | FMN  | C2'-C3'-C4'-C5' |
| 2   | A     | 4000 | FMN  | C2'-C3'-C4'-C5' |
| 2   | F     | 4000 | FMN  | C2'-C3'-C4'-C5' |
| 2   | D     | 4000 | FMN  | C2'-C3'-C4'-C5' |
| 2   | E     | 4000 | FMN  | C2'-C3'-C4'-C5' |
| 2   | B     | 4000 | FMN  | C2'-C3'-C4'-O4' |
| 2   | C     | 4000 | FMN  | C2'-C3'-C4'-O4' |
| 2   | A     | 4000 | FMN  | C2'-C3'-C4'-O4' |
| 2   | F     | 4000 | FMN  | C2'-C3'-C4'-O4' |
| 2   | D     | 4000 | FMN  | C2'-C3'-C4'-O4' |
| 2   | E     | 4000 | FMN  | C2'-C3'-C4'-O4' |
| 2   | B     | 4000 | FMN  | C4'-C5'-O5'-P   |
| 2   | C     | 4000 | FMN  | C4'-C5'-O5'-P   |
| 2   | A     | 4000 | FMN  | C4'-C5'-O5'-P   |
| 2   | F     | 4000 | FMN  | C4'-C5'-O5'-P   |
| 2   | D     | 4000 | FMN  | C4'-C5'-O5'-P   |
| 2   | E     | 4000 | FMN  | C4'-C5'-O5'-P   |
| 2   | B     | 4000 | FMN  | O3'-C3'-C4'-O4' |
| 2   | C     | 4000 | FMN  | O3'-C3'-C4'-O4' |
| 2   | A     | 4000 | FMN  | O3'-C3'-C4'-O4' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | F     | 4000 | FMN  | O3'-C3'-C4'-O4' |
| 2   | D     | 4000 | FMN  | O3'-C3'-C4'-O4' |
| 2   | E     | 4000 | FMN  | O3'-C3'-C4'-O4' |

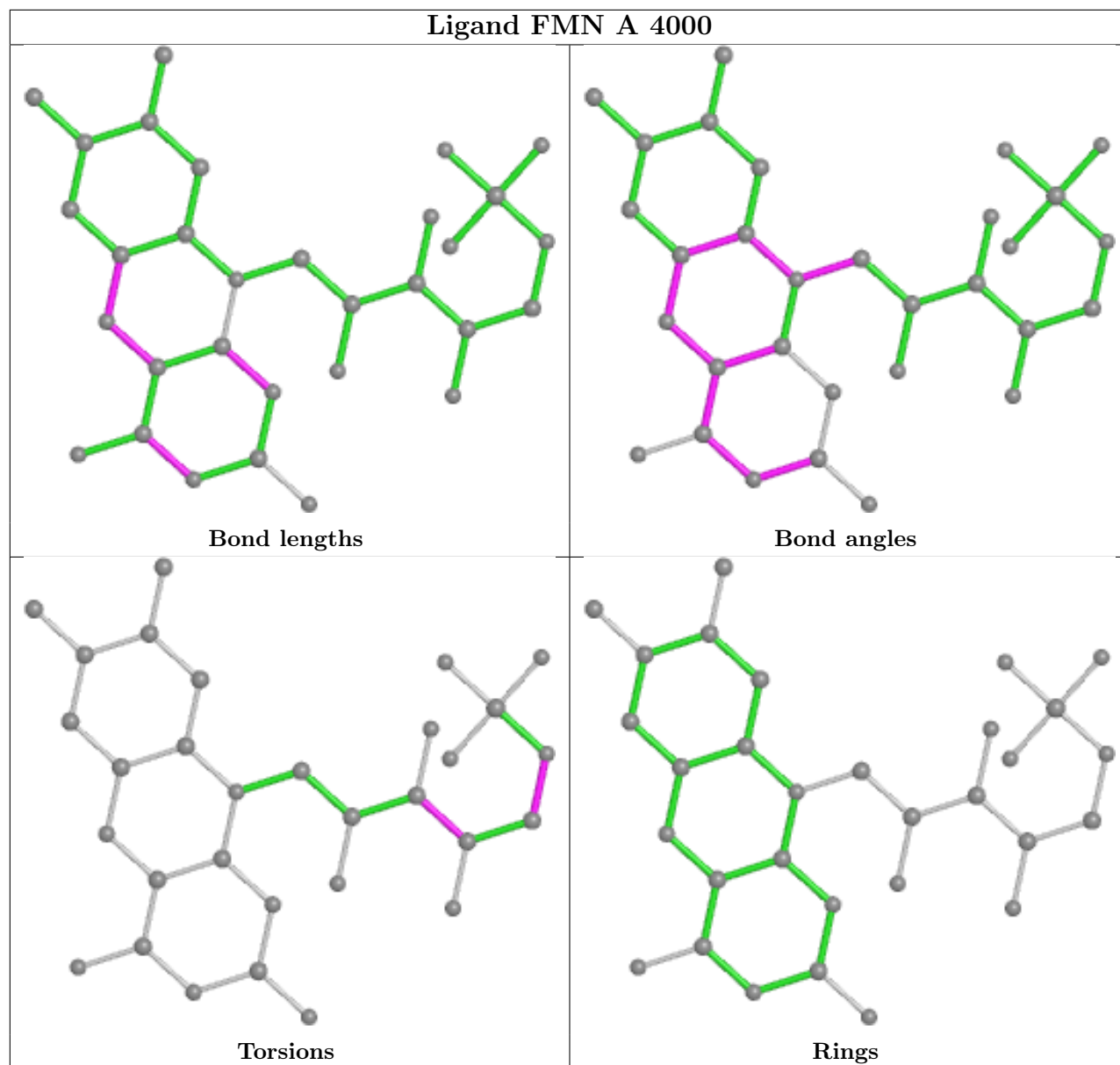
There are no ring outliers.

3 monomers are involved in 14 short contacts:

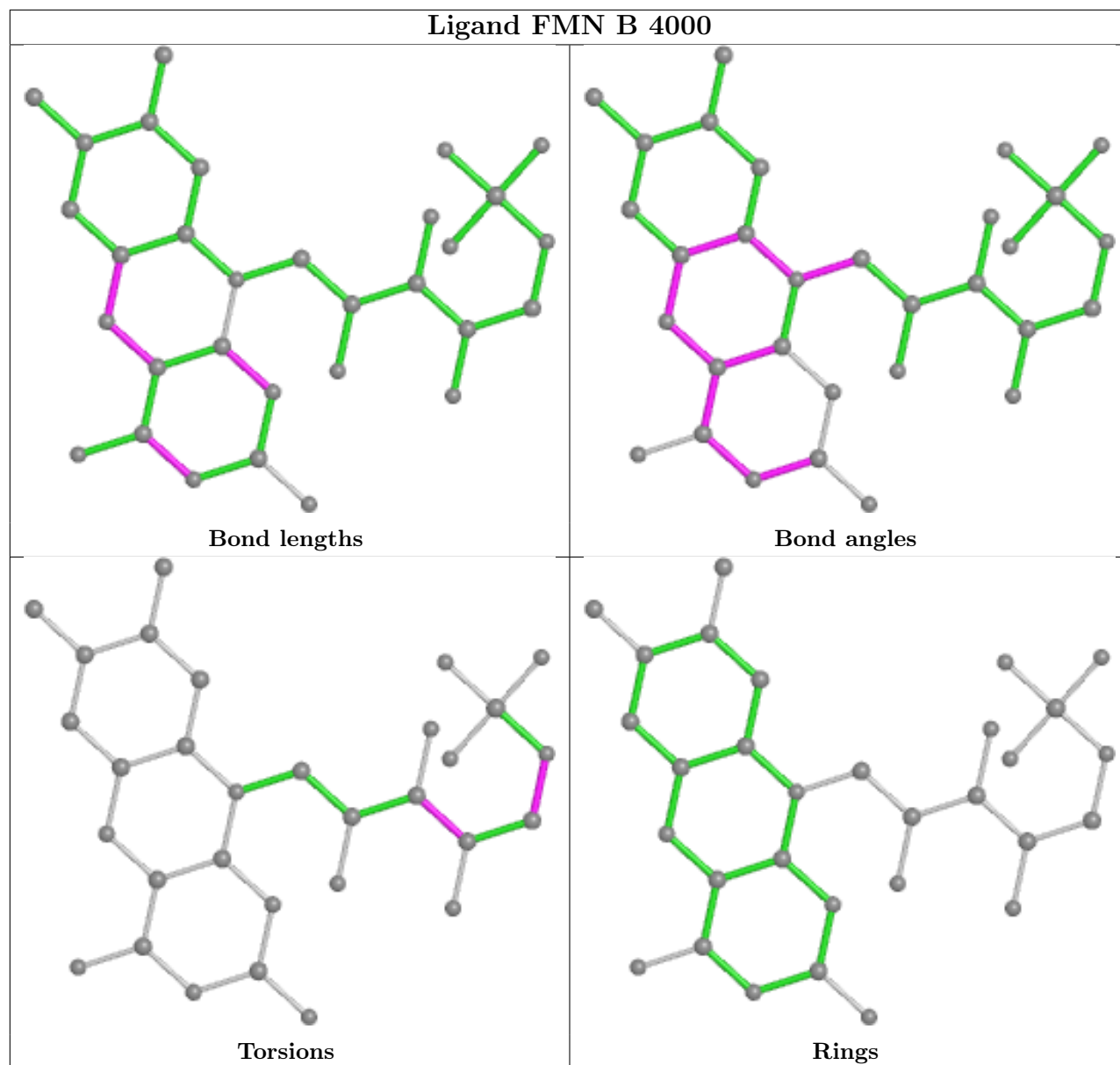
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | A     | 4000 | FMN  | 5       | 0            |
| 2   | B     | 4000 | FMN  | 5       | 0            |
| 2   | C     | 4000 | FMN  | 4       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

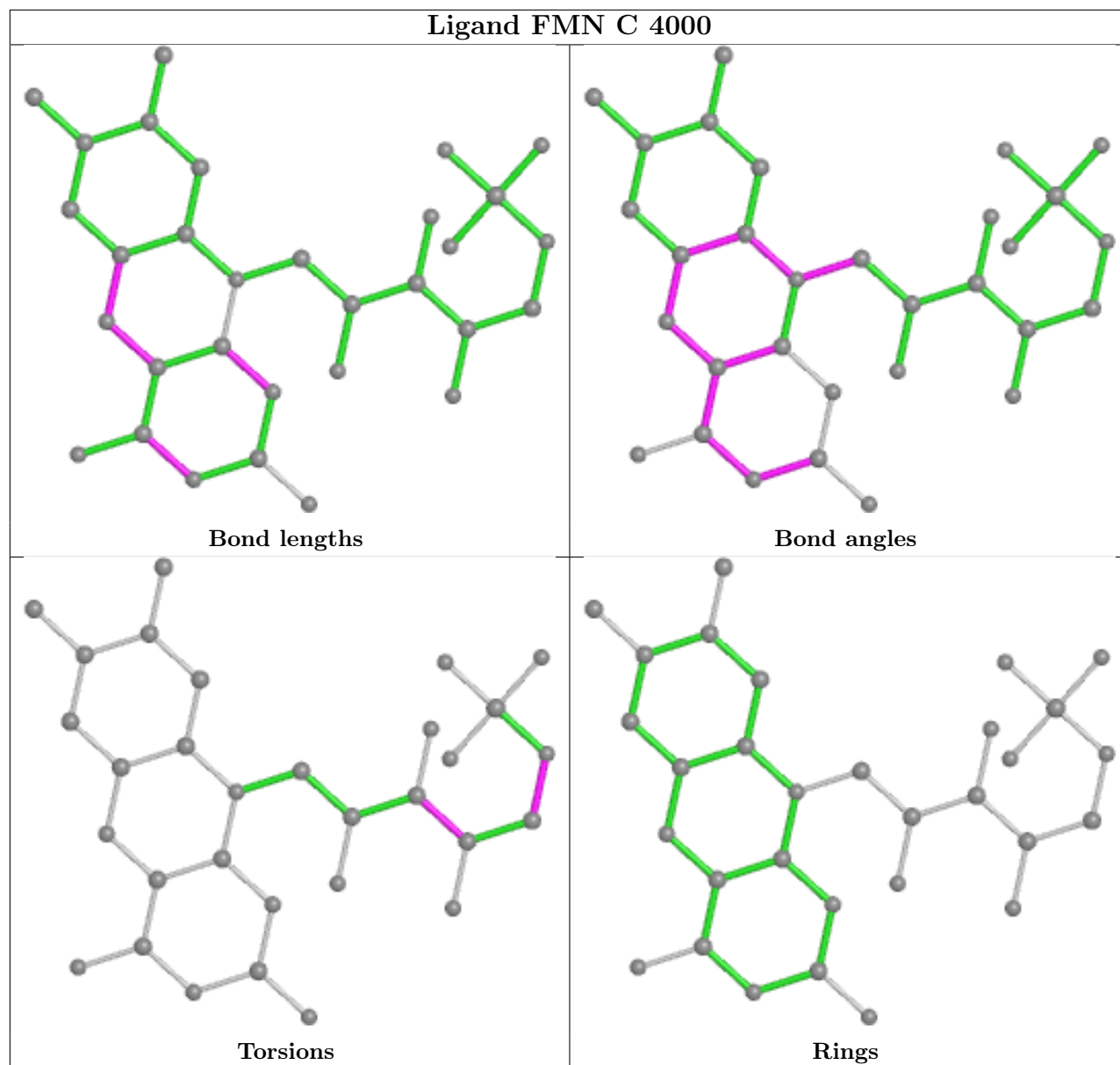
## Ligand FMN A 4000



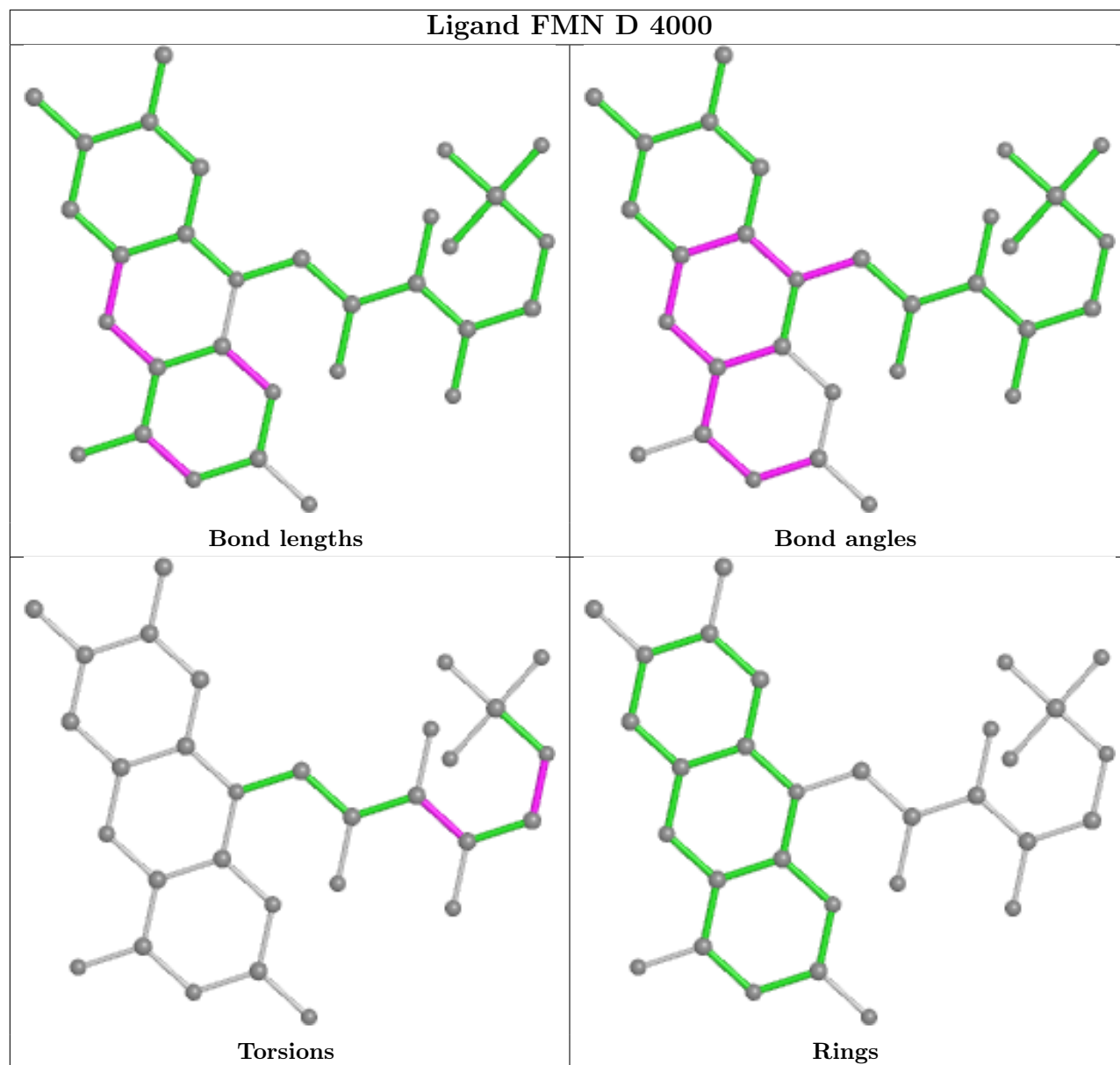
## Ligand FMN B 4000



## Ligand FMN C 4000

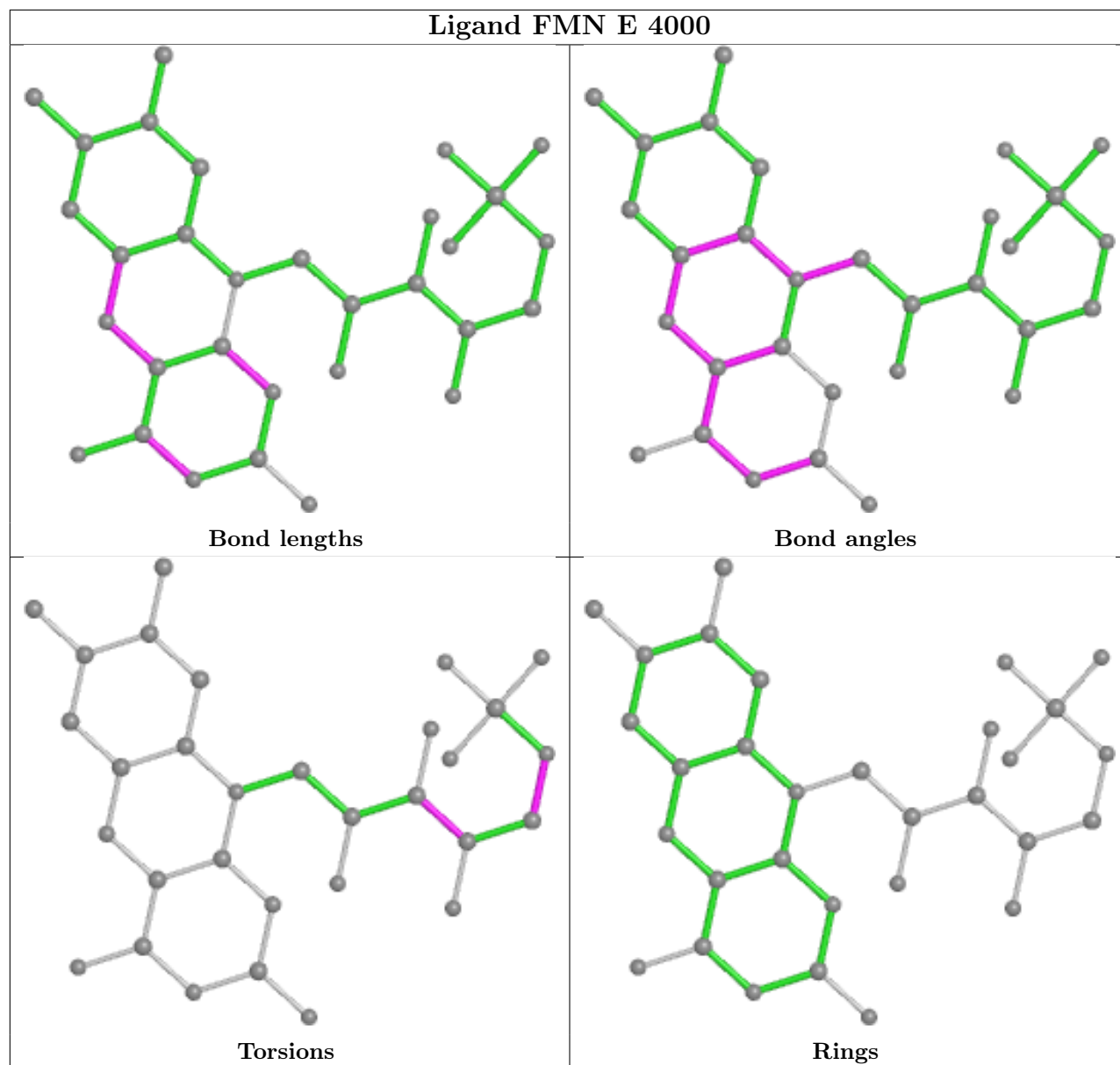


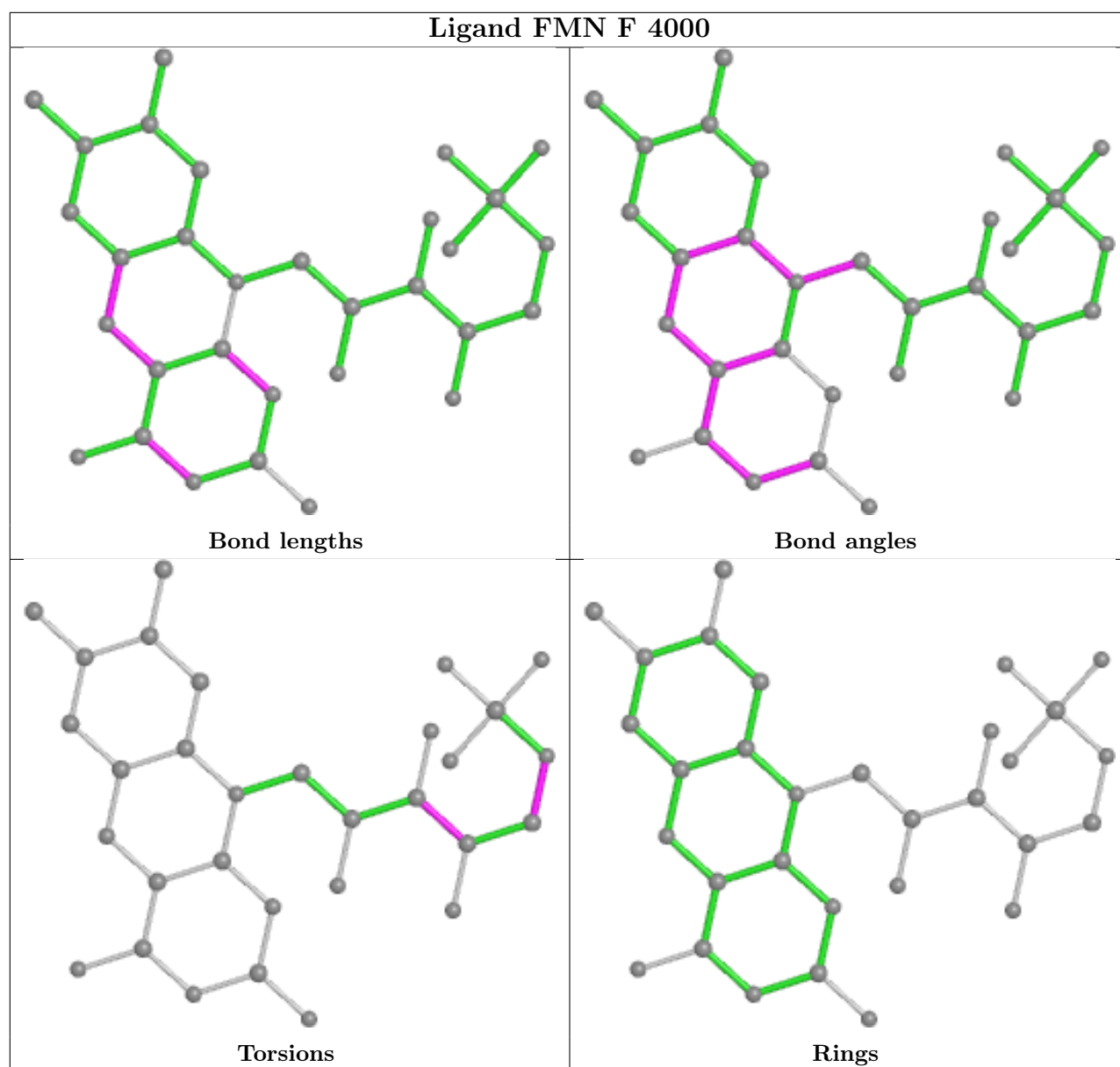
## Ligand FMN D 4000





## Ligand FMN E 4000





## 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.