



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:32 PM GMT

PDB ID : 4F5X  
Title : Location of the dsRNA-dependent polymerase, VP1, in rotavirus particles  
Authors : Estrozi, L.F.; Settembre, E.C.; Goret, G.; McClain, B.; Zhang, X.; Chen, J.Z.; Grigorieff, N.; Harrison, S.C.  
Deposited on : 2012-05-13  
Resolution : 5.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : **FAILED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

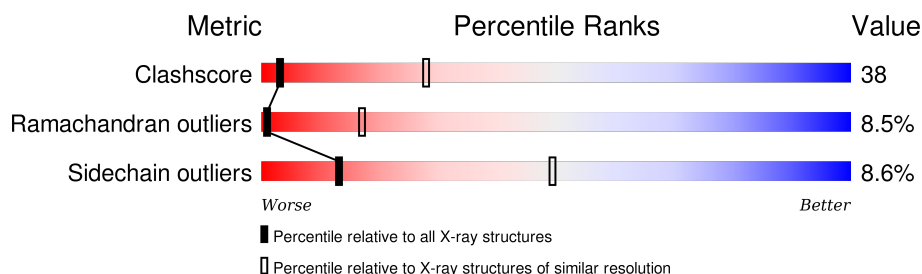
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.00 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 102246                      | 1019 (6.22-3.66)                                      |
| Ramachandran outliers | 100387                      | 1158 (6.22-3.60)                                      |
| Sidechain outliers    | 100360                      | 1136 (6.22-3.60)                                      |










The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS failed to run properly.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 880    | <div> <div>16%</div> <div>49%</div> <div>21%</div> <div>•</div> <div>11%</div> </div> |
| 1   | B     | 880    | <div> <div>19%</div> <div>49%</div> <div>22%</div> <div>•</div> <div>8%</div> </div>  |
| 2   | C     | 397    | <div> <div>60%</div> <div>31%</div> <div>8%</div> <div>•</div> </div>                 |
| 2   | D     | 397    | <div> <div>57%</div> <div>32%</div> <div>9%</div> <div>•</div> </div>                 |
| 2   | E     | 397    | <div> <div>58%</div> <div>33%</div> <div>8%</div> <div>•</div> </div>                 |
| 2   | F     | 397    | <div> <div>59%</div> <div>34%</div> <div>7%</div> <div>•</div> </div>                 |
| 2   | G     | 397    | <div> <div>62%</div> <div>30%</div> <div>7%</div> <div>•</div> </div>                 |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 2   | H     | 397    |  60% 32% 7% .   |
| 2   | I     | 397    |  58% 33% 9%     |
| 2   | J     | 397    |  58% 34% 8% .   |
| 2   | K     | 397    |  59% 33% 8% .   |
| 2   | L     | 397    |  57% 35% 7% .   |
| 2   | M     | 397    |  58% 35% 6% .   |
| 2   | N     | 397    |  56% 34% 9% .   |
| 2   | O     | 397    |  57% 33% 9% .   |
| 3   | W     | 1089   |  40% 44% 5% 10% |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 62014 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called VP2 protein.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 781      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6374  | 4049 | 1099 | 1190 | 36 |         |         |       |
| 1   | B     | 810      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6624  | 4211 | 1138 | 1239 | 36 |         |         |       |

- Molecule 2 is a protein called Intermediate capsid protein VP6.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | C     | 397      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3162  | 2001 | 550 | 596 | 15 |         |         |       |
| 2   | D     | 397      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3162  | 2001 | 550 | 596 | 15 |         |         |       |
| 2   | E     | 397      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3162  | 2001 | 550 | 596 | 15 |         |         |       |
| 2   | F     | 397      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3162  | 2001 | 550 | 596 | 15 |         |         |       |
| 2   | G     | 397      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3162  | 2001 | 550 | 596 | 15 |         |         |       |
| 2   | H     | 397      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3162  | 2001 | 550 | 596 | 15 |         |         |       |
| 2   | I     | 397      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3162  | 2001 | 550 | 596 | 15 |         |         |       |
| 2   | J     | 397      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3162  | 2001 | 550 | 596 | 15 |         |         |       |
| 2   | K     | 397      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3162  | 2001 | 550 | 596 | 15 |         |         |       |
| 2   | L     | 397      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3162  | 2001 | 550 | 596 | 15 |         |         |       |
| 2   | M     | 397      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3162  | 2001 | 550 | 596 | 15 |         |         |       |
| 2   | N     | 397      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3162  | 2001 | 550 | 596 | 15 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | O     | 397      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3162  | 2001 | 550 | 596 | 15 |         |         |       |

- Molecule 3 is a protein called RNA-directed RNA polymerase.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3   | W     | 975      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7905  | 5081 | 1308 | 1482 | 34 |         |         |       |

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

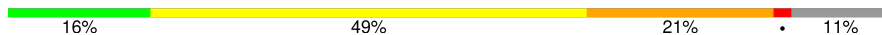
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | O     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | I     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | L     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | C     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | F     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

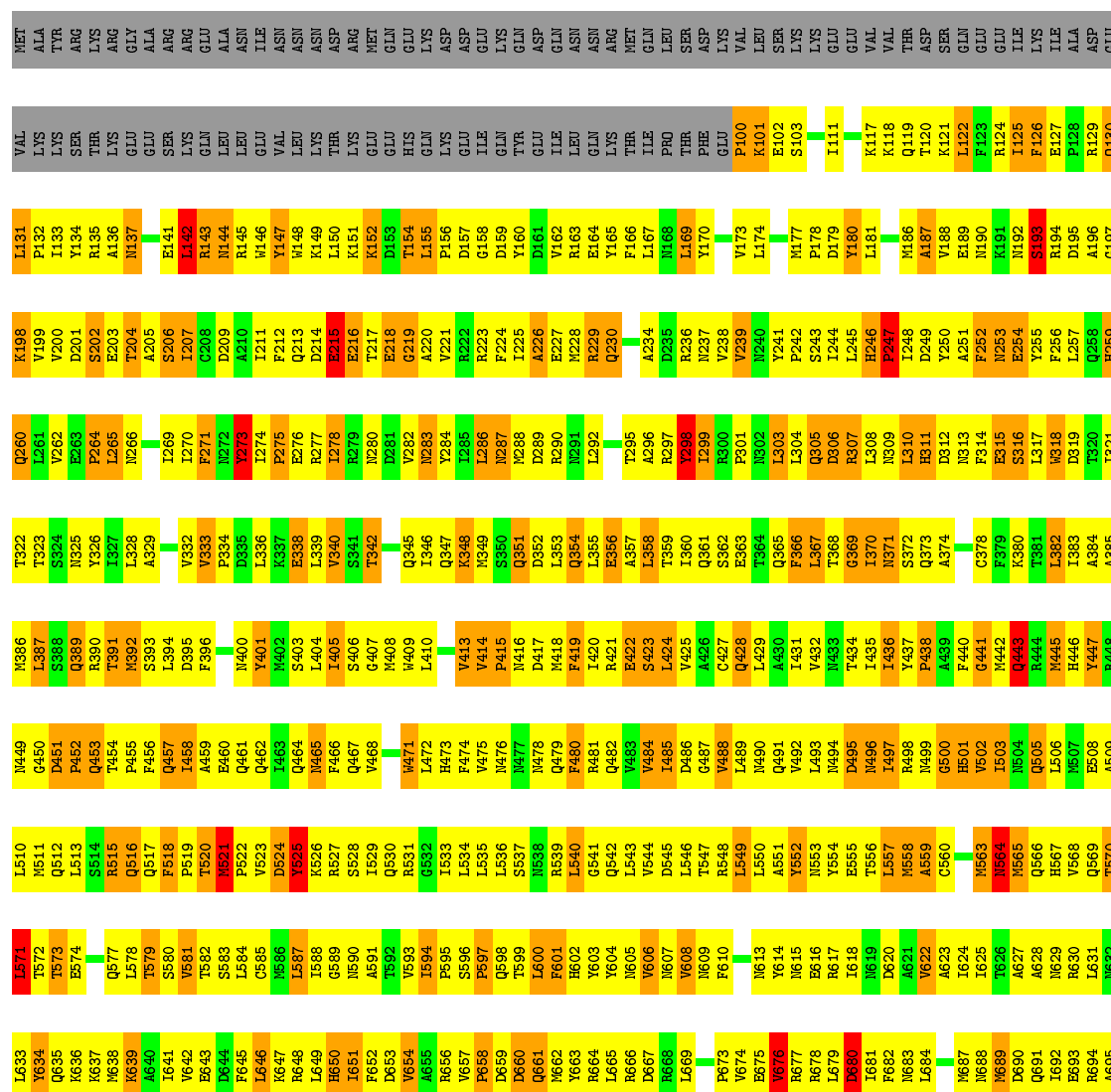
### 3 Residue-property plots

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

Note EDS failed to run properly.

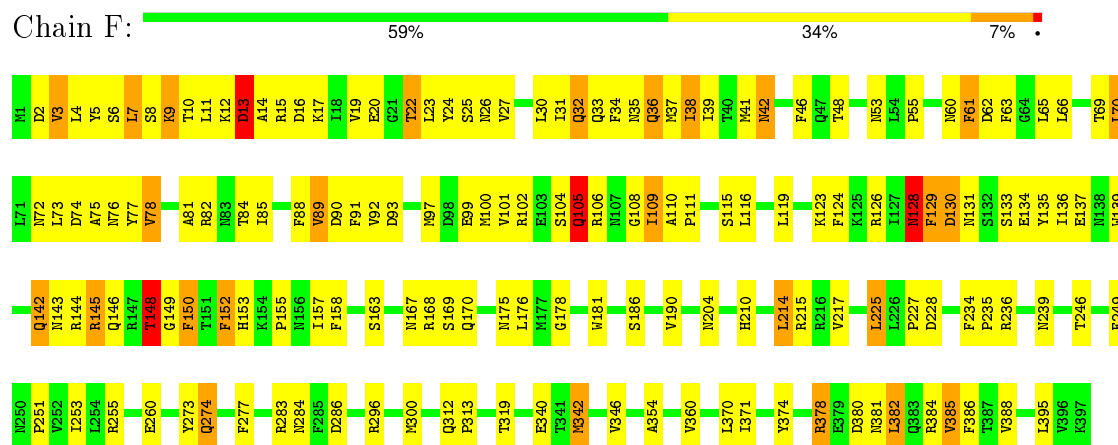
- Molecule 1: VP2 protein

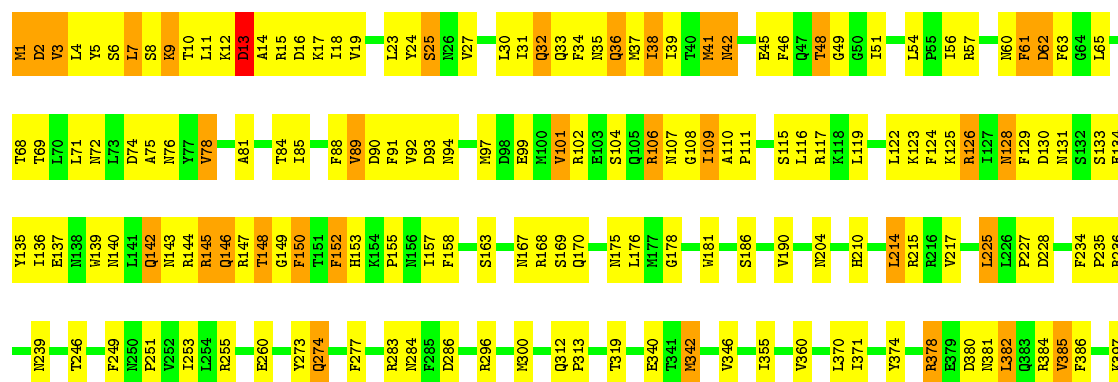
Chain A: 



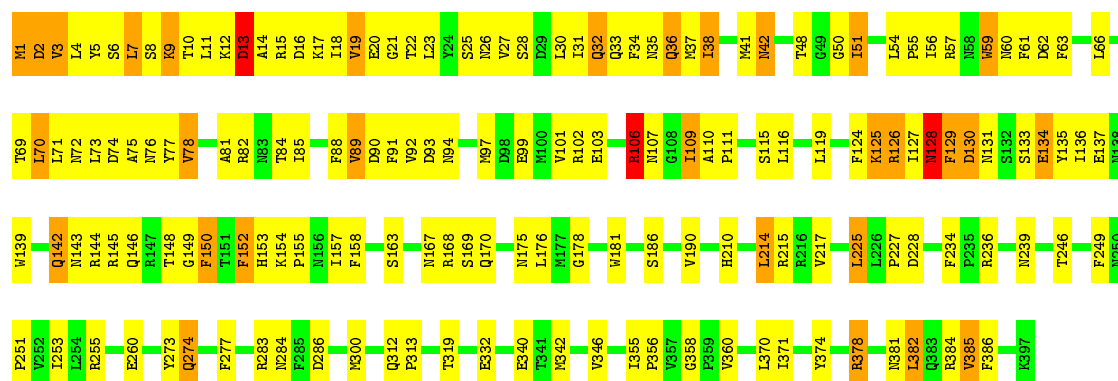
|      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|
| S696 | D697 | A758 | V757 | S821 | S769 | S821 |
| K698 | L759 | A758 | A758 | L622 | S770 | L622 |
| L760 | L760 | A758 | A758 | K824 | S771 | K824 |
| A700 | A700 | A758 | A758 | L760 | I772 | L760 |
| A701 | A701 | A758 | A758 | L760 | S773 | L760 |
| G702 | G702 | A758 | A758 | L760 | A774 | L760 |
| L703 | L703 | A758 | A758 | L760 | L775 | L760 |
| L704 | L704 | A758 | A758 | L760 | L776 | L760 |
| L705 | L705 | A758 | A758 | L760 | L777 | L760 |
| L706 | L706 | A758 | A758 | L760 | L778 | L760 |
| L707 | L707 | A758 | A758 | L760 | L779 | L760 |
| L708 | L708 | A758 | A758 | L760 | L780 | L760 |
| L709 | L709 | A758 | A758 | L760 | L781 | L760 |
| L710 | L710 | A758 | A758 | L760 | L782 | L760 |
| L711 | L711 | A758 | A758 | L760 | L783 | L760 |
| L712 | L712 | A758 | A758 | L760 | L784 | L760 |
| L713 | L713 | A758 | A758 | L760 | L785 | L760 |
| L714 | L714 | A758 | A758 | L760 | L786 | L760 |
| L715 | L715 | A758 | A758 | L760 | L787 | L760 |
| L716 | L716 | A758 | A758 | L760 | L788 | L760 |
| L717 | L717 | A758 | A758 | L760 | L789 | L760 |
| L718 | L718 | A758 | A758 | L760 | L790 | L760 |
| L719 | L719 | A758 | A758 | L760 | L791 | L760 |
| L720 | L720 | A758 | A758 | L760 | L792 | L760 |
| L721 | L721 | A758 | A758 | L760 | L793 | L760 |
| L722 | L722 | A758 | A758 | L760 | L794 | L760 |
| L723 | L723 | A758 | A758 | L760 | L795 | L760 |
| L724 | L724 | A758 | A758 | L760 | L796 | L760 |
| L725 | L725 | A758 | A758 | L760 | L797 | L760 |
| L726 | L726 | A758 | A758 | L760 | L798 | L760 |
| L727 | L727 | A758 | A758 | L760 | L799 | L760 |
| L728 | L728 | A758 | A758 | L760 | L800 | L760 |
| L729 | L729 | A758 | A758 | L760 | L801 | L760 |
| L730 | L730 | A758 | A758 | L760 | L802 | L760 |
| L731 | L731 | A758 | A758 | L760 | L803 | L760 |
| L732 | L732 | A758 | A758 | L760 | L804 | L760 |
| L733 | L733 | A758 | A758 | L760 | L805 | L760 |
| L734 | L734 | A758 | A758 | L760 | L806 | L760 |
| L735 | L735 | A758 | A758 | L760 | L807 | L760 |
| L736 | L736 | A758 | A758 | L760 | L808 | L760 |
| L737 | L737 | A758 | A758 | L760 | L809 | L760 |
| L738 | L738 | A758 | A758 | L760 | L810 | L760 |
| L739 | L739 | A758 | A758 | L760 | L811 | L760 |
| L740 | L740 | A758 | A758 | L760 | L812 | L760 |
| L741 | L741 | A758 | A758 | L760 | L813 | L760 |
| L742 | L742 | A758 | A758 | L760 | L814 | L760 |
| L743 | L743 | A758 | A758 | L760 | L815 | L760 |
| L744 | L744 | A758 | A758 | L760 | L816 | L760 |
| L745 | L745 | A758 | A758 | L760 | L817 | L760 |
| L746 | L746 | A758 | A758 | L760 | L818 | L760 |
| L747 | L747 | A758 | A758 | L760 | L819 | L760 |
| L748 | L748 | A758 | A758 | L760 | L820 | L760 |
| L749 | L749 | A758 | A758 | L760 | L821 | L760 |
| L750 | L750 | A758 | A758 | L760 | L822 | L760 |
| L751 | L751 | A758 | A758 | L760 | L823 | L760 |
| L752 | L752 | A758 | A758 | L760 | L824 | L760 |
| L753 | L753 | A758 | A758 | L760 | L825 | L760 |
| L754 | L754 | A758 | A758 | L760 | L826 | L760 |
| L755 | L755 | A758 | A758 | L760 | L827 | L760 |
| L756 | L756 | A758 | A758 | L760 | L828 | L760 |
| L757 | L757 | A758 | A758 | L760 | L829 | L760 |
| L758 | L758 | A758 | A758 | L760 | L830 | L760 |
| L759 | L759 | A758 | A758 | L760 | L831 | L760 |
| L760 | L760 | A758 | A758 | L760 | L832 | L760 |
| L761 | L761 | A758 | A758 | L760 | L833 | L760 |
| L762 | L762 | A758 | A758 | L760 | L834 | L760 |
| L763 | L763 | A758 | A758 | L760 | L835 | L760 |
| L764 | L764 | A758 | A758 | L760 | L836 | L760 |
| L765 | L765 | A758 | A758 | L760 | L837 | L760 |
| L766 | L766 | A758 | A758 | L760 | L838 | L760 |
| L767 | L767 | A758 | A758 | L760 | L839 | L760 |
| L768 | L768 | A758 | A758 | L760 | L840 | L760 |
| L769 | L769 | A758 | A758 | L760 | L841 | L760 |
| L770 | L770 | A758 | A758 | L760 | L842 | L760 |
| L771 | L771 | A758 | A758 | L760 | L843 | L760 |
| L772 | L772 | A758 | A758 | L760 | L844 | L760 |
| L773 | L773 | A758 | A758 | L760 | L845 | L760 |
| L774 | L774 | A758 | A758 | L760 | L846 | L760 |
| L775 | L775 | A758 | A758 | L760 | L847 | L760 |
| L776 | L776 | A758 | A758 | L760 | L848 | L760 |
| L777 | L777 | A758 | A758 | L760 | L849 | L760 |
| L778 | L778 | A758 | A758 | L760 | L850 | L760 |
| L779 | L779 | A758 | A758 | L760 | L851 | L760 |
| L780 | L780 | A758 | A758 | L760 | L852 | L760 |
| L781 | L781 | A758 | A758 | L760 | L853 | L760 |
| L782 | L782 | A758 | A758 | L760 | L854 | L760 |
| L783 | L783 | A758 | A758 | L760 | L855 | L760 |
| L784 | L784 | A758 | A758 | L760 | L856 | L760 |
| L785 | L785 | A758 | A758 | L760 | L857 | L760 |
| L786 | L786 | A758 | A758 | L760 | L858 | L760 |
| L787 | L787 | A758 | A758 | L760 | L859 | L760 |
| L788 | L788 | A758 | A758 | L760 | L860 | L760 |
| L789 | L789 | A758 | A758 | L760 | L861 | L760 |
| L790 | L790 | A758 | A758 | L760 | L862 | L760 |
| L791 | L791 | A758 | A758 | L760 | L863 | L760 |
| L792 | L792 | A758 | A758 | L760 | L864 | L760 |
| L793 | L793 | A758 | A758 | L760 | L865 | L760 |
| L794 | L794 | A758 | A758 | L760 | L866 | L760 |
| L795 | L795 | A758 | A758 | L760 | L867 | L760 |
| L796 | L796 | A758 | A758 | L760 | L868 | L760 |
| L797 | L797 | A758 | A758 | L760 | L869 | L760 |
| L798 | L798 | A758 | A758 | L760 | L870 | L760 |
| L799 | L799 | A758 | A758 | L760 | L871 | L760 |
| L800 | L800 | A758 | A758 | L760 | L872 | L760 |
| L801 | L801 | A758 | A758 | L760 | L873 | L760 |
| L802 | L802 | A758 | A758 | L760 | L874 | L760 |
| L803 | L803 | A758 | A758 | L760 | L875 | L760 |
| L804 | L804 | A758 | A758 | L760 | L876 | L760 |
| L805 | L805 | A758 | A758 | L760 | L877 | L760 |
| L806 | L806 | A758 | A758 | L760 | L878 | L760 |
| L807 | L807 | A758 | A758 | L760 | L879 | L760 |
| L808 | L808 | A758 | A758 | L760 | L880 | L760 |
| L809 | L809 | A758 | A758 | L760 | L881 | L760 |
| L810 | L810 | A758 | A758 | L760 | L882 | L760 |
| L811 | L811 | A758 | A758 | L760 | L883 | L760 |
| L812 | L812 | A758 | A758 | L760 | L884 | L760 |
| L813 | L813 | A758 | A758 | L760 | L885 | L760 |
| L814 | L814 | A758 | A758 | L760 | L886 | L760 |
| L815 | L815 | A758 | A758 | L760 | L887 | L760 |
| L816 | L816 | A758 | A758 | L760 | L888 | L760 |
| L817 | L817 | A758 | A758 | L760 | L889 | L760 |
| L818 | L818 | A758 | A758 | L760 | L890 | L760 |
| L819 | L819 | A758 | A758 | L760 | L891 | L760 |
| L820 | L820 | A758 | A758 | L760 | L892 | L760 |
| L821 | L821 | A758 | A758 | L760 | L893 | L760 |
| L822 | L822 | A758 | A758 | L760 | L894 | L760 |
| L823 | L823 | A758 | A758 | L760 | L895 | L760 |
| L824 | L824 | A758 | A758 | L760 | L896 | L760 |
| L825 | L825 | A758 | A758 | L760 | L897 | L760 |
| L826 | L826 | A758 | A758 | L760 | L898 | L760 |
| L827 | L827 | A758 | A758 | L760 | L899 | L760 |
| L828 | L828 | A758 | A758 | L760 | L900 | L760 |
| L829 | L829 | A758 | A758 | L760 | L901 | L760 |
| L830 | L830 | A758 | A758 | L760 | L902 | L760 |
| L831 | L831 | A758 | A758 | L760 | L903 | L760 |
| L832 | L832 | A758 | A758 | L760 | L904 | L760 |
| L833 | L833 | A758 | A758 | L760 | L905 | L760 |
| L834 | L834 | A758 | A758 | L760 | L906 | L760 |
| L835 | L835 | A758 | A758 | L760 | L907 | L760 |
| L836 | L836 | A758 | A758 | L760 | L908 | L760 |
| L837 | L837 | A758 | A758 | L760 | L909 | L760 |
| L838 | L838 | A758 | A758 | L760 | L910 | L760 |
| L839 | L839 | A758 | A758 | L760 | L911 | L760 |
| L840 | L840 | A758 | A758 | L760 | L912 | L760 |
| L841 | L841 | A758 | A758 | L760 | L913 | L760 |
| L842 | L842 | A758 | A758 | L760 | L914 | L760 |
| L843 | L843 | A758 | A758 | L760 | L915 | L760 |
| L844 | L844 | A758 | A758 | L760 | L916 | L760 |
| L845 | L845 | A758 | A758 | L760 | L917 | L760 |
| L846 | L846 | A758 | A758 | L760 | L918 | L760 |
| L847 | L847 | A758 | A758 | L760 | L919 | L760 |
| L848 | L848 | A758 | A758 | L760 | L920 | L760 |
| L849 | L849 | A758 | A758 | L760 | L921 | L760 |
| L850 | L850 | A758 | A758 | L760 | L922 | L760 |
| L851 | L851 | A758 | A758 | L760 | L923 | L760 |
| L852 | L852 | A758 | A758 | L760 | L924 | L760 |
| L853 | L853 | A758 | A758 | L760 | L925 | L760 |
| L854 | L854 | A758 | A758 | L760 | L926 | L760 |
| L855 | L855 | A758 | A758 | L760 | L927 | L760 |
| L856 | L856 | A758 | A758 | L760 | L928 | L760 |
| L857 | L857 | A758 | A758 | L760 | L929 | L760 |
| L858 | L858 | A758 | A758 | L760 | L930 | L760 |
| L859 | L859 | A758 | A758 | L760 | L931 | L760 |
| L860 | L860 | A758 | A758 | L760 | L932 | L760 |
| L861 | L861 | A758 | A758 | L760 | L933 | L760 |
| L862 | L862 | A758 | A758 | L760 | L934 | L760 |
| L863 | L863 | A758 | A758 | L760 | L935 | L760 |
| L864 | L864 | A758 | A758 | L760 | L936 | L760 |
| L865 | L865 | A758 | A758 | L760 | L937 | L760 |
| L866 | L866 | A758 | A758 | L760 | L938 | L760 |
| L867 | L867 | A758 | A758 | L760 | L939 | L760 |
| L868 | L868 | A758 | A758 | L760 | L940 | L760 |
| L869 | L869 | A758 | A758 | L760 | L941 | L760 |
| L870 | L870 | A758 | A758 | L760 | L942 | L760 |
| L871 | L871 | A758 | A758 | L760 | L943 | L760 |
| L872 | L872 | A758 | A758 | L760 | L944 | L760 |
| L873 | L873 | A758 | A758 | L760 | L945 | L760 |
| L874 | L874 | A758 | A758 | L760 | L946 | L760 |
| L875 | L875 | A758 | A758 | L760 | L947 | L760 |
| L876 | L876 | A758 | A758 | L760 | L948 | L760 |
| L877 | L877 | A758 | A758 | L760 | L949 | L760 |
| L878 | L878 | A758 | A758 | L760 | L950 | L760 |
| L879 | L879 | A758 | A758 | L760 | L951 | L760 |
| L880 | L880 | A758 | A758 | L760 | L952 | L760 |
| L881 | L881 | A758 | A758 | L760 | L953 | L760 |
| L882 | L882 | A758 | A758 | L760 | L954 | L760 |
| L883 | L883 | A758 | A758 | L760 | L955 | L760 |
| L884 | L884 | A758 | A758 | L760 | L956 | L760 |
| L885 | L885 | A758 | A758 | L760 | L957 | L760 |
| L886 | L886 | A758 | A758 | L760 | L958 | L760 |
| L887 | L887 | A758 | A758 | L760 | L959 | L760 |
| L888 | L888 | A758 | A758 | L760 | L960 | L760 |
| L889 | L889 | A758 | A758 | L760 | L961 | L760 |
| L890 | L890 | A758 | A758 | L760 | L962 | L760 |
| L891 | L891 | A758 | A758 | L760 | L963 | L760 |
| L892 | L892 | A758 | A758 | L760 | L964 | L760 |
| L893 | L893 | A758 | A758 | L760 | L965 | L760 |
| L894 | L894 | A758 | A758 | L760 | L966 | L760 |
| L895 | L895 | A758 | A758 | L760 | L967 | L760 |
| L896 | L896 | A758 | A758 | L760 | L968 | L760 |
| L897 | L897 | A758 | A758 | L760 | L969 |      |



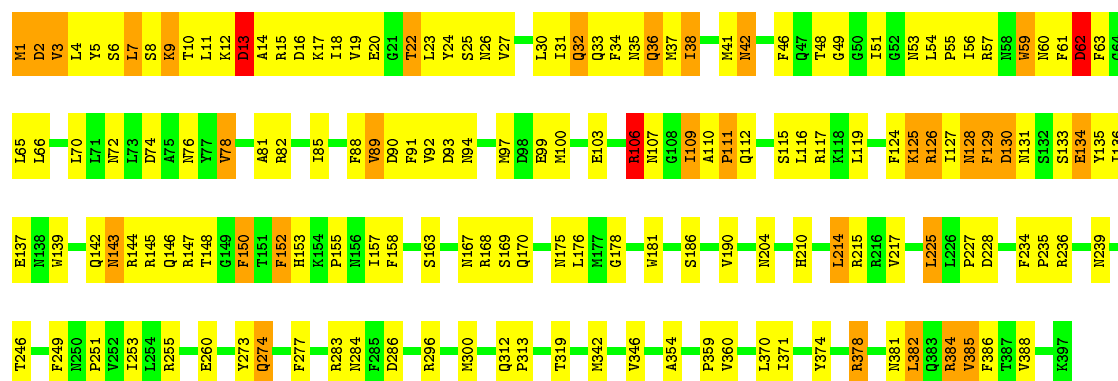




- Molecule 2: Intermediate capsid protein VP6

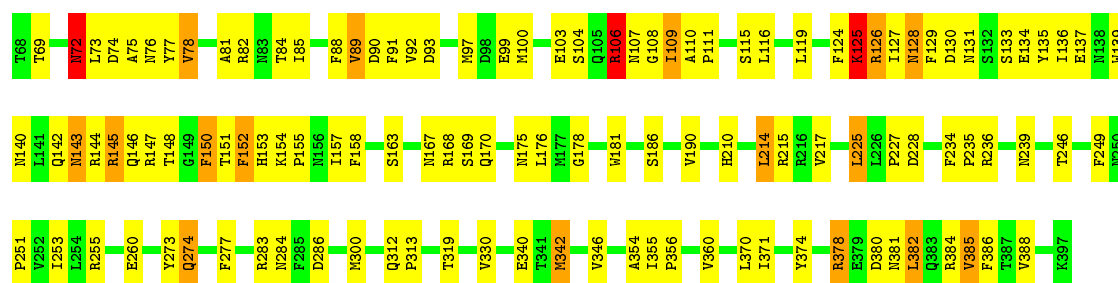


- Molecule 2: Intermediate capsid protein VP6



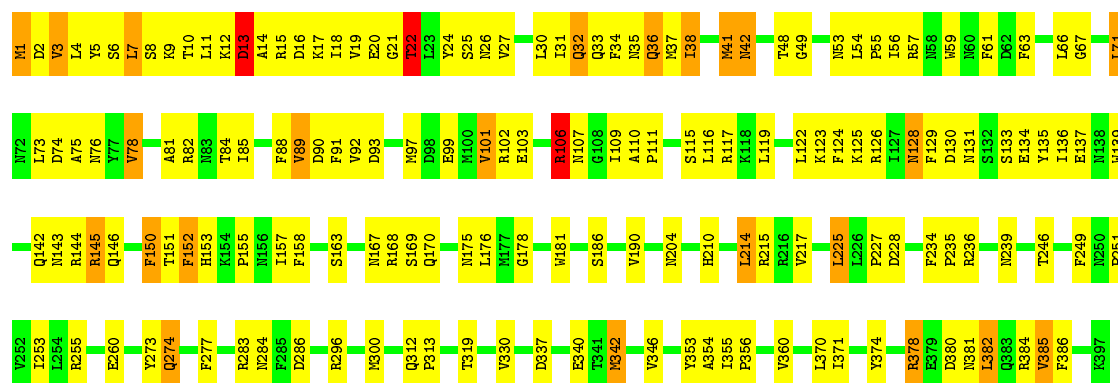
- Molecule 2: Intermediate capsid protein VP6





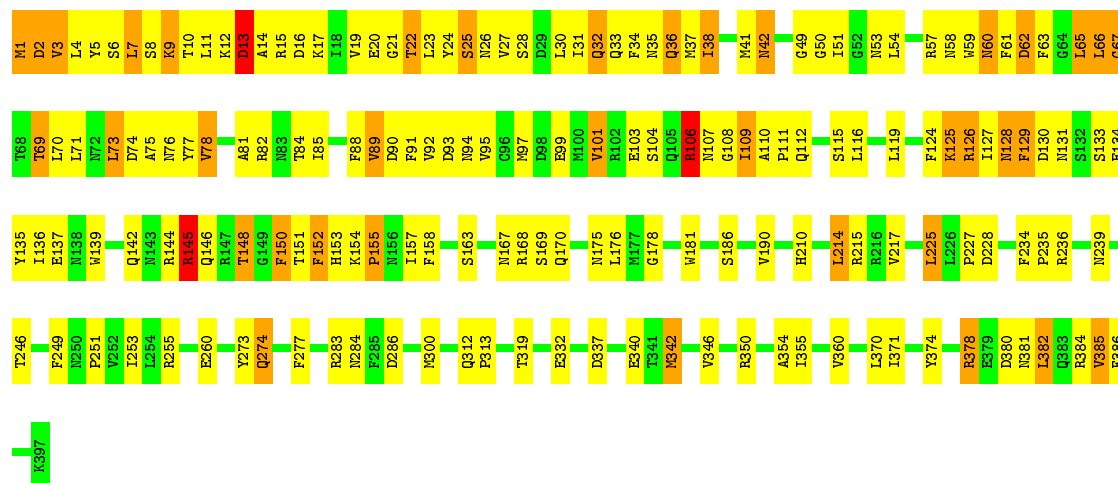
• Molecule 2: Intermediate capsid protein VP6

Chain M: 58% 35% 6%



• Molecule 2: Intermediate capsid protein VP6

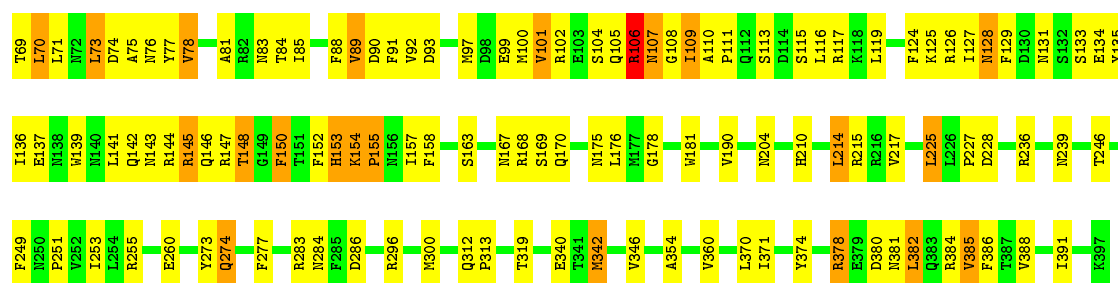
Chain N: 56% 34% 9%



• Molecule 2: Intermediate capsid protein VP6

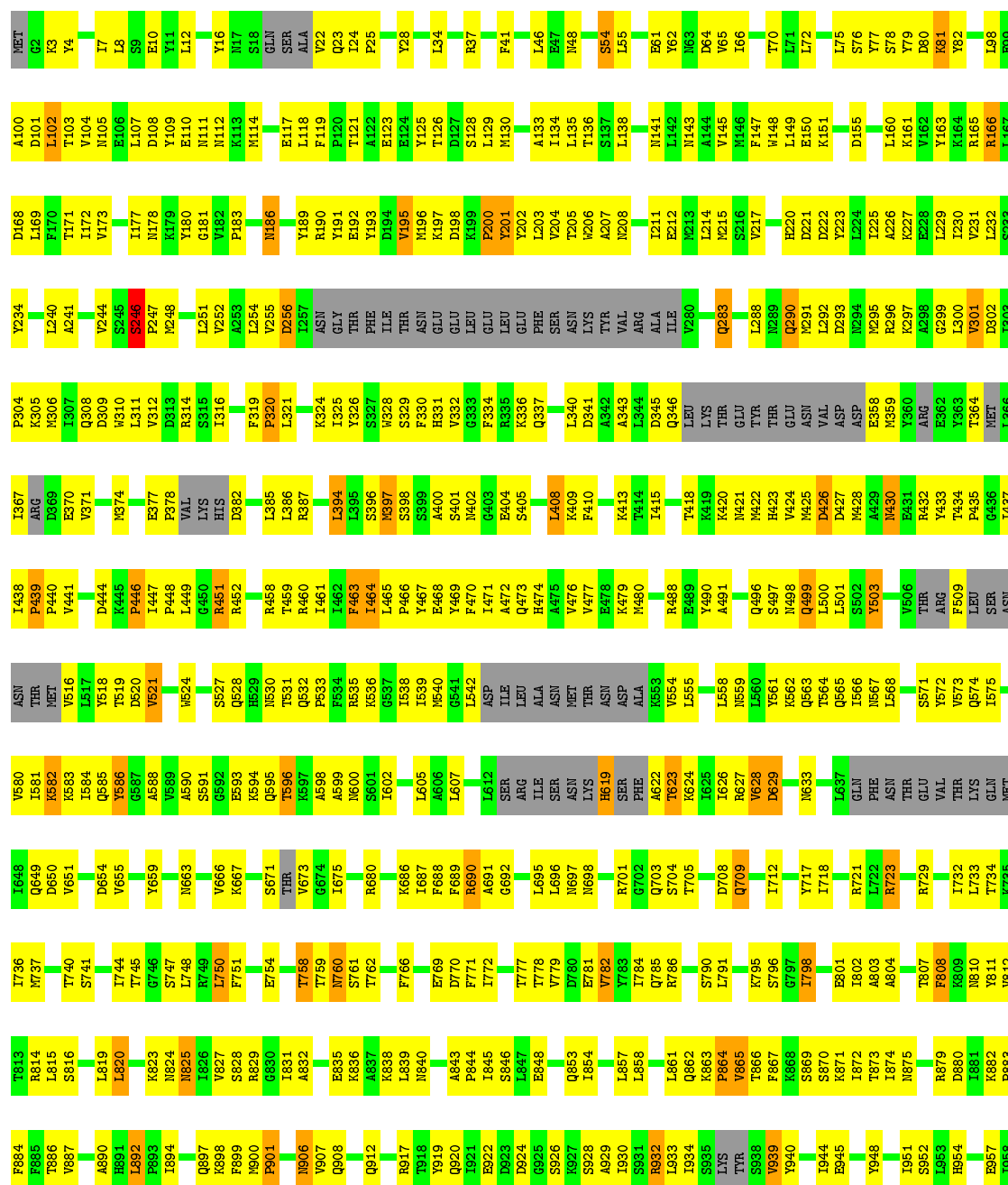
Chain O: 57% 33% 9%





• Molecule 3: RNA-directed RNA polymerase

Chain W: 40% 44% 5% 10%



|     |     |      |      |     |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |     |       |       |       |       |     |     |     |     |     |
|-----|-----|------|------|-----|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-------|-------|-------|-------|-----|-----|-----|-----|-----|
| LYS | ILE | PRO  | ALA  | VAL | THR  | F1031 | H1034 | A1037 | I1042 | M1043 | K1047 | N1048 | G1049 | S1050 | W1051 | I1052 | S1053 | L1054 | Y1058 | P1059 | M1063 | K1068 | K1069 | M1070 | W1071 | M1072 | I1073 | T1074 | R1077 | S1078 | P1079 | Y1080 | T1081 | M1082 | A1083 | M1084 | F1085 | F1086 | GLN   | GLU   | PRO   |       |       |     |       |       |       |       |     |     |     |     |     |
| GLN | LEU | Y961 | I962 | ILE | S964 | L965  | G966  | PRO   | LYS   | ILE   | ASP   | ALA   | ASP   | THR   | TYR   | VAL   | GLY   | SER   | LYS   | ILE   | Y981  | S982  | ARG   | D984  | R985  | Y986  | R987  | I988  | S991  | Y992  | L996  | I999  | M1000 | Y1001 | G1002 | C1003 | Y1004 | Q1005 | L1006 | F1009 | M1010 | D1013 | L1014 | GLU | K1016 | L1017 | I1018 | R1019 | ILE | PRO | PHE | LYS | GLY |

## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

| Property   | Value   | Source    |
|--|---|-----------|
| Space group  | P 21 21 21  | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 740.75Å 1198.07Å 1345.41Å<br>90.00° 90.00° 90.00°           | Depositor |
| Resolution (Å)   | 30.00 – 5.00  | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (30.00-5.00)                                | Depositor |
| $R_{merge}$  | (Not available)   | Depositor |
| $R_{sym}$  | (Not available)   | Depositor |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>               | 0.49 (at 3.78Å)   | Xtriage   |
| Refinement program                                       | CNS   | Depositor |
| R, $R_{free}$  | 0.293 , 0.296   | Depositor |
| Wilson B-factor (Å <sup>2</sup> )                        | 167.1   | Xtriage   |
| Anisotropy   | 0.043   | Xtriage   |
| Estimated twinning fraction                              | No twinning to report.                                      | Xtriage   |
| L-test for twinning <sup>2</sup>                         | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.29$ | Xtriage   |
| Outliers   | 4 of 2393850 reflections (0.000%)                           | Xtriage   |
| Total number of atoms                                    | 62014   | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 146.0   | wwPDB-VP  |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.48         | 0/6491      | 0.84        | 9/8806 (0.1%)   |
| 1   | B     | 0.50         | 0/6745      | 0.82        | 10/9149 (0.1%)  |
| 2   | C     | 0.51         | 0/3232      | 0.78        | 5/4397 (0.1%)   |
| 2   | D     | 0.51         | 0/3232      | 0.78        | 5/4397 (0.1%)   |
| 2   | E     | 0.51         | 0/3232      | 0.77        | 5/4397 (0.1%)   |
| 2   | F     | 0.50         | 0/3232      | 0.76        | 5/4397 (0.1%)   |
| 2   | G     | 0.50         | 0/3232      | 0.77        | 5/4397 (0.1%)   |
| 2   | H     | 0.50         | 0/3232      | 0.76        | 5/4397 (0.1%)   |
| 2   | I     | 0.50         | 0/3232      | 0.77        | 5/4397 (0.1%)   |
| 2   | J     | 0.51         | 0/3232      | 0.78        | 5/4397 (0.1%)   |
| 2   | K     | 0.51         | 0/3232      | 0.77        | 5/4397 (0.1%)   |
| 2   | L     | 0.51         | 0/3232      | 0.77        | 5/4397 (0.1%)   |
| 2   | M     | 0.51         | 0/3232      | 0.77        | 5/4397 (0.1%)   |
| 2   | N     | 0.51         | 0/3232      | 0.77        | 5/4397 (0.1%)   |
| 2   | O     | 0.52         | 0/3232      | 0.79        | 7/4397 (0.2%)   |
| 3   | W     | 0.41         | 0/8045      | 0.62        | 3/10847 (0.0%)  |
| All | All   | 0.49         | 0/63297     | 0.77        | 89/85963 (0.1%) |

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                   | 1                   |

There are no bond length outliers.

All (89) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 273  | TYR  | CB-CG-CD2 | 10.70 | 127.42      | 121.00   |
| 1   | A     | 273  | TYR  | CB-CG-CD1 | -9.86 | 115.08      | 121.00   |
| 1   | A     | 273  | TYR  | CA-CB-CG  | 9.85  | 132.12      | 113.40   |
| 1   | B     | 273  | TYR  | CB-CG-CD1 | 9.85  | 126.91      | 121.00   |
| 1   | B     | 273  | TYR  | CB-CG-CD2 | -9.21 | 115.48      | 121.00   |
| 1   | B     | 273  | TYR  | CA-CB-CG  | 9.02  | 130.53      | 113.40   |
| 1   | A     | 367  | LEU  | N-CA-C    | -7.59 | 90.51       | 111.00   |
| 1   | A     | 298  | TYR  | N-CA-C    | 7.41  | 131.01      | 111.00   |
| 2   | L     | 384  | ARG  | NE-CZ-NH2 | 7.00  | 123.80      | 120.30   |
| 2   | H     | 384  | ARG  | NE-CZ-NH2 | 6.92  | 123.76      | 120.30   |
| 2   | F     | 384  | ARG  | NE-CZ-NH2 | 6.86  | 123.73      | 120.30   |
| 2   | I     | 384  | ARG  | NE-CZ-NH2 | 6.80  | 123.70      | 120.30   |
| 2   | K     | 384  | ARG  | NE-CZ-NH2 | 6.75  | 123.67      | 120.30   |
| 1   | A     | 639  | LYS  | N-CA-C    | -6.67 | 92.98       | 111.00   |
| 2   | D     | 236  | ARG  | NE-CZ-NH2 | 6.67  | 123.64      | 120.30   |
| 2   | C     | 384  | ARG  | NE-CZ-NH2 | 6.67  | 123.64      | 120.30   |
| 2   | O     | 384  | ARG  | NE-CZ-NH2 | 6.66  | 123.63      | 120.30   |
| 2   | N     | 384  | ARG  | NE-CZ-NH2 | 6.62  | 123.61      | 120.30   |
| 2   | E     | 384  | ARG  | NE-CZ-NH2 | 6.59  | 123.59      | 120.30   |
| 2   | F     | 236  | ARG  | NE-CZ-NH2 | 6.57  | 123.58      | 120.30   |
| 2   | D     | 384  | ARG  | NE-CZ-NH2 | 6.57  | 123.58      | 120.30   |
| 2   | C     | 283  | ARG  | NE-CZ-NH2 | 6.51  | 123.56      | 120.30   |
| 2   | L     | 236  | ARG  | NE-CZ-NH2 | 6.51  | 123.56      | 120.30   |
| 2   | H     | 236  | ARG  | NE-CZ-NH2 | 6.51  | 123.55      | 120.30   |
| 2   | M     | 283  | ARG  | NE-CZ-NH2 | 6.46  | 123.53      | 120.30   |
| 2   | J     | 283  | ARG  | NE-CZ-NH2 | 6.42  | 123.51      | 120.30   |
| 2   | M     | 236  | ARG  | NE-CZ-NH2 | 6.41  | 123.51      | 120.30   |
| 2   | J     | 384  | ARG  | NE-CZ-NH2 | 6.40  | 123.50      | 120.30   |
| 2   | M     | 384  | ARG  | NE-CZ-NH2 | 6.38  | 123.49      | 120.30   |
| 2   | J     | 236  | ARG  | NE-CZ-NH2 | 6.38  | 123.49      | 120.30   |
| 2   | I     | 236  | ARG  | NE-CZ-NH2 | 6.37  | 123.49      | 120.30   |
| 2   | G     | 236  | ARG  | NE-CZ-NH2 | 6.35  | 123.47      | 120.30   |
| 2   | N     | 236  | ARG  | NE-CZ-NH2 | 6.34  | 123.47      | 120.30   |
| 3   | W     | 1082 | ASN  | N-CA-C    | 6.33  | 128.08      | 111.00   |
| 2   | D     | 283  | ARG  | NE-CZ-NH2 | 6.30  | 123.45      | 120.30   |
| 2   | O     | 283  | ARG  | NE-CZ-NH2 | 6.27  | 123.44      | 120.30   |
| 2   | N     | 283  | ARG  | NE-CZ-NH2 | 6.26  | 123.43      | 120.30   |
| 2   | G     | 384  | ARG  | NE-CZ-NH2 | 6.25  | 123.43      | 120.30   |
| 2   | O     | 236  | ARG  | NE-CZ-NH2 | 6.25  | 123.42      | 120.30   |
| 2   | E     | 236  | ARG  | NE-CZ-NH2 | 6.23  | 123.42      | 120.30   |
| 2   | C     | 236  | ARG  | NE-CZ-NH2 | 6.23  | 123.42      | 120.30   |
| 2   | K     | 236  | ARG  | NE-CZ-NH2 | 6.19  | 123.40      | 120.30   |
| 2   | G     | 283  | ARG  | NE-CZ-NH2 | 6.17  | 123.39      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | E     | 283  | ARG  | NE-CZ-NH2 | 6.13  | 123.37      | 120.30   |
| 2   | F     | 283  | ARG  | NE-CZ-NH2 | 6.12  | 123.36      | 120.30   |
| 1   | B     | 636  | LYS  | N-CA-C    | -6.10 | 94.53       | 111.00   |
| 2   | K     | 283  | ARG  | NE-CZ-NH2 | 6.08  | 123.34      | 120.30   |
| 2   | L     | 283  | ARG  | NE-CZ-NH2 | 6.08  | 123.34      | 120.30   |
| 2   | H     | 283  | ARG  | NE-CZ-NH2 | 6.06  | 123.33      | 120.30   |
| 2   | I     | 283  | ARG  | NE-CZ-NH2 | 6.03  | 123.31      | 120.30   |
| 2   | O     | 154  | LYS  | N-CA-C    | -5.98 | 94.86       | 111.00   |
| 2   | O     | 300  | MET  | CG-SD-CE  | 5.80  | 109.48      | 100.20   |
| 2   | C     | 300  | MET  | CG-SD-CE  | 5.80  | 109.47      | 100.20   |
| 2   | F     | 300  | MET  | CG-SD-CE  | 5.79  | 109.47      | 100.20   |
| 2   | I     | 300  | MET  | CG-SD-CE  | 5.78  | 109.44      | 100.20   |
| 2   | N     | 300  | MET  | CG-SD-CE  | 5.76  | 109.42      | 100.20   |
| 2   | L     | 300  | MET  | CG-SD-CE  | 5.76  | 109.41      | 100.20   |
| 1   | B     | 497  | ILE  | N-CA-C    | -5.75 | 95.47       | 111.00   |
| 2   | M     | 300  | MET  | CG-SD-CE  | 5.75  | 109.41      | 100.20   |
| 2   | D     | 300  | MET  | CG-SD-CE  | 5.75  | 109.39      | 100.20   |
| 2   | J     | 300  | MET  | CG-SD-CE  | 5.74  | 109.39      | 100.20   |
| 2   | G     | 300  | MET  | CG-SD-CE  | 5.73  | 109.37      | 100.20   |
| 2   | H     | 300  | MET  | CG-SD-CE  | 5.72  | 109.36      | 100.20   |
| 2   | K     | 300  | MET  | CG-SD-CE  | 5.70  | 109.31      | 100.20   |
| 1   | B     | 76   | LEU  | CA-CB-CG  | 5.69  | 128.40      | 115.30   |
| 2   | E     | 300  | MET  | CG-SD-CE  | 5.63  | 109.21      | 100.20   |
| 3   | W     | 1077 | ARG  | N-CA-C    | 5.57  | 126.05      | 111.00   |
| 1   | B     | 273  | TYR  | CB-CA-C   | -5.50 | 99.39       | 110.40   |
| 1   | B     | 811  | LEU  | N-CA-C    | -5.48 | 96.21       | 111.00   |
| 2   | M     | 342  | MET  | CG-SD-CE  | 5.35  | 108.75      | 100.20   |
| 2   | D     | 342  | MET  | CG-SD-CE  | 5.32  | 108.70      | 100.20   |
| 2   | G     | 342  | MET  | CG-SD-CE  | 5.29  | 108.67      | 100.20   |
| 1   | A     | 317  | LEU  | CA-CB-CG  | -5.27 | 103.18      | 115.30   |
| 2   | J     | 342  | MET  | CG-SD-CE  | 5.27  | 108.63      | 100.20   |
| 1   | B     | 317  | LEU  | CA-CB-CG  | -5.25 | 103.24      | 115.30   |
| 2   | L     | 342  | MET  | CG-SD-CE  | 5.23  | 108.57      | 100.20   |
| 2   | O     | 153  | HIS  | N-CA-C    | 5.22  | 125.09      | 111.00   |
| 2   | E     | 342  | MET  | CG-SD-CE  | 5.21  | 108.54      | 100.20   |
| 2   | N     | 342  | MET  | CG-SD-CE  | 5.21  | 108.53      | 100.20   |
| 2   | F     | 342  | MET  | CG-SD-CE  | 5.19  | 108.51      | 100.20   |
| 2   | O     | 342  | MET  | CG-SD-CE  | 5.19  | 108.50      | 100.20   |
| 2   | I     | 342  | MET  | CG-SD-CE  | 5.18  | 108.49      | 100.20   |
| 1   | B     | 82   | HIS  | N-CA-C    | -5.17 | 97.05       | 111.00   |
| 2   | C     | 342  | MET  | CG-SD-CE  | 5.16  | 108.46      | 100.20   |
| 3   | W     | 1085 | PHE  | N-CA-C    | 5.16  | 124.92      | 111.00   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | K     | 342 | MET  | CG-SD-CE | 5.15  | 108.44      | 100.20   |
| 2   | H     | 342 | MET  | CG-SD-CE | 5.14  | 108.43      | 100.20   |
| 1   | A     | 842 | LEU  | CA-CB-CG | -5.07 | 103.64      | 115.30   |
| 1   | A     | 719 | GLY  | N-CA-C   | -5.06 | 100.46      | 113.10   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 273 | TYR  | Sidechain |

## 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     | 6374  | 0        | 6394     | 1006    | 0            |
| 1   | B     | 6624  | 0        | 6652     | 1133    | 0            |
| 2   | C     | 3162  | 0        | 3101     | 170     | 0            |
| 2   | D     | 3162  | 0        | 3101     | 179     | 0            |
| 2   | E     | 3162  | 0        | 3101     | 164     | 0            |
| 2   | F     | 3162  | 0        | 3101     | 160     | 0            |
| 2   | G     | 3162  | 0        | 3101     | 149     | 0            |
| 2   | H     | 3162  | 0        | 3101     | 175     | 0            |
| 2   | I     | 3162  | 0        | 3101     | 215     | 0            |
| 2   | J     | 3162  | 0        | 3101     | 187     | 0            |
| 2   | K     | 3162  | 0        | 3101     | 166     | 0            |
| 2   | L     | 3162  | 0        | 3101     | 178     | 0            |
| 2   | M     | 3162  | 0        | 3101     | 173     | 0            |
| 2   | N     | 3162  | 0        | 3101     | 191     | 0            |
| 2   | O     | 3162  | 0        | 3101     | 163     | 0            |
| 3   | W     | 7905  | 0        | 7966     | 543     | 0            |
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | F     | 1     | 0        | 0        | 0       | 0            |
| 4   | I     | 1     | 0        | 0        | 0       | 0            |
| 4   | L     | 1     | 0        | 0        | 0       | 0            |
| 4   | O     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 62014 | 0        | 61325    | 4691    | 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 38.

All (4691) 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:B:75:VAL:HG22  | 3:W:673:VAL:CG1  | 1.63                     | 1.28              |
| 1:B:771:VAL:HB   | 1:B:809:PHE:HB3  | 1.23                     | 1.18              |
| 1:B:75:VAL:CG2   | 3:W:673:VAL:HG12 | 1.72                     | 1.18              |
| 1:A:333:VAL:HG11 | 1:A:380:LYS:HA   | 1.27                     | 1.15              |
| 1:A:428:GLN:OE1  | 1:A:456:PHE:HB2  | 1.46                     | 1.13              |
| 1:A:563:MET:HA   | 1:A:563:MET:HE3  | 1.22                     | 1.12              |
| 2:G:145:ARG:HB3  | 2:G:145:ARG:HH11 | 1.10                     | 1.12              |
| 2:H:83:ASN:ND2   | 2:I:122:LEU:HB2  | 1.65                     | 1.11              |
| 1:A:451:ASP:HB3  | 1:A:452:PRO:HD2  | 1.14                     | 1.11              |
| 1:B:432:VAL:HA   | 1:B:436:ILE:HD11 | 1.18                     | 1.11              |
| 1:B:734:ASN:HB3  | 1:B:737:GLU:HB2  | 1.28                     | 1.10              |
| 1:B:718:TYR:HB3  | 1:B:721:VAL:HG21 | 1.33                     | 1.10              |
| 1:B:548:ARG:NH1  | 1:B:878:ASN:H    | 1.50                     | 1.09              |
| 1:A:270:ILE:HD11 | 1:A:292:LEU:HD11 | 1.31                     | 1.09              |
| 2:L:22:THR:HG23  | 2:L:73:LEU:HD12  | 1.35                     | 1.08              |
| 1:A:699:ILE:HG12 | 1:A:700:ALA:H    | 1.18                     | 1.07              |
| 2:G:145:ARG:HD2  | 2:I:143:ASN:HA   | 1.34                     | 1.07              |
| 1:A:318:TRP:HA   | 1:A:321:ILE:HD12 | 1.34                     | 1.07              |
| 1:B:200:VAL:HG21 | 1:B:243:SER:HB3  | 1.13                     | 1.07              |
| 2:N:106:ARG:H    | 2:N:106:ARG:HD3  | 1.17                     | 1.06              |
| 1:B:790:ARG:HA   | 1:B:790:ARG:HE   | 0.98                     | 1.06              |
| 1:B:318:TRP:HA   | 1:B:321:ILE:HD12 | 1.37                     | 1.06              |
| 1:A:658:PRO:HG2  | 1:B:348:LYS:HG2  | 1.38                     | 1.05              |
| 1:B:498:ARG:HB2  | 2:I:32:GLN:HE22  | 1.15                     | 1.05              |
| 1:B:510:LEU:HD11 | 1:B:537:SER:HA   | 1.36                     | 1.04              |
| 1:A:721:VAL:HG12 | 1:A:722:ASN:H    | 1.18                     | 1.04              |
| 1:A:199:VAL:HG12 | 1:A:200:VAL:H    | 1.20                     | 1.04              |
| 1:B:457:GLN:HG3  | 1:B:458:ILE:H    | 1.22                     | 1.03              |
| 1:B:646:LEU:HA   | 1:B:649:LEU:HD12 | 1.40                     | 1.03              |
| 1:A:428:GLN:NE2  | 1:A:455:PRO:HB2  | 1.73                     | 1.03              |
| 1:B:274:ILE:HG23 | 1:B:278:ILE:HD11 | 1.40                     | 1.03              |
| 1:A:451:ASP:CB   | 1:A:452:PRO:HD2  | 1.84                     | 1.03              |
| 1:B:444:ARG:HH21 | 1:B:520:THR:HG23 | 1.20                     | 1.02              |
| 1:A:510:LEU:HD22 | 1:A:540:LEU:HD13 | 1.39                     | 1.02              |
| 1:A:310:LEU:HD12 | 1:A:310:LEU:H    | 1.21                     | 1.02              |
| 1:B:457:GLN:HB2  | 1:B:476:ASN:ND2  | 1.75                     | 1.02              |
| 1:A:513:LEU:HA   | 1:A:516:GLN:NE2  | 1.75                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:224:PHE:O    | 1:B:228:MET:HG2  | 1.61                     | 1.01              |
| 1:B:573:THR:HG22 | 1:B:574:GLU:H    | 0.88                     | 1.01              |
| 1:A:521:MET:HB3  | 1:A:522:PRO:HD3  | 1.39                     | 1.01              |
| 1:B:790:ARG:HE   | 1:B:790:ARG:CA   | 1.70                     | 1.00              |
| 1:A:506:LEU:HD23 | 1:A:544:VAL:HA   | 1.40                     | 1.00              |
| 2:C:106:ARG:HD3  | 2:C:106:ARG:H    | 1.26                     | 1.00              |
| 1:A:367:LEU:HD21 | 3:W:929:ALA:HA   | 1.44                     | 0.99              |
| 1:B:573:THR:HG22 | 1:B:574:GLU:N    | 1.71                     | 0.99              |
| 1:A:705:ILE:HA   | 1:A:823:THR:HG22 | 1.43                     | 0.99              |
| 1:B:674:VAL:HG21 | 1:B:679:LEU:HD13 | 1.44                     | 0.99              |
| 1:B:510:LEU:HD22 | 1:B:540:LEU:HD13 | 1.42                     | 0.99              |
| 1:B:473:HIS:HB2  | 2:I:126:ARG:HH22 | 1.21                     | 0.99              |
| 1:B:573:THR:CG2  | 1:B:574:GLU:H    | 1.71                     | 0.99              |
| 2:L:42:ASN:HA    | 2:L:61:PHE:HB2   | 1.43                     | 0.98              |
| 1:B:371:ASN:HD22 | 1:B:583:SER:HB3  | 1.28                     | 0.98              |
| 1:B:204:THR:HG23 | 1:B:244:ILE:HG22 | 1.44                     | 0.98              |
| 2:H:106:ARG:H    | 2:H:106:ARG:HD3  | 1.26                     | 0.98              |
| 1:A:275:PRO:HB2  | 1:A:278:ILE:HD11 | 1.45                     | 0.98              |
| 1:B:435:ILE:HG22 | 1:B:436:ILE:H    | 1.29                     | 0.98              |
| 1:B:265:LEU:HB3  | 1:B:296:ALA:HB1  | 1.46                     | 0.98              |
| 2:J:106:ARG:HD3  | 2:J:106:ARG:H    | 1.23                     | 0.97              |
| 1:B:743:ASP:C    | 1:B:744:TYR:HD2  | 1.67                     | 0.97              |
| 1:B:700:ALA:HB2  | 1:B:827:LYS:HB2  | 1.45                     | 0.97              |
| 1:B:700:ALA:CB   | 1:B:827:LYS:HB2  | 1.95                     | 0.97              |
| 1:A:540:LEU:O    | 1:A:544:VAL:HG23 | 1.64                     | 0.97              |
| 1:A:270:ILE:HG23 | 1:A:854:LEU:HD21 | 1.46                     | 0.96              |
| 3:W:441:VAL:HB   | 3:W:447:ILE:HD11 | 1.46                     | 0.96              |
| 1:A:192:ASN:O    | 1:A:193:SER:HB3  | 1.65                     | 0.96              |
| 2:H:83:ASN:HD21  | 2:I:122:LEU:HB2  | 1.30                     | 0.96              |
| 1:B:200:VAL:HG21 | 1:B:243:SER:CB   | 1.96                     | 0.96              |
| 1:A:660:ASP:HB3  | 1:B:539:ARG:HD2  | 1.43                     | 0.96              |
| 1:A:588:ILE:HG22 | 1:A:589:GLY:H    | 1.28                     | 0.96              |
| 1:B:717:MET:HE1  | 1:B:830:PRO:HD2  | 1.48                     | 0.95              |
| 1:B:458:ILE:HD12 | 1:B:459:ALA:N    | 1.81                     | 0.95              |
| 1:B:435:ILE:O    | 1:B:438:PRO:HD2  | 1.67                     | 0.95              |
| 3:W:385:LEU:HD23 | 3:W:479:LYS:HE2  | 1.48                     | 0.95              |
| 2:I:145:ARG:NH1  | 2:I:145:ARG:HB3  | 1.82                     | 0.95              |
| 3:W:651:VAL:O    | 3:W:655:VAL:HG23 | 1.66                     | 0.95              |
| 1:A:563:MET:HA   | 1:A:563:MET:CE   | 1.98                     | 0.94              |
| 1:A:510:LEU:HD11 | 1:A:537:SER:HA   | 1.46                     | 0.94              |
| 1:B:446:HIS:O    | 1:B:447:TYR:HB2  | 1.68                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:27:VAL:O     | 2:O:31:ILE:HG12  | 1.66                     | 0.93              |
| 1:A:779:ASP:HA   | 1:A:798:ILE:CD1  | 1.98                     | 0.93              |
| 1:B:764:PRO:O    | 1:B:765:PHE:HB3  | 1.65                     | 0.93              |
| 1:B:518:PHE:HB3  | 1:B:519:PRO:HD2  | 1.49                     | 0.93              |
| 1:B:790:ARG:HA   | 1:B:790:ARG:NE   | 1.84                     | 0.92              |
| 1:A:428:GLN:HE21 | 1:A:455:PRO:HB2  | 1.30                     | 0.92              |
| 2:G:145:ARG:HB3  | 2:G:145:ARG:NH1  | 1.84                     | 0.92              |
| 1:B:126:PHE:HD2  | 1:B:126:PHE:H    | 1.09                     | 0.92              |
| 3:W:8:LEU:HD12   | 3:W:737:MET:HG2  | 1.49                     | 0.92              |
| 1:B:722:ASN:HD22 | 1:B:824:LYS:HA   | 1.35                     | 0.92              |
| 1:B:190:ASN:HD21 | 1:B:193:SER:HB3  | 1.31                     | 0.92              |
| 2:G:6:SER:OG     | 2:G:128:ASN:HA   | 1.70                     | 0.92              |
| 1:B:513:LEU:HA   | 1:B:516:GLN:NE2  | 1.85                     | 0.91              |
| 1:B:428:GLN:HB2  | 1:B:456:PHE:CD1  | 2.05                     | 0.91              |
| 1:A:779:ASP:HA   | 1:A:798:ILE:HD12 | 1.50                     | 0.91              |
| 1:B:803:ASN:H    | 1:B:807:ASN:HD21 | 1.17                     | 0.91              |
| 1:A:661:GLN:HE21 | 1:B:348:LYS:NZ   | 1.67                     | 0.91              |
| 1:B:454:THR:HG21 | 1:B:476:ASN:ND2  | 1.86                     | 0.91              |
| 1:B:166:PHE:HE2  | 1:B:689:MET:HA   | 1.34                     | 0.91              |
| 1:B:459:ALA:HB1  | 1:B:463:ILE:HD11 | 1.51                     | 0.90              |
| 1:A:588:ILE:HG22 | 1:A:589:GLY:N    | 1.85                     | 0.90              |
| 2:L:88:PHE:O     | 2:L:92:VAL:HG23  | 1.72                     | 0.90              |
| 1:A:339:LEU:HD22 | 1:A:588:ILE:HA   | 1.53                     | 0.90              |
| 1:A:126:PHE:N    | 1:A:126:PHE:HD2  | 1.68                     | 0.90              |
| 2:L:106:ARG:H    | 2:L:106:ARG:HD3  | 1.37                     | 0.90              |
| 2:N:145:ARG:O    | 2:N:146:GLN:HG3  | 1.71                     | 0.90              |
| 2:C:88:PHE:O     | 2:C:92:VAL:HG23  | 1.72                     | 0.89              |
| 1:B:509:ALA:O    | 1:B:513:LEU:HG   | 1.71                     | 0.89              |
| 1:A:244:ILE:HD13 | 1:A:835:PHE:HE1  | 1.38                     | 0.89              |
| 1:A:169:LEU:O    | 1:A:173:VAL:HG23 | 1.73                     | 0.89              |
| 1:A:660:ASP:HB3  | 1:B:539:ARG:HH11 | 1.38                     | 0.89              |
| 1:A:358:LEU:HD21 | 3:W:986:TYR:CE2  | 2.08                     | 0.89              |
| 2:K:106:ARG:H    | 2:K:106:ARG:HD3  | 1.37                     | 0.89              |
| 1:A:855:LEU:O    | 1:A:857:PHE:N    | 2.06                     | 0.88              |
| 1:B:457:GLN:O    | 1:B:459:ALA:N    | 2.05                     | 0.88              |
| 1:A:371:ASN:C    | 1:A:373:GLN:H    | 1.71                     | 0.88              |
| 1:A:486:ASP:HB2  | 1:A:490:ASN:HD22 | 1.38                     | 0.88              |
| 1:B:874:MET:O    | 1:B:875:ARG:HB2  | 1.73                     | 0.88              |
| 2:M:88:PHE:O     | 2:M:92:VAL:HG23  | 1.74                     | 0.88              |
| 1:B:99:GLU:HB3   | 1:B:100:PRO:HD3  | 1.54                     | 0.88              |
| 1:B:658:PRO:HB2  | 1:B:661:GLN:HG2  | 1.56                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:106:ARG:HD3  | 2:J:106:ARG:N    | 1.87                     | 0.88              |
| 1:A:194:ARG:HH11 | 1:A:229:ARG:HG2  | 1.39                     | 0.88              |
| 1:B:803:ASN:H    | 1:B:807:ASN:ND2  | 1.72                     | 0.87              |
| 3:W:438:ILE:HG22 | 3:W:468:GLU:HB3  | 1.55                     | 0.87              |
| 1:B:182:LEU:HD11 | 1:B:847:THR:H    | 1.38                     | 0.87              |
| 1:B:297:ARG:HG3  | 1:B:848:PHE:HD2  | 1.40                     | 0.87              |
| 1:A:428:GLN:HB2  | 1:A:456:PHE:CD1  | 2.09                     | 0.86              |
| 1:A:509:ALA:O    | 1:A:513:LEU:HG   | 1.75                     | 0.86              |
| 1:B:447:TYR:O    | 1:B:448:ARG:HG2  | 1.73                     | 0.86              |
| 2:O:88:PHE:O     | 2:O:92:VAL:HG23  | 1.72                     | 0.86              |
| 2:D:88:PHE:O     | 2:D:92:VAL:HG23  | 1.73                     | 0.86              |
| 2:I:76:ASN:H     | 2:M:76:ASN:HB2   | 1.37                     | 0.86              |
| 3:W:98:LEU:HD11  | 3:W:172:ILE:HG23 | 1.56                     | 0.86              |
| 1:B:513:LEU:HA   | 1:B:516:GLN:CD   | 1.95                     | 0.86              |
| 3:W:499:GLN:HG3  | 3:W:1086:PHE:HB2 | 1.55                     | 0.86              |
| 1:B:451:ASP:H    | 1:B:452:PRO:HD3  | 1.39                     | 0.86              |
| 1:B:413:VAL:HG12 | 1:B:414:VAL:N    | 1.88                     | 0.86              |
| 2:N:88:PHE:O     | 2:N:92:VAL:HG23  | 1.74                     | 0.86              |
| 1:B:473:HIS:HB2  | 2:I:126:ARG:NH2  | 1.91                     | 0.86              |
| 1:B:745:ALA:HB1  | 1:B:748:THR:HB   | 1.57                     | 0.86              |
| 2:H:88:PHE:O     | 2:H:92:VAL:HG23  | 1.73                     | 0.86              |
| 2:I:24:TYR:O     | 2:I:27:VAL:HG22  | 1.74                     | 0.86              |
| 1:B:540:LEU:O    | 1:B:544:VAL:HG23 | 1.75                     | 0.86              |
| 1:B:182:LEU:HD23 | 1:B:183:LEU:H    | 1.40                     | 0.86              |
| 1:A:275:PRO:HB2  | 1:A:278:ILE:CD1  | 2.04                     | 0.86              |
| 1:A:150:LEU:HD12 | 1:A:696:SER:HB2  | 1.58                     | 0.86              |
| 2:E:88:PHE:O     | 2:E:92:VAL:HG23  | 1.75                     | 0.86              |
| 2:J:88:PHE:O     | 2:J:92:VAL:HG23  | 1.75                     | 0.85              |
| 1:A:451:ASP:HB3  | 1:A:452:PRO:CD   | 2.03                     | 0.85              |
| 2:I:88:PHE:O     | 2:I:92:VAL:HG23  | 1.76                     | 0.85              |
| 1:B:590:ASN:HD22 | 1:B:590:ASN:N    | 1.74                     | 0.85              |
| 1:B:366:PHE:C    | 1:B:368:THR:H    | 1.76                     | 0.85              |
| 3:W:605:LEU:HB2  | 3:W:628:VAL:HG11 | 1.57                     | 0.85              |
| 2:C:150:PHE:HB2  | 2:C:152:PHE:CE1  | 2.11                     | 0.85              |
| 2:F:88:PHE:O     | 2:F:92:VAL:HG23  | 1.75                     | 0.85              |
| 1:A:366:PHE:C    | 1:A:368:THR:H    | 1.76                     | 0.85              |
| 2:M:106:ARG:H    | 2:M:106:ARG:HD3  | 1.40                     | 0.85              |
| 1:B:126:PHE:HD2  | 1:B:126:PHE:N    | 1.73                     | 0.85              |
| 2:G:88:PHE:O     | 2:G:92:VAL:HG23  | 1.75                     | 0.85              |
| 2:M:6:SER:OG     | 2:M:128:ASN:HA   | 1.76                     | 0.85              |
| 2:H:6:SER:OG     | 2:H:128:ASN:HA   | 1.77                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:723:ILE:HG22 | 1:B:724:ALA:H    | 1.40                     | 0.84              |
| 1:A:239:VAL:HG22 | 1:A:846:LEU:HG   | 1.58                     | 0.84              |
| 3:W:248:MET:HE3  | 3:W:248:MET:O    | 1.77                     | 0.84              |
| 1:B:518:PHE:HD2  | 2:H:69:THR:HB    | 1.40                     | 0.84              |
| 1:B:306:ASP:O    | 1:B:308:LEU:N    | 2.10                     | 0.84              |
| 2:K:88:PHE:O     | 2:K:92:VAL:HG23  | 1.76                     | 0.84              |
| 1:B:825:VAL:HG12 | 1:B:826:TYR:N    | 1.91                     | 0.84              |
| 1:B:701:GLN:HB2  | 1:B:826:TYR:HD2  | 1.40                     | 0.84              |
| 1:A:660:ASP:HB3  | 1:B:539:ARG:CD   | 2.05                     | 0.84              |
| 1:B:415:PRO:HG2  | 1:B:480:PHE:HD1  | 1.42                     | 0.84              |
| 2:L:144:ARG:O    | 2:L:145:ARG:HB2  | 1.74                     | 0.84              |
| 1:A:125:ILE:N    | 1:A:125:ILE:HD12 | 1.92                     | 0.84              |
| 1:B:735:LEU:HG   | 1:B:760:VAL:O    | 1.78                     | 0.84              |
| 1:A:570:THR:HG22 | 1:A:571:LEU:H    | 1.42                     | 0.84              |
| 1:B:498:ARG:NH1  | 2:J:25:SER:HB3   | 1.92                     | 0.84              |
| 1:B:200:VAL:CG2  | 1:B:243:SER:HB3  | 2.05                     | 0.84              |
| 1:B:471:TRP:HB2  | 1:B:512:GLN:OE1  | 1.77                     | 0.84              |
| 1:B:503:ILE:HD11 | 1:B:548:ARG:HG2  | 1.58                     | 0.84              |
| 1:A:126:PHE:CD2  | 1:A:126:PHE:N    | 2.42                     | 0.84              |
| 2:I:76:ASN:HB2   | 2:M:76:ASN:HB2   | 1.57                     | 0.84              |
| 2:F:82:ARG:NH1   | 2:H:144:ARG:HD2  | 1.93                     | 0.84              |
| 1:A:771:VAL:HG13 | 1:A:772:ILE:H    | 1.43                     | 0.84              |
| 1:B:428:GLN:HG2  | 1:B:429:LEU:N    | 1.92                     | 0.83              |
| 1:B:435:ILE:HG22 | 1:B:436:ILE:N    | 1.93                     | 0.83              |
| 2:L:23:LEU:HD21  | 2:N:36:GLN:OE1   | 1.76                     | 0.83              |
| 1:A:361:GLN:HB2  | 1:A:528:SER:OG   | 1.78                     | 0.83              |
| 3:W:296:ARG:NH2  | 3:W:308:GLN:HE21 | 1.75                     | 0.83              |
| 3:W:248:MET:HG2  | 3:W:326:TYR:CD2  | 2.13                     | 0.83              |
| 3:W:520:ASP:HB2  | 3:W:667:LYS:HE3  | 1.59                     | 0.83              |
| 3:W:254:LEU:HB3  | 3:W:314:ARG:HD2  | 1.58                     | 0.83              |
| 2:I:23:LEU:HD23  | 2:I:24:TYR:N     | 1.94                     | 0.83              |
| 1:B:454:THR:HG21 | 1:B:476:ASN:HD21 | 1.39                     | 0.83              |
| 1:A:158:GLY:H    | 1:A:762:ALA:HB3  | 1.43                     | 0.83              |
| 3:W:4:TYR:HD1    | 3:W:733:LEU:HD22 | 1.41                     | 0.83              |
| 1:B:126:PHE:N    | 1:B:126:PHE:CD2  | 2.43                     | 0.83              |
| 1:A:474:PHE:O    | 1:A:478:ASN:HB2  | 1.77                     | 0.83              |
| 1:A:216:GLU:CD   | 1:A:216:GLU:H    | 1.81                     | 0.83              |
| 1:B:799:LEU:HD22 | 1:B:800:TYR:N    | 1.93                     | 0.83              |
| 1:B:457:GLN:HB2  | 1:B:476:ASN:CG   | 1.98                     | 0.83              |
| 1:A:471:TRP:HB2  | 1:A:512:GLN:OE1  | 1.79                     | 0.83              |
| 1:A:524:ASP:O    | 1:A:526:LYS:N    | 2.10                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:647:LYS:HG3  | 1:A:654:VAL:HG21 | 1.59                     | 0.83              |
| 3:W:539:ILE:HG23 | 3:W:562:LYS:HG3  | 1.61                     | 0.82              |
| 3:W:750:LEU:HD21 | 3:W:861:LEU:HD22 | 1.60                     | 0.82              |
| 2:O:6:SER:OG     | 2:O:128:ASN:HA   | 1.80                     | 0.82              |
| 2:I:38:ILE:HG22  | 2:I:42:ASN:HD21  | 1.42                     | 0.82              |
| 1:B:516:GLN:HA   | 1:B:518:PHE:HE1  | 1.41                     | 0.82              |
| 1:B:590:ASN:H    | 1:B:590:ASN:HD22 | 1.25                     | 0.82              |
| 1:A:461:GLN:HA   | 2:F:32:GLN:HE22  | 1.43                     | 0.82              |
| 1:B:428:GLN:HA   | 1:B:431:ILE:HD12 | 1.61                     | 0.82              |
| 2:F:150:PHE:HB2  | 2:F:152:PHE:CE1  | 2.15                     | 0.82              |
| 1:B:722:ASN:HB2  | 1:B:824:LYS:HB3  | 1.62                     | 0.81              |
| 1:A:486:ASP:HB2  | 1:A:490:ASN:ND2  | 1.94                     | 0.81              |
| 2:H:109:ILE:HG13 | 2:H:109:ILE:O    | 1.79                     | 0.81              |
| 1:A:734:ASN:HB3  | 1:A:737:GLU:HG2  | 1.61                     | 0.81              |
| 1:B:454:THR:CG2  | 1:B:476:ASN:HD21 | 1.92                     | 0.81              |
| 1:B:769:SER:HB3  | 1:B:807:ASN:OD1  | 1.80                     | 0.81              |
| 1:A:406:SER:O    | 1:A:409:TRP:HB3  | 1.81                     | 0.81              |
| 2:L:22:THR:HB    | 2:N:128:ASN:O    | 1.79                     | 0.81              |
| 3:W:367:ILE:O    | 3:W:371:VAL:HG23 | 1.80                     | 0.81              |
| 1:B:494:ASN:ND2  | 1:B:495:ASP:H    | 1.79                     | 0.81              |
| 1:A:712:LEU:HB3  | 1:A:721:VAL:O    | 1.79                     | 0.81              |
| 1:B:218:GLU:HG3  | 1:B:221:VAL:HG23 | 1.62                     | 0.81              |
| 1:B:193:SER:HB2  | 1:B:226:ALA:HA   | 1.62                     | 0.81              |
| 1:B:725:ARG:H    | 1:B:725:ARG:HD2  | 1.44                     | 0.81              |
| 1:B:537:SER:O    | 1:B:540:LEU:HB3  | 1.81                     | 0.81              |
| 1:B:498:ARG:HB2  | 2:I:32:GLN:NE2   | 1.94                     | 0.81              |
| 1:B:511:MET:CE   | 2:J:70:LEU:HG    | 2.09                     | 0.81              |
| 2:H:76:ASN:HB2   | 2:J:76:ASN:HB2   | 1.60                     | 0.81              |
| 1:A:459:ALA:O    | 1:A:462:GLN:HB2  | 1.81                     | 0.81              |
| 2:I:76:ASN:CB    | 2:M:76:ASN:HB2   | 2.11                     | 0.81              |
| 1:B:118:LYS:HG2  | 1:B:119:GLN:H    | 1.46                     | 0.81              |
| 1:A:712:LEU:HG   | 1:A:819:PRO:HB2  | 1.61                     | 0.81              |
| 1:B:315:GLU:HB3  | 1:B:571:LEU:HD11 | 1.61                     | 0.80              |
| 2:O:67:GLY:O     | 2:O:69:THR:N     | 2.14                     | 0.80              |
| 3:W:906:ASN:HD22 | 3:W:907:VAL:H    | 1.26                     | 0.80              |
| 2:E:24:TYR:O     | 2:E:27:VAL:HG22  | 1.82                     | 0.80              |
| 2:D:128:ASN:O    | 2:E:22:THR:HB    | 1.82                     | 0.80              |
| 1:A:660:ASP:O    | 1:A:662:MET:N    | 2.14                     | 0.80              |
| 1:B:510:LEU:CD1  | 1:B:537:SER:HA   | 2.11                     | 0.80              |
| 1:A:699:ILE:HG12 | 1:A:700:ALA:N    | 1.97                     | 0.80              |
| 1:A:362:SER:HB2  | 1:A:365:GLN:NE2  | 1.97                     | 0.80              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:L:150:PHE:HB2   | 2:L:152:PHE:CE1  | 2.17                     | 0.80              |
| 1:A:546:LEU:HD21  | 1:A:588:ILE:CD1  | 2.12                     | 0.80              |
| 1:A:270:ILE:CD1   | 1:A:292:LEU:HD11 | 2.10                     | 0.80              |
| 1:B:239:VAL:HG23  | 1:B:844:SER:O    | 1.81                     | 0.80              |
| 1:A:126:PHE:H     | 1:A:126:PHE:HD2  | 1.26                     | 0.80              |
| 1:A:370:ILE:HD11  | 3:W:933:LEU:O    | 1.81                     | 0.80              |
| 2:N:144:ARG:O     | 2:N:145:ARG:HB2  | 1.81                     | 0.80              |
| 1:A:769:SER:HB3   | 1:A:807:ASN:OD1  | 1.82                     | 0.80              |
| 1:B:869:VAL:CG1   | 1:B:873:ASN:HA   | 2.11                     | 0.80              |
| 3:W:78:SER:O      | 3:W:747:SER:HB2  | 1.81                     | 0.80              |
| 1:B:506:LEU:HD23  | 1:B:544:VAL:HA   | 1.62                     | 0.79              |
| 1:B:393:SER:O     | 1:B:394:LEU:HD23 | 1.82                     | 0.79              |
| 1:B:743:ASP:CG    | 1:B:745:ALA:H    | 1.85                     | 0.79              |
| 1:A:437:TYR:N     | 1:A:438:PRO:HD2  | 1.97                     | 0.79              |
| 1:A:303:LEU:HA    | 1:A:615:ASN:ND2  | 1.97                     | 0.79              |
| 1:A:694:ARG:HG2   | 1:A:701:GLN:HE22 | 1.46                     | 0.79              |
| 1:A:199:VAL:HG12  | 1:A:200:VAL:N    | 1.97                     | 0.79              |
| 1:B:790:ARG:HG3   | 1:B:791:LYS:H    | 1.48                     | 0.79              |
| 2:L:104:SER:O     | 2:L:108:GLY:HA3  | 1.82                     | 0.79              |
| 2:I:57:ARG:HH11   | 2:I:94:ASN:HD21  | 1.31                     | 0.79              |
| 1:A:869:VAL:HG11  | 1:A:873:ASN:HA   | 1.64                     | 0.79              |
| 1:B:744:TYR:CD2   | 1:B:744:TYR:N    | 2.38                     | 0.79              |
| 2:K:6:SER:OG      | 2:K:128:ASN:HA   | 1.82                     | 0.79              |
| 1:A:721:VAL:HG12  | 1:A:722:ASN:N    | 1.98                     | 0.79              |
| 3:W:836:LYS:HA    | 3:W:839:LEU:HD12 | 1.64                     | 0.79              |
| 1:A:370:ILE:HG13  | 3:W:933:LEU:CD1  | 2.13                     | 0.79              |
| 1:B:457:GLN:HG3   | 1:B:458:ILE:N    | 1.98                     | 0.79              |
| 1:B:465:ASN:HD22  | 1:B:468:VAL:HG23 | 1.47                     | 0.79              |
| 1:A:480:PHE:CD2   | 1:A:493:LEU:HB3  | 2.18                     | 0.79              |
| 1:B:673:PRO:O     | 1:B:674:VAL:HG13 | 1.83                     | 0.79              |
| 2:H:2:ASP:HB2     | 2:H:128:ASN:HD21 | 1.46                     | 0.79              |
| 1:A:606:VAL:HG23  | 1:A:607:ASN:H    | 1.46                     | 0.79              |
| 3:W:1018:ILE:HD12 | 3:W:1037:ALA:HB1 | 1.65                     | 0.79              |
| 1:B:124:ARG:C     | 1:B:125:ILE:HD12 | 2.02                     | 0.79              |
| 2:N:50:GLY:O      | 2:N:51:ILE:HG23  | 1.83                     | 0.79              |
| 1:B:277:ARG:O     | 1:B:278:ILE:HG12 | 1.83                     | 0.79              |
| 1:A:869:VAL:CG1   | 1:A:873:ASN:HA   | 2.12                     | 0.79              |
| 3:W:843:ALA:HB3   | 3:W:844:PRO:HD3  | 1.64                     | 0.79              |
| 1:B:272:ASN:C     | 1:B:274:ILE:H    | 1.87                     | 0.78              |
| 1:B:548:ARG:HH11  | 1:B:878:ASN:H    | 1.28                     | 0.78              |
| 1:B:743:ASP:C     | 1:B:744:TYR:CD2  | 2.54                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:128:ASN:O    | 2:K:22:THR:HB    | 1.83                     | 0.78              |
| 1:B:75:VAL:HG22  | 3:W:673:VAL:HG12 | 0.83                     | 0.78              |
| 1:A:445:MET:C    | 1:A:447:TYR:H    | 1.84                     | 0.78              |
| 2:M:145:ARG:O    | 2:M:146:GLN:HG3  | 1.83                     | 0.78              |
| 3:W:296:ARG:HH22 | 3:W:308:GLN:HE21 | 1.29                     | 0.78              |
| 1:A:428:GLN:HG2  | 1:A:429:LEU:N    | 1.98                     | 0.78              |
| 1:A:305:GLN:O    | 1:A:307:ARG:HG3  | 1.82                     | 0.78              |
| 1:B:523:VAL:C    | 1:B:525:TYR:H    | 1.85                     | 0.78              |
| 1:A:118:LYS:HG2  | 1:A:119:GLN:N    | 1.98                     | 0.78              |
| 1:A:480:PHE:HD2  | 1:A:493:LEU:HB3  | 1.49                     | 0.78              |
| 1:B:549:LEU:HD13 | 1:B:877:MET:HE1  | 1.64                     | 0.78              |
| 1:B:606:VAL:HG23 | 1:B:607:ASN:H    | 1.46                     | 0.78              |
| 1:A:639:LYS:O    | 1:A:643:GLU:HG3  | 1.84                     | 0.78              |
| 3:W:1001:TYR:HD1 | 3:W:1084:ASN:HB3 | 1.49                     | 0.78              |
| 2:I:42:ASN:HA    | 2:I:61:PHE:HB2   | 1.66                     | 0.78              |
| 1:B:702:GLY:HA3  | 1:B:759:LEU:O    | 1.84                     | 0.77              |
| 1:B:717:MET:CE   | 1:B:830:PRO:HD2  | 2.15                     | 0.77              |
| 2:N:144:ARG:NH2  | 2:N:146:GLN:HE22 | 1.81                     | 0.77              |
| 3:W:212:GLU:HB2  | 3:W:696:LEU:HD12 | 1.65                     | 0.77              |
| 1:B:562:THR:HB   | 1:B:611:HIS:CD2  | 2.20                     | 0.77              |
| 1:B:374:ALA:HB1  | 1:B:580:SER:HB3  | 1.66                     | 0.77              |
| 3:W:186:ASN:HD22 | 3:W:186:ASN:H    | 1.32                     | 0.77              |
| 1:B:779:ASP:HA   | 1:B:798:ILE:CD1  | 2.14                     | 0.77              |
| 1:B:406:SER:O    | 1:B:409:TRP:HB3  | 1.84                     | 0.77              |
| 2:I:128:ASN:HD22 | 2:J:19:VAL:HB    | 1.49                     | 0.77              |
| 2:H:106:ARG:CD   | 2:H:106:ARG:H    | 1.98                     | 0.77              |
| 2:K:93:ASP:O     | 2:K:97:MET:HG3   | 1.85                     | 0.77              |
| 2:E:93:ASP:O     | 2:E:97:MET:HG3   | 1.84                     | 0.77              |
| 2:M:22:THR:HG23  | 2:M:73:LEU:HD12  | 1.66                     | 0.77              |
| 1:B:764:PRO:O    | 1:B:765:PHE:CB   | 2.33                     | 0.77              |
| 3:W:704:SER:HB2  | 3:W:709:GLN:HE22 | 1.47                     | 0.77              |
| 1:A:471:TRP:O    | 1:A:475:VAL:HG23 | 1.85                     | 0.77              |
| 1:B:169:LEU:O    | 1:B:173:VAL:HG23 | 1.84                     | 0.77              |
| 1:B:855:LEU:O    | 1:B:857:PHE:N    | 2.17                     | 0.77              |
| 1:B:204:THR:CG2  | 1:B:244:ILE:HG22 | 2.14                     | 0.77              |
| 2:H:93:ASP:O     | 2:H:97:MET:HG3   | 1.85                     | 0.77              |
| 1:A:371:ASN:C    | 1:A:373:GLN:N    | 2.37                     | 0.76              |
| 1:B:503:ILE:O    | 1:B:505:GLN:HG2  | 1.85                     | 0.76              |
| 1:B:573:THR:O    | 1:B:574:GLU:HG2  | 1.84                     | 0.76              |
| 1:B:744:TYR:HD2  | 1:B:744:TYR:N    | 1.77                     | 0.76              |
| 1:B:166:PHE:CE2  | 1:B:689:MET:HA   | 2.20                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:218:GLU:HG3  | 1:B:221:VAL:CG2  | 2.15                     | 0.76              |
| 2:F:17:LYS:HG2   | 2:H:130:ASP:HA   | 1.67                     | 0.76              |
| 3:W:217:VAL:HG13 | 3:W:222:ASP:HB2  | 1.66                     | 0.76              |
| 1:A:614:TYR:O    | 1:A:618:ILE:HG12 | 1.85                     | 0.76              |
| 1:A:405:ILE:HG21 | 1:A:536:LEU:HG   | 1.67                     | 0.76              |
| 1:B:200:VAL:HG23 | 1:B:242:PRO:O    | 1.86                     | 0.76              |
| 1:B:731:GLN:HG2  | 2:D:62:ASP:HB2   | 1.67                     | 0.76              |
| 1:A:548:ARG:HH12 | 1:A:878:ASN:H    | 1.34                     | 0.76              |
| 1:A:588:ILE:CG2  | 1:A:589:GLY:H    | 1.99                     | 0.76              |
| 1:A:122:LEU:HG   | 1:A:201:ASP:OD2  | 1.84                     | 0.76              |
| 1:A:461:GLN:HA   | 2:F:32:GLN:NE2   | 2.00                     | 0.76              |
| 1:B:133:ILE:HD12 | 1:B:145:ARG:HB2  | 1.66                     | 0.76              |
| 1:B:678:ARG:O    | 1:B:681:ILE:HG22 | 1.85                     | 0.76              |
| 2:D:67:GLY:O     | 2:D:68:THR:HG23  | 1.85                     | 0.76              |
| 2:C:24:TYR:O     | 2:C:27:VAL:HG22  | 1.86                     | 0.76              |
| 2:I:110:ALA:HB1  | 2:I:111:PRO:CD   | 2.16                     | 0.76              |
| 1:B:701:GLN:HA   | 1:B:761:GLY:O    | 1.85                     | 0.76              |
| 1:A:158:GLY:H    | 1:A:762:ALA:CB   | 1.99                     | 0.76              |
| 1:B:199:VAL:HG12 | 1:B:200:VAL:N    | 2.00                     | 0.76              |
| 2:G:93:ASP:O     | 2:G:97:MET:HG3   | 1.85                     | 0.76              |
| 1:A:678:ARG:O    | 1:A:681:ILE:HG22 | 1.86                     | 0.76              |
| 1:A:503:ILE:HD13 | 1:A:547:THR:HB   | 1.68                     | 0.76              |
| 1:B:675:GLU:HB3  | 1:B:678:ARG:HG2  | 1.68                     | 0.76              |
| 1:A:428:GLN:HA   | 1:A:431:ILE:HD12 | 1.68                     | 0.76              |
| 1:A:244:ILE:HD13 | 1:A:835:PHE:CE1  | 2.21                     | 0.76              |
| 2:I:93:ASP:O     | 2:I:97:MET:HG3   | 1.86                     | 0.76              |
| 1:B:361:GLN:HE22 | 3:W:624:LYS:NZ   | 1.84                     | 0.76              |
| 1:B:96:PRO:O     | 1:B:652:PHE:HB3  | 1.84                     | 0.76              |
| 1:A:310:LEU:CD1  | 1:A:310:LEU:H    | 1.97                     | 0.75              |
| 1:B:518:PHE:CB   | 1:B:519:PRO:HD2  | 2.14                     | 0.75              |
| 2:C:145:ARG:HB3  | 2:C:145:ARG:NH1  | 2.02                     | 0.75              |
| 2:F:104:SER:HB3  | 2:F:108:GLY:CA   | 2.16                     | 0.75              |
| 1:B:781:THR:O    | 1:B:783:PHE:N    | 2.19                     | 0.75              |
| 1:A:371:ASN:HA   | 1:A:374:ALA:HB3  | 1.68                     | 0.75              |
| 1:A:457:GLN:HB2  | 1:A:476:ASN:HD21 | 1.52                     | 0.75              |
| 2:L:19:VAL:HG23  | 2:N:128:ASN:HB3  | 1.69                     | 0.75              |
| 2:J:93:ASP:O     | 2:J:97:MET:HG3   | 1.87                     | 0.75              |
| 1:B:498:ARG:CB   | 2:I:32:GLN:HE22  | 1.97                     | 0.75              |
| 1:B:251:ALA:HA   | 2:N:69:THR:HG21  | 1.69                     | 0.75              |
| 1:A:694:ARG:HG2  | 1:A:701:GLN:NE2  | 2.01                     | 0.74              |
| 3:W:520:ASP:HB3  | 3:W:667:LYS:HB3  | 1.69                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:38:ILE:HG22  | 2:C:42:ASN:HD21  | 1.51                     | 0.74              |
| 1:B:698:LYS:O    | 1:B:699:ILE:HB   | 1.86                     | 0.74              |
| 2:I:76:ASN:HB2   | 2:M:76:ASN:CB    | 2.17                     | 0.74              |
| 1:B:491:GLN:HG3  | 1:B:565:MET:H    | 1.50                     | 0.74              |
| 1:A:537:SER:O    | 1:A:540:LEU:HB3  | 1.87                     | 0.74              |
| 1:A:148:TRP:CZ3  | 1:A:246:HIS:HB2  | 2.22                     | 0.74              |
| 2:J:128:ASN:HB3  | 2:K:19:VAL:HG23  | 1.69                     | 0.74              |
| 3:W:708:ASP:HB3  | 3:W:1080:TYR:CE1 | 2.21                     | 0.74              |
| 3:W:820:LEU:HB3  | 3:W:824:ASN:HD22 | 1.51                     | 0.74              |
| 2:N:57:ARG:HH11  | 2:N:94:ASN:HD21  | 1.33                     | 0.74              |
| 1:A:492:VAL:HG13 | 1:A:558:MET:SD   | 2.27                     | 0.74              |
| 1:B:482:GLN:HB2  | 1:B:493:LEU:HD22 | 1.70                     | 0.74              |
| 1:B:675:GLU:HB3  | 1:B:678:ARG:CG   | 2.17                     | 0.74              |
| 1:B:688:ASN:O    | 1:B:692:ILE:HD12 | 1.87                     | 0.74              |
| 1:A:647:LYS:CG   | 1:A:654:VAL:HG21 | 2.17                     | 0.74              |
| 3:W:825:ASN:HA   | 3:W:828:SER:HB2  | 1.69                     | 0.74              |
| 1:B:614:TYR:O    | 1:B:618:ILE:HG12 | 1.87                     | 0.74              |
| 3:W:165:ARG:HD3  | 3:W:223:TYR:HB2  | 1.68                     | 0.74              |
| 2:O:150:PHE:HB2  | 2:O:152:PHE:CE1  | 2.23                     | 0.74              |
| 1:B:293:PRO:C    | 1:B:295:THR:H    | 1.90                     | 0.74              |
| 2:I:75:ALA:HB3   | 2:M:76:ASN:HA    | 1.68                     | 0.74              |
| 2:D:23:LEU:HD23  | 2:D:24:TYR:N     | 2.03                     | 0.74              |
| 2:D:93:ASP:O     | 2:D:97:MET:HG3   | 1.87                     | 0.74              |
| 2:L:93:ASP:O     | 2:L:97:MET:HG3   | 1.88                     | 0.74              |
| 1:A:286:LEU:HD23 | 1:A:286:LEU:H    | 1.52                     | 0.74              |
| 1:B:190:ASN:ND2  | 1:B:193:SER:HB3  | 2.03                     | 0.74              |
| 1:B:783:PHE:HD1  | 1:B:783:PHE:H    | 1.33                     | 0.74              |
| 1:A:784:ALA:O    | 1:A:787:VAL:HG23 | 1.88                     | 0.74              |
| 2:H:105:GLN:C    | 2:H:107:ASN:H    | 1.91                     | 0.74              |
| 1:A:802:ILE:HA   | 1:A:807:ASN:HD21 | 1.52                     | 0.74              |
| 2:D:24:TYR:O     | 2:D:27:VAL:HG22  | 1.88                     | 0.74              |
| 2:C:82:ARG:CZ    | 2:E:144:ARG:HD2  | 2.18                     | 0.74              |
| 1:A:428:GLN:HB2  | 1:A:456:PHE:HD1  | 1.51                     | 0.74              |
| 1:A:405:ILE:CG2  | 1:A:536:LEU:HG   | 2.18                     | 0.74              |
| 2:E:54:LEU:HD12  | 2:E:55:PRO:HD2   | 1.70                     | 0.74              |
| 1:A:301:PRO:O    | 1:A:303:LEU:HD23 | 1.87                     | 0.74              |
| 1:B:510:LEU:HD11 | 1:B:537:SER:CA   | 2.15                     | 0.74              |
| 2:D:6:SER:OG     | 2:D:128:ASN:HA   | 1.87                     | 0.74              |
| 1:A:252:PHE:HD2  | 1:A:684:LEU:HD21 | 1.52                     | 0.74              |
| 1:A:164:GLU:O    | 1:A:167:LEU:HB3  | 1.87                     | 0.74              |
| 1:B:433:ASN:ND2  | 1:B:446:HIS:HB3  | 2.02                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:368:THR:HG22 | 1:B:371:ASN:HD21 | 1.51                     | 0.73              |
| 3:W:473:GLN:OE1  | 3:W:595:GLN:HG2  | 1.88                     | 0.73              |
| 2:J:150:PHE:HB2  | 2:J:152:PHE:CE1  | 2.22                     | 0.73              |
| 1:B:254:GLU:HG2  | 2:N:69:THR:HB    | 1.68                     | 0.73              |
| 1:A:275:PRO:CB   | 1:A:278:ILE:HD11 | 2.18                     | 0.73              |
| 1:A:117:LYS:O    | 1:A:179:ASP:HB2  | 1.88                     | 0.73              |
| 2:G:106:ARG:H    | 2:G:106:ARG:HD3  | 1.53                     | 0.73              |
| 1:A:711:GLN:C    | 1:A:712:LEU:HD23 | 2.08                     | 0.73              |
| 2:M:144:ARG:HD2  | 2:N:82:ARG:NH1   | 2.02                     | 0.73              |
| 1:A:660:ASP:CB   | 1:B:539:ARG:HD2  | 2.19                     | 0.73              |
| 2:H:109:ILE:HB   | 2:H:380:ASP:HB3  | 1.68                     | 0.73              |
| 1:A:277:ARG:HD3  | 1:A:559:ALA:HB2  | 1.71                     | 0.73              |
| 1:B:257:LEU:O    | 1:B:260:GLN:HG3  | 1.88                     | 0.73              |
| 2:F:42:ASN:HA    | 2:F:61:PHE:HB2   | 1.70                     | 0.73              |
| 2:C:93:ASP:O     | 2:C:97:MET:HG3   | 1.87                     | 0.73              |
| 1:A:310:LEU:HD12 | 1:A:310:LEU:N    | 2.00                     | 0.73              |
| 1:B:540:LEU:HD23 | 1:B:541:GLY:N    | 2.03                     | 0.73              |
| 1:B:457:GLN:C    | 1:B:459:ALA:H    | 1.91                     | 0.73              |
| 3:W:708:ASP:O    | 3:W:712:ILE:HG13 | 1.88                     | 0.73              |
| 2:N:93:ASP:O     | 2:N:97:MET:HG3   | 1.87                     | 0.73              |
| 1:A:499:ASN:HA   | 1:A:505:GLN:NE2  | 2.04                     | 0.73              |
| 2:N:24:TYR:O     | 2:N:27:VAL:HG22  | 1.89                     | 0.73              |
| 1:B:265:LEU:HB3  | 1:B:296:ALA:CB   | 2.17                     | 0.73              |
| 2:I:145:ARG:HH11 | 2:I:145:ARG:HB3  | 1.50                     | 0.73              |
| 1:B:111:ILE:C    | 1:B:113:PRO:HD3  | 2.09                     | 0.73              |
| 1:B:703:VAL:HG13 | 1:B:824:LYS:O    | 1.89                     | 0.73              |
| 1:A:286:LEU:HD23 | 1:A:286:LEU:N    | 2.04                     | 0.73              |
| 1:A:245:LEU:HB3  | 1:A:249:ASP:HB2  | 1.71                     | 0.73              |
| 3:W:906:ASN:HD22 | 3:W:907:VAL:N    | 1.85                     | 0.73              |
| 2:M:93:ASP:O     | 2:M:97:MET:HG3   | 1.88                     | 0.73              |
| 2:F:93:ASP:O     | 2:F:97:MET:HG3   | 1.87                     | 0.73              |
| 1:B:771:VAL:HB   | 1:B:809:PHE:CB   | 2.11                     | 0.73              |
| 1:B:770:SER:HB2  | 1:B:773:SER:OG   | 1.88                     | 0.73              |
| 1:A:631:LEU:HB3  | 1:A:633:LEU:HD13 | 1.69                     | 0.73              |
| 1:A:661:GLN:HE21 | 1:B:348:LYS:HZ1  | 1.37                     | 0.73              |
| 1:B:503:ILE:O    | 1:B:505:GLN:N    | 2.22                     | 0.73              |
| 1:B:491:GLN:CD   | 1:B:564:ASN:HB3  | 2.08                     | 0.73              |
| 1:B:674:VAL:HG23 | 1:B:679:LEU:HD22 | 1.69                     | 0.73              |
| 2:J:11:LEU:O     | 2:J:14:ALA:HB3   | 1.89                     | 0.73              |
| 2:F:145:ARG:O    | 2:F:146:GLN:HG2  | 1.89                     | 0.73              |
| 1:B:701:GLN:O    | 1:B:826:TYR:HB3  | 1.89                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:277:ARG:O    | 1:B:279:ARG:N    | 2.20                     | 0.73              |
| 2:D:63:PHE:CD2   | 2:D:84:THR:HG23  | 2.24                     | 0.73              |
| 2:H:27:VAL:O     | 2:H:31:ILE:HG12  | 1.88                     | 0.73              |
| 2:F:23:LEU:HD21  | 2:H:36:GLN:OE1   | 1.89                     | 0.73              |
| 1:B:436:ILE:HG13 | 1:B:437:TYR:H    | 1.54                     | 0.72              |
| 1:B:471:TRP:O    | 1:B:475:VAL:HG23 | 1.88                     | 0.72              |
| 2:H:106:ARG:N    | 2:H:106:ARG:HD3  | 2.03                     | 0.72              |
| 1:B:712:LEU:CD1  | 1:B:722:ASN:HB3  | 2.18                     | 0.72              |
| 1:A:643:GLU:HG2  | 1:A:662:MET:HE3  | 1.72                     | 0.72              |
| 1:B:498:ARG:HH12 | 2:J:25:SER:HB3   | 1.52                     | 0.72              |
| 1:B:442:MET:CE   | 1:B:463:ILE:HG12 | 2.19                     | 0.72              |
| 1:B:521:MET:HB2  | 1:B:522:PRO:CD   | 2.19                     | 0.72              |
| 3:W:473:GLN:HG2  | 3:W:561:TYR:CE1  | 2.23                     | 0.72              |
| 3:W:394:LEU:HD21 | 3:W:424:VAL:HG11 | 1.69                     | 0.72              |
| 1:A:510:LEU:CD1  | 1:A:537:SER:HA   | 2.20                     | 0.72              |
| 1:B:799:LEU:HD22 | 1:B:800:TYR:H    | 1.52                     | 0.72              |
| 1:B:516:GLN:HA   | 1:B:518:PHE:CE1  | 2.25                     | 0.72              |
| 1:B:492:VAL:HG11 | 1:B:558:MET:HG2  | 1.71                     | 0.72              |
| 1:A:370:ILE:HG13 | 3:W:933:LEU:HD12 | 1.71                     | 0.72              |
| 1:B:435:ILE:C    | 1:B:436:ILE:HG12 | 2.08                     | 0.72              |
| 2:J:106:ARG:HG2  | 2:J:107:ASN:H    | 1.54                     | 0.72              |
| 1:B:630:ARG:O    | 1:B:631:LEU:HG   | 1.90                     | 0.72              |
| 3:W:627:ARG:HH11 | 3:W:627:ARG:HG2  | 1.54                     | 0.72              |
| 1:A:629:ASN:O    | 1:A:631:LEU:N    | 2.17                     | 0.72              |
| 1:B:615:ASN:O    | 1:B:618:ILE:HB   | 1.90                     | 0.72              |
| 1:A:420:ILE:HG12 | 1:A:423:SER:HB2  | 1.69                     | 0.72              |
| 2:M:122:LEU:HB2  | 2:O:83:ASN:ND2   | 2.04                     | 0.72              |
| 2:J:144:ARG:HD2  | 2:K:82:ARG:NH1   | 2.05                     | 0.72              |
| 1:A:496:ASN:HD22 | 1:A:498:ARG:HB2  | 1.53                     | 0.72              |
| 2:F:22:THR:HB    | 2:H:128:ASN:O    | 1.89                     | 0.72              |
| 1:B:444:ARG:NH2  | 1:B:520:THR:HG23 | 2.03                     | 0.72              |
| 3:W:370:GLU:O    | 3:W:374:MET:HG3  | 1.88                     | 0.72              |
| 1:B:156:PRO:HB2  | 1:B:161:ASP:HB3  | 1.72                     | 0.72              |
| 1:A:239:VAL:CG2  | 1:A:846:LEU:HG   | 2.19                     | 0.72              |
| 1:A:613:ASN:HD22 | 1:A:649:LEU:CD2  | 2.03                     | 0.72              |
| 3:W:447:ILE:HD12 | 3:W:447:ILE:N    | 2.05                     | 0.72              |
| 1:A:605:ASN:O    | 1:A:608:VAL:HB   | 1.90                     | 0.72              |
| 3:W:331:HIS:NE2  | 3:W:692:GLY:HA2  | 2.05                     | 0.72              |
| 3:W:430:ASN:HB3  | 3:W:432:ARG:HG3  | 1.71                     | 0.72              |
| 1:B:825:VAL:HG12 | 1:B:826:TYR:H    | 1.53                     | 0.72              |
| 1:B:551:ALA:O    | 1:B:555:GLU:HB2  | 1.90                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:721:VAL:CG1  | 1:A:722:ASN:H    | 2.01                     | 0.72              |
| 1:A:146:TRP:O    | 1:A:833:PHE:HB3  | 1.89                     | 0.72              |
| 2:I:135:TYR:OH   | 2:I:340:GLU:OE1  | 2.06                     | 0.72              |
| 2:D:145:ARG:O    | 2:D:146:GLN:HG3  | 1.90                     | 0.72              |
| 1:B:473:HIS:HB3  | 2:I:126:ARG:HH12 | 1.54                     | 0.71              |
| 1:A:445:MET:O    | 1:A:447:TYR:N    | 2.23                     | 0.71              |
| 2:D:11:LEU:O     | 2:D:14:ALA:HB3   | 1.90                     | 0.71              |
| 3:W:101:ASP:O    | 3:W:104:VAL:HG23 | 1.90                     | 0.71              |
| 1:B:355:LEU:HG   | 1:B:356:GLU:N    | 2.05                     | 0.71              |
| 1:B:480:PHE:CE2  | 1:B:493:LEU:HB2  | 2.24                     | 0.71              |
| 1:B:442:MET:HE1  | 1:B:463:ILE:HG12 | 1.71                     | 0.71              |
| 1:A:735:LEU:HG   | 1:A:760:VAL:O    | 1.89                     | 0.71              |
| 1:A:764:PRO:O    | 1:A:797:PRO:HD2  | 1.91                     | 0.71              |
| 1:B:422:GLU:HA   | 1:B:425:VAL:HG23 | 1.72                     | 0.71              |
| 2:O:93:ASP:O     | 2:O:97:MET:HG3   | 1.90                     | 0.71              |
| 2:J:130:ASP:HA   | 2:K:17:LYS:HG2   | 1.71                     | 0.71              |
| 2:L:6:SER:OG     | 2:L:128:ASN:HA   | 1.91                     | 0.71              |
| 1:B:156:PRO:CB   | 1:B:161:ASP:HB3  | 2.20                     | 0.71              |
| 2:C:144:ARG:HD2  | 2:D:82:ARG:CZ    | 2.20                     | 0.71              |
| 1:B:428:GLN:OE1  | 1:B:456:PHE:HB2  | 1.90                     | 0.71              |
| 2:I:11:LEU:O     | 2:I:14:ALA:HB3   | 1.91                     | 0.71              |
| 1:B:194:ARG:O    | 1:B:196:ALA:N    | 2.23                     | 0.71              |
| 1:A:709:ASP:HB3  | 1:A:820:THR:HG23 | 1.73                     | 0.71              |
| 1:A:246:HIS:HB3  | 1:A:249:ASP:OD2  | 1.90                     | 0.71              |
| 3:W:293:ASP:HA   | 3:W:296:ARG:HD2  | 1.72                     | 0.71              |
| 3:W:22:VAL:HG22  | 3:W:77:TYR:HB3   | 1.72                     | 0.71              |
| 2:I:150:PHE:HB2  | 2:I:152:PHE:CE1  | 2.25                     | 0.71              |
| 2:K:11:LEU:O     | 2:K:14:ALA:HB3   | 1.91                     | 0.71              |
| 1:B:791:LYS:O    | 1:B:792:VAL:HG22 | 1.91                     | 0.71              |
| 1:B:166:PHE:CE2  | 1:B:689:MET:HG3  | 2.24                     | 0.71              |
| 1:A:236:ARG:HB2  | 1:A:238:VAL:HG23 | 1.72                     | 0.71              |
| 1:A:530:GLN:HA   | 1:A:533:ILE:HD12 | 1.71                     | 0.71              |
| 1:B:605:ASN:O    | 1:B:608:VAL:HB   | 1.91                     | 0.71              |
| 2:K:38:ILE:HG22  | 2:K:42:ASN:HD21  | 1.56                     | 0.71              |
| 2:N:11:LEU:O     | 2:N:14:ALA:HB3   | 1.91                     | 0.71              |
| 2:N:38:ILE:HG22  | 2:N:42:ASN:HD21  | 1.56                     | 0.71              |
| 1:A:194:ARG:NH1  | 1:A:229:ARG:HG2  | 2.05                     | 0.71              |
| 1:B:277:ARG:HG2  | 1:B:278:ILE:H    | 1.54                     | 0.71              |
| 2:O:11:LEU:O     | 2:O:14:ALA:HB3   | 1.90                     | 0.71              |
| 2:H:116:LEU:HD12 | 2:H:119:LEU:HB2  | 1.73                     | 0.71              |
| 2:G:36:GLN:OE1   | 2:H:23:LEU:HD21  | 1.91                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:283:ASN:O    | 1:A:863:VAL:HG23 | 1.91                     | 0.71              |
| 1:B:712:LEU:HD12 | 1:B:722:ASN:HB3  | 1.72                     | 0.71              |
| 1:B:548:ARG:HH12 | 1:B:878:ASN:H    | 1.35                     | 0.71              |
| 1:A:510:LEU:HD11 | 1:A:537:SER:CA   | 2.21                     | 0.71              |
| 2:M:11:LEU:O     | 2:M:14:ALA:HB3   | 1.91                     | 0.71              |
| 2:G:4:LEU:HA     | 2:G:7:LEU:HD12   | 1.73                     | 0.71              |
| 1:A:496:ASN:ND2  | 1:A:498:ARG:HB2  | 2.06                     | 0.71              |
| 2:K:53:ASN:HD22  | 2:K:354:ALA:HB3  | 1.56                     | 0.71              |
| 1:A:415:PRO:HG2  | 1:A:480:PHE:CD1  | 2.26                     | 0.70              |
| 1:A:501:HIS:C    | 1:A:503:ILE:HG13 | 2.11                     | 0.70              |
| 1:B:374:ALA:HB1  | 1:B:580:SER:HA   | 1.71                     | 0.70              |
| 2:L:82:ARG:CZ    | 2:N:144:ARG:HD2  | 2.21                     | 0.70              |
| 1:A:312:ASP:O    | 1:A:313:ASN:HB3  | 1.90                     | 0.70              |
| 1:A:102:GLU:O    | 3:W:555:LEU:HD11 | 1.90                     | 0.70              |
| 3:W:340:LEU:O    | 3:W:340:LEU:HD12 | 1.90                     | 0.70              |
| 2:D:4:LEU:HA     | 2:D:7:LEU:HD12   | 1.73                     | 0.70              |
| 2:M:150:PHE:HB2  | 2:M:152:PHE:CE1  | 2.26                     | 0.70              |
| 1:B:164:GLU:O    | 1:B:167:LEU:HB3  | 1.90                     | 0.70              |
| 1:A:615:ASN:O    | 1:A:618:ILE:HB   | 1.89                     | 0.70              |
| 1:B:518:PHE:CD2  | 2:H:69:THR:HB    | 2.24                     | 0.70              |
| 1:B:477:ASN:ND2  | 2:I:39:ILE:HG21  | 2.06                     | 0.70              |
| 2:J:106:ARG:H    | 2:J:106:ARG:CD   | 2.03                     | 0.70              |
| 2:J:109:ILE:HD12 | 2:J:109:ILE:O    | 1.91                     | 0.70              |
| 1:B:511:MET:HE1  | 2:J:70:LEU:HG    | 1.72                     | 0.70              |
| 2:N:4:LEU:HA     | 2:N:7:LEU:HD12   | 1.73                     | 0.70              |
| 1:B:259:HIS:CD2  | 1:B:677:ARG:HG3  | 2.25                     | 0.70              |
| 2:J:12:LYS:C     | 2:J:14:ALA:H     | 1.94                     | 0.70              |
| 2:C:11:LEU:O     | 2:C:14:ALA:HB3   | 1.90                     | 0.70              |
| 2:K:54:LEU:HD12  | 2:K:55:PRO:HD2   | 1.71                     | 0.70              |
| 1:A:551:ALA:O    | 1:A:555:GLU:HB2  | 1.92                     | 0.70              |
| 1:A:506:LEU:CD2  | 1:A:544:VAL:HA   | 2.18                     | 0.70              |
| 1:B:230:GLN:HA   | 1:B:242:PRO:HD3  | 1.73                     | 0.70              |
| 1:A:467:GLN:HB2  | 1:A:515:ARG:HD2  | 1.72                     | 0.70              |
| 1:B:508:GLU:HG2  | 1:B:512:GLN:NE2  | 2.07                     | 0.70              |
| 1:A:762:ALA:O    | 1:A:763:LEU:HG   | 1.92                     | 0.70              |
| 1:B:790:ARG:HG3  | 1:B:791:LYS:N    | 2.05                     | 0.70              |
| 1:A:131:LEU:HD12 | 1:A:132:PRO:HD2  | 1.74                     | 0.70              |
| 2:J:116:LEU:HD12 | 2:J:119:LEU:HB2  | 1.74                     | 0.70              |
| 2:N:167:ASN:HD22 | 2:N:178:GLY:HA2  | 1.57                     | 0.70              |
| 1:A:783:PHE:H    | 1:A:783:PHE:HD1  | 1.38                     | 0.70              |
| 2:G:167:ASN:HD22 | 2:G:178:GLY:HA2  | 1.57                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:153:HIS:NE2  | 2:E:153:HIS:NE2  | 2.39                     | 0.70              |
| 2:C:167:ASN:HD22 | 2:C:178:GLY:HA2  | 1.57                     | 0.70              |
| 1:A:482:GLN:OE1  | 1:A:493:LEU:HD22 | 1.90                     | 0.70              |
| 2:I:12:LYS:C     | 2:I:14:ALA:H     | 1.95                     | 0.70              |
| 1:B:786:ILE:HG13 | 1:B:787:VAL:H    | 1.56                     | 0.70              |
| 1:B:262:VAL:CG1  | 1:B:297:ARG:HB3  | 2.21                     | 0.70              |
| 1:A:560:CYS:HB2  | 1:A:603:TYR:HD2  | 1.57                     | 0.70              |
| 2:K:167:ASN:HD22 | 2:K:178:GLY:HA2  | 1.57                     | 0.70              |
| 2:O:154:LYS:N    | 2:O:155:PRO:CD   | 2.54                     | 0.70              |
| 1:B:393:SER:N    | 1:B:573:THR:HG23 | 2.06                     | 0.70              |
| 1:B:857:PHE:HD1  | 1:B:857:PHE:H    | 1.40                     | 0.70              |
| 2:C:4:LEU:HA     | 2:C:7:LEU:HD12   | 1.74                     | 0.70              |
| 2:O:167:ASN:HD22 | 2:O:178:GLY:HA2  | 1.57                     | 0.70              |
| 2:J:167:ASN:HD22 | 2:J:178:GLY:HA2  | 1.57                     | 0.70              |
| 2:J:38:ILE:HG22  | 2:J:42:ASN:HD21  | 1.56                     | 0.70              |
| 1:B:721:VAL:CG1  | 1:B:799:LEU:HD21 | 2.22                     | 0.70              |
| 1:A:396:PHE:HB3  | 1:A:578:LEU:CD1  | 2.22                     | 0.70              |
| 1:A:401:TYR:HA   | 1:A:404:LEU:HD13 | 1.73                     | 0.70              |
| 1:A:436:ILE:HD11 | 1:A:437:TYR:CD1  | 2.27                     | 0.70              |
| 2:C:6:SER:OG     | 2:C:128:ASN:HA   | 1.92                     | 0.70              |
| 2:E:38:ILE:HG22  | 2:E:42:ASN:HD21  | 1.57                     | 0.70              |
| 3:W:999:ILE:HD11 | 3:W:1009:PHE:CD1 | 2.27                     | 0.70              |
| 1:B:318:TRP:CA   | 1:B:321:ILE:HD12 | 2.19                     | 0.69              |
| 1:B:791:LYS:O    | 1:B:792:VAL:HG13 | 1.91                     | 0.69              |
| 1:A:781:THR:O    | 1:A:783:PHE:N    | 2.24                     | 0.69              |
| 1:B:670:ARG:O    | 1:B:671:LEU:HD23 | 1.92                     | 0.69              |
| 2:O:4:LEU:HA     | 2:O:7:LEU:HD12   | 1.74                     | 0.69              |
| 2:D:239:ASN:HD22 | 2:D:246:THR:HG22 | 1.57                     | 0.69              |
| 1:B:590:ASN:H    | 1:B:590:ASN:ND2  | 1.90                     | 0.69              |
| 2:F:104:SER:HB3  | 2:F:108:GLY:HA2  | 1.74                     | 0.69              |
| 2:C:22:THR:OG1   | 2:C:26:ASN:ND2   | 2.25                     | 0.69              |
| 2:O:106:ARG:HD3  | 2:O:106:ARG:H    | 1.56                     | 0.69              |
| 3:W:434:THR:HG21 | 3:W:437:ILE:HD12 | 1.74                     | 0.69              |
| 1:A:548:ARG:HH11 | 1:A:877:MET:HA   | 1.56                     | 0.69              |
| 2:N:106:ARG:N    | 2:N:106:ARG:HD3  | 2.01                     | 0.69              |
| 1:B:182:LEU:HD11 | 1:B:847:THR:N    | 2.07                     | 0.69              |
| 3:W:248:MET:HA   | 3:W:251:LEU:HD12 | 1.73                     | 0.69              |
| 1:A:437:TYR:H    | 1:A:438:PRO:HD2  | 1.56                     | 0.69              |
| 2:L:11:LEU:O     | 2:L:14:ALA:HB3   | 1.93                     | 0.69              |
| 2:L:239:ASN:HD22 | 2:L:246:THR:HG22 | 1.58                     | 0.69              |
| 2:C:239:ASN:HD22 | 2:C:246:THR:HG22 | 1.58                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:150:PHE:HB2  | 2:D:152:PHE:CE1  | 2.27                     | 0.69              |
| 2:K:150:PHE:HB2  | 2:K:152:PHE:CE1  | 2.27                     | 0.69              |
| 1:A:306:ASP:C    | 1:A:308:LEU:H    | 1.95                     | 0.69              |
| 2:J:22:THR:O     | 2:J:72:ASN:HA    | 1.92                     | 0.69              |
| 1:A:275:PRO:HB2  | 1:A:278:ILE:CG1  | 2.22                     | 0.69              |
| 2:H:12:LYS:C     | 2:H:14:ALA:H     | 1.95                     | 0.69              |
| 3:W:840:ASN:HA   | 3:W:845:ILE:CG2  | 2.23                     | 0.69              |
| 2:F:110:ALA:HB1  | 2:F:111:PRO:CD   | 2.22                     | 0.69              |
| 2:I:167:ASN:HD22 | 2:I:178:GLY:HA2  | 1.57                     | 0.69              |
| 2:I:109:ILE:HD12 | 2:I:109:ILE:O    | 1.90                     | 0.69              |
| 2:G:11:LEU:O     | 2:G:14:ALA:HB3   | 1.92                     | 0.69              |
| 2:E:11:LEU:O     | 2:E:14:ALA:HB3   | 1.91                     | 0.69              |
| 2:M:167:ASN:HD22 | 2:M:178:GLY:HA2  | 1.57                     | 0.69              |
| 1:A:634:TYR:HB2  | 1:B:875:ARG:HH22 | 1.57                     | 0.69              |
| 1:B:366:PHE:C    | 1:B:368:THR:N    | 2.46                     | 0.69              |
| 1:B:374:ALA:HB1  | 1:B:580:SER:CB   | 2.23                     | 0.69              |
| 3:W:535:ARG:CZ   | 3:W:568:LEU:HD13 | 2.22                     | 0.69              |
| 2:E:5:TYR:CE2    | 2:E:131:ASN:HA   | 2.27                     | 0.69              |
| 2:F:167:ASN:HD22 | 2:F:178:GLY:HA2  | 1.57                     | 0.69              |
| 2:N:116:LEU:HD12 | 2:N:119:LEU:HB2  | 1.74                     | 0.69              |
| 1:B:772:ILE:HG23 | 1:B:773:SER:N    | 2.06                     | 0.69              |
| 1:A:588:ILE:CG2  | 1:A:589:GLY:N    | 2.56                     | 0.69              |
| 1:A:666:ARG:CG   | 1:A:667:ASP:N    | 2.55                     | 0.69              |
| 1:A:540:LEU:HD23 | 1:A:541:GLY:N    | 2.08                     | 0.69              |
| 1:A:803:ASN:HD22 | 1:A:805:ASP:HB3  | 1.58                     | 0.69              |
| 3:W:519:THR:HG22 | 3:W:520:ASP:N    | 2.08                     | 0.69              |
| 1:A:322:THR:HG22 | 1:A:390:ARG:HB2  | 1.75                     | 0.69              |
| 1:A:451:ASP:CB   | 1:A:452:PRO:CD   | 2.68                     | 0.69              |
| 1:B:783:PHE:N    | 1:B:783:PHE:CD1  | 2.60                     | 0.69              |
| 1:B:563:MET:HA   | 1:B:563:MET:HE3  | 1.73                     | 0.69              |
| 1:B:368:THR:HA   | 1:B:579:THR:HG23 | 1.75                     | 0.69              |
| 1:A:689:MET:HA   | 1:A:692:ILE:HD13 | 1.73                     | 0.69              |
| 1:A:664:ARG:HD3  | 1:B:538:ASN:OD1  | 1.92                     | 0.69              |
| 2:D:106:ARG:H    | 2:D:106:ARG:HD3  | 1.58                     | 0.69              |
| 2:E:109:ILE:HB   | 2:E:380:ASP:HB3  | 1.74                     | 0.69              |
| 2:E:150:PHE:HB2  | 2:E:152:PHE:CE1  | 2.27                     | 0.69              |
| 1:B:812:VAL:HG13 | 1:B:813:ALA:H    | 1.57                     | 0.69              |
| 1:A:546:LEU:HD21 | 1:A:588:ILE:HD13 | 1.73                     | 0.69              |
| 1:A:757:VAL:HG12 | 1:A:758:ALA:H    | 1.57                     | 0.69              |
| 2:G:12:LYS:C     | 2:G:14:ALA:H     | 1.96                     | 0.69              |
| 1:B:118:LYS:HG2  | 1:B:119:GLN:N    | 2.08                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:118:LYS:HG2  | 1:A:119:GLN:H    | 1.57                     | 0.69              |
| 1:B:594:ILE:HD12 | 1:B:594:ILE:C    | 2.13                     | 0.69              |
| 1:B:752:LEU:C    | 1:B:754:ASN:H    | 1.95                     | 0.69              |
| 2:E:116:LEU:HD12 | 2:E:119:LEU:HB2  | 1.73                     | 0.69              |
| 2:F:11:LEU:O     | 2:F:14:ALA:HB3   | 1.93                     | 0.69              |
| 1:B:457:GLN:CG   | 1:B:458:ILE:H    | 1.89                     | 0.69              |
| 2:I:6:SER:OG     | 2:I:128:ASN:HA   | 1.92                     | 0.69              |
| 2:M:12:LYS:C     | 2:M:14:ALA:H     | 1.96                     | 0.69              |
| 1:B:633:LEU:O    | 1:B:633:LEU:HD23 | 1.92                     | 0.69              |
| 2:K:106:ARG:HG2  | 2:K:107:ASN:H    | 1.56                     | 0.69              |
| 1:A:100:PRO:HB2  | 3:W:558:LEU:HD11 | 1.75                     | 0.69              |
| 3:W:535:ARG:NH2  | 3:W:568:LEU:HD13 | 2.07                     | 0.69              |
| 2:L:167:ASN:HD22 | 2:L:178:GLY:HA2  | 1.57                     | 0.69              |
| 3:W:105:ASN:ND2  | 3:W:111:ASN:HA   | 2.08                     | 0.69              |
| 2:H:239:ASN:HD22 | 2:H:246:THR:HG22 | 1.58                     | 0.69              |
| 1:B:364:THR:CG2  | 3:W:622:ALA:HA   | 2.22                     | 0.69              |
| 2:O:109:ILE:O    | 2:O:109:ILE:HD12 | 1.92                     | 0.69              |
| 2:K:144:ARG:O    | 2:K:145:ARG:HB2  | 1.92                     | 0.69              |
| 3:W:147:PHE:HE1  | 3:W:151:LYS:HE3  | 1.58                     | 0.69              |
| 2:M:116:LEU:HD12 | 2:M:119:LEU:HB2  | 1.75                     | 0.69              |
| 1:B:805:ASP:O    | 1:B:807:ASN:N    | 2.26                     | 0.68              |
| 1:A:306:ASP:O    | 1:A:308:LEU:N    | 2.25                     | 0.68              |
| 1:A:570:THR:HG22 | 1:A:571:LEU:N    | 2.07                     | 0.68              |
| 1:A:658:PRO:HG3  | 1:B:345:GLN:HA   | 1.75                     | 0.68              |
| 1:B:166:PHE:O    | 1:B:169:LEU:HB2  | 1.93                     | 0.68              |
| 2:E:12:LYS:C     | 2:E:14:ALA:H     | 1.96                     | 0.68              |
| 1:A:661:GLN:NE2  | 1:B:348:LYS:NZ   | 2.39                     | 0.68              |
| 2:H:106:ARG:O    | 2:H:107:ASN:HB2  | 1.93                     | 0.68              |
| 1:B:264:PRO:O    | 1:B:265:LEU:HB2  | 1.92                     | 0.68              |
| 1:A:366:PHE:N    | 1:A:366:PHE:CD1  | 2.60                     | 0.68              |
| 1:A:807:ASN:O    | 1:A:809:PHE:N    | 2.26                     | 0.68              |
| 2:J:4:LEU:HA     | 2:J:7:LEU:HD12   | 1.75                     | 0.68              |
| 2:F:6:SER:OG     | 2:F:128:ASN:HA   | 1.92                     | 0.68              |
| 2:L:116:LEU:HD12 | 2:L:119:LEU:HB2  | 1.75                     | 0.68              |
| 2:N:12:LYS:C     | 2:N:14:ALA:H     | 1.94                     | 0.68              |
| 2:D:12:LYS:C     | 2:D:14:ALA:H     | 1.95                     | 0.68              |
| 2:F:4:LEU:HA     | 2:F:7:LEU:HD12   | 1.75                     | 0.68              |
| 2:E:167:ASN:HD22 | 2:E:178:GLY:HA2  | 1.57                     | 0.68              |
| 2:L:110:ALA:HB1  | 2:L:111:PRO:CD   | 2.23                     | 0.68              |
| 1:B:548:ARG:NH1  | 1:B:878:ASN:N    | 2.35                     | 0.68              |
| 2:H:11:LEU:O     | 2:H:14:ALA:HB3   | 1.93                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:153:HIS:NE2  | 2:H:153:HIS:NE2  | 2.41                     | 0.68              |
| 2:C:116:LEU:HD12 | 2:C:119:LEU:HB2  | 1.75                     | 0.68              |
| 2:N:239:ASN:HD22 | 2:N:246:THR:HG22 | 1.58                     | 0.68              |
| 2:D:116:LEU:HD12 | 2:D:119:LEU:HB2  | 1.75                     | 0.68              |
| 2:F:116:LEU:HD12 | 2:F:119:LEU:HB2  | 1.75                     | 0.68              |
| 1:A:318:TRP:CA   | 1:A:321:ILE:HD12 | 2.19                     | 0.68              |
| 2:I:116:LEU:HD12 | 2:I:119:LEU:HB2  | 1.75                     | 0.68              |
| 1:B:180:TYR:HD1  | 1:B:181:LEU:N    | 1.91                     | 0.68              |
| 3:W:186:ASN:HD21 | 3:W:190:ARG:H    | 1.39                     | 0.68              |
| 2:M:153:HIS:NE2  | 2:N:153:HIS:NE2  | 2.40                     | 0.68              |
| 2:I:239:ASN:HD22 | 2:I:246:THR:HG22 | 1.59                     | 0.68              |
| 1:A:396:PHE:HB3  | 1:A:578:LEU:HD12 | 1.76                     | 0.68              |
| 1:A:660:ASP:CB   | 1:B:539:ARG:HH11 | 2.04                     | 0.68              |
| 1:B:545:ASP:HB3  | 1:B:877:MET:SD   | 2.34                     | 0.68              |
| 1:B:431:ILE:HA   | 1:B:435:ILE:HD12 | 1.76                     | 0.68              |
| 2:M:4:LEU:HA     | 2:M:7:LEU:HD12   | 1.75                     | 0.68              |
| 1:B:855:LEU:O    | 1:B:858:VAL:HG23 | 1.94                     | 0.68              |
| 3:W:691:ALA:HB2  | 3:W:723:ARG:HB3  | 1.75                     | 0.68              |
| 1:A:659:ASP:O    | 1:A:662:MET:HB2  | 1.94                     | 0.68              |
| 2:I:4:LEU:HA     | 2:I:7:LEU:HD12   | 1.74                     | 0.68              |
| 2:H:4:LEU:HA     | 2:H:7:LEU:HD12   | 1.76                     | 0.68              |
| 3:W:324:LYS:HG2  | 3:W:328:TRP:CD1  | 2.29                     | 0.68              |
| 2:N:65:LEU:O     | 2:N:66:LEU:HD23  | 1.94                     | 0.68              |
| 1:B:498:ARG:HB3  | 1:B:505:GLN:HE22 | 1.59                     | 0.68              |
| 1:B:869:VAL:HG11 | 1:B:873:ASN:HA   | 1.74                     | 0.68              |
| 2:O:12:LYS:C     | 2:O:14:ALA:H     | 1.96                     | 0.68              |
| 2:I:135:TYR:CZ   | 2:I:342:MET:HE3  | 2.28                     | 0.68              |
| 2:H:167:ASN:HD22 | 2:H:178:GLY:HA2  | 1.57                     | 0.68              |
| 2:J:239:ASN:HD22 | 2:J:246:THR:HG22 | 1.58                     | 0.68              |
| 1:A:587:LEU:HD13 | 1:A:587:LEU:O    | 1.94                     | 0.68              |
| 1:B:492:VAL:HG11 | 1:B:558:MET:CG   | 2.22                     | 0.68              |
| 2:K:12:LYS:C     | 2:K:14:ALA:H     | 1.96                     | 0.68              |
| 1:B:246:HIS:CD2  | 1:B:248:ILE:H    | 2.11                     | 0.68              |
| 1:B:530:GLN:HA   | 1:B:533:ILE:HD12 | 1.76                     | 0.68              |
| 1:A:136:ALA:O    | 1:A:137:ASN:HB3  | 1.94                     | 0.68              |
| 2:M:239:ASN:HD22 | 2:M:246:THR:HG22 | 1.59                     | 0.68              |
| 1:B:143:ARG:HG3  | 1:B:216:GLU:OE2  | 1.92                     | 0.68              |
| 1:A:101:LYS:HZ2  | 3:W:382:ASP:N    | 1.92                     | 0.68              |
| 2:D:167:ASN:HD22 | 2:D:178:GLY:HA2  | 1.57                     | 0.68              |
| 1:A:589:GLY:O    | 1:A:591:ALA:N    | 2.26                     | 0.67              |
| 1:B:499:ASN:O    | 1:B:500:GLY:C    | 2.33                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:76:ASN:HB2   | 2:J:76:ASN:CB    | 2.23                     | 0.67              |
| 3:W:686:LYS:HB2  | 3:W:688:PHE:HE2  | 1.58                     | 0.67              |
| 2:I:9:LYS:O      | 2:I:13:ASP:HB2   | 1.94                     | 0.67              |
| 1:B:721:VAL:HG12 | 1:B:722:ASN:N    | 2.08                     | 0.67              |
| 1:B:125:ILE:N    | 1:B:125:ILE:HD12 | 2.10                     | 0.67              |
| 3:W:438:ILE:HD11 | 3:W:563:GLN:HB3  | 1.75                     | 0.67              |
| 2:D:144:ARG:O    | 2:D:145:ARG:HB2  | 1.94                     | 0.67              |
| 2:C:12:LYS:C     | 2:C:14:ALA:H     | 1.96                     | 0.67              |
| 2:F:12:LYS:C     | 2:F:14:ALA:H     | 1.96                     | 0.67              |
| 1:B:258:GLN:HB3  | 2:N:71:LEU:HB2   | 1.76                     | 0.67              |
| 2:G:239:ASN:HD22 | 2:G:246:THR:HG22 | 1.58                     | 0.67              |
| 1:A:188:VAL:O    | 1:A:198:LYS:HA   | 1.93                     | 0.67              |
| 2:K:117:ARG:HH21 | 2:M:57:ARG:NH1   | 1.90                     | 0.67              |
| 1:A:270:ILE:HG23 | 1:A:854:LEU:CD2  | 2.22                     | 0.67              |
| 3:W:217:VAL:HG13 | 3:W:222:ASP:CB   | 2.25                     | 0.67              |
| 1:A:306:ASP:HB3  | 1:A:310:LEU:CD1  | 2.24                     | 0.67              |
| 1:B:745:ALA:O    | 1:B:748:THR:N    | 2.28                     | 0.67              |
| 2:F:19:VAL:HG23  | 2:H:128:ASN:HB3  | 1.77                     | 0.67              |
| 2:H:76:ASN:H     | 2:J:76:ASN:HB2   | 1.60                     | 0.67              |
| 2:L:4:LEU:HA     | 2:L:7:LEU:HD12   | 1.75                     | 0.67              |
| 1:B:605:ASN:HD21 | 1:B:855:LEU:HD12 | 1.58                     | 0.67              |
| 2:D:38:ILE:HD12  | 2:D:65:LEU:HD23  | 1.75                     | 0.67              |
| 2:E:4:LEU:HA     | 2:E:7:LEU:HD12   | 1.75                     | 0.67              |
| 2:I:104:SER:O    | 2:I:108:GLY:HA3  | 1.94                     | 0.67              |
| 2:K:116:LEU:HD12 | 2:K:119:LEU:HB2  | 1.76                     | 0.67              |
| 2:N:73:LEU:HD23  | 2:N:73:LEU:N     | 2.09                     | 0.67              |
| 1:A:310:LEU:O    | 1:A:318:TRP:HD1  | 1.76                     | 0.67              |
| 1:B:183:LEU:HD12 | 1:B:844:SER:HB3  | 1.77                     | 0.67              |
| 1:A:136:ALA:O    | 1:A:137:ASN:CB   | 2.43                     | 0.67              |
| 2:I:63:PHE:CD2   | 2:I:84:THR:HG23  | 2.28                     | 0.67              |
| 2:O:239:ASN:HD22 | 2:O:246:THR:HG22 | 1.58                     | 0.67              |
| 1:A:571:LEU:O    | 1:A:571:LEU:HD13 | 1.94                     | 0.67              |
| 1:B:869:VAL:HG22 | 1:B:875:ARG:HA   | 1.76                     | 0.67              |
| 2:F:239:ASN:HD22 | 2:F:246:THR:HG22 | 1.58                     | 0.67              |
| 2:K:239:ASN:HD22 | 2:K:246:THR:HG22 | 1.58                     | 0.67              |
| 1:B:782:VAL:HG11 | 1:B:796:LYS:O    | 1.94                     | 0.67              |
| 1:B:361:GLN:HE22 | 3:W:624:LYS:HZ1  | 1.42                     | 0.67              |
| 2:O:9:LYS:O      | 2:O:13:ASP:HB2   | 1.95                     | 0.67              |
| 1:B:666:ARG:CG   | 1:B:667:ASP:N    | 2.57                     | 0.67              |
| 2:K:4:LEU:HA     | 2:K:7:LEU:HD12   | 1.75                     | 0.67              |
| 2:I:76:ASN:N     | 2:M:76:ASN:HB2   | 2.09                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:154:THR:O    | 1:B:155:LEU:HD23 | 1.94                     | 0.67              |
| 1:B:108:LEU:N    | 1:B:108:LEU:HD22 | 2.10                     | 0.67              |
| 1:B:371:ASN:ND2  | 1:B:583:SER:HB3  | 2.06                     | 0.67              |
| 1:A:367:LEU:CD2  | 3:W:929:ALA:HA   | 2.22                     | 0.67              |
| 1:A:839:MET:HG2  | 1:A:840:HIS:H    | 1.60                     | 0.67              |
| 1:A:223:ARG:O    | 1:A:226:ALA:HB3  | 1.95                     | 0.67              |
| 1:A:219:GLY:O    | 1:A:221:VAL:N    | 2.28                     | 0.67              |
| 2:K:9:LYS:O      | 2:K:13:ASP:HB2   | 1.95                     | 0.67              |
| 2:G:116:LEU:HD12 | 2:G:119:LEU:HB2  | 1.76                     | 0.67              |
| 1:B:700:ALA:HB1  | 1:B:827:LYS:HB2  | 1.75                     | 0.67              |
| 1:B:771:VAL:HG12 | 1:B:772:ILE:N    | 2.09                     | 0.67              |
| 1:A:503:ILE:C    | 1:A:505:GLN:H    | 1.98                     | 0.67              |
| 1:A:521:MET:HB3  | 1:A:522:PRO:CD   | 2.22                     | 0.67              |
| 1:B:200:VAL:HG12 | 1:B:201:ASP:N    | 2.08                     | 0.67              |
| 1:A:650:HIS:O    | 1:A:651:ILE:HB   | 1.94                     | 0.67              |
| 3:W:778:THR:O    | 3:W:782:VAL:HG22 | 1.93                     | 0.67              |
| 1:B:523:VAL:C    | 1:B:525:TYR:N    | 2.47                     | 0.66              |
| 1:A:252:PHE:CD2  | 1:A:684:LEU:HD21 | 2.30                     | 0.66              |
| 2:O:116:LEU:HD12 | 2:O:119:LEU:HB2  | 1.76                     | 0.66              |
| 1:A:524:ASP:OD1  | 1:A:525:TYR:N    | 2.27                     | 0.66              |
| 1:B:229:ARG:HD2  | 1:B:230:GLN:HE22 | 1.60                     | 0.66              |
| 1:B:672:LEU:HB3  | 1:B:673:PRO:HD2  | 1.77                     | 0.66              |
| 2:D:99:GLU:OE1   | 2:D:116:LEU:HD22 | 1.94                     | 0.66              |
| 2:D:99:GLU:HG2   | 2:D:99:GLU:O     | 1.94                     | 0.66              |
| 2:O:49:GLY:HA2   | 2:O:54:LEU:HD23  | 1.77                     | 0.66              |
| 1:B:825:VAL:CG1  | 1:B:826:TYR:N    | 2.57                     | 0.66              |
| 1:A:563:MET:CA   | 1:A:563:MET:HE3  | 2.14                     | 0.66              |
| 3:W:1006:LEU:HG  | 3:W:1086:PHE:HE1 | 1.60                     | 0.66              |
| 2:E:239:ASN:HD22 | 2:E:246:THR:HG22 | 1.59                     | 0.66              |
| 1:B:724:ALA:HB2  | 1:B:824:LYS:HE3  | 1.77                     | 0.66              |
| 1:A:508:GLU:HG2  | 1:A:512:GLN:NE2  | 2.10                     | 0.66              |
| 1:A:246:HIS:CD2  | 1:A:248:ILE:H    | 2.14                     | 0.66              |
| 2:E:14:ALA:O     | 2:E:18:ILE:HD12  | 1.95                     | 0.66              |
| 2:C:153:HIS:NE2  | 2:E:153:HIS:NE2  | 2.43                     | 0.66              |
| 3:W:967:ILE:H    | 3:W:967:ILE:HD12 | 1.59                     | 0.66              |
| 1:A:701:GLN:HG2  | 1:A:826:TYR:CD2  | 2.31                     | 0.66              |
| 1:B:374:ALA:HB1  | 1:B:580:SER:CA   | 2.25                     | 0.66              |
| 3:W:440:PRO:HA   | 3:W:567:ASN:HD22 | 1.61                     | 0.66              |
| 3:W:296:ARG:NH2  | 3:W:308:GLN:NE2  | 2.43                     | 0.66              |
| 2:L:153:HIS:NE2  | 2:M:153:HIS:NE2  | 2.44                     | 0.66              |
| 1:A:653:ASP:HB3  | 1:A:656:ARG:HB2  | 1.77                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:454:THR:HB   | 1:A:457:GLN:HB3  | 1.78                     | 0.66              |
| 1:A:513:LEU:O    | 1:A:516:GLN:OE1  | 2.14                     | 0.66              |
| 1:B:396:PHE:HB2  | 1:B:578:LEU:HD11 | 1.77                     | 0.66              |
| 2:E:23:LEU:HD23  | 2:E:24:TYR:N     | 2.11                     | 0.66              |
| 2:N:150:PHE:HB2  | 2:N:152:PHE:CE1  | 2.30                     | 0.66              |
| 2:N:9:LYS:O      | 2:N:13:ASP:HB2   | 1.96                     | 0.66              |
| 1:B:825:VAL:CG1  | 1:B:826:TYR:H    | 2.08                     | 0.66              |
| 1:A:277:ARG:HD3  | 1:A:559:ALA:CB   | 2.25                     | 0.66              |
| 1:B:594:ILE:HB   | 1:B:595:PRO:CD   | 2.26                     | 0.66              |
| 1:B:349:MET:O    | 1:B:353:LEU:HB2  | 1.94                     | 0.66              |
| 2:N:4:LEU:HA     | 2:N:7:LEU:CD1    | 2.26                     | 0.66              |
| 2:L:12:LYS:C     | 2:L:14:ALA:H     | 1.96                     | 0.66              |
| 2:C:2:ASP:HB2    | 2:C:128:ASN:HD21 | 1.60                     | 0.66              |
| 2:J:5:TYR:CE2    | 2:J:131:ASN:HA   | 2.31                     | 0.66              |
| 1:A:729:GLY:C    | 1:A:730:PHE:HD1  | 1.98                     | 0.66              |
| 2:M:9:LYS:O      | 2:M:13:ASP:HB2   | 1.96                     | 0.66              |
| 1:B:140:LYS:O    | 1:B:142:LEU:N    | 2.29                     | 0.66              |
| 1:B:504:ASN:O    | 1:B:507:MET:N    | 2.29                     | 0.66              |
| 1:A:521:MET:CE   | 1:A:521:MET:HA   | 2.26                     | 0.66              |
| 2:G:145:ARG:CB   | 2:G:145:ARG:HH11 | 2.00                     | 0.66              |
| 1:B:445:MET:O    | 1:B:447:TYR:N    | 2.23                     | 0.66              |
| 2:I:110:ALA:HB1  | 2:I:111:PRO:HD2  | 1.77                     | 0.66              |
| 2:C:22:THR:HG23  | 2:C:73:LEU:HD12  | 1.78                     | 0.66              |
| 1:B:194:ARG:HA   | 1:B:194:ARG:NE   | 2.11                     | 0.66              |
| 1:B:170:TYR:HE1  | 1:B:681:ILE:HG23 | 1.60                     | 0.66              |
| 2:O:4:LEU:HA     | 2:O:7:LEU:CD1    | 2.26                     | 0.66              |
| 1:A:166:PHE:O    | 1:A:169:LEU:HB2  | 1.96                     | 0.65              |
| 2:C:150:PHE:HB2  | 2:C:152:PHE:HE1  | 1.61                     | 0.65              |
| 2:I:109:ILE:HB   | 2:I:380:ASP:HB3  | 1.79                     | 0.65              |
| 2:N:150:PHE:HB2  | 2:N:152:PHE:HE1  | 1.61                     | 0.65              |
| 2:D:9:LYS:O      | 2:D:13:ASP:HB2   | 1.94                     | 0.65              |
| 2:F:26:ASN:OD1   | 2:H:33:GLN:HB2   | 1.97                     | 0.65              |
| 2:G:128:ASN:O    | 2:H:22:THR:HB    | 1.95                     | 0.65              |
| 1:A:603:TYR:O    | 1:A:606:VAL:HG22 | 1.96                     | 0.65              |
| 3:W:394:LEU:HD22 | 3:W:815:LEU:HD21 | 1.77                     | 0.65              |
| 2:C:4:LEU:HA     | 2:C:7:LEU:CD1    | 2.27                     | 0.65              |
| 2:C:54:LEU:HD12  | 2:C:55:PRO:HD2   | 1.77                     | 0.65              |
| 1:B:322:THR:HB   | 1:B:390:ARG:HH11 | 1.61                     | 0.65              |
| 1:A:508:GLU:C    | 1:A:512:GLN:HE21 | 2.00                     | 0.65              |
| 1:A:755:GLN:O    | 1:A:757:VAL:HG23 | 1.96                     | 0.65              |
| 1:B:642:VAL:O    | 1:B:646:LEU:HG   | 1.96                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:396:PHE:HE1  | 1:B:398:THR:HA   | 1.60                     | 0.65              |
| 2:J:12:LYS:HG2   | 2:J:16:ASP:OD2   | 1.95                     | 0.65              |
| 2:M:144:ARG:HD2  | 2:N:82:ARG:CZ    | 2.27                     | 0.65              |
| 2:K:46:PHE:HE2   | 2:K:119:LEU:HD21 | 1.62                     | 0.65              |
| 2:D:109:ILE:HB   | 2:D:380:ASP:HB3  | 1.78                     | 0.65              |
| 2:G:9:LYS:O      | 2:G:13:ASP:HB2   | 1.96                     | 0.65              |
| 1:A:849:THR:HB   | 1:A:851:TYR:HE1  | 1.61                     | 0.65              |
| 3:W:135:LEU:HD13 | 3:W:709:GLN:OE1  | 1.96                     | 0.65              |
| 2:C:9:LYS:O      | 2:C:13:ASP:HB2   | 1.96                     | 0.65              |
| 1:A:871:PHE:O    | 1:A:871:PHE:HD1  | 1.80                     | 0.65              |
| 1:A:711:GLN:O    | 1:A:712:LEU:HD23 | 1.96                     | 0.65              |
| 1:B:708:ARG:O    | 1:B:709:ASP:C    | 2.35                     | 0.65              |
| 1:A:501:HIS:O    | 1:A:503:ILE:HG13 | 1.97                     | 0.65              |
| 2:G:4:LEU:HA     | 2:G:7:LEU:CD1    | 2.26                     | 0.65              |
| 2:I:150:PHE:HB2  | 2:I:152:PHE:CZ   | 2.32                     | 0.65              |
| 2:D:22:THR:O     | 2:D:72:ASN:HA    | 1.95                     | 0.65              |
| 1:B:805:ASP:C    | 1:B:807:ASN:H    | 1.99                     | 0.65              |
| 1:A:622:VAL:HG11 | 1:A:673:PRO:O    | 1.97                     | 0.65              |
| 1:A:642:VAL:O    | 1:A:646:LEU:HG   | 1.96                     | 0.65              |
| 1:A:516:GLN:N    | 1:A:516:GLN:OE1  | 2.28                     | 0.65              |
| 3:W:704:SER:HB2  | 3:W:709:GLN:NE2  | 2.12                     | 0.65              |
| 2:I:130:ASP:HA   | 2:J:17:LYS:HG2   | 1.78                     | 0.65              |
| 2:I:153:HIS:NE2  | 2:K:153:HIS:NE2  | 2.45                     | 0.65              |
| 2:H:9:LYS:O      | 2:H:13:ASP:HB2   | 1.97                     | 0.65              |
| 1:A:589:GLY:C    | 1:A:591:ALA:H    | 1.99                     | 0.65              |
| 1:A:658:PRO:CG   | 1:B:348:LYS:HG2  | 2.23                     | 0.65              |
| 1:A:782:VAL:O    | 1:A:785:GLN:HG2  | 1.97                     | 0.65              |
| 1:B:170:TYR:CE1  | 1:B:681:ILE:HG23 | 2.31                     | 0.65              |
| 1:A:142:LEU:O    | 1:A:144:ASN:N    | 2.28                     | 0.65              |
| 1:B:401:TYR:HA   | 1:B:404:LEU:HD13 | 1.79                     | 0.65              |
| 1:A:779:ASP:CA   | 1:A:798:ILE:HD12 | 2.26                     | 0.65              |
| 1:B:315:GLU:CB   | 1:B:571:LEU:HD11 | 2.25                     | 0.65              |
| 1:B:236:ARG:O    | 1:B:237:ASN:HB2  | 1.97                     | 0.65              |
| 3:W:207:ALA:O    | 3:W:211:ILE:HG13 | 1.96                     | 0.65              |
| 2:N:12:LYS:HG2   | 2:N:16:ASP:OD2   | 1.96                     | 0.65              |
| 1:B:96:PRO:HG2   | 1:B:657:VAL:HG22 | 1.79                     | 0.65              |
| 1:A:271:PHE:HA   | 1:A:274:ILE:HD12 | 1.79                     | 0.65              |
| 1:B:298:TYR:HD1  | 1:B:299:ILE:N    | 1.94                     | 0.65              |
| 2:I:4:LEU:HA     | 2:I:7:LEU:CD1    | 2.27                     | 0.64              |
| 1:B:378:CYS:HB2  | 1:B:580:SER:HB2  | 1.79                     | 0.64              |
| 2:F:9:LYS:O      | 2:F:13:ASP:HB2   | 1.97                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:9:LYS:O      | 2:E:13:ASP:HB2   | 1.97                     | 0.64              |
| 2:J:57:ARG:HH11  | 2:J:94:ASN:HD21  | 1.46                     | 0.64              |
| 1:A:793:ASP:C    | 1:A:795:LEU:H    | 2.00                     | 0.64              |
| 2:D:4:LEU:HA     | 2:D:7:LEU:CD1    | 2.27                     | 0.64              |
| 1:B:603:TYR:O    | 1:B:606:VAL:HG22 | 1.97                     | 0.64              |
| 2:D:106:ARG:HG2  | 2:D:107:ASN:H    | 1.62                     | 0.64              |
| 1:B:314:PHE:CZ   | 1:B:664:ARG:HG2  | 2.32                     | 0.64              |
| 2:L:9:LYS:O      | 2:L:13:ASP:HB2   | 1.96                     | 0.64              |
| 1:A:802:ILE:HA   | 1:A:807:ASN:ND2  | 2.12                     | 0.64              |
| 2:O:104:SER:HB3  | 2:O:108:GLY:HA2  | 1.79                     | 0.64              |
| 3:W:191:TYR:CE2  | 3:W:204:VAL:HG11 | 2.31                     | 0.64              |
| 3:W:777:THR:HG21 | 3:W:882:LYS:NZ   | 2.11                     | 0.64              |
| 2:L:27:VAL:O     | 2:L:31:ILE:HG12  | 1.97                     | 0.64              |
| 1:A:863:VAL:HG12 | 1:A:864:GLU:H    | 1.61                     | 0.64              |
| 2:D:110:ALA:HB1  | 2:D:111:PRO:CD   | 2.28                     | 0.64              |
| 1:A:714:ARG:HA   | 1:A:720:TYR:HB3  | 1.78                     | 0.64              |
| 1:A:414:VAL:HB   | 1:A:419:PHE:HE1  | 1.62                     | 0.64              |
| 1:B:491:GLN:NE2  | 1:B:566:GLN:HG2  | 2.12                     | 0.64              |
| 1:B:457:GLN:CG   | 1:B:458:ILE:N    | 2.53                     | 0.64              |
| 1:B:182:LEU:CD2  | 1:B:183:LEU:H    | 2.08                     | 0.64              |
| 1:B:606:VAL:HG23 | 1:B:607:ASN:N    | 2.11                     | 0.64              |
| 2:J:144:ARG:NH2  | 2:J:146:GLN:HE22 | 1.96                     | 0.64              |
| 1:A:834:ASP:O    | 1:A:838:SER:HB2  | 1.97                     | 0.64              |
| 1:B:718:TYR:HB3  | 1:B:721:VAL:CG2  | 2.18                     | 0.64              |
| 1:A:548:ARG:HB3  | 1:A:876:ILE:HG23 | 1.78                     | 0.64              |
| 2:K:12:LYS:HG2   | 2:K:16:ASP:OD2   | 1.97                     | 0.64              |
| 1:B:645:PHE:HD2  | 1:B:646:LEU:HD23 | 1.62                     | 0.64              |
| 1:A:246:HIS:O    | 1:A:249:ASP:N    | 2.31                     | 0.64              |
| 3:W:906:ASN:ND2  | 3:W:907:VAL:N    | 2.44                     | 0.64              |
| 2:J:4:LEU:HA     | 2:J:7:LEU:CD1    | 2.28                     | 0.64              |
| 2:F:109:ILE:HB   | 2:F:380:ASP:HB3  | 1.79                     | 0.64              |
| 3:W:532:GLN:HB2  | 3:W:533:PRO:HD3  | 1.78                     | 0.64              |
| 2:J:9:LYS:O      | 2:J:13:ASP:HB2   | 1.98                     | 0.64              |
| 2:M:139:TRP:NE1  | 2:M:143:ASN:ND2  | 2.46                     | 0.64              |
| 1:B:703:VAL:HG22 | 1:B:825:VAL:HG22 | 1.78                     | 0.64              |
| 1:A:378:CYS:SG   | 1:A:584:LEU:HD13 | 2.38                     | 0.64              |
| 2:N:128:ASN:O    | 2:N:129:PHE:HB3  | 1.98                     | 0.64              |
| 1:A:246:HIS:HD2  | 1:A:248:ILE:HB   | 1.63                     | 0.64              |
| 2:M:42:ASN:HA    | 2:M:61:PHE:HB3   | 1.80                     | 0.64              |
| 2:F:38:ILE:HG22  | 2:F:42:ASN:HD21  | 1.62                     | 0.64              |
| 1:B:721:VAL:HG12 | 1:B:722:ASN:H    | 1.63                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:389:GLN:OE1  | 1:B:389:GLN:HA   | 1.98                     | 0.64              |
| 1:B:492:VAL:HG13 | 1:B:565:MET:SD   | 2.38                     | 0.64              |
| 2:M:12:LYS:HG2   | 2:M:16:ASP:OD2   | 1.98                     | 0.64              |
| 1:B:182:LEU:HD11 | 1:B:847:THR:HA   | 1.78                     | 0.64              |
| 1:A:606:VAL:HG23 | 1:A:607:ASN:N    | 2.13                     | 0.64              |
| 3:W:890:ALA:HB2  | 3:W:1053:SER:HB2 | 1.79                     | 0.64              |
| 1:A:360:ILE:HG23 | 1:A:363:GLU:HB2  | 1.78                     | 0.64              |
| 2:G:106:ARG:HG2  | 2:G:107:ASN:H    | 1.62                     | 0.64              |
| 2:D:54:LEU:HD12  | 2:D:55:PRO:HD2   | 1.79                     | 0.64              |
| 2:K:4:LEU:HA     | 2:K:7:LEU:CD1    | 2.28                     | 0.64              |
| 2:O:14:ALA:O     | 2:O:18:ILE:HD12  | 1.97                     | 0.64              |
| 2:D:12:LYS:HG2   | 2:D:16:ASP:OD2   | 1.98                     | 0.64              |
| 3:W:509:PHE:CD2  | 3:W:624:LYS:HB3  | 2.32                     | 0.64              |
| 2:E:4:LEU:HA     | 2:E:7:LEU:CD1    | 2.28                     | 0.64              |
| 3:W:387:ARG:HB3  | 3:W:387:ARG:HH11 | 1.63                     | 0.64              |
| 2:H:57:ARG:HH11  | 2:H:94:ASN:HD21  | 1.44                     | 0.64              |
| 1:A:371:ASN:HB3  | 1:A:583:SER:HB2  | 1.80                     | 0.63              |
| 1:B:491:GLN:HE22 | 1:B:566:GLN:HG2  | 1.63                     | 0.63              |
| 1:B:498:ARG:CB   | 1:B:505:GLN:HE22 | 2.10                     | 0.63              |
| 2:I:19:VAL:CG2   | 2:K:128:ASN:HB3  | 2.27                     | 0.63              |
| 1:A:158:GLY:N    | 1:A:762:ALA:HB3  | 2.13                     | 0.63              |
| 2:L:12:LYS:HG2   | 2:L:16:ASP:OD2   | 1.98                     | 0.63              |
| 2:M:27:VAL:O     | 2:M:31:ILE:HG12  | 1.97                     | 0.63              |
| 2:J:110:ALA:HB1  | 2:J:111:PRO:CD   | 2.28                     | 0.63              |
| 3:W:741:SER:HB3  | 3:W:751:PHE:CD1  | 2.33                     | 0.63              |
| 1:B:346:ILE:O    | 1:B:349:MET:HB3  | 1.97                     | 0.63              |
| 1:B:442:MET:HG2  | 1:B:443:GLN:H    | 1.63                     | 0.63              |
| 2:J:71:LEU:HG    | 2:J:72:ASN:OD1   | 1.98                     | 0.63              |
| 2:M:4:LEU:HA     | 2:M:7:LEU:CD1    | 2.28                     | 0.63              |
| 1:B:645:PHE:CD2  | 1:B:646:LEU:HD23 | 2.33                     | 0.63              |
| 1:A:772:ILE:O    | 1:A:775:ILE:HG13 | 1.98                     | 0.63              |
| 2:F:4:LEU:HA     | 2:F:7:LEU:CD1    | 2.29                     | 0.63              |
| 1:B:772:ILE:O    | 1:B:775:ILE:HB   | 1.98                     | 0.63              |
| 1:A:491:GLN:OE1  | 1:A:564:ASN:HB3  | 1.99                     | 0.63              |
| 1:B:396:PHE:CE1  | 1:B:398:THR:HA   | 2.33                     | 0.63              |
| 2:I:145:ARG:HH11 | 2:I:145:ARG:CB   | 2.12                     | 0.63              |
| 2:F:110:ALA:HB1  | 2:F:111:PRO:HD2  | 1.80                     | 0.63              |
| 1:B:730:PHE:N    | 1:B:730:PHE:CD1  | 2.67                     | 0.63              |
| 1:B:722:ASN:ND2  | 1:B:824:LYS:HA   | 2.10                     | 0.63              |
| 1:B:415:PRO:CB   | 1:B:480:PHE:HB2  | 2.28                     | 0.63              |
| 1:B:503:ILE:HD11 | 1:B:548:ARG:CG   | 2.26                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:305:GLN:HG3  | 1:B:564:ASN:HD21 | 1.62                     | 0.63              |
| 1:A:721:VAL:HG11 | 1:A:799:LEU:HD22 | 1.81                     | 0.63              |
| 1:A:839:MET:HE2  | 1:A:839:MET:C    | 2.19                     | 0.63              |
| 1:A:560:CYS:HB2  | 1:A:603:TYR:CD2  | 2.33                     | 0.63              |
| 2:F:12:LYS:HG2   | 2:F:16:ASP:OD2   | 1.99                     | 0.63              |
| 2:D:109:ILE:HD12 | 2:D:109:ILE:O    | 1.99                     | 0.63              |
| 3:W:872:ILE:HD11 | 3:W:1072:ASN:HB2 | 1.80                     | 0.63              |
| 2:O:141:LEU:HD12 | 2:O:148:THR:HG21 | 1.80                     | 0.63              |
| 1:B:498:ARG:HD3  | 2:I:32:GLN:HE21  | 1.63                     | 0.63              |
| 3:W:324:LYS:O    | 3:W:328:TRP:HD1  | 1.82                     | 0.63              |
| 2:F:104:SER:O    | 2:F:105:GLN:HB2  | 1.98                     | 0.63              |
| 1:A:262:VAL:HG12 | 1:A:297:ARG:HB3  | 1.80                     | 0.63              |
| 3:W:729:ARG:NH1  | 3:W:770:ASP:OD1  | 2.31                     | 0.63              |
| 2:L:346:VAL:HG21 | 2:L:385:VAL:HG13 | 1.81                     | 0.63              |
| 1:B:701:GLN:HB2  | 1:B:826:TYR:CD2  | 2.29                     | 0.63              |
| 1:B:735:LEU:HD21 | 1:B:759:LEU:HB3  | 1.80                     | 0.63              |
| 1:B:492:VAL:HG11 | 1:B:558:MET:SD   | 2.38                     | 0.63              |
| 1:B:231:ARG:HB3  | 1:B:240:ASN:HB2  | 1.80                     | 0.63              |
| 1:B:587:LEU:HG   | 1:B:587:LEU:O    | 1.97                     | 0.63              |
| 1:B:422:GLU:HA   | 1:B:425:VAL:CG2  | 2.29                     | 0.63              |
| 1:A:513:LEU:HA   | 1:A:516:GLN:HE22 | 1.64                     | 0.63              |
| 2:L:24:TYR:O     | 2:L:27:VAL:HG22  | 1.98                     | 0.63              |
| 2:O:12:LYS:HG2   | 2:O:16:ASP:OD2   | 1.99                     | 0.63              |
| 3:W:470:PHE:HE1  | 3:W:594:LYS:HD3  | 1.64                     | 0.63              |
| 2:C:12:LYS:HG2   | 2:C:16:ASP:OD2   | 1.99                     | 0.63              |
| 2:O:85:ILE:O     | 2:O:89:VAL:HG23  | 1.99                     | 0.63              |
| 2:L:85:ILE:O     | 2:L:89:VAL:HG23  | 1.99                     | 0.63              |
| 1:B:818:VAL:HG12 | 1:B:819:PRO:HD2  | 1.80                     | 0.63              |
| 1:B:549:LEU:HD13 | 1:B:877:MET:CE   | 2.28                     | 0.63              |
| 1:A:795:LEU:O    | 1:A:797:PRO:HD3  | 1.98                     | 0.63              |
| 2:N:106:ARG:H    | 2:N:106:ARG:CD   | 1.99                     | 0.63              |
| 2:O:147:ARG:HG2  | 2:O:148:THR:N    | 2.13                     | 0.63              |
| 2:K:346:VAL:HG21 | 2:K:385:VAL:HG13 | 1.81                     | 0.63              |
| 1:B:127:GLU:OE1  | 1:B:151:LYS:HE2  | 1.98                     | 0.63              |
| 1:A:436:ILE:HD12 | 1:A:436:ILE:C    | 2.18                     | 0.63              |
| 1:A:601:PHE:HD1  | 1:A:601:PHE:H    | 1.46                     | 0.63              |
| 1:A:416:ASN:HB3  | 1:A:424:LEU:CD2  | 2.29                     | 0.62              |
| 1:B:274:ILE:HG23 | 1:B:278:ILE:CD1  | 2.24                     | 0.62              |
| 2:I:12:LYS:HG2   | 2:I:16:ASP:OD2   | 1.99                     | 0.62              |
| 1:A:328:LEU:HD11 | 1:A:606:VAL:HG21 | 1.80                     | 0.62              |
| 3:W:161:LYS:O    | 3:W:165:ARG:HG3  | 1.98                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:W:147:PHE:CE1  | 3:W:151:LYS:HE3  | 2.33                     | 0.62              |
| 2:I:85:ILE:O     | 2:I:89:VAL:HG23  | 1.99                     | 0.62              |
| 2:N:346:VAL:HG21 | 2:N:385:VAL:HG13 | 1.81                     | 0.62              |
| 2:N:49:GLY:HA2   | 2:N:54:LEU:HD23  | 1.81                     | 0.62              |
| 1:B:704:ILE:O    | 1:B:823:THR:OG1  | 2.17                     | 0.62              |
| 1:B:812:VAL:HG22 | 1:B:813:ALA:N    | 2.13                     | 0.62              |
| 1:B:305:GLN:HE21 | 1:B:564:ASN:CG   | 2.03                     | 0.62              |
| 1:B:199:VAL:CG1  | 1:B:200:VAL:N    | 2.62                     | 0.62              |
| 1:A:721:VAL:HG13 | 1:A:800:TYR:O    | 1.98                     | 0.62              |
| 1:B:451:ASP:N    | 1:B:452:PRO:HD3  | 2.13                     | 0.62              |
| 1:B:494:ASN:ND2  | 1:B:495:ASP:N    | 2.46                     | 0.62              |
| 1:B:95:ILE:HG22  | 1:B:97:THR:OG1   | 1.99                     | 0.62              |
| 2:J:346:VAL:HG21 | 2:J:385:VAL:HG13 | 1.81                     | 0.62              |
| 1:A:810:TYR:O    | 1:A:812:VAL:N    | 2.32                     | 0.62              |
| 2:O:346:VAL:HG21 | 2:O:385:VAL:HG13 | 1.81                     | 0.62              |
| 1:A:545:ASP:HA   | 1:A:548:ARG:HD2  | 1.80                     | 0.62              |
| 1:A:472:LEU:O    | 1:A:476:ASN:HB2  | 1.99                     | 0.62              |
| 1:A:360:ILE:CG2  | 1:A:363:GLU:HB2  | 2.29                     | 0.62              |
| 2:J:144:ARG:HD2  | 2:K:82:ARG:CZ    | 2.28                     | 0.62              |
| 2:K:48:THR:HG22  | 2:K:115:SER:OG   | 1.98                     | 0.62              |
| 1:B:596:SER:HB2  | 1:B:599:THR:OG1  | 1.99                     | 0.62              |
| 2:H:346:VAL:HG21 | 2:H:385:VAL:HG13 | 1.81                     | 0.62              |
| 2:O:135:TYR:OH   | 2:O:340:GLU:OE1  | 2.17                     | 0.62              |
| 3:W:781:GLU:O    | 3:W:785:GLN:HB2  | 1.98                     | 0.62              |
| 3:W:408:LEU:HD13 | 3:W:415:ILE:HG13 | 1.79                     | 0.62              |
| 1:B:723:ILE:O    | 1:B:824:LYS:HD2  | 2.00                     | 0.62              |
| 1:A:503:ILE:CD1  | 1:A:547:THR:HB   | 2.29                     | 0.62              |
| 1:B:122:LEU:HD11 | 1:B:200:VAL:CG1  | 2.29                     | 0.62              |
| 1:B:681:ILE:O    | 1:B:684:LEU:HB3  | 1.99                     | 0.62              |
| 2:C:21:GLY:O     | 2:C:22:THR:O     | 2.17                     | 0.62              |
| 1:B:497:ILE:HG12 | 2:I:68:THR:HG23  | 1.82                     | 0.62              |
| 1:B:791:LYS:C    | 1:B:792:VAL:HG13 | 2.20                     | 0.62              |
| 1:B:394:LEU:C    | 1:B:396:PHE:H    | 2.02                     | 0.62              |
| 2:H:109:ILE:CG1  | 2:H:109:ILE:O    | 2.48                     | 0.62              |
| 2:L:4:LEU:HA     | 2:L:7:LEU:CD1    | 2.28                     | 0.62              |
| 2:C:8:SER:O      | 2:C:11:LEU:N     | 2.33                     | 0.62              |
| 2:E:116:LEU:HA   | 2:E:119:LEU:HD12 | 1.81                     | 0.62              |
| 2:I:346:VAL:HG21 | 2:I:385:VAL:HG13 | 1.81                     | 0.62              |
| 1:B:432:VAL:HA   | 1:B:436:ILE:CD1  | 2.12                     | 0.62              |
| 1:A:763:LEU:HD23 | 1:A:764:PRO:HD3  | 1.80                     | 0.62              |
| 3:W:463:PHE:HD2  | 3:W:465:LEU:HD21 | 1.65                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:692:ILE:H    | 1:B:692:ILE:HD12 | 1.63                     | 0.62              |
| 3:W:906:ASN:ND2  | 3:W:907:VAL:H    | 1.95                     | 0.62              |
| 3:W:1001:TYR:CD1 | 3:W:1084:ASN:HB3 | 2.33                     | 0.62              |
| 2:J:85:ILE:O     | 2:J:89:VAL:HG23  | 1.99                     | 0.62              |
| 1:B:435:ILE:O    | 1:B:436:ILE:HG12 | 2.00                     | 0.62              |
| 1:B:371:ASN:HA   | 1:B:374:ALA:HB3  | 1.82                     | 0.62              |
| 3:W:324:LYS:O    | 3:W:328:TRP:CD1  | 2.53                     | 0.62              |
| 3:W:161:LYS:HB3  | 3:W:165:ARG:HH12 | 1.64                     | 0.62              |
| 1:A:738:LEU:C    | 1:A:740:ARG:H    | 2.02                     | 0.62              |
| 1:A:556:THR:O    | 1:A:557:LEU:C    | 2.38                     | 0.62              |
| 1:A:596:SER:O    | 1:A:600:LEU:HD12 | 1.99                     | 0.62              |
| 2:I:23:LEU:HD23  | 2:I:24:TYR:H     | 1.65                     | 0.62              |
| 2:J:22:THR:HG22  | 2:J:73:LEU:HD12  | 1.81                     | 0.62              |
| 2:N:8:SER:O      | 2:N:11:LEU:N     | 2.33                     | 0.62              |
| 2:L:38:ILE:HD12  | 2:L:65:LEU:CD2   | 2.29                     | 0.62              |
| 2:H:4:LEU:HA     | 2:H:7:LEU:CD1    | 2.28                     | 0.62              |
| 2:H:76:ASN:CB    | 2:J:76:ASN:HB2   | 2.30                     | 0.62              |
| 2:F:346:VAL:HG21 | 2:F:385:VAL:HG13 | 1.81                     | 0.62              |
| 2:O:23:LEU:HD23  | 2:O:24:TYR:N     | 2.14                     | 0.62              |
| 1:B:634:TYR:O    | 1:B:635:GLN:HG2  | 1.99                     | 0.62              |
| 2:L:62:ASP:CG    | 2:L:62:ASP:O     | 2.37                     | 0.62              |
| 2:H:12:LYS:HG2   | 2:H:16:ASP:OD2   | 2.00                     | 0.62              |
| 2:G:46:PHE:HE2   | 2:G:119:LEU:HD21 | 1.63                     | 0.62              |
| 3:W:758:THR:HG22 | 3:W:766:PHE:O    | 2.00                     | 0.62              |
| 2:M:346:VAL:HG21 | 2:M:385:VAL:HG13 | 1.81                     | 0.62              |
| 1:B:722:ASN:O    | 1:B:824:LYS:HB2  | 1.99                     | 0.62              |
| 1:B:240:ASN:HA   | 1:B:842:LEU:O    | 2.00                     | 0.62              |
| 1:A:692:ILE:H    | 1:A:692:ILE:HD12 | 1.64                     | 0.62              |
| 3:W:247:PRO:HG3  | 3:W:291:MET:HB3  | 1.81                     | 0.62              |
| 2:D:27:VAL:O     | 2:D:31:ILE:HG12  | 1.99                     | 0.62              |
| 2:L:109:ILE:HD12 | 2:L:109:ILE:O    | 1.99                     | 0.62              |
| 1:B:503:ILE:HG21 | 1:B:544:VAL:HG13 | 1.80                     | 0.61              |
| 3:W:928:SER:HB2  | 3:W:984:ASP:OD1  | 2.00                     | 0.61              |
| 2:E:12:LYS:HG2   | 2:E:16:ASP:OD2   | 1.99                     | 0.61              |
| 3:W:225:ILE:HD13 | 3:W:325:ILE:HD13 | 1.81                     | 0.61              |
| 1:B:508:GLU:CD   | 2:J:71:LEU:HB3   | 2.20                     | 0.61              |
| 2:L:22:THR:HG23  | 2:L:73:LEU:CD1   | 2.23                     | 0.61              |
| 2:G:27:VAL:O     | 2:G:31:ILE:HG12  | 2.01                     | 0.61              |
| 2:M:145:ARG:CZ   | 2:M:145:ARG:HB3  | 2.31                     | 0.61              |
| 2:M:116:LEU:HA   | 2:M:119:LEU:HD12 | 1.82                     | 0.61              |
| 2:N:66:LEU:HD13  | 2:N:77:TYR:OH    | 2.00                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:568:VAL:HG12 | 1:A:569:GLN:N    | 2.14                     | 0.61              |
| 1:B:863:VAL:HG12 | 1:B:864:GLU:H    | 1.65                     | 0.61              |
| 1:B:415:PRO:HG2  | 1:B:480:PHE:CD1  | 2.30                     | 0.61              |
| 1:A:447:TYR:OH   | 1:A:458:ILE:HG23 | 2.01                     | 0.61              |
| 1:B:428:GLN:HB2  | 1:B:456:PHE:HD1  | 1.61                     | 0.61              |
| 1:B:194:ARG:HA   | 1:B:194:ARG:CZ   | 2.30                     | 0.61              |
| 1:B:182:LEU:HD21 | 1:B:846:LEU:HA   | 1.82                     | 0.61              |
| 1:B:94:THR:O     | 1:B:316:SER:HB3  | 2.01                     | 0.61              |
| 1:A:362:SER:CB   | 1:A:365:GLN:NE2  | 2.63                     | 0.61              |
| 2:D:23:LEU:HD23  | 2:D:24:TYR:H     | 1.62                     | 0.61              |
| 2:E:8:SER:O      | 2:E:11:LEU:N     | 2.34                     | 0.61              |
| 1:A:225:ILE:HA   | 1:A:228:MET:HE1  | 1.83                     | 0.61              |
| 2:E:346:VAL:HG21 | 2:E:385:VAL:HG13 | 1.81                     | 0.61              |
| 2:D:346:VAL:HG21 | 2:D:385:VAL:HG13 | 1.81                     | 0.61              |
| 2:K:8:SER:O      | 2:K:11:LEU:N     | 2.34                     | 0.61              |
| 2:O:38:ILE:HG22  | 2:O:42:ASN:HD21  | 1.64                     | 0.61              |
| 1:B:744:TYR:O    | 1:B:745:ALA:HB3  | 2.00                     | 0.61              |
| 2:G:12:LYS:HG2   | 2:G:16:ASP:OD2   | 1.99                     | 0.61              |
| 2:J:116:LEU:HA   | 2:J:119:LEU:HD12 | 1.82                     | 0.61              |
| 2:G:128:ASN:HB3  | 2:H:19:VAL:HG23  | 1.81                     | 0.61              |
| 2:G:38:ILE:HG22  | 2:G:42:ASN:HD21  | 1.64                     | 0.61              |
| 2:O:8:SER:O      | 2:O:11:LEU:N     | 2.34                     | 0.61              |
| 1:B:521:MET:HB2  | 1:B:522:PRO:HD2  | 1.81                     | 0.61              |
| 2:L:8:SER:O      | 2:L:11:LEU:N     | 2.33                     | 0.61              |
| 2:I:116:LEU:HA   | 2:I:119:LEU:HD12 | 1.82                     | 0.61              |
| 1:A:389:GLN:O    | 1:A:389:GLN:HG3  | 2.00                     | 0.61              |
| 2:M:63:PHE:CD2   | 2:M:84:THR:HG23  | 2.35                     | 0.61              |
| 1:A:506:LEU:HD21 | 1:A:543:LEU:C    | 2.20                     | 0.61              |
| 1:B:297:ARG:HG3  | 1:B:848:PHE:CD2  | 2.29                     | 0.61              |
| 3:W:463:PHE:CD1  | 3:W:590:ALA:HB3  | 2.35                     | 0.61              |
| 3:W:292:LEU:O    | 3:W:296:ARG:HG3  | 2.00                     | 0.61              |
| 2:D:85:ILE:O     | 2:D:89:VAL:HG23  | 2.01                     | 0.61              |
| 1:B:545:ASP:HA   | 1:B:548:ARG:HD2  | 1.82                     | 0.61              |
| 1:A:443:GLN:CD   | 1:A:521:MET:HG2  | 2.21                     | 0.61              |
| 3:W:917:ARG:HD2  | 3:W:919:TYR:CE1  | 2.36                     | 0.61              |
| 3:W:779:VAL:O    | 3:W:782:VAL:HG23 | 2.00                     | 0.61              |
| 1:B:496:ASN:HB3  | 1:B:498:ARG:HB3  | 1.83                     | 0.61              |
| 3:W:967:ILE:HD12 | 3:W:967:ILE:N    | 2.15                     | 0.61              |
| 1:A:443:GLN:O    | 1:A:445:MET:N    | 2.34                     | 0.61              |
| 1:A:450:GLY:O    | 1:A:451:ASP:HB2  | 2.01                     | 0.61              |
| 2:O:150:PHE:CD1  | 2:O:150:PHE:N    | 2.69                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:147:ARG:O    | 2:O:148:THR:HB   | 1.99                     | 0.61              |
| 1:A:282:VAL:O    | 1:A:284:TYR:N    | 2.34                     | 0.61              |
| 1:A:257:LEU:HD13 | 1:A:843:THR:O    | 2.01                     | 0.61              |
| 2:L:72:ASN:ND2   | 2:N:126:ARG:HH11 | 1.99                     | 0.61              |
| 1:A:125:ILE:HD13 | 1:A:126:PHE:HE2  | 1.66                     | 0.61              |
| 2:J:6:SER:OG     | 2:J:128:ASN:HA   | 2.00                     | 0.61              |
| 2:O:116:LEU:HA   | 2:O:119:LEU:HD12 | 1.82                     | 0.61              |
| 3:W:145:VAL:HG21 | 3:W:211:ILE:HG23 | 1.82                     | 0.61              |
| 2:I:19:VAL:HG23  | 2:K:128:ASN:HB3  | 1.83                     | 0.61              |
| 1:A:701:GLN:HB3  | 1:A:826:TYR:HD2  | 1.66                     | 0.61              |
| 3:W:98:LEU:CD1   | 3:W:172:ILE:HG23 | 2.30                     | 0.61              |
| 2:J:8:SER:O      | 2:J:11:LEU:N     | 2.34                     | 0.61              |
| 1:B:523:VAL:O    | 1:B:525:TYR:N    | 2.34                     | 0.61              |
| 1:B:96:PRO:O     | 1:B:320:THR:HG21 | 1.99                     | 0.61              |
| 2:K:152:PHE:CD1  | 2:K:152:PHE:N    | 2.69                     | 0.61              |
| 2:N:116:LEU:HA   | 2:N:119:LEU:HD12 | 1.82                     | 0.61              |
| 3:W:573:VAL:HG21 | 3:W:586:TYR:CD1  | 2.36                     | 0.61              |
| 2:E:135:TYR:CZ   | 2:E:342:MET:HE3  | 2.36                     | 0.61              |
| 2:G:346:VAL:HG21 | 2:G:385:VAL:HG13 | 1.81                     | 0.61              |
| 1:A:570:THR:CG2  | 1:A:571:LEU:H    | 2.12                     | 0.60              |
| 1:A:660:ASP:O    | 1:A:661:GLN:C    | 2.38                     | 0.60              |
| 1:B:482:GLN:CB   | 1:B:493:LEU:HD22 | 2.30                     | 0.60              |
| 1:A:817:TRP:CG   | 1:A:818:VAL:N    | 2.65                     | 0.60              |
| 1:B:180:TYR:CD1  | 1:B:181:LEU:N    | 2.68                     | 0.60              |
| 1:B:133:ILE:CD1  | 1:B:145:ARG:HB2  | 2.31                     | 0.60              |
| 2:E:150:PHE:HB2  | 2:E:152:PHE:CZ   | 2.37                     | 0.60              |
| 2:N:109:ILE:HB   | 2:N:380:ASP:HB3  | 1.82                     | 0.60              |
| 1:B:333:VAL:HG11 | 1:B:380:LYS:HA   | 1.83                     | 0.60              |
| 1:A:434:THR:HG22 | 1:A:434:THR:O    | 2.00                     | 0.60              |
| 1:A:319:ASP:OD2  | 1:A:571:LEU:HB3  | 2.00                     | 0.60              |
| 1:A:631:LEU:HB3  | 1:A:633:LEU:CD1  | 2.31                     | 0.60              |
| 1:B:527:ARG:O    | 1:B:531:ARG:CG   | 2.49                     | 0.60              |
| 1:B:503:ILE:HD13 | 1:B:544:VAL:CG1  | 2.31                     | 0.60              |
| 1:A:817:TRP:CH2  | 1:A:819:PRO:HA   | 2.36                     | 0.60              |
| 1:A:403:SER:HA   | 1:A:582:THR:OG1  | 2.00                     | 0.60              |
| 2:L:150:PHE:HB2  | 2:L:152:PHE:HE1  | 1.60                     | 0.60              |
| 1:B:779:ASP:HA   | 1:B:798:ILE:HD11 | 1.82                     | 0.60              |
| 1:B:156:PRO:HB2  | 1:B:161:ASP:CB   | 2.30                     | 0.60              |
| 1:B:364:THR:HG21 | 3:W:622:ALA:HA   | 1.83                     | 0.60              |
| 2:F:109:ILE:O    | 2:F:109:ILE:HD12 | 2.01                     | 0.60              |
| 2:H:142:GLN:HE21 | 2:H:143:ASN:N    | 1.98                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:49:GLY:HA2   | 2:M:54:LEU:CD2   | 2.31                     | 0.60              |
| 2:C:346:VAL:HG21 | 2:C:385:VAL:HG13 | 1.81                     | 0.60              |
| 1:A:308:LEU:O    | 1:A:309:ASN:C    | 2.39                     | 0.60              |
| 1:A:757:VAL:HG12 | 1:A:758:ALA:N    | 2.17                     | 0.60              |
| 1:A:779:ASP:HA   | 1:A:798:ILE:HD11 | 1.80                     | 0.60              |
| 1:A:122:LEU:HD11 | 1:A:200:VAL:HG12 | 1.82                     | 0.60              |
| 1:B:684:LEU:O    | 1:B:687:MET:HG2  | 2.02                     | 0.60              |
| 1:B:118:LYS:CG   | 1:B:119:GLN:H    | 2.13                     | 0.60              |
| 1:A:625:ILE:O    | 1:A:628:ALA:HB3  | 2.00                     | 0.60              |
| 2:D:133:SER:O    | 2:D:135:TYR:N    | 2.35                     | 0.60              |
| 2:M:8:SER:O      | 2:M:11:LEU:N     | 2.34                     | 0.60              |
| 2:M:5:TYR:CE2    | 2:M:131:ASN:HA   | 2.37                     | 0.60              |
| 2:N:12:LYS:C     | 2:N:14:ALA:N     | 2.54                     | 0.60              |
| 1:A:355:LEU:HD13 | 1:A:363:GLU:HG2  | 1.83                     | 0.60              |
| 2:I:153:HIS:NE2  | 2:J:153:HIS:NE2  | 2.50                     | 0.60              |
| 3:W:100:ALA:O    | 3:W:102:LEU:HD13 | 2.02                     | 0.60              |
| 2:E:57:ARG:HH11  | 2:E:94:ASN:HD21  | 1.49                     | 0.60              |
| 1:B:424:LEU:O    | 1:B:424:LEU:HD12 | 2.01                     | 0.60              |
| 1:B:275:PRO:HD2  | 1:B:278:ILE:HD11 | 1.83                     | 0.60              |
| 1:B:492:VAL:O    | 1:B:493:LEU:C    | 2.40                     | 0.60              |
| 1:B:875:ARG:HD3  | 1:B:878:ASN:HD22 | 1.66                     | 0.60              |
| 2:O:24:TYR:HB2   | 2:O:71:LEU:HD12  | 1.83                     | 0.60              |
| 2:L:116:LEU:HA   | 2:L:119:LEU:HD12 | 1.83                     | 0.60              |
| 2:E:133:SER:O    | 2:E:135:TYR:N    | 2.35                     | 0.60              |
| 1:B:389:GLN:NE2  | 1:B:567:HIS:HA   | 2.17                     | 0.60              |
| 2:N:27:VAL:O     | 2:N:30:LEU:N     | 2.34                     | 0.60              |
| 2:H:8:SER:O      | 2:H:11:LEU:N     | 2.34                     | 0.60              |
| 1:A:803:ASN:C    | 1:A:805:ASP:H    | 2.05                     | 0.60              |
| 2:D:8:SER:O      | 2:D:11:LEU:N     | 2.34                     | 0.60              |
| 1:A:437:TYR:CD2  | 1:A:442:MET:HG3  | 2.36                     | 0.60              |
| 1:B:604:TYR:O    | 1:B:608:VAL:HG23 | 2.00                     | 0.60              |
| 2:N:157:ILE:HG12 | 2:N:214:LEU:HD13 | 1.84                     | 0.60              |
| 1:B:874:MET:O    | 1:B:875:ARG:CB   | 2.50                     | 0.60              |
| 2:L:73:LEU:HD22  | 2:L:77:TYR:CD2   | 2.36                     | 0.60              |
| 1:B:371:ASN:HD22 | 1:B:583:SER:CB   | 2.10                     | 0.60              |
| 1:B:674:VAL:CG2  | 1:B:679:LEU:HD13 | 2.27                     | 0.60              |
| 1:B:745:ALA:O    | 1:B:746:GLN:C    | 2.40                     | 0.60              |
| 2:H:23:LEU:H     | 2:H:26:ASN:ND2   | 2.00                     | 0.60              |
| 1:A:203:GLU:O    | 1:A:207:ILE:HG13 | 2.02                     | 0.60              |
| 2:M:145:ARG:NH1  | 2:M:145:ARG:HB3  | 2.16                     | 0.60              |
| 2:F:104:SER:HB3  | 2:F:108:GLY:HA3  | 1.84                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:68:THR:HG22  | 2:I:69:THR:N     | 2.16                     | 0.60              |
| 2:E:85:ILE:O     | 2:E:89:VAL:HG23  | 2.01                     | 0.60              |
| 1:A:326:TYR:CD1  | 1:A:384:ALA:HB1  | 2.36                     | 0.60              |
| 1:A:492:VAL:CG1  | 1:A:558:MET:SD   | 2.90                     | 0.60              |
| 1:A:546:LEU:CD1  | 1:A:584:LEU:HD23 | 2.32                     | 0.60              |
| 1:A:666:ARG:HG3  | 1:A:667:ASP:N    | 2.14                     | 0.60              |
| 1:B:274:ILE:CG2  | 1:B:278:ILE:HD11 | 2.25                     | 0.60              |
| 1:B:387:LEU:HD23 | 1:B:554:TYR:CE1  | 2.36                     | 0.60              |
| 1:B:508:GLU:C    | 1:B:512:GLN:HE21 | 2.05                     | 0.60              |
| 2:K:5:TYR:CE2    | 2:K:131:ASN:HA   | 2.37                     | 0.60              |
| 1:B:371:ASN:C    | 1:B:373:GLN:N    | 2.52                     | 0.60              |
| 1:B:743:ASP:OD2  | 1:B:745:ALA:HA   | 2.01                     | 0.60              |
| 3:W:473:GLN:HE22 | 3:W:593:GLU:HB3  | 1.66                     | 0.60              |
| 2:D:116:LEU:HA   | 2:D:119:LEU:HD12 | 1.82                     | 0.60              |
| 2:K:116:LEU:HA   | 2:K:119:LEU:HD12 | 1.84                     | 0.60              |
| 1:A:225:ILE:HA   | 1:A:228:MET:CE   | 2.32                     | 0.60              |
| 2:J:110:ALA:HB1  | 2:J:111:PRO:HD2  | 1.83                     | 0.60              |
| 2:G:157:ILE:HG12 | 2:G:214:LEU:HD13 | 1.84                     | 0.60              |
| 2:M:274:GLN:N    | 2:M:274:GLN:HE21 | 2.00                     | 0.60              |
| 2:C:133:SER:O    | 2:C:135:TYR:N    | 2.34                     | 0.60              |
| 2:F:133:SER:O    | 2:F:135:TYR:N    | 2.35                     | 0.60              |
| 1:A:237:ASN:OD1  | 1:A:237:ASN:O    | 2.20                     | 0.60              |
| 1:A:727:LEU:O    | 1:A:727:LEU:HD12 | 2.02                     | 0.60              |
| 1:B:723:ILE:O    | 1:B:724:ALA:HB2  | 2.01                     | 0.60              |
| 1:B:502:VAL:O    | 1:B:504:ASN:N    | 2.35                     | 0.60              |
| 1:B:435:ILE:CG2  | 1:B:436:ILE:H    | 2.09                     | 0.60              |
| 1:B:180:TYR:CD1  | 1:B:180:TYR:C    | 2.75                     | 0.60              |
| 2:D:38:ILE:HG22  | 2:D:42:ASN:HD21  | 1.67                     | 0.60              |
| 2:E:157:ILE:HG12 | 2:E:214:LEU:HD13 | 1.84                     | 0.60              |
| 2:J:133:SER:O    | 2:J:135:TYR:N    | 2.35                     | 0.60              |
| 2:J:274:GLN:N    | 2:J:274:GLN:HE21 | 2.00                     | 0.60              |
| 1:A:535:LEU:O    | 1:A:539:ARG:HG2  | 2.02                     | 0.60              |
| 1:B:555:GLU:OE2  | 1:B:871:PHE:HE2  | 1.85                     | 0.60              |
| 3:W:933:LEU:HD23 | 3:W:962:LEU:HD22 | 1.84                     | 0.60              |
| 3:W:463:PHE:CE1  | 3:W:590:ALA:HB3  | 2.37                     | 0.60              |
| 2:O:8:SER:C      | 2:O:10:THR:N     | 2.55                     | 0.60              |
| 3:W:708:ASP:HB3  | 3:W:1080:TYR:CZ  | 2.37                     | 0.60              |
| 1:B:601:PHE:H    | 1:B:601:PHE:HD1  | 1.47                     | 0.60              |
| 3:W:165:ARG:HE   | 3:W:220:HIS:HA   | 1.67                     | 0.60              |
| 2:M:152:PHE:CD1  | 2:M:152:PHE:N    | 2.70                     | 0.60              |
| 2:F:157:ILE:HG12 | 2:F:214:LEU:HD13 | 1.84                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:5:TYR:CE2    | 2:H:131:ASN:HA   | 2.37                     | 0.60              |
| 2:K:133:SER:O    | 2:K:135:TYR:N    | 2.35                     | 0.60              |
| 2:G:73:LEU:HD22  | 2:G:77:TYR:CD2   | 2.37                     | 0.60              |
| 1:B:482:GLN:O    | 1:B:482:GLN:HG3  | 2.02                     | 0.59              |
| 1:B:535:LEU:O    | 1:B:539:ARG:HG2  | 2.01                     | 0.59              |
| 1:A:445:MET:C    | 1:A:447:TYR:N    | 2.54                     | 0.59              |
| 1:B:508:GLU:OE2  | 2:J:71:LEU:HB3   | 2.02                     | 0.59              |
| 2:D:128:ASN:ND2  | 2:E:19:VAL:HG21  | 2.17                     | 0.59              |
| 1:A:604:TYR:O    | 1:A:608:VAL:HG23 | 2.01                     | 0.59              |
| 2:G:111:PRO:HB3  | 2:G:116:LEU:HD23 | 1.83                     | 0.59              |
| 2:H:133:SER:O    | 2:H:135:TYR:N    | 2.35                     | 0.59              |
| 2:C:85:ILE:O     | 2:C:89:VAL:HG23  | 2.01                     | 0.59              |
| 2:C:274:GLN:HE21 | 2:C:274:GLN:N    | 2.00                     | 0.59              |
| 1:A:577:GLN:O    | 1:A:581:VAL:HG23 | 2.01                     | 0.59              |
| 1:B:513:LEU:HA   | 1:B:516:GLN:OE1  | 2.01                     | 0.59              |
| 2:L:19:VAL:CG2   | 2:N:128:ASN:HB3  | 2.32                     | 0.59              |
| 1:A:366:PHE:C    | 1:A:368:THR:N    | 2.48                     | 0.59              |
| 2:M:24:TYR:O     | 2:M:27:VAL:HG22  | 2.02                     | 0.59              |
| 2:H:152:PHE:N    | 2:H:152:PHE:CD1  | 2.69                     | 0.59              |
| 2:I:157:ILE:HG12 | 2:I:214:LEU:HD13 | 1.84                     | 0.59              |
| 2:D:76:ASN:HB2   | 2:L:76:ASN:HB2   | 1.83                     | 0.59              |
| 1:A:548:ARG:HH11 | 1:A:877:MET:CA   | 2.14                     | 0.59              |
| 1:B:124:ARG:HB2  | 1:B:249:ASP:CG   | 2.22                     | 0.59              |
| 1:A:744:TYR:O    | 1:A:746:GLN:N    | 2.35                     | 0.59              |
| 1:A:747:ILE:HD11 | 1:A:786:ILE:HG21 | 1.85                     | 0.59              |
| 1:A:246:HIS:CD2  | 1:A:248:ILE:HB   | 2.36                     | 0.59              |
| 1:B:112:LYS:N    | 1:B:113:PRO:HD3  | 2.18                     | 0.59              |
| 3:W:816:SER:HB3  | 3:W:820:LEU:HD11 | 1.82                     | 0.59              |
| 2:C:131:ASN:HD22 | 2:C:131:ASN:N    | 1.99                     | 0.59              |
| 1:B:401:TYR:O    | 1:B:404:LEU:HB2  | 2.02                     | 0.59              |
| 1:B:863:VAL:HG12 | 1:B:864:GLU:N    | 2.17                     | 0.59              |
| 2:G:85:ILE:O     | 2:G:89:VAL:HG23  | 2.01                     | 0.59              |
| 2:N:85:ILE:O     | 2:N:89:VAL:HG23  | 2.02                     | 0.59              |
| 2:N:274:GLN:HE21 | 2:N:274:GLN:N    | 2.00                     | 0.59              |
| 2:H:274:GLN:HE21 | 2:H:274:GLN:N    | 2.00                     | 0.59              |
| 1:B:363:GLU:HA   | 1:B:363:GLU:OE1  | 2.02                     | 0.59              |
| 2:M:133:SER:O    | 2:M:135:TYR:N    | 2.35                     | 0.59              |
| 1:B:543:LEU:HD23 | 1:B:546:LEU:HD12 | 1.84                     | 0.59              |
| 1:A:703:VAL:HG21 | 1:A:797:PRO:HB3  | 1.84                     | 0.59              |
| 2:J:8:SER:C      | 2:J:10:THR:N     | 2.55                     | 0.59              |
| 2:F:23:LEU:HD11  | 2:H:36:GLN:HB2   | 1.85                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:415:PRO:HB3  | 1:A:479:GLN:HA   | 1.84                     | 0.59              |
| 1:A:545:ASP:O    | 1:A:548:ARG:N    | 2.35                     | 0.59              |
| 1:B:383:ILE:HD11 | 1:B:550:LEU:CD2  | 2.32                     | 0.59              |
| 1:A:521:MET:HA   | 1:A:521:MET:HE2  | 1.84                     | 0.59              |
| 1:A:700:ALA:O    | 1:A:701:GLN:HB2  | 2.02                     | 0.59              |
| 1:A:839:MET:HG2  | 1:A:840:HIS:N    | 2.16                     | 0.59              |
| 2:L:157:ILE:HG12 | 2:L:214:LEU:HD13 | 1.84                     | 0.59              |
| 2:D:70:LEU:HD12  | 2:D:71:LEU:N     | 2.17                     | 0.59              |
| 2:L:53:ASN:HD22  | 2:L:354:ALA:HB3  | 1.66                     | 0.59              |
| 1:B:141:GLU:O    | 1:B:142:LEU:HB2  | 2.03                     | 0.59              |
| 1:A:371:ASN:O    | 1:A:373:GLN:N    | 2.36                     | 0.59              |
| 1:A:548:ARG:NH1  | 1:A:877:MET:HA   | 2.17                     | 0.59              |
| 1:B:368:THR:O    | 1:B:371:ASN:ND2  | 2.36                     | 0.59              |
| 1:B:393:SER:HB3  | 1:B:573:THR:HG21 | 1.84                     | 0.59              |
| 2:M:74:ASP:OD2   | 2:M:76:ASN:HB3   | 2.03                     | 0.59              |
| 1:A:770:SER:O    | 1:A:771:VAL:C    | 2.40                     | 0.59              |
| 2:C:8:SER:C      | 2:C:10:THR:N     | 2.55                     | 0.59              |
| 2:H:135:TYR:CZ   | 2:H:342:MET:HE3  | 2.38                     | 0.59              |
| 2:M:135:TYR:OH   | 2:M:340:GLU:OE1  | 2.20                     | 0.59              |
| 2:D:104:SER:O    | 2:D:108:GLY:HA3  | 2.02                     | 0.59              |
| 2:O:274:GLN:N    | 2:O:274:GLN:HE21 | 2.00                     | 0.59              |
| 3:W:791:LEU:HD23 | 3:W:791:LEU:H    | 1.65                     | 0.59              |
| 1:A:160:TYR:CZ   | 1:A:635:GLN:HB2  | 2.38                     | 0.59              |
| 1:B:498:ARG:HH22 | 2:J:25:SER:H     | 1.49                     | 0.59              |
| 1:B:190:ASN:HD21 | 1:B:193:SER:CB   | 2.10                     | 0.59              |
| 1:A:803:ASN:H    | 1:A:807:ASN:ND2  | 2.00                     | 0.59              |
| 2:L:130:ASP:HA   | 2:M:17:LYS:HG2   | 1.83                     | 0.59              |
| 2:C:5:TYR:CE2    | 2:C:131:ASN:HA   | 2.36                     | 0.59              |
| 2:J:157:ILE:HG12 | 2:J:214:LEU:HD13 | 1.84                     | 0.59              |
| 2:K:157:ILE:HG12 | 2:K:214:LEU:HD13 | 1.84                     | 0.59              |
| 3:W:134:ILE:HG23 | 3:W:136:THR:HG22 | 1.85                     | 0.59              |
| 2:D:157:ILE:HG12 | 2:D:214:LEU:HD13 | 1.84                     | 0.59              |
| 1:A:413:VAL:HG12 | 1:A:414:VAL:N    | 2.17                     | 0.59              |
| 2:G:8:SER:C      | 2:G:10:THR:N     | 2.56                     | 0.59              |
| 1:A:368:THR:HG21 | 1:A:582:THR:HB   | 1.83                     | 0.59              |
| 3:W:687:ILE:CG2  | 3:W:900:MET:HG2  | 2.32                     | 0.59              |
| 2:D:76:ASN:H     | 2:L:76:ASN:HB2   | 1.67                     | 0.59              |
| 2:E:274:GLN:HE21 | 2:E:274:GLN:N    | 2.00                     | 0.59              |
| 2:H:157:ILE:HG12 | 2:H:214:LEU:HD13 | 1.84                     | 0.59              |
| 2:J:124:PHE:O    | 2:J:127:ILE:HG13 | 2.03                     | 0.59              |
| 1:A:464:GLN:HG3  | 2:F:39:ILE:HD11  | 1.84                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:322:THR:HG21 | 1:A:390:ARG:HA   | 1.83                     | 0.59              |
| 1:A:545:ASP:HA   | 1:A:548:ARG:CD   | 2.33                     | 0.59              |
| 1:A:467:GLN:HE21 | 1:A:511:MET:HG2  | 1.67                     | 0.59              |
| 1:A:520:THR:HG21 | 1:A:526:LYS:HD3  | 1.85                     | 0.59              |
| 1:A:409:TRP:HH2  | 1:A:547:THR:HG1  | 1.50                     | 0.59              |
| 1:A:784:ALA:O    | 1:A:785:GLN:C    | 2.41                     | 0.59              |
| 1:A:771:VAL:HG22 | 1:A:772:ILE:N    | 2.18                     | 0.59              |
| 1:A:216:GLU:CD   | 1:A:216:GLU:N    | 2.55                     | 0.59              |
| 2:O:4:LEU:HG     | 2:O:391:ILE:HG21 | 1.85                     | 0.59              |
| 2:J:12:LYS:C     | 2:J:14:ALA:N     | 2.55                     | 0.59              |
| 2:F:8:SER:O      | 2:F:11:LEU:N     | 2.36                     | 0.59              |
| 3:W:586:TYR:CE2  | 3:W:588:ALA:HB3  | 2.37                     | 0.59              |
| 2:H:85:ILE:O     | 2:H:89:VAL:HG23  | 2.03                     | 0.59              |
| 2:L:274:GLN:HE21 | 2:L:274:GLN:N    | 2.00                     | 0.59              |
| 2:G:152:PHE:N    | 2:G:152:PHE:CD1  | 2.71                     | 0.59              |
| 2:F:274:GLN:N    | 2:F:274:GLN:HE21 | 2.00                     | 0.59              |
| 1:B:833:PHE:CZ   | 1:B:835:PHE:HA   | 2.38                     | 0.59              |
| 2:G:71:LEU:HG    | 2:G:72:ASN:N     | 2.17                     | 0.59              |
| 3:W:460:ARG:HH11 | 3:W:460:ARG:HG3  | 1.67                     | 0.59              |
| 1:B:803:ASN:N    | 1:B:807:ASN:ND2  | 2.48                     | 0.59              |
| 1:A:546:LEU:HD11 | 1:A:588:ILE:HD12 | 1.83                     | 0.59              |
| 1:A:629:ASN:C    | 1:A:631:LEU:H    | 2.02                     | 0.59              |
| 1:A:401:TYR:O    | 1:A:404:LEU:HB2  | 2.02                     | 0.59              |
| 2:K:8:SER:C      | 2:K:10:THR:N     | 2.55                     | 0.59              |
| 1:A:722:ASN:HD22 | 1:A:824:LYS:HA   | 1.68                     | 0.59              |
| 1:A:242:PRO:HA   | 1:A:841:MET:SD   | 2.42                     | 0.59              |
| 2:O:12:LYS:C     | 2:O:14:ALA:N     | 2.57                     | 0.59              |
| 2:M:38:ILE:HG22  | 2:M:42:ASN:HD21  | 1.67                     | 0.59              |
| 2:I:152:PHE:N    | 2:I:152:PHE:CD1  | 2.70                     | 0.59              |
| 3:W:105:ASN:HB3  | 3:W:110:GLU:HB2  | 1.85                     | 0.59              |
| 1:A:810:TYR:CD1  | 1:A:811:LEU:N    | 2.71                     | 0.59              |
| 2:N:109:ILE:O    | 2:N:109:ILE:HD12 | 2.03                     | 0.59              |
| 2:M:135:TYR:CZ   | 2:M:342:MET:HE3  | 2.37                     | 0.59              |
| 2:O:100:MET:HG3  | 2:O:388:VAL:HG11 | 1.85                     | 0.59              |
| 3:W:319:PHE:N    | 3:W:320:PRO:CD   | 2.66                     | 0.58              |
| 1:A:571:LEU:HD23 | 1:B:531:ARG:NH2  | 2.17                     | 0.58              |
| 1:B:326:TYR:CD1  | 1:B:384:ALA:HB1  | 2.37                     | 0.58              |
| 1:B:745:ALA:HB1  | 1:B:748:THR:CB   | 2.31                     | 0.58              |
| 1:A:803:ASN:O    | 1:A:805:ASP:N    | 2.36                     | 0.58              |
| 1:A:437:TYR:CE2  | 1:A:442:MET:HG3  | 2.37                     | 0.58              |
| 2:H:116:LEU:HA   | 2:H:119:LEU:HD12 | 1.84                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:153:HIS:NE2  | 2:H:153:HIS:NE2  | 2.51                     | 0.58              |
| 2:F:116:LEU:HA   | 2:F:119:LEU:HD12 | 1.85                     | 0.58              |
| 3:W:343:ALA:O    | 3:W:346:GLN:HG3  | 2.03                     | 0.58              |
| 1:B:285:ILE:C    | 1:B:286:LEU:HD13 | 2.22                     | 0.58              |
| 1:A:484:VAL:HG12 | 1:A:485:ILE:H    | 1.68                     | 0.58              |
| 1:A:571:LEU:HD23 | 1:B:531:ARG:CZ   | 2.32                     | 0.58              |
| 1:B:875:ARG:HD3  | 1:B:878:ASN:ND2  | 2.18                     | 0.58              |
| 1:A:428:GLN:NE2  | 1:A:455:PRO:CB   | 2.59                     | 0.58              |
| 1:A:508:GLU:O    | 1:A:512:GLN:HG3  | 2.02                     | 0.58              |
| 1:B:437:TYR:CD2  | 1:B:443:GLN:HB3  | 2.38                     | 0.58              |
| 1:B:463:ILE:HG21 | 1:B:468:VAL:HG11 | 1.84                     | 0.58              |
| 2:H:22:THR:HG23  | 2:H:73:LEU:HD12  | 1.83                     | 0.58              |
| 2:C:12:LYS:C     | 2:C:14:ALA:N     | 2.56                     | 0.58              |
| 2:G:274:GLN:HE21 | 2:G:274:GLN:N    | 2.00                     | 0.58              |
| 2:C:157:ILE:HG12 | 2:C:214:LEU:HD13 | 1.84                     | 0.58              |
| 1:A:661:GLN:HG3  | 1:B:348:LYS:HZ1  | 1.67                     | 0.58              |
| 1:A:503:ILE:C    | 1:A:505:GLN:N    | 2.55                     | 0.58              |
| 1:B:190:ASN:O    | 1:B:192:ASN:N    | 2.37                     | 0.58              |
| 1:B:223:ARG:O    | 1:B:226:ALA:HB3  | 2.03                     | 0.58              |
| 2:L:5:TYR:CE2    | 2:L:131:ASN:HA   | 2.37                     | 0.58              |
| 1:B:111:ILE:HG22 | 1:B:113:PRO:HD3  | 1.84                     | 0.58              |
| 1:A:420:ILE:CD1  | 1:A:422:GLU:HG3  | 2.33                     | 0.58              |
| 1:B:421:ARG:O    | 1:B:425:VAL:HG23 | 2.02                     | 0.58              |
| 2:E:152:PHE:N    | 2:E:152:PHE:CD1  | 2.71                     | 0.58              |
| 2:M:85:ILE:O     | 2:M:89:VAL:HG23  | 2.02                     | 0.58              |
| 2:K:260:GLU:HG2  | 2:K:274:GLN:HG3  | 1.85                     | 0.58              |
| 2:M:157:ILE:HG12 | 2:M:214:LEU:HD13 | 1.84                     | 0.58              |
| 2:D:274:GLN:N    | 2:D:274:GLN:HE21 | 2.00                     | 0.58              |
| 2:I:10:THR:O     | 2:I:14:ALA:HB2   | 2.04                     | 0.58              |
| 3:W:105:ASN:HB2  | 3:W:111:ASN:CG   | 2.23                     | 0.58              |
| 2:K:145:ARG:O    | 2:K:146:GLN:HG2  | 2.02                     | 0.58              |
| 1:A:197:GLY:O    | 1:A:198:LYS:C    | 2.42                     | 0.58              |
| 2:G:133:SER:O    | 2:G:135:TYR:N    | 2.35                     | 0.58              |
| 2:L:17:LYS:HG2   | 2:N:130:ASP:HA   | 1.84                     | 0.58              |
| 2:D:130:ASP:HA   | 2:E:17:LYS:HG2   | 1.84                     | 0.58              |
| 2:F:5:TYR:CE2    | 2:F:131:ASN:HA   | 2.38                     | 0.58              |
| 2:G:12:LYS:C     | 2:G:14:ALA:N     | 2.57                     | 0.58              |
| 1:A:244:ILE:O    | 1:A:245:LEU:HD23 | 2.03                     | 0.58              |
| 1:B:218:GLU:O    | 1:B:221:VAL:HG23 | 2.03                     | 0.58              |
| 3:W:470:PHE:CE1  | 3:W:594:LYS:HD3  | 2.39                     | 0.58              |
| 1:A:259:HIS:CD2  | 1:A:677:ARG:HG3  | 2.38                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:116:LEU:HA   | 2:G:119:LEU:HD12 | 1.84                     | 0.58              |
| 2:L:74:ASP:OD2   | 2:L:76:ASN:HB3   | 2.03                     | 0.58              |
| 2:F:130:ASP:HA   | 2:G:17:LYS:HG2   | 1.85                     | 0.58              |
| 2:O:157:ILE:HG12 | 2:O:214:LEU:HD13 | 1.84                     | 0.58              |
| 1:A:160:TYR:OH   | 1:A:635:GLN:HB2  | 2.04                     | 0.58              |
| 1:B:508:GLU:O    | 1:B:512:GLN:HG3  | 2.04                     | 0.58              |
| 2:M:128:ASN:O    | 2:N:22:THR:HB    | 2.03                     | 0.58              |
| 2:H:8:SER:C      | 2:H:10:THR:N     | 2.56                     | 0.58              |
| 2:E:22:THR:HG23  | 2:E:73:LEU:HD12  | 1.86                     | 0.58              |
| 1:A:180:TYR:CD1  | 1:A:180:TYR:C    | 2.75                     | 0.58              |
| 2:K:49:GLY:HA3   | 2:K:55:PRO:O     | 2.03                     | 0.58              |
| 1:A:188:VAL:HG12 | 1:A:189:GLU:N    | 2.17                     | 0.58              |
| 2:N:133:SER:O    | 2:N:135:TYR:N    | 2.36                     | 0.58              |
| 3:W:126:THR:O    | 3:W:126:THR:HG23 | 2.03                     | 0.58              |
| 1:B:772:ILE:CG2  | 1:B:773:SER:N    | 2.66                     | 0.58              |
| 1:A:744:TYR:C    | 1:A:746:GLN:H    | 2.07                     | 0.58              |
| 1:B:371:ASN:HB3  | 1:B:583:SER:HB2  | 1.86                     | 0.58              |
| 2:K:85:ILE:O     | 2:K:89:VAL:HG23  | 2.02                     | 0.58              |
| 3:W:22:VAL:CG2   | 3:W:77:TYR:HB3   | 2.34                     | 0.58              |
| 2:C:116:LEU:HA   | 2:C:119:LEU:HD12 | 1.84                     | 0.58              |
| 2:J:5:TYR:HE2    | 2:J:131:ASN:HA   | 1.69                     | 0.58              |
| 2:O:260:GLU:HG2  | 2:O:274:GLN:HG3  | 1.86                     | 0.58              |
| 3:W:744:ILE:HG13 | 3:W:858:LEU:HD13 | 1.85                     | 0.58              |
| 2:I:260:GLU:HG2  | 2:I:274:GLN:HG3  | 1.86                     | 0.58              |
| 2:F:85:ILE:O     | 2:F:89:VAL:HG23  | 2.04                     | 0.58              |
| 1:B:416:ASN:O    | 1:B:418:MET:N    | 2.36                     | 0.58              |
| 2:M:12:LYS:C     | 2:M:14:ALA:N     | 2.57                     | 0.58              |
| 1:B:340:VAL:HB   | 1:B:587:LEU:HD12 | 1.84                     | 0.58              |
| 2:G:8:SER:O      | 2:G:11:LEU:N     | 2.36                     | 0.58              |
| 1:A:613:ASN:HD22 | 1:A:649:LEU:HD23 | 1.69                     | 0.58              |
| 3:W:28:TYR:CD2   | 3:W:72:LEU:HD13  | 2.37                     | 0.58              |
| 3:W:542:LEU:HD23 | 3:W:558:LEU:HD23 | 1.86                     | 0.58              |
| 3:W:623:THR:HG21 | 3:W:626:ILE:HD11 | 1.86                     | 0.58              |
| 2:E:8:SER:C      | 2:E:10:THR:N     | 2.55                     | 0.58              |
| 2:J:116:LEU:HD12 | 2:J:119:LEU:HD12 | 1.86                     | 0.58              |
| 2:N:116:LEU:HD12 | 2:N:119:LEU:HD12 | 1.86                     | 0.58              |
| 2:F:260:GLU:HG2  | 2:F:274:GLN:HG3  | 1.86                     | 0.58              |
| 2:L:133:SER:O    | 2:L:135:TYR:N    | 2.36                     | 0.58              |
| 1:B:696:SER:O    | 1:B:827:LYS:HE3  | 2.04                     | 0.58              |
| 1:A:303:LEU:HA   | 1:A:615:ASN:HD22 | 1.67                     | 0.58              |
| 1:A:304:LEU:N    | 1:A:615:ASN:HD21 | 2.02                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:459:ALA:O    | 1:B:463:ILE:HG13 | 2.03                     | 0.58              |
| 2:K:12:LYS:C     | 2:K:14:ALA:N     | 2.56                     | 0.58              |
| 1:B:190:ASN:HB2  | 1:B:199:VAL:HG23 | 1.85                     | 0.58              |
| 1:A:365:GLN:HB2  | 1:A:366:PHE:CZ   | 2.39                     | 0.58              |
| 3:W:906:ASN:ND2  | 3:W:907:VAL:HG23 | 2.18                     | 0.58              |
| 2:J:10:THR:O     | 2:J:14:ALA:HB2   | 2.04                     | 0.58              |
| 2:D:68:THR:O     | 2:D:69:THR:C     | 2.41                     | 0.58              |
| 1:A:420:ILE:CG1  | 1:A:423:SER:HB2  | 2.32                     | 0.58              |
| 2:C:7:LEU:O      | 2:C:11:LEU:HG    | 2.04                     | 0.58              |
| 2:O:133:SER:O    | 2:O:135:TYR:N    | 2.36                     | 0.58              |
| 1:A:568:VAL:HG12 | 1:A:569:GLN:H    | 1.68                     | 0.58              |
| 2:C:260:GLU:HG2  | 2:C:274:GLN:HG3  | 1.86                     | 0.58              |
| 1:A:390:ARG:HD2  | 1:A:570:THR:HG21 | 1.84                     | 0.58              |
| 1:B:491:GLN:HE22 | 1:B:566:GLN:CG   | 2.16                     | 0.58              |
| 1:A:803:ASN:H    | 1:A:807:ASN:HD22 | 1.50                     | 0.58              |
| 3:W:292:LEU:HD23 | 3:W:295:MET:CE   | 2.34                     | 0.58              |
| 3:W:519:THR:CG2  | 3:W:520:ASP:N    | 2.67                     | 0.58              |
| 2:I:38:ILE:HG22  | 2:I:42:ASN:ND2   | 2.16                     | 0.57              |
| 2:L:104:SER:HB3  | 2:L:108:GLY:HA2  | 1.86                     | 0.57              |
| 2:L:12:LYS:C     | 2:L:14:ALA:N     | 2.56                     | 0.57              |
| 2:K:53:ASN:HD22  | 2:K:354:ALA:CB   | 2.17                     | 0.57              |
| 3:W:449:LEU:HD13 | 3:W:573:VAL:HG13 | 1.85                     | 0.57              |
| 2:K:274:GLN:HE21 | 2:K:274:GLN:N    | 2.01                     | 0.57              |
| 2:I:274:GLN:HE21 | 2:I:274:GLN:N    | 2.00                     | 0.57              |
| 1:B:140:LYS:C    | 1:B:142:LEU:H    | 2.06                     | 0.57              |
| 1:A:527:ARG:O    | 1:A:531:ARG:CG   | 2.51                     | 0.57              |
| 2:I:8:SER:O      | 2:I:11:LEU:N     | 2.36                     | 0.57              |
| 1:B:199:VAL:CG1  | 1:B:200:VAL:H    | 2.17                     | 0.57              |
| 1:A:681:ILE:O    | 1:A:684:LEU:HB3  | 2.03                     | 0.57              |
| 2:I:133:SER:O    | 2:I:135:TYR:N    | 2.36                     | 0.57              |
| 2:F:12:LYS:C     | 2:F:14:ALA:N     | 2.56                     | 0.57              |
| 2:M:260:GLU:HG2  | 2:M:274:GLN:HG3  | 1.86                     | 0.57              |
| 2:D:260:GLU:HG2  | 2:D:274:GLN:HG3  | 1.86                     | 0.57              |
| 1:A:548:ARG:NH1  | 1:A:878:ASN:H    | 2.01                     | 0.57              |
| 1:B:415:PRO:HB2  | 1:B:480:PHE:HB2  | 1.86                     | 0.57              |
| 1:B:434:THR:HG22 | 1:B:434:THR:O    | 2.04                     | 0.57              |
| 1:B:472:LEU:O    | 1:B:476:ASN:HB2  | 2.04                     | 0.57              |
| 2:I:12:LYS:C     | 2:I:14:ALA:N     | 2.56                     | 0.57              |
| 2:K:8:SER:O      | 2:K:10:THR:N     | 2.38                     | 0.57              |
| 2:K:10:THR:O     | 2:K:14:ALA:HB2   | 2.05                     | 0.57              |
| 2:M:8:SER:C      | 2:M:10:THR:N     | 2.55                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:254:GLU:HG2  | 2:N:69:THR:CB    | 2.34                     | 0.57              |
| 2:G:10:THR:O     | 2:G:14:ALA:HB2   | 2.05                     | 0.57              |
| 1:B:494:ASN:CG   | 1:B:495:ASP:H    | 2.07                     | 0.57              |
| 2:F:144:ARG:HD2  | 2:G:82:ARG:NH1   | 2.19                     | 0.57              |
| 2:E:260:GLU:HG2  | 2:E:274:GLN:HG3  | 1.86                     | 0.57              |
| 2:N:76:ASN:HB2   | 2:O:76:ASN:H     | 1.69                     | 0.57              |
| 2:K:62:ASP:O     | 2:K:62:ASP:CG    | 2.42                     | 0.57              |
| 2:I:8:SER:C      | 2:I:10:THR:N     | 2.56                     | 0.57              |
| 2:L:144:ARG:O    | 2:L:145:ARG:CB   | 2.48                     | 0.57              |
| 2:F:8:SER:C      | 2:F:10:THR:N     | 2.55                     | 0.57              |
| 3:W:690:ARG:HB3  | 3:W:690:ARG:HH11 | 1.68                     | 0.57              |
| 1:A:342:THR:HG21 | 3:W:967:ILE:HG22 | 1.87                     | 0.57              |
| 1:A:503:ILE:HG22 | 1:A:506:LEU:HB2  | 1.86                     | 0.57              |
| 2:K:7:LEU:O      | 2:K:11:LEU:HG    | 2.04                     | 0.57              |
| 2:L:145:ARG:O    | 2:L:146:GLN:HG3  | 2.04                     | 0.57              |
| 1:A:771:VAL:CG1  | 1:A:809:PHE:HB3  | 2.34                     | 0.57              |
| 2:L:7:LEU:O      | 2:L:11:LEU:HG    | 2.05                     | 0.57              |
| 2:C:116:LEU:HD12 | 2:C:119:LEU:HD12 | 1.86                     | 0.57              |
| 1:A:738:LEU:O    | 1:A:740:ARG:N    | 2.37                     | 0.57              |
| 1:A:127:GLU:OE2  | 1:A:151:LYS:HG2  | 2.03                     | 0.57              |
| 1:B:817:TRP:CD1  | 1:B:818:VAL:N    | 2.73                     | 0.57              |
| 2:N:5:TYR:CE2    | 2:N:131:ASN:HA   | 2.39                     | 0.57              |
| 1:B:786:ILE:HG13 | 1:B:787:VAL:HG23 | 1.87                     | 0.57              |
| 1:A:783:PHE:O    | 1:A:786:ILE:HD12 | 2.05                     | 0.57              |
| 3:W:561:TYR:OH   | 3:W:595:GLN:HB3  | 2.04                     | 0.57              |
| 2:E:149:GLY:C    | 2:E:150:PHE:CD1  | 2.77                     | 0.57              |
| 1:B:117:LYS:HB2  | 1:B:179:ASP:OD2  | 2.04                     | 0.57              |
| 3:W:208:ASN:HB2  | 3:W:697:ASN:HD21 | 1.68                     | 0.57              |
| 1:B:703:VAL:HG12 | 1:B:704:ILE:N    | 2.20                     | 0.57              |
| 1:B:477:ASN:O    | 1:B:478:ASN:C    | 2.43                     | 0.57              |
| 1:B:518:PHE:N    | 1:B:518:PHE:CD1  | 2.72                     | 0.57              |
| 1:B:535:LEU:O    | 1:B:539:ARG:CG   | 2.52                     | 0.57              |
| 1:B:246:HIS:HB3  | 1:B:249:ASP:OD2  | 2.05                     | 0.57              |
| 1:A:259:HIS:ND1  | 1:A:260:GLN:N    | 2.52                     | 0.57              |
| 1:A:131:LEU:HD12 | 1:A:132:PRO:CD   | 2.35                     | 0.57              |
| 2:C:128:ASN:HB3  | 2:D:19:VAL:CG2   | 2.35                     | 0.57              |
| 2:G:116:LEU:HD12 | 2:G:119:LEU:HD12 | 1.87                     | 0.57              |
| 2:G:260:GLU:HG2  | 2:G:274:GLN:HG3  | 1.86                     | 0.57              |
| 3:W:951:ILE:HG12 | 3:W:985:LYS:HA   | 1.85                     | 0.57              |
| 1:B:701:GLN:O    | 1:B:702:GLY:O    | 2.23                     | 0.57              |
| 1:A:163:ARG:HH22 | 1:A:736:GLU:CD   | 2.07                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:473:HIS:CB   | 2:I:126:ARG:HH22 | 2.08                     | 0.57              |
| 1:B:340:VAL:HB   | 1:B:587:LEU:CD1  | 2.35                     | 0.57              |
| 2:I:145:ARG:O    | 2:I:146:GLN:HG3  | 2.04                     | 0.57              |
| 2:M:106:ARG:H    | 2:M:106:ARG:CD   | 2.14                     | 0.57              |
| 2:O:150:PHE:HB2  | 2:O:152:PHE:HE1  | 1.70                     | 0.57              |
| 2:I:116:LEU:HD12 | 2:I:119:LEU:HD12 | 1.86                     | 0.57              |
| 3:W:853:GLN:HE21 | 3:W:857:LEU:HB2  | 1.69                     | 0.57              |
| 1:B:839:MET:C    | 1:B:839:MET:SD   | 2.83                     | 0.57              |
| 1:B:277:ARG:C    | 1:B:278:ILE:HG12 | 2.23                     | 0.57              |
| 1:B:492:VAL:CG1  | 1:B:558:MET:SD   | 2.93                     | 0.57              |
| 1:A:512:GLN:O    | 1:A:516:GLN:HG3  | 2.05                     | 0.57              |
| 1:A:710:MET:CE   | 1:A:824:LYS:HE2  | 2.35                     | 0.57              |
| 1:A:122:LEU:HD11 | 1:A:201:ASP:HB2  | 1.85                     | 0.57              |
| 1:A:420:ILE:CD1  | 1:A:423:SER:HB2  | 2.35                     | 0.57              |
| 1:A:187:ALA:O    | 1:A:188:VAL:HG23 | 2.04                     | 0.57              |
| 3:W:872:ILE:O    | 3:W:1073:ILE:HA  | 2.05                     | 0.57              |
| 2:J:260:GLU:HG2  | 2:J:274:GLN:HG3  | 1.86                     | 0.57              |
| 2:N:260:GLU:HG2  | 2:N:274:GLN:HG3  | 1.85                     | 0.57              |
| 3:W:572:TYR:CE1  | 3:W:585:GLN:HG3  | 2.40                     | 0.57              |
| 1:A:370:ILE:H    | 3:W:933:LEU:HD11 | 1.70                     | 0.57              |
| 1:B:271:PHE:O    | 1:B:274:ILE:HB   | 2.05                     | 0.57              |
| 1:B:673:PRO:C    | 1:B:674:VAL:HG22 | 2.26                     | 0.57              |
| 2:G:5:TYR:CE2    | 2:G:131:ASN:HA   | 2.40                     | 0.57              |
| 2:G:24:TYR:O     | 2:G:27:VAL:HG22  | 2.03                     | 0.57              |
| 2:C:150:PHE:HB2  | 2:C:152:PHE:CZ   | 2.40                     | 0.57              |
| 2:H:7:LEU:O      | 2:H:11:LEU:HG    | 2.05                     | 0.57              |
| 2:L:144:ARG:HD2  | 2:M:82:ARG:NH1   | 2.20                     | 0.57              |
| 2:E:27:VAL:O     | 2:E:31:ILE:HG12  | 2.05                     | 0.57              |
| 3:W:491:ALA:HB3  | 3:W:629:ASP:OD1  | 2.05                     | 0.57              |
| 2:E:35:ASN:HA    | 2:E:38:ILE:HD12  | 1.87                     | 0.57              |
| 3:W:225:ILE:CD1  | 3:W:325:ILE:HD13 | 2.33                     | 0.57              |
| 1:B:312:ASP:O    | 1:B:313:ASN:HB2  | 2.05                     | 0.57              |
| 3:W:226:ALA:O    | 3:W:230:ILE:HG13 | 2.04                     | 0.57              |
| 1:B:775:ILE:HD12 | 1:B:775:ILE:N    | 2.20                     | 0.56              |
| 1:B:272:ASN:C    | 1:B:274:ILE:N    | 2.54                     | 0.56              |
| 2:K:14:ALA:O     | 2:K:18:ILE:HD12  | 2.05                     | 0.56              |
| 1:B:254:GLU:CG   | 2:N:69:THR:HB    | 2.35                     | 0.56              |
| 1:B:790:ARG:CA   | 1:B:790:ARG:NE   | 2.47                     | 0.56              |
| 3:W:440:PRO:HA   | 3:W:567:ASN:ND2  | 2.19                     | 0.56              |
| 2:G:61:PHE:HA    | 2:G:63:PHE:HE1   | 1.70                     | 0.56              |
| 2:D:8:SER:C      | 2:D:10:THR:N     | 2.54                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:128:ASN:HB3  | 2:E:19:VAL:HG23  | 1.87                     | 0.56              |
| 1:A:180:TYR:HD1  | 1:A:181:LEU:N    | 2.03                     | 0.56              |
| 2:D:116:LEU:HD12 | 2:D:119:LEU:HD12 | 1.85                     | 0.56              |
| 2:G:135:TYR:OH   | 2:G:340:GLU:OE1  | 2.23                     | 0.56              |
| 2:N:74:ASP:OD2   | 2:N:76:ASN:HB3   | 2.05                     | 0.56              |
| 1:B:137:ASN:OD1  | 1:B:137:ASN:O    | 2.22                     | 0.56              |
| 1:A:597:PRO:HB3  | 1:A:860:ALA:CB   | 2.35                     | 0.56              |
| 2:H:42:ASN:OD1   | 2:H:62:ASP:HA    | 2.05                     | 0.56              |
| 1:A:332:VAL:HG13 | 1:A:599:THR:CG2  | 2.36                     | 0.56              |
| 1:A:703:VAL:HG22 | 1:A:825:VAL:HG22 | 1.87                     | 0.56              |
| 1:B:97:THR:HA    | 1:B:320:THR:HG23 | 1.86                     | 0.56              |
| 2:E:12:LYS:C     | 2:E:14:ALA:N     | 2.56                     | 0.56              |
| 1:A:226:ALA:O    | 1:A:228:MET:N    | 2.32                     | 0.56              |
| 2:M:139:TRP:HE1  | 2:M:143:ASN:HD21 | 1.52                     | 0.56              |
| 2:O:110:ALA:HB1  | 2:O:111:PRO:CD   | 2.35                     | 0.56              |
| 1:B:390:ARG:HG3  | 1:B:391:THR:H    | 1.69                     | 0.56              |
| 1:B:556:THR:O    | 1:B:557:LEU:C    | 2.44                     | 0.56              |
| 1:A:305:GLN:O    | 1:A:307:ARG:N    | 2.38                     | 0.56              |
| 2:N:24:TYR:O     | 2:N:26:ASN:N     | 2.38                     | 0.56              |
| 1:B:393:SER:N    | 1:B:573:THR:CG2  | 2.68                     | 0.56              |
| 1:B:368:THR:O    | 1:B:369:GLY:O    | 2.23                     | 0.56              |
| 3:W:984:ASP:O    | 3:W:988:ILE:HG12 | 2.05                     | 0.56              |
| 1:A:275:PRO:O    | 1:A:278:ILE:HG13 | 2.05                     | 0.56              |
| 1:B:409:TRP:CH2  | 1:B:413:VAL:HG21 | 2.40                     | 0.56              |
| 1:A:649:LEU:O    | 1:A:650:HIS:O    | 2.24                     | 0.56              |
| 2:D:10:THR:O     | 2:D:14:ALA:HB2   | 2.05                     | 0.56              |
| 2:D:8:SER:O      | 2:D:10:THR:N     | 2.38                     | 0.56              |
| 3:W:477:VAL:HA   | 3:W:480:MET:CE   | 2.35                     | 0.56              |
| 2:J:152:PHE:CD1  | 2:J:152:PHE:N    | 2.71                     | 0.56              |
| 1:A:420:ILE:HD12 | 1:A:422:GLU:HG3  | 1.87                     | 0.56              |
| 2:K:35:ASN:HA    | 2:K:38:ILE:HD12  | 1.87                     | 0.56              |
| 2:I:116:LEU:CD1  | 2:I:119:LEU:HD12 | 2.36                     | 0.56              |
| 1:A:135:ARG:O    | 1:A:136:ALA:C    | 2.44                     | 0.56              |
| 2:H:260:GLU:HG2  | 2:H:274:GLN:HG3  | 1.85                     | 0.56              |
| 1:A:765:PHE:CD1  | 1:A:765:PHE:C    | 2.79                     | 0.56              |
| 3:W:329:SER:O    | 3:W:332:VAL:HG22 | 2.05                     | 0.56              |
| 1:A:308:LEU:HB2  | 1:A:614:TYR:OH   | 2.06                     | 0.56              |
| 1:A:410:LEU:O    | 1:A:413:VAL:HB   | 2.05                     | 0.56              |
| 1:A:587:LEU:C    | 1:A:588:ILE:HG13 | 2.24                     | 0.56              |
| 1:B:870:ALA:C    | 1:B:872:ASP:N    | 2.56                     | 0.56              |
| 2:G:2:ASP:HB2    | 2:G:128:ASN:HD21 | 1.71                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:10:THR:O     | 2:H:14:ALA:HB2   | 2.06                     | 0.56              |
| 2:J:74:ASP:OD2   | 2:J:76:ASN:HB3   | 2.04                     | 0.56              |
| 2:D:12:LYS:C     | 2:D:14:ALA:N     | 2.56                     | 0.56              |
| 2:H:27:VAL:CG2   | 2:H:31:ILE:HD11  | 2.35                     | 0.56              |
| 2:M:150:PHE:CD1  | 2:M:150:PHE:N    | 2.74                     | 0.56              |
| 1:A:729:GLY:C    | 1:A:730:PHE:CD1  | 2.78                     | 0.56              |
| 3:W:948:TYR:O    | 3:W:951:ILE:HG22 | 2.05                     | 0.56              |
| 1:A:209:ASP:O    | 1:A:213:GLN:HG3  | 2.05                     | 0.56              |
| 3:W:112:ASN:ND2  | 3:W:234:TYR:CE1  | 2.74                     | 0.56              |
| 2:M:110:ALA:HB1  | 2:M:111:PRO:CD   | 2.36                     | 0.56              |
| 3:W:334:PHE:HB2  | 3:W:336:LYS:HE3  | 1.87                     | 0.56              |
| 1:B:153:ASP:O    | 1:B:153:ASP:OD1  | 2.22                     | 0.56              |
| 2:M:10:THR:O     | 2:M:14:ALA:HB2   | 2.05                     | 0.56              |
| 2:M:7:LEU:O      | 2:M:11:LEU:HG    | 2.06                     | 0.56              |
| 1:B:303:LEU:HD13 | 1:B:562:THR:HG21 | 1.88                     | 0.56              |
| 1:B:618:ILE:O    | 1:B:622:VAL:HG23 | 2.06                     | 0.56              |
| 2:L:38:ILE:HD12  | 2:L:65:LEU:HD23  | 1.86                     | 0.56              |
| 1:A:190:ASN:OD1  | 1:A:192:ASN:N    | 2.38                     | 0.56              |
| 2:N:144:ARG:O    | 2:N:145:ARG:CB   | 2.52                     | 0.56              |
| 2:O:116:LEU:HD12 | 2:O:119:LEU:HD12 | 1.87                     | 0.56              |
| 3:W:528:GLN:O    | 3:W:531:THR:HG22 | 2.06                     | 0.56              |
| 3:W:208:ASN:HB2  | 3:W:697:ASN:ND2  | 2.20                     | 0.56              |
| 2:H:108:GLY:C    | 2:H:110:ALA:H    | 2.09                     | 0.56              |
| 3:W:1059:PRO:O   | 3:W:1063:MET:HG3 | 2.06                     | 0.56              |
| 1:B:246:HIS:ND1  | 1:B:247:PRO:HD2  | 2.20                     | 0.56              |
| 3:W:385:LEU:CD2  | 3:W:479:LYS:HE2  | 2.31                     | 0.56              |
| 1:A:245:LEU:HB3  | 1:A:249:ASP:CB   | 2.34                     | 0.56              |
| 2:I:76:ASN:H     | 2:M:76:ASN:CB    | 2.13                     | 0.56              |
| 3:W:499:GLN:NE2  | 3:W:680:ARG:HH11 | 2.02                     | 0.56              |
| 2:F:150:PHE:HB2  | 2:F:152:PHE:HE1  | 1.70                     | 0.56              |
| 2:L:8:SER:C      | 2:L:10:THR:N     | 2.55                     | 0.56              |
| 2:E:5:TYR:HE2    | 2:E:131:ASN:HA   | 1.69                     | 0.56              |
| 2:E:109:ILE:HD12 | 2:E:109:ILE:O    | 2.05                     | 0.56              |
| 2:L:260:GLU:HG2  | 2:L:274:GLN:HG3  | 1.86                     | 0.56              |
| 1:B:203:GLU:O    | 1:B:207:ILE:HG13 | 2.05                     | 0.56              |
| 2:N:10:THR:O     | 2:N:14:ALA:HB2   | 2.06                     | 0.56              |
| 1:B:392:MET:HA   | 1:B:573:THR:HG23 | 1.87                     | 0.56              |
| 2:D:38:ILE:HD12  | 2:D:65:LEU:CD2   | 2.35                     | 0.56              |
| 2:C:35:ASN:HA    | 2:C:38:ILE:HD12  | 1.88                     | 0.56              |
| 2:M:150:PHE:HB2  | 2:M:152:PHE:CZ   | 2.41                     | 0.56              |
| 2:E:8:SER:O      | 2:E:10:THR:N     | 2.39                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:7:LEU:O      | 2:F:11:LEU:HG     | 2.06                     | 0.56              |
| 2:F:116:LEU:HD12 | 2:F:119:LEU:HD12  | 1.88                     | 0.56              |
| 3:W:781:GLU:O    | 3:W:784:ILE:HG22  | 2.05                     | 0.56              |
| 2:K:99:GLU:O     | 2:K:384:ARG:NH1   | 2.39                     | 0.56              |
| 3:W:930:ILE:O    | 3:W:934:ILE:HG13  | 2.06                     | 0.56              |
| 1:A:319:ASP:OD2  | 1:A:571:LEU:CB    | 2.53                     | 0.56              |
| 1:B:496:ASN:HB3  | 1:B:498:ARG:CB    | 2.35                     | 0.56              |
| 1:B:305:GLN:HE21 | 1:B:564:ASN:ND2   | 2.04                     | 0.56              |
| 1:A:857:PHE:H    | 1:A:857:PHE:HD1   | 1.52                     | 0.56              |
| 2:O:35:ASN:HA    | 2:O:38:ILE:HD12   | 1.88                     | 0.56              |
| 2:O:7:LEU:O      | 2:O:11:LEU:HG     | 2.06                     | 0.56              |
| 2:M:35:ASN:HA    | 2:M:38:ILE:HD12   | 1.86                     | 0.56              |
| 2:M:116:LEU:HD12 | 2:M:119:LEU:HD12  | 1.86                     | 0.56              |
| 1:B:153:ASP:CG   | 1:B:153:ASP:O     | 2.43                     | 0.56              |
| 2:K:57:ARG:NH1   | 2:K:94:ASN:HD21   | 2.03                     | 0.56              |
| 3:W:119:PHE:CG   | 3:W:125:TYR:HA    | 2.40                     | 0.56              |
| 2:E:99:GLU:HG3   | 2:E:99:GLU:O      | 2.05                     | 0.56              |
| 1:A:404:LEU:CD2  | 1:A:435:ILE:HD11  | 2.36                     | 0.56              |
| 1:A:852:SER:O    | 1:A:853:ASP:HB3   | 2.04                     | 0.56              |
| 3:W:563:GLN:OE1  | 3:W:566:ILE:HB    | 2.06                     | 0.56              |
| 1:A:461:GLN:HB3  | 2:F:32:GLN:NE2    | 2.20                     | 0.56              |
| 2:D:128:ASN:HB3  | 2:E:19:VAL:CG2    | 2.36                     | 0.56              |
| 2:J:8:SER:O      | 2:J:10:THR:N      | 2.39                     | 0.56              |
| 2:J:35:ASN:HA    | 2:J:38:ILE:HD12   | 1.87                     | 0.56              |
| 2:E:38:ILE:HG22  | 2:E:42:ASN:ND2    | 2.19                     | 0.56              |
| 3:W:1009:PHE:C   | 3:W:1010:ASN:HD22 | 2.09                     | 0.56              |
| 1:B:364:THR:HG23 | 3:W:622:ALA:HA    | 1.87                     | 0.56              |
| 1:A:389:GLN:O    | 1:A:389:GLN:CG    | 2.54                     | 0.56              |
| 1:A:389:GLN:NE2  | 1:A:568:VAL:H     | 2.04                     | 0.56              |
| 2:J:50:GLY:O     | 2:J:51:ILE:HB     | 2.05                     | 0.56              |
| 1:B:498:ARG:HG3  | 1:B:505:GLN:OE1   | 2.05                     | 0.56              |
| 1:B:516:GLN:O    | 1:B:517:GLN:NE2   | 2.39                     | 0.56              |
| 1:A:503:ILE:CG2  | 1:A:506:LEU:HB2   | 2.36                     | 0.56              |
| 2:N:7:LEU:O      | 2:N:11:LEU:HG     | 2.06                     | 0.56              |
| 2:D:7:LEU:O      | 2:D:11:LEU:HG     | 2.06                     | 0.56              |
| 3:W:223:TYR:O    | 3:W:227:LYS:HB2   | 2.06                     | 0.56              |
| 1:B:325:ASN:O    | 1:B:328:LEU:HB3   | 2.05                     | 0.56              |
| 1:B:712:LEU:CB   | 1:B:819:PRO:HB2   | 2.36                     | 0.55              |
| 1:A:490:ASN:HB3  | 1:A:492:VAL:HG23  | 1.88                     | 0.55              |
| 1:A:332:VAL:HG13 | 1:A:599:THR:HG22  | 1.87                     | 0.55              |
| 1:B:563:MET:SD   | 1:B:611:HIS:CD2   | 2.99                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:W:441:VAL:HG22 | 3:W:567:ASN:HB3  | 1.86                     | 0.55              |
| 2:I:145:ARG:CZ   | 2:I:145:ARG:HB3  | 2.35                     | 0.55              |
| 1:B:763:LEU:HD22 | 1:B:764:PRO:CD   | 2.36                     | 0.55              |
| 1:A:440:PHE:O    | 1:A:442:MET:N    | 2.38                     | 0.55              |
| 2:I:57:ARG:NH1   | 2:I:94:ASN:HD21  | 2.02                     | 0.55              |
| 2:D:152:PHE:CD1  | 2:D:152:PHE:N    | 2.73                     | 0.55              |
| 1:B:707:TYR:HE2  | 1:B:754:ASN:OD1  | 1.89                     | 0.55              |
| 2:F:10:THR:O     | 2:F:14:ALA:HB2   | 2.05                     | 0.55              |
| 1:B:266:ASN:O    | 1:B:267:ASN:C    | 2.45                     | 0.55              |
| 3:W:255:VAL:O    | 3:W:673:VAL:HG21 | 2.06                     | 0.55              |
| 1:A:414:VAL:O    | 1:A:416:ASN:N    | 2.38                     | 0.55              |
| 1:B:260:GLN:O    | 1:B:262:VAL:N    | 2.39                     | 0.55              |
| 2:E:129:PHE:CD1  | 2:E:129:PHE:C    | 2.80                     | 0.55              |
| 1:A:314:PHE:O    | 1:A:316:SER:N    | 2.38                     | 0.55              |
| 1:A:738:LEU:HA   | 1:A:741:THR:HG22 | 1.88                     | 0.55              |
| 1:B:363:GLU:O    | 1:B:363:GLU:HG3  | 2.05                     | 0.55              |
| 1:A:346:ILE:O    | 1:A:349:MET:HB3  | 2.06                     | 0.55              |
| 3:W:309:ASP:O    | 3:W:312:VAL:HG22 | 2.06                     | 0.55              |
| 2:F:53:ASN:HD22  | 2:F:354:ALA:HB3  | 1.71                     | 0.55              |
| 3:W:524:TRP:NE1  | 3:W:607:LEU:HD13 | 2.21                     | 0.55              |
| 1:A:396:PHE:CB   | 1:A:578:LEU:HD12 | 2.37                     | 0.55              |
| 1:A:535:LEU:O    | 1:A:539:ARG:CG   | 2.55                     | 0.55              |
| 1:B:433:ASN:HD21 | 1:B:446:HIS:HB3  | 1.71                     | 0.55              |
| 2:N:8:SER:C      | 2:N:10:THR:N     | 2.55                     | 0.55              |
| 3:W:750:LEU:HD21 | 3:W:861:LEU:CD2  | 2.34                     | 0.55              |
| 2:O:8:SER:O      | 2:O:10:THR:N     | 2.40                     | 0.55              |
| 2:F:144:ARG:O    | 2:F:145:ARG:HB2  | 2.06                     | 0.55              |
| 2:C:153:HIS:CD2  | 2:E:153:HIS:NE2  | 2.75                     | 0.55              |
| 2:N:116:LEU:CD1  | 2:N:119:LEU:HD12 | 2.36                     | 0.55              |
| 1:B:127:GLU:HB3  | 1:B:151:LYS:HE3  | 1.87                     | 0.55              |
| 3:W:573:VAL:HG23 | 3:W:586:TYR:HB2  | 1.88                     | 0.55              |
| 2:N:99:GLU:O     | 2:N:99:GLU:HG3   | 2.06                     | 0.55              |
| 3:W:761:SER:OG   | 3:W:762:THR:N    | 2.38                     | 0.55              |
| 2:I:35:ASN:HA    | 2:I:38:ILE:HD12  | 1.87                     | 0.55              |
| 1:B:428:GLN:HG3  | 1:B:456:PHE:HD1  | 1.70                     | 0.55              |
| 1:A:725:ARG:HB3  | 1:A:828:GLN:OE1  | 2.06                     | 0.55              |
| 1:A:275:PRO:HB2  | 1:A:278:ILE:HG13 | 1.87                     | 0.55              |
| 2:H:12:LYS:C     | 2:H:14:ALA:N     | 2.56                     | 0.55              |
| 2:J:116:LEU:CD1  | 2:J:119:LEU:HD12 | 2.36                     | 0.55              |
| 3:W:530:ASN:O    | 3:W:533:PRO:HD2  | 2.06                     | 0.55              |
| 1:A:804:SER:HB2  | 1:A:810:TYR:CB   | 2.35                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:W:301:VAL:C    | 3:W:304:PRO:HD2  | 2.26                     | 0.55              |
| 2:C:99:GLU:HG3   | 2:C:99:GLU:O     | 2.07                     | 0.55              |
| 1:B:868:ALA:C    | 1:B:876:ILE:HG23 | 2.26                     | 0.55              |
| 2:N:6:SER:OG     | 2:N:128:ASN:HA   | 2.05                     | 0.55              |
| 1:A:822:THR:C    | 1:A:823:THR:HG23 | 2.26                     | 0.55              |
| 1:B:413:VAL:HG12 | 1:B:414:VAL:H    | 1.69                     | 0.55              |
| 1:A:150:LEU:HD12 | 1:A:696:SER:CB   | 2.34                     | 0.55              |
| 2:J:128:ASN:HB3  | 2:K:19:VAL:CG2   | 2.36                     | 0.55              |
| 2:J:14:ALA:C     | 2:J:16:ASP:H     | 2.10                     | 0.55              |
| 2:G:106:ARG:N    | 2:G:106:ARG:HD3  | 2.22                     | 0.55              |
| 3:W:109:TYR:HD1  | 3:W:129:LEU:HD13 | 1.70                     | 0.55              |
| 1:B:723:ILE:HG22 | 1:B:724:ALA:N    | 2.16                     | 0.55              |
| 1:B:804:SER:HA   | 1:B:810:TYR:CZ   | 2.42                     | 0.55              |
| 1:A:383:ILE:HD11 | 1:A:550:LEU:HD23 | 1.89                     | 0.55              |
| 1:B:508:GLU:HG2  | 1:B:512:GLN:HE21 | 1.71                     | 0.55              |
| 1:A:744:TYR:C    | 1:A:746:GLN:N    | 2.60                     | 0.55              |
| 1:B:675:GLU:HB3  | 1:B:678:ARG:HG3  | 1.88                     | 0.55              |
| 1:B:675:GLU:O    | 1:B:676:VAL:C    | 2.44                     | 0.55              |
| 2:L:35:ASN:HA    | 2:L:38:ILE:HD12  | 1.87                     | 0.55              |
| 2:G:63:PHE:N     | 2:G:63:PHE:CD1   | 2.74                     | 0.55              |
| 2:O:10:THR:O     | 2:O:14:ALA:HB2   | 2.06                     | 0.55              |
| 1:B:650:HIS:O    | 1:B:652:PHE:N    | 2.39                     | 0.55              |
| 2:C:145:ARG:O    | 2:C:146:GLN:HG3  | 2.06                     | 0.55              |
| 2:C:144:ARG:HD2  | 2:D:82:ARG:NH1   | 2.20                     | 0.55              |
| 2:H:116:LEU:HD12 | 2:H:119:LEU:HD12 | 1.89                     | 0.55              |
| 2:F:8:SER:O      | 2:F:10:THR:N     | 2.39                     | 0.55              |
| 2:L:116:LEU:HD12 | 2:L:119:LEU:HD12 | 1.87                     | 0.55              |
| 2:D:116:LEU:CD1  | 2:D:119:LEU:HD12 | 2.36                     | 0.55              |
| 3:W:882:LYS:HB3  | 3:W:883:PRO:HD3  | 1.89                     | 0.55              |
| 3:W:451:ARG:HH21 | 3:W:459:THR:HG21 | 1.72                     | 0.55              |
| 2:O:144:ARG:O    | 2:O:145:ARG:HG2  | 2.07                     | 0.55              |
| 1:B:625:ILE:O    | 1:B:628:ALA:HB3  | 2.06                     | 0.55              |
| 1:B:784:ALA:O    | 1:B:785:GLN:O    | 2.25                     | 0.55              |
| 1:B:371:ASN:O    | 1:B:373:GLN:N    | 2.39                     | 0.55              |
| 2:L:8:SER:O      | 2:L:10:THR:N     | 2.39                     | 0.55              |
| 2:C:82:ARG:NH1   | 2:E:144:ARG:HD2  | 2.21                     | 0.55              |
| 3:W:473:GLN:O    | 3:W:477:VAL:HG23 | 2.06                     | 0.55              |
| 2:C:10:THR:O     | 2:C:14:ALA:HB2   | 2.06                     | 0.55              |
| 2:O:49:GLY:HA2   | 2:O:54:LEU:CD2   | 2.37                     | 0.55              |
| 2:I:89:VAL:O     | 2:I:91:PHE:N     | 2.40                     | 0.55              |
| 3:W:584:ILE:HG13 | 3:W:585:GLN:O    | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:732:GLN:O    | 1:A:733:ILE:HG23 | 2.06                     | 0.55              |
| 2:H:99:GLU:HG3   | 2:H:99:GLU:O     | 2.07                     | 0.55              |
| 2:I:60:ASN:C     | 2:I:61:PHE:CD1   | 2.80                     | 0.55              |
| 1:A:510:LEU:HD22 | 1:A:540:LEU:CD1  | 2.26                     | 0.55              |
| 1:A:563:MET:O    | 1:A:565:MET:N    | 2.40                     | 0.55              |
| 1:B:122:LEU:HG   | 1:B:201:ASP:CG   | 2.27                     | 0.55              |
| 1:B:160:TYR:OH   | 1:B:635:GLN:HG3  | 2.07                     | 0.55              |
| 1:B:763:LEU:O    | 1:B:764:PRO:O    | 2.25                     | 0.55              |
| 2:C:152:PHE:N    | 2:C:152:PHE:CD1  | 2.74                     | 0.55              |
| 2:H:8:SER:O      | 2:H:10:THR:N     | 2.40                     | 0.55              |
| 3:W:559:ASN:HA   | 3:W:562:LYS:NZ   | 2.22                     | 0.55              |
| 1:B:113:PRO:HG2  | 1:B:609:ASN:HB3  | 1.89                     | 0.55              |
| 2:K:35:ASN:HA    | 2:K:38:ILE:CD1   | 2.37                     | 0.55              |
| 2:J:38:ILE:HG22  | 2:J:42:ASN:ND2   | 2.22                     | 0.55              |
| 2:I:153:HIS:NE2  | 2:J:153:HIS:CD2  | 2.75                     | 0.55              |
| 3:W:952:SER:OG   | 3:W:1071:TRP:HE3 | 1.90                     | 0.55              |
| 2:I:101:VAL:HB   | 2:I:355:ILE:HG21 | 1.88                     | 0.55              |
| 1:B:787:VAL:O    | 1:B:788:LYS:C    | 2.46                     | 0.55              |
| 2:G:8:SER:O      | 2:G:10:THR:N     | 2.40                     | 0.55              |
| 2:L:10:THR:O     | 2:L:14:ALA:HB2   | 2.06                     | 0.55              |
| 2:L:116:LEU:CD1  | 2:L:119:LEU:HD12 | 2.37                     | 0.55              |
| 3:W:449:LEU:HD21 | 3:W:461:ILE:CD1  | 2.37                     | 0.55              |
| 2:M:99:GLU:HG3   | 2:M:99:GLU:O     | 2.07                     | 0.55              |
| 2:N:35:ASN:HA    | 2:N:38:ILE:HD12  | 1.89                     | 0.55              |
| 1:B:698:LYS:O    | 1:B:699:ILE:CB   | 2.53                     | 0.55              |
| 2:F:152:PHE:CD1  | 2:F:152:PHE:N    | 2.74                     | 0.55              |
| 1:B:360:ILE:HD12 | 1:B:360:ILE:N    | 2.22                     | 0.55              |
| 1:B:654:VAL:O    | 1:B:656:ARG:N    | 2.39                     | 0.55              |
| 2:F:144:ARG:O    | 2:F:145:ARG:CB   | 2.55                     | 0.55              |
| 2:E:7:LEU:O      | 2:E:11:LEU:HG    | 2.07                     | 0.55              |
| 2:C:167:ASN:ND2  | 2:C:178:GLY:HA2  | 2.23                     | 0.55              |
| 2:C:109:ILE:HG23 | 2:C:110:ALA:H    | 1.70                     | 0.55              |
| 2:C:116:LEU:CD1  | 2:C:119:LEU:HD12 | 2.36                     | 0.55              |
| 1:A:500:GLY:O    | 1:A:502:VAL:N    | 2.36                     | 0.55              |
| 3:W:864:PRO:O    | 3:W:865:VAL:HG12 | 2.07                     | 0.55              |
| 1:A:525:TYR:O    | 1:A:529:ILE:HG13 | 2.05                     | 0.54              |
| 2:N:8:SER:O      | 2:N:10:THR:N     | 2.40                     | 0.54              |
| 1:B:195:ASP:O    | 1:B:197:GLY:N    | 2.39                     | 0.54              |
| 1:B:245:LEU:HD12 | 1:B:250:TYR:HA   | 1.89                     | 0.54              |
| 1:A:705:ILE:HG22 | 1:A:757:VAL:O    | 2.07                     | 0.54              |
| 2:L:82:ARG:NH1   | 2:N:144:ARG:HD2  | 2.22                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:116:LEU:HD12 | 2:E:119:LEU:HD12 | 1.88                     | 0.54              |
| 2:J:131:ASN:N    | 2:J:131:ASN:HD22 | 2.04                     | 0.54              |
| 1:A:142:LEU:O    | 1:A:143:ARG:HG2  | 2.08                     | 0.54              |
| 3:W:536:LYS:O    | 3:W:540:MET:HG3  | 2.07                     | 0.54              |
| 1:A:717:MET:HE1  | 1:A:830:PRO:O    | 2.07                     | 0.54              |
| 1:B:388:SER:O    | 1:B:389:GLN:HB2  | 2.07                     | 0.54              |
| 2:I:124:PHE:O    | 2:I:126:ARG:N    | 2.39                     | 0.54              |
| 2:I:8:SER:O      | 2:I:10:THR:N     | 2.40                     | 0.54              |
| 2:O:35:ASN:HA    | 2:O:38:ILE:CD1   | 2.37                     | 0.54              |
| 2:G:35:ASN:HA    | 2:G:38:ILE:HD12  | 1.89                     | 0.54              |
| 3:W:186:ASN:ND2  | 3:W:190:ARG:H    | 2.06                     | 0.54              |
| 1:B:779:ASP:HA   | 1:B:798:ILE:HG13 | 1.89                     | 0.54              |
| 3:W:476:VAL:O    | 3:W:480:MET:HG3  | 2.07                     | 0.54              |
| 2:D:144:ARG:HD2  | 2:E:82:ARG:CZ    | 2.36                     | 0.54              |
| 2:C:22:THR:HB    | 2:E:128:ASN:O    | 2.08                     | 0.54              |
| 2:J:35:ASN:HA    | 2:J:38:ILE:CD1   | 2.37                     | 0.54              |
| 2:I:153:HIS:CD2  | 2:K:153:HIS:NE2  | 2.75                     | 0.54              |
| 3:W:346:GLN:HG2  | 3:W:586:TYR:CZ   | 2.42                     | 0.54              |
| 2:C:135:TYR:OH   | 2:C:340:GLU:OE1  | 2.24                     | 0.54              |
| 1:A:742:GLY:HA3  | 1:B:285:ILE:HD11 | 1.89                     | 0.54              |
| 3:W:398:SER:HA   | 3:W:838:LYS:HE2  | 1.90                     | 0.54              |
| 3:W:582:LYS:HG2  | 3:W:583:LYS:H    | 1.71                     | 0.54              |
| 1:A:393:SER:HB2  | 1:A:573:THR:HG21 | 1.90                     | 0.54              |
| 1:A:871:PHE:O    | 1:A:871:PHE:CD1  | 2.60                     | 0.54              |
| 2:M:8:SER:O      | 2:M:10:THR:N     | 2.40                     | 0.54              |
| 1:A:120:THR:HA   | 1:A:186:MET:HE1  | 1.88                     | 0.54              |
| 3:W:8:LEU:HD12   | 3:W:737:MET:CG   | 2.31                     | 0.54              |
| 1:A:166:PHE:CE2  | 1:A:689:MET:HG3  | 2.42                     | 0.54              |
| 1:A:863:VAL:HG12 | 1:A:864:GLU:N    | 2.22                     | 0.54              |
| 2:H:116:LEU:CD1  | 2:H:119:LEU:HD12 | 2.38                     | 0.54              |
| 2:E:35:ASN:HA    | 2:E:38:ILE:CD1   | 2.37                     | 0.54              |
| 2:O:116:LEU:CD1  | 2:O:119:LEU:HD12 | 2.37                     | 0.54              |
| 1:A:730:PHE:CD1  | 1:A:730:PHE:N    | 2.75                     | 0.54              |
| 3:W:449:LEU:HD11 | 3:W:461:ILE:HD12 | 1.89                     | 0.54              |
| 2:H:150:PHE:HB2  | 2:H:152:PHE:CE1  | 2.43                     | 0.54              |
| 1:A:151:LYS:O    | 1:A:152:LYS:HB2  | 2.06                     | 0.54              |
| 2:O:144:ARG:O    | 2:O:146:GLN:N    | 2.41                     | 0.54              |
| 1:A:717:MET:SD   | 1:A:829:VAL:HG22 | 2.47                     | 0.54              |
| 2:I:49:GLY:HA2   | 2:I:54:LEU:HD21  | 1.90                     | 0.54              |
| 3:W:166:ARG:HH11 | 3:W:166:ARG:HG2  | 1.72                     | 0.54              |
| 1:A:643:GLU:HG2  | 1:A:662:MET:CE   | 2.37                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:42:ASN:HA    | 2:N:61:PHE:HB2   | 1.88                     | 0.54              |
| 3:W:186:ASN:HD22 | 3:W:186:ASN:N    | 1.96                     | 0.54              |
| 3:W:491:ALA:HB2  | 3:W:627:ARG:HD2  | 1.88                     | 0.54              |
| 2:C:8:SER:O      | 2:C:10:THR:N     | 2.40                     | 0.54              |
| 2:C:16:ASP:HB3   | 2:E:131:ASN:O    | 2.06                     | 0.54              |
| 1:B:404:LEU:O    | 1:B:407:GLY:N    | 2.40                     | 0.54              |
| 2:D:110:ALA:HB1  | 2:D:111:PRO:HD2  | 1.89                     | 0.54              |
| 2:F:65:LEU:O     | 2:F:66:LEU:HD23  | 2.08                     | 0.54              |
| 1:A:111:ILE:HG23 | 1:A:111:ILE:O    | 2.07                     | 0.54              |
| 1:A:633:LEU:C    | 1:A:635:GLN:H    | 2.11                     | 0.54              |
| 1:A:663:TYR:O    | 1:A:666:ARG:HG2  | 2.08                     | 0.54              |
| 1:B:323:THR:O    | 1:B:326:TYR:HB3  | 2.08                     | 0.54              |
| 1:B:326:TYR:CD1  | 1:B:384:ALA:CB   | 2.91                     | 0.54              |
| 1:B:506:LEU:HD21 | 1:B:543:LEU:C    | 2.27                     | 0.54              |
| 1:B:481:ARG:HG2  | 2:I:65:LEU:HD12  | 1.89                     | 0.54              |
| 1:A:530:GLN:HA   | 1:A:533:ILE:CD1  | 2.37                     | 0.54              |
| 1:B:370:ILE:O    | 1:B:373:GLN:HB3  | 2.08                     | 0.54              |
| 2:H:74:ASP:OD2   | 2:H:76:ASN:HB3   | 2.07                     | 0.54              |
| 2:F:35:ASN:HA    | 2:F:38:ILE:HD12  | 1.90                     | 0.54              |
| 2:E:10:THR:O     | 2:E:14:ALA:HB2   | 2.07                     | 0.54              |
| 3:W:134:ILE:HG13 | 3:W:698:ASN:OD1  | 2.08                     | 0.54              |
| 3:W:772:ILE:CD1  | 3:W:1047:LYS:HB2 | 2.37                     | 0.54              |
| 3:W:248:MET:HE2  | 3:W:252:VAL:HG12 | 1.89                     | 0.54              |
| 2:J:7:LEU:O      | 2:J:11:LEU:HG    | 2.06                     | 0.54              |
| 2:I:167:ASN:ND2  | 2:I:178:GLY:HA2  | 2.22                     | 0.54              |
| 2:E:116:LEU:CD1  | 2:E:119:LEU:HD12 | 2.38                     | 0.54              |
| 2:E:167:ASN:ND2  | 2:E:178:GLY:HA2  | 2.22                     | 0.54              |
| 1:B:666:ARG:HG3  | 1:B:667:ASP:N    | 2.20                     | 0.54              |
| 3:W:364:THR:OG1  | 3:W:533:PRO:HB3  | 2.07                     | 0.54              |
| 2:O:158:PHE:HE2  | 2:O:214:LEU:HD22 | 1.73                     | 0.54              |
| 2:N:110:ALA:HB1  | 2:N:111:PRO:CD   | 2.37                     | 0.54              |
| 1:B:875:ARG:CD   | 1:B:878:ASN:HD22 | 2.20                     | 0.54              |
| 1:A:501:HIS:C    | 1:A:503:ILE:H    | 2.09                     | 0.54              |
| 1:B:428:GLN:HG2  | 1:B:429:LEU:H    | 1.71                     | 0.54              |
| 2:O:14:ALA:C     | 2:O:16:ASP:H     | 2.11                     | 0.54              |
| 2:D:14:ALA:C     | 2:D:16:ASP:H     | 2.11                     | 0.54              |
| 3:W:1082:ASN:O   | 3:W:1084:ASN:N   | 2.40                     | 0.54              |
| 2:C:35:ASN:HA    | 2:C:38:ILE:CD1   | 2.38                     | 0.54              |
| 3:W:816:SER:HB3  | 3:W:820:LEU:CD1  | 2.38                     | 0.54              |
| 3:W:473:GLN:HB3  | 3:W:594:LYS:HB3  | 1.90                     | 0.54              |
| 2:H:35:ASN:HA    | 2:H:38:ILE:HD12  | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:14:ALA:C     | 2:C:16:ASP:H     | 2.10                     | 0.54              |
| 2:M:139:TRP:HE1  | 2:M:143:ASN:ND2  | 2.04                     | 0.54              |
| 2:I:106:ARG:HD3  | 2:I:106:ARG:H    | 1.72                     | 0.54              |
| 3:W:195:VAL:HG23 | 3:W:196:MET:H    | 1.73                     | 0.54              |
| 1:A:217:THR:O    | 1:A:217:THR:HG22 | 2.07                     | 0.54              |
| 2:J:99:GLU:HG3   | 2:J:99:GLU:O     | 2.08                     | 0.54              |
| 1:A:311:HIS:HB3  | 1:A:318:TRP:NE1  | 2.23                     | 0.54              |
| 1:A:645:PHE:HD2  | 1:A:646:LEU:HD23 | 1.72                     | 0.54              |
| 1:B:501:HIS:C    | 1:B:503:ILE:N    | 2.60                     | 0.54              |
| 2:K:14:ALA:C     | 2:K:16:ASP:H     | 2.11                     | 0.54              |
| 1:A:701:GLN:HG2  | 1:A:826:TYR:CE2  | 2.43                     | 0.54              |
| 1:A:650:HIS:O    | 1:A:651:ILE:CB   | 2.56                     | 0.54              |
| 2:M:167:ASN:ND2  | 2:M:178:GLY:HA2  | 2.23                     | 0.54              |
| 1:A:738:LEU:C    | 1:A:740:ARG:N    | 2.62                     | 0.54              |
| 3:W:573:VAL:CG1  | 3:W:575:ILE:HG13 | 2.38                     | 0.54              |
| 2:F:158:PHE:HE2  | 2:F:214:LEU:HD22 | 1.73                     | 0.54              |
| 3:W:736:ILE:O    | 3:W:740:THR:HG23 | 2.07                     | 0.54              |
| 1:B:771:VAL:CG1  | 1:B:772:ILE:N    | 2.71                     | 0.54              |
| 1:B:427:CYS:O    | 1:B:431:ILE:HG13 | 2.08                     | 0.54              |
| 2:L:72:ASN:ND2   | 2:N:126:ARG:NH1  | 2.56                     | 0.54              |
| 1:A:178:PRO:HD2  | 1:A:256:PHE:CE2  | 2.43                     | 0.54              |
| 2:L:128:ASN:O    | 2:M:22:THR:HB    | 2.08                     | 0.54              |
| 2:D:167:ASN:ND2  | 2:D:178:GLY:HA2  | 2.23                     | 0.54              |
| 2:G:116:LEU:CD1  | 2:G:119:LEU:HD12 | 2.38                     | 0.54              |
| 2:K:158:PHE:HE2  | 2:K:214:LEU:HD22 | 1.73                     | 0.54              |
| 1:A:298:TYR:O    | 1:A:299:ILE:HB   | 2.06                     | 0.54              |
| 1:B:457:GLN:CB   | 1:B:476:ASN:ND2  | 2.63                     | 0.54              |
| 2:I:7:LEU:O      | 2:I:11:LEU:HG    | 2.08                     | 0.54              |
| 2:D:35:ASN:HA    | 2:D:38:ILE:HD12  | 1.89                     | 0.54              |
| 1:B:653:ASP:O    | 1:B:654:VAL:C    | 2.46                     | 0.54              |
| 2:N:167:ASN:ND2  | 2:N:178:GLY:HA2  | 2.22                     | 0.54              |
| 2:J:27:VAL:O     | 2:J:30:LEU:N     | 2.40                     | 0.54              |
| 2:M:116:LEU:CD1  | 2:M:119:LEU:HD12 | 2.37                     | 0.54              |
| 2:C:67:GLY:C     | 2:C:69:THR:H     | 2.09                     | 0.54              |
| 1:A:273:TYR:O    | 1:A:273:TYR:CD2  | 2.61                     | 0.54              |
| 1:B:503:ILE:HD13 | 1:B:544:VAL:HG12 | 1.88                     | 0.53              |
| 1:B:457:GLN:O    | 1:B:458:ILE:HG13 | 2.08                     | 0.53              |
| 1:B:125:ILE:CD1  | 1:B:125:ILE:N    | 2.71                     | 0.53              |
| 1:B:125:ILE:HB   | 1:B:126:PHE:CD2  | 2.43                     | 0.53              |
| 1:B:393:SER:CB   | 1:B:573:THR:HG21 | 2.38                     | 0.53              |
| 2:H:23:LEU:N     | 2:H:26:ASN:ND2   | 2.57                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:W:186:ASN:HD21 | 3:W:190:ARG:N    | 2.05                     | 0.53              |
| 2:M:35:ASN:HA    | 2:M:38:ILE:CD1   | 2.38                     | 0.53              |
| 2:F:116:LEU:CD1  | 2:F:119:LEU:HD12 | 2.38                     | 0.53              |
| 2:K:116:LEU:HD12 | 2:K:119:LEU:HD12 | 1.89                     | 0.53              |
| 1:A:804:SER:HB2  | 1:A:810:TYR:HA   | 1.89                     | 0.53              |
| 3:W:410:PHE:HD1  | 3:W:807:THR:HG21 | 1.73                     | 0.53              |
| 1:B:862:THR:HG22 | 1:B:863:VAL:O    | 2.09                     | 0.53              |
| 2:H:135:TYR:OH   | 2:H:340:GLU:OE1  | 2.25                     | 0.53              |
| 2:I:158:PHE:HE2  | 2:I:214:LEU:HD22 | 1.73                     | 0.53              |
| 2:G:150:PHE:HB2  | 2:G:152:PHE:CE1  | 2.43                     | 0.53              |
| 2:G:22:THR:OG1   | 2:G:26:ASN:ND2   | 2.41                     | 0.53              |
| 2:E:74:ASP:OD2   | 2:E:76:ASN:HB3   | 2.08                     | 0.53              |
| 1:A:306:ASP:C    | 1:A:308:LEU:N    | 2.56                     | 0.53              |
| 1:B:467:GLN:HB3  | 1:B:512:GLN:HG2  | 1.90                     | 0.53              |
| 2:N:14:ALA:C     | 2:N:16:ASP:H     | 2.10                     | 0.53              |
| 1:B:252:PHE:O    | 1:B:254:GLU:N    | 2.40                     | 0.53              |
| 2:G:128:ASN:HB3  | 2:H:19:VAL:CG2   | 2.37                     | 0.53              |
| 3:W:222:ASP:OD1  | 3:W:324:LYS:HD3  | 2.08                     | 0.53              |
| 2:K:167:ASN:ND2  | 2:K:178:GLY:HA2  | 2.22                     | 0.53              |
| 2:K:150:PHE:HB2  | 2:K:152:PHE:CZ   | 2.42                     | 0.53              |
| 3:W:796:SER:OG   | 3:W:845:ILE:HG23 | 2.09                     | 0.53              |
| 2:L:153:HIS:NE2  | 2:N:153:HIS:NE2  | 2.55                     | 0.53              |
| 2:G:46:PHE:CE2   | 2:G:119:LEU:HD21 | 2.43                     | 0.53              |
| 2:N:89:VAL:O     | 2:N:91:PHE:N     | 2.41                     | 0.53              |
| 1:B:140:LYS:C    | 1:B:142:LEU:N    | 2.60                     | 0.53              |
| 1:B:449:ASN:HD21 | 1:B:455:PRO:CG   | 2.21                     | 0.53              |
| 2:O:24:TYR:O     | 2:O:27:VAL:HG22  | 2.09                     | 0.53              |
| 2:N:49:GLY:HA2   | 2:N:54:LEU:CD2   | 2.39                     | 0.53              |
| 2:N:158:PHE:HE2  | 2:N:214:LEU:HD22 | 1.73                     | 0.53              |
| 2:D:70:LEU:HD12  | 2:D:71:LEU:H     | 1.74                     | 0.53              |
| 2:C:158:PHE:HE2  | 2:C:214:LEU:HD22 | 1.73                     | 0.53              |
| 2:G:130:ASP:HA   | 2:H:17:LYS:HG2   | 1.90                     | 0.53              |
| 2:K:215:ARG:HG3  | 2:K:371:ILE:O    | 2.09                     | 0.53              |
| 2:I:35:ASN:HA    | 2:I:38:ILE:CD1   | 2.38                     | 0.53              |
| 1:A:503:ILE:HG22 | 1:A:506:LEU:H    | 1.73                     | 0.53              |
| 1:A:705:ILE:HG12 | 1:A:705:ILE:O    | 2.07                     | 0.53              |
| 2:L:38:ILE:O     | 2:L:42:ASN:OD1   | 2.27                     | 0.53              |
| 2:J:150:PHE:HB2  | 2:J:152:PHE:CZ   | 2.42                     | 0.53              |
| 2:E:116:LEU:HA   | 2:E:119:LEU:CD1  | 2.38                     | 0.53              |
| 2:D:99:GLU:CD    | 2:D:116:LEU:HD22 | 2.28                     | 0.53              |
| 3:W:221:ASP:O    | 3:W:225:ILE:HG13 | 2.09                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:211:ILE:O    | 1:B:213:GLN:N     | 2.41                     | 0.53              |
| 2:O:215:ARG:HG3  | 2:O:371:ILE:O     | 2.09                     | 0.53              |
| 3:W:240:LEU:O    | 3:W:244:VAL:HG23  | 2.09                     | 0.53              |
| 2:F:99:GLU:HG3   | 2:F:99:GLU:O      | 2.08                     | 0.53              |
| 1:A:542:GLN:O    | 1:A:545:ASP:HB2   | 2.08                     | 0.53              |
| 1:B:122:LEU:HD11 | 1:B:200:VAL:HG12  | 1.88                     | 0.53              |
| 1:B:199:VAL:HG12 | 1:B:200:VAL:H     | 1.70                     | 0.53              |
| 1:B:246:HIS:CE1  | 1:B:247:PRO:HD2   | 2.44                     | 0.53              |
| 1:B:170:TYR:CE1  | 1:B:681:ILE:CG2   | 2.92                     | 0.53              |
| 2:L:63:PHE:N     | 2:L:63:PHE:CD1    | 2.75                     | 0.53              |
| 1:B:182:LEU:HD23 | 1:B:183:LEU:N     | 2.15                     | 0.53              |
| 1:B:94:THR:HG23  | 1:B:658:PRO:HG3   | 1.90                     | 0.53              |
| 1:A:771:VAL:O    | 1:A:772:ILE:C     | 2.46                     | 0.53              |
| 3:W:293:ASP:O    | 3:W:297:LYS:HG2   | 2.08                     | 0.53              |
| 1:B:361:GLN:NE2  | 3:W:624:LYS:NZ    | 2.54                     | 0.53              |
| 2:D:144:ARG:HD2  | 2:E:82:ARG:NH1    | 2.23                     | 0.53              |
| 2:J:116:LEU:HA   | 2:J:119:LEU:CD1   | 2.38                     | 0.53              |
| 3:W:387:ARG:HB3  | 3:W:387:ARG:NH1   | 2.22                     | 0.53              |
| 3:W:873:THR:HA   | 3:W:1073:ILE:HG23 | 1.89                     | 0.53              |
| 1:B:497:ILE:HG23 | 2:I:68:THR:HG23   | 1.89                     | 0.53              |
| 2:L:158:PHE:HE2  | 2:L:214:LEU:HD22  | 1.73                     | 0.53              |
| 2:H:158:PHE:HE2  | 2:H:214:LEU:HD22  | 1.73                     | 0.53              |
| 2:N:215:ARG:HG3  | 2:N:371:ILE:O     | 2.09                     | 0.53              |
| 2:G:99:GLU:O     | 2:G:99:GLU:HG3    | 2.09                     | 0.53              |
| 2:I:215:ARG:HG3  | 2:I:371:ILE:O     | 2.09                     | 0.53              |
| 1:B:770:SER:HB3  | 1:B:772:ILE:HG22  | 1.90                     | 0.53              |
| 1:A:311:HIS:NE2  | 1:A:566:GLN:NE2   | 2.54                     | 0.53              |
| 1:A:546:LEU:HD22 | 1:A:584:LEU:HD21  | 1.90                     | 0.53              |
| 1:B:498:ARG:HG3  | 1:B:505:GLN:HE22  | 1.73                     | 0.53              |
| 1:B:428:GLN:CG   | 1:B:456:PHE:HD1   | 2.21                     | 0.53              |
| 1:B:200:VAL:HB   | 1:B:204:THR:HG21  | 1.89                     | 0.53              |
| 1:A:560:CYS:CB   | 1:A:603:TYR:HD2   | 2.21                     | 0.53              |
| 1:B:133:ILE:HD11 | 1:B:147:TYR:CE1   | 2.43                     | 0.53              |
| 1:B:298:TYR:CD1  | 1:B:299:ILE:N     | 2.75                     | 0.53              |
| 3:W:864:PRO:HB3  | 3:W:867:PHE:HE2   | 1.73                     | 0.53              |
| 3:W:12:LEU:HD22  | 3:W:16:TYR:HE2    | 1.73                     | 0.53              |
| 1:A:642:VAL:HG13 | 1:A:665:LEU:HD23  | 1.90                     | 0.53              |
| 2:K:131:ASN:HD22 | 2:K:131:ASN:N     | 2.05                     | 0.53              |
| 2:N:35:ASN:HA    | 2:N:38:ILE:CD1    | 2.38                     | 0.53              |
| 3:W:426:ASP:HB3  | 3:W:432:ARG:NH2   | 2.24                     | 0.53              |
| 2:O:167:ASN:ND2  | 2:O:178:GLY:HA2   | 2.22                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:116:LEU:HA   | 2:D:119:LEU:CD1  | 2.39                     | 0.53              |
| 2:G:158:PHE:HE2  | 2:G:214:LEU:HD22 | 1.73                     | 0.53              |
| 2:E:158:PHE:HE2  | 2:E:214:LEU:HD22 | 1.73                     | 0.53              |
| 2:J:158:PHE:HE2  | 2:J:214:LEU:HD22 | 1.73                     | 0.53              |
| 3:W:345:ASP:HB2  | 3:W:458:ARG:CZ   | 2.39                     | 0.53              |
| 2:L:215:ARG:HG3  | 2:L:371:ILE:O    | 2.09                     | 0.53              |
| 1:A:487:GLY:O    | 1:A:488:VAL:HG23 | 2.08                     | 0.53              |
| 1:B:498:ARG:CB   | 2:I:32:GLN:NE2   | 2.66                     | 0.53              |
| 1:A:491:GLN:HB3  | 1:A:564:ASN:HB3  | 1.90                     | 0.53              |
| 1:B:436:ILE:O    | 1:B:438:PRO:N    | 2.42                     | 0.53              |
| 1:B:458:ILE:HD12 | 1:B:458:ILE:C    | 2.29                     | 0.53              |
| 1:B:577:GLN:C    | 1:B:579:THR:N    | 2.60                     | 0.53              |
| 2:I:144:ARG:HD2  | 2:J:82:ARG:NH1   | 2.24                     | 0.53              |
| 1:A:238:VAL:HG12 | 1:A:239:VAL:N    | 2.24                     | 0.53              |
| 1:A:647:LYS:C    | 1:A:649:LEU:H    | 2.12                     | 0.53              |
| 2:F:144:ARG:HD2  | 2:G:82:ARG:CZ    | 2.38                     | 0.53              |
| 2:F:14:ALA:C     | 2:F:16:ASP:H     | 2.11                     | 0.53              |
| 2:I:116:LEU:HA   | 2:I:119:LEU:CD1  | 2.38                     | 0.53              |
| 1:B:400:ASN:ND2  | 1:B:403:SER:OG   | 2.41                     | 0.53              |
| 2:O:74:ASP:OD2   | 2:O:76:ASN:HB3   | 2.09                     | 0.53              |
| 3:W:985:LYS:HB3  | 3:W:985:LYS:NZ   | 2.24                     | 0.53              |
| 3:W:7:ILE:HA     | 3:W:10:GLU:OE1   | 2.08                     | 0.53              |
| 2:E:110:ALA:HB1  | 2:E:111:PRO:CD   | 2.39                     | 0.53              |
| 2:I:99:GLU:O     | 2:I:99:GLU:HG3   | 2.09                     | 0.53              |
| 1:A:550:LEU:O    | 1:A:551:ALA:C    | 2.47                     | 0.53              |
| 1:A:876:ILE:HG22 | 1:A:877:MET:HG2  | 1.89                     | 0.53              |
| 1:B:548:ARG:HD3  | 1:B:877:MET:H    | 1.73                     | 0.53              |
| 1:A:853:ASP:O    | 1:A:854:LEU:CB   | 2.56                     | 0.53              |
| 2:N:31:ILE:O     | 2:N:34:PHE:HB3   | 2.09                     | 0.53              |
| 1:B:786:ILE:O    | 1:B:788:LYS:N    | 2.41                     | 0.53              |
| 1:B:371:ASN:C    | 1:B:373:GLN:H    | 2.11                     | 0.53              |
| 1:A:771:VAL:HA   | 1:A:802:ILE:HD11 | 1.91                     | 0.53              |
| 3:W:232:LEU:HD21 | 3:W:299:GLY:HA3  | 1.90                     | 0.53              |
| 3:W:519:THR:CG2  | 3:W:520:ASP:H    | 2.21                     | 0.53              |
| 1:A:325:ASN:O    | 1:A:328:LEU:HB3  | 2.09                     | 0.53              |
| 2:M:145:ARG:NH1  | 2:M:145:ARG:CB   | 2.71                     | 0.53              |
| 3:W:161:LYS:CB   | 3:W:165:ARG:HH12 | 2.21                     | 0.53              |
| 3:W:627:ARG:HG2  | 3:W:627:ARG:NH1  | 2.16                     | 0.53              |
| 2:H:167:ASN:ND2  | 2:H:178:GLY:HA2  | 2.23                     | 0.53              |
| 2:K:116:LEU:CD1  | 2:K:119:LEU:HD12 | 2.39                     | 0.53              |
| 2:K:46:PHE:CE2   | 2:K:119:LEU:HD21 | 2.41                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:271:PHE:O    | 1:A:274:ILE:HD12 | 2.08                     | 0.53              |
| 2:O:89:VAL:O     | 2:O:91:PHE:N     | 2.42                     | 0.53              |
| 2:M:158:PHE:HE2  | 2:M:214:LEU:HD22 | 1.74                     | 0.53              |
| 2:H:215:ARG:HG3  | 2:H:371:ILE:O    | 2.09                     | 0.53              |
| 2:C:215:ARG:HG3  | 2:C:371:ILE:O    | 2.09                     | 0.53              |
| 1:B:755:GLN:O    | 1:B:757:VAL:HG23 | 2.08                     | 0.53              |
| 2:K:65:LEU:C     | 2:K:66:LEU:HG    | 2.29                     | 0.53              |
| 1:A:661:GLN:NE2  | 1:B:348:LYS:HZ2  | 2.06                     | 0.53              |
| 1:B:387:LEU:O    | 1:B:389:GLN:N    | 2.42                     | 0.53              |
| 1:B:501:HIS:ND1  | 1:B:548:ARG:HG2  | 2.24                     | 0.53              |
| 1:B:508:GLU:OE2  | 2:J:70:LEU:HD23  | 2.09                     | 0.53              |
| 1:B:642:VAL:O    | 1:B:645:PHE:HB3  | 2.09                     | 0.53              |
| 1:B:182:LEU:CD2  | 1:B:183:LEU:N    | 2.71                     | 0.53              |
| 2:D:35:ASN:HA    | 2:D:38:ILE:CD1   | 2.39                     | 0.53              |
| 1:B:654:VAL:HG12 | 1:B:655:ALA:N    | 2.24                     | 0.53              |
| 2:F:167:ASN:ND2  | 2:F:178:GLY:HA2  | 2.22                     | 0.53              |
| 1:B:708:ARG:O    | 1:B:710:MET:N    | 2.42                     | 0.53              |
| 3:W:109:TYR:HA   | 3:W:118:LEU:CD2  | 2.39                     | 0.53              |
| 2:J:215:ARG:HG3  | 2:J:371:ILE:O    | 2.09                     | 0.53              |
| 2:M:215:ARG:HG3  | 2:M:371:ILE:O    | 2.09                     | 0.53              |
| 2:G:215:ARG:HG3  | 2:G:371:ILE:O    | 2.09                     | 0.53              |
| 3:W:421:ASN:OD1  | 3:W:422:MET:N    | 2.42                     | 0.53              |
| 2:O:99:GLU:O     | 2:O:99:GLU:HG3   | 2.09                     | 0.53              |
| 1:A:323:THR:O    | 1:A:326:TYR:HB3  | 2.08                     | 0.52              |
| 1:B:499:ASN:O    | 1:B:500:GLY:O    | 2.27                     | 0.52              |
| 1:B:504:ASN:O    | 1:B:505:GLN:C    | 2.46                     | 0.52              |
| 1:A:401:TYR:N    | 1:A:401:TYR:CD1  | 2.75                     | 0.52              |
| 1:A:428:GLN:CD   | 1:A:456:PHE:HB2  | 2.27                     | 0.52              |
| 1:B:437:TYR:HD2  | 1:B:443:GLN:HB3  | 1.73                     | 0.52              |
| 2:I:14:ALA:C     | 2:I:16:ASP:H     | 2.11                     | 0.52              |
| 1:A:721:VAL:CG1  | 1:A:799:LEU:HD22 | 2.39                     | 0.52              |
| 1:B:742:GLY:O    | 1:B:744:TYR:CE2  | 2.62                     | 0.52              |
| 2:K:89:VAL:O     | 2:K:91:PHE:N     | 2.43                     | 0.52              |
| 2:L:152:PHE:N    | 2:L:152:PHE:CD1  | 2.77                     | 0.52              |
| 1:A:606:VAL:O    | 1:A:607:ASN:C    | 2.46                     | 0.52              |
| 1:B:654:VAL:O    | 1:B:657:VAL:HG23 | 2.08                     | 0.52              |
| 2:J:129:PHE:CD1  | 2:J:129:PHE:C    | 2.82                     | 0.52              |
| 1:A:297:ARG:HG3  | 1:A:848:PHE:CE2  | 2.43                     | 0.52              |
| 2:J:139:TRP:CD1  | 2:J:139:TRP:C    | 2.83                     | 0.52              |
| 3:W:168:ASP:O    | 3:W:171:THR:HB   | 2.09                     | 0.52              |
| 1:A:794:THR:HG22 | 1:A:794:THR:O    | 2.08                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:135:ARG:O    | 1:B:138:GLY:N    | 2.43                     | 0.52              |
| 1:A:424:LEU:HD12 | 1:A:424:LEU:O    | 2.08                     | 0.52              |
| 1:A:618:ILE:HD13 | 1:A:645:PHE:CZ   | 2.44                     | 0.52              |
| 1:B:326:TYR:CE1  | 1:B:384:ALA:HB3  | 2.44                     | 0.52              |
| 1:B:466:PHE:O    | 1:B:467:GLN:C    | 2.47                     | 0.52              |
| 1:A:722:ASN:C    | 1:A:723:ILE:HG13 | 2.29                     | 0.52              |
| 2:L:61:PHE:O     | 2:L:62:ASP:HB3   | 2.07                     | 0.52              |
| 1:A:255:TYR:O    | 1:A:259:HIS:HB3  | 2.08                     | 0.52              |
| 1:B:663:TYR:O    | 1:B:666:ARG:HG2  | 2.09                     | 0.52              |
| 3:W:420:LYS:HA   | 3:W:423:HIS:CD2  | 2.44                     | 0.52              |
| 2:M:48:THR:O     | 2:M:56:ILE:HA    | 2.10                     | 0.52              |
| 1:A:329:ALA:O    | 1:A:333:VAL:HG23 | 2.10                     | 0.52              |
| 1:A:340:VAL:HB   | 1:A:587:LEU:CD2  | 2.39                     | 0.52              |
| 1:A:658:PRO:HB2  | 1:A:660:ASP:OD1  | 2.09                     | 0.52              |
| 1:B:311:HIS:CD2  | 1:B:566:GLN:OE1  | 2.62                     | 0.52              |
| 1:B:525:TYR:O    | 1:B:529:ILE:HG13 | 2.08                     | 0.52              |
| 2:D:42:ASN:HA    | 2:D:61:PHE:HB2   | 1.92                     | 0.52              |
| 3:W:823:LYS:HE2  | 3:W:825:ASN:OD1  | 2.09                     | 0.52              |
| 2:E:14:ALA:C     | 2:E:16:ASP:H     | 2.11                     | 0.52              |
| 2:M:116:LEU:HA   | 2:M:119:LEU:CD1  | 2.38                     | 0.52              |
| 2:O:116:LEU:HA   | 2:O:119:LEU:CD1  | 2.39                     | 0.52              |
| 2:C:381:ASN:O    | 2:C:385:VAL:HB   | 2.10                     | 0.52              |
| 2:H:150:PHE:HB2  | 2:H:152:PHE:CZ   | 2.44                     | 0.52              |
| 2:D:158:PHE:HE2  | 2:D:214:LEU:HD22 | 1.74                     | 0.52              |
| 2:O:110:ALA:HB1  | 2:O:111:PRO:HD2  | 1.90                     | 0.52              |
| 2:D:215:ARG:HG3  | 2:D:371:ILE:O    | 2.09                     | 0.52              |
| 3:W:496:GLN:HB3  | 3:W:920:GLN:HB2  | 1.91                     | 0.52              |
| 2:M:101:VAL:HG23 | 2:M:102:ARG:N    | 2.24                     | 0.52              |
| 1:A:326:TYR:CD1  | 1:A:384:ALA:CB   | 2.92                     | 0.52              |
| 1:A:555:GLU:OE2  | 1:A:871:PHE:CE2  | 2.63                     | 0.52              |
| 1:B:418:MET:HB3  | 1:B:567:HIS:NE2  | 2.24                     | 0.52              |
| 1:B:431:ILE:O    | 1:B:435:ILE:HB   | 2.09                     | 0.52              |
| 2:O:23:LEU:HB3   | 2:O:26:ASN:HD21  | 1.73                     | 0.52              |
| 1:A:200:VAL:O    | 1:A:204:THR:OG1  | 2.17                     | 0.52              |
| 2:G:35:ASN:HA    | 2:G:38:ILE:CD1   | 2.39                     | 0.52              |
| 1:B:689:MET:HA   | 1:B:692:ILE:HD13 | 1.91                     | 0.52              |
| 2:I:74:ASP:OD2   | 2:I:76:ASN:HB3   | 2.08                     | 0.52              |
| 1:A:361:GLN:HG3  | 1:A:362:SER:H    | 1.75                     | 0.52              |
| 2:M:31:ILE:O     | 2:M:34:PHE:HB3   | 2.09                     | 0.52              |
| 2:D:24:TYR:CZ    | 2:D:68:THR:HG22  | 2.44                     | 0.52              |
| 2:J:150:PHE:HB2  | 2:J:152:PHE:HE1  | 1.73                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:167:ASN:ND2  | 2:L:178:GLY:HA2  | 2.22                     | 0.52              |
| 3:W:879:ARG:HG3  | 3:W:879:ARG:HH11 | 1.75                     | 0.52              |
| 1:B:277:ARG:NH1  | 1:B:559:ALA:HB2  | 2.25                     | 0.52              |
| 3:W:967:ILE:H    | 3:W:967:ILE:CD1  | 2.23                     | 0.52              |
| 1:B:340:VAL:O    | 1:B:587:LEU:HD11 | 2.09                     | 0.52              |
| 2:F:150:PHE:HB2  | 2:F:152:PHE:CZ   | 2.44                     | 0.52              |
| 2:L:8:SER:C      | 2:L:10:THR:H     | 2.13                     | 0.52              |
| 1:A:421:ARG:O    | 1:A:425:VAL:HG23 | 2.10                     | 0.52              |
| 2:K:53:ASN:ND2   | 2:K:354:ALA:HB3  | 2.25                     | 0.52              |
| 2:N:116:LEU:HA   | 2:N:119:LEU:CD1  | 2.39                     | 0.52              |
| 1:A:314:PHE:O    | 1:A:315:GLU:C    | 2.48                     | 0.52              |
| 2:F:381:ASN:O    | 2:F:385:VAL:HB   | 2.10                     | 0.52              |
| 3:W:321:LEU:O    | 3:W:325:ILE:HG12 | 2.10                     | 0.52              |
| 3:W:573:VAL:HG12 | 3:W:575:ILE:HG13 | 1.91                     | 0.52              |
| 2:G:381:ASN:O    | 2:G:385:VAL:HB   | 2.10                     | 0.52              |
| 2:D:74:ASP:OD2   | 2:D:76:ASN:HB3   | 2.09                     | 0.52              |
| 1:A:742:GLY:O    | 1:A:743:ASP:O    | 2.28                     | 0.52              |
| 1:A:872:ASP:OD2  | 1:A:874:MET:HB2  | 2.10                     | 0.52              |
| 1:B:811:LEU:HD23 | 1:B:811:LEU:N    | 2.24                     | 0.52              |
| 1:B:527:ARG:HH11 | 1:B:527:ARG:HG3  | 1.74                     | 0.52              |
| 1:B:527:ARG:O    | 1:B:531:ARG:HG2  | 2.08                     | 0.52              |
| 1:B:558:MET:O    | 1:B:561:VAL:HG23 | 2.09                     | 0.52              |
| 1:A:286:LEU:O    | 1:A:287:ASN:HB2  | 2.09                     | 0.52              |
| 1:B:396:PHE:C    | 1:B:396:PHE:CD1  | 2.83                     | 0.52              |
| 1:B:763:LEU:HD22 | 1:B:764:PRO:HD2  | 1.92                     | 0.52              |
| 2:G:7:LEU:O      | 2:G:11:LEU:HG    | 2.09                     | 0.52              |
| 2:M:21:GLY:O     | 2:M:22:THR:O     | 2.28                     | 0.52              |
| 3:W:820:LEU:HD13 | 3:W:824:ASN:HB2  | 1.91                     | 0.52              |
| 3:W:538:ILE:HD13 | 3:W:595:GLN:OE1  | 2.10                     | 0.52              |
| 2:O:107:ASN:CG   | 2:O:107:ASN:O    | 2.48                     | 0.52              |
| 2:H:57:ARG:NH1   | 2:H:94:ASN:HD21  | 2.07                     | 0.52              |
| 1:A:464:GLN:O    | 1:A:465:ASN:HB2  | 2.08                     | 0.52              |
| 3:W:744:ILE:N    | 3:W:744:ILE:HD12 | 2.24                     | 0.52              |
| 2:E:215:ARG:HG3  | 2:E:371:ILE:O    | 2.09                     | 0.52              |
| 2:F:215:ARG:HG3  | 2:F:371:ILE:O    | 2.09                     | 0.52              |
| 1:B:326:TYR:HD1  | 1:B:384:ALA:HB1  | 1.75                     | 0.52              |
| 2:I:14:ALA:O     | 2:I:18:ILE:HD12  | 2.10                     | 0.52              |
| 2:N:12:LYS:O     | 2:N:14:ALA:N     | 2.43                     | 0.52              |
| 1:A:721:VAL:HG13 | 1:A:800:TYR:C    | 2.29                     | 0.52              |
| 1:B:632:ASN:O    | 1:B:634:TYR:N    | 2.38                     | 0.52              |
| 2:G:14:ALA:C     | 2:G:16:ASP:H     | 2.11                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:803:ASN:C    | 1:A:805:ASP:N     | 2.63                     | 0.52              |
| 1:B:570:THR:HG22 | 1:B:571:LEU:H     | 1.75                     | 0.52              |
| 2:D:8:SER:C      | 2:D:10:THR:H      | 2.13                     | 0.52              |
| 3:W:564:THR:O    | 3:W:568:LEU:HG    | 2.09                     | 0.52              |
| 3:W:428:MET:SD   | 3:W:811:TYR:HD1   | 2.32                     | 0.52              |
| 2:J:167:ASN:ND2  | 2:J:178:GLY:HA2   | 2.23                     | 0.52              |
| 2:L:381:ASN:O    | 2:L:385:VAL:HB    | 2.10                     | 0.52              |
| 2:K:381:ASN:O    | 2:K:385:VAL:HB    | 2.10                     | 0.52              |
| 2:N:381:ASN:O    | 2:N:385:VAL:HB    | 2.10                     | 0.52              |
| 2:J:381:ASN:O    | 2:J:385:VAL:HB    | 2.10                     | 0.52              |
| 2:O:381:ASN:O    | 2:O:385:VAL:HB    | 2.10                     | 0.52              |
| 2:F:5:TYR:HE2    | 2:F:131:ASN:HA    | 1.75                     | 0.52              |
| 1:B:211:ILE:O    | 1:B:212:PHE:C     | 2.48                     | 0.52              |
| 3:W:114:MET:HB2  | 3:W:117:GLU:HG2   | 1.92                     | 0.52              |
| 2:F:129:PHE:C    | 2:F:129:PHE:CD1   | 2.83                     | 0.52              |
| 1:B:812:VAL:HG23 | 1:B:817:TRP:CZ3   | 2.45                     | 0.52              |
| 1:B:550:LEU:O    | 1:B:551:ALA:C     | 2.49                     | 0.52              |
| 1:A:786:ILE:O    | 1:A:789:LEU:N     | 2.43                     | 0.52              |
| 2:L:31:ILE:O     | 2:L:34:PHE:HB3    | 2.10                     | 0.52              |
| 2:D:23:LEU:HD22  | 2:D:25:SER:OG     | 2.10                     | 0.52              |
| 2:D:41:MET:O     | 2:D:42:ASN:C      | 2.47                     | 0.52              |
| 2:M:89:VAL:O     | 2:M:91:PHE:N      | 2.43                     | 0.52              |
| 1:B:723:ILE:CG2  | 1:B:724:ALA:H     | 2.13                     | 0.52              |
| 1:A:323:THR:OG1  | 1:A:390:ARG:NH1   | 2.43                     | 0.52              |
| 1:A:163:ARG:NH2  | 1:A:736:GLU:OE2   | 2.42                     | 0.52              |
| 1:B:444:ARG:HH22 | 1:B:520:THR:HA    | 1.75                     | 0.52              |
| 1:B:540:LEU:HA   | 1:B:543:LEU:HB2   | 1.92                     | 0.52              |
| 1:A:467:GLN:HB3  | 1:A:512:GLN:HG2   | 1.92                     | 0.52              |
| 2:M:14:ALA:C     | 2:M:16:ASP:H      | 2.11                     | 0.52              |
| 2:M:8:SER:C      | 2:M:10:THR:H      | 2.13                     | 0.52              |
| 2:L:35:ASN:HA    | 2:L:38:ILE:CD1    | 2.39                     | 0.52              |
| 2:L:106:ARG:N    | 2:L:106:ARG:HD3   | 2.17                     | 0.52              |
| 2:H:14:ALA:C     | 2:H:16:ASP:H      | 2.11                     | 0.52              |
| 2:L:110:ALA:HB1  | 2:L:111:PRO:HD2   | 1.92                     | 0.52              |
| 1:B:314:PHE:N    | 1:B:314:PHE:CD1   | 2.77                     | 0.52              |
| 2:K:99:GLU:O     | 2:K:99:GLU:HG3    | 2.10                     | 0.52              |
| 3:W:772:ILE:HG23 | 3:W:1043:ASN:HD22 | 1.75                     | 0.52              |
| 2:H:139:TRP:CD1  | 2:H:139:TRP:C     | 2.83                     | 0.52              |
| 2:M:131:ASN:N    | 2:M:131:ASN:HD22  | 2.07                     | 0.52              |
| 1:B:293:PRO:C    | 1:B:295:THR:N     | 2.60                     | 0.52              |
| 2:H:128:ASN:O    | 2:H:129:PHE:HB3   | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:35:ASN:HA    | 2:F:38:ILE:CD1   | 2.40                     | 0.52              |
| 2:F:135:TYR:OH   | 2:F:340:GLU:OE1  | 2.28                     | 0.52              |
| 1:A:310:LEU:O    | 1:A:318:TRP:CD1  | 2.62                     | 0.51              |
| 1:B:322:THR:O    | 1:B:323:THR:C    | 2.48                     | 0.51              |
| 1:A:540:LEU:C    | 1:A:540:LEU:HD23 | 2.30                     | 0.51              |
| 1:B:563:MET:HA   | 1:B:563:MET:CE   | 2.39                     | 0.51              |
| 1:A:769:SER:O    | 1:A:771:VAL:N    | 2.43                     | 0.51              |
| 1:B:530:GLN:HA   | 1:B:533:ILE:CD1  | 2.40                     | 0.51              |
| 1:B:606:VAL:O    | 1:B:607:ASN:C    | 2.47                     | 0.51              |
| 2:M:27:VAL:CG2   | 2:M:31:ILE:HD11  | 2.40                     | 0.51              |
| 3:W:101:ASP:C    | 3:W:103:THR:H    | 2.13                     | 0.51              |
| 2:C:116:LEU:HA   | 2:C:119:LEU:CD1  | 2.40                     | 0.51              |
| 1:B:235:ASP:O    | 1:B:236:ARG:HB2  | 2.10                     | 0.51              |
| 3:W:880:ASP:O    | 3:W:883:PRO:HD2  | 2.10                     | 0.51              |
| 2:O:133:SER:O    | 2:O:136:ILE:HG22 | 2.10                     | 0.51              |
| 2:J:89:VAL:O     | 2:J:91:PHE:N     | 2.43                     | 0.51              |
| 1:B:286:LEU:N    | 1:B:286:LEU:HD22 | 2.25                     | 0.51              |
| 1:A:269:ILE:HG21 | 1:A:298:TYR:HE2  | 1.76                     | 0.51              |
| 1:A:431:ILE:HG23 | 1:A:435:ILE:HD12 | 1.91                     | 0.51              |
| 2:I:139:TRP:CD1  | 2:I:139:TRP:C    | 2.84                     | 0.51              |
| 1:B:378:CYS:SG   | 1:B:581:VAL:HA   | 2.50                     | 0.51              |
| 1:A:125:ILE:CD1  | 1:A:125:ILE:N    | 2.63                     | 0.51              |
| 2:J:11:LEU:O     | 2:J:15:ARG:N     | 2.39                     | 0.51              |
| 2:C:27:VAL:O     | 2:C:30:LEU:N     | 2.38                     | 0.51              |
| 3:W:227:LYS:O    | 3:W:231:VAL:HG23 | 2.10                     | 0.51              |
| 1:B:422:GLU:O    | 1:B:425:VAL:N    | 2.43                     | 0.51              |
| 3:W:408:LEU:N    | 3:W:408:LEU:HD12 | 2.24                     | 0.51              |
| 3:W:177:ILE:HD13 | 3:W:203:LEU:HD11 | 1.90                     | 0.51              |
| 2:D:105:GLN:NE2  | 2:D:359:PRO:O    | 2.43                     | 0.51              |
| 2:H:145:ARG:O    | 2:H:146:GLN:HG3  | 2.10                     | 0.51              |
| 2:K:74:ASP:OD2   | 2:K:76:ASN:HB3   | 2.10                     | 0.51              |
| 3:W:808:PHE:O    | 3:W:812:VAL:HG23 | 2.09                     | 0.51              |
| 1:A:326:TYR:CE1  | 1:A:384:ALA:HB3  | 2.45                     | 0.51              |
| 2:I:128:ASN:HD22 | 2:J:19:VAL:CB    | 2.21                     | 0.51              |
| 2:G:6:SER:HG     | 2:G:128:ASN:HA   | 1.72                     | 0.51              |
| 1:A:647:LYS:O    | 1:A:649:LEU:N    | 2.43                     | 0.51              |
| 2:H:76:ASN:N     | 2:J:76:ASN:HB2   | 2.24                     | 0.51              |
| 2:D:6:SER:O      | 2:D:8:SER:N      | 2.44                     | 0.51              |
| 1:B:133:ILE:HD11 | 1:B:147:TYR:HE1  | 1.76                     | 0.51              |
| 2:C:24:TYR:OH    | 2:C:68:THR:HG22  | 2.10                     | 0.51              |
| 1:A:259:HIS:HD1  | 1:A:260:GLN:N    | 2.07                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:K:41:MET:O     | 2:K:42:ASN:C      | 2.49                     | 0.51              |
| 2:L:116:LEU:HA   | 2:L:119:LEU:CD1   | 2.40                     | 0.51              |
| 2:M:381:ASN:O    | 2:M:385:VAL:HB    | 2.10                     | 0.51              |
| 2:E:135:TYR:OH   | 2:E:340:GLU:OE1   | 2.28                     | 0.51              |
| 3:W:803:ALA:HA   | 3:W:808:PHE:CD2   | 2.46                     | 0.51              |
| 2:H:148:THR:OG1  | 2:H:332:GLU:HG2   | 2.10                     | 0.51              |
| 1:A:645:PHE:CD2  | 1:A:646:LEU:HD23  | 2.44                     | 0.51              |
| 1:B:460:GLU:HG3  | 1:B:473:HIS:HD2   | 1.76                     | 0.51              |
| 1:B:498:ARG:CG   | 1:B:505:GLN:HE22  | 2.23                     | 0.51              |
| 1:B:498:ARG:HG3  | 1:B:505:GLN:NE2   | 2.26                     | 0.51              |
| 1:A:519:PRO:O    | 1:A:520:THR:HG23  | 2.10                     | 0.51              |
| 1:B:442:MET:SD   | 1:B:463:ILE:HA    | 2.49                     | 0.51              |
| 1:B:639:LYS:O    | 1:B:642:VAL:HG23  | 2.10                     | 0.51              |
| 1:B:699:ILE:HG13 | 1:B:763:LEU:O     | 2.10                     | 0.51              |
| 3:W:1005:GLN:CG  | 3:W:1006:LEU:HD12 | 2.41                     | 0.51              |
| 1:B:779:ASP:HA   | 1:B:798:ILE:CG1   | 2.39                     | 0.51              |
| 1:A:420:ILE:HG12 | 1:A:423:SER:CB    | 2.38                     | 0.51              |
| 2:E:6:SER:O      | 2:E:8:SER:N       | 2.44                     | 0.51              |
| 2:D:381:ASN:O    | 2:D:385:VAL:HB    | 2.10                     | 0.51              |
| 2:E:89:VAL:O     | 2:E:91:PHE:N      | 2.44                     | 0.51              |
| 2:H:5:TYR:HE2    | 2:H:131:ASN:HA    | 1.75                     | 0.51              |
| 2:G:89:VAL:O     | 2:G:91:PHE:N      | 2.44                     | 0.51              |
| 1:B:89:GLU:C     | 1:B:91:LEU:N      | 2.61                     | 0.51              |
| 2:C:74:ASP:OD2   | 2:C:76:ASN:HB3    | 2.11                     | 0.51              |
| 1:A:631:LEU:O    | 1:A:633:LEU:HD12  | 2.10                     | 0.51              |
| 1:A:661:GLN:HG3  | 1:B:348:LYS:NZ    | 2.26                     | 0.51              |
| 1:B:548:ARG:HH11 | 1:B:878:ASN:N     | 2.04                     | 0.51              |
| 2:N:41:MET:O     | 2:N:42:ASN:C      | 2.49                     | 0.51              |
| 1:A:773:SER:HB3  | 1:A:778:LEU:HD12  | 1.91                     | 0.51              |
| 3:W:820:LEU:HD13 | 3:W:824:ASN:CB    | 2.40                     | 0.51              |
| 2:H:31:ILE:O     | 2:H:34:PHE:HB3    | 2.11                     | 0.51              |
| 2:O:106:ARG:HD3  | 2:O:106:ARG:N     | 2.23                     | 0.51              |
| 1:B:594:ILE:C    | 1:B:594:ILE:CD1   | 2.79                     | 0.51              |
| 1:B:705:ILE:HG22 | 1:B:707:TYR:CE1   | 2.45                     | 0.51              |
| 2:D:89:VAL:O     | 2:D:91:PHE:N      | 2.43                     | 0.51              |
| 2:N:133:SER:O    | 2:N:136:ILE:HG22  | 2.11                     | 0.51              |
| 3:W:126:THR:OG1  | 3:W:128:SER:HB3   | 2.11                     | 0.51              |
| 2:K:155:PRO:O    | 2:K:186:SER:HB3   | 2.10                     | 0.51              |
| 1:B:104:ILE:HD12 | 1:B:327:ILE:HD12  | 1.92                     | 0.51              |
| 2:M:253:ILE:HD13 | 2:M:319:THR:HB    | 1.93                     | 0.51              |
| 2:D:139:TRP:C    | 2:D:139:TRP:CD1   | 2.84                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:272:ASN:O    | 1:B:274:ILE:N     | 2.43                     | 0.51              |
| 1:B:481:ARG:NH2  | 1:B:496:ASN:HD21  | 2.08                     | 0.51              |
| 1:A:427:CYS:O    | 1:A:431:ILE:HG13  | 2.11                     | 0.51              |
| 1:A:443:GLN:NE2  | 1:A:521:MET:HB3   | 2.25                     | 0.51              |
| 1:B:431:ILE:HG23 | 1:B:435:ILE:HD12  | 1.93                     | 0.51              |
| 1:B:178:PRO:HD2  | 1:B:256:PHE:CE2   | 2.45                     | 0.51              |
| 3:W:1005:GLN:HG3 | 3:W:1006:LEU:HD12 | 1.92                     | 0.51              |
| 2:E:31:ILE:O     | 2:E:34:PHE:HB3    | 2.09                     | 0.51              |
| 1:A:252:PHE:O    | 1:A:254:GLU:N     | 2.44                     | 0.51              |
| 1:A:496:ASN:O    | 1:A:497:ILE:C     | 2.49                     | 0.51              |
| 2:K:116:LEU:HA   | 2:K:119:LEU:CD1   | 2.41                     | 0.51              |
| 2:L:89:VAL:O     | 2:L:91:PHE:N      | 2.43                     | 0.51              |
| 3:W:582:LYS:CG   | 3:W:583:LYS:H     | 2.24                     | 0.51              |
| 3:W:596:THR:O    | 3:W:600:ASN:HB2   | 2.10                     | 0.51              |
| 1:B:305:GLN:NE2  | 1:B:564:ASN:ND2   | 2.58                     | 0.51              |
| 1:A:158:GLY:O    | 1:A:162:VAL:HG23  | 2.09                     | 0.51              |
| 1:A:159:ASP:O    | 1:A:162:VAL:HB    | 2.11                     | 0.51              |
| 2:O:31:ILE:O     | 2:O:34:PHE:HB3    | 2.11                     | 0.51              |
| 1:B:302:ASN:O    | 1:B:303:LEU:HD23  | 2.11                     | 0.51              |
| 2:H:105:GLN:C    | 2:H:107:ASN:N     | 2.58                     | 0.51              |
| 2:K:106:ARG:HD3  | 2:K:106:ARG:N     | 2.17                     | 0.51              |
| 2:F:8:SER:C      | 2:F:10:THR:H      | 2.14                     | 0.51              |
| 2:C:110:ALA:HB1  | 2:C:111:PRO:CD    | 2.41                     | 0.51              |
| 2:O:54:LEU:HD12  | 2:O:55:PRO:HD2    | 1.93                     | 0.51              |
| 2:F:109:ILE:CB   | 2:F:380:ASP:HB3   | 2.40                     | 0.51              |
| 2:H:381:ASN:O    | 2:H:385:VAL:HB    | 2.10                     | 0.51              |
| 3:W:410:PHE:HE2  | 3:W:415:ILE:HD11  | 1.76                     | 0.51              |
| 3:W:166:ARG:HG2  | 3:W:166:ARG:NH1   | 2.25                     | 0.51              |
| 2:D:360:VAL:O    | 2:D:378:ARG:HD3   | 2.11                     | 0.51              |
| 3:W:41:PHE:HB2   | 3:W:62:TYR:CD1    | 2.45                     | 0.51              |
| 2:K:253:ILE:HD13 | 2:K:319:THR:HB    | 1.93                     | 0.51              |
| 1:A:814:ASN:O    | 1:A:815:TYR:C     | 2.48                     | 0.51              |
| 2:O:253:ILE:HD13 | 2:O:319:THR:HB    | 1.93                     | 0.51              |
| 2:J:253:ILE:HD13 | 2:J:319:THR:HB    | 1.92                     | 0.51              |
| 1:A:326:TYR:HD1  | 1:A:384:ALA:HB1   | 1.75                     | 0.51              |
| 1:B:481:ARG:CZ   | 1:B:496:ASN:OD1   | 2.59                     | 0.51              |
| 1:B:491:GLN:O    | 1:B:491:GLN:HG3   | 2.10                     | 0.51              |
| 1:A:793:ASP:C    | 1:A:795:LEU:N     | 2.63                     | 0.51              |
| 2:O:41:MET:O     | 2:O:42:ASN:C      | 2.49                     | 0.51              |
| 1:B:658:PRO:HD2  | 1:B:661:GLN:HG3   | 1.93                     | 0.51              |
| 2:M:106:ARG:HG2  | 2:M:107:ASN:H     | 1.75                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:12:LYS:O     | 2:J:14:ALA:N     | 2.43                     | 0.51              |
| 2:L:14:ALA:C     | 2:L:16:ASP:H     | 2.12                     | 0.51              |
| 2:M:24:TYR:O     | 2:M:26:ASN:N     | 2.44                     | 0.51              |
| 2:C:42:ASN:HA    | 2:C:61:PHE:HB2   | 1.92                     | 0.51              |
| 2:F:23:LEU:HD11  | 2:H:36:GLN:OE1   | 2.10                     | 0.51              |
| 2:H:35:ASN:HA    | 2:H:38:ILE:CD1   | 2.41                     | 0.51              |
| 2:G:111:PRO:HB3  | 2:G:116:LEU:CD2  | 2.41                     | 0.51              |
| 2:I:381:ASN:O    | 2:I:385:VAL:HB   | 2.10                     | 0.51              |
| 2:E:381:ASN:O    | 2:E:385:VAL:HB   | 2.10                     | 0.51              |
| 3:W:343:ALA:CB   | 3:W:575:ILE:HD13 | 2.41                     | 0.51              |
| 2:J:360:VAL:O    | 2:J:378:ARG:HD3  | 2.11                     | 0.51              |
| 2:F:360:VAL:O    | 2:F:378:ARG:HD3  | 2.11                     | 0.51              |
| 2:M:360:VAL:O    | 2:M:378:ARG:HD3  | 2.11                     | 0.51              |
| 2:M:109:ILE:HB   | 2:M:380:ASP:HB3  | 1.93                     | 0.51              |
| 2:L:99:GLU:HG3   | 2:L:99:GLU:O     | 2.10                     | 0.51              |
| 2:C:139:TRP:CD1  | 2:C:139:TRP:C    | 2.83                     | 0.51              |
| 1:B:712:LEU:HD11 | 1:B:722:ASN:HB3  | 1.93                     | 0.51              |
| 1:A:631:LEU:CB   | 1:A:633:LEU:HD13 | 2.38                     | 0.51              |
| 1:B:869:VAL:N    | 1:B:876:ILE:HG23 | 2.26                     | 0.51              |
| 3:W:962:LEU:O    | 3:W:967:ILE:HD13 | 2.11                     | 0.51              |
| 1:B:577:GLN:C    | 1:B:579:THR:H    | 2.14                     | 0.51              |
| 1:A:368:THR:HG22 | 1:A:368:THR:O    | 2.09                     | 0.51              |
| 1:A:130:GLN:O    | 1:A:131:LEU:HB3  | 2.10                     | 0.51              |
| 2:C:17:LYS:HG2   | 2:E:130:ASP:HA   | 1.92                     | 0.51              |
| 3:W:330:PHE:CE1  | 3:W:690:ARG:NE   | 2.79                     | 0.51              |
| 3:W:899:PHE:C    | 3:W:901:PRO:HD3  | 2.31                     | 0.51              |
| 2:C:89:VAL:O     | 2:C:91:PHE:N     | 2.43                     | 0.51              |
| 2:F:89:VAL:O     | 2:F:91:PHE:N     | 2.44                     | 0.51              |
| 2:G:253:ILE:HD13 | 2:G:319:THR:HB   | 1.93                     | 0.51              |
| 2:G:360:VAL:O    | 2:G:378:ARG:HD3  | 2.11                     | 0.51              |
| 2:L:139:TRP:C    | 2:L:139:TRP:CD1  | 2.84                     | 0.51              |
| 1:B:140:LYS:HE2  | 1:B:805:ASP:OD2  | 2.10                     | 0.51              |
| 1:A:546:LEU:HD11 | 1:A:584:LEU:HD23 | 1.93                     | 0.51              |
| 1:A:618:ILE:O    | 1:A:622:VAL:HG23 | 2.11                     | 0.51              |
| 1:A:501:HIS:C    | 1:A:503:ILE:N    | 2.62                     | 0.51              |
| 1:A:527:ARG:O    | 1:A:531:ARG:HG2  | 2.10                     | 0.51              |
| 2:N:60:ASN:C     | 2:N:61:PHE:CD1   | 2.84                     | 0.51              |
| 1:A:701:GLN:O    | 1:A:761:GLY:O    | 2.29                     | 0.51              |
| 2:O:23:LEU:C     | 2:O:23:LEU:HD23  | 2.31                     | 0.51              |
| 1:A:362:SER:HB2  | 1:A:365:GLN:HE22 | 1.72                     | 0.51              |
| 2:O:8:SER:C      | 2:O:10:THR:H     | 2.14                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:128:ASN:HB3  | 2:D:19:VAL:HG23  | 1.93                     | 0.51              |
| 3:W:687:ILE:HG23 | 3:W:687:ILE:O    | 2.11                     | 0.51              |
| 2:G:116:LEU:HA   | 2:G:119:LEU:CD1  | 2.40                     | 0.51              |
| 2:J:153:HIS:NE2  | 2:K:153:HIS:NE2  | 2.59                     | 0.51              |
| 3:W:659:TYR:CG   | 3:W:666:VAL:HG21 | 2.46                     | 0.51              |
| 2:F:74:ASP:OD2   | 2:F:76:ASN:HB3   | 2.11                     | 0.51              |
| 2:G:103:GLU:HG3  | 2:G:359:PRO:HD2  | 1.93                     | 0.51              |
| 2:F:63:PHE:CD2   | 2:F:84:THR:HG23  | 2.46                     | 0.51              |
| 1:B:805:ASP:C    | 1:B:807:ASN:N    | 2.65                     | 0.50              |
| 1:A:555:GLU:OE1  | 1:A:871:PHE:HD2  | 1.93                     | 0.50              |
| 1:B:509:ALA:O    | 1:B:513:LEU:CG   | 2.50                     | 0.50              |
| 1:B:539:ARG:O    | 1:B:542:GLN:N    | 2.44                     | 0.50              |
| 1:A:508:GLU:O    | 1:A:512:GLN:NE2  | 2.45                     | 0.50              |
| 2:K:11:LEU:O     | 2:K:15:ARG:N     | 2.38                     | 0.50              |
| 1:B:178:PRO:HD2  | 1:B:256:PHE:CD2  | 2.45                     | 0.50              |
| 2:H:12:LYS:O     | 2:H:14:ALA:N     | 2.44                     | 0.50              |
| 1:A:676:VAL:O    | 1:A:680:ASP:HB2  | 2.10                     | 0.50              |
| 2:H:116:LEU:HA   | 2:H:119:LEU:CD1  | 2.40                     | 0.50              |
| 2:C:129:PHE:CD1  | 2:C:129:PHE:C    | 2.85                     | 0.50              |
| 3:W:330:PHE:CZ   | 3:W:690:ARG:CZ   | 2.94                     | 0.50              |
| 2:C:49:GLY:HA2   | 2:C:54:LEU:HD23  | 1.93                     | 0.50              |
| 2:N:135:TYR:OH   | 2:N:340:GLU:OE1  | 2.25                     | 0.50              |
| 2:L:135:TYR:CZ   | 2:L:342:MET:HE3  | 2.45                     | 0.50              |
| 2:F:253:ILE:HD13 | 2:F:319:THR:HB   | 1.93                     | 0.50              |
| 3:W:358:GLU:HG3  | 3:W:359:MET:H    | 1.76                     | 0.50              |
| 1:B:527:ARG:O    | 1:B:531:ARG:HG3  | 2.10                     | 0.50              |
| 1:A:467:GLN:NE2  | 1:A:511:MET:HG2  | 2.25                     | 0.50              |
| 1:A:452:PRO:O    | 1:A:453:GLN:CB   | 2.58                     | 0.50              |
| 1:B:449:ASN:ND2  | 1:B:455:PRO:CG   | 2.75                     | 0.50              |
| 2:L:23:LEU:HD11  | 2:N:36:GLN:HB2   | 1.92                     | 0.50              |
| 1:B:392:MET:C    | 1:B:573:THR:HG23 | 2.32                     | 0.50              |
| 1:B:671:LEU:O    | 1:B:672:LEU:HD23 | 2.10                     | 0.50              |
| 1:B:182:LEU:HD11 | 1:B:847:THR:CA   | 2.40                     | 0.50              |
| 2:G:8:SER:C      | 2:G:10:THR:H     | 2.14                     | 0.50              |
| 2:I:133:SER:O    | 2:I:136:ILE:HG22 | 2.11                     | 0.50              |
| 2:C:133:SER:O    | 2:C:136:ILE:HG22 | 2.12                     | 0.50              |
| 2:D:155:PRO:O    | 2:D:186:SER:HB3  | 2.11                     | 0.50              |
| 2:K:360:VAL:O    | 2:K:378:ARG:HD3  | 2.11                     | 0.50              |
| 3:W:703:GLN:H    | 3:W:703:GLN:NE2  | 2.08                     | 0.50              |
| 1:B:518:PHE:CB   | 1:B:519:PRO:CD   | 2.89                     | 0.50              |
| 1:B:878:ASN:OD1  | 1:B:878:ASN:O    | 2.29                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:520:THR:O    | 1:A:521:MET:HE3  | 2.11                     | 0.50              |
| 2:N:8:SER:C      | 2:N:10:THR:H     | 2.14                     | 0.50              |
| 2:N:23:LEU:O     | 2:N:26:ASN:ND2   | 2.43                     | 0.50              |
| 2:L:150:PHE:CD1  | 2:L:150:PHE:N    | 2.78                     | 0.50              |
| 2:L:6:SER:O      | 2:L:8:SER:N      | 2.44                     | 0.50              |
| 2:F:61:PHE:N     | 2:F:61:PHE:CD1   | 2.79                     | 0.50              |
| 2:E:8:SER:C      | 2:E:10:THR:H     | 2.14                     | 0.50              |
| 1:B:298:TYR:HE1  | 1:B:300:ARG:HA   | 1.77                     | 0.50              |
| 2:H:89:VAL:O     | 2:H:91:PHE:N     | 2.44                     | 0.50              |
| 2:L:155:PRO:O    | 2:L:186:SER:HB3  | 2.11                     | 0.50              |
| 2:K:60:ASN:C     | 2:K:61:PHE:CD1   | 2.85                     | 0.50              |
| 3:W:892:LEU:HB2  | 3:W:1051:TRP:CD1 | 2.47                     | 0.50              |
| 2:D:253:ILE:HD13 | 2:D:319:THR:HB   | 1.93                     | 0.50              |
| 2:E:56:ILE:HG22  | 2:E:56:ILE:O     | 2.11                     | 0.50              |
| 1:B:712:LEU:HB2  | 1:B:819:PRO:HB2  | 1.94                     | 0.50              |
| 1:A:545:ASP:OD1  | 1:A:877:MET:HA   | 2.11                     | 0.50              |
| 1:B:498:ARG:HD3  | 2:I:32:GLN:NE2   | 2.26                     | 0.50              |
| 2:I:31:ILE:O     | 2:I:34:PHE:HB3   | 2.11                     | 0.50              |
| 1:B:457:GLN:C    | 1:B:458:ILE:HG13 | 2.31                     | 0.50              |
| 2:N:106:ARG:HG2  | 2:N:107:ASN:H    | 1.77                     | 0.50              |
| 1:A:822:THR:O    | 1:A:823:THR:HG23 | 2.12                     | 0.50              |
| 1:A:199:VAL:CG1  | 1:A:200:VAL:H    | 2.07                     | 0.50              |
| 3:W:385:LEU:HD13 | 3:W:939:VAL:CG2  | 2.42                     | 0.50              |
| 3:W:8:LEU:HA     | 3:W:737:MET:SD   | 2.52                     | 0.50              |
| 2:G:31:ILE:O     | 2:G:34:PHE:HB3   | 2.11                     | 0.50              |
| 2:G:6:SER:O      | 2:G:8:SER:N      | 2.44                     | 0.50              |
| 1:A:436:ILE:CD1  | 1:A:437:TYR:CD1  | 2.94                     | 0.50              |
| 2:C:12:LYS:O     | 2:C:14:ALA:N     | 2.45                     | 0.50              |
| 2:N:66:LEU:HD13  | 2:N:77:TYR:CZ    | 2.46                     | 0.50              |
| 1:B:596:SER:O    | 1:B:599:THR:HB   | 2.11                     | 0.50              |
| 2:L:133:SER:O    | 2:L:136:ILE:HG22 | 2.12                     | 0.50              |
| 2:L:253:ILE:HD13 | 2:L:319:THR:HB   | 1.93                     | 0.50              |
| 2:H:253:ILE:HD13 | 2:H:319:THR:HB   | 1.93                     | 0.50              |
| 3:W:54:SER:OG    | 3:W:55:LEU:N     | 2.44                     | 0.50              |
| 2:N:139:TRP:C    | 2:N:139:TRP:CD1  | 2.84                     | 0.50              |
| 1:B:826:TYR:O    | 1:B:827:LYS:C    | 2.50                     | 0.50              |
| 1:A:634:TYR:HD1  | 1:A:635:GLN:HG3  | 1.76                     | 0.50              |
| 2:I:124:PHE:C    | 2:I:126:ARG:H    | 2.14                     | 0.50              |
| 1:B:428:GLN:NE2  | 1:B:455:PRO:HB2  | 2.26                     | 0.50              |
| 2:D:12:LYS:O     | 2:D:14:ALA:N     | 2.45                     | 0.50              |
| 2:J:8:SER:C      | 2:J:10:THR:H     | 2.14                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:W:397:MET:HA   | 3:W:400:ALA:HB2  | 1.93                     | 0.50              |
| 2:C:46:PHE:HE2   | 2:C:119:LEU:HD21 | 1.75                     | 0.50              |
| 1:A:389:GLN:OE1  | 1:A:567:HIS:HA   | 2.11                     | 0.50              |
| 2:D:100:MET:HG3  | 2:D:388:VAL:HG11 | 1.93                     | 0.50              |
| 2:L:360:VAL:O    | 2:L:378:ARG:HD3  | 2.11                     | 0.50              |
| 2:G:124:PHE:O    | 2:G:127:ILE:HG13 | 2.11                     | 0.50              |
| 2:C:360:VAL:O    | 2:C:378:ARG:HD3  | 2.11                     | 0.50              |
| 2:D:124:PHE:O    | 2:D:127:ILE:HG13 | 2.11                     | 0.50              |
| 2:L:125:LYS:O    | 2:L:127:ILE:N    | 2.42                     | 0.50              |
| 2:F:139:TRP:CD1  | 2:F:139:TRP:C    | 2.85                     | 0.50              |
| 1:B:387:LEU:HD23 | 1:B:554:TYR:HE1  | 1.74                     | 0.50              |
| 2:I:6:SER:O      | 2:I:8:SER:N      | 2.44                     | 0.50              |
| 1:B:176:GLU:O    | 1:B:178:PRO:HD3  | 2.11                     | 0.50              |
| 1:B:578:LEU:HA   | 1:B:581:VAL:CG2  | 2.42                     | 0.50              |
| 2:F:73:LEU:HD22  | 2:F:77:TYR:CD2   | 2.46                     | 0.50              |
| 2:O:11:LEU:O     | 2:O:15:ARG:N     | 2.40                     | 0.50              |
| 2:J:6:SER:O      | 2:J:8:SER:N      | 2.45                     | 0.50              |
| 2:L:11:LEU:O     | 2:L:15:ARG:N     | 2.39                     | 0.50              |
| 2:C:14:ALA:C     | 2:C:16:ASP:N     | 2.65                     | 0.50              |
| 2:G:167:ASN:ND2  | 2:G:178:GLY:HA2  | 2.22                     | 0.50              |
| 2:E:150:PHE:CD1  | 2:E:150:PHE:N    | 2.80                     | 0.50              |
| 2:E:151:THR:C    | 2:E:152:PHE:CD1  | 2.84                     | 0.50              |
| 2:E:139:TRP:C    | 2:E:139:TRP:CD1  | 2.84                     | 0.50              |
| 3:W:898:LYS:HE2  | 3:W:908:GLN:HG2  | 1.94                     | 0.50              |
| 1:A:214:ASP:O    | 1:A:215:GLU:C    | 2.50                     | 0.50              |
| 2:E:253:ILE:HD13 | 2:E:319:THR:HB   | 1.93                     | 0.50              |
| 2:G:139:TRP:C    | 2:G:139:TRP:CD1  | 2.85                     | 0.50              |
| 1:B:810:TYR:HA   | 1:B:812:VAL:HG12 | 1.92                     | 0.50              |
| 1:A:332:VAL:HG11 | 1:A:557:LEU:HD21 | 1.93                     | 0.50              |
| 1:B:499:ASN:N    | 1:B:505:GLN:NE2  | 2.60                     | 0.50              |
| 1:B:463:ILE:HG21 | 1:B:468:VAL:CG1  | 2.41                     | 0.50              |
| 2:I:8:SER:C      | 2:I:10:THR:H     | 2.14                     | 0.50              |
| 1:B:618:ILE:HD13 | 1:B:645:PHE:CZ   | 2.47                     | 0.50              |
| 1:B:170:TYR:CE1  | 1:B:682:PHE:HB2  | 2.47                     | 0.50              |
| 2:L:35:ASN:O     | 2:L:36:GLN:C     | 2.50                     | 0.50              |
| 1:A:229:ARG:O    | 1:A:242:PRO:CG   | 2.60                     | 0.50              |
| 1:B:536:LEU:HD22 | 1:B:536:LEU:N    | 2.27                     | 0.50              |
| 2:C:31:ILE:O     | 2:C:34:PHE:HB3   | 2.12                     | 0.50              |
| 1:A:675:GLU:O    | 1:A:676:VAL:C    | 2.50                     | 0.50              |
| 2:F:6:SER:O      | 2:F:8:SER:N      | 2.45                     | 0.50              |
| 1:B:364:THR:O    | 1:B:364:THR:HG22 | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:133:SER:O    | 2:D:136:ILE:HG22 | 2.11                     | 0.50              |
| 3:W:607:LEU:HD21 | 3:W:659:TYR:HE1  | 1.75                     | 0.50              |
| 2:K:124:PHE:O    | 2:K:126:ARG:N    | 2.45                     | 0.50              |
| 2:I:360:VAL:O    | 2:I:378:ARG:HD3  | 2.11                     | 0.50              |
| 2:N:104:SER:O    | 2:N:108:GLY:HA3  | 2.12                     | 0.50              |
| 1:B:141:GLU:O    | 1:B:142:LEU:CB   | 2.60                     | 0.50              |
| 1:A:309:ASN:HA   | 1:A:311:HIS:CE1  | 2.47                     | 0.50              |
| 1:B:477:ASN:O    | 1:B:479:GLN:N    | 2.44                     | 0.50              |
| 1:B:510:LEU:HD12 | 1:B:513:LEU:HD12 | 1.94                     | 0.50              |
| 1:A:660:ASP:CA   | 1:B:539:ARG:HH11 | 2.24                     | 0.50              |
| 2:J:23:LEU:O     | 2:J:26:ASN:ND2   | 2.45                     | 0.50              |
| 2:I:12:LYS:O     | 2:I:14:ALA:N     | 2.45                     | 0.50              |
| 1:A:704:ILE:HG23 | 1:A:758:ALA:HB2  | 1.94                     | 0.50              |
| 1:B:392:MET:HB3  | 1:B:574:GLU:O    | 2.10                     | 0.50              |
| 3:W:4:TYR:C      | 3:W:4:TYR:CD2    | 2.84                     | 0.50              |
| 1:A:603:TYR:O    | 1:A:606:VAL:CG2  | 2.60                     | 0.50              |
| 1:B:113:PRO:HD2  | 1:B:609:ASN:HB3  | 1.94                     | 0.50              |
| 2:I:150:PHE:CD1  | 2:I:150:PHE:N    | 2.79                     | 0.50              |
| 1:A:297:ARG:HG3  | 1:A:848:PHE:CD2  | 2.46                     | 0.50              |
| 3:W:777:THR:HG21 | 3:W:882:LYS:HZ1  | 1.74                     | 0.50              |
| 2:E:101:VAL:HG23 | 2:E:102:ARG:N    | 2.27                     | 0.50              |
| 1:A:289:ASP:C    | 1:A:290:ARG:HG2  | 2.32                     | 0.50              |
| 2:N:360:VAL:O    | 2:N:378:ARG:HD3  | 2.11                     | 0.50              |
| 3:W:452:ARG:HH11 | 3:W:452:ARG:HG3  | 1.76                     | 0.50              |
| 3:W:255:VAL:HG12 | 3:W:256:ASP:O    | 2.12                     | 0.50              |
| 1:A:369:GLY:O    | 1:A:370:ILE:C    | 2.49                     | 0.50              |
| 1:B:444:ARG:HH21 | 1:B:520:THR:CG2  | 2.09                     | 0.50              |
| 1:A:503:ILE:O    | 1:A:503:ILE:HG22 | 2.12                     | 0.50              |
| 1:B:436:ILE:CG1  | 1:B:437:TYR:H    | 2.21                     | 0.50              |
| 2:K:8:SER:C      | 2:K:10:THR:H     | 2.14                     | 0.50              |
| 2:O:30:LEU:O     | 2:O:31:ILE:C     | 2.51                     | 0.50              |
| 1:B:306:ASP:C    | 1:B:308:LEU:H    | 2.08                     | 0.50              |
| 1:A:613:ASN:HD22 | 1:A:649:LEU:HD21 | 1.75                     | 0.50              |
| 2:E:24:TYR:O     | 2:E:26:ASN:N     | 2.43                     | 0.50              |
| 2:J:144:ARG:O    | 2:J:145:ARG:HB2  | 2.12                     | 0.50              |
| 2:F:153:HIS:NE2  | 2:G:153:HIS:CD2  | 2.80                     | 0.50              |
| 2:G:124:PHE:O    | 2:G:126:ARG:N    | 2.45                     | 0.50              |
| 2:E:360:VAL:O    | 2:E:378:ARG:HD3  | 2.11                     | 0.50              |
| 2:J:63:PHE:CD1   | 2:J:63:PHE:N     | 2.80                     | 0.50              |
| 2:C:253:ILE:HD13 | 2:C:319:THR:HB   | 1.93                     | 0.50              |
| 2:N:253:ILE:HD13 | 2:N:319:THR:HB   | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:155:PRO:O    | 2:G:186:SER:HB3  | 2.12                     | 0.50              |
| 2:G:74:ASP:OD2   | 2:G:76:ASN:HB3   | 2.12                     | 0.50              |
| 1:A:310:LEU:CD1  | 1:A:310:LEU:N    | 2.69                     | 0.49              |
| 1:A:311:HIS:HA   | 1:A:318:TRP:CD1  | 2.47                     | 0.49              |
| 1:A:555:GLU:OE1  | 1:A:871:PHE:CD2  | 2.66                     | 0.49              |
| 1:B:305:GLN:NE2  | 1:B:564:ASN:CG   | 2.65                     | 0.49              |
| 1:B:394:LEU:C    | 1:B:396:PHE:N    | 2.65                     | 0.49              |
| 3:W:466:PRO:HD2  | 3:W:469:TYR:CD2  | 2.46                     | 0.49              |
| 1:A:774:LEU:HD12 | 1:A:774:LEU:O    | 2.11                     | 0.49              |
| 2:O:6:SER:O      | 2:O:8:SER:N      | 2.45                     | 0.49              |
| 2:J:14:ALA:C     | 2:J:16:ASP:N     | 2.65                     | 0.49              |
| 1:A:674:VAL:HG12 | 1:A:678:ARG:HB2  | 1.93                     | 0.49              |
| 1:A:392:MET:O    | 1:A:420:ILE:HG23 | 2.11                     | 0.49              |
| 3:W:145:VAL:CG2  | 3:W:211:ILE:HG23 | 2.42                     | 0.49              |
| 3:W:532:GLN:O    | 3:W:536:LYS:HG3  | 2.12                     | 0.49              |
| 1:A:284:TYR:OH   | 1:A:594:ILE:HG23 | 2.12                     | 0.49              |
| 2:K:133:SER:O    | 2:K:136:ILE:HG22 | 2.12                     | 0.49              |
| 1:A:465:ASN:HB3  | 1:A:468:VAL:HB   | 1.94                     | 0.49              |
| 1:B:134:TYR:CD2  | 1:B:803:ASN:HB2  | 2.47                     | 0.49              |
| 1:A:390:ARG:HG3  | 1:A:391:THR:N    | 2.26                     | 0.49              |
| 1:B:322:THR:HG21 | 1:B:390:ARG:HA   | 1.94                     | 0.49              |
| 1:A:404:LEU:O    | 1:A:405:ILE:C    | 2.50                     | 0.49              |
| 1:A:503:ILE:HG22 | 1:A:506:LEU:CB   | 2.42                     | 0.49              |
| 2:O:35:ASN:HD21  | 2:O:66:LEU:HD12  | 1.77                     | 0.49              |
| 1:A:779:ASP:N    | 1:A:779:ASP:OD1  | 2.43                     | 0.49              |
| 1:B:639:LYS:O    | 1:B:642:VAL:N    | 2.44                     | 0.49              |
| 2:C:106:ARG:HD3  | 2:C:106:ARG:N    | 2.10                     | 0.49              |
| 2:O:14:ALA:C     | 2:O:16:ASP:N     | 2.66                     | 0.49              |
| 2:C:60:ASN:C     | 2:C:61:PHE:CD1   | 2.85                     | 0.49              |
| 2:F:116:LEU:HA   | 2:F:119:LEU:CD1  | 2.42                     | 0.49              |
| 1:A:141:GLU:O    | 1:A:142:LEU:HB2  | 2.11                     | 0.49              |
| 3:W:531:THR:HG23 | 3:W:532:GLN:N    | 2.27                     | 0.49              |
| 2:M:139:TRP:C    | 2:M:139:TRP:CD1  | 2.84                     | 0.49              |
| 2:G:133:SER:O    | 2:G:136:ILE:HG22 | 2.12                     | 0.49              |
| 1:B:267:ASN:N    | 1:B:292:LEU:HD12 | 2.27                     | 0.49              |
| 2:H:101:VAL:HB   | 2:H:355:ILE:HG21 | 1.94                     | 0.49              |
| 2:H:360:VAL:O    | 2:H:378:ARG:HD3  | 2.11                     | 0.49              |
| 1:A:230:GLN:NE2  | 1:A:230:GLN:O    | 2.45                     | 0.49              |
| 1:B:159:ASP:OD2  | 1:B:761:GLY:HA3  | 2.11                     | 0.49              |
| 1:B:735:LEU:CD2  | 1:B:759:LEU:HB3  | 2.42                     | 0.49              |
| 1:A:415:PRO:HD2  | 1:A:480:PHE:HE1  | 1.76                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:277:ARG:CB   | 1:B:277:ARG:NH1  | 2.75                     | 0.49              |
| 1:B:480:PHE:O    | 1:B:481:ARG:C    | 2.49                     | 0.49              |
| 1:B:501:HIS:C    | 1:B:503:ILE:H    | 2.15                     | 0.49              |
| 1:A:501:HIS:O    | 1:A:503:ILE:N    | 2.37                     | 0.49              |
| 1:A:527:ARG:HH11 | 1:A:527:ARG:HG3  | 1.77                     | 0.49              |
| 1:B:428:GLN:HE22 | 1:B:455:PRO:HB2  | 1.77                     | 0.49              |
| 1:B:590:ASN:ND2  | 1:B:590:ASN:N    | 2.46                     | 0.49              |
| 3:W:246:SER:OG   | 3:W:247:PRO:HD3  | 2.12                     | 0.49              |
| 2:E:22:THR:CG2   | 2:E:73:LEU:HD12  | 2.42                     | 0.49              |
| 2:K:31:ILE:O     | 2:K:34:PHE:HB3   | 2.11                     | 0.49              |
| 2:C:8:SER:C      | 2:C:10:THR:H     | 2.14                     | 0.49              |
| 2:E:12:LYS:O     | 2:E:14:ALA:N     | 2.45                     | 0.49              |
| 3:W:126:THR:C    | 3:W:128:SER:H    | 2.15                     | 0.49              |
| 1:B:498:ARG:HH12 | 2:J:25:SER:CB    | 2.23                     | 0.49              |
| 1:B:869:VAL:HG13 | 1:B:873:ASN:HA   | 1.92                     | 0.49              |
| 1:B:428:GLN:CB   | 1:B:456:PHE:HD1  | 2.24                     | 0.49              |
| 1:B:698:LYS:C    | 1:B:699:ILE:HD13 | 2.33                     | 0.49              |
| 1:B:698:LYS:O    | 1:B:699:ILE:HD13 | 2.12                     | 0.49              |
| 2:G:14:ALA:C     | 2:G:16:ASP:N     | 2.66                     | 0.49              |
| 1:A:688:ASN:O    | 1:A:689:MET:C    | 2.51                     | 0.49              |
| 1:B:450:GLY:O    | 1:B:451:ASP:HB2  | 2.11                     | 0.49              |
| 2:H:8:SER:C      | 2:H:10:THR:H     | 2.14                     | 0.49              |
| 1:A:771:VAL:HG12 | 1:A:809:PHE:HB3  | 1.93                     | 0.49              |
| 2:M:133:SER:O    | 2:M:136:ILE:HG22 | 2.13                     | 0.49              |
| 1:A:149:LYS:NZ   | 1:A:697:ASP:OD1  | 2.45                     | 0.49              |
| 2:O:139:TRP:CD1  | 2:O:139:TRP:C    | 2.85                     | 0.49              |
| 1:B:812:VAL:HA   | 1:B:817:TRP:HZ3  | 1.78                     | 0.49              |
| 1:A:333:VAL:CG1  | 1:A:380:LYS:HA   | 2.19                     | 0.49              |
| 1:A:415:PRO:HG2  | 1:A:480:PHE:HD1  | 1.73                     | 0.49              |
| 1:B:305:GLN:O    | 1:B:307:ARG:N    | 2.46                     | 0.49              |
| 2:K:12:LYS:O     | 2:K:14:ALA:N     | 2.45                     | 0.49              |
| 2:K:14:ALA:C     | 2:K:16:ASP:N     | 2.65                     | 0.49              |
| 2:N:22:THR:OG1   | 2:N:26:ASN:ND2   | 2.40                     | 0.49              |
| 1:B:122:LEU:O    | 1:B:123:PHE:HB3  | 2.12                     | 0.49              |
| 1:A:178:PRO:HD2  | 1:A:256:PHE:HE2  | 1.77                     | 0.49              |
| 2:J:144:ARG:NH2  | 2:J:146:GLN:NE2  | 2.61                     | 0.49              |
| 1:A:718:TYR:CD1  | 1:A:718:TYR:N    | 2.80                     | 0.49              |
| 3:W:345:ASP:HB2  | 3:W:458:ARG:NH1  | 2.25                     | 0.49              |
| 2:O:63:PHE:CD1   | 2:O:63:PHE:N     | 2.81                     | 0.49              |
| 1:B:174:LEU:O    | 1:B:177:MET:HB2  | 2.12                     | 0.49              |
| 3:W:759:THR:HG23 | 3:W:759:THR:O    | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:150:LEU:HD12 | 1:B:696:SER:HA   | 1.93                     | 0.49              |
| 1:B:603:TYR:O    | 1:B:606:VAL:CG2  | 2.61                     | 0.49              |
| 1:B:856:ALA:C    | 1:B:858:VAL:H    | 2.14                     | 0.49              |
| 2:C:6:SER:O      | 2:C:8:SER:N      | 2.45                     | 0.49              |
| 2:J:115:SER:O    | 2:J:119:LEU:HG   | 2.13                     | 0.49              |
| 2:C:153:HIS:CE1  | 2:D:153:HIS:CD2  | 3.01                     | 0.49              |
| 2:J:30:LEU:O     | 2:J:31:ILE:C     | 2.51                     | 0.49              |
| 2:J:31:ILE:O     | 2:J:34:PHE:HB3   | 2.13                     | 0.49              |
| 2:F:12:LYS:O     | 2:F:14:ALA:N     | 2.45                     | 0.49              |
| 3:W:803:ALA:HA   | 3:W:808:PHE:CG   | 2.47                     | 0.49              |
| 2:H:155:PRO:O    | 2:H:186:SER:HB3  | 2.13                     | 0.49              |
| 2:O:360:VAL:O    | 2:O:378:ARG:HD3  | 2.11                     | 0.49              |
| 1:B:807:ASN:C    | 1:B:809:PHE:N    | 2.66                     | 0.49              |
| 1:A:548:ARG:O    | 1:A:551:ALA:HB3  | 2.12                     | 0.49              |
| 1:B:544:VAL:HG11 | 1:B:548:ARG:HH21 | 1.78                     | 0.49              |
| 1:A:457:GLN:O    | 1:A:459:ALA:N    | 2.45                     | 0.49              |
| 1:A:452:PRO:O    | 1:A:453:GLN:HB3  | 2.13                     | 0.49              |
| 1:B:457:GLN:C    | 1:B:459:ALA:N    | 2.57                     | 0.49              |
| 2:I:5:TYR:CE2    | 2:I:131:ASN:HA   | 2.47                     | 0.49              |
| 1:A:854:LEU:O    | 1:A:856:ALA:N    | 2.46                     | 0.49              |
| 2:M:5:TYR:HE2    | 2:M:131:ASN:HA   | 1.77                     | 0.49              |
| 2:N:14:ALA:C     | 2:N:16:ASP:N     | 2.65                     | 0.49              |
| 2:F:150:PHE:CD1  | 2:F:150:PHE:N    | 2.80                     | 0.49              |
| 2:C:35:ASN:O     | 2:C:36:GLN:C     | 2.51                     | 0.49              |
| 2:C:153:HIS:O    | 2:C:154:LYS:C    | 2.50                     | 0.49              |
| 2:E:115:SER:O    | 2:E:119:LEU:HG   | 2.13                     | 0.49              |
| 2:F:14:ALA:C     | 2:F:16:ASP:N     | 2.66                     | 0.49              |
| 2:G:153:HIS:NE2  | 2:H:153:HIS:CD2  | 2.81                     | 0.49              |
| 1:A:389:GLN:HE22 | 1:A:568:VAL:H    | 1.60                     | 0.49              |
| 2:L:139:TRP:HE1  | 2:L:143:ASN:HD22 | 1.61                     | 0.49              |
| 1:A:147:TYR:CD1  | 1:A:147:TYR:N    | 2.80                     | 0.49              |
| 2:I:253:ILE:HD13 | 2:I:319:THR:HB   | 1.93                     | 0.49              |
| 1:A:539:ARG:O    | 1:A:542:GLN:N    | 2.44                     | 0.49              |
| 1:A:662:MET:O    | 1:A:665:LEU:CB   | 2.61                     | 0.49              |
| 2:I:14:ALA:C     | 2:I:16:ASP:N     | 2.66                     | 0.49              |
| 1:A:820:THR:O    | 1:A:820:THR:HG22 | 2.13                     | 0.49              |
| 1:B:580:SER:O    | 1:B:581:VAL:C    | 2.51                     | 0.49              |
| 1:B:182:LEU:HD21 | 1:B:846:LEU:HD12 | 1.95                     | 0.49              |
| 1:B:184:LYS:C    | 1:B:186:MET:H    | 2.15                     | 0.49              |
| 2:E:21:GLY:O     | 2:E:22:THR:O     | 2.31                     | 0.49              |
| 2:J:2:ASP:HB2    | 2:J:128:ASN:HD21 | 1.77                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:854:LEU:CD2  | 1:B:855:LEU:N    | 2.76                     | 0.49              |
| 2:O:109:ILE:HB   | 2:O:380:ASP:HB3  | 1.94                     | 0.49              |
| 2:E:110:ALA:HB1  | 2:E:111:PRO:HD2  | 1.95                     | 0.49              |
| 3:W:748:LEU:O    | 3:W:748:LEU:HD23 | 2.13                     | 0.49              |
| 1:B:487:GLY:O    | 1:B:488:VAL:HB   | 2.13                     | 0.49              |
| 2:F:72:ASN:ND2   | 2:H:126:ARG:NH1  | 2.60                     | 0.49              |
| 1:A:652:PHE:CD1  | 1:A:652:PHE:N    | 2.80                     | 0.49              |
| 1:B:288:MET:HA   | 1:B:288:MET:CE   | 2.42                     | 0.49              |
| 1:B:139:GLU:O    | 1:B:141:GLU:N    | 2.46                     | 0.49              |
| 1:B:501:HIS:O    | 1:B:503:ILE:HG13 | 2.12                     | 0.49              |
| 1:B:428:GLN:O    | 1:B:432:VAL:HG23 | 2.13                     | 0.49              |
| 1:B:676:VAL:O    | 1:B:680:ASP:HB2  | 2.13                     | 0.49              |
| 1:B:845:ASN:HB3  | 1:B:848:PHE:HE1  | 1.77                     | 0.49              |
| 1:A:192:ASN:O    | 1:A:193:SER:CB   | 2.49                     | 0.49              |
| 2:I:144:ARG:NH2  | 2:I:146:GLN:HE22 | 2.10                     | 0.49              |
| 2:G:42:ASN:HA    | 2:G:61:PHE:HB2   | 1.94                     | 0.49              |
| 2:H:6:SER:O      | 2:H:8:SER:N      | 2.46                     | 0.49              |
| 2:L:12:LYS:O     | 2:L:14:ALA:N     | 2.45                     | 0.49              |
| 2:D:35:ASN:O     | 2:D:36:GLN:C     | 2.51                     | 0.49              |
| 2:J:150:PHE:N    | 2:J:150:PHE:CD1  | 2.81                     | 0.49              |
| 2:J:35:ASN:O     | 2:J:36:GLN:C     | 2.51                     | 0.49              |
| 2:F:46:PHE:CE2   | 2:F:119:LEU:HD21 | 2.48                     | 0.49              |
| 3:W:76:SER:O     | 3:W:748:LEU:HA   | 2.12                     | 0.49              |
| 3:W:23:GLN:O     | 3:W:25:PRO:HD3   | 2.13                     | 0.49              |
| 2:J:101:VAL:HG23 | 2:J:102:ARG:N    | 2.27                     | 0.49              |
| 2:F:101:VAL:HG23 | 2:F:102:ARG:N    | 2.27                     | 0.49              |
| 2:K:139:TRP:C    | 2:K:139:TRP:CD1  | 2.85                     | 0.49              |
| 3:W:488:ARG:NH2  | 3:W:501:LEU:HD11 | 2.28                     | 0.49              |
| 3:W:255:VAL:HG22 | 3:W:314:ARG:O    | 2.13                     | 0.49              |
| 1:A:311:HIS:HE2  | 1:A:566:GLN:HE22 | 1.59                     | 0.49              |
| 1:A:646:LEU:HD23 | 1:A:646:LEU:N    | 2.28                     | 0.49              |
| 1:A:666:ARG:HG2  | 1:A:667:ASP:H    | 1.78                     | 0.49              |
| 1:B:277:ARG:NH1  | 1:B:277:ARG:HB2  | 2.28                     | 0.49              |
| 1:B:473:HIS:CB   | 2:I:126:ARG:NH2  | 2.69                     | 0.49              |
| 2:M:12:LYS:O     | 2:M:14:ALA:N     | 2.46                     | 0.49              |
| 1:B:587:LEU:O    | 1:B:587:LEU:CG   | 2.60                     | 0.49              |
| 2:C:106:ARG:HG2  | 2:C:107:ASN:H    | 1.77                     | 0.49              |
| 2:G:12:LYS:O     | 2:G:14:ALA:N     | 2.46                     | 0.49              |
| 3:W:232:LEU:HD22 | 3:W:300:LEU:HD12 | 1.95                     | 0.49              |
| 3:W:212:GLU:CB   | 3:W:696:LEU:HD12 | 2.39                     | 0.49              |
| 1:B:422:GLU:N    | 1:B:422:GLU:OE1  | 2.46                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:597:PRO:HB3  | 1:A:860:ALA:HB3  | 1.94                     | 0.49              |
| 3:W:591:SER:HB2  | 3:W:596:THR:HG21 | 1.95                     | 0.49              |
| 2:K:59:TRP:CD1   | 2:K:59:TRP:N     | 2.79                     | 0.49              |
| 1:A:404:LEU:O    | 1:A:407:GLY:N    | 2.46                     | 0.48              |
| 2:O:69:THR:O     | 2:O:70:LEU:O     | 2.31                     | 0.48              |
| 1:B:785:GLN:O    | 1:B:787:VAL:N    | 2.46                     | 0.48              |
| 1:A:122:LEU:HD11 | 1:A:201:ASP:CB   | 2.43                     | 0.48              |
| 1:B:302:ASN:ND2  | 1:B:615:ASN:HB3  | 2.27                     | 0.48              |
| 2:L:41:MET:O     | 2:L:42:ASN:C     | 2.51                     | 0.48              |
| 1:A:179:ASP:HA   | 1:A:677:ARG:NH2  | 2.27                     | 0.48              |
| 2:E:14:ALA:C     | 2:E:16:ASP:N     | 2.66                     | 0.48              |
| 2:G:115:SER:O    | 2:G:119:LEU:HG   | 2.13                     | 0.48              |
| 1:A:271:PHE:CA   | 1:A:274:ILE:HD12 | 2.43                     | 0.48              |
| 2:I:49:GLY:HA2   | 2:I:54:LEU:CD2   | 2.43                     | 0.48              |
| 3:W:1047:LYS:O   | 3:W:1048:ASN:ND2 | 2.46                     | 0.48              |
| 3:W:80:ASP:O     | 3:W:81:LYS:HG3   | 2.13                     | 0.48              |
| 2:G:129:PHE:C    | 2:G:129:PHE:CD1  | 2.86                     | 0.48              |
| 1:A:322:THR:O    | 1:A:323:THR:C    | 2.50                     | 0.48              |
| 1:B:473:HIS:O    | 1:B:477:ASN:ND2  | 2.46                     | 0.48              |
| 1:A:529:ILE:O    | 1:A:533:ILE:HG13 | 2.12                     | 0.48              |
| 1:B:436:ILE:O    | 1:B:437:TYR:C    | 2.51                     | 0.48              |
| 2:K:6:SER:O      | 2:K:8:SER:N      | 2.46                     | 0.48              |
| 2:M:6:SER:O      | 2:M:8:SER:N      | 2.45                     | 0.48              |
| 1:B:789:LEU:O    | 1:B:790:ARG:C    | 2.51                     | 0.48              |
| 1:B:583:SER:O    | 1:B:587:LEU:HB3  | 2.12                     | 0.48              |
| 2:L:14:ALA:C     | 2:L:16:ASP:N     | 2.67                     | 0.48              |
| 2:M:38:ILE:HG22  | 2:M:42:ASN:ND2   | 2.27                     | 0.48              |
| 3:W:477:VAL:HA   | 3:W:480:MET:HE3  | 1.94                     | 0.48              |
| 2:K:30:LEU:O     | 2:K:31:ILE:C     | 2.52                     | 0.48              |
| 2:L:109:ILE:HB   | 2:L:380:ASP:HB3  | 1.94                     | 0.48              |
| 2:L:135:TYR:OH   | 2:L:340:GLU:OE1  | 2.30                     | 0.48              |
| 3:W:396:SER:O    | 3:W:398:SER:N    | 2.46                     | 0.48              |
| 2:O:48:THR:O     | 2:O:56:ILE:HA    | 2.12                     | 0.48              |
| 2:N:53:ASN:ND2   | 2:N:354:ALA:HB3  | 2.28                     | 0.48              |
| 1:B:477:ASN:HD21 | 2:I:39:ILE:HG21  | 1.77                     | 0.48              |
| 2:G:144:ARG:O    | 2:G:145:ARG:HB2  | 2.14                     | 0.48              |
| 2:I:19:VAL:HG21  | 2:K:128:ASN:HB3  | 1.94                     | 0.48              |
| 2:M:131:ASN:O    | 2:N:16:ASP:HB3   | 2.13                     | 0.48              |
| 1:B:765:PHE:CZ   | 1:B:767:THR:HG23 | 2.48                     | 0.48              |
| 3:W:498:ASN:HB2  | 3:W:1086:PHE:CE2 | 2.48                     | 0.48              |
| 2:H:14:ALA:C     | 2:H:16:ASP:N     | 2.66                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:522:PRO:O    | 1:B:525:TYR:HB2   | 2.14                     | 0.48              |
| 2:C:130:ASP:C    | 2:C:131:ASN:HD22  | 2.17                     | 0.48              |
| 3:W:1009:PHE:HE2 | 3:W:1042:ILE:HG13 | 1.78                     | 0.48              |
| 1:A:434:THR:O    | 1:A:434:THR:CG2   | 2.61                     | 0.48              |
| 2:J:135:TYR:OH   | 2:J:340:GLU:OE1   | 2.30                     | 0.48              |
| 2:H:149:GLY:C    | 2:H:150:PHE:CD1   | 2.87                     | 0.48              |
| 2:O:144:ARG:C    | 2:O:145:ARG:HG2   | 2.33                     | 0.48              |
| 1:B:486:ASP:O    | 1:B:488:VAL:N     | 2.46                     | 0.48              |
| 2:M:123:LYS:HG3  | 2:M:124:PHE:CE1   | 2.49                     | 0.48              |
| 1:A:384:ALA:O    | 1:A:385:ALA:C     | 2.50                     | 0.48              |
| 1:A:390:ARG:HE   | 1:A:574:GLU:HG2   | 1.78                     | 0.48              |
| 1:B:275:PRO:HD2  | 1:B:278:ILE:CD1   | 2.43                     | 0.48              |
| 1:B:329:ALA:HB3  | 1:B:384:ALA:CB    | 2.43                     | 0.48              |
| 1:B:442:MET:O    | 1:B:443:GLN:C     | 2.50                     | 0.48              |
| 1:B:228:MET:O    | 1:B:228:MET:HG3   | 2.12                     | 0.48              |
| 1:B:231:ARG:CB   | 1:B:240:ASN:HB2   | 2.42                     | 0.48              |
| 1:A:704:ILE:O    | 1:A:823:THR:HB    | 2.14                     | 0.48              |
| 1:A:122:LEU:HD23 | 1:A:122:LEU:N     | 2.28                     | 0.48              |
| 3:W:466:PRO:HD2  | 3:W:469:TYR:HD2   | 1.79                     | 0.48              |
| 3:W:186:ASN:ND2  | 3:W:186:ASN:H     | 2.07                     | 0.48              |
| 2:L:5:TYR:HE2    | 2:L:130:ASP:O     | 1.97                     | 0.48              |
| 1:B:422:GLU:O    | 1:B:425:VAL:HB    | 2.12                     | 0.48              |
| 2:K:35:ASN:O     | 2:K:36:GLN:C      | 2.51                     | 0.48              |
| 2:J:36:GLN:OE1   | 2:K:23:LEU:HD21   | 2.13                     | 0.48              |
| 2:E:133:SER:O    | 2:E:136:ILE:HG22  | 2.13                     | 0.48              |
| 3:W:769:GLU:HG2  | 3:W:772:ILE:HD12  | 1.95                     | 0.48              |
| 1:A:486:ASP:OD2  | 1:A:490:ASN:HB2   | 2.13                     | 0.48              |
| 1:A:545:ASP:OD1  | 1:A:548:ARG:NH1   | 2.46                     | 0.48              |
| 1:A:545:ASP:O    | 1:A:546:LEU:C     | 2.51                     | 0.48              |
| 1:A:305:GLN:OE1  | 1:A:564:ASN:ND2   | 2.44                     | 0.48              |
| 1:B:176:GLU:O    | 1:B:178:PRO:CD    | 2.61                     | 0.48              |
| 2:O:42:ASN:HA    | 2:O:61:PHE:HB2    | 1.95                     | 0.48              |
| 1:B:392:MET:CA   | 1:B:573:THR:HG23  | 2.43                     | 0.48              |
| 2:H:22:THR:OG1   | 2:H:26:ASN:ND2    | 2.46                     | 0.48              |
| 2:O:14:ALA:O     | 2:O:18:ILE:CD1    | 2.61                     | 0.48              |
| 2:I:48:THR:O     | 2:I:56:ILE:HA     | 2.13                     | 0.48              |
| 1:B:521:MET:CB   | 1:B:522:PRO:CD    | 2.90                     | 0.48              |
| 1:B:113:PRO:CD   | 1:B:609:ASN:HB3   | 2.43                     | 0.48              |
| 2:H:35:ASN:O     | 2:H:36:GLN:C      | 2.51                     | 0.48              |
| 2:H:115:SER:O    | 2:H:119:LEU:HG    | 2.13                     | 0.48              |
| 2:E:6:SER:OG     | 2:E:128:ASN:HA    | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:108:LEU:C    | 1:B:110:ASP:N    | 2.67                     | 0.48              |
| 1:A:226:ALA:C    | 1:A:228:MET:H    | 2.15                     | 0.48              |
| 1:A:484:VAL:CG1  | 1:A:485:ILE:H    | 2.25                     | 0.48              |
| 2:D:125:LYS:O    | 2:D:127:ILE:N    | 2.46                     | 0.48              |
| 1:A:170:TYR:CE1  | 1:A:682:PHE:HB2  | 2.49                     | 0.48              |
| 2:J:155:PRO:O    | 2:J:186:SER:HB3  | 2.14                     | 0.48              |
| 1:A:659:ASP:O    | 1:A:660:ASP:O    | 2.32                     | 0.48              |
| 1:A:404:LEU:CB   | 1:A:435:ILE:HD11 | 2.43                     | 0.48              |
| 1:A:428:GLN:CB   | 1:A:456:PHE:HD1  | 2.22                     | 0.48              |
| 1:A:460:GLU:C    | 1:A:462:GLN:H    | 2.16                     | 0.48              |
| 1:A:516:GLN:CD   | 1:A:516:GLN:H    | 2.11                     | 0.48              |
| 2:M:128:ASN:HD22 | 2:N:19:VAL:HB    | 1.79                     | 0.48              |
| 2:N:35:ASN:O     | 2:N:36:GLN:C     | 2.51                     | 0.48              |
| 1:B:782:VAL:O    | 1:B:785:GLN:HB2  | 2.14                     | 0.48              |
| 1:A:822:THR:O    | 1:A:823:THR:OG1  | 2.22                     | 0.48              |
| 2:C:150:PHE:CD1  | 2:C:150:PHE:N    | 2.82                     | 0.48              |
| 1:A:865:PRO:O    | 1:A:867:ASN:N    | 2.47                     | 0.48              |
| 1:A:118:LYS:CG   | 1:A:119:GLN:N    | 2.73                     | 0.48              |
| 2:D:24:TYR:CE1   | 2:D:68:THR:HG22  | 2.48                     | 0.48              |
| 2:D:31:ILE:O     | 2:D:34:PHE:HB3   | 2.13                     | 0.48              |
| 3:W:825:ASN:HA   | 3:W:828:SER:CB   | 2.41                     | 0.48              |
| 2:E:35:ASN:O     | 2:E:36:GLN:C     | 2.52                     | 0.48              |
| 2:D:150:PHE:HB2  | 2:D:152:PHE:HE1  | 1.77                     | 0.48              |
| 3:W:796:SER:C    | 3:W:798:ILE:H    | 2.16                     | 0.48              |
| 2:F:53:ASN:ND2   | 2:F:354:ALA:HB3  | 2.28                     | 0.48              |
| 1:B:104:ILE:HD12 | 1:B:327:ILE:CD1  | 2.44                     | 0.48              |
| 2:G:54:LEU:HD12  | 2:G:55:PRO:HD2   | 1.96                     | 0.48              |
| 2:O:32:GLN:O     | 2:O:33:GLN:C     | 2.52                     | 0.48              |
| 1:B:723:ILE:O    | 1:B:724:ALA:CB   | 2.61                     | 0.48              |
| 1:A:627:ALA:O    | 1:A:631:LEU:HG   | 2.13                     | 0.48              |
| 1:A:629:ASN:C    | 1:A:631:LEU:N    | 2.61                     | 0.48              |
| 1:B:415:PRO:O    | 1:B:416:ASN:C    | 2.52                     | 0.48              |
| 1:B:305:GLN:CG   | 1:B:564:ASN:HD21 | 2.26                     | 0.48              |
| 1:A:458:ILE:O    | 1:A:462:GLN:HG2  | 2.13                     | 0.48              |
| 1:B:459:ALA:HB1  | 1:B:463:ILE:CD1  | 2.36                     | 0.48              |
| 2:N:6:SER:O      | 2:N:8:SER:N      | 2.47                     | 0.48              |
| 1:B:190:ASN:O    | 1:B:190:ASN:CG   | 2.52                     | 0.48              |
| 1:B:220:ALA:O    | 1:B:223:ARG:HB2  | 2.14                     | 0.48              |
| 1:B:785:GLN:O    | 1:B:786:ILE:C    | 2.51                     | 0.48              |
| 2:L:30:LEU:O     | 2:L:31:ILE:C     | 2.52                     | 0.48              |
| 2:G:23:LEU:HD23  | 2:G:24:TYR:N     | 2.28                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:363:GLU:C    | 1:A:366:PHE:HE1  | 2.16                     | 0.48              |
| 3:W:248:MET:O    | 3:W:252:VAL:HG13 | 2.14                     | 0.48              |
| 2:E:23:LEU:O     | 2:E:26:ASN:ND2   | 2.47                     | 0.48              |
| 2:C:30:LEU:O     | 2:C:31:ILE:C     | 2.52                     | 0.48              |
| 2:F:144:ARG:O    | 2:F:145:ARG:HG3  | 2.14                     | 0.48              |
| 3:W:626:ILE:O    | 3:W:627:ARG:NH1  | 2.43                     | 0.48              |
| 2:K:150:PHE:N    | 2:K:150:PHE:CD1  | 2.82                     | 0.48              |
| 2:I:45:GLU:C     | 2:I:46:PHE:CD1   | 2.87                     | 0.48              |
| 2:C:63:PHE:CD1   | 2:C:63:PHE:N     | 2.81                     | 0.48              |
| 1:B:775:ILE:CD1  | 1:B:775:ILE:N    | 2.76                     | 0.48              |
| 1:A:589:GLY:C    | 1:A:591:ALA:N    | 2.66                     | 0.48              |
| 2:I:128:ASN:O    | 2:J:22:THR:HB    | 2.14                     | 0.48              |
| 1:B:745:ALA:HA   | 1:B:748:THR:OG1  | 2.13                     | 0.48              |
| 3:W:499:GLN:HE21 | 3:W:499:GLN:HB3  | 1.50                     | 0.48              |
| 1:B:452:PRO:O    | 1:B:453:GLN:OE1  | 2.32                     | 0.48              |
| 2:M:22:THR:HG23  | 2:M:73:LEU:CD1   | 2.39                     | 0.48              |
| 1:B:655:ALA:C    | 1:B:657:VAL:H    | 2.17                     | 0.48              |
| 1:B:594:ILE:HB   | 1:B:595:PRO:HD2  | 1.94                     | 0.48              |
| 2:D:70:LEU:CG    | 2:D:71:LEU:N     | 2.76                     | 0.48              |
| 1:A:145:ARG:HB3  | 1:A:147:TYR:CE1  | 2.49                     | 0.48              |
| 1:B:319:ASP:OD2  | 1:B:572:THR:N    | 2.46                     | 0.48              |
| 1:B:233:GLN:HB2  | 1:B:238:VAL:HB   | 1.96                     | 0.48              |
| 3:W:433:TYR:CE1  | 3:W:435:PRO:HD3  | 2.49                     | 0.48              |
| 1:B:811:LEU:HA   | 1:B:814:ASN:HD22 | 1.79                     | 0.48              |
| 1:B:712:LEU:HB3  | 1:B:819:PRO:HB2  | 1.96                     | 0.48              |
| 1:B:517:GLN:N    | 1:B:518:PHE:CE1  | 2.79                     | 0.48              |
| 2:I:37:MET:O     | 2:I:38:ILE:C     | 2.53                     | 0.48              |
| 1:B:466:PHE:CD1  | 2:H:80:THR:HG22  | 2.48                     | 0.48              |
| 1:A:817:TRP:CZ3  | 1:A:819:PRO:HA   | 2.49                     | 0.48              |
| 3:W:464:ILE:HG22 | 3:W:464:ILE:O    | 2.14                     | 0.48              |
| 2:L:106:ARG:HG2  | 2:L:107:ASN:H    | 1.78                     | 0.48              |
| 1:A:239:VAL:HG21 | 1:A:845:ASN:O    | 2.13                     | 0.48              |
| 1:A:769:SER:O    | 1:A:770:SER:C    | 2.51                     | 0.48              |
| 3:W:519:THR:HG22 | 3:W:520:ASP:H    | 1.74                     | 0.48              |
| 2:D:14:ALA:C     | 2:D:16:ASP:N     | 2.66                     | 0.48              |
| 1:A:328:LEU:HG   | 1:A:603:TYR:HE1  | 1.79                     | 0.48              |
| 1:B:536:LEU:CD2  | 1:B:536:LEU:N    | 2.77                     | 0.48              |
| 3:W:1082:ASN:O   | 3:W:1084:ASN:CG  | 2.52                     | 0.48              |
| 2:C:145:ARG:HB3  | 2:C:145:ARG:CZ   | 2.43                     | 0.48              |
| 1:B:214:ASP:O    | 1:B:216:GLU:N    | 2.47                     | 0.48              |
| 2:J:346:VAL:CG2  | 2:J:385:VAL:HG13 | 2.44                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:283:ASN:O    | 1:B:863:VAL:HG23 | 2.13                     | 0.48              |
| 1:A:484:VAL:HG12 | 1:A:485:ILE:N    | 2.28                     | 0.48              |
| 3:W:951:ILE:HG23 | 3:W:1071:TRP:HZ3 | 1.79                     | 0.48              |
| 2:F:31:ILE:O     | 2:F:34:PHE:HB3   | 2.13                     | 0.48              |
| 2:L:50:GLY:HA2   | 2:L:56:ILE:HD11  | 1.95                     | 0.48              |
| 1:A:660:ASP:C    | 1:A:662:MET:N    | 2.66                     | 0.48              |
| 1:B:384:ALA:O    | 1:B:385:ALA:C    | 2.50                     | 0.48              |
| 1:B:478:ASN:C    | 1:B:480:PHE:H    | 2.17                     | 0.48              |
| 1:B:540:LEU:C    | 1:B:540:LEU:HD23 | 2.34                     | 0.48              |
| 2:I:35:ASN:O     | 2:I:36:GLN:C     | 2.52                     | 0.48              |
| 2:I:41:MET:O     | 2:I:42:ASN:C     | 2.52                     | 0.48              |
| 1:A:527:ARG:O    | 1:A:531:ARG:HG3  | 2.13                     | 0.48              |
| 1:B:447:TYR:OH   | 1:B:458:ILE:HD11 | 2.13                     | 0.48              |
| 1:B:449:ASN:HD21 | 1:B:455:PRO:HG3  | 1.78                     | 0.48              |
| 2:J:19:VAL:O     | 2:J:21:GLY:N     | 2.47                     | 0.48              |
| 2:M:14:ALA:C     | 2:M:16:ASP:N     | 2.66                     | 0.48              |
| 1:A:694:ARG:HD2  | 1:A:828:GLN:HG3  | 1.96                     | 0.48              |
| 1:B:126:PHE:HB3  | 1:B:149:LYS:O    | 2.14                     | 0.48              |
| 2:O:35:ASN:O     | 2:O:36:GLN:C     | 2.52                     | 0.48              |
| 1:B:639:LYS:O    | 1:B:640:ALA:C    | 2.52                     | 0.48              |
| 3:W:447:ILE:HG22 | 3:W:448:PRO:O    | 2.14                     | 0.48              |
| 1:A:365:GLN:C    | 1:A:366:PHE:CG   | 2.88                     | 0.48              |
| 1:A:436:ILE:HD11 | 1:A:437:TYR:CE1  | 2.49                     | 0.48              |
| 1:B:533:ILE:O    | 1:B:536:LEU:HB2  | 2.14                     | 0.48              |
| 2:M:30:LEU:O     | 2:M:31:ILE:C     | 2.52                     | 0.48              |
| 2:M:35:ASN:O     | 2:M:36:GLN:C     | 2.51                     | 0.48              |
| 3:W:472:ALA:O    | 3:W:561:TYR:HD1  | 1.96                     | 0.48              |
| 2:F:38:ILE:HG22  | 2:F:42:ASN:ND2   | 2.27                     | 0.48              |
| 1:A:314:PHE:N    | 1:A:314:PHE:CD1  | 2.82                     | 0.48              |
| 3:W:107:LEU:HB2  | 3:W:110:GLU:HG3  | 1.96                     | 0.48              |
| 2:K:115:SER:O    | 2:K:119:LEU:HG   | 2.14                     | 0.48              |
| 1:B:236:ARG:O    | 1:B:237:ASN:CB   | 2.61                     | 0.48              |
| 2:O:346:VAL:CG2  | 2:O:385:VAL:HG13 | 2.44                     | 0.48              |
| 2:I:346:VAL:CG2  | 2:I:385:VAL:HG13 | 2.44                     | 0.48              |
| 2:J:133:SER:O    | 2:J:136:ILE:HG22 | 2.13                     | 0.48              |
| 1:A:356:GLU:O    | 3:W:982:SER:HB2  | 2.14                     | 0.48              |
| 1:B:89:GLU:C     | 1:B:91:LEU:H     | 2.16                     | 0.48              |
| 2:L:139:TRP:HE1  | 2:L:143:ASN:ND2  | 2.11                     | 0.48              |
| 2:O:63:PHE:CD2   | 2:O:84:THR:HG23  | 2.49                     | 0.48              |
| 2:N:42:ASN:HA    | 2:N:61:PHE:CB    | 2.44                     | 0.47              |
| 1:B:122:LEU:HD11 | 1:B:200:VAL:HG11 | 1.94                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:12:LYS:O     | 2:O:14:ALA:N     | 2.46                     | 0.47              |
| 2:I:48:THR:HG21  | 2:I:94:ASN:HB3   | 1.96                     | 0.47              |
| 2:M:41:MET:O     | 2:M:42:ASN:C     | 2.52                     | 0.47              |
| 2:D:66:LEU:O     | 2:D:67:GLY:O     | 2.31                     | 0.47              |
| 2:C:131:ASN:ND2  | 2:C:131:ASN:N    | 2.62                     | 0.47              |
| 2:E:131:ASN:HD22 | 2:E:131:ASN:N    | 2.11                     | 0.47              |
| 2:N:152:PHE:N    | 2:N:152:PHE:CD1  | 2.82                     | 0.47              |
| 1:B:405:ILE:O    | 1:B:408:MET:HB2  | 2.14                     | 0.47              |
| 2:L:346:VAL:CG2  | 2:L:385:VAL:HG13 | 2.44                     | 0.47              |
| 2:N:99:GLU:OE2   | 2:N:112:GLN:HG2  | 2.13                     | 0.47              |
| 3:W:772:ILE:HG23 | 3:W:1043:ASN:ND2 | 2.29                     | 0.47              |
| 3:W:195:VAL:HG23 | 3:W:196:MET:N    | 2.29                     | 0.47              |
| 3:W:497:SER:HB2  | 3:W:501:LEU:HD23 | 1.95                     | 0.47              |
| 2:J:48:THR:O     | 2:J:56:ILE:HA    | 2.13                     | 0.47              |
| 1:A:540:LEU:HA   | 1:A:543:LEU:HB2  | 1.96                     | 0.47              |
| 2:G:35:ASN:O     | 2:G:36:GLN:C     | 2.52                     | 0.47              |
| 2:H:22:THR:HG23  | 2:H:73:LEU:CD1   | 2.43                     | 0.47              |
| 3:W:906:ASN:HD21 | 3:W:907:VAL:HG23 | 1.79                     | 0.47              |
| 3:W:595:GLN:O    | 3:W:599:ALA:N    | 2.38                     | 0.47              |
| 2:C:5:TYR:HE2    | 2:C:131:ASN:HA   | 1.80                     | 0.47              |
| 2:M:115:SER:O    | 2:M:119:LEU:HG   | 2.14                     | 0.47              |
| 3:W:387:ARG:HH11 | 3:W:387:ARG:CB   | 2.25                     | 0.47              |
| 3:W:405:SER:HA   | 3:W:418:THR:HA   | 1.97                     | 0.47              |
| 1:B:822:THR:HG22 | 1:B:822:THR:O    | 2.14                     | 0.47              |
| 2:H:51:ILE:O     | 2:H:51:ILE:HG23  | 2.14                     | 0.47              |
| 1:A:306:ASP:HB3  | 1:A:310:LEU:HD11 | 1.95                     | 0.47              |
| 1:A:383:ILE:O    | 1:A:384:ALA:C    | 2.53                     | 0.47              |
| 1:A:539:ARG:NH2  | 1:A:588:ILE:O    | 2.47                     | 0.47              |
| 1:A:660:ASP:O    | 1:A:663:TYR:N    | 2.47                     | 0.47              |
| 1:B:493:LEU:HD11 | 1:B:567:HIS:HB2  | 1.95                     | 0.47              |
| 2:I:33:GLN:HA    | 2:J:23:LEU:HD12  | 1.95                     | 0.47              |
| 1:A:503:ILE:HG12 | 1:A:547:THR:HG21 | 1.96                     | 0.47              |
| 1:B:511:MET:HE3  | 2:J:70:LEU:HG    | 1.94                     | 0.47              |
| 2:M:11:LEU:O     | 2:M:15:ARG:N     | 2.41                     | 0.47              |
| 1:A:701:GLN:HB3  | 1:A:826:TYR:CD2  | 2.46                     | 0.47              |
| 1:B:295:THR:O    | 1:B:297:ARG:HG2  | 2.14                     | 0.47              |
| 1:B:296:ALA:C    | 1:B:297:ARG:HG2  | 2.35                     | 0.47              |
| 3:W:441:VAL:O    | 3:W:571:SER:HA   | 2.14                     | 0.47              |
| 1:A:437:TYR:N    | 1:A:438:PRO:CD   | 2.73                     | 0.47              |
| 2:D:32:GLN:O     | 2:D:33:GLN:C     | 2.52                     | 0.47              |
| 3:W:535:ARG:HH11 | 3:W:565:GLN:NE2  | 2.12                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:35:ASN:O     | 2:F:36:GLN:C     | 2.53                     | 0.47              |
| 1:B:638:MET:HE1  | 1:B:666:ARG:HH12 | 1.78                     | 0.47              |
| 2:H:133:SER:O    | 2:H:136:ILE:HG22 | 2.14                     | 0.47              |
| 2:F:30:LEU:O     | 2:F:31:ILE:C     | 2.53                     | 0.47              |
| 1:A:636:LYS:O    | 1:A:637:LYS:C    | 2.52                     | 0.47              |
| 1:B:460:GLU:HG3  | 1:B:473:HIS:CD2  | 2.49                     | 0.47              |
| 1:B:513:LEU:HA   | 1:B:516:GLN:HE22 | 1.71                     | 0.47              |
| 1:A:827:LYS:O    | 1:A:828:GLN:O    | 2.32                     | 0.47              |
| 1:A:710:MET:HE1  | 1:A:824:LYS:HE2  | 1.97                     | 0.47              |
| 2:N:32:GLN:O     | 2:N:33:GLN:C     | 2.53                     | 0.47              |
| 3:W:385:LEU:HD13 | 3:W:939:VAL:HG22 | 1.96                     | 0.47              |
| 2:E:30:LEU:O     | 2:E:31:ILE:C     | 2.51                     | 0.47              |
| 2:M:37:MET:O     | 2:M:38:ILE:C     | 2.53                     | 0.47              |
| 1:B:355:LEU:HG   | 1:B:356:GLU:H    | 1.76                     | 0.47              |
| 2:O:153:HIS:O    | 2:O:154:LYS:C    | 2.52                     | 0.47              |
| 3:W:382:ASP:O    | 3:W:387:ARG:HD2  | 2.14                     | 0.47              |
| 1:A:714:ARG:HG2  | 1:A:720:TYR:HD2  | 1.79                     | 0.47              |
| 2:G:346:VAL:CG2  | 2:G:385:VAL:HG13 | 2.45                     | 0.47              |
| 2:H:151:THR:C    | 2:H:152:PHE:CD1  | 2.88                     | 0.47              |
| 2:D:48:THR:O     | 2:D:56:ILE:HA    | 2.14                     | 0.47              |
| 1:B:735:LEU:HD21 | 1:B:759:LEU:CB   | 2.45                     | 0.47              |
| 1:A:311:HIS:N    | 1:A:311:HIS:ND1  | 2.63                     | 0.47              |
| 1:B:513:LEU:O    | 1:B:516:GLN:OE1  | 2.32                     | 0.47              |
| 1:B:481:ARG:HG2  | 2:I:65:LEU:CD1   | 2.44                     | 0.47              |
| 2:N:23:LEU:HD23  | 2:N:24:TYR:N     | 2.29                     | 0.47              |
| 1:A:148:TRP:CH2  | 1:A:246:HIS:HB2  | 2.49                     | 0.47              |
| 1:B:95:ILE:O     | 1:B:97:THR:N     | 2.46                     | 0.47              |
| 2:C:115:SER:O    | 2:C:119:LEU:HG   | 2.15                     | 0.47              |
| 1:B:666:ARG:HG2  | 1:B:667:ASP:H    | 1.79                     | 0.47              |
| 2:O:115:SER:O    | 2:O:119:LEU:HG   | 2.14                     | 0.47              |
| 2:J:129:PHE:O    | 2:J:131:ASN:ND2  | 2.47                     | 0.47              |
| 2:F:133:SER:O    | 2:F:136:ILE:HG22 | 2.14                     | 0.47              |
| 1:A:742:GLY:CA   | 1:B:285:ILE:HD11 | 2.44                     | 0.47              |
| 2:E:32:GLN:O     | 2:E:33:GLN:C     | 2.52                     | 0.47              |
| 2:K:125:LYS:O    | 2:K:127:ILE:N    | 2.45                     | 0.47              |
| 1:A:338:GLU:O    | 1:A:338:GLU:HG3  | 2.14                     | 0.47              |
| 1:A:596:SER:HB3  | 1:A:599:THR:OG1  | 2.15                     | 0.47              |
| 1:A:527:ARG:HH11 | 1:A:531:ARG:HH21 | 1.63                     | 0.47              |
| 1:A:723:ILE:O    | 1:A:824:LYS:HD2  | 2.14                     | 0.47              |
| 2:I:144:ARG:O    | 2:I:145:ARG:HB2  | 2.15                     | 0.47              |
| 1:B:593:VAL:HG12 | 1:B:594:ILE:N    | 2.30                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:153:HIS:O    | 2:G:154:LYS:C    | 2.53                     | 0.47              |
| 2:N:152:PHE:HD2  | 2:N:337:ASP:HB3  | 1.78                     | 0.47              |
| 2:E:346:VAL:CG2  | 2:E:385:VAL:HG13 | 2.44                     | 0.47              |
| 3:W:1058:TYR:HD2 | 3:W:1063:MET:HG2 | 1.79                     | 0.47              |
| 2:K:100:MET:HG3  | 2:K:388:VAL:HG11 | 1.95                     | 0.47              |
| 2:M:53:ASN:O     | 2:M:353:TYR:HD2  | 1.97                     | 0.47              |
| 2:F:78:VAL:O     | 2:F:81:ALA:HB3   | 2.14                     | 0.47              |
| 1:B:721:VAL:CG1  | 1:B:722:ASN:N    | 2.77                     | 0.47              |
| 2:I:124:PHE:C    | 2:I:126:ARG:N    | 2.68                     | 0.47              |
| 1:B:548:ARG:O    | 1:B:551:ALA:HB3  | 2.15                     | 0.47              |
| 1:A:454:THR:HB   | 1:A:457:GLN:CB   | 2.44                     | 0.47              |
| 1:A:508:GLU:HG2  | 1:A:512:GLN:HE21 | 1.75                     | 0.47              |
| 1:A:516:GLN:C    | 1:A:518:PHE:H    | 2.18                     | 0.47              |
| 2:I:139:TRP:HE1  | 2:I:143:ASN:HD22 | 1.62                     | 0.47              |
| 1:A:450:GLY:O    | 1:A:451:ASP:CB   | 2.62                     | 0.47              |
| 2:N:11:LEU:O     | 2:N:15:ARG:N     | 2.39                     | 0.47              |
| 2:N:124:PHE:O    | 2:N:127:ILE:HG13 | 2.15                     | 0.47              |
| 1:A:699:ILE:HA   | 1:A:763:LEU:O    | 2.14                     | 0.47              |
| 1:B:122:LEU:O    | 1:B:253:ASN:OD1  | 2.32                     | 0.47              |
| 1:B:583:SER:O    | 1:B:584:LEU:C    | 2.53                     | 0.47              |
| 2:L:37:MET:O     | 2:L:38:ILE:C     | 2.53                     | 0.47              |
| 2:H:23:LEU:N     | 2:H:26:ASN:HD22  | 2.12                     | 0.47              |
| 1:A:248:ILE:O    | 1:A:251:ALA:HB3  | 2.14                     | 0.47              |
| 1:B:308:LEU:HA   | 1:B:308:LEU:HD23 | 1.73                     | 0.47              |
| 1:A:772:ILE:HA   | 1:A:775:ILE:CD1  | 2.45                     | 0.47              |
| 1:A:133:ILE:O    | 1:A:134:TYR:HD2  | 1.97                     | 0.47              |
| 1:B:725:ARG:H    | 1:B:725:ARG:CD   | 2.22                     | 0.47              |
| 2:M:27:VAL:HG21  | 2:M:31:ILE:HD11  | 1.97                     | 0.47              |
| 2:L:128:ASN:ND2  | 2:M:19:VAL:HG21  | 2.30                     | 0.47              |
| 1:B:852:SER:O    | 1:B:854:LEU:N    | 2.46                     | 0.47              |
| 2:N:115:SER:O    | 2:N:119:LEU:HG   | 2.15                     | 0.47              |
| 3:W:687:ILE:HG22 | 3:W:899:PHE:O    | 2.15                     | 0.47              |
| 3:W:449:LEU:HD22 | 3:W:573:VAL:HG11 | 1.95                     | 0.47              |
| 1:B:211:ILE:C    | 1:B:213:GLN:N    | 2.67                     | 0.47              |
| 2:J:63:PHE:CD2   | 2:J:84:THR:HG23  | 2.50                     | 0.47              |
| 2:F:72:ASN:ND2   | 2:H:126:ARG:HH11 | 2.12                     | 0.47              |
| 3:W:24:ILE:HG21  | 3:W:46:LEU:CD1   | 2.44                     | 0.47              |
| 2:K:32:GLN:O     | 2:K:33:GLN:C     | 2.53                     | 0.47              |
| 2:F:142:GLN:HE21 | 2:F:143:ASN:N    | 2.12                     | 0.47              |
| 3:W:633:ASN:O    | 3:W:633:ASN:OD1  | 2.33                     | 0.47              |
| 3:W:1068:LYS:HE3 | 3:W:1068:LYS:HA  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:32:GLN:O     | 2:L:33:GLN:C     | 2.52                     | 0.47              |
| 3:W:1013:ASP:O   | 3:W:1016:LYS:HG2 | 2.15                     | 0.47              |
| 1:A:205:ALA:O    | 1:A:206:SER:C    | 2.52                     | 0.47              |
| 1:A:494:ASN:CG   | 1:A:495:ASP:N    | 2.67                     | 0.47              |
| 2:I:102:ARG:HG2  | 2:I:102:ARG:HH11 | 1.80                     | 0.47              |
| 1:A:578:LEU:HA   | 1:A:581:VAL:CG2  | 2.44                     | 0.47              |
| 1:B:480:PHE:CE2  | 1:B:493:LEU:CB   | 2.96                     | 0.47              |
| 1:B:549:LEU:HA   | 1:B:549:LEU:HD12 | 1.64                     | 0.47              |
| 1:A:428:GLN:CD   | 1:A:456:PHE:N    | 2.67                     | 0.47              |
| 1:A:510:LEU:HD12 | 1:A:513:LEU:HD12 | 1.96                     | 0.47              |
| 1:A:510:LEU:CD2  | 1:A:540:LEU:HD13 | 2.29                     | 0.47              |
| 1:B:458:ILE:HD12 | 1:B:459:ALA:CA   | 2.45                     | 0.47              |
| 1:A:763:LEU:HD23 | 1:A:764:PRO:CD   | 2.44                     | 0.47              |
| 2:G:30:LEU:O     | 2:G:31:ILE:C     | 2.52                     | 0.47              |
| 1:A:647:LYS:C    | 1:A:649:LEU:N    | 2.68                     | 0.47              |
| 1:B:360:ILE:O    | 1:B:361:GLN:HB2  | 2.15                     | 0.47              |
| 1:B:73:LEU:HB2   | 3:W:509:PHE:O    | 2.15                     | 0.47              |
| 2:D:115:SER:O    | 2:D:119:LEU:HG   | 2.15                     | 0.47              |
| 2:F:46:PHE:HE2   | 2:F:119:LEU:HD21 | 1.80                     | 0.47              |
| 2:I:115:SER:O    | 2:I:119:LEU:HG   | 2.14                     | 0.47              |
| 2:O:104:SER:O    | 2:O:108:GLY:HA3  | 2.15                     | 0.47              |
| 2:N:346:VAL:CG2  | 2:N:385:VAL:HG13 | 2.44                     | 0.47              |
| 2:D:346:VAL:CG2  | 2:D:385:VAL:HG13 | 2.44                     | 0.47              |
| 1:A:594:ILE:HG12 | 1:A:595:PRO:HD2  | 1.95                     | 0.47              |
| 3:W:41:PHE:HD1   | 3:W:62:TYR:CD2   | 2.33                     | 0.47              |
| 2:K:103:GLU:HG3  | 2:K:359:PRO:HD2  | 1.95                     | 0.47              |
| 2:L:100:MET:HG3  | 2:L:388:VAL:HG11 | 1.95                     | 0.47              |
| 2:O:73:LEU:HD22  | 2:O:77:TYR:CD2   | 2.50                     | 0.47              |
| 1:A:332:VAL:O    | 1:A:333:VAL:C    | 2.53                     | 0.47              |
| 1:A:663:TYR:O    | 1:A:666:ARG:N    | 2.47                     | 0.47              |
| 2:I:23:LEU:HD22  | 2:I:25:SER:OG    | 2.14                     | 0.47              |
| 2:C:106:ARG:H    | 2:C:106:ARG:CD   | 2.10                     | 0.47              |
| 1:A:277:ARG:CD   | 1:A:559:ALA:HB2  | 2.43                     | 0.47              |
| 1:B:845:ASN:HB3  | 1:B:848:PHE:CE1  | 2.49                     | 0.47              |
| 1:A:803:ASN:ND2  | 1:A:806:SER:H    | 2.13                     | 0.47              |
| 2:M:32:GLN:O     | 2:M:33:GLN:C     | 2.52                     | 0.47              |
| 1:B:854:LEU:O    | 1:B:856:ALA:N    | 2.47                     | 0.47              |
| 1:B:653:ASP:O    | 1:B:653:ASP:CG   | 2.52                     | 0.47              |
| 2:K:27:VAL:O     | 2:K:31:ILE:HG12  | 2.15                     | 0.47              |
| 2:E:5:TYR:HE2    | 2:E:130:ASP:O    | 1.98                     | 0.47              |
| 2:J:27:VAL:HG21  | 2:J:31:ILE:HD11  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:135:TYR:CZ   | 2:O:342:MET:HE3  | 2.50                     | 0.47              |
| 3:W:134:ILE:CG2  | 3:W:136:THR:HG22 | 2.45                     | 0.47              |
| 2:F:53:ASN:HD22  | 2:F:354:ALA:CB   | 2.26                     | 0.47              |
| 1:A:217:THR:O    | 1:A:218:GLU:HB2  | 2.13                     | 0.47              |
| 1:B:503:ILE:O    | 1:B:504:ASN:C    | 2.54                     | 0.47              |
| 1:B:519:PRO:O    | 1:B:520:THR:OG1  | 2.32                     | 0.47              |
| 1:B:383:ILE:HD11 | 1:B:550:LEU:HD23 | 1.97                     | 0.47              |
| 2:N:37:MET:O     | 2:N:38:ILE:C     | 2.53                     | 0.47              |
| 2:O:65:LEU:O     | 2:O:66:LEU:HD23  | 2.15                     | 0.47              |
| 1:A:122:LEU:CD1  | 1:A:201:ASP:HB2  | 2.45                     | 0.47              |
| 1:B:645:PHE:HD2  | 1:B:646:LEU:CD2  | 2.25                     | 0.47              |
| 2:G:32:GLN:O     | 2:G:33:GLN:C     | 2.53                     | 0.47              |
| 2:C:150:PHE:HA   | 2:D:397:LYS:NZ   | 2.30                     | 0.47              |
| 2:H:11:LEU:O     | 2:H:15:ARG:N     | 2.39                     | 0.47              |
| 1:A:461:GLN:CA   | 2:F:32:GLN:NE2   | 2.75                     | 0.47              |
| 1:B:112:LYS:N    | 1:B:113:PRO:CD   | 2.78                     | 0.47              |
| 1:B:752:LEU:C    | 1:B:754:ASN:N    | 2.63                     | 0.47              |
| 2:H:346:VAL:CG2  | 2:H:385:VAL:HG13 | 2.44                     | 0.47              |
| 1:A:356:GLU:HB3  | 1:A:357:ALA:H    | 1.30                     | 0.47              |
| 1:B:87:GLN:C     | 1:B:89:GLU:N     | 2.68                     | 0.47              |
| 2:K:109:ILE:HG13 | 2:K:110:ALA:N    | 2.29                     | 0.47              |
| 3:W:215:MET:CE   | 3:W:215:MET:HA   | 2.45                     | 0.47              |
| 1:B:354:GLN:HA   | 1:B:354:GLN:OE1  | 2.15                     | 0.47              |
| 1:B:479:GLN:O    | 1:B:480:PHE:HB3  | 2.16                     | 0.46              |
| 2:I:36:GLN:HE22  | 2:I:126:ARG:HD3  | 1.80                     | 0.46              |
| 2:I:42:ASN:OD1   | 2:I:62:ASP:N     | 2.48                     | 0.46              |
| 1:A:286:LEU:H    | 1:A:286:LEU:CD2  | 2.10                     | 0.46              |
| 2:N:124:PHE:O    | 2:N:126:ARG:N    | 2.49                     | 0.46              |
| 2:N:30:LEU:O     | 2:N:31:ILE:C     | 2.54                     | 0.46              |
| 2:L:27:VAL:CG2   | 2:L:31:ILE:HD11  | 2.45                     | 0.46              |
| 1:A:169:LEU:HA   | 1:A:169:LEU:HD12 | 1.62                     | 0.46              |
| 1:B:409:TRP:O    | 1:B:412:THR:HB   | 2.16                     | 0.46              |
| 3:W:300:LEU:N    | 3:W:300:LEU:HD12 | 2.30                     | 0.46              |
| 2:D:128:ASN:HD22 | 2:E:19:VAL:HG21  | 1.80                     | 0.46              |
| 3:W:827:VAL:HG13 | 3:W:940:TYR:CZ   | 2.50                     | 0.46              |
| 3:W:400:ALA:HB2  | 3:W:470:PHE:CE2  | 2.50                     | 0.46              |
| 1:A:180:TYR:CD1  | 1:A:181:LEU:N    | 2.83                     | 0.46              |
| 2:C:129:PHE:CE1  | 2:C:130:ASP:HB2  | 2.50                     | 0.46              |
| 2:E:41:MET:O     | 2:E:42:ASN:C     | 2.52                     | 0.46              |
| 3:W:402:ASN:N    | 3:W:420:LYS:HD2  | 2.30                     | 0.46              |
| 2:F:27:VAL:O     | 2:F:30:LEU:N     | 2.47                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:W:283:GLN:HG2  | 3:W:649:GLN:HG3  | 1.97                     | 0.46              |
| 3:W:924:ASP:C    | 3:W:944:ILE:HD13 | 2.35                     | 0.46              |
| 2:L:57:ARG:HB3   | 2:L:59:TRP:CZ2   | 2.49                     | 0.46              |
| 2:F:106:ARG:NH1  | 2:F:106:ARG:HB2  | 2.30                     | 0.46              |
| 1:A:419:PHE:CD1  | 1:A:419:PHE:N    | 2.82                     | 0.46              |
| 2:I:128:ASN:HB3  | 2:J:19:VAL:CG2   | 2.44                     | 0.46              |
| 2:M:14:ALA:O     | 2:M:18:ILE:HD12  | 2.16                     | 0.46              |
| 1:A:760:VAL:HG12 | 1:A:761:GLY:N    | 2.30                     | 0.46              |
| 1:A:746:GLN:O    | 1:A:750:MET:HG3  | 2.14                     | 0.46              |
| 2:I:144:ARG:O    | 2:I:145:ARG:CB   | 2.64                     | 0.46              |
| 2:E:54:LEU:HD12  | 2:E:55:PRO:CD    | 2.42                     | 0.46              |
| 2:D:150:PHE:N    | 2:D:150:PHE:CD1  | 2.83                     | 0.46              |
| 3:W:449:LEU:HD21 | 3:W:461:ILE:HD12 | 1.97                     | 0.46              |
| 1:B:75:VAL:HG12  | 1:B:75:VAL:O     | 2.16                     | 0.46              |
| 1:A:386:MET:HE3  | 1:A:414:VAL:HG13 | 1.96                     | 0.46              |
| 2:I:32:GLN:O     | 2:I:33:GLN:C     | 2.54                     | 0.46              |
| 1:A:499:ASN:CA   | 1:A:505:GLN:NE2  | 2.77                     | 0.46              |
| 1:A:854:LEU:CD2  | 1:A:855:LEU:N    | 2.78                     | 0.46              |
| 1:A:856:ALA:O    | 1:A:858:VAL:N    | 2.41                     | 0.46              |
| 1:B:369:GLY:C    | 1:B:371:ASN:N    | 2.69                     | 0.46              |
| 1:A:250:TYR:HB2  | 1:A:840:HIS:CD2  | 2.50                     | 0.46              |
| 2:E:73:LEU:HD22  | 2:E:77:TYR:CD2   | 2.50                     | 0.46              |
| 1:A:253:ASN:O    | 1:A:256:PHE:HB2  | 2.14                     | 0.46              |
| 1:B:420:ILE:O    | 1:B:422:GLU:N    | 2.48                     | 0.46              |
| 2:C:110:ALA:HB1  | 2:C:111:PRO:HD2  | 1.97                     | 0.46              |
| 2:L:153:HIS:O    | 2:L:154:LYS:C    | 2.54                     | 0.46              |
| 2:N:66:LEU:O     | 2:N:67:GLY:C     | 2.53                     | 0.46              |
| 1:B:282:VAL:O    | 1:B:284:TYR:N    | 2.48                     | 0.46              |
| 2:N:76:ASN:HB2   | 2:O:76:ASN:HB2   | 1.97                     | 0.46              |
| 3:W:109:TYR:HA   | 3:W:118:LEU:HD21 | 1.98                     | 0.46              |
| 2:C:62:ASP:H     | 2:C:63:PHE:HD1   | 1.62                     | 0.46              |
| 2:F:100:MET:HG3  | 2:F:388:VAL:HG11 | 1.97                     | 0.46              |
| 1:B:820:THR:HG22 | 1:B:820:THR:O    | 2.15                     | 0.46              |
| 1:B:818:VAL:HA   | 1:B:819:PRO:HD3  | 1.75                     | 0.46              |
| 1:B:500:GLY:HA3  | 1:B:871:PHE:HZ   | 1.80                     | 0.46              |
| 1:A:428:GLN:HG3  | 1:A:456:PHE:HA   | 1.97                     | 0.46              |
| 2:I:1:MET:C      | 2:I:3:VAL:N      | 2.67                     | 0.46              |
| 2:M:128:ASN:HB3  | 2:N:19:VAL:HG23  | 1.97                     | 0.46              |
| 1:A:722:ASN:HB3  | 1:A:824:LYS:HA   | 1.96                     | 0.46              |
| 1:A:363:GLU:HA   | 1:A:366:PHE:HE1  | 1.80                     | 0.46              |
| 3:W:295:MET:O    | 3:W:300:LEU:HB2  | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:W:1080:TYR:C   | 3:W:1082:ASN:H   | 2.19                     | 0.46              |
| 2:D:38:ILE:HG22  | 2:D:42:ASN:ND2   | 2.30                     | 0.46              |
| 2:H:27:VAL:HG21  | 2:H:31:ILE:HD11  | 1.96                     | 0.46              |
| 2:C:19:VAL:HG23  | 2:E:128:ASN:HB3  | 1.98                     | 0.46              |
| 2:F:115:SER:O    | 2:F:119:LEU:HG   | 2.14                     | 0.46              |
| 2:L:153:HIS:NE2  | 2:M:153:HIS:CD2  | 2.84                     | 0.46              |
| 2:H:150:PHE:N    | 2:H:150:PHE:CD1  | 2.84                     | 0.46              |
| 3:W:129:LEU:HB2  | 3:W:201:TYR:OH   | 2.15                     | 0.46              |
| 2:J:32:GLN:O     | 2:J:33:GLN:C     | 2.54                     | 0.46              |
| 2:K:63:PHE:N     | 2:K:63:PHE:CD1   | 2.82                     | 0.46              |
| 1:A:548:ARG:HB2  | 1:A:877:MET:HE2  | 1.98                     | 0.46              |
| 1:A:405:ILE:HG21 | 1:A:536:LEU:CG   | 2.43                     | 0.46              |
| 2:O:60:ASN:C     | 2:O:61:PHE:CD1   | 2.89                     | 0.46              |
| 1:A:775:ILE:C    | 1:A:777:LYS:H    | 2.19                     | 0.46              |
| 2:O:1:MET:O      | 2:O:2:ASP:C      | 2.53                     | 0.46              |
| 2:D:14:ALA:O     | 2:D:18:ILE:HD12  | 2.16                     | 0.46              |
| 2:K:54:LEU:HD12  | 2:K:55:PRO:CD    | 2.41                     | 0.46              |
| 2:N:150:PHE:N    | 2:N:150:PHE:CD1  | 2.84                     | 0.46              |
| 2:J:153:HIS:O    | 2:J:154:LYS:C    | 2.53                     | 0.46              |
| 1:B:298:TYR:C    | 1:B:298:TYR:CD1  | 2.88                     | 0.46              |
| 2:O:141:LEU:CD1  | 2:O:148:THR:HG21 | 2.46                     | 0.46              |
| 1:A:151:LYS:O    | 1:A:152:LYS:CB   | 2.63                     | 0.46              |
| 1:A:145:ARG:HB3  | 1:A:147:TYR:HE1  | 1.79                     | 0.46              |
| 3:W:801:GLU:O    | 3:W:804:ALA:HB3  | 2.15                     | 0.46              |
| 2:J:148:THR:OG1  | 2:J:332:GLU:HG2  | 2.15                     | 0.46              |
| 1:B:739:MET:C    | 1:B:741:THR:H    | 2.19                     | 0.46              |
| 3:W:922:GLU:OE1  | 3:W:926:SER:N    | 2.49                     | 0.46              |
| 1:A:639:LYS:HE3  | 1:A:659:ASP:OD1  | 2.15                     | 0.46              |
| 1:B:490:ASN:O    | 1:B:492:VAL:HG23 | 2.15                     | 0.46              |
| 2:I:61:PHE:N     | 2:I:61:PHE:CD1   | 2.83                     | 0.46              |
| 1:A:454:THR:HG22 | 1:A:457:GLN:H    | 1.80                     | 0.46              |
| 1:A:122:LEU:CG   | 1:A:201:ASP:HB2  | 2.46                     | 0.46              |
| 1:B:366:PHE:O    | 1:B:368:THR:N    | 2.48                     | 0.46              |
| 1:A:772:ILE:O    | 1:A:773:SER:C    | 2.54                     | 0.46              |
| 1:B:605:ASN:ND2  | 1:B:855:LEU:HD12 | 2.30                     | 0.46              |
| 1:A:197:GLY:O    | 1:A:198:LYS:O    | 2.34                     | 0.46              |
| 3:W:180:TYR:CE1  | 3:W:200:PRO:HD3  | 2.51                     | 0.46              |
| 2:O:139:TRP:NE1  | 2:O:143:ASN:ND2  | 2.63                     | 0.46              |
| 1:A:299:ILE:O    | 1:A:301:PRO:HD3  | 2.15                     | 0.46              |
| 1:A:329:ALA:HB3  | 1:A:384:ALA:CB   | 2.46                     | 0.46              |
| 1:B:413:VAL:CG1  | 1:B:414:VAL:H    | 2.26                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:22:THR:CG2   | 2:F:73:LEU:HD12  | 2.45                     | 0.46              |
| 1:B:608:VAL:O    | 1:B:609:ASN:C    | 2.54                     | 0.46              |
| 1:B:857:PHE:CD1  | 1:B:857:PHE:N    | 2.72                     | 0.46              |
| 2:D:61:PHE:N     | 2:D:61:PHE:CD1   | 2.84                     | 0.46              |
| 3:W:426:ASP:O    | 3:W:430:ASN:HB2  | 2.15                     | 0.46              |
| 3:W:101:ASP:O    | 3:W:103:THR:N    | 2.48                     | 0.46              |
| 1:A:314:PHE:CZ   | 1:A:664:ARG:HG2  | 2.51                     | 0.46              |
| 1:A:601:PHE:O    | 1:A:602:HIS:C    | 2.54                     | 0.46              |
| 2:F:346:VAL:CG2  | 2:F:385:VAL:HG13 | 2.44                     | 0.46              |
| 3:W:865:VAL:HG22 | 3:W:865:VAL:O    | 2.16                     | 0.46              |
| 2:D:123:LYS:HG3  | 2:D:124:PHE:CE1  | 2.50                     | 0.46              |
| 1:A:620:ASP:O    | 1:A:624:ILE:HG13 | 2.15                     | 0.46              |
| 2:L:49:GLY:HA2   | 2:L:54:LEU:HD23  | 1.98                     | 0.46              |
| 3:W:760:ASN:ND2  | 3:W:760:ASN:C    | 2.67                     | 0.46              |
| 2:K:129:PHE:C    | 2:K:129:PHE:CD1  | 2.89                     | 0.46              |
| 1:B:770:SER:O    | 1:B:773:SER:HB2  | 2.15                     | 0.46              |
| 1:A:660:ASP:HB3  | 1:B:539:ARG:NH1  | 2.20                     | 0.46              |
| 1:B:478:ASN:O    | 1:B:480:PHE:N    | 2.45                     | 0.46              |
| 1:A:404:LEU:HB3  | 1:A:435:ILE:HD11 | 1.98                     | 0.46              |
| 1:A:506:LEU:HD23 | 1:A:544:VAL:CA   | 2.29                     | 0.46              |
| 2:N:61:PHE:CD1   | 2:N:61:PHE:N     | 2.84                     | 0.46              |
| 1:B:373:GLN:O    | 1:B:376:ASN:N    | 2.49                     | 0.46              |
| 3:W:465:LEU:HB3  | 3:W:469:TYR:CD2  | 2.50                     | 0.46              |
| 2:G:41:MET:O     | 2:G:42:ASN:C     | 2.54                     | 0.46              |
| 2:F:22:THR:HG23  | 2:F:73:LEU:HD12  | 1.98                     | 0.46              |
| 1:B:601:PHE:HB3  | 1:B:855:LEU:HD13 | 1.98                     | 0.46              |
| 1:B:854:LEU:O    | 1:B:855:LEU:C    | 2.54                     | 0.46              |
| 2:C:41:MET:O     | 2:C:42:ASN:C     | 2.53                     | 0.46              |
| 3:W:535:ARG:HH11 | 3:W:565:GLN:HE22 | 1.63                     | 0.46              |
| 2:L:153:HIS:CD2  | 2:N:153:HIS:NE2  | 2.83                     | 0.46              |
| 2:M:346:VAL:CG2  | 2:M:385:VAL:HG13 | 2.45                     | 0.46              |
| 2:C:346:VAL:CG2  | 2:C:385:VAL:HG13 | 2.44                     | 0.46              |
| 3:W:112:ASN:OD1  | 3:W:202:TYR:HB2  | 2.16                     | 0.46              |
| 1:A:706:ALA:C    | 1:A:708:ARG:H    | 2.19                     | 0.46              |
| 1:A:708:ARG:HD2  | 1:A:708:ARG:HA   | 1.80                     | 0.46              |
| 3:W:310:TRP:CZ2  | 3:W:319:PHE:HD1  | 2.34                     | 0.46              |
| 1:B:727:LEU:HG   | 1:B:727:LEU:O    | 2.15                     | 0.46              |
| 1:B:345:GLN:HG3  | 1:B:349:MET:CE   | 2.46                     | 0.46              |
| 1:B:510:LEU:HD13 | 1:B:540:LEU:HB2  | 1.98                     | 0.46              |
| 1:B:383:ILE:HD11 | 1:B:550:LEU:HD22 | 1.97                     | 0.46              |
| 2:O:37:MET:O     | 2:O:38:ILE:C     | 2.54                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:783:PHE:O    | 1:B:784:ALA:C    | 2.54                     | 0.46              |
| 1:A:779:ASP:OD2  | 1:A:822:THR:O    | 2.34                     | 0.46              |
| 1:B:239:VAL:CG2  | 1:B:845:ASN:O    | 2.63                     | 0.46              |
| 1:B:848:PHE:O    | 1:B:849:THR:OG1  | 2.28                     | 0.46              |
| 3:W:438:ILE:HD11 | 3:W:563:GLN:CB   | 2.45                     | 0.46              |
| 1:A:846:LEU:HA   | 1:A:846:LEU:HD23 | 1.65                     | 0.46              |
| 1:A:461:GLN:CB   | 2:F:32:GLN:NE2   | 2.79                     | 0.46              |
| 1:B:118:LYS:CG   | 1:B:119:GLN:N    | 2.73                     | 0.46              |
| 2:L:104:SER:HB3  | 2:L:108:GLY:CA   | 2.46                     | 0.46              |
| 1:A:867:ASN:O    | 1:A:867:ASN:CG   | 2.54                     | 0.46              |
| 2:J:27:VAL:CG2   | 2:J:31:ILE:HD11  | 2.45                     | 0.46              |
| 1:B:314:PHE:HZ   | 1:B:664:ARG:HG2  | 1.78                     | 0.46              |
| 2:O:22:THR:CG2   | 2:O:73:LEU:HD12  | 2.46                     | 0.46              |
| 2:J:142:GLN:HE21 | 2:J:143:ASN:N    | 2.13                     | 0.46              |
| 3:W:160:LEU:O    | 3:W:163:TYR:HB3  | 2.16                     | 0.46              |
| 2:I:155:PRO:O    | 2:I:186:SER:HB3  | 2.16                     | 0.46              |
| 2:I:382:LEU:HD22 | 2:I:386:PHE:CE2  | 2.51                     | 0.46              |
| 1:A:428:GLN:OE1  | 1:A:456:PHE:CB   | 2.38                     | 0.46              |
| 1:A:509:ALA:O    | 1:A:513:LEU:CG   | 2.55                     | 0.46              |
| 1:A:821:SER:OG   | 1:A:822:THR:N    | 2.46                     | 0.46              |
| 1:B:340:VAL:O    | 1:B:341:SER:C    | 2.54                     | 0.46              |
| 2:H:106:ARG:O    | 2:H:107:ASN:CB   | 2.62                     | 0.46              |
| 1:A:245:LEU:O    | 1:A:246:HIS:HB2  | 2.16                     | 0.46              |
| 1:B:94:THR:O     | 1:B:94:THR:HG22  | 2.16                     | 0.46              |
| 2:D:30:LEU:O     | 2:D:31:ILE:C     | 2.53                     | 0.46              |
| 2:I:135:TYR:CE1  | 2:I:342:MET:HE3  | 2.51                     | 0.46              |
| 3:W:105:ASN:HD22 | 3:W:111:ASN:HA   | 1.76                     | 0.46              |
| 2:H:239:ASN:ND2  | 2:H:246:THR:HG22 | 2.30                     | 0.46              |
| 2:F:239:ASN:ND2  | 2:F:246:THR:HG22 | 2.29                     | 0.46              |
| 2:K:346:VAL:CG2  | 2:K:385:VAL:HG13 | 2.44                     | 0.46              |
| 3:W:467:TYR:C    | 3:W:467:TYR:CD1  | 2.89                     | 0.46              |
| 1:B:613:ASN:O    | 1:B:617:ARG:HG2  | 2.16                     | 0.46              |
| 3:W:598:ALA:O    | 3:W:602:ILE:HG13 | 2.16                     | 0.46              |
| 3:W:290:GLN:HB2  | 3:W:290:GLN:HE21 | 1.54                     | 0.46              |
| 2:N:1:MET:C      | 2:N:3:VAL:N      | 2.69                     | 0.45              |
| 2:N:1:MET:O      | 2:N:2:ASP:C      | 2.55                     | 0.45              |
| 1:B:637:LYS:HA   | 1:B:641:ILE:HD11 | 1.97                     | 0.45              |
| 1:B:170:TYR:CZ   | 1:B:682:PHE:HB2  | 2.52                     | 0.45              |
| 1:B:675:GLU:O    | 1:B:677:ARG:N    | 2.49                     | 0.45              |
| 2:G:5:TYR:HE2    | 2:G:131:ASN:HA   | 1.80                     | 0.45              |
| 2:J:37:MET:O     | 2:J:38:ILE:C     | 2.54                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:137:ASN:CG   | 1:B:137:ASN:O    | 2.55                     | 0.45              |
| 2:H:62:ASP:H     | 2:H:63:PHE:HD1   | 1.63                     | 0.45              |
| 3:W:396:SER:OG   | 3:W:474:HIS:NE2  | 2.49                     | 0.45              |
| 2:J:382:LEU:HD22 | 2:J:386:PHE:CE2  | 2.52                     | 0.45              |
| 2:K:382:LEU:HD22 | 2:K:386:PHE:CE2  | 2.51                     | 0.45              |
| 1:A:549:LEU:HA   | 1:A:549:LEU:HD12 | 1.65                     | 0.45              |
| 1:B:772:ILE:HG22 | 1:B:809:PHE:CE2  | 2.51                     | 0.45              |
| 1:A:416:ASN:C    | 1:A:418:MET:N    | 2.70                     | 0.45              |
| 2:I:30:LEU:O     | 2:I:31:ILE:C     | 2.52                     | 0.45              |
| 2:I:36:GLN:HB2   | 2:J:23:LEU:HD11  | 1.97                     | 0.45              |
| 2:I:1:MET:O      | 2:I:2:ASP:C      | 2.54                     | 0.45              |
| 1:B:508:GLU:OE2  | 2:J:70:LEU:CD2   | 2.65                     | 0.45              |
| 2:L:73:LEU:HD22  | 2:L:77:TYR:HD2   | 1.77                     | 0.45              |
| 1:B:583:SER:OG   | 1:B:584:LEU:N    | 2.48                     | 0.45              |
| 2:H:21:GLY:O     | 2:H:22:THR:O     | 2.34                     | 0.45              |
| 3:W:186:ASN:O    | 3:W:189:TYR:N    | 2.48                     | 0.45              |
| 2:F:17:LYS:HE2   | 2:H:130:ASP:OD2  | 2.16                     | 0.45              |
| 2:I:136:ILE:HG23 | 2:I:137:GLU:N    | 2.31                     | 0.45              |
| 2:L:115:SER:O    | 2:L:119:LEU:HG   | 2.15                     | 0.45              |
| 3:W:690:ARG:O    | 3:W:723:ARG:NH1  | 2.49                     | 0.45              |
| 3:W:872:ILE:HG13 | 3:W:1072:ASN:O   | 2.17                     | 0.45              |
| 2:I:89:VAL:C     | 2:I:91:PHE:H     | 2.19                     | 0.45              |
| 1:B:282:VAL:HG13 | 1:B:283:ASN:N    | 2.31                     | 0.45              |
| 2:C:135:TYR:CZ   | 2:C:342:MET:HE3  | 2.52                     | 0.45              |
| 3:W:422:MET:HA   | 3:W:425:MET:HG3  | 1.99                     | 0.45              |
| 3:W:302:ASP:O    | 3:W:306:MET:HG3  | 2.17                     | 0.45              |
| 2:M:382:LEU:HD22 | 2:M:386:PHE:CE2  | 2.52                     | 0.45              |
| 2:G:109:ILE:O    | 2:G:109:ILE:HD12 | 2.17                     | 0.45              |
| 1:B:542:GLN:OE1  | 1:B:542:GLN:N    | 2.49                     | 0.45              |
| 1:B:872:ASP:CG   | 1:B:874:MET:H    | 2.20                     | 0.45              |
| 1:B:498:ARG:CZ   | 2:J:25:SER:HB3   | 2.47                     | 0.45              |
| 1:A:353:LEU:HD22 | 1:A:531:ARG:HB3  | 1.98                     | 0.45              |
| 1:A:526:LYS:HG3  | 1:A:527:ARG:N    | 2.31                     | 0.45              |
| 2:L:22:THR:CG2   | 2:L:73:LEU:HD12  | 2.24                     | 0.45              |
| 2:N:24:TYR:CE1   | 2:N:31:ILE:HG13  | 2.51                     | 0.45              |
| 1:B:633:LEU:O    | 1:B:635:GLN:N    | 2.48                     | 0.45              |
| 1:A:688:ASN:O    | 1:A:691:GLN:N    | 2.49                     | 0.45              |
| 2:F:32:GLN:O     | 2:F:33:GLN:C     | 2.54                     | 0.45              |
| 3:W:819:LEU:C    | 3:W:820:LEU:HD23 | 2.37                     | 0.45              |
| 1:A:608:VAL:O    | 1:A:609:ASN:C    | 2.55                     | 0.45              |
| 2:K:24:TYR:O     | 2:K:27:VAL:HG22  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:239:ASN:ND2  | 2:L:246:THR:HG22 | 2.29                     | 0.45              |
| 1:B:594:ILE:HD12 | 1:B:594:ILE:O    | 2.17                     | 0.45              |
| 3:W:125:TYR:HE1  | 3:W:201:TYR:HE1  | 1.63                     | 0.45              |
| 2:M:53:ASN:HD22  | 2:M:354:ALA:HB3  | 1.81                     | 0.45              |
| 1:A:706:ALA:O    | 1:A:708:ARG:N    | 2.45                     | 0.45              |
| 2:E:190:VAL:HG21 | 2:E:210:HIS:HB2  | 1.99                     | 0.45              |
| 2:C:124:PHE:O    | 2:C:127:ILE:HG13 | 2.16                     | 0.45              |
| 3:W:64:ASP:OD2   | 3:W:65:VAL:N     | 2.48                     | 0.45              |
| 2:J:78:VAL:O     | 2:J:81:ALA:N     | 2.40                     | 0.45              |
| 2:H:382:LEU:HD22 | 2:H:386:PHE:CE2  | 2.51                     | 0.45              |
| 2:C:59:TRP:N     | 2:C:59:TRP:CD1   | 2.83                     | 0.45              |
| 1:B:159:ASP:O    | 1:B:162:VAL:HB   | 2.16                     | 0.45              |
| 1:A:466:PHE:O    | 1:A:467:GLN:C    | 2.54                     | 0.45              |
| 1:A:518:PHE:CB   | 1:A:519:PRO:CD   | 2.94                     | 0.45              |
| 1:A:266:ASN:C    | 1:A:292:LEU:HD12 | 2.36                     | 0.45              |
| 3:W:479:LYS:HD3  | 3:W:479:LYS:HA   | 1.85                     | 0.45              |
| 1:A:688:ASN:O    | 1:A:690:ASP:N    | 2.50                     | 0.45              |
| 1:B:119:GLN:CG   | 1:B:181:LEU:HD11 | 2.46                     | 0.45              |
| 2:D:1:MET:C      | 2:D:3:VAL:N      | 2.70                     | 0.45              |
| 2:J:1:MET:C      | 2:J:3:VAL:N      | 2.68                     | 0.45              |
| 2:M:144:ARG:O    | 2:M:145:ARG:HB2  | 2.17                     | 0.45              |
| 3:W:705:THR:O    | 3:W:709:GLN:HB2  | 2.16                     | 0.45              |
| 2:D:37:MET:O     | 2:D:38:ILE:C     | 2.55                     | 0.45              |
| 2:C:37:MET:O     | 2:C:38:ILE:C     | 2.55                     | 0.45              |
| 1:B:420:ILE:O    | 1:B:421:ARG:C    | 2.54                     | 0.45              |
| 2:L:89:VAL:C     | 2:L:91:PHE:H     | 2.20                     | 0.45              |
| 3:W:180:TYR:CD1  | 3:W:200:PRO:HD3  | 2.51                     | 0.45              |
| 1:B:589:GLY:C    | 1:B:591:ALA:H    | 2.20                     | 0.45              |
| 1:B:434:THR:O    | 1:B:435:ILE:CG1  | 2.65                     | 0.45              |
| 1:A:857:PHE:CD1  | 1:A:857:PHE:N    | 2.83                     | 0.45              |
| 3:W:247:PRO:O    | 3:W:251:LEU:HG   | 2.17                     | 0.45              |
| 1:B:854:LEU:HD22 | 1:B:855:LEU:H    | 1.82                     | 0.45              |
| 3:W:161:LYS:HB3  | 3:W:165:ARG:NH1  | 2.28                     | 0.45              |
| 2:N:110:ALA:HB1  | 2:N:111:PRO:HD2  | 1.99                     | 0.45              |
| 2:D:382:LEU:HD22 | 2:D:386:PHE:CE2  | 2.52                     | 0.45              |
| 3:W:944:ILE:HG23 | 3:W:945:GLU:N    | 2.30                     | 0.45              |
| 1:B:205:ALA:O    | 1:B:206:SER:C    | 2.55                     | 0.45              |
| 2:C:382:LEU:HD22 | 2:C:386:PHE:CE2  | 2.51                     | 0.45              |
| 2:D:190:VAL:HG21 | 2:D:210:HIS:HB2  | 1.99                     | 0.45              |
| 2:I:225:LEU:HD13 | 2:I:277:PHE:HD2  | 1.82                     | 0.45              |
| 2:M:130:ASP:HA   | 2:N:17:LYS:HG2   | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:482:GLN:OE1  | 1:A:493:LEU:CD2  | 2.64                     | 0.45              |
| 1:A:712:LEU:CG   | 1:A:819:PRO:HB2  | 2.40                     | 0.45              |
| 1:A:822:THR:O    | 1:A:823:THR:CB   | 2.64                     | 0.45              |
| 1:B:646:LEU:N    | 1:B:646:LEU:HD23 | 2.32                     | 0.45              |
| 1:A:367:LEU:CD2  | 3:W:932:ARG:HB2  | 2.46                     | 0.45              |
| 2:H:107:ASN:ND2  | 2:H:109:ILE:HG23 | 2.32                     | 0.45              |
| 1:A:246:HIS:O    | 1:A:247:PRO:C    | 2.54                     | 0.45              |
| 3:W:4:TYR:CD1    | 3:W:733:LEU:HD22 | 2.33                     | 0.45              |
| 1:B:852:SER:O    | 1:B:853:ASP:HB3  | 2.16                     | 0.45              |
| 2:D:24:TYR:O     | 2:D:26:ASN:N     | 2.50                     | 0.45              |
| 3:W:477:VAL:HA   | 3:W:480:MET:HE2  | 1.99                     | 0.45              |
| 2:C:128:ASN:O    | 2:D:22:THR:HB    | 2.17                     | 0.45              |
| 2:H:32:GLN:O     | 2:H:33:GLN:C     | 2.54                     | 0.45              |
| 1:A:804:SER:HB2  | 1:A:810:TYR:CA   | 2.47                     | 0.45              |
| 3:W:410:PHE:CE2  | 3:W:415:ILE:HD11 | 2.52                     | 0.45              |
| 3:W:501:LEU:HD12 | 3:W:501:LEU:O    | 2.17                     | 0.45              |
| 2:H:190:VAL:HG21 | 2:H:210:HIS:HB2  | 1.99                     | 0.45              |
| 2:M:155:PRO:HA   | 2:M:337:ASP:HB2  | 1.99                     | 0.45              |
| 2:C:190:VAL:HG21 | 2:C:210:HIS:HB2  | 1.99                     | 0.45              |
| 2:D:78:VAL:O     | 2:D:81:ALA:HB3   | 2.17                     | 0.45              |
| 3:W:874:ILE:CG2  | 3:W:875:ASN:N    | 2.80                     | 0.45              |
| 2:E:312:GLN:HB3  | 2:E:313:PRO:HA   | 1.99                     | 0.45              |
| 2:L:190:VAL:HG21 | 2:L:210:HIS:HB2  | 1.99                     | 0.45              |
| 1:B:772:ILE:O    | 1:B:773:SER:C    | 2.54                     | 0.45              |
| 1:A:319:ASP:OD2  | 1:A:571:LEU:N    | 2.49                     | 0.45              |
| 1:A:546:LEU:HD13 | 1:A:584:LEU:HD23 | 1.97                     | 0.45              |
| 1:B:554:TYR:O    | 1:B:558:MET:HB2  | 2.17                     | 0.45              |
| 2:N:23:LEU:HD22  | 2:N:25:SER:OG    | 2.17                     | 0.45              |
| 1:B:577:GLN:O    | 1:B:579:THR:N    | 2.50                     | 0.45              |
| 2:H:105:GLN:O    | 2:H:107:ASN:N    | 2.50                     | 0.45              |
| 1:B:742:GLY:O    | 1:B:744:TYR:HE2  | 1.98                     | 0.45              |
| 3:W:448:PRO:HB2  | 3:W:464:ILE:HB   | 1.99                     | 0.45              |
| 1:B:601:PHE:CD1  | 1:B:601:PHE:N    | 2.80                     | 0.45              |
| 1:B:419:PHE:O    | 1:B:420:ILE:C    | 2.54                     | 0.45              |
| 2:E:11:LEU:O     | 2:E:15:ARG:N     | 2.41                     | 0.45              |
| 2:D:54:LEU:HD12  | 2:D:55:PRO:CD    | 2.46                     | 0.45              |
| 2:G:150:PHE:HB2  | 2:G:152:PHE:CZ   | 2.51                     | 0.45              |
| 2:M:110:ALA:HB1  | 2:M:111:PRO:HD2  | 1.99                     | 0.45              |
| 2:H:312:GLN:HB3  | 2:H:313:PRO:HA   | 1.99                     | 0.45              |
| 1:B:85:GLU:O     | 1:B:86:ILE:C     | 2.54                     | 0.45              |
| 1:A:155:LEU:HA   | 1:A:156:PRO:HD3  | 1.55                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:60:ASN:C     | 2:J:61:PHE:CD1   | 2.90                     | 0.45              |
| 2:E:382:LEU:HD22 | 2:E:386:PHE:CE2  | 2.51                     | 0.45              |
| 2:L:382:LEU:HD22 | 2:L:386:PHE:CE2  | 2.52                     | 0.45              |
| 2:F:190:VAL:HG21 | 2:F:210:HIS:HB2  | 1.99                     | 0.45              |
| 1:A:339:LEU:O    | 1:A:340:VAL:C    | 2.55                     | 0.45              |
| 1:A:580:SER:O    | 1:A:581:VAL:C    | 2.55                     | 0.45              |
| 2:I:42:ASN:OD1   | 2:I:61:PHE:HB3   | 2.16                     | 0.45              |
| 1:A:454:THR:O    | 1:A:457:GLN:HB3  | 2.17                     | 0.45              |
| 1:A:503:ILE:O    | 1:A:505:GLN:N    | 2.50                     | 0.45              |
| 1:A:506:LEU:CD2  | 1:A:544:VAL:CA   | 2.94                     | 0.45              |
| 1:A:452:PRO:O    | 1:A:453:GLN:OE1  | 2.35                     | 0.45              |
| 2:I:145:ARG:O    | 2:I:146:GLN:CG   | 2.65                     | 0.45              |
| 1:B:601:PHE:O    | 1:B:602:HIS:C    | 2.53                     | 0.45              |
| 1:A:252:PHE:CD2  | 1:A:684:LEU:CD2  | 3.00                     | 0.45              |
| 3:W:538:ILE:HD12 | 3:W:565:GLN:NE2  | 2.31                     | 0.45              |
| 2:J:41:MET:O     | 2:J:42:ASN:C     | 2.54                     | 0.45              |
| 2:E:37:MET:O     | 2:E:38:ILE:C     | 2.54                     | 0.45              |
| 3:W:840:ASN:OD1  | 3:W:846:SER:HA   | 2.16                     | 0.45              |
| 1:B:400:ASN:O    | 1:B:404:LEU:CD1  | 2.65                     | 0.45              |
| 2:D:225:LEU:HD13 | 2:D:277:PHE:HD2  | 1.82                     | 0.45              |
| 3:W:695:LEU:HD21 | 3:W:732:ILE:CD1  | 2.47                     | 0.45              |
| 2:O:217:VAL:HG22 | 2:O:286:ASP:HB3  | 1.99                     | 0.45              |
| 2:G:382:LEU:HD22 | 2:G:386:PHE:CE2  | 2.51                     | 0.45              |
| 2:J:225:LEU:HD13 | 2:J:277:PHE:HD2  | 1.82                     | 0.45              |
| 2:F:312:GLN:HB3  | 2:F:313:PRO:HA   | 1.99                     | 0.45              |
| 2:H:48:THR:O     | 2:H:56:ILE:HA    | 2.17                     | 0.45              |
| 2:E:154:LYS:N    | 2:E:327:GLU:O    | 2.42                     | 0.45              |
| 2:M:225:LEU:HD13 | 2:M:277:PHE:HD2  | 1.82                     | 0.45              |
| 1:B:771:VAL:HG21 | 1:B:809:PHE:O    | 2.17                     | 0.45              |
| 1:A:583:SER:OG   | 1:A:584:LEU:N    | 2.50                     | 0.45              |
| 1:B:277:ARG:HH11 | 1:B:277:ARG:HB3  | 1.80                     | 0.45              |
| 1:B:496:ASN:HB3  | 1:B:499:ASN:H    | 1.82                     | 0.45              |
| 2:J:70:LEU:HD22  | 2:J:72:ASN:O     | 2.16                     | 0.45              |
| 1:A:762:ALA:C    | 1:A:763:LEU:HG   | 2.37                     | 0.45              |
| 1:B:786:ILE:HG22 | 1:B:792:VAL:HG12 | 1.98                     | 0.45              |
| 1:A:783:PHE:N    | 1:A:783:PHE:CD1  | 2.72                     | 0.45              |
| 1:A:186:MET:HG3  | 1:A:200:VAL:HG13 | 1.98                     | 0.45              |
| 1:B:573:THR:CG2  | 1:B:574:GLU:N    | 2.45                     | 0.45              |
| 2:O:131:ASN:N    | 2:O:131:ASN:HD22 | 2.14                     | 0.45              |
| 1:B:119:GLN:NE2  | 1:B:181:LEU:HD11 | 2.32                     | 0.45              |
| 2:H:30:LEU:O     | 2:H:31:ILE:C     | 2.53                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:89:VAL:C     | 2:J:91:PHE:H     | 2.21                     | 0.45              |
| 2:C:136:ILE:HG23 | 2:C:137:GLU:N    | 2.32                     | 0.45              |
| 2:N:89:VAL:C     | 2:N:91:PHE:H     | 2.21                     | 0.45              |
| 2:O:273:TYR:C    | 2:O:274:GLN:HE21 | 2.21                     | 0.45              |
| 2:I:273:TYR:C    | 2:I:274:GLN:HE21 | 2.20                     | 0.45              |
| 3:W:301:VAL:O    | 3:W:304:PRO:HD2  | 2.17                     | 0.45              |
| 2:C:127:ILE:O    | 2:C:127:ILE:HG22 | 2.15                     | 0.45              |
| 2:I:217:VAL:HG22 | 2:I:286:ASP:HB3  | 1.99                     | 0.45              |
| 2:O:190:VAL:HG21 | 2:O:210:HIS:HB2  | 1.99                     | 0.45              |
| 2:O:225:LEU:HD13 | 2:O:277:PHE:HD2  | 1.82                     | 0.45              |
| 2:F:382:LEU:HD22 | 2:F:386:PHE:CE2  | 2.52                     | 0.45              |
| 2:E:225:LEU:HD13 | 2:E:277:PHE:HD2  | 1.82                     | 0.45              |
| 2:M:312:GLN:HB3  | 2:M:313:PRO:HA   | 1.99                     | 0.45              |
| 2:F:225:LEU:HD13 | 2:F:277:PHE:HD2  | 1.82                     | 0.45              |
| 1:B:772:ILE:CG2  | 1:B:809:PHE:HE2  | 2.29                     | 0.45              |
| 1:A:269:ILE:HG21 | 1:A:298:TYR:CE2  | 2.51                     | 0.45              |
| 1:A:428:GLN:HG2  | 1:A:429:LEU:H    | 1.79                     | 0.45              |
| 1:B:467:GLN:HE21 | 1:B:511:MET:HG2  | 1.82                     | 0.45              |
| 1:B:846:LEU:HD12 | 1:B:847:THR:N    | 2.32                     | 0.45              |
| 2:M:42:ASN:HA    | 2:M:61:PHE:CB    | 2.46                     | 0.45              |
| 2:C:32:GLN:O     | 2:C:33:GLN:C     | 2.54                     | 0.45              |
| 1:A:224:PHE:O    | 1:A:225:ILE:C    | 2.55                     | 0.45              |
| 1:B:596:SER:O    | 1:B:597:PRO:C    | 2.55                     | 0.45              |
| 2:N:135:TYR:CZ   | 2:N:342:MET:HE3  | 2.53                     | 0.45              |
| 2:H:126:ARG:C    | 2:H:127:ILE:HG13 | 2.37                     | 0.45              |
| 2:G:190:VAL:HG21 | 2:G:210:HIS:HB2  | 1.99                     | 0.45              |
| 2:K:190:VAL:HG21 | 2:K:210:HIS:HB2  | 1.99                     | 0.45              |
| 2:C:217:VAL:HG22 | 2:C:286:ASP:HB3  | 1.99                     | 0.45              |
| 2:J:217:VAL:HG22 | 2:J:286:ASP:HB3  | 1.99                     | 0.45              |
| 2:J:312:GLN:HB3  | 2:J:313:PRO:HA   | 1.99                     | 0.45              |
| 2:N:382:LEU:HD22 | 2:N:386:PHE:CE2  | 2.52                     | 0.45              |
| 1:A:866:ILE:HG22 | 1:A:866:ILE:O    | 2.17                     | 0.45              |
| 1:A:587:LEU:O    | 1:A:587:LEU:HD22 | 2.17                     | 0.44              |
| 1:B:428:GLN:CB   | 1:B:456:PHE:CD1  | 2.90                     | 0.44              |
| 2:L:60:ASN:C     | 2:L:61:PHE:CD1   | 2.91                     | 0.44              |
| 1:B:763:LEU:HD22 | 1:B:764:PRO:HD3  | 1.99                     | 0.44              |
| 1:A:118:LYS:CG   | 1:A:119:GLN:H    | 2.29                     | 0.44              |
| 1:A:680:ASP:HA   | 1:A:683:ASN:HD22 | 1.81                     | 0.44              |
| 1:A:117:LYS:HB2  | 1:A:179:ASP:CG   | 2.37                     | 0.44              |
| 1:A:420:ILE:HD11 | 1:A:423:SER:HB2  | 1.99                     | 0.44              |
| 2:K:37:MET:O     | 2:K:38:ILE:C     | 2.55                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:1:MET:C      | 2:C:3:VAL:N      | 2.70                     | 0.44              |
| 3:W:105:ASN:HB2  | 3:W:111:ASN:OD1  | 2.18                     | 0.44              |
| 2:J:153:HIS:NE2  | 2:K:153:HIS:CD2  | 2.84                     | 0.44              |
| 2:D:136:ILE:HG23 | 2:D:137:GLU:N    | 2.32                     | 0.44              |
| 2:G:273:TYR:C    | 2:G:274:GLN:HE21 | 2.20                     | 0.44              |
| 2:G:312:GLN:HB3  | 2:G:313:PRO:HA   | 1.99                     | 0.44              |
| 2:I:190:VAL:HG21 | 2:I:210:HIS:HB2  | 1.99                     | 0.44              |
| 2:G:78:VAL:O     | 2:G:81:ALA:HB3   | 2.18                     | 0.44              |
| 2:E:44:ASN:HB3   | 2:E:46:PHE:HE1   | 1.81                     | 0.44              |
| 2:L:225:LEU:HD13 | 2:L:277:PHE:HD2  | 1.82                     | 0.44              |
| 2:D:217:VAL:HG22 | 2:D:286:ASP:HB3  | 1.99                     | 0.44              |
| 3:W:580:VAL:HG12 | 3:W:581:ILE:N    | 2.32                     | 0.44              |
| 2:K:225:LEU:HD13 | 2:K:277:PHE:HD2  | 1.82                     | 0.44              |
| 2:L:312:GLN:HB3  | 2:L:313:PRO:HA   | 1.99                     | 0.44              |
| 1:A:348:LYS:O    | 1:A:351:GLN:HB2  | 2.17                     | 0.44              |
| 2:I:140:ASN:O    | 2:I:143:ASN:N    | 2.50                     | 0.44              |
| 1:B:463:ILE:HD12 | 1:B:472:LEU:CD1  | 2.47                     | 0.44              |
| 1:A:270:ILE:HD11 | 1:A:292:LEU:CD1  | 2.23                     | 0.44              |
| 1:A:286:LEU:O    | 1:A:287:ASN:CB   | 2.65                     | 0.44              |
| 1:B:226:ALA:O    | 1:B:228:MET:N    | 2.50                     | 0.44              |
| 1:B:248:ILE:O    | 1:B:251:ALA:HB3  | 2.17                     | 0.44              |
| 1:B:374:ALA:O    | 1:B:580:SER:HB2  | 2.17                     | 0.44              |
| 2:O:1:MET:C      | 2:O:3:VAL:N      | 2.68                     | 0.44              |
| 2:J:1:MET:O      | 2:J:2:ASP:C      | 2.54                     | 0.44              |
| 1:B:420:ILE:O    | 1:B:420:ILE:HG23 | 2.18                     | 0.44              |
| 2:C:22:THR:HG23  | 2:C:73:LEU:CD1   | 2.46                     | 0.44              |
| 3:W:437:ILE:O    | 3:W:439:PRO:HD3  | 2.17                     | 0.44              |
| 2:M:239:ASN:ND2  | 2:M:246:THR:HG22 | 2.30                     | 0.44              |
| 1:A:101:LYS:C    | 1:A:103:SER:H    | 2.20                     | 0.44              |
| 2:C:54:LEU:HD12  | 2:C:55:PRO:CD    | 2.44                     | 0.44              |
| 1:A:296:ALA:C    | 1:A:297:ARG:HG2  | 2.38                     | 0.44              |
| 2:F:273:TYR:C    | 2:F:274:GLN:HE21 | 2.21                     | 0.44              |
| 1:B:148:TRP:HE1  | 1:B:833:PHE:HD1  | 1.64                     | 0.44              |
| 2:F:78:VAL:O     | 2:F:81:ALA:N     | 2.43                     | 0.44              |
| 2:N:225:LEU:HD13 | 2:N:277:PHE:HD2  | 1.82                     | 0.44              |
| 2:O:382:LEU:HD22 | 2:O:386:PHE:CE2  | 2.51                     | 0.44              |
| 1:A:556:THR:O    | 1:A:558:MET:N    | 2.51                     | 0.44              |
| 1:A:660:ASP:OD1  | 1:A:661:GLN:N    | 2.50                     | 0.44              |
| 1:B:447:TYR:C    | 1:B:448:ARG:HG2  | 2.38                     | 0.44              |
| 1:B:368:THR:HG22 | 1:B:371:ASN:ND2  | 2.26                     | 0.44              |
| 1:B:674:VAL:O    | 1:B:675:GLU:C    | 2.54                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:183:LEU:HD12 | 1:B:844:SER:CB   | 2.47                     | 0.44              |
| 1:A:229:ARG:O    | 1:A:242:PRO:HG3  | 2.18                     | 0.44              |
| 2:C:27:VAL:O     | 2:C:30:LEU:HB3   | 2.17                     | 0.44              |
| 1:A:674:VAL:HB   | 1:A:679:LEU:HB2  | 1.99                     | 0.44              |
| 2:F:153:HIS:CD2  | 2:H:153:HIS:NE2  | 2.86                     | 0.44              |
| 2:K:239:ASN:ND2  | 2:K:246:THR:HG22 | 2.29                     | 0.44              |
| 2:C:89:VAL:C     | 2:C:91:PHE:H     | 2.21                     | 0.44              |
| 2:L:136:ILE:HG23 | 2:L:137:GLU:N    | 2.32                     | 0.44              |
| 2:C:69:THR:OG1   | 2:C:70:LEU:N     | 2.49                     | 0.44              |
| 1:B:757:VAL:HG12 | 1:B:758:ALA:N    | 2.32                     | 0.44              |
| 2:K:111:PRO:O    | 2:K:112:GLN:HG2  | 2.17                     | 0.44              |
| 2:K:78:VAL:O     | 2:K:81:ALA:N     | 2.40                     | 0.44              |
| 1:B:382:LEU:HA   | 1:B:382:LEU:HD12 | 1.62                     | 0.44              |
| 1:B:158:GLY:O    | 1:B:159:ASP:C    | 2.56                     | 0.44              |
| 1:B:250:TYR:HB2  | 1:B:840:HIS:CD2  | 2.53                     | 0.44              |
| 1:B:790:ARG:CG   | 1:B:791:LYS:N    | 2.71                     | 0.44              |
| 2:L:34:PHE:O     | 2:L:37:MET:HB3   | 2.17                     | 0.44              |
| 2:C:152:PHE:O    | 2:C:328:SER:HA   | 2.17                     | 0.44              |
| 2:E:66:LEU:HB3   | 2:E:77:TYR:OH    | 2.16                     | 0.44              |
| 1:B:361:GLN:NE2  | 3:W:624:LYS:HZ1  | 2.12                     | 0.44              |
| 2:C:145:ARG:CB   | 2:C:145:ARG:HH11 | 2.30                     | 0.44              |
| 3:W:223:TYR:CZ   | 3:W:227:LYS:HD2  | 2.53                     | 0.44              |
| 3:W:473:GLN:NE2  | 3:W:593:GLU:HB3  | 2.29                     | 0.44              |
| 1:B:630:ARG:O    | 1:B:631:LEU:CG   | 2.62                     | 0.44              |
| 2:K:27:VAL:CG2   | 2:K:31:ILE:HD11  | 2.48                     | 0.44              |
| 2:E:1:MET:C      | 2:E:3:VAL:N      | 2.68                     | 0.44              |
| 1:B:751:LEU:O    | 1:B:754:ASN:HA   | 2.16                     | 0.44              |
| 2:F:48:THR:HG22  | 2:F:115:SER:OG   | 2.18                     | 0.44              |
| 2:O:89:VAL:C     | 2:O:91:PHE:H     | 2.21                     | 0.44              |
| 1:A:804:SER:CB   | 1:A:810:TYR:HA   | 2.48                     | 0.44              |
| 2:J:89:VAL:C     | 2:J:91:PHE:N     | 2.71                     | 0.44              |
| 1:A:597:PRO:HB3  | 1:A:860:ALA:HB1  | 1.99                     | 0.44              |
| 2:C:63:PHE:CD2   | 2:C:84:THR:HG23  | 2.52                     | 0.44              |
| 2:J:225:LEU:HD13 | 2:J:277:PHE:CD2  | 2.53                     | 0.44              |
| 2:N:190:VAL:HG21 | 2:N:210:HIS:HB2  | 1.99                     | 0.44              |
| 2:E:78:VAL:O     | 2:E:81:ALA:HB3   | 2.17                     | 0.44              |
| 1:A:557:LEU:O    | 1:A:558:MET:C    | 2.55                     | 0.44              |
| 1:B:277:ARG:CB   | 1:B:277:ARG:HH11 | 2.30                     | 0.44              |
| 1:B:498:ARG:HH11 | 1:B:502:VAL:HG11 | 1.83                     | 0.44              |
| 1:A:513:LEU:CA   | 1:A:516:GLN:NE2  | 2.65                     | 0.44              |
| 1:B:446:HIS:O    | 1:B:447:TYR:CB   | 2.49                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:1:MET:O      | 2:K:2:ASP:C      | 2.54                     | 0.44              |
| 2:K:1:MET:C      | 2:K:3:VAL:N      | 2.68                     | 0.44              |
| 2:N:38:ILE:HG22  | 2:N:42:ASN:ND2   | 2.29                     | 0.44              |
| 3:W:448:PRO:HD2  | 3:W:464:ILE:O    | 2.17                     | 0.44              |
| 2:F:82:ARG:CZ    | 2:H:144:ARG:HD2  | 2.47                     | 0.44              |
| 3:W:232:LEU:CD2  | 3:W:300:LEU:HD12 | 2.46                     | 0.44              |
| 2:H:37:MET:O     | 2:H:38:ILE:C     | 2.55                     | 0.44              |
| 1:A:130:GLN:NE2  | 1:A:146:TRP:CZ2  | 2.85                     | 0.44              |
| 2:M:150:PHE:O    | 2:M:330:VAL:HG13 | 2.17                     | 0.44              |
| 3:W:840:ASN:HA   | 3:W:845:ILE:HG21 | 1.97                     | 0.44              |
| 1:B:707:TYR:N    | 1:B:707:TYR:CD1  | 2.85                     | 0.44              |
| 2:G:239:ASN:ND2  | 2:G:246:THR:HG22 | 2.29                     | 0.44              |
| 2:J:273:TYR:C    | 2:J:274:GLN:HE21 | 2.20                     | 0.44              |
| 2:K:136:ILE:HG23 | 2:K:137:GLU:N    | 2.32                     | 0.44              |
| 2:D:75:ALA:HB3   | 2:L:76:ASN:HA    | 2.00                     | 0.44              |
| 2:M:136:ILE:HG23 | 2:M:137:GLU:N    | 2.33                     | 0.44              |
| 2:L:273:TYR:C    | 2:L:274:GLN:HE21 | 2.21                     | 0.44              |
| 3:W:241:ALA:HB2  | 3:W:332:VAL:HG21 | 2.00                     | 0.44              |
| 2:I:101:VAL:HG11 | 2:I:355:ILE:HG13 | 1.99                     | 0.44              |
| 1:A:870:ALA:C    | 1:A:872:ASP:H    | 2.20                     | 0.44              |
| 2:N:78:VAL:O     | 2:N:81:ALA:HB3   | 2.17                     | 0.44              |
| 1:B:727:LEU:HD23 | 1:B:826:TYR:CE1  | 2.53                     | 0.44              |
| 1:A:488:VAL:O    | 1:A:490:ASN:N    | 2.51                     | 0.44              |
| 2:H:67:GLY:O     | 2:H:69:THR:N     | 2.51                     | 0.44              |
| 2:I:24:TYR:N     | 2:I:71:LEU:O     | 2.51                     | 0.44              |
| 1:A:516:GLN:OE1  | 1:A:517:GLN:N    | 2.50                     | 0.44              |
| 1:B:449:ASN:ND2  | 1:B:455:PRO:HG3  | 2.33                     | 0.44              |
| 1:A:701:GLN:CG   | 1:A:826:TYR:CD2  | 3.00                     | 0.44              |
| 1:B:393:SER:HA   | 1:B:423:SER:CB   | 2.47                     | 0.44              |
| 1:B:680:ASP:HA   | 1:B:683:ASN:HD22 | 1.82                     | 0.44              |
| 2:G:33:GLN:HB2   | 2:H:26:ASN:OD1   | 2.16                     | 0.44              |
| 1:A:771:VAL:HG13 | 1:A:772:ILE:N    | 2.22                     | 0.44              |
| 2:F:37:MET:O     | 2:F:38:ILE:C     | 2.56                     | 0.44              |
| 2:F:41:MET:O     | 2:F:42:ASN:C     | 2.56                     | 0.44              |
| 3:W:424:VAL:O    | 3:W:428:MET:HG3  | 2.17                     | 0.44              |
| 2:F:11:LEU:O     | 2:F:15:ARG:N     | 2.40                     | 0.44              |
| 2:O:136:ILE:HG23 | 2:O:137:GLU:N    | 2.32                     | 0.44              |
| 2:M:273:TYR:C    | 2:M:274:GLN:HE21 | 2.20                     | 0.44              |
| 1:A:727:LEU:O    | 1:A:727:LEU:CD1  | 2.65                     | 0.44              |
| 2:E:273:TYR:C    | 2:E:274:GLN:HE21 | 2.21                     | 0.44              |
| 2:K:273:TYR:C    | 2:K:274:GLN:HE21 | 2.21                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:W:948:TYR:OH   | 3:W:1071:TRP:HA  | 2.18                     | 0.44              |
| 2:M:225:LEU:HD13 | 2:M:277:PHE:CD2  | 2.53                     | 0.44              |
| 2:E:225:LEU:HD13 | 2:E:277:PHE:CD2  | 2.53                     | 0.44              |
| 2:F:249:PHE:CE2  | 2:F:251:PRO:HG3  | 2.53                     | 0.44              |
| 2:O:125:LYS:C    | 2:O:127:ILE:H    | 2.21                     | 0.44              |
| 2:N:63:PHE:N     | 2:N:63:PHE:CD1   | 2.85                     | 0.44              |
| 3:W:148:TRP:CE3  | 3:W:149:LEU:HD23 | 2.52                     | 0.44              |
| 2:G:104:SER:O    | 2:G:108:GLY:CA   | 2.66                     | 0.44              |
| 3:W:123:GLU:CD   | 3:W:123:GLU:N    | 2.71                     | 0.44              |
| 1:B:519:PRO:O    | 1:B:520:THR:CB   | 2.66                     | 0.44              |
| 1:B:428:GLN:HA   | 1:B:431:ILE:CD1  | 2.42                     | 0.44              |
| 2:K:14:ALA:O     | 2:K:16:ASP:N     | 2.51                     | 0.44              |
| 1:A:795:LEU:HA   | 1:A:795:LEU:HD12 | 1.74                     | 0.44              |
| 2:G:23:LEU:C     | 2:G:23:LEU:HD23  | 2.38                     | 0.44              |
| 1:A:312:ASP:O    | 1:A:313:ASN:CB   | 2.63                     | 0.44              |
| 2:M:151:THR:C    | 2:M:152:PHE:CD1  | 2.91                     | 0.44              |
| 2:C:3:VAL:O      | 2:C:4:LEU:C      | 2.56                     | 0.44              |
| 2:O:153:HIS:CD2  | 2:O:154:LYS:N    | 2.86                     | 0.44              |
| 2:I:46:PHE:HE2   | 2:I:119:LEU:HD21 | 1.83                     | 0.44              |
| 3:W:770:ASP:O    | 3:W:771:PHE:HB2  | 2.18                     | 0.44              |
| 2:H:142:GLN:NE2  | 2:H:143:ASN:N    | 2.65                     | 0.44              |
| 2:K:110:ALA:HB1  | 2:K:111:PRO:HD2  | 2.00                     | 0.44              |
| 2:J:78:VAL:O     | 2:J:81:ALA:HB3   | 2.17                     | 0.44              |
| 2:I:225:LEU:HD13 | 2:I:277:PHE:CD2  | 2.53                     | 0.44              |
| 2:O:225:LEU:HD13 | 2:O:277:PHE:CD2  | 2.53                     | 0.44              |
| 2:N:217:VAL:HG22 | 2:N:286:ASP:HB3  | 2.00                     | 0.44              |
| 2:H:217:VAL:HG22 | 2:H:286:ASP:HB3  | 2.00                     | 0.44              |
| 2:M:249:PHE:CE2  | 2:M:251:PRO:HG3  | 2.53                     | 0.44              |
| 2:H:249:PHE:CE2  | 2:H:251:PRO:HG3  | 2.53                     | 0.44              |
| 2:O:169:SER:HA   | 2:O:176:LEU:HD23 | 2.00                     | 0.44              |
| 2:K:312:GLN:HB3  | 2:K:313:PRO:HA   | 1.99                     | 0.44              |
| 2:D:249:PHE:CE2  | 2:D:251:PRO:HG3  | 2.53                     | 0.44              |
| 2:D:73:LEU:N     | 2:D:73:LEU:HD23  | 2.33                     | 0.44              |
| 1:B:738:LEU:HD12 | 1:B:738:LEU:HA   | 1.82                     | 0.44              |
| 1:B:305:GLN:OE1  | 1:B:305:GLN:HA   | 2.18                     | 0.44              |
| 2:I:122:LEU:C    | 2:I:124:PHE:H    | 2.21                     | 0.44              |
| 1:B:508:GLU:O    | 1:B:512:GLN:NE2  | 2.48                     | 0.44              |
| 2:K:14:ALA:C     | 2:K:18:ILE:HD12  | 2.39                     | 0.44              |
| 2:D:66:LEU:HD23  | 2:D:66:LEU:HA    | 1.72                     | 0.44              |
| 1:B:155:LEU:HA   | 1:B:156:PRO:HD3  | 1.81                     | 0.44              |
| 1:B:108:LEU:CD2  | 1:B:108:LEU:N    | 2.79                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:404:LEU:O    | 1:B:405:ILE:C    | 2.55                     | 0.44              |
| 3:W:758:THR:HG22 | 3:W:766:PHE:C    | 2.37                     | 0.44              |
| 1:B:282:VAL:HG13 | 1:B:283:ASN:H    | 1.83                     | 0.44              |
| 1:A:625:ILE:HG13 | 1:A:625:ILE:H    | 1.62                     | 0.44              |
| 1:B:487:GLY:O    | 1:B:488:VAL:CB   | 2.66                     | 0.44              |
| 2:L:225:LEU:HD13 | 2:L:277:PHE:CD2  | 2.53                     | 0.44              |
| 2:K:227:PRO:HD3  | 2:K:277:PHE:CG   | 2.53                     | 0.44              |
| 2:F:169:SER:HA   | 2:F:176:LEU:HD23 | 2.00                     | 0.44              |
| 2:J:103:GLU:OE1  | 2:J:358:GLY:HA3  | 2.18                     | 0.44              |
| 2:O:312:GLN:HB3  | 2:O:313:PRO:HA   | 1.99                     | 0.44              |
| 2:G:169:SER:HA   | 2:G:176:LEU:HD23 | 2.00                     | 0.44              |
| 2:C:249:PHE:CE2  | 2:C:251:PRO:HG3  | 2.53                     | 0.44              |
| 2:M:217:VAL:HG22 | 2:M:286:ASP:HB3  | 1.99                     | 0.44              |
| 2:E:217:VAL:HG22 | 2:E:286:ASP:HB3  | 2.00                     | 0.44              |
| 3:W:897:GLN:N    | 3:W:897:GLN:OE1  | 2.49                     | 0.44              |
| 1:A:160:TYR:HE1  | 1:A:633:LEU:HA   | 1.83                     | 0.44              |
| 1:A:618:ILE:HD13 | 1:A:645:PHE:HZ   | 1.83                     | 0.44              |
| 1:B:353:LEU:HD23 | 1:B:353:LEU:O    | 2.18                     | 0.44              |
| 1:B:473:HIS:HB3  | 2:I:126:ARG:NH1  | 2.26                     | 0.44              |
| 1:B:496:ASN:HD22 | 1:B:498:ARG:HB2  | 1.83                     | 0.44              |
| 1:B:543:LEU:O    | 1:B:546:LEU:HB2  | 2.18                     | 0.44              |
| 1:B:870:ALA:O    | 1:B:871:PHE:C    | 2.55                     | 0.44              |
| 2:N:21:GLY:O     | 2:N:22:THR:C     | 2.56                     | 0.44              |
| 1:B:122:LEU:HD12 | 1:B:124:ARG:HH22 | 1.82                     | 0.44              |
| 1:B:790:ARG:CG   | 1:B:791:LYS:H    | 2.18                     | 0.44              |
| 1:A:799:LEU:HD22 | 1:A:800:TYR:H    | 1.82                     | 0.44              |
| 1:B:675:GLU:O    | 1:B:678:ARG:N    | 2.51                     | 0.44              |
| 2:L:63:PHE:CD2   | 2:L:84:THR:HG23  | 2.53                     | 0.44              |
| 2:G:37:MET:O     | 2:G:38:ILE:C     | 2.55                     | 0.44              |
| 1:A:245:LEU:O    | 1:A:246:HIS:CB   | 2.66                     | 0.44              |
| 2:K:89:VAL:C     | 2:K:91:PHE:N     | 2.71                     | 0.44              |
| 2:D:5:TYR:CE2    | 2:D:131:ASN:HA   | 2.52                     | 0.44              |
| 3:W:832:ALA:O    | 3:W:836:LYS:HG3  | 2.17                     | 0.44              |
| 1:B:111:ILE:HG22 | 1:B:113:PRO:CD   | 2.48                     | 0.44              |
| 1:A:181:LEU:H    | 1:A:260:GLN:HE21 | 1.65                     | 0.44              |
| 2:K:49:GLY:HA2   | 2:K:54:LEU:HD23  | 1.99                     | 0.44              |
| 2:O:106:ARG:HG2  | 2:O:107:ASN:H    | 1.83                     | 0.44              |
| 2:I:63:PHE:N     | 2:I:63:PHE:CD1   | 2.86                     | 0.44              |
| 2:C:273:TYR:C    | 2:C:274:GLN:HE21 | 2.21                     | 0.44              |
| 2:G:150:PHE:N    | 2:G:150:PHE:CD1  | 2.86                     | 0.44              |
| 1:B:207:ILE:O    | 1:B:210:ALA:HB3  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:78:VAL:O     | 2:H:81:ALA:HB3   | 2.17                     | 0.44              |
| 2:O:78:VAL:O     | 2:O:81:ALA:HB3   | 2.18                     | 0.44              |
| 1:B:101:LYS:HB2  | 1:B:102:GLU:H    | 1.68                     | 0.44              |
| 2:N:169:SER:HA   | 2:N:176:LEU:HD23 | 2.00                     | 0.44              |
| 2:E:125:LYS:C    | 2:E:127:ILE:H    | 2.21                     | 0.44              |
| 2:E:249:PHE:CE2  | 2:E:251:PRO:HG3  | 2.53                     | 0.44              |
| 2:G:100:MET:HG3  | 2:G:388:VAL:HG11 | 1.99                     | 0.44              |
| 2:D:169:SER:HA   | 2:D:176:LEU:HD23 | 2.00                     | 0.44              |
| 2:M:190:VAL:HG21 | 2:M:210:HIS:HB2  | 1.99                     | 0.44              |
| 3:W:894:ILE:O    | 3:W:894:ILE:HG13 | 2.17                     | 0.44              |
| 1:B:321:ILE:O    | 1:B:322:THR:C    | 2.57                     | 0.43              |
| 1:B:510:LEU:O    | 1:B:513:LEU:N    | 2.51                     | 0.43              |
| 1:B:506:LEU:CD2  | 1:B:544:VAL:HA   | 2.39                     | 0.43              |
| 1:A:428:GLN:HE22 | 1:A:455:PRO:HB2  | 1.74                     | 0.43              |
| 2:N:2:ASP:HB2    | 2:N:128:ASN:HD21 | 1.83                     | 0.43              |
| 1:B:293:PRO:O    | 1:B:295:THR:N    | 2.50                     | 0.43              |
| 3:W:1006:LEU:HG  | 3:W:1086:PHE:CE1 | 2.49                     | 0.43              |
| 2:O:3:VAL:O      | 2:O:4:LEU:C      | 2.56                     | 0.43              |
| 1:B:529:ILE:O    | 1:B:533:ILE:HG13 | 2.18                     | 0.43              |
| 1:A:119:GLN:NE2  | 1:A:178:PRO:HG2  | 2.33                     | 0.43              |
| 2:L:3:VAL:O      | 2:L:4:LEU:C      | 2.56                     | 0.43              |
| 3:W:824:ASN:O    | 3:W:827:VAL:N    | 2.46                     | 0.43              |
| 2:N:155:PRO:O    | 2:N:186:SER:HB3  | 2.17                     | 0.43              |
| 2:N:151:THR:C    | 2:N:152:PHE:CD1  | 2.91                     | 0.43              |
| 3:W:527:SER:O    | 3:W:530:ASN:N    | 2.48                     | 0.43              |
| 2:I:89:VAL:C     | 2:I:91:PHE:N     | 2.70                     | 0.43              |
| 2:E:89:VAL:C     | 2:E:91:PHE:H     | 2.22                     | 0.43              |
| 2:J:125:LYS:O    | 2:J:127:ILE:N    | 2.42                     | 0.43              |
| 2:M:89:VAL:C     | 2:M:91:PHE:H     | 2.21                     | 0.43              |
| 2:D:273:TYR:C    | 2:D:274:GLN:HE21 | 2.21                     | 0.43              |
| 3:W:981:TYR:CZ   | 3:W:985:LYS:HD2  | 2.53                     | 0.43              |
| 2:H:41:MET:O     | 2:H:42:ASN:C     | 2.56                     | 0.43              |
| 2:O:227:PRO:HD3  | 2:O:277:PHE:CG   | 2.53                     | 0.43              |
| 2:N:62:ASP:H     | 2:N:63:PHE:HD1   | 1.66                     | 0.43              |
| 2:G:225:LEU:HD13 | 2:G:277:PHE:CD2  | 2.53                     | 0.43              |
| 2:D:312:GLN:HB3  | 2:D:313:PRO:HA   | 1.99                     | 0.43              |
| 2:H:225:LEU:HD13 | 2:H:277:PHE:CD2  | 2.53                     | 0.43              |
| 2:H:225:LEU:HD13 | 2:H:277:PHE:HD2  | 1.82                     | 0.43              |
| 2:L:217:VAL:HG22 | 2:L:286:ASP:HB3  | 2.00                     | 0.43              |
| 2:C:225:LEU:HD13 | 2:C:277:PHE:HD2  | 1.82                     | 0.43              |
| 1:B:138:GLY:O    | 1:B:804:SER:HB3  | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:333:VAL:HB   | 1:A:380:LYS:HG2  | 2.00                     | 0.43              |
| 1:A:416:ASN:C    | 1:A:418:MET:H    | 2.21                     | 0.43              |
| 1:B:498:ARG:CD   | 2:I:32:GLN:NE2   | 2.82                     | 0.43              |
| 1:B:503:ILE:HG12 | 1:B:547:THR:HB   | 2.00                     | 0.43              |
| 1:B:491:GLN:CG   | 1:B:564:ASN:HB3  | 2.48                     | 0.43              |
| 2:I:36:GLN:CB    | 2:J:23:LEU:HD11  | 2.48                     | 0.43              |
| 1:A:854:LEU:O    | 1:A:855:LEU:C    | 2.56                     | 0.43              |
| 1:B:190:ASN:O    | 1:B:192:ASN:O    | 2.35                     | 0.43              |
| 1:A:722:ASN:ND2  | 1:A:823:THR:O    | 2.51                     | 0.43              |
| 1:B:635:GLN:C    | 1:B:636:LYS:O    | 2.50                     | 0.43              |
| 1:B:341:SER:O    | 1:B:342:THR:C    | 2.57                     | 0.43              |
| 1:B:374:ALA:CB   | 1:B:580:SER:HB3  | 2.44                     | 0.43              |
| 2:L:35:ASN:O     | 2:L:37:MET:N     | 2.51                     | 0.43              |
| 2:G:61:PHE:N     | 2:G:61:PHE:CD1   | 2.86                     | 0.43              |
| 2:L:14:ALA:O     | 2:L:18:ILE:HD12  | 2.18                     | 0.43              |
| 2:M:22:THR:OG1   | 2:M:26:ASN:ND2   | 2.45                     | 0.43              |
| 3:W:825:ASN:O    | 3:W:829:ARG:HG2  | 2.18                     | 0.43              |
| 3:W:595:GLN:O    | 3:W:599:ALA:HB3  | 2.18                     | 0.43              |
| 2:E:1:MET:O      | 2:E:2:ASP:C      | 2.56                     | 0.43              |
| 2:C:153:HIS:NE2  | 2:D:153:HIS:NE2  | 2.66                     | 0.43              |
| 2:C:239:ASN:ND2  | 2:C:246:THR:HG22 | 2.29                     | 0.43              |
| 2:D:99:GLU:CD    | 2:D:116:LEU:CD2  | 2.86                     | 0.43              |
| 1:A:187:ALA:O    | 1:A:188:VAL:CG2  | 2.66                     | 0.43              |
| 1:A:141:GLU:O    | 1:A:142:LEU:CB   | 2.65                     | 0.43              |
| 1:A:810:TYR:C    | 1:A:812:VAL:N    | 2.71                     | 0.43              |
| 3:W:951:ILE:HG13 | 3:W:985:LYS:HG2  | 1.99                     | 0.43              |
| 2:C:227:PRO:HD3  | 2:C:277:PHE:CG   | 2.53                     | 0.43              |
| 3:W:377:GLU:N    | 3:W:378:PRO:CD   | 2.81                     | 0.43              |
| 2:C:312:GLN:HB3  | 2:C:313:PRO:HA   | 1.99                     | 0.43              |
| 2:M:169:SER:HA   | 2:M:176:LEU:HD23 | 2.00                     | 0.43              |
| 3:W:786:ARG:HD3  | 3:W:869:SER:HB2  | 1.99                     | 0.43              |
| 2:K:217:VAL:HG22 | 2:K:286:ASP:HB3  | 2.00                     | 0.43              |
| 2:O:249:PHE:CE2  | 2:O:251:PRO:HG3  | 2.53                     | 0.43              |
| 1:A:396:PHE:HD2  | 1:A:578:LEU:HD11 | 1.84                     | 0.43              |
| 1:A:591:ALA:O    | 1:A:877:MET:SD   | 2.76                     | 0.43              |
| 1:B:309:ASN:HA   | 1:B:311:HIS:CE1  | 2.54                     | 0.43              |
| 1:A:501:HIS:CA   | 1:A:503:ILE:HG13 | 2.48                     | 0.43              |
| 2:K:5:TYR:HE2    | 2:K:131:ASN:HA   | 1.79                     | 0.43              |
| 2:K:3:VAL:O      | 2:K:4:LEU:C      | 2.56                     | 0.43              |
| 2:M:128:ASN:HB3  | 2:N:19:VAL:CG2   | 2.48                     | 0.43              |
| 1:B:791:LYS:HB3  | 1:B:792:VAL:H    | 1.59                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:751:LEU:HD21 | 1:A:783:PHE:O    | 2.18                     | 0.43              |
| 1:A:772:ILE:O    | 1:A:774:LEU:N    | 2.51                     | 0.43              |
| 1:A:769:SER:CB   | 1:A:807:ASN:OD1  | 2.60                     | 0.43              |
| 2:J:3:VAL:O      | 2:J:4:LEU:C      | 2.56                     | 0.43              |
| 3:W:165:ARG:HH11 | 3:W:165:ARG:HG3  | 1.84                     | 0.43              |
| 1:A:181:LEU:N    | 1:A:260:GLN:HE21 | 2.16                     | 0.43              |
| 2:D:63:PHE:N     | 2:D:63:PHE:CD1   | 2.86                     | 0.43              |
| 1:A:143:ARG:HG3  | 1:A:144:ASN:N    | 2.34                     | 0.43              |
| 3:W:586:TYR:HE2  | 3:W:588:ALA:HB3  | 1.81                     | 0.43              |
| 2:N:136:ILE:HG23 | 2:N:137:GLU:N    | 2.33                     | 0.43              |
| 3:W:854:ILE:O    | 3:W:858:LEU:HG   | 2.17                     | 0.43              |
| 1:A:215:GLU:CD   | 1:A:215:GLU:H    | 2.21                     | 0.43              |
| 3:W:81:LYS:O     | 3:W:82:TYR:HB2   | 2.19                     | 0.43              |
| 2:N:227:PRO:HD3  | 2:N:277:PHE:CG   | 2.53                     | 0.43              |
| 2:E:78:VAL:O     | 2:E:81:ALA:N     | 2.41                     | 0.43              |
| 2:G:225:LEU:HD13 | 2:G:277:PHE:HD2  | 1.82                     | 0.43              |
| 2:H:227:PRO:HD3  | 2:H:277:PHE:CG   | 2.53                     | 0.43              |
| 2:G:53:ASN:ND2   | 2:G:354:ALA:HB3  | 2.33                     | 0.43              |
| 2:F:217:VAL:HG22 | 2:F:286:ASP:HB3  | 1.99                     | 0.43              |
| 3:W:954:HIS:HB2  | 3:W:957:GLU:HG3  | 1.99                     | 0.43              |
| 2:I:169:SER:HA   | 2:I:176:LEU:HD23 | 2.00                     | 0.43              |
| 1:A:383:ILE:O    | 1:A:386:MET:N    | 2.52                     | 0.43              |
| 1:B:510:LEU:HA   | 1:B:513:LEU:HD12 | 1.99                     | 0.43              |
| 1:B:510:LEU:HD22 | 1:B:540:LEU:CD1  | 2.30                     | 0.43              |
| 1:B:542:GLN:O    | 1:B:543:LEU:C    | 2.57                     | 0.43              |
| 1:A:750:MET:CE   | 1:A:757:VAL:HG21 | 2.48                     | 0.43              |
| 1:A:781:THR:HG22 | 1:A:782:VAL:N    | 2.34                     | 0.43              |
| 2:L:42:ASN:CA    | 2:L:61:PHE:HB2   | 2.30                     | 0.43              |
| 2:I:146:GLN:O    | 2:I:148:THR:HG23 | 2.19                     | 0.43              |
| 2:G:6:SER:C      | 2:G:8:SER:N      | 2.72                     | 0.43              |
| 2:M:24:TYR:N     | 2:M:71:LEU:O     | 2.49                     | 0.43              |
| 2:C:1:MET:O      | 2:C:2:ASP:C      | 2.56                     | 0.43              |
| 1:B:595:PRO:HB2  | 1:B:600:LEU:HD11 | 2.00                     | 0.43              |
| 2:N:153:HIS:O    | 2:N:154:LYS:C    | 2.57                     | 0.43              |
| 2:L:89:VAL:C     | 2:L:91:PHE:N     | 2.71                     | 0.43              |
| 1:B:312:ASP:CG   | 1:B:312:ASP:O    | 2.56                     | 0.43              |
| 2:I:227:PRO:HD3  | 2:I:277:PHE:CG   | 2.53                     | 0.43              |
| 2:E:227:PRO:HD3  | 2:E:277:PHE:CG   | 2.53                     | 0.43              |
| 2:F:227:PRO:HD3  | 2:F:277:PHE:CG   | 2.53                     | 0.43              |
| 2:K:225:LEU:HD13 | 2:K:277:PHE:CD2  | 2.53                     | 0.43              |
| 2:N:225:LEU:HD13 | 2:N:277:PHE:CD2  | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:249:PHE:CE2  | 2:G:251:PRO:HG3  | 2.53                     | 0.43              |
| 3:W:650:ASP:O    | 3:W:654:ASP:OD1  | 2.36                     | 0.43              |
| 2:I:312:GLN:HB3  | 2:I:313:PRO:HA   | 1.99                     | 0.43              |
| 2:H:169:SER:HA   | 2:H:176:LEU:HD23 | 2.00                     | 0.43              |
| 2:N:101:VAL:HG11 | 2:N:355:ILE:HG13 | 2.01                     | 0.43              |
| 2:E:142:GLN:HE21 | 2:E:143:ASN:N    | 2.16                     | 0.43              |
| 1:B:703:VAL:CG1  | 1:B:704:ILE:N    | 2.81                     | 0.43              |
| 1:B:772:ILE:O    | 1:B:775:ILE:N    | 2.51                     | 0.43              |
| 1:A:415:PRO:O    | 1:A:417:ASP:N    | 2.43                     | 0.43              |
| 1:A:546:LEU:HD23 | 1:A:546:LEU:HA   | 1.86                     | 0.43              |
| 1:A:583:SER:O    | 1:A:584:LEU:C    | 2.56                     | 0.43              |
| 1:A:548:ARG:HH11 | 1:A:877:MET:H    | 1.67                     | 0.43              |
| 1:B:309:ASN:HA   | 1:B:311:HIS:NE2  | 2.33                     | 0.43              |
| 1:B:540:LEU:HD23 | 1:B:541:GLY:CA   | 2.48                     | 0.43              |
| 2:I:34:PHE:O     | 2:I:37:MET:HB3   | 2.18                     | 0.43              |
| 1:A:408:MET:HG2  | 1:A:471:TRP:CH2  | 2.53                     | 0.43              |
| 2:N:24:TYR:HE1   | 2:N:31:ILE:HG13  | 1.83                     | 0.43              |
| 1:A:799:LEU:HD23 | 1:A:799:LEU:HA   | 1.68                     | 0.43              |
| 2:G:38:ILE:H     | 2:G:38:ILE:HG13  | 1.59                     | 0.43              |
| 2:N:145:ARG:HE   | 2:N:145:ARG:HA   | 1.83                     | 0.43              |
| 1:A:243:SER:O    | 1:A:839:MET:HG2  | 2.19                     | 0.43              |
| 1:B:451:ASP:H    | 1:B:452:PRO:CD   | 2.20                     | 0.43              |
| 2:H:1:MET:O      | 2:H:2:ASP:C      | 2.57                     | 0.43              |
| 2:K:89:VAL:C     | 2:K:91:PHE:H     | 2.21                     | 0.43              |
| 3:W:296:ARG:HH22 | 3:W:308:GLN:NE2  | 2.05                     | 0.43              |
| 2:E:24:TYR:HE1   | 2:E:31:ILE:HG13  | 1.83                     | 0.43              |
| 3:W:427:ASP:OD1  | 3:W:432:ARG:NH2  | 2.52                     | 0.43              |
| 2:F:3:VAL:O      | 2:F:4:LEU:C      | 2.56                     | 0.43              |
| 3:W:686:LYS:HD3  | 3:W:901:PRO:HG2  | 2.01                     | 0.43              |
| 1:B:706:ALA:C    | 1:B:708:ARG:N    | 2.72                     | 0.43              |
| 1:A:714:ARG:HG2  | 1:A:720:TYR:CD2  | 2.54                     | 0.43              |
| 2:M:63:PHE:HD2   | 2:M:84:THR:HG23  | 1.81                     | 0.43              |
| 2:E:136:ILE:HG23 | 2:E:137:GLU:N    | 2.34                     | 0.43              |
| 1:A:717:MET:HE3  | 1:A:829:VAL:HG13 | 2.01                     | 0.43              |
| 2:M:123:LYS:HG3  | 2:M:124:PHE:CD1  | 2.53                     | 0.43              |
| 2:M:155:PRO:HA   | 2:M:337:ASP:CB   | 2.49                     | 0.43              |
| 2:F:225:LEU:HD13 | 2:F:277:PHE:CD2  | 2.53                     | 0.43              |
| 2:N:63:PHE:CD2   | 2:N:84:THR:HG23  | 2.54                     | 0.43              |
| 2:E:125:LYS:O    | 2:E:127:ILE:N    | 2.51                     | 0.43              |
| 2:L:249:PHE:CE2  | 2:L:251:PRO:HG3  | 2.53                     | 0.43              |
| 2:L:169:SER:HA   | 2:L:176:LEU:HD23 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:312:GLN:HB3  | 2:N:313:PRO:HA   | 1.99                     | 0.43              |
| 2:C:78:VAL:O     | 2:C:81:ALA:HB3   | 2.17                     | 0.43              |
| 2:E:60:ASN:C     | 2:E:61:PHE:CD1   | 2.91                     | 0.43              |
| 2:G:217:VAL:HG22 | 2:G:286:ASP:HB3  | 1.99                     | 0.43              |
| 2:J:169:SER:HA   | 2:J:176:LEU:HD23 | 2.00                     | 0.43              |
| 1:B:772:ILE:CG2  | 1:B:773:SER:H    | 2.29                     | 0.43              |
| 1:A:298:TYR:C    | 1:A:298:TYR:CD1  | 2.91                     | 0.43              |
| 1:B:383:ILE:O    | 1:B:386:MET:N    | 2.51                     | 0.43              |
| 1:A:353:LEU:C    | 1:A:354:GLN:HG2  | 2.37                     | 0.43              |
| 1:A:501:HIS:HA   | 1:A:503:ILE:HG13 | 2.01                     | 0.43              |
| 1:A:521:MET:CB   | 1:A:522:PRO:HD3  | 2.26                     | 0.43              |
| 1:A:563:MET:O    | 1:A:564:ASN:C    | 2.56                     | 0.43              |
| 1:B:224:PHE:CD1  | 2:O:71:LEU:HD13  | 2.54                     | 0.43              |
| 1:B:231:ARG:HD2  | 1:B:231:ARG:HA   | 1.77                     | 0.43              |
| 1:A:675:GLU:HB3  | 1:A:678:ARG:HG2  | 2.01                     | 0.43              |
| 2:E:152:PHE:O    | 2:E:328:SER:HA   | 2.19                     | 0.43              |
| 2:G:89:VAL:C     | 2:G:91:PHE:H     | 2.22                     | 0.43              |
| 2:G:151:THR:C    | 2:G:152:PHE:CD1  | 2.92                     | 0.43              |
| 2:O:62:ASP:H     | 2:O:63:PHE:HD1   | 1.66                     | 0.43              |
| 2:F:163:SER:HB3  | 2:F:181:TRP:CZ2  | 2.54                     | 0.43              |
| 3:W:1077:ARG:O   | 3:W:1078:SER:C   | 2.57                     | 0.43              |
| 3:W:386:LEU:HB3  | 3:W:554:VAL:HG22 | 2.00                     | 0.43              |
| 3:W:133:ALA:HB1  | 3:W:701:ARG:HG3  | 1.99                     | 0.43              |
| 1:B:770:SER:O    | 1:B:771:VAL:C    | 2.57                     | 0.43              |
| 1:A:428:GLN:O    | 1:A:432:VAL:HG23 | 2.19                     | 0.43              |
| 2:G:145:ARG:HE   | 2:I:142:GLN:NE2  | 2.17                     | 0.43              |
| 1:B:434:THR:C    | 1:B:435:ILE:HG13 | 2.37                     | 0.43              |
| 1:B:508:GLU:OE1  | 2:J:71:LEU:HB3   | 2.18                     | 0.43              |
| 1:B:743:ASP:CG   | 1:B:744:TYR:N    | 2.72                     | 0.43              |
| 3:W:447:ILE:CG2  | 3:W:464:ILE:H    | 2.31                     | 0.43              |
| 1:A:693:GLU:O    | 1:A:695:ALA:O    | 2.37                     | 0.43              |
| 2:D:11:LEU:O     | 2:D:15:ARG:N     | 2.40                     | 0.43              |
| 2:J:14:ALA:O     | 2:J:16:ASP:N     | 2.50                     | 0.43              |
| 2:H:35:ASN:O     | 2:H:37:MET:N     | 2.52                     | 0.43              |
| 2:N:154:LYS:N    | 2:N:155:PRO:CD   | 2.82                     | 0.43              |
| 1:B:666:ARG:HG2  | 1:B:667:ASP:N    | 2.32                     | 0.43              |
| 2:D:89:VAL:C     | 2:D:91:PHE:H     | 2.22                     | 0.43              |
| 2:J:136:ILE:HG23 | 2:J:137:GLU:N    | 2.33                     | 0.43              |
| 2:H:273:TYR:C    | 2:H:274:GLN:HE21 | 2.21                     | 0.43              |
| 2:C:78:VAL:O     | 2:C:81:ALA:N     | 2.40                     | 0.43              |
| 2:E:169:SER:HA   | 2:E:176:LEU:HD23 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:620:ASP:O    | 1:B:624:ILE:HG13 | 2.19                     | 0.43              |
| 1:A:387:LEU:HD23 | 1:A:554:TYR:CE1  | 2.54                     | 0.43              |
| 2:L:78:VAL:O     | 2:L:81:ALA:HB3   | 2.18                     | 0.43              |
| 1:A:370:ILE:O    | 1:A:374:ALA:HB2  | 2.19                     | 0.43              |
| 1:A:393:SER:C    | 1:A:394:LEU:HG   | 2.38                     | 0.43              |
| 1:A:571:LEU:HD22 | 1:A:571:LEU:HA   | 1.74                     | 0.43              |
| 1:B:871:PHE:CD1  | 1:B:872:ASP:N    | 2.87                     | 0.43              |
| 1:B:433:ASN:C    | 1:B:435:ILE:H    | 2.22                     | 0.43              |
| 2:I:11:LEU:O     | 2:I:15:ARG:N     | 2.38                     | 0.43              |
| 2:I:4:LEU:O      | 2:I:5:TYR:C      | 2.57                     | 0.43              |
| 2:N:125:LYS:C    | 2:N:127:ILE:H    | 2.22                     | 0.43              |
| 2:N:3:VAL:O      | 2:N:4:LEU:C      | 2.56                     | 0.43              |
| 1:A:709:ASP:O    | 1:A:710:MET:HB3  | 2.18                     | 0.43              |
| 1:A:785:GLN:O    | 1:A:786:ILE:C    | 2.57                     | 0.43              |
| 1:B:658:PRO:HB2  | 1:B:661:GLN:CG   | 2.39                     | 0.43              |
| 2:M:74:ASP:O     | 2:M:75:ALA:C     | 2.57                     | 0.43              |
| 3:W:169:LEU:HG   | 3:W:223:TYR:CE1  | 2.54                     | 0.43              |
| 3:W:811:TYR:CZ   | 3:W:815:LEU:HD11 | 2.54                     | 0.43              |
| 3:W:500:LEU:HD12 | 3:W:917:ARG:O    | 2.18                     | 0.43              |
| 3:W:951:ILE:CG1  | 3:W:985:LYS:HA   | 2.47                     | 0.43              |
| 3:W:173:VAL:O    | 3:W:177:ILE:HG12 | 2.19                     | 0.43              |
| 1:B:776:ALA:O    | 1:B:778:LEU:N    | 2.52                     | 0.43              |
| 2:N:249:PHE:CE2  | 2:N:251:PRO:HG3  | 2.53                     | 0.43              |
| 2:J:190:VAL:HG21 | 2:J:210:HIS:HB2  | 1.99                     | 0.43              |
| 2:C:53:ASN:HD22  | 2:C:354:ALA:HB3  | 1.83                     | 0.43              |
| 1:A:396:PHE:HB3  | 1:A:578:LEU:HG   | 2.00                     | 0.43              |
| 1:A:393:SER:HB2  | 1:A:573:THR:CG2  | 2.48                     | 0.43              |
| 1:B:870:ALA:O    | 1:B:872:ASP:N    | 2.52                     | 0.43              |
| 2:I:27:VAL:O     | 2:I:30:LEU:HB3   | 2.19                     | 0.43              |
| 1:A:510:LEU:HD13 | 1:A:540:LEU:HB2  | 2.01                     | 0.43              |
| 2:I:16:ASP:HB3   | 2:K:131:ASN:O    | 2.18                     | 0.43              |
| 2:M:1:MET:C      | 2:M:3:VAL:N      | 2.71                     | 0.43              |
| 2:G:3:VAL:O      | 2:G:4:LEU:C      | 2.56                     | 0.43              |
| 1:B:409:TRP:CZ3  | 1:B:413:VAL:HG23 | 2.54                     | 0.43              |
| 1:B:218:GLU:OE1  | 1:B:836:ARG:NH2  | 2.51                     | 0.43              |
| 2:N:50:GLY:O     | 2:N:51:ILE:CG2   | 2.61                     | 0.43              |
| 2:C:35:ASN:O     | 2:C:37:MET:N     | 2.52                     | 0.43              |
| 1:A:420:ILE:HD12 | 1:A:422:GLU:CG   | 2.49                     | 0.43              |
| 1:A:481:ARG:HH12 | 1:A:497:ILE:CD1  | 2.32                     | 0.43              |
| 2:C:14:ALA:O     | 2:C:16:ASP:N     | 2.52                     | 0.43              |
| 2:O:89:VAL:C     | 2:O:91:PHE:N     | 2.71                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:W:754:GLU:O    | 3:W:758:THR:OG1  | 2.35                     | 0.43              |
| 2:D:89:VAL:C     | 2:D:91:PHE:N     | 2.72                     | 0.43              |
| 2:H:135:TYR:CE1  | 2:H:342:MET:HE3  | 2.54                     | 0.43              |
| 2:C:89:VAL:C     | 2:C:91:PHE:N     | 2.72                     | 0.43              |
| 2:H:89:VAL:C     | 2:H:91:PHE:N     | 2.73                     | 0.43              |
| 1:B:625:ILE:H    | 1:B:625:ILE:HG13 | 1.60                     | 0.43              |
| 1:A:815:TYR:HD1  | 1:A:815:TYR:H    | 1.62                     | 0.43              |
| 3:W:181:GLY:O    | 3:W:183:PRO:HD3  | 2.19                     | 0.43              |
| 2:K:163:SER:HB3  | 2:K:181:TRP:CZ2  | 2.54                     | 0.43              |
| 2:E:70:LEU:HB3   | 2:E:72:ASN:O     | 2.19                     | 0.43              |
| 3:W:138:LEU:HA   | 3:W:141:ASN:HD22 | 1.84                     | 0.43              |
| 2:J:66:LEU:HD23  | 2:J:66:LEU:HA    | 1.81                     | 0.43              |
| 1:B:134:TYR:N    | 1:B:134:TYR:CD1  | 2.86                     | 0.43              |
| 1:B:810:TYR:C    | 1:B:812:VAL:HG12 | 2.38                     | 0.43              |
| 1:A:319:ASP:OD2  | 1:A:572:THR:N    | 2.52                     | 0.43              |
| 1:A:339:LEU:HD13 | 1:A:588:ILE:HG12 | 2.00                     | 0.43              |
| 1:A:396:PHE:HB3  | 1:A:578:LEU:CG   | 2.47                     | 0.43              |
| 1:A:656:ARG:HB3  | 1:B:347:GLN:NE2  | 2.34                     | 0.43              |
| 1:B:477:ASN:ND2  | 2:I:39:ILE:CG2   | 2.81                     | 0.43              |
| 1:B:126:PHE:CB   | 1:B:149:LYS:O    | 2.67                     | 0.43              |
| 2:M:34:PHE:O     | 2:M:37:MET:HB3   | 2.19                     | 0.43              |
| 2:E:49:GLY:HA2   | 2:E:54:LEU:HD23  | 2.01                     | 0.43              |
| 3:W:428:MET:SD   | 3:W:811:TYR:CD1  | 3.11                     | 0.43              |
| 1:A:496:ASN:O    | 1:A:498:ARG:N    | 2.51                     | 0.43              |
| 2:I:149:GLY:C    | 2:I:150:PHE:CD1  | 2.92                     | 0.43              |
| 2:K:27:VAL:O     | 2:K:30:LEU:N     | 2.52                     | 0.43              |
| 2:J:34:PHE:O     | 2:J:37:MET:HB3   | 2.18                     | 0.43              |
| 2:J:35:ASN:O     | 2:J:37:MET:N     | 2.52                     | 0.43              |
| 3:W:500:LEU:HD22 | 3:W:899:PHE:HE1  | 1.83                     | 0.43              |
| 3:W:729:ARG:HD2  | 3:W:770:ASP:OD2  | 2.19                     | 0.43              |
| 2:F:89:VAL:C     | 2:F:91:PHE:H     | 2.22                     | 0.43              |
| 2:M:56:ILE:O     | 2:M:56:ILE:HG22  | 2.19                     | 0.43              |
| 3:W:496:GLN:O    | 3:W:920:GLN:HG2  | 2.18                     | 0.43              |
| 1:B:89:GLU:O     | 1:B:91:LEU:N     | 2.52                     | 0.43              |
| 2:D:225:LEU:HD13 | 2:D:277:PHE:CD2  | 2.53                     | 0.43              |
| 2:O:163:SER:HB3  | 2:O:181:TRP:CZ2  | 2.54                     | 0.43              |
| 1:A:598:GLN:HG3  | 1:A:598:GLN:H    | 1.61                     | 0.43              |
| 1:B:305:GLN:HG3  | 1:B:489:LEU:CD2  | 2.49                     | 0.42              |
| 1:B:548:ARG:CD   | 1:B:877:MET:H    | 2.31                     | 0.42              |
| 2:N:27:VAL:O     | 2:N:28:SER:C     | 2.58                     | 0.42              |
| 2:N:35:ASN:O     | 2:N:37:MET:N     | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:249:ASP:O    | 1:B:250:TYR:C    | 2.58                     | 0.42              |
| 1:B:251:ALA:HA   | 2:N:69:THR:CG2   | 2.42                     | 0.42              |
| 2:O:23:LEU:CD2   | 2:O:24:TYR:N     | 2.82                     | 0.42              |
| 2:L:38:ILE:H     | 2:L:38:ILE:HG13  | 1.55                     | 0.42              |
| 1:B:698:LYS:C    | 1:B:699:ILE:CD1  | 2.87                     | 0.42              |
| 1:B:99:GLU:HB3   | 1:B:100:PRO:CD   | 2.35                     | 0.42              |
| 1:A:355:LEU:HA   | 1:A:355:LEU:HD23 | 1.79                     | 0.42              |
| 3:W:324:LYS:HG2  | 3:W:328:TRP:NE1  | 2.33                     | 0.42              |
| 2:C:34:PHE:O     | 2:C:37:MET:HB3   | 2.19                     | 0.42              |
| 2:C:38:ILE:HG13  | 2:C:38:ILE:H     | 1.58                     | 0.42              |
| 3:W:426:ASP:HB3  | 3:W:432:ARG:HH21 | 1.84                     | 0.42              |
| 2:D:150:PHE:HB2  | 2:D:152:PHE:CZ   | 2.53                     | 0.42              |
| 3:W:900:MET:N    | 3:W:901:PRO:HD3  | 2.34                     | 0.42              |
| 2:H:89:VAL:C     | 2:H:91:PHE:H     | 2.22                     | 0.42              |
| 2:F:89:VAL:C     | 2:F:91:PHE:N     | 2.72                     | 0.42              |
| 3:W:109:TYR:OH   | 3:W:337:GLN:HB2  | 2.19                     | 0.42              |
| 3:W:521:VAL:HG11 | 3:W:607:LEU:CD2  | 2.49                     | 0.42              |
| 3:W:863:LYS:HA   | 3:W:864:PRO:HD3  | 1.70                     | 0.42              |
| 3:W:745:THR:OG1  | 3:W:748:LEU:HB3  | 2.19                     | 0.42              |
| 2:K:125:LYS:C    | 2:K:127:ILE:H    | 2.22                     | 0.42              |
| 2:D:227:PRO:HD3  | 2:D:277:PHE:CG   | 2.53                     | 0.42              |
| 2:J:227:PRO:HD3  | 2:J:277:PHE:CG   | 2.53                     | 0.42              |
| 2:E:154:LYS:HG2  | 2:E:186:SER:OG   | 2.19                     | 0.42              |
| 1:B:795:LEU:O    | 1:B:797:PRO:HD3  | 2.18                     | 0.42              |
| 2:F:148:THR:HB   | 2:F:149:GLY:H    | 1.64                     | 0.42              |
| 2:I:249:PHE:CE2  | 2:I:251:PRO:HG3  | 2.53                     | 0.42              |
| 2:J:249:PHE:CE2  | 2:J:251:PRO:HG3  | 2.53                     | 0.42              |
| 2:I:163:SER:HB3  | 2:I:181:TRP:CZ2  | 2.54                     | 0.42              |
| 1:B:701:GLN:N    | 1:B:701:GLN:CD   | 2.72                     | 0.42              |
| 1:A:587:LEU:HD22 | 1:A:587:LEU:C    | 2.39                     | 0.42              |
| 1:A:633:LEU:C    | 1:A:635:GLN:N    | 2.72                     | 0.42              |
| 1:B:346:ILE:HA   | 1:B:349:MET:HB2  | 2.01                     | 0.42              |
| 1:B:491:GLN:NE2  | 1:B:566:GLN:CG   | 2.79                     | 0.42              |
| 1:B:498:ARG:CD   | 2:I:32:GLN:HE21  | 2.32                     | 0.42              |
| 2:I:61:PHE:O     | 2:I:62:ASP:HB3   | 2.19                     | 0.42              |
| 2:I:14:ALA:C     | 2:I:18:ILE:HD12  | 2.39                     | 0.42              |
| 1:B:393:SER:H    | 1:B:573:THR:CG2  | 2.31                     | 0.42              |
| 3:W:441:VAL:HB   | 3:W:447:ILE:CD1  | 2.33                     | 0.42              |
| 1:A:124:ARG:C    | 1:A:125:ILE:HD12 | 2.37                     | 0.42              |
| 1:B:413:VAL:O    | 1:B:414:VAL:C    | 2.58                     | 0.42              |
| 1:B:308:LEU:HB3  | 1:B:310:LEU:CD2  | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:613:ASN:O    | 1:A:617:ARG:HG2  | 2.19                     | 0.42              |
| 2:D:14:ALA:O     | 2:D:16:ASP:N     | 2.52                     | 0.42              |
| 2:D:3:VAL:O      | 2:D:4:LEU:C      | 2.57                     | 0.42              |
| 2:C:4:LEU:O      | 2:C:5:TYR:C      | 2.58                     | 0.42              |
| 2:E:6:SER:C      | 2:E:8:SER:N      | 2.73                     | 0.42              |
| 2:E:150:PHE:HB2  | 2:E:152:PHE:HE1  | 1.81                     | 0.42              |
| 2:M:89:VAL:C     | 2:M:91:PHE:N     | 2.72                     | 0.42              |
| 2:I:51:ILE:O     | 2:I:54:LEU:HB3   | 2.19                     | 0.42              |
| 1:A:273:TYR:O    | 1:A:273:TYR:HD2  | 2.01                     | 0.42              |
| 2:M:227:PRO:HD3  | 2:M:277:PHE:CG   | 2.53                     | 0.42              |
| 2:L:227:PRO:HD3  | 2:L:277:PHE:CG   | 2.53                     | 0.42              |
| 2:G:227:PRO:HD3  | 2:G:277:PHE:CG   | 2.54                     | 0.42              |
| 2:C:225:LEU:HD13 | 2:C:277:PHE:CD2  | 2.53                     | 0.42              |
| 2:O:113:SER:O    | 2:O:117:ARG:HG3  | 2.18                     | 0.42              |
| 2:J:54:LEU:HD12  | 2:J:55:PRO:HD2   | 2.00                     | 0.42              |
| 2:K:169:SER:HA   | 2:K:176:LEU:HD23 | 2.00                     | 0.42              |
| 2:C:163:SER:HB3  | 2:C:181:TRP:CZ2  | 2.54                     | 0.42              |
| 2:C:169:SER:HA   | 2:C:176:LEU:HD23 | 2.00                     | 0.42              |
| 2:K:249:PHE:CE2  | 2:K:251:PRO:HG3  | 2.53                     | 0.42              |
| 1:A:370:ILE:O    | 1:A:374:ALA:CB   | 2.68                     | 0.42              |
| 1:A:391:THR:O    | 1:A:573:THR:HA   | 2.19                     | 0.42              |
| 1:A:548:ARG:NH1  | 1:A:877:MET:CA   | 2.78                     | 0.42              |
| 2:I:36:GLN:NE2   | 2:I:126:ARG:HD3  | 2.34                     | 0.42              |
| 1:A:510:LEU:HA   | 1:A:513:LEU:HD12 | 2.01                     | 0.42              |
| 1:B:636:LYS:O    | 1:B:637:LYS:CB   | 2.66                     | 0.42              |
| 2:L:106:ARG:H    | 2:L:106:ARG:CD   | 2.20                     | 0.42              |
| 1:A:775:ILE:C    | 1:A:777:LYS:N    | 2.71                     | 0.42              |
| 1:A:864:GLU:CD   | 1:A:865:PRO:HD2  | 2.40                     | 0.42              |
| 3:W:1034:HIS:O   | 3:W:1037:ALA:HB3 | 2.20                     | 0.42              |
| 2:D:27:VAL:CG2   | 2:D:31:ILE:HD11  | 2.49                     | 0.42              |
| 2:D:35:ASN:O     | 2:D:37:MET:N     | 2.53                     | 0.42              |
| 2:H:38:ILE:HG13  | 2:H:38:ILE:H     | 1.57                     | 0.42              |
| 2:C:26:ASN:N     | 2:C:26:ASN:OD1   | 2.52                     | 0.42              |
| 2:N:116:LEU:O    | 2:N:119:LEU:N    | 2.48                     | 0.42              |
| 2:C:111:PRO:HB3  | 2:C:116:LEU:HD23 | 2.01                     | 0.42              |
| 1:A:265:LEU:HB3  | 1:A:296:ALA:HB1  | 2.00                     | 0.42              |
| 1:B:380:LYS:O    | 1:B:381:THR:C    | 2.58                     | 0.42              |
| 2:N:273:TYR:C    | 2:N:274:GLN:HE21 | 2.21                     | 0.42              |
| 2:L:140:ASN:O    | 2:L:143:ASN:N    | 2.50                     | 0.42              |
| 2:I:17:LYS:HG2   | 2:K:130:ASP:HA   | 2.01                     | 0.42              |
| 3:W:409:LYS:HA   | 3:W:413:LYS:O    | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:69:THR:O     | 2:F:70:LEU:C     | 2.56                     | 0.42              |
| 2:E:63:PHE:N     | 2:E:63:PHE:CD1   | 2.87                     | 0.42              |
| 3:W:319:PHE:N    | 3:W:320:PRO:HD2  | 2.34                     | 0.42              |
| 1:A:321:ILE:O    | 1:A:322:THR:C    | 2.58                     | 0.42              |
| 1:A:383:ILE:HD11 | 1:A:550:LEU:CD2  | 2.49                     | 0.42              |
| 1:A:660:ASP:CA   | 1:B:539:ARG:NH1  | 2.83                     | 0.42              |
| 1:A:666:ARG:HA   | 1:A:669:LEU:HD12 | 2.00                     | 0.42              |
| 1:A:548:ARG:HH11 | 1:A:877:MET:N    | 2.17                     | 0.42              |
| 1:B:482:GLN:CA   | 1:B:493:LEU:HD22 | 2.49                     | 0.42              |
| 1:B:557:LEU:O    | 1:B:558:MET:C    | 2.58                     | 0.42              |
| 1:B:443:GLN:C    | 1:B:445:MET:H    | 2.21                     | 0.42              |
| 1:B:192:ASN:O    | 1:B:193:SER:HB3  | 2.19                     | 0.42              |
| 1:B:789:LEU:O    | 1:B:790:ARG:O    | 2.37                     | 0.42              |
| 2:L:24:TYR:O     | 2:L:26:ASN:N     | 2.52                     | 0.42              |
| 2:L:62:ASP:H     | 2:L:63:PHE:HD1   | 1.66                     | 0.42              |
| 1:B:239:VAL:CG2  | 1:B:844:SER:O    | 2.61                     | 0.42              |
| 1:B:853:ASP:O    | 1:B:854:LEU:CB   | 2.67                     | 0.42              |
| 2:E:4:LEU:O      | 2:E:5:TYR:C      | 2.57                     | 0.42              |
| 2:C:46:PHE:CE2   | 2:C:119:LEU:HD21 | 2.54                     | 0.42              |
| 2:J:131:ASN:ND2  | 2:J:131:ASN:N    | 2.67                     | 0.42              |
| 1:B:300:ARG:HA   | 1:B:301:PRO:HD3  | 1.76                     | 0.42              |
| 3:W:777:THR:HG23 | 3:W:882:LYS:HD2  | 2.00                     | 0.42              |
| 3:W:880:ASP:OD2  | 3:W:1069:LYS:HE3 | 2.19                     | 0.42              |
| 1:A:714:ARG:CG   | 1:A:720:TYR:HD2  | 2.32                     | 0.42              |
| 2:F:136:ILE:HG23 | 2:F:137:GLU:N    | 2.34                     | 0.42              |
| 2:K:139:TRP:HE1  | 2:K:143:ASN:HD22 | 1.66                     | 0.42              |
| 2:E:227:PRO:O    | 2:E:228:ASP:HB2  | 2.19                     | 0.42              |
| 2:C:227:PRO:O    | 2:C:228:ASP:HB2  | 2.20                     | 0.42              |
| 1:B:879:GLU:O    | 1:B:880:LEU:OXT  | 2.37                     | 0.42              |
| 2:F:168:ARG:HD2  | 2:F:175:ASN:O    | 2.20                     | 0.42              |
| 2:L:163:SER:HB3  | 2:L:181:TRP:CZ2  | 2.54                     | 0.42              |
| 2:N:163:SER:HB3  | 2:N:181:TRP:CZ2  | 2.54                     | 0.42              |
| 2:N:168:ARG:HD2  | 2:N:175:ASN:O    | 2.20                     | 0.42              |
| 2:F:123:LYS:HG3  | 2:F:124:PHE:CD1  | 2.53                     | 0.42              |
| 2:J:163:SER:HB3  | 2:J:181:TRP:CZ2  | 2.54                     | 0.42              |
| 3:W:61:GLU:O     | 3:W:61:GLU:HG2   | 2.19                     | 0.42              |
| 1:A:319:ASP:OD2  | 1:A:570:THR:HG22 | 2.19                     | 0.42              |
| 1:A:570:THR:CG2  | 1:A:571:LEU:N    | 2.74                     | 0.42              |
| 2:M:14:ALA:O     | 2:M:16:ASP:N     | 2.52                     | 0.42              |
| 2:N:21:GLY:O     | 2:N:22:THR:O     | 2.36                     | 0.42              |
| 2:N:34:PHE:O     | 2:N:37:MET:HB3   | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:400:ASN:O    | 1:A:403:SER:HB2  | 2.20                     | 0.42              |
| 2:E:24:TYR:CE1   | 2:E:31:ILE:HG13  | 2.54                     | 0.42              |
| 2:M:145:ARG:CB   | 2:M:145:ARG:HH11 | 2.32                     | 0.42              |
| 1:B:113:PRO:CG   | 1:B:609:ASN:HB3  | 2.49                     | 0.42              |
| 2:C:128:ASN:O    | 2:C:129:PHE:HB2  | 2.20                     | 0.42              |
| 2:K:23:LEU:H     | 2:K:26:ASN:ND2   | 2.17                     | 0.42              |
| 3:W:108:ASP:HA   | 3:W:111:ASN:HD22 | 1.83                     | 0.42              |
| 2:F:153:HIS:NE2  | 2:G:153:HIS:NE2  | 2.67                     | 0.42              |
| 2:G:89:VAL:C     | 2:G:91:PHE:N     | 2.73                     | 0.42              |
| 1:B:146:TRP:O    | 1:B:833:PHE:HB3  | 2.20                     | 0.42              |
| 2:G:136:ILE:HG23 | 2:G:137:GLU:N    | 2.33                     | 0.42              |
| 3:W:358:GLU:HG3  | 3:W:359:MET:N    | 2.33                     | 0.42              |
| 3:W:64:ASP:OD2   | 3:W:65:VAL:HG23  | 2.20                     | 0.42              |
| 2:O:227:PRO:O    | 2:O:228:ASP:HB2  | 2.20                     | 0.42              |
| 2:L:227:PRO:O    | 2:L:228:ASP:HB2  | 2.20                     | 0.42              |
| 2:G:163:SER:HB3  | 2:G:181:TRP:CZ2  | 2.54                     | 0.42              |
| 2:L:66:LEU:HB3   | 2:L:67:GLY:H     | 1.66                     | 0.42              |
| 2:I:168:ARG:HD2  | 2:I:175:ASN:O    | 2.20                     | 0.42              |
| 2:M:78:VAL:O     | 2:M:81:ALA:HB3   | 2.19                     | 0.42              |
| 1:A:546:LEU:HD21 | 1:A:588:ILE:HD12 | 1.99                     | 0.42              |
| 1:A:876:ILE:O    | 1:A:877:MET:CB   | 2.68                     | 0.42              |
| 1:B:555:GLU:OE2  | 1:B:871:PHE:CE2  | 2.69                     | 0.42              |
| 1:A:351:GLN:O    | 1:A:353:LEU:N    | 2.53                     | 0.42              |
| 1:A:443:GLN:HE22 | 1:A:522:PRO:HG3  | 1.84                     | 0.42              |
| 1:B:465:ASN:O    | 1:B:466:PHE:C    | 2.58                     | 0.42              |
| 2:M:3:VAL:O      | 2:M:4:LEU:C      | 2.57                     | 0.42              |
| 1:B:195:ASP:O    | 1:B:196:ALA:C    | 2.58                     | 0.42              |
| 1:B:199:VAL:HG13 | 1:B:242:PRO:O    | 2.20                     | 0.42              |
| 1:A:200:VAL:CG2  | 1:A:241:TYR:HD2  | 2.32                     | 0.42              |
| 2:O:6:SER:C      | 2:O:8:SER:N      | 2.73                     | 0.42              |
| 2:J:74:ASP:O     | 2:J:75:ALA:C     | 2.57                     | 0.42              |
| 2:J:6:SER:C      | 2:J:8:SER:N      | 2.73                     | 0.42              |
| 1:A:259:HIS:O    | 1:A:260:GLN:C    | 2.56                     | 0.42              |
| 3:W:999:ILE:HD11 | 3:W:1009:PHE:HD1 | 1.81                     | 0.42              |
| 2:C:9:LYS:HE3    | 2:C:13:ASP:OD1   | 2.19                     | 0.42              |
| 1:A:271:PHE:HA   | 1:A:274:ILE:CD1  | 2.47                     | 0.42              |
| 1:A:594:ILE:HG23 | 1:A:595:PRO:HD2  | 2.01                     | 0.42              |
| 1:A:593:VAL:HG12 | 1:A:594:ILE:N    | 2.35                     | 0.42              |
| 2:J:227:PRO:O    | 2:J:228:ASP:HB2  | 2.20                     | 0.42              |
| 2:N:101:VAL:HG12 | 2:N:350:ARG:HG2  | 2.01                     | 0.42              |
| 2:E:163:SER:HB3  | 2:E:181:TRP:CZ2  | 2.54                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:78:VAL:O     | 2:I:81:ALA:HB3   | 2.20                     | 0.42              |
| 2:G:168:ARG:HD2  | 2:G:175:ASN:O    | 2.20                     | 0.42              |
| 2:E:59:TRP:N     | 2:E:59:TRP:CD1   | 2.87                     | 0.42              |
| 1:B:390:ARG:HG3  | 1:B:391:THR:N    | 2.34                     | 0.42              |
| 1:B:496:ASN:HD22 | 1:B:498:ARG:CB   | 2.32                     | 0.42              |
| 1:A:571:LEU:CD2  | 1:B:531:ARG:CZ   | 2.97                     | 0.42              |
| 1:A:409:TRP:CH2  | 1:A:547:THR:OG1  | 2.71                     | 0.42              |
| 1:A:853:ASP:O    | 1:A:854:LEU:HB2  | 2.18                     | 0.42              |
| 1:B:243:SER:HB3  | 1:B:842:LEU:HD12 | 2.01                     | 0.42              |
| 1:A:709:ASP:OD2  | 1:A:820:THR:HG21 | 2.20                     | 0.42              |
| 1:A:125:ILE:H    | 1:A:125:ILE:HD12 | 1.77                     | 0.42              |
| 1:A:839:MET:CG   | 1:A:840:HIS:N    | 2.83                     | 0.42              |
| 1:B:409:TRP:CZ3  | 1:B:413:VAL:CG2  | 3.02                     | 0.42              |
| 1:A:775:ILE:HG13 | 1:A:775:ILE:H    | 1.35                     | 0.42              |
| 3:W:72:LEU:HG    | 3:W:861:LEU:HG   | 2.00                     | 0.42              |
| 3:W:840:ASN:HA   | 3:W:845:ILE:HG22 | 1.99                     | 0.42              |
| 2:G:9:LYS:HE3    | 2:G:13:ASP:OD1   | 2.19                     | 0.42              |
| 2:H:136:ILE:HG23 | 2:H:137:GLU:N    | 2.34                     | 0.42              |
| 1:A:211:ILE:C    | 1:A:213:GLN:H    | 2.23                     | 0.42              |
| 3:W:3:LYS:O      | 3:W:7:ILE:HG13   | 2.18                     | 0.42              |
| 3:W:114:MET:HB2  | 3:W:117:GLU:CG   | 2.50                     | 0.42              |
| 2:F:227:PRO:O    | 2:F:228:ASP:HB2  | 2.20                     | 0.42              |
| 2:N:227:PRO:O    | 2:N:228:ASP:HB2  | 2.19                     | 0.42              |
| 2:K:78:VAL:O     | 2:K:81:ALA:HB3   | 2.19                     | 0.42              |
| 2:E:168:ARG:HD2  | 2:E:175:ASN:O    | 2.20                     | 0.42              |
| 2:L:168:ARG:HD2  | 2:L:175:ASN:O    | 2.20                     | 0.42              |
| 1:B:482:GLN:O    | 1:B:483:VAL:CG2  | 2.68                     | 0.42              |
| 1:B:546:LEU:HD23 | 1:B:546:LEU:HA   | 1.81                     | 0.42              |
| 1:A:517:GLN:HG3  | 1:A:517:GLN:O    | 2.20                     | 0.42              |
| 2:O:23:LEU:HG    | 2:O:24:TYR:H     | 1.85                     | 0.42              |
| 2:L:42:ASN:HB3   | 2:L:62:ASP:N     | 2.35                     | 0.42              |
| 2:L:61:PHE:N     | 2:L:61:PHE:CD1   | 2.88                     | 0.42              |
| 1:A:440:PHE:O    | 1:A:441:GLY:C    | 2.58                     | 0.42              |
| 3:W:824:ASN:ND2  | 3:W:964:SER:HB2  | 2.35                     | 0.42              |
| 2:F:145:ARG:C    | 2:F:146:GLN:HG2  | 2.40                     | 0.42              |
| 1:A:850:VAL:C    | 1:A:851:TYR:CD1  | 2.93                     | 0.42              |
| 2:E:9:LYS:HE3    | 2:E:13:ASP:OD1   | 2.20                     | 0.42              |
| 3:W:200:PRO:O    | 3:W:201:TYR:C    | 2.58                     | 0.42              |
| 2:G:253:ILE:HG13 | 2:H:234:PHE:CE1  | 2.55                     | 0.42              |
| 2:L:125:LYS:C    | 2:L:127:ILE:H    | 2.22                     | 0.42              |
| 2:O:124:PHE:O    | 2:O:127:ILE:HG13 | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:355:ILE:HA   | 2:M:356:PRO:HD3  | 1.96                     | 0.42              |
| 2:M:163:SER:HB3  | 2:M:181:TRP:CZ2  | 2.55                     | 0.42              |
| 2:C:155:PRO:HA   | 2:C:337:ASP:HB2  | 2.02                     | 0.42              |
| 1:A:707:TYR:N    | 1:A:707:TYR:CD1  | 2.88                     | 0.42              |
| 1:A:487:GLY:O    | 1:A:488:VAL:CB   | 2.68                     | 0.42              |
| 1:B:454:THR:CG2  | 1:B:476:ASN:ND2  | 2.61                     | 0.42              |
| 2:J:73:LEU:HD22  | 2:J:77:TYR:CD2   | 2.54                     | 0.42              |
| 2:M:14:ALA:C     | 2:M:18:ILE:HD12  | 2.40                     | 0.42              |
| 2:M:7:LEU:HG     | 2:M:7:LEU:H      | 1.53                     | 0.42              |
| 2:N:14:ALA:O     | 2:N:16:ASP:N     | 2.53                     | 0.42              |
| 2:N:4:LEU:O      | 2:N:5:TYR:C      | 2.58                     | 0.42              |
| 1:B:253:ASN:O    | 1:B:256:PHE:HB2  | 2.20                     | 0.42              |
| 1:B:646:LEU:H    | 1:B:646:LEU:HG   | 1.51                     | 0.42              |
| 1:B:183:LEU:O    | 1:B:184:LYS:C    | 2.57                     | 0.42              |
| 1:B:310:LEU:H    | 1:B:310:LEU:HG   | 1.44                     | 0.42              |
| 1:A:216:GLU:N    | 1:A:216:GLU:OE1  | 2.50                     | 0.42              |
| 1:B:570:THR:HG22 | 1:B:571:LEU:N    | 2.34                     | 0.42              |
| 1:B:856:ALA:C    | 1:B:858:VAL:N    | 2.72                     | 0.42              |
| 3:W:827:VAL:O    | 3:W:831:ILE:HG13 | 2.20                     | 0.42              |
| 2:E:129:PHE:CE1  | 2:E:130:ASP:HB3  | 2.54                     | 0.42              |
| 2:E:3:VAL:O      | 2:E:4:LEU:C      | 2.57                     | 0.42              |
| 2:O:153:HIS:C    | 2:O:155:PRO:N    | 2.71                     | 0.42              |
| 2:I:397:LYS:NZ   | 2:K:150:PHE:HA   | 2.34                     | 0.42              |
| 2:I:104:SER:HB3  | 2:I:108:GLY:HA2  | 2.02                     | 0.42              |
| 2:K:9:LYS:HE3    | 2:K:13:ASP:OD1   | 2.20                     | 0.42              |
| 1:A:141:GLU:O    | 1:A:142:LEU:HD12 | 2.20                     | 0.42              |
| 2:J:253:ILE:HG13 | 2:K:234:PHE:CE1  | 2.55                     | 0.42              |
| 3:W:922:GLU:HG3  | 3:W:991:SER:OG   | 2.20                     | 0.42              |
| 2:K:227:PRO:O    | 2:K:228:ASP:HB2  | 2.20                     | 0.42              |
| 2:E:61:PHE:CD1   | 2:E:61:PHE:N     | 2.87                     | 0.42              |
| 2:D:163:SER:HB3  | 2:D:181:TRP:CZ2  | 2.54                     | 0.42              |
| 3:W:516:VAL:HG21 | 3:W:675:ILE:HG21 | 2.01                     | 0.42              |
| 3:W:214:LEU:C    | 3:W:214:LEU:HD12 | 2.40                     | 0.42              |
| 1:A:492:VAL:CG1  | 1:A:493:LEU:N    | 2.82                     | 0.42              |
| 1:B:544:VAL:HG12 | 1:B:548:ARG:HE   | 1.83                     | 0.42              |
| 2:I:35:ASN:O     | 2:I:37:MET:N     | 2.52                     | 0.42              |
| 2:K:4:LEU:O      | 2:K:5:TYR:C      | 2.58                     | 0.42              |
| 1:A:201:ASP:O    | 1:A:204:THR:N    | 2.52                     | 0.42              |
| 1:B:746:GLN:HE22 | 2:D:64:GLY:HA2   | 1.85                     | 0.42              |
| 2:G:23:LEU:HD23  | 2:G:25:SER:H     | 1.85                     | 0.42              |
| 2:I:74:ASP:O     | 2:I:75:ALA:C     | 2.57                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:695:ALA:O    | 1:A:696:SER:HB3  | 2.20                     | 0.42              |
| 2:H:3:VAL:O      | 2:H:4:LEU:C      | 2.58                     | 0.42              |
| 1:A:134:TYR:CE1  | 1:A:803:ASN:CG   | 2.93                     | 0.42              |
| 2:O:1:MET:HG3    | 2:O:2:ASP:N      | 2.34                     | 0.42              |
| 3:W:169:LEU:HG   | 3:W:223:TYR:HE1  | 1.85                     | 0.42              |
| 2:K:35:ASN:O     | 2:K:37:MET:N     | 2.53                     | 0.42              |
| 2:E:14:ALA:O     | 2:E:16:ASP:N     | 2.52                     | 0.42              |
| 2:O:239:ASN:ND2  | 2:O:246:THR:HG22 | 2.29                     | 0.42              |
| 1:A:810:TYR:O    | 1:A:813:ALA:N    | 2.53                     | 0.42              |
| 2:H:152:PHE:O    | 2:H:328:SER:HA   | 2.19                     | 0.42              |
| 1:B:148:TRP:NE1  | 1:B:833:PHE:HD1  | 2.18                     | 0.42              |
| 1:B:287:ASN:HD22 | 1:B:287:ASN:HA   | 1.60                     | 0.42              |
| 2:K:61:PHE:CD1   | 2:K:61:PHE:N     | 2.88                     | 0.42              |
| 2:M:227:PRO:O    | 2:M:228:ASP:HB2  | 2.20                     | 0.42              |
| 3:W:516:VAL:N    | 3:W:671:SER:O    | 2.52                     | 0.42              |
| 2:D:51:ILE:O     | 2:D:52:GLY:C     | 2.58                     | 0.42              |
| 2:H:163:SER:HB3  | 2:H:181:TRP:CZ2  | 2.54                     | 0.42              |
| 2:C:168:ARG:HD2  | 2:C:175:ASN:O    | 2.20                     | 0.42              |
| 2:K:51:ILE:O     | 2:K:51:ILE:HG23  | 2.20                     | 0.42              |
| 2:N:59:TRP:CD1   | 2:N:59:TRP:N     | 2.88                     | 0.42              |
| 1:B:501:HIS:O    | 1:B:503:ILE:N    | 2.53                     | 0.41              |
| 2:I:27:VAL:O     | 2:I:31:ILE:HG12  | 2.19                     | 0.41              |
| 3:W:962:LEU:HD22 | 3:W:967:ILE:HG12 | 2.02                     | 0.41              |
| 1:A:853:ASP:OD1  | 1:A:854:LEU:N    | 2.53                     | 0.41              |
| 1:A:162:VAL:O    | 1:A:165:TYR:HB3  | 2.20                     | 0.41              |
| 1:B:224:PHE:CE1  | 2:O:71:LEU:N     | 2.87                     | 0.41              |
| 3:W:441:VAL:HG11 | 3:W:465:LEU:HD22 | 2.02                     | 0.41              |
| 1:B:526:LYS:O    | 1:B:530:GLN:HG2  | 2.20                     | 0.41              |
| 3:W:542:LEU:HD11 | 3:W:561:TYR:HD2  | 1.85                     | 0.41              |
| 1:A:129:ARG:HG2  | 1:A:130:GLN:H    | 1.84                     | 0.41              |
| 2:E:239:ASN:ND2  | 2:E:246:THR:HG22 | 2.30                     | 0.41              |
| 2:E:89:VAL:C     | 2:E:91:PHE:N     | 2.73                     | 0.41              |
| 2:N:89:VAL:C     | 2:N:91:PHE:N     | 2.71                     | 0.41              |
| 2:N:76:ASN:HA    | 2:O:75:ALA:HB3   | 2.01                     | 0.41              |
| 2:O:125:LYS:O    | 2:O:127:ILE:N    | 2.51                     | 0.41              |
| 2:C:235:PRO:HA   | 2:C:249:PHE:O    | 2.20                     | 0.41              |
| 2:H:227:PRO:O    | 2:H:228:ASP:HB2  | 2.20                     | 0.41              |
| 2:L:235:PRO:HA   | 2:L:249:PHE:O    | 2.20                     | 0.41              |
| 2:E:106:ARG:HB3  | 2:E:107:ASN:H    | 1.54                     | 0.41              |
| 1:A:174:LEU:HA   | 1:A:177:MET:HB2  | 2.01                     | 0.41              |
| 2:L:124:PHE:O    | 2:L:126:ARG:N    | 2.53                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:842:LEU:HD23 | 1:A:842:LEU:HA   | 1.76                     | 0.41              |
| 1:A:493:LEU:HD11 | 1:A:566:GLN:O    | 2.20                     | 0.41              |
| 1:A:656:ARG:O    | 1:A:657:VAL:HG23 | 2.20                     | 0.41              |
| 1:B:383:ILE:O    | 1:B:384:ALA:C    | 2.57                     | 0.41              |
| 1:A:404:LEU:HD22 | 1:A:435:ILE:HD11 | 2.02                     | 0.41              |
| 1:B:466:PHE:CE1  | 2:H:80:THR:HG22  | 2.55                     | 0.41              |
| 2:O:38:ILE:HG22  | 2:O:42:ASN:ND2   | 2.33                     | 0.41              |
| 1:B:371:ASN:O    | 1:B:372:SER:C    | 2.58                     | 0.41              |
| 1:A:275:PRO:C    | 1:A:277:ARG:H    | 2.23                     | 0.41              |
| 1:A:275:PRO:CG   | 1:A:278:ILE:HD11 | 2.50                     | 0.41              |
| 1:A:124:ARG:HD2  | 1:A:203:GLU:OE1  | 2.20                     | 0.41              |
| 2:C:142:GLN:OE1  | 2:N:145:ARG:NH1  | 2.48                     | 0.41              |
| 1:B:406:SER:O    | 1:B:409:TRP:N    | 2.51                     | 0.41              |
| 2:D:1:MET:O      | 2:D:2:ASP:C      | 2.56                     | 0.41              |
| 2:D:4:LEU:O      | 2:D:5:TYR:C      | 2.58                     | 0.41              |
| 1:A:314:PHE:HZ   | 1:A:664:ARG:HG2  | 1.84                     | 0.41              |
| 2:D:116:LEU:O    | 2:D:119:LEU:N    | 2.50                     | 0.41              |
| 1:A:848:PHE:C    | 1:A:849:THR:OG1  | 2.58                     | 0.41              |
| 3:W:729:ARG:HH11 | 3:W:770:ASP:CG   | 2.22                     | 0.41              |
| 2:D:133:SER:O    | 2:D:134:GLU:C    | 2.59                     | 0.41              |
| 2:D:70:LEU:CD1   | 2:D:71:LEU:N     | 2.82                     | 0.41              |
| 2:E:74:ASP:O     | 2:E:75:ALA:C     | 2.58                     | 0.41              |
| 2:F:234:PHE:CE1  | 2:H:253:ILE:HG13 | 2.55                     | 0.41              |
| 2:G:125:LYS:C    | 2:G:127:ILE:H    | 2.24                     | 0.41              |
| 2:C:234:PHE:CE1  | 2:E:253:ILE:HG13 | 2.55                     | 0.41              |
| 2:F:27:VAL:O     | 2:F:31:ILE:HG12  | 2.20                     | 0.41              |
| 2:M:155:PRO:O    | 2:M:186:SER:HB3  | 2.20                     | 0.41              |
| 2:K:168:ARG:HD2  | 2:K:175:ASN:O    | 2.20                     | 0.41              |
| 2:H:168:ARG:HD2  | 2:H:175:ASN:O    | 2.20                     | 0.41              |
| 1:B:721:VAL:CG1  | 1:B:722:ASN:H    | 2.30                     | 0.41              |
| 1:A:382:LEU:O    | 1:A:385:ALA:HB3  | 2.20                     | 0.41              |
| 2:G:144:ARG:O    | 2:G:145:ARG:CB   | 2.67                     | 0.41              |
| 1:B:456:PHE:O    | 1:B:457:GLN:O    | 2.38                     | 0.41              |
| 2:I:14:ALA:O     | 2:I:16:ASP:N     | 2.53                     | 0.41              |
| 2:M:6:SER:C      | 2:M:8:SER:N      | 2.73                     | 0.41              |
| 1:B:646:LEU:O    | 1:B:649:LEU:HB2  | 2.20                     | 0.41              |
| 1:A:236:ARG:HB2  | 1:A:238:VAL:CG2  | 2.47                     | 0.41              |
| 1:A:647:LYS:HG2  | 1:A:654:VAL:HG21 | 1.99                     | 0.41              |
| 2:O:4:LEU:O      | 2:O:5:TYR:C      | 2.58                     | 0.41              |
| 2:L:151:THR:C    | 2:L:152:PHE:CD1  | 2.94                     | 0.41              |
| 2:L:6:SER:C      | 2:L:8:SER:N      | 2.73                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:34:PHE:O     | 2:K:37:MET:HB3   | 2.20                     | 0.41              |
| 2:E:128:ASN:O    | 2:E:129:PHE:CB   | 2.68                     | 0.41              |
| 2:E:35:ASN:O     | 2:E:37:MET:N     | 2.53                     | 0.41              |
| 2:N:239:ASN:ND2  | 2:N:246:THR:HG22 | 2.29                     | 0.41              |
| 2:M:153:HIS:NE2  | 2:N:153:HIS:CD2  | 2.88                     | 0.41              |
| 2:J:239:ASN:ND2  | 2:J:246:THR:HG22 | 2.29                     | 0.41              |
| 3:W:718:ILE:HG23 | 3:W:771:PHE:CE1  | 2.55                     | 0.41              |
| 3:W:449:LEU:HD21 | 3:W:461:ILE:HD13 | 2.02                     | 0.41              |
| 2:M:253:ILE:HG13 | 2:N:234:PHE:CE1  | 2.55                     | 0.41              |
| 1:A:170:TYR:CZ   | 1:A:682:PHE:HB2  | 2.55                     | 0.41              |
| 2:L:48:THR:O     | 2:L:56:ILE:HA    | 2.20                     | 0.41              |
| 2:G:235:PRO:HA   | 2:G:249:PHE:O    | 2.21                     | 0.41              |
| 3:W:992:TYR:CE2  | 3:W:996:LEU:HD11 | 2.56                     | 0.41              |
| 2:D:168:ARG:HD2  | 2:D:175:ASN:O    | 2.20                     | 0.41              |
| 2:N:148:THR:OG1  | 2:N:332:GLU:HG2  | 2.20                     | 0.41              |
| 1:A:414:VAL:C    | 1:A:416:ASN:H    | 2.22                     | 0.41              |
| 1:A:163:ARG:NE   | 1:A:631:LEU:O    | 2.54                     | 0.41              |
| 1:B:275:PRO:HB2  | 1:B:278:ILE:HD13 | 2.03                     | 0.41              |
| 1:B:322:THR:HG22 | 1:B:390:ARG:HD3  | 2.02                     | 0.41              |
| 1:B:449:ASN:ND2  | 1:B:455:PRO:HB3  | 2.36                     | 0.41              |
| 2:O:61:PHE:N     | 2:O:61:PHE:CD1   | 2.87                     | 0.41              |
| 1:B:743:ASP:OD2  | 1:B:745:ALA:CA   | 2.68                     | 0.41              |
| 2:G:35:ASN:O     | 2:G:37:MET:N     | 2.54                     | 0.41              |
| 3:W:438:ILE:HD11 | 3:W:563:GLN:CG   | 2.50                     | 0.41              |
| 1:A:807:ASN:C    | 1:A:809:PHE:N    | 2.73                     | 0.41              |
| 2:D:14:ALA:C     | 2:D:18:ILE:HD12  | 2.41                     | 0.41              |
| 2:M:35:ASN:O     | 2:M:37:MET:N     | 2.53                     | 0.41              |
| 2:D:34:PHE:O     | 2:D:37:MET:HB3   | 2.20                     | 0.41              |
| 2:J:149:GLY:C    | 2:J:150:PHE:CD1  | 2.94                     | 0.41              |
| 2:C:153:HIS:CD2  | 2:E:153:HIS:CE1  | 3.08                     | 0.41              |
| 2:F:6:SER:C      | 2:F:8:SER:N      | 2.73                     | 0.41              |
| 2:O:74:ASP:O     | 2:O:75:ALA:C     | 2.58                     | 0.41              |
| 2:C:253:ILE:HG13 | 2:D:234:PHE:CE1  | 2.55                     | 0.41              |
| 2:N:78:VAL:O     | 2:N:81:ALA:N     | 2.39                     | 0.41              |
| 1:B:776:ALA:O    | 1:B:777:LYS:C    | 2.58                     | 0.41              |
| 3:W:34:LEU:O     | 3:W:37:ARG:HB2   | 2.20                     | 0.41              |
| 2:M:66:LEU:O     | 2:M:67:GLY:C     | 2.58                     | 0.41              |
| 3:W:619:HIS:ND1  | 3:W:619:HIS:N    | 2.65                     | 0.41              |
| 1:B:735:LEU:CG   | 1:B:760:VAL:O    | 2.59                     | 0.41              |
| 1:B:807:ASN:C    | 1:B:809:PHE:H    | 2.23                     | 0.41              |
| 1:B:812:VAL:C    | 1:B:814:ASN:H    | 2.23                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:542:GLN:N    | 1:A:542:GLN:OE1  | 2.53                     | 0.41              |
| 2:G:11:LEU:HA    | 2:G:14:ALA:HB3   | 2.02                     | 0.41              |
| 2:G:34:PHE:O     | 2:G:37:MET:HB3   | 2.20                     | 0.41              |
| 3:W:292:LEU:HD13 | 3:W:308:GLN:NE2  | 2.35                     | 0.41              |
| 2:D:6:SER:C      | 2:D:8:SER:N      | 2.73                     | 0.41              |
| 2:H:34:PHE:O     | 2:H:37:MET:HB3   | 2.20                     | 0.41              |
| 2:H:9:LYS:HE3    | 2:H:13:ASP:OD1   | 2.20                     | 0.41              |
| 2:L:9:LYS:HE3    | 2:L:13:ASP:OD1   | 2.21                     | 0.41              |
| 3:W:191:TYR:CZ   | 3:W:204:VAL:HG11 | 2.56                     | 0.41              |
| 2:D:74:ASP:O     | 2:D:75:ALA:C     | 2.59                     | 0.41              |
| 2:N:74:ASP:O     | 2:N:75:ALA:C     | 2.58                     | 0.41              |
| 2:D:253:ILE:HG13 | 2:E:234:PHE:CE1  | 2.55                     | 0.41              |
| 3:W:908:GLN:O    | 3:W:912:GLN:HG3  | 2.21                     | 0.41              |
| 3:W:467:TYR:O    | 3:W:471:ILE:HD13 | 2.20                     | 0.41              |
| 2:D:227:PRO:O    | 2:D:228:ASP:HB2  | 2.20                     | 0.41              |
| 2:O:53:ASN:HD22  | 2:O:354:ALA:HB3  | 1.86                     | 0.41              |
| 1:B:191:LYS:HD3  | 1:B:191:LYS:HA   | 1.90                     | 0.41              |
| 1:B:712:LEU:HG   | 1:B:721:VAL:O    | 2.19                     | 0.41              |
| 1:B:493:LEU:CD1  | 1:B:567:HIS:HB2  | 2.50                     | 0.41              |
| 2:I:3:VAL:O      | 2:I:4:LEU:C      | 2.57                     | 0.41              |
| 1:A:855:LEU:O    | 1:A:856:ALA:C    | 2.56                     | 0.41              |
| 1:B:190:ASN:HB2  | 1:B:199:VAL:CG2  | 2.50                     | 0.41              |
| 1:B:786:ILE:O    | 1:B:787:VAL:C    | 2.59                     | 0.41              |
| 2:O:14:ALA:O     | 2:O:16:ASP:N     | 2.52                     | 0.41              |
| 1:B:270:ILE:HG23 | 1:B:854:LEU:HD21 | 2.03                     | 0.41              |
| 2:D:239:ASN:ND2  | 2:D:246:THR:HG22 | 2.29                     | 0.41              |
| 2:I:239:ASN:ND2  | 2:I:246:THR:HG22 | 2.30                     | 0.41              |
| 3:W:934:ILE:HG23 | 3:W:965:LEU:CD1  | 2.49                     | 0.41              |
| 3:W:772:ILE:HD11 | 3:W:1047:LYS:HB2 | 2.02                     | 0.41              |
| 2:I:234:PHE:CE1  | 2:K:253:ILE:HG13 | 2.55                     | 0.41              |
| 2:I:253:ILE:HG13 | 2:J:234:PHE:CE1  | 2.55                     | 0.41              |
| 3:W:574:GLN:HG2  | 3:W:581:ILE:CG2  | 2.50                     | 0.41              |
| 2:I:235:PRO:HA   | 2:I:249:PHE:O    | 2.21                     | 0.41              |
| 2:J:59:TRP:N     | 2:J:59:TRP:CD1   | 2.86                     | 0.41              |
| 3:W:255:VAL:HG23 | 3:W:310:TRP:CH2  | 2.56                     | 0.41              |
| 1:A:396:PHE:CD2  | 1:A:578:LEU:HD11 | 2.56                     | 0.41              |
| 1:A:304:LEU:H    | 1:A:615:ASN:ND2  | 2.19                     | 0.41              |
| 1:A:405:ILE:O    | 1:A:408:MET:HB2  | 2.21                     | 0.41              |
| 2:L:21:GLY:O     | 2:L:22:THR:O     | 2.38                     | 0.41              |
| 1:B:178:PRO:CD   | 1:B:256:PHE:CE2  | 3.04                     | 0.41              |
| 2:O:35:ASN:O     | 2:O:37:MET:N     | 2.53                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:166:PHE:CE2  | 1:B:689:MET:CA   | 2.99                     | 0.41              |
| 2:J:11:LEU:HA    | 2:J:14:ALA:HB3   | 2.03                     | 0.41              |
| 2:J:14:ALA:O     | 2:J:18:ILE:HD12  | 2.21                     | 0.41              |
| 1:B:521:MET:SD   | 1:B:521:MET:N    | 2.94                     | 0.41              |
| 1:A:178:PRO:CD   | 1:A:256:PHE:HE2  | 2.32                     | 0.41              |
| 2:C:61:PHE:CD1   | 2:C:61:PHE:N     | 2.89                     | 0.41              |
| 1:A:679:LEU:O    | 1:A:681:ILE:N    | 2.54                     | 0.41              |
| 2:C:6:SER:C      | 2:C:8:SER:N      | 2.74                     | 0.41              |
| 1:B:136:ALA:O    | 1:B:137:ASN:HB3  | 2.21                     | 0.41              |
| 1:A:345:GLN:HG3  | 1:A:349:MET:CE   | 2.51                     | 0.41              |
| 3:W:229:LEU:HD21 | 3:W:244:VAL:HG21 | 2.01                     | 0.41              |
| 2:F:253:ILE:HG13 | 2:G:234:PHE:CE1  | 2.55                     | 0.41              |
| 3:W:54:SER:O     | 3:W:55:LEU:HD23  | 2.20                     | 0.41              |
| 2:D:124:PHE:CD1  | 2:D:124:PHE:N    | 2.89                     | 0.41              |
| 2:K:110:ALA:HB1  | 2:K:111:PRO:CD   | 2.50                     | 0.41              |
| 2:M:235:PRO:HA   | 2:M:249:PHE:O    | 2.21                     | 0.41              |
| 2:G:227:PRO:O    | 2:G:228:ASP:HB2  | 2.20                     | 0.41              |
| 3:W:205:THR:HG23 | 3:W:206:TRP:N    | 2.36                     | 0.41              |
| 1:B:552:TYR:O    | 1:B:553:ASN:C    | 2.58                     | 0.41              |
| 1:B:515:ARG:O    | 1:B:515:ARG:HG3  | 2.21                     | 0.41              |
| 1:B:721:VAL:HG12 | 1:B:799:LEU:HD21 | 1.98                     | 0.41              |
| 1:A:310:LEU:HD11 | 1:A:614:TYR:OH   | 2.21                     | 0.41              |
| 1:A:503:ILE:HG13 | 1:A:503:ILE:H    | 1.72                     | 0.41              |
| 2:L:23:LEU:HD22  | 2:L:72:ASN:OD1   | 2.21                     | 0.41              |
| 2:N:7:LEU:H      | 2:N:7:LEU:HG     | 1.54                     | 0.41              |
| 1:A:701:GLN:CB   | 1:A:826:TYR:HD2  | 2.33                     | 0.41              |
| 1:B:252:PHE:O    | 1:B:253:ASN:C    | 2.59                     | 0.41              |
| 1:A:120:THR:HB   | 1:A:121:LYS:H    | 1.66                     | 0.41              |
| 2:L:35:ASN:OD1   | 2:L:65:LEU:HD22  | 2.21                     | 0.41              |
| 2:G:14:ALA:O     | 2:G:16:ASP:N     | 2.54                     | 0.41              |
| 2:H:6:SER:C      | 2:H:8:SER:N      | 2.74                     | 0.41              |
| 2:L:150:PHE:O    | 2:L:330:VAL:HG13 | 2.20                     | 0.41              |
| 2:C:145:ARG:CB   | 2:C:145:ARG:NH1  | 2.79                     | 0.41              |
| 3:W:690:ARG:HH11 | 3:W:690:ARG:CB   | 2.34                     | 0.41              |
| 2:D:9:LYS:HE3    | 2:D:13:ASP:OD1   | 2.21                     | 0.41              |
| 2:I:153:HIS:CD2  | 2:K:153:HIS:CE1  | 3.08                     | 0.41              |
| 2:J:136:ILE:HD12 | 2:J:139:TRP:HB3  | 2.03                     | 0.41              |
| 1:B:286:LEU:O    | 1:B:287:ASN:ND2  | 2.54                     | 0.41              |
| 3:W:200:PRO:O    | 3:W:203:LEU:N    | 2.54                     | 0.41              |
| 3:W:802:ILE:O    | 3:W:808:PHE:HB2  | 2.21                     | 0.41              |
| 2:L:253:ILE:HG13 | 2:M:234:PHE:CE1  | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:124:PHE:CD1  | 2:M:124:PHE:N    | 2.89                     | 0.41              |
| 2:H:235:PRO:HA   | 2:H:249:PHE:O    | 2.21                     | 0.41              |
| 2:C:100:MET:HG3  | 2:C:388:VAL:HG11 | 2.01                     | 0.41              |
| 2:M:168:ARG:HD2  | 2:M:175:ASN:O    | 2.20                     | 0.41              |
| 2:O:168:ARG:HD2  | 2:O:175:ASN:O    | 2.20                     | 0.41              |
| 3:W:887:VAL:HG12 | 3:W:1054:LEU:HG  | 2.02                     | 0.41              |
| 1:B:159:ASP:OD2  | 1:B:761:GLY:CA   | 2.69                     | 0.41              |
| 1:B:771:VAL:O    | 1:B:775:ILE:HD13 | 2.21                     | 0.41              |
| 1:A:374:ALA:HB1  | 1:A:580:SER:HA   | 2.02                     | 0.41              |
| 1:B:349:MET:HB2  | 1:B:349:MET:HE2  | 1.88                     | 0.41              |
| 1:B:489:LEU:HD23 | 1:B:489:LEU:C    | 2.41                     | 0.41              |
| 1:A:382:LEU:HD12 | 1:A:382:LEU:HA   | 1.60                     | 0.41              |
| 1:A:622:VAL:O    | 1:A:623:ALA:C    | 2.59                     | 0.41              |
| 1:B:492:VAL:O    | 1:B:493:LEU:O    | 2.38                     | 0.41              |
| 1:A:472:LEU:HD23 | 1:A:472:LEU:N    | 2.36                     | 0.41              |
| 1:A:287:ASN:O    | 1:A:858:VAL:HA   | 2.20                     | 0.41              |
| 2:N:124:PHE:C    | 2:N:126:ARG:H    | 2.24                     | 0.41              |
| 2:O:34:PHE:O     | 2:O:35:ASN:C     | 2.59                     | 0.41              |
| 2:O:23:LEU:CG    | 2:O:24:TYR:N     | 2.83                     | 0.41              |
| 1:B:791:LYS:O    | 1:B:792:VAL:CG1  | 2.66                     | 0.41              |
| 1:A:782:VAL:CG2  | 1:A:798:ILE:HD11 | 2.51                     | 0.41              |
| 1:A:756:PRO:C    | 1:A:757:VAL:CG2  | 2.89                     | 0.41              |
| 2:L:26:ASN:OD1   | 2:N:33:GLN:HB2   | 2.21                     | 0.41              |
| 1:B:763:LEU:HD23 | 1:B:763:LEU:HA   | 1.80                     | 0.41              |
| 3:W:499:GLN:NE2  | 3:W:689:PHE:HE1  | 2.19                     | 0.41              |
| 1:A:368:THR:HG23 | 1:A:579:THR:O    | 2.21                     | 0.41              |
| 2:O:5:TYR:CE2    | 2:O:131:ASN:HA   | 2.55                     | 0.41              |
| 2:E:23:LEU:HD22  | 2:E:25:SER:OG    | 2.21                     | 0.41              |
| 2:D:128:ASN:HD22 | 2:E:19:VAL:CG2   | 2.34                     | 0.41              |
| 1:A:862:THR:HG22 | 1:A:863:VAL:N    | 2.36                     | 0.41              |
| 1:A:283:ASN:HD21 | 1:A:869:VAL:H    | 1.69                     | 0.41              |
| 2:L:4:LEU:O      | 2:L:5:TYR:C      | 2.59                     | 0.41              |
| 2:L:14:ALA:O     | 2:L:16:ASP:N     | 2.54                     | 0.41              |
| 2:D:31:ILE:O     | 2:D:32:GLN:C     | 2.59                     | 0.41              |
| 2:C:33:GLN:O     | 2:C:36:GLN:HB3   | 2.21                     | 0.41              |
| 3:W:169:LEU:HD21 | 3:W:227:LYS:HG3  | 2.03                     | 0.41              |
| 2:O:152:PHE:CD1  | 2:O:152:PHE:N    | 2.89                     | 0.41              |
| 2:J:27:VAL:O     | 2:J:28:SER:C     | 2.57                     | 0.41              |
| 2:I:397:LYS:HZ1  | 2:K:150:PHE:HA   | 1.86                     | 0.41              |
| 3:W:503:TYR:HB2  | 3:W:687:ILE:HD13 | 2.02                     | 0.41              |
| 2:I:9:LYS:HE3    | 2:I:13:ASP:OD1   | 2.20                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:24:TYR:C     | 2:F:26:ASN:H      | 2.24                     | 0.41              |
| 2:F:9:LYS:HE3    | 2:F:13:ASP:OD1    | 2.21                     | 0.41              |
| 2:J:9:LYS:HE3    | 2:J:13:ASP:OD1    | 2.21                     | 0.41              |
| 2:O:147:ARG:O    | 2:O:148:THR:CB    | 2.66                     | 0.41              |
| 1:A:601:PHE:CD1  | 1:A:601:PHE:N     | 2.80                     | 0.41              |
| 2:F:135:TYR:CZ   | 2:F:342:MET:HE3   | 2.56                     | 0.41              |
| 2:H:91:PHE:O     | 2:H:95:VAL:HG23   | 2.21                     | 0.41              |
| 3:W:884:PHE:CG   | 3:W:1058:TYR:CD1  | 3.09                     | 0.41              |
| 2:I:106:ARG:HG2  | 2:I:107:ASN:H     | 1.84                     | 0.41              |
| 3:W:802:ILE:HG13 | 3:W:808:PHE:HD2   | 1.85                     | 0.41              |
| 2:I:72:ASN:CG    | 2:K:126:ARG:NH1   | 2.74                     | 0.41              |
| 1:A:202:SER:O    | 1:A:205:ALA:HB3   | 2.21                     | 0.41              |
| 2:I:227:PRO:O    | 2:I:228:ASP:HB2   | 2.20                     | 0.41              |
| 2:D:235:PRO:HA   | 2:D:249:PHE:O     | 2.21                     | 0.41              |
| 3:W:1078:SER:HA  | 3:W:1079:PRO:HD3  | 1.76                     | 0.41              |
| 3:W:133:ALA:CB   | 3:W:701:ARG:HG3   | 2.50                     | 0.41              |
| 3:W:675:ILE:C    | 3:W:675:ILE:HD12  | 2.41                     | 0.41              |
| 3:W:810:ASN:O    | 3:W:814:ARG:HB2   | 2.20                     | 0.41              |
| 3:W:871:LYS:HD3  | 3:W:1074:THR:HG21 | 2.01                     | 0.41              |
| 2:L:1:MET:O      | 2:L:2:ASP:C       | 2.59                     | 0.41              |
| 1:A:552:TYR:O    | 1:A:553:ASN:C     | 2.59                     | 0.41              |
| 2:J:168:ARG:HD2  | 2:J:175:ASN:O     | 2.20                     | 0.41              |
| 1:A:370:ILE:HD11 | 3:W:933:LEU:HA    | 2.01                     | 0.41              |
| 1:B:415:PRO:HB3  | 1:B:480:PHE:HB2   | 2.01                     | 0.41              |
| 2:I:16:ASP:HB3   | 2:K:131:ASN:C     | 2.42                     | 0.41              |
| 2:N:34:PHE:O     | 2:N:35:ASN:C      | 2.59                     | 0.41              |
| 1:A:763:LEU:HA   | 1:A:764:PRO:HD3   | 1.68                     | 0.41              |
| 1:B:229:ARG:HD2  | 1:B:230:GLN:NE2   | 2.31                     | 0.41              |
| 3:W:929:ALA:N    | 3:W:984:ASP:OD2   | 2.53                     | 0.41              |
| 1:B:672:LEU:O    | 1:B:673:PRO:O     | 2.38                     | 0.41              |
| 2:L:42:ASN:CB    | 2:L:62:ASP:HA     | 2.51                     | 0.41              |
| 1:B:451:ASP:N    | 1:B:452:PRO:CD    | 2.82                     | 0.41              |
| 2:H:14:ALA:O     | 2:H:16:ASP:N      | 2.54                     | 0.41              |
| 1:A:771:VAL:HG12 | 1:A:809:PHE:CB    | 2.51                     | 0.41              |
| 2:D:34:PHE:O     | 2:D:35:ASN:C      | 2.59                     | 0.41              |
| 1:A:609:ASN:O    | 1:A:610:PHE:C     | 2.59                     | 0.41              |
| 2:C:5:TYR:HE2    | 2:C:130:ASP:O     | 2.04                     | 0.41              |
| 2:J:27:VAL:O     | 2:J:31:ILE:HG12   | 2.20                     | 0.41              |
| 1:B:379:PHE:O    | 1:B:380:LYS:C     | 2.59                     | 0.41              |
| 1:B:207:ILE:H    | 1:B:207:ILE:HG13  | 1.62                     | 0.41              |
| 2:C:67:GLY:C     | 2:C:69:THR:N      | 2.72                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:74:ASP:O     | 2:F:75:ALA:C     | 2.59                     | 0.41              |
| 1:B:288:MET:HE1  | 1:B:288:MET:HA   | 2.02                     | 0.41              |
| 2:N:235:PRO:HA   | 2:N:249:PHE:O    | 2.21                     | 0.41              |
| 2:K:235:PRO:HA   | 2:K:249:PHE:O    | 2.21                     | 0.41              |
| 2:H:123:LYS:HG3  | 2:H:124:PHE:CD1  | 2.56                     | 0.41              |
| 2:C:204:ASN:HB3  | 2:C:296:ARG:HB3  | 2.03                     | 0.41              |
| 2:D:204:ASN:HB3  | 2:D:296:ARG:HB3  | 2.03                     | 0.41              |
| 1:B:411:LEU:HA   | 1:B:411:LEU:HD23 | 1.83                     | 0.41              |
| 1:A:726:ASN:HD22 | 1:A:726:ASN:HA   | 1.60                     | 0.41              |
| 1:B:869:VAL:HG13 | 1:B:873:ASN:CA   | 2.51                     | 0.40              |
| 2:I:11:LEU:HA    | 2:I:14:ALA:HB3   | 2.02                     | 0.40              |
| 1:B:743:ASP:OD1  | 1:B:744:TYR:N    | 2.53                     | 0.40              |
| 2:I:144:ARG:HD2  | 2:J:82:ARG:CZ    | 2.51                     | 0.40              |
| 3:W:490:TYR:HA   | 3:W:628:VAL:HG22 | 2.02                     | 0.40              |
| 2:L:131:ASN:HD22 | 2:L:131:ASN:N    | 2.19                     | 0.40              |
| 1:B:854:LEU:HD22 | 1:B:855:LEU:N    | 2.36                     | 0.40              |
| 2:D:38:ILE:HG13  | 2:D:38:ILE:H     | 1.57                     | 0.40              |
| 2:H:34:PHE:O     | 2:H:35:ASN:C     | 2.60                     | 0.40              |
| 2:D:144:ARG:O    | 2:D:145:ARG:CB   | 2.65                     | 0.40              |
| 2:K:38:ILE:H     | 2:K:38:ILE:HG13  | 1.58                     | 0.40              |
| 3:W:798:ILE:HB   | 3:W:845:ILE:HG12 | 2.03                     | 0.40              |
| 2:I:116:LEU:O    | 2:I:119:LEU:N    | 2.50                     | 0.40              |
| 3:W:917:ARG:HD2  | 3:W:919:TYR:CZ   | 2.56                     | 0.40              |
| 1:B:401:TYR:N    | 1:B:401:TYR:CD1  | 2.74                     | 0.40              |
| 2:J:110:ALA:CB   | 2:J:111:PRO:CD   | 2.96                     | 0.40              |
| 3:W:873:THR:HA   | 3:W:1073:ILE:CG2 | 2.50                     | 0.40              |
| 1:A:594:ILE:HA   | 1:A:595:PRO:HD3  | 1.86                     | 0.40              |
| 2:J:133:SER:O    | 2:J:134:GLU:C    | 2.59                     | 0.40              |
| 2:J:126:ARG:NH1  | 2:K:72:ASN:ND2   | 2.69                     | 0.40              |
| 3:W:524:TRP:CD1  | 3:W:607:LEU:HD22 | 2.55                     | 0.40              |
| 2:L:234:PHE:CE1  | 2:N:253:ILE:HG13 | 2.55                     | 0.40              |
| 2:E:235:PRO:HA   | 2:E:249:PHE:O    | 2.21                     | 0.40              |
| 3:W:444:ASP:C    | 3:W:446:PRO:HD3  | 2.41                     | 0.40              |
| 2:J:355:ILE:HA   | 2:J:356:PRO:HD3  | 1.96                     | 0.40              |
| 1:B:747:ILE:H    | 1:B:747:ILE:HG22 | 1.51                     | 0.40              |
| 1:B:150:LEU:CD1  | 1:B:696:SER:HA   | 2.50                     | 0.40              |
| 1:B:543:LEU:O    | 1:B:544:VAL:C    | 2.58                     | 0.40              |
| 1:B:558:MET:O    | 1:B:559:ALA:C    | 2.60                     | 0.40              |
| 1:A:793:ASP:N    | 1:A:793:ASP:OD1  | 2.54                     | 0.40              |
| 1:B:224:PHE:HE1  | 2:O:70:LEU:C     | 2.24                     | 0.40              |
| 1:A:785:GLN:HB2  | 1:A:786:ILE:H    | 1.60                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:200:VAL:O    | 1:A:201:ASP:HB3  | 2.21                     | 0.40              |
| 1:B:847:THR:O    | 1:B:847:THR:HG22 | 2.20                     | 0.40              |
| 1:A:249:ASP:O    | 1:A:250:TYR:C    | 2.60                     | 0.40              |
| 2:E:65:LEU:C     | 2:E:66:LEU:HG    | 2.42                     | 0.40              |
| 1:A:283:ASN:ND2  | 1:A:869:VAL:H    | 2.18                     | 0.40              |
| 2:L:153:HIS:CE1  | 2:M:153:HIS:CD2  | 3.09                     | 0.40              |
| 1:A:264:PRO:O    | 1:A:265:LEU:HB2  | 2.22                     | 0.40              |
| 1:A:714:ARG:O    | 1:A:715:ASP:C    | 2.59                     | 0.40              |
| 1:A:594:ILE:HG23 | 1:A:595:PRO:N    | 2.36                     | 0.40              |
| 2:E:91:PHE:O     | 2:E:95:VAL:HG23  | 2.22                     | 0.40              |
| 2:H:152:PHE:HB3  | 2:H:337:ASP:CB   | 2.51                     | 0.40              |
| 2:D:214:LEU:N    | 2:D:214:LEU:HD23 | 2.36                     | 0.40              |
| 2:F:65:LEU:HB3   | 2:F:66:LEU:H     | 1.69                     | 0.40              |
| 3:W:62:TYR:O     | 3:W:66:ILE:HG12  | 2.22                     | 0.40              |
| 2:G:104:SER:O    | 2:G:108:GLY:HA2  | 2.21                     | 0.40              |
| 2:I:204:ASN:HB3  | 2:I:296:ARG:HB3  | 2.03                     | 0.40              |
| 3:W:193:TYR:O    | 3:W:197:LYS:HB2  | 2.21                     | 0.40              |
| 2:H:65:LEU:O     | 2:H:66:LEU:HD23  | 2.22                     | 0.40              |
| 3:W:75:LEU:N     | 3:W:75:LEU:HD12  | 2.37                     | 0.40              |
| 1:A:338:GLU:O    | 1:A:339:LEU:HG   | 2.22                     | 0.40              |
| 1:A:542:GLN:HA   | 1:A:545:ASP:OD2  | 2.20                     | 0.40              |
| 1:A:506:LEU:HD21 | 1:A:544:VAL:N    | 2.36                     | 0.40              |
| 1:A:451:ASP:O    | 1:A:452:PRO:O    | 2.39                     | 0.40              |
| 2:M:131:ASN:ND2  | 2:M:131:ASN:N    | 2.70                     | 0.40              |
| 2:M:11:LEU:HA    | 2:M:14:ALA:HB3   | 2.04                     | 0.40              |
| 1:B:622:VAL:O    | 1:B:623:ALA:C    | 2.59                     | 0.40              |
| 1:B:743:ASP:OD2  | 1:B:745:ALA:N    | 2.54                     | 0.40              |
| 2:I:145:ARG:NH1  | 2:I:145:ARG:CB   | 2.65                     | 0.40              |
| 2:G:4:LEU:O      | 2:G:5:TYR:C      | 2.59                     | 0.40              |
| 2:H:23:LEU:H     | 2:H:26:ASN:HD21  | 1.67                     | 0.40              |
| 1:A:362:SER:HA   | 1:A:365:GLN:HE21 | 1.87                     | 0.40              |
| 2:K:88:PHE:O     | 2:K:91:PHE:HB3   | 2.22                     | 0.40              |
| 3:W:539:ILE:HG23 | 3:W:562:LYS:CG   | 2.42                     | 0.40              |
| 2:F:14:ALA:O     | 2:F:16:ASP:N     | 2.54                     | 0.40              |
| 3:W:687:ILE:O    | 3:W:687:ILE:CG2  | 2.69                     | 0.40              |
| 2:K:48:THR:O     | 2:K:56:ILE:HA    | 2.20                     | 0.40              |
| 2:O:9:LYS:HE3    | 2:O:13:ASP:OD1   | 2.21                     | 0.40              |
| 1:A:715:ASP:O    | 1:A:718:TYR:O    | 2.39                     | 0.40              |
| 1:B:497:ILE:HG23 | 2:I:68:THR:CG2   | 2.52                     | 0.40              |
| 2:E:136:ILE:HD12 | 2:E:139:TRP:HB3  | 2.04                     | 0.40              |
| 2:J:124:PHE:O    | 2:J:126:ARG:N    | 2.54                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:214:LEU:HD23 | 2:C:214:LEU:N    | 2.37                     | 0.40              |
| 1:A:707:TYR:H    | 1:A:707:TYR:HD1  | 1.69                     | 0.40              |
| 2:F:155:PRO:O    | 2:F:186:SER:HB3  | 2.21                     | 0.40              |
| 2:F:204:ASN:HB3  | 2:F:296:ARG:HB3  | 2.03                     | 0.40              |
| 2:M:204:ASN:HB3  | 2:M:296:ARG:HB3  | 2.04                     | 0.40              |
| 2:O:204:ASN:HB3  | 2:O:296:ARG:HB3  | 2.03                     | 0.40              |
| 1:B:804:SER:O    | 1:B:805:ASP:HB2  | 2.22                     | 0.40              |
| 1:A:304:LEU:N    | 1:A:615:ASN:ND2  | 2.67                     | 0.40              |
| 1:A:657:VAL:HA   | 1:A:658:PRO:HD3  | 1.64                     | 0.40              |
| 1:A:163:ARG:NH2  | 1:A:736:GLU:OE1  | 2.52                     | 0.40              |
| 1:B:870:ALA:C    | 1:B:872:ASP:H    | 2.21                     | 0.40              |
| 2:I:31:ILE:O     | 2:I:32:GLN:C     | 2.59                     | 0.40              |
| 1:A:536:LEU:HD22 | 1:A:536:LEU:N    | 2.36                     | 0.40              |
| 2:K:11:LEU:HA    | 2:K:14:ALA:HB3   | 2.03                     | 0.40              |
| 1:A:854:LEU:HD22 | 1:A:855:LEU:H    | 1.86                     | 0.40              |
| 1:B:190:ASN:HB3  | 1:B:197:GLY:O    | 2.21                     | 0.40              |
| 1:B:244:ILE:O    | 1:B:244:ILE:HG23 | 2.22                     | 0.40              |
| 2:O:34:PHE:O     | 2:O:37:MET:HB3   | 2.21                     | 0.40              |
| 1:B:639:LYS:O    | 1:B:641:ILE:N    | 2.55                     | 0.40              |
| 1:B:239:VAL:HG21 | 1:B:845:ASN:O    | 2.21                     | 0.40              |
| 2:D:11:LEU:HA    | 2:D:14:ALA:HB3   | 2.03                     | 0.40              |
| 3:W:844:PRO:O    | 3:W:848:GLU:HB2  | 2.20                     | 0.40              |
| 2:M:31:ILE:O     | 2:M:32:GLN:C     | 2.60                     | 0.40              |
| 2:F:11:LEU:HB2   | 2:F:395:LEU:HD21 | 2.04                     | 0.40              |
| 2:K:133:SER:O    | 2:K:134:GLU:C    | 2.60                     | 0.40              |
| 2:N:91:PHE:O     | 2:N:95:VAL:HG23  | 2.21                     | 0.40              |
| 2:O:100:MET:HG3  | 2:O:388:VAL:CG1  | 2.51                     | 0.40              |
| 2:H:108:GLY:C    | 2:H:110:ALA:N    | 2.75                     | 0.40              |
| 2:O:144:ARG:O    | 2:O:145:ARG:CG   | 2.69                     | 0.40              |
| 3:W:865:VAL:HG13 | 3:W:866:THR:HG23 | 2.02                     | 0.40              |
| 2:D:124:PHE:O    | 2:D:126:ARG:N    | 2.54                     | 0.40              |
| 2:L:59:TRP:CD1   | 2:L:59:TRP:N     | 2.88                     | 0.40              |
| 1:A:154:THR:O    | 1:A:155:LEU:C    | 2.59                     | 0.40              |
| 3:W:288:LEU:O    | 3:W:288:LEU:HD12 | 2.20                     | 0.40              |
| 3:W:255:VAL:HG11 | 3:W:316:ILE:HB   | 2.02                     | 0.40              |
| 1:A:303:LEU:HA   | 1:A:615:ASN:HD21 | 1.82                     | 0.40              |
| 1:B:477:ASN:C    | 1:B:479:GLN:N    | 2.75                     | 0.40              |
| 1:B:556:THR:HG22 | 1:B:557:LEU:N    | 2.36                     | 0.40              |
| 1:A:510:LEU:HA   | 1:A:513:LEU:CD1  | 2.51                     | 0.40              |
| 1:A:536:LEU:CD2  | 1:A:536:LEU:N    | 2.85                     | 0.40              |
| 2:M:4:LEU:O      | 2:M:5:TYR:C      | 2.58                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:373:GLN:O    | 1:B:374:ALA:C    | 2.59                     | 0.40              |
| 1:B:746:GLN:O    | 1:B:750:MET:HG3  | 2.21                     | 0.40              |
| 3:W:463:PHE:O    | 3:W:464:ILE:HG12 | 2.21                     | 0.40              |
| 2:G:131:ASN:N    | 2:G:131:ASN:HD22 | 2.20                     | 0.40              |
| 2:G:34:PHE:O     | 2:G:35:ASN:C     | 2.60                     | 0.40              |
| 2:D:128:ASN:O    | 2:D:129:PHE:HB3  | 2.21                     | 0.40              |
| 1:A:421:ARG:C    | 1:A:423:SER:H    | 2.25                     | 0.40              |
| 1:A:131:LEU:HA   | 1:A:132:PRO:HD3  | 1.90                     | 0.40              |
| 2:C:14:ALA:O     | 2:C:18:ILE:HD12  | 2.21                     | 0.40              |
| 2:K:116:LEU:O    | 2:K:119:LEU:N    | 2.50                     | 0.40              |
| 2:L:74:ASP:O     | 2:L:75:ALA:C     | 2.59                     | 0.40              |
| 3:W:982:SER:O    | 3:W:985:LYS:HB2  | 2.21                     | 0.40              |
| 1:B:87:GLN:C     | 1:B:89:GLU:H     | 2.25                     | 0.40              |
| 2:D:378:ARG:O    | 2:D:382:LEU:HB2  | 2.22                     | 0.40              |
| 1:A:815:TYR:CD1  | 1:A:815:TYR:N    | 2.85                     | 0.40              |
| 2:F:235:PRO:HA   | 2:F:249:PHE:O    | 2.21                     | 0.40              |
| 2:O:101:VAL:HG23 | 2:O:102:ARG:N    | 2.36                     | 0.40              |
| 2:L:355:ILE:HA   | 2:L:356:PRO:HD3  | 1.96                     | 0.40              |
| 2:K:204:ASN:HB3  | 2:K:296:ARG:HB3  | 2.04                     | 0.40              |
| 2:E:100:MET:HG3  | 2:E:388:VAL:HG11 | 2.04                     | 0.40              |
| 1:A:359:THR:HG22 | 1:A:359:THR:O    | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed   | Outliers  | Percentiles |    |
|-----|-------|----------------|-----------|-----------|-----------|-------------|----|
| 1   | A     | 779/880 (88%)  | 431 (55%) | 199 (26%) | 149 (19%) | 0           | 3  |
| 1   | B     | 808/880 (92%)  | 458 (57%) | 204 (25%) | 146 (18%) | 0           | 3  |
| 2   | C     | 395/397 (100%) | 318 (80%) | 54 (14%)  | 23 (6%)   | 2           | 27 |
| 2   | D     | 395/397 (100%) | 315 (80%) | 50 (13%)  | 30 (8%)   | 1           | 20 |

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| Mol | Chain | Analysed        | Favoured   | Allowed    | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|------------|----------|-------------|----|
| 2   | E     | 395/397 (100%)  | 323 (82%)  | 49 (12%)   | 23 (6%)  | 2           | 27 |
| 2   | F     | 395/397 (100%)  | 324 (82%)  | 47 (12%)   | 24 (6%)  | 2           | 26 |
| 2   | G     | 395/397 (100%)  | 323 (82%)  | 49 (12%)   | 23 (6%)  | 2           | 27 |
| 2   | H     | 395/397 (100%)  | 323 (82%)  | 50 (13%)   | 22 (6%)  | 2           | 28 |
| 2   | I     | 395/397 (100%)  | 320 (81%)  | 51 (13%)   | 24 (6%)  | 2           | 26 |
| 2   | J     | 395/397 (100%)  | 320 (81%)  | 53 (13%)   | 22 (6%)  | 2           | 28 |
| 2   | K     | 395/397 (100%)  | 318 (80%)  | 52 (13%)   | 25 (6%)  | 2           | 26 |
| 2   | L     | 395/397 (100%)  | 322 (82%)  | 47 (12%)   | 26 (7%)  | 1           | 24 |
| 2   | M     | 395/397 (100%)  | 322 (82%)  | 52 (13%)   | 21 (5%)  | 2           | 30 |
| 2   | N     | 395/397 (100%)  | 317 (80%)  | 50 (13%)   | 28 (7%)  | 1           | 22 |
| 2   | O     | 395/397 (100%)  | 317 (80%)  | 47 (12%)   | 31 (8%)  | 1           | 19 |
| 3   | W     | 933/1089 (86%)  | 807 (86%)  | 93 (10%)   | 33 (4%)  | 4           | 40 |
| All | All   | 7655/8010 (96%) | 5858 (76%) | 1147 (15%) | 650 (8%) | 1           | 17 |

All (650) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 101 | LYS  |
| 1   | A     | 130 | GLN  |
| 1   | A     | 193 | SER  |
| 1   | A     | 198 | LYS  |
| 1   | A     | 220 | ALA  |
| 1   | A     | 234 | ALA  |
| 1   | A     | 246 | HIS  |
| 1   | A     | 252 | PHE  |
| 1   | A     | 260 | GLN  |
| 1   | A     | 275 | PRO  |
| 1   | A     | 283 | ASN  |
| 1   | A     | 287 | ASN  |
| 1   | A     | 306 | ASP  |
| 1   | A     | 315 | GLU  |
| 1   | A     | 338 | GLU  |
| 1   | A     | 340 | VAL  |
| 1   | A     | 356 | GLU  |
| 1   | A     | 358 | LEU  |
| 1   | A     | 370 | ILE  |
| 1   | A     | 413 | VAL  |
| 1   | A     | 443 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 446 | HIS  |
| 1   | A     | 451 | ASP  |
| 1   | A     | 452 | PRO  |
| 1   | A     | 453 | GLN  |
| 1   | A     | 484 | VAL  |
| 1   | A     | 485 | ILE  |
| 1   | A     | 488 | VAL  |
| 1   | A     | 489 | LEU  |
| 1   | A     | 501 | HIS  |
| 1   | A     | 523 | VAL  |
| 1   | A     | 558 | MET  |
| 1   | A     | 564 | ASN  |
| 1   | A     | 570 | THR  |
| 1   | A     | 573 | THR  |
| 1   | A     | 585 | CYS  |
| 1   | A     | 650 | HIS  |
| 1   | A     | 651 | ILE  |
| 1   | A     | 660 | ASP  |
| 1   | A     | 661 | GLN  |
| 1   | A     | 689 | MET  |
| 1   | A     | 701 | GLN  |
| 1   | A     | 715 | ASP  |
| 1   | A     | 743 | ASP  |
| 1   | A     | 745 | ALA  |
| 1   | A     | 770 | SER  |
| 1   | A     | 771 | VAL  |
| 1   | A     | 772 | ILE  |
| 1   | A     | 781 | THR  |
| 1   | A     | 782 | VAL  |
| 1   | A     | 785 | GLN  |
| 1   | A     | 786 | ILE  |
| 1   | A     | 808 | ASP  |
| 1   | A     | 811 | LEU  |
| 1   | A     | 814 | ASN  |
| 1   | A     | 828 | GLN  |
| 1   | A     | 854 | LEU  |
| 1   | A     | 855 | LEU  |
| 1   | A     | 856 | ALA  |
| 1   | A     | 857 | PHE  |
| 1   | B     | 191 | LYS  |
| 1   | B     | 194 | ARG  |
| 1   | B     | 195 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 196 | ALA  |
| 1   | B     | 200 | VAL  |
| 1   | B     | 215 | GLU  |
| 1   | B     | 218 | GLU  |
| 1   | B     | 226 | ALA  |
| 1   | B     | 227 | GLU  |
| 1   | B     | 252 | PHE  |
| 1   | B     | 306 | ASP  |
| 1   | B     | 355 | LEU  |
| 1   | B     | 361 | GLN  |
| 1   | B     | 369 | GLY  |
| 1   | B     | 400 | ASN  |
| 1   | B     | 417 | ASP  |
| 1   | B     | 446 | HIS  |
| 1   | B     | 447 | TYR  |
| 1   | B     | 451 | ASP  |
| 1   | B     | 457 | GLN  |
| 1   | B     | 458 | ILE  |
| 1   | B     | 479 | GLN  |
| 1   | B     | 481 | ARG  |
| 1   | B     | 503 | ILE  |
| 1   | B     | 504 | ASN  |
| 1   | B     | 574 | GLU  |
| 1   | B     | 585 | CYS  |
| 1   | B     | 634 | TYR  |
| 1   | B     | 640 | ALA  |
| 1   | B     | 651 | ILE  |
| 1   | B     | 655 | ALA  |
| 1   | B     | 673 | PRO  |
| 1   | B     | 699 | ILE  |
| 1   | B     | 702 | GLY  |
| 1   | B     | 724 | ALA  |
| 1   | B     | 764 | PRO  |
| 1   | B     | 765 | PHE  |
| 1   | B     | 777 | LYS  |
| 1   | B     | 782 | VAL  |
| 1   | B     | 785 | GLN  |
| 1   | B     | 786 | ILE  |
| 1   | B     | 790 | ARG  |
| 1   | B     | 792 | VAL  |
| 1   | B     | 805 | ASP  |
| 1   | B     | 806 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 855 | LEU  |
| 1   | B     | 856 | ALA  |
| 1   | B     | 875 | ARG  |
| 2   | C     | 22  | THR  |
| 2   | C     | 70  | LEU  |
| 2   | C     | 134 | GLU  |
| 2   | D     | 25  | SER  |
| 2   | D     | 70  | LEU  |
| 2   | D     | 126 | ARG  |
| 2   | D     | 128 | ASN  |
| 2   | D     | 134 | GLU  |
| 2   | D     | 148 | THR  |
| 2   | E     | 22  | THR  |
| 2   | E     | 25  | SER  |
| 2   | E     | 106 | ARG  |
| 2   | E     | 134 | GLU  |
| 2   | F     | 22  | THR  |
| 2   | F     | 62  | ASP  |
| 2   | F     | 70  | LEU  |
| 2   | F     | 105 | GLN  |
| 2   | F     | 134 | GLU  |
| 2   | F     | 145 | ARG  |
| 2   | F     | 148 | THR  |
| 2   | G     | 20  | GLU  |
| 2   | G     | 22  | THR  |
| 2   | G     | 134 | GLU  |
| 2   | G     | 148 | THR  |
| 2   | H     | 22  | THR  |
| 2   | H     | 107 | ASN  |
| 2   | H     | 134 | GLU  |
| 2   | I     | 25  | SER  |
| 2   | I     | 62  | ASP  |
| 2   | I     | 134 | GLU  |
| 2   | I     | 148 | THR  |
| 2   | J     | 20  | GLU  |
| 2   | J     | 70  | LEU  |
| 2   | J     | 106 | ARG  |
| 2   | J     | 134 | GLU  |
| 2   | K     | 22  | THR  |
| 2   | K     | 70  | LEU  |
| 2   | K     | 126 | ARG  |
| 2   | K     | 128 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | K     | 134  | GLU  |
| 2   | K     | 148  | THR  |
| 2   | L     | 22   | THR  |
| 2   | L     | 62   | ASP  |
| 2   | L     | 126  | ARG  |
| 2   | L     | 134  | GLU  |
| 2   | L     | 145  | ARG  |
| 2   | L     | 148  | THR  |
| 2   | M     | 22   | THR  |
| 2   | M     | 25   | SER  |
| 2   | M     | 128  | ASN  |
| 2   | M     | 134  | GLU  |
| 2   | N     | 22   | THR  |
| 2   | N     | 25   | SER  |
| 2   | N     | 70   | LEU  |
| 2   | N     | 128  | ASN  |
| 2   | N     | 134  | GLU  |
| 2   | N     | 148  | THR  |
| 2   | O     | 65   | LEU  |
| 2   | O     | 68   | THR  |
| 2   | O     | 70   | LEU  |
| 2   | O     | 134  | GLU  |
| 2   | O     | 145  | ARG  |
| 2   | O     | 148  | THR  |
| 3   | W     | 54   | SER  |
| 3   | W     | 397  | MET  |
| 3   | W     | 401  | SER  |
| 3   | W     | 864  | PRO  |
| 3   | W     | 1082 | ASN  |
| 3   | W     | 1083 | ALA  |
| 3   | W     | 1084 | ASN  |
| 1   | A     | 143  | ARG  |
| 1   | A     | 202  | SER  |
| 1   | A     | 215  | GLU  |
| 1   | A     | 219  | GLY  |
| 1   | A     | 226  | ALA  |
| 1   | A     | 227  | GLU  |
| 1   | A     | 253  | ASN  |
| 1   | A     | 264  | PRO  |
| 1   | A     | 307  | ARG  |
| 1   | A     | 336  | LEU  |
| 1   | A     | 352  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 369 | GLY  |
| 1   | A     | 415 | PRO  |
| 1   | A     | 438 | PRO  |
| 1   | A     | 441 | GLY  |
| 1   | A     | 458 | ILE  |
| 1   | A     | 465 | ASN  |
| 1   | A     | 503 | ILE  |
| 1   | A     | 559 | ALA  |
| 1   | A     | 571 | LEU  |
| 1   | A     | 590 | ASN  |
| 1   | A     | 608 | VAL  |
| 1   | A     | 630 | ARG  |
| 1   | A     | 654 | VAL  |
| 1   | A     | 680 | ASP  |
| 1   | A     | 739 | MET  |
| 1   | A     | 804 | SER  |
| 1   | A     | 815 | TYR  |
| 1   | A     | 823 | THR  |
| 1   | A     | 847 | THR  |
| 1   | A     | 866 | ILE  |
| 1   | B     | 73  | LEU  |
| 1   | B     | 141 | GLU  |
| 1   | B     | 142 | LEU  |
| 1   | B     | 212 | PHE  |
| 1   | B     | 230 | GLN  |
| 1   | B     | 253 | ASN  |
| 1   | B     | 261 | LEU  |
| 1   | B     | 264 | PRO  |
| 1   | B     | 265 | LEU  |
| 1   | B     | 278 | ILE  |
| 1   | B     | 282 | VAL  |
| 1   | B     | 283 | ASN  |
| 1   | B     | 307 | ARG  |
| 1   | B     | 313 | ASN  |
| 1   | B     | 338 | GLU  |
| 1   | B     | 388 | SER  |
| 1   | B     | 436 | ILE  |
| 1   | B     | 438 | PRO  |
| 1   | B     | 443 | GLN  |
| 1   | B     | 452 | PRO  |
| 1   | B     | 465 | ASN  |
| 1   | B     | 478 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 487 | GLY  |
| 1   | B     | 488 | VAL  |
| 1   | B     | 489 | LEU  |
| 1   | B     | 493 | LEU  |
| 1   | B     | 496 | ASN  |
| 1   | B     | 500 | GLY  |
| 1   | B     | 520 | THR  |
| 1   | B     | 524 | ASP  |
| 1   | B     | 608 | VAL  |
| 1   | B     | 631 | LEU  |
| 1   | B     | 637 | LYS  |
| 1   | B     | 638 | MET  |
| 1   | B     | 654 | VAL  |
| 1   | B     | 674 | VAL  |
| 1   | B     | 676 | VAL  |
| 1   | B     | 787 | VAL  |
| 1   | B     | 854 | LEU  |
| 2   | C     | 7   | LEU  |
| 2   | C     | 20  | GLU  |
| 2   | C     | 25  | SER  |
| 2   | C     | 62  | ASP  |
| 2   | C     | 106 | ARG  |
| 2   | C     | 130 | ASP  |
| 2   | C     | 148 | THR  |
| 2   | D     | 7   | LEU  |
| 2   | D     | 20  | GLU  |
| 2   | D     | 42  | ASN  |
| 2   | D     | 65  | LEU  |
| 2   | D     | 67  | GLY  |
| 2   | D     | 69  | THR  |
| 2   | D     | 72  | ASN  |
| 2   | D     | 90  | ASP  |
| 2   | D     | 106 | ARG  |
| 2   | D     | 147 | ARG  |
| 2   | E     | 7   | LEU  |
| 2   | E     | 62  | ASP  |
| 2   | E     | 90  | ASP  |
| 2   | E     | 126 | ARG  |
| 2   | E     | 128 | ASN  |
| 2   | E     | 130 | ASP  |
| 2   | E     | 148 | THR  |
| 2   | F     | 7   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 25  | SER  |
| 2   | F     | 128 | ASN  |
| 2   | G     | 7   | LEU  |
| 2   | G     | 25  | SER  |
| 2   | G     | 125 | LYS  |
| 2   | G     | 126 | ARG  |
| 2   | H     | 7   | LEU  |
| 2   | H     | 25  | SER  |
| 2   | H     | 42  | ASN  |
| 2   | H     | 51  | ILE  |
| 2   | H     | 62  | ASP  |
| 2   | H     | 68  | THR  |
| 2   | H     | 109 | ILE  |
| 2   | H     | 128 | ASN  |
| 2   | I     | 7   | LEU  |
| 2   | I     | 90  | ASP  |
| 2   | I     | 125 | LYS  |
| 2   | I     | 147 | ARG  |
| 2   | J     | 7   | LEU  |
| 2   | J     | 51  | ILE  |
| 2   | J     | 62  | ASP  |
| 2   | J     | 90  | ASP  |
| 2   | J     | 126 | ARG  |
| 2   | J     | 128 | ASN  |
| 2   | J     | 130 | ASP  |
| 2   | K     | 7   | LEU  |
| 2   | K     | 20  | GLU  |
| 2   | K     | 62  | ASP  |
| 2   | K     | 106 | ARG  |
| 2   | K     | 125 | LYS  |
| 2   | L     | 7   | LEU  |
| 2   | L     | 25  | SER  |
| 2   | L     | 69  | THR  |
| 2   | L     | 72  | ASN  |
| 2   | L     | 106 | ARG  |
| 2   | L     | 128 | ASN  |
| 2   | L     | 147 | ARG  |
| 2   | M     | 7   | LEU  |
| 2   | M     | 42  | ASN  |
| 2   | M     | 90  | ASP  |
| 2   | N     | 7   | LEU  |
| 2   | N     | 42  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | N     | 62   | ASP  |
| 2   | N     | 65   | LEU  |
| 2   | N     | 90   | ASP  |
| 2   | N     | 145  | ARG  |
| 2   | O     | 7    | LEU  |
| 2   | O     | 22   | THR  |
| 2   | O     | 25   | SER  |
| 2   | O     | 62   | ASP  |
| 2   | O     | 90   | ASP  |
| 2   | O     | 105  | GLN  |
| 3   | W     | 102  | LEU  |
| 3   | W     | 201  | TYR  |
| 3   | W     | 521  | VAL  |
| 3   | W     | 825  | ASN  |
| 3   | W     | 862  | GLN  |
| 3   | W     | 865  | VAL  |
| 3   | W     | 1002 | GLY  |
| 1   | A     | 137  | ASN  |
| 1   | A     | 142  | LEU  |
| 1   | A     | 218  | GLU  |
| 1   | A     | 254  | GLU  |
| 1   | A     | 265  | LEU  |
| 1   | A     | 276  | GLU  |
| 1   | A     | 496  | ASN  |
| 1   | A     | 497  | ILE  |
| 1   | A     | 521  | MET  |
| 1   | A     | 525  | TYR  |
| 1   | A     | 579  | THR  |
| 1   | A     | 597  | PRO  |
| 1   | A     | 648  | ARG  |
| 1   | A     | 658  | PRO  |
| 1   | A     | 676  | VAL  |
| 1   | A     | 687  | MET  |
| 1   | A     | 696  | SER  |
| 1   | A     | 773  | SER  |
| 1   | A     | 816  | ASP  |
| 1   | A     | 849  | THR  |
| 1   | B     | 237  | ASN  |
| 1   | B     | 254  | GLU  |
| 1   | B     | 273  | TYR  |
| 1   | B     | 359  | THR  |
| 1   | B     | 387  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 421 | ARG  |
| 1   | B     | 549 | LEU  |
| 1   | B     | 579 | THR  |
| 1   | B     | 581 | VAL  |
| 1   | B     | 590 | ASN  |
| 1   | B     | 635 | GLN  |
| 1   | B     | 656 | ARG  |
| 1   | B     | 670 | ARG  |
| 1   | B     | 675 | GLU  |
| 1   | B     | 794 | THR  |
| 1   | B     | 849 | THR  |
| 2   | C     | 13  | ASP  |
| 2   | C     | 42  | ASN  |
| 2   | C     | 69  | THR  |
| 2   | C     | 90  | ASP  |
| 2   | C     | 126 | ARG  |
| 2   | D     | 13  | ASP  |
| 2   | D     | 32  | GLN  |
| 2   | D     | 62  | ASP  |
| 2   | D     | 68  | THR  |
| 2   | D     | 125 | LYS  |
| 2   | E     | 13  | ASP  |
| 2   | E     | 32  | GLN  |
| 2   | E     | 70  | LEU  |
| 2   | F     | 13  | ASP  |
| 2   | F     | 32  | GLN  |
| 2   | F     | 90  | ASP  |
| 2   | F     | 126 | ARG  |
| 2   | F     | 130 | ASP  |
| 2   | G     | 13  | ASP  |
| 2   | G     | 32  | GLN  |
| 2   | G     | 42  | ASN  |
| 2   | G     | 90  | ASP  |
| 2   | G     | 128 | ASN  |
| 2   | H     | 13  | ASP  |
| 2   | H     | 32  | GLN  |
| 2   | H     | 90  | ASP  |
| 2   | I     | 13  | ASP  |
| 2   | I     | 32  | GLN  |
| 2   | I     | 126 | ARG  |
| 2   | I     | 128 | ASN  |
| 2   | I     | 146 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | J     | 13  | ASP  |
| 2   | J     | 42  | ASN  |
| 2   | K     | 13  | ASP  |
| 2   | K     | 25  | SER  |
| 2   | K     | 32  | GLN  |
| 2   | K     | 90  | ASP  |
| 2   | K     | 111 | PRO  |
| 2   | L     | 13  | ASP  |
| 2   | L     | 20  | GLU  |
| 2   | L     | 41  | MET  |
| 2   | L     | 90  | ASP  |
| 2   | L     | 125 | LYS  |
| 2   | M     | 13  | ASP  |
| 2   | M     | 106 | ARG  |
| 2   | N     | 13  | ASP  |
| 2   | N     | 67  | GLY  |
| 2   | N     | 106 | ARG  |
| 2   | N     | 125 | LYS  |
| 2   | N     | 155 | PRO  |
| 2   | O     | 20  | GLU  |
| 2   | O     | 24  | TYR  |
| 2   | O     | 32  | GLN  |
| 2   | O     | 42  | ASN  |
| 2   | O     | 73  | LEU  |
| 2   | O     | 106 | ARG  |
| 2   | O     | 126 | ARG  |
| 2   | O     | 155 | PRO  |
| 3   | W     | 81  | LYS  |
| 3   | W     | 582 | LYS  |
| 3   | W     | 870 | SER  |
| 1   | A     | 131 | LEU  |
| 1   | A     | 144 | ASN  |
| 1   | A     | 155 | LEU  |
| 1   | A     | 187 | ALA  |
| 1   | A     | 195 | ASP  |
| 1   | A     | 206 | SER  |
| 1   | A     | 212 | PHE  |
| 1   | A     | 299 | ILE  |
| 1   | A     | 333 | VAL  |
| 1   | A     | 372 | SER  |
| 1   | A     | 387 | LEU  |
| 1   | A     | 457 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 518 | PHE  |
| 1   | A     | 524 | ASP  |
| 1   | A     | 549 | LEU  |
| 1   | A     | 552 | TYR  |
| 1   | A     | 557 | LEU  |
| 1   | A     | 581 | VAL  |
| 1   | A     | 700 | ALA  |
| 1   | A     | 730 | PHE  |
| 1   | A     | 853 | ASP  |
| 1   | A     | 877 | MET  |
| 1   | B     | 85  | GLU  |
| 1   | B     | 101 | LYS  |
| 1   | B     | 185 | ASP  |
| 1   | B     | 193 | SER  |
| 1   | B     | 206 | SER  |
| 1   | B     | 294 | SER  |
| 1   | B     | 302 | ASN  |
| 1   | B     | 372 | SER  |
| 1   | B     | 442 | MET  |
| 1   | B     | 466 | PHE  |
| 1   | B     | 483 | VAL  |
| 1   | B     | 552 | TYR  |
| 1   | B     | 564 | ASN  |
| 1   | B     | 597 | PRO  |
| 1   | B     | 639 | LYS  |
| 1   | B     | 680 | ASP  |
| 1   | B     | 731 | GLN  |
| 2   | C     | 32  | GLN  |
| 2   | C     | 38  | ILE  |
| 2   | C     | 89  | VAL  |
| 2   | D     | 38  | ILE  |
| 2   | D     | 41  | MET  |
| 2   | D     | 89  | VAL  |
| 2   | D     | 123 | LYS  |
| 2   | D     | 145 | ARG  |
| 2   | E     | 38  | ILE  |
| 2   | F     | 20  | GLU  |
| 2   | F     | 38  | ILE  |
| 2   | F     | 42  | ASN  |
| 2   | G     | 38  | ILE  |
| 2   | G     | 130 | ASP  |
| 2   | G     | 145 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 36  | GLN  |
| 2   | H     | 38  | ILE  |
| 2   | H     | 89  | VAL  |
| 2   | H     | 106 | ARG  |
| 2   | I     | 36  | GLN  |
| 2   | I     | 38  | ILE  |
| 2   | I     | 42  | ASN  |
| 2   | I     | 89  | VAL  |
| 2   | I     | 145 | ARG  |
| 2   | J     | 32  | GLN  |
| 2   | J     | 36  | GLN  |
| 2   | J     | 38  | ILE  |
| 2   | J     | 89  | VAL  |
| 2   | K     | 9   | LYS  |
| 2   | K     | 36  | GLN  |
| 2   | K     | 38  | ILE  |
| 2   | K     | 89  | VAL  |
| 2   | L     | 32  | GLN  |
| 2   | L     | 36  | GLN  |
| 2   | L     | 38  | ILE  |
| 2   | M     | 20  | GLU  |
| 2   | M     | 32  | GLN  |
| 2   | M     | 38  | ILE  |
| 2   | M     | 55  | PRO  |
| 2   | M     | 89  | VAL  |
| 2   | M     | 126 | ARG  |
| 2   | N     | 20  | GLU  |
| 2   | N     | 32  | GLN  |
| 2   | N     | 36  | GLN  |
| 2   | N     | 38  | ILE  |
| 2   | N     | 89  | VAL  |
| 2   | N     | 126 | ARG  |
| 2   | O     | 13  | ASP  |
| 2   | O     | 38  | ILE  |
| 2   | O     | 89  | VAL  |
| 2   | O     | 128 | ASN  |
| 3   | W     | 256 | ASP  |
| 3   | W     | 463 | PHE  |
| 3   | W     | 464 | ILE  |
| 3   | W     | 596 | THR  |
| 3   | W     | 760 | ASN  |
| 3   | W     | 790 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | W     | 795 | LYS  |
| 1   | A     | 152 | LYS  |
| 1   | A     | 196 | ALA  |
| 1   | A     | 351 | GLN  |
| 1   | B     | 86  | ILE  |
| 1   | B     | 103 | SER  |
| 1   | B     | 207 | ILE  |
| 1   | B     | 277 | ARG  |
| 1   | B     | 399 | THR  |
| 1   | B     | 416 | ASN  |
| 1   | B     | 437 | TYR  |
| 1   | B     | 827 | LYS  |
| 2   | C     | 36  | GLN  |
| 2   | C     | 145 | ARG  |
| 2   | D     | 9   | LYS  |
| 2   | D     | 36  | GLN  |
| 2   | E     | 36  | GLN  |
| 2   | E     | 55  | PRO  |
| 2   | E     | 89  | VAL  |
| 2   | F     | 9   | LYS  |
| 2   | F     | 36  | GLN  |
| 2   | F     | 89  | VAL  |
| 2   | G     | 36  | GLN  |
| 2   | G     | 89  | VAL  |
| 2   | G     | 123 | LYS  |
| 2   | G     | 155 | PRO  |
| 2   | H     | 9   | LYS  |
| 2   | H     | 130 | ASP  |
| 2   | I     | 9   | LYS  |
| 2   | I     | 41  | MET  |
| 2   | J     | 125 | LYS  |
| 2   | K     | 42  | ASN  |
| 2   | K     | 130 | ASP  |
| 2   | L     | 9   | LYS  |
| 2   | L     | 65  | LEU  |
| 2   | L     | 89  | VAL  |
| 2   | M     | 36  | GLN  |
| 2   | M     | 41  | MET  |
| 2   | M     | 145 | ARG  |
| 2   | N     | 9   | LYS  |
| 2   | N     | 69  | THR  |
| 2   | O     | 9   | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | O     | 36   | GLN  |
| 2   | O     | 41   | MET  |
| 3   | W     | 192  | GLU  |
| 3   | W     | 586  | TYR  |
| 1   | A     | 207  | ILE  |
| 1   | A     | 422  | GLU  |
| 1   | A     | 622  | VAL  |
| 1   | A     | 733  | ILE  |
| 1   | A     | 819  | PRO  |
| 1   | B     | 521  | MET  |
| 1   | B     | 557  | LEU  |
| 1   | B     | 622  | VAL  |
| 1   | B     | 677  | ARG  |
| 1   | B     | 781  | THR  |
| 1   | B     | 857  | PHE  |
| 2   | C     | 3    | VAL  |
| 2   | E     | 9    | LYS  |
| 2   | E     | 20   | GLU  |
| 2   | E     | 42   | ASN  |
| 2   | F     | 55   | PRO  |
| 2   | G     | 3    | VAL  |
| 2   | G     | 9    | LYS  |
| 2   | I     | 123  | LYS  |
| 2   | J     | 3    | VAL  |
| 2   | J     | 9    | LYS  |
| 2   | J     | 69   | THR  |
| 2   | K     | 3    | VAL  |
| 2   | K     | 147  | ARG  |
| 2   | L     | 3    | VAL  |
| 2   | N     | 3    | VAL  |
| 2   | O     | 3    | VAL  |
| 3   | W     | 1078 | SER  |
| 1   | A     | 247  | PRO  |
| 1   | A     | 334  | PRO  |
| 1   | B     | 519  | PRO  |
| 1   | B     | 723  | ILE  |
| 1   | B     | 865  | PRO  |
| 2   | D     | 3    | VAL  |
| 2   | E     | 3    | VAL  |
| 2   | F     | 3    | VAL  |
| 2   | H     | 3    | VAL  |
| 2   | I     | 3    | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 3   | VAL  |
| 3   | W     | 200 | PRO  |
| 3   | W     | 246 | SER  |
| 3   | W     | 301 | VAL  |
| 3   | W     | 901 | PRO  |
| 1   | A     | 502 | VAL  |
| 1   | A     | 606 | VAL  |
| 1   | B     | 415 | PRO  |
| 2   | E     | 78  | VAL  |
| 2   | I     | 78  | VAL  |
| 2   | I     | 101 | VAL  |
| 2   | L     | 78  | VAL  |
| 2   | N     | 78  | VAL  |
| 3   | W     | 798 | ILE  |
| 1   | A     | 405 | ILE  |
| 1   | A     | 699 | ILE  |
| 1   | B     | 128 | PRO  |
| 1   | B     | 370 | ILE  |
| 1   | B     | 405 | ILE  |
| 1   | B     | 413 | VAL  |
| 2   | C     | 78  | VAL  |
| 2   | F     | 78  | VAL  |
| 2   | H     | 78  | VAL  |
| 2   | J     | 78  | VAL  |
| 2   | K     | 78  | VAL  |
| 2   | M     | 78  | VAL  |
| 2   | M     | 101 | VAL  |
| 2   | N     | 101 | VAL  |
| 2   | O     | 51  | ILE  |
| 2   | O     | 78  | VAL  |
| 2   | O     | 101 | VAL  |
| 3   | W     | 446 | PRO  |
| 1   | A     | 500 | GLY  |
| 1   | B     | 435 | ILE  |
| 1   | B     | 606 | VAL  |
| 2   | C     | 67  | GLY  |
| 2   | D     | 78  | VAL  |
| 2   | G     | 78  | VAL  |
| 1   | A     | 787 | VAL  |
| 1   | B     | 246 | HIS  |
| 1   | B     | 544 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 715/809 (88%)   | 603 (84%)  | 112 (16%) | 3           | 23 |
| 1   | B     | 744/809 (92%)   | 635 (85%)  | 109 (15%) | 4           | 25 |
| 2   | C     | 350/350 (100%)  | 325 (93%)  | 25 (7%)   | 18          | 57 |
| 2   | D     | 350/350 (100%)  | 322 (92%)  | 28 (8%)   | 15          | 52 |
| 2   | E     | 350/350 (100%)  | 325 (93%)  | 25 (7%)   | 18          | 57 |
| 2   | F     | 350/350 (100%)  | 327 (93%)  | 23 (7%)   | 21          | 59 |
| 2   | G     | 350/350 (100%)  | 327 (93%)  | 23 (7%)   | 21          | 59 |
| 2   | H     | 350/350 (100%)  | 329 (94%)  | 21 (6%)   | 24          | 62 |
| 2   | I     | 350/350 (100%)  | 327 (93%)  | 23 (7%)   | 21          | 59 |
| 2   | J     | 350/350 (100%)  | 327 (93%)  | 23 (7%)   | 21          | 59 |
| 2   | K     | 350/350 (100%)  | 327 (93%)  | 23 (7%)   | 21          | 59 |
| 2   | L     | 350/350 (100%)  | 321 (92%)  | 29 (8%)   | 14          | 51 |
| 2   | M     | 350/350 (100%)  | 325 (93%)  | 25 (7%)   | 18          | 57 |
| 2   | N     | 350/350 (100%)  | 324 (93%)  | 26 (7%)   | 17          | 55 |
| 2   | O     | 350/350 (100%)  | 329 (94%)  | 21 (6%)   | 24          | 62 |
| 3   | W     | 885/990 (89%)   | 828 (94%)  | 57 (6%)   | 22          | 60 |
| All | All   | 6894/7158 (96%) | 6301 (91%) | 593 (9%)  | 13          | 49 |

All (593) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 100 | PRO  |
| 1   | A     | 122 | LEU  |
| 1   | A     | 125 | ILE  |
| 1   | A     | 126 | PHE  |
| 1   | A     | 142 | LEU  |
| 1   | A     | 147 | TYR  |
| 1   | A     | 154 | THR  |
| 1   | A     | 157 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 169 | LEU  |
| 1   | A     | 180 | TYR  |
| 1   | A     | 193 | SER  |
| 1   | A     | 204 | THR  |
| 1   | A     | 215 | GLU  |
| 1   | A     | 216 | GLU  |
| 1   | A     | 229 | ARG  |
| 1   | A     | 230 | GLN  |
| 1   | A     | 239 | VAL  |
| 1   | A     | 247 | PRO  |
| 1   | A     | 259 | HIS  |
| 1   | A     | 271 | PHE  |
| 1   | A     | 273 | TYR  |
| 1   | A     | 278 | ILE  |
| 1   | A     | 280 | ASN  |
| 1   | A     | 286 | LEU  |
| 1   | A     | 288 | MET  |
| 1   | A     | 295 | THR  |
| 1   | A     | 298 | TYR  |
| 1   | A     | 303 | LEU  |
| 1   | A     | 305 | GLN  |
| 1   | A     | 310 | LEU  |
| 1   | A     | 311 | HIS  |
| 1   | A     | 316 | SER  |
| 1   | A     | 318 | TRP  |
| 1   | A     | 342 | THR  |
| 1   | A     | 347 | GLN  |
| 1   | A     | 348 | LYS  |
| 1   | A     | 354 | GLN  |
| 1   | A     | 366 | PHE  |
| 1   | A     | 371 | ASN  |
| 1   | A     | 382 | LEU  |
| 1   | A     | 389 | GLN  |
| 1   | A     | 391 | THR  |
| 1   | A     | 392 | MET  |
| 1   | A     | 395 | ASP  |
| 1   | A     | 401 | TYR  |
| 1   | A     | 414 | VAL  |
| 1   | A     | 419 | PHE  |
| 1   | A     | 423 | SER  |
| 1   | A     | 424 | LEU  |
| 1   | A     | 428 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 436 | ILE  |
| 1   | A     | 443 | GLN  |
| 1   | A     | 445 | MET  |
| 1   | A     | 447 | TYR  |
| 1   | A     | 449 | ASN  |
| 1   | A     | 471 | TRP  |
| 1   | A     | 473 | HIS  |
| 1   | A     | 480 | PHE  |
| 1   | A     | 495 | ASP  |
| 1   | A     | 505 | GLN  |
| 1   | A     | 515 | ARG  |
| 1   | A     | 516 | GLN  |
| 1   | A     | 520 | THR  |
| 1   | A     | 521 | MET  |
| 1   | A     | 525 | TYR  |
| 1   | A     | 534 | LEU  |
| 1   | A     | 540 | LEU  |
| 1   | A     | 563 | MET  |
| 1   | A     | 564 | ASN  |
| 1   | A     | 565 | MET  |
| 1   | A     | 571 | LEU  |
| 1   | A     | 587 | LEU  |
| 1   | A     | 594 | ILE  |
| 1   | A     | 600 | LEU  |
| 1   | A     | 601 | PHE  |
| 1   | A     | 616 | GLU  |
| 1   | A     | 634 | TYR  |
| 1   | A     | 638 | MET  |
| 1   | A     | 641 | ILE  |
| 1   | A     | 646 | LEU  |
| 1   | A     | 676 | VAL  |
| 1   | A     | 680 | ASP  |
| 1   | A     | 701 | GLN  |
| 1   | A     | 704 | ILE  |
| 1   | A     | 707 | TYR  |
| 1   | A     | 717 | MET  |
| 1   | A     | 718 | TYR  |
| 1   | A     | 720 | TYR  |
| 1   | A     | 723 | ILE  |
| 1   | A     | 726 | ASN  |
| 1   | A     | 730 | PHE  |
| 1   | A     | 743 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 744 | TYR  |
| 1   | A     | 747 | ILE  |
| 1   | A     | 753 | ASN  |
| 1   | A     | 759 | LEU  |
| 1   | A     | 765 | PHE  |
| 1   | A     | 771 | VAL  |
| 1   | A     | 775 | ILE  |
| 1   | A     | 782 | VAL  |
| 1   | A     | 793 | ASP  |
| 1   | A     | 798 | ILE  |
| 1   | A     | 799 | LEU  |
| 1   | A     | 802 | ILE  |
| 1   | A     | 816 | ASP  |
| 1   | A     | 829 | VAL  |
| 1   | A     | 837 | ASN  |
| 1   | A     | 839 | MET  |
| 1   | A     | 848 | PHE  |
| 1   | A     | 849 | THR  |
| 1   | A     | 861 | ASP  |
| 1   | A     | 872 | ASP  |
| 1   | B     | 74  | GLU  |
| 1   | B     | 126 | PHE  |
| 1   | B     | 134 | TYR  |
| 1   | B     | 135 | ARG  |
| 1   | B     | 153 | ASP  |
| 1   | B     | 157 | ASP  |
| 1   | B     | 169 | LEU  |
| 1   | B     | 180 | TYR  |
| 1   | B     | 182 | LEU  |
| 1   | B     | 190 | ASN  |
| 1   | B     | 194 | ARG  |
| 1   | B     | 201 | ASP  |
| 1   | B     | 204 | THR  |
| 1   | B     | 215 | GLU  |
| 1   | B     | 217 | THR  |
| 1   | B     | 239 | VAL  |
| 1   | B     | 271 | PHE  |
| 1   | B     | 286 | LEU  |
| 1   | B     | 287 | ASN  |
| 1   | B     | 298 | TYR  |
| 1   | B     | 310 | LEU  |
| 1   | B     | 311 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 312 | ASP  |
| 1   | B     | 314 | PHE  |
| 1   | B     | 316 | SER  |
| 1   | B     | 318 | TRP  |
| 1   | B     | 336 | LEU  |
| 1   | B     | 347 | GLN  |
| 1   | B     | 348 | LYS  |
| 1   | B     | 352 | ASP  |
| 1   | B     | 353 | LEU  |
| 1   | B     | 358 | LEU  |
| 1   | B     | 382 | LEU  |
| 1   | B     | 389 | GLN  |
| 1   | B     | 392 | MET  |
| 1   | B     | 396 | PHE  |
| 1   | B     | 397 | VAL  |
| 1   | B     | 401 | TYR  |
| 1   | B     | 424 | LEU  |
| 1   | B     | 428 | GLN  |
| 1   | B     | 436 | ILE  |
| 1   | B     | 451 | ASP  |
| 1   | B     | 453 | GLN  |
| 1   | B     | 457 | GLN  |
| 1   | B     | 471 | TRP  |
| 1   | B     | 476 | ASN  |
| 1   | B     | 494 | ASN  |
| 1   | B     | 495 | ASP  |
| 1   | B     | 497 | ILE  |
| 1   | B     | 498 | ARG  |
| 1   | B     | 499 | ASN  |
| 1   | B     | 505 | GLN  |
| 1   | B     | 518 | PHE  |
| 1   | B     | 521 | MET  |
| 1   | B     | 525 | TYR  |
| 1   | B     | 534 | LEU  |
| 1   | B     | 540 | LEU  |
| 1   | B     | 542 | GLN  |
| 1   | B     | 560 | CYS  |
| 1   | B     | 562 | THR  |
| 1   | B     | 590 | ASN  |
| 1   | B     | 600 | LEU  |
| 1   | B     | 601 | PHE  |
| 1   | B     | 616 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 634 | TYR  |
| 1   | B     | 638 | MET  |
| 1   | B     | 641 | ILE  |
| 1   | B     | 646 | LEU  |
| 1   | B     | 652 | PHE  |
| 1   | B     | 660 | ASP  |
| 1   | B     | 674 | VAL  |
| 1   | B     | 676 | VAL  |
| 1   | B     | 680 | ASP  |
| 1   | B     | 697 | ASP  |
| 1   | B     | 707 | TYR  |
| 1   | B     | 709 | ASP  |
| 1   | B     | 710 | MET  |
| 1   | B     | 725 | ARG  |
| 1   | B     | 727 | LEU  |
| 1   | B     | 728 | ASP  |
| 1   | B     | 730 | PHE  |
| 1   | B     | 734 | ASN  |
| 1   | B     | 744 | TYR  |
| 1   | B     | 747 | ILE  |
| 1   | B     | 759 | LEU  |
| 1   | B     | 765 | PHE  |
| 1   | B     | 771 | VAL  |
| 1   | B     | 774 | LEU  |
| 1   | B     | 782 | VAL  |
| 1   | B     | 783 | PHE  |
| 1   | B     | 786 | ILE  |
| 1   | B     | 789 | LEU  |
| 1   | B     | 790 | ARG  |
| 1   | B     | 791 | LYS  |
| 1   | B     | 798 | ILE  |
| 1   | B     | 799 | LEU  |
| 1   | B     | 808 | ASP  |
| 1   | B     | 810 | TYR  |
| 1   | B     | 812 | VAL  |
| 1   | B     | 818 | VAL  |
| 1   | B     | 823 | THR  |
| 1   | B     | 832 | GLN  |
| 1   | B     | 836 | ARG  |
| 1   | B     | 839 | MET  |
| 1   | B     | 841 | MET  |
| 1   | B     | 857 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 871 | PHE  |
| 1   | B     | 872 | ASP  |
| 1   | B     | 876 | ILE  |
| 2   | C     | 1   | MET  |
| 2   | C     | 2   | ASP  |
| 2   | C     | 13  | ASP  |
| 2   | C     | 22  | THR  |
| 2   | C     | 26  | ASN  |
| 2   | C     | 59  | TRP  |
| 2   | C     | 68  | THR  |
| 2   | C     | 106 | ARG  |
| 2   | C     | 128 | ASN  |
| 2   | C     | 129 | PHE  |
| 2   | C     | 142 | GLN  |
| 2   | C     | 147 | ARG  |
| 2   | C     | 150 | PHE  |
| 2   | C     | 152 | PHE  |
| 2   | C     | 170 | GLN  |
| 2   | C     | 214 | LEU  |
| 2   | C     | 225 | LEU  |
| 2   | C     | 255 | ARG  |
| 2   | C     | 274 | GLN  |
| 2   | C     | 284 | ASN  |
| 2   | C     | 370 | LEU  |
| 2   | C     | 374 | TYR  |
| 2   | C     | 378 | ARG  |
| 2   | C     | 382 | LEU  |
| 2   | C     | 385 | VAL  |
| 2   | D     | 1   | MET  |
| 2   | D     | 2   | ASP  |
| 2   | D     | 13  | ASP  |
| 2   | D     | 19  | VAL  |
| 2   | D     | 68  | THR  |
| 2   | D     | 70  | LEU  |
| 2   | D     | 73  | LEU  |
| 2   | D     | 103 | GLU  |
| 2   | D     | 106 | ARG  |
| 2   | D     | 109 | ILE  |
| 2   | D     | 117 | ARG  |
| 2   | D     | 129 | PHE  |
| 2   | D     | 142 | GLN  |
| 2   | D     | 143 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 147 | ARG  |
| 2   | D     | 150 | PHE  |
| 2   | D     | 152 | PHE  |
| 2   | D     | 170 | GLN  |
| 2   | D     | 214 | LEU  |
| 2   | D     | 225 | LEU  |
| 2   | D     | 255 | ARG  |
| 2   | D     | 274 | GLN  |
| 2   | D     | 284 | ASN  |
| 2   | D     | 370 | LEU  |
| 2   | D     | 374 | TYR  |
| 2   | D     | 378 | ARG  |
| 2   | D     | 382 | LEU  |
| 2   | D     | 385 | VAL  |
| 2   | E     | 1   | MET  |
| 2   | E     | 2   | ASP  |
| 2   | E     | 13  | ASP  |
| 2   | E     | 26  | ASN  |
| 2   | E     | 59  | TRP  |
| 2   | E     | 69  | THR  |
| 2   | E     | 103 | GLU  |
| 2   | E     | 109 | ILE  |
| 2   | E     | 128 | ASN  |
| 2   | E     | 129 | PHE  |
| 2   | E     | 142 | GLN  |
| 2   | E     | 148 | THR  |
| 2   | E     | 150 | PHE  |
| 2   | E     | 152 | PHE  |
| 2   | E     | 170 | GLN  |
| 2   | E     | 214 | LEU  |
| 2   | E     | 225 | LEU  |
| 2   | E     | 255 | ARG  |
| 2   | E     | 274 | GLN  |
| 2   | E     | 284 | ASN  |
| 2   | E     | 370 | LEU  |
| 2   | E     | 374 | TYR  |
| 2   | E     | 378 | ARG  |
| 2   | E     | 382 | LEU  |
| 2   | E     | 385 | VAL  |
| 2   | F     | 2   | ASP  |
| 2   | F     | 13  | ASP  |
| 2   | F     | 60  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 61  | PHE  |
| 2   | F     | 105 | GLN  |
| 2   | F     | 109 | ILE  |
| 2   | F     | 128 | ASN  |
| 2   | F     | 129 | PHE  |
| 2   | F     | 142 | GLN  |
| 2   | F     | 148 | THR  |
| 2   | F     | 150 | PHE  |
| 2   | F     | 152 | PHE  |
| 2   | F     | 170 | GLN  |
| 2   | F     | 214 | LEU  |
| 2   | F     | 225 | LEU  |
| 2   | F     | 255 | ARG  |
| 2   | F     | 274 | GLN  |
| 2   | F     | 284 | ASN  |
| 2   | F     | 370 | LEU  |
| 2   | F     | 374 | TYR  |
| 2   | F     | 378 | ARG  |
| 2   | F     | 382 | LEU  |
| 2   | F     | 385 | VAL  |
| 2   | G     | 2   | ASP  |
| 2   | G     | 13  | ASP  |
| 2   | G     | 26  | ASN  |
| 2   | G     | 63  | PHE  |
| 2   | G     | 106 | ARG  |
| 2   | G     | 109 | ILE  |
| 2   | G     | 117 | ARG  |
| 2   | G     | 129 | PHE  |
| 2   | G     | 142 | GLN  |
| 2   | G     | 143 | ASN  |
| 2   | G     | 145 | ARG  |
| 2   | G     | 152 | PHE  |
| 2   | G     | 170 | GLN  |
| 2   | G     | 214 | LEU  |
| 2   | G     | 225 | LEU  |
| 2   | G     | 255 | ARG  |
| 2   | G     | 274 | GLN  |
| 2   | G     | 284 | ASN  |
| 2   | G     | 370 | LEU  |
| 2   | G     | 374 | TYR  |
| 2   | G     | 378 | ARG  |
| 2   | G     | 382 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | G     | 385 | VAL  |
| 2   | H     | 1   | MET  |
| 2   | H     | 2   | ASP  |
| 2   | H     | 13  | ASP  |
| 2   | H     | 103 | GLU  |
| 2   | H     | 106 | ARG  |
| 2   | H     | 128 | ASN  |
| 2   | H     | 129 | PHE  |
| 2   | H     | 142 | GLN  |
| 2   | H     | 150 | PHE  |
| 2   | H     | 152 | PHE  |
| 2   | H     | 170 | GLN  |
| 2   | H     | 214 | LEU  |
| 2   | H     | 225 | LEU  |
| 2   | H     | 255 | ARG  |
| 2   | H     | 274 | GLN  |
| 2   | H     | 284 | ASN  |
| 2   | H     | 370 | LEU  |
| 2   | H     | 374 | TYR  |
| 2   | H     | 378 | ARG  |
| 2   | H     | 382 | LEU  |
| 2   | H     | 385 | VAL  |
| 2   | I     | 1   | MET  |
| 2   | I     | 2   | ASP  |
| 2   | I     | 13  | ASP  |
| 2   | I     | 48  | THR  |
| 2   | I     | 61  | PHE  |
| 2   | I     | 106 | ARG  |
| 2   | I     | 109 | ILE  |
| 2   | I     | 117 | ARG  |
| 2   | I     | 129 | PHE  |
| 2   | I     | 142 | GLN  |
| 2   | I     | 150 | PHE  |
| 2   | I     | 152 | PHE  |
| 2   | I     | 170 | GLN  |
| 2   | I     | 214 | LEU  |
| 2   | I     | 225 | LEU  |
| 2   | I     | 255 | ARG  |
| 2   | I     | 274 | GLN  |
| 2   | I     | 284 | ASN  |
| 2   | I     | 370 | LEU  |
| 2   | I     | 374 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | I     | 378 | ARG  |
| 2   | I     | 382 | LEU  |
| 2   | I     | 385 | VAL  |
| 2   | J     | 1   | MET  |
| 2   | J     | 2   | ASP  |
| 2   | J     | 13  | ASP  |
| 2   | J     | 19  | VAL  |
| 2   | J     | 59  | TRP  |
| 2   | J     | 106 | ARG  |
| 2   | J     | 109 | ILE  |
| 2   | J     | 128 | ASN  |
| 2   | J     | 129 | PHE  |
| 2   | J     | 142 | GLN  |
| 2   | J     | 150 | PHE  |
| 2   | J     | 152 | PHE  |
| 2   | J     | 170 | GLN  |
| 2   | J     | 214 | LEU  |
| 2   | J     | 225 | LEU  |
| 2   | J     | 255 | ARG  |
| 2   | J     | 274 | GLN  |
| 2   | J     | 284 | ASN  |
| 2   | J     | 370 | LEU  |
| 2   | J     | 374 | TYR  |
| 2   | J     | 378 | ARG  |
| 2   | J     | 382 | LEU  |
| 2   | J     | 385 | VAL  |
| 2   | K     | 1   | MET  |
| 2   | K     | 2   | ASP  |
| 2   | K     | 13  | ASP  |
| 2   | K     | 59  | TRP  |
| 2   | K     | 62  | ASP  |
| 2   | K     | 106 | ARG  |
| 2   | K     | 109 | ILE  |
| 2   | K     | 129 | PHE  |
| 2   | K     | 142 | GLN  |
| 2   | K     | 143 | ASN  |
| 2   | K     | 150 | PHE  |
| 2   | K     | 152 | PHE  |
| 2   | K     | 170 | GLN  |
| 2   | K     | 214 | LEU  |
| 2   | K     | 225 | LEU  |
| 2   | K     | 255 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | K     | 274 | GLN  |
| 2   | K     | 284 | ASN  |
| 2   | K     | 370 | LEU  |
| 2   | K     | 374 | TYR  |
| 2   | K     | 378 | ARG  |
| 2   | K     | 382 | LEU  |
| 2   | K     | 385 | VAL  |
| 2   | L     | 1   | MET  |
| 2   | L     | 2   | ASP  |
| 2   | L     | 13  | ASP  |
| 2   | L     | 19  | VAL  |
| 2   | L     | 22  | THR  |
| 2   | L     | 25  | SER  |
| 2   | L     | 59  | TRP  |
| 2   | L     | 62  | ASP  |
| 2   | L     | 72  | ASN  |
| 2   | L     | 103 | GLU  |
| 2   | L     | 106 | ARG  |
| 2   | L     | 109 | ILE  |
| 2   | L     | 125 | LYS  |
| 2   | L     | 129 | PHE  |
| 2   | L     | 142 | GLN  |
| 2   | L     | 143 | ASN  |
| 2   | L     | 150 | PHE  |
| 2   | L     | 152 | PHE  |
| 2   | L     | 170 | GLN  |
| 2   | L     | 214 | LEU  |
| 2   | L     | 225 | LEU  |
| 2   | L     | 255 | ARG  |
| 2   | L     | 274 | GLN  |
| 2   | L     | 284 | ASN  |
| 2   | L     | 370 | LEU  |
| 2   | L     | 374 | TYR  |
| 2   | L     | 378 | ARG  |
| 2   | L     | 382 | LEU  |
| 2   | L     | 385 | VAL  |
| 2   | M     | 1   | MET  |
| 2   | M     | 2   | ASP  |
| 2   | M     | 13  | ASP  |
| 2   | M     | 22  | THR  |
| 2   | M     | 59  | TRP  |
| 2   | M     | 71  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 103 | GLU  |
| 2   | M     | 106 | ARG  |
| 2   | M     | 117 | ARG  |
| 2   | M     | 125 | LYS  |
| 2   | M     | 129 | PHE  |
| 2   | M     | 142 | GLN  |
| 2   | M     | 150 | PHE  |
| 2   | M     | 152 | PHE  |
| 2   | M     | 170 | GLN  |
| 2   | M     | 214 | LEU  |
| 2   | M     | 225 | LEU  |
| 2   | M     | 255 | ARG  |
| 2   | M     | 274 | GLN  |
| 2   | M     | 284 | ASN  |
| 2   | M     | 370 | LEU  |
| 2   | M     | 374 | TYR  |
| 2   | M     | 378 | ARG  |
| 2   | M     | 382 | LEU  |
| 2   | M     | 385 | VAL  |
| 2   | N     | 1   | MET  |
| 2   | N     | 2   | ASP  |
| 2   | N     | 13  | ASP  |
| 2   | N     | 58  | ASN  |
| 2   | N     | 60  | ASN  |
| 2   | N     | 66  | LEU  |
| 2   | N     | 73  | LEU  |
| 2   | N     | 103 | GLU  |
| 2   | N     | 106 | ARG  |
| 2   | N     | 109 | ILE  |
| 2   | N     | 129 | PHE  |
| 2   | N     | 142 | GLN  |
| 2   | N     | 145 | ARG  |
| 2   | N     | 150 | PHE  |
| 2   | N     | 152 | PHE  |
| 2   | N     | 170 | GLN  |
| 2   | N     | 214 | LEU  |
| 2   | N     | 225 | LEU  |
| 2   | N     | 255 | ARG  |
| 2   | N     | 274 | GLN  |
| 2   | N     | 284 | ASN  |
| 2   | N     | 370 | LEU  |
| 2   | N     | 374 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 378 | ARG  |
| 2   | N     | 382 | LEU  |
| 2   | N     | 385 | VAL  |
| 2   | O     | 2   | ASP  |
| 2   | O     | 13  | ASP  |
| 2   | O     | 23  | LEU  |
| 2   | O     | 25  | SER  |
| 2   | O     | 106 | ARG  |
| 2   | O     | 107 | ASN  |
| 2   | O     | 109 | ILE  |
| 2   | O     | 129 | PHE  |
| 2   | O     | 142 | GLN  |
| 2   | O     | 150 | PHE  |
| 2   | O     | 170 | GLN  |
| 2   | O     | 214 | LEU  |
| 2   | O     | 225 | LEU  |
| 2   | O     | 255 | ARG  |
| 2   | O     | 274 | GLN  |
| 2   | O     | 284 | ASN  |
| 2   | O     | 370 | LEU  |
| 2   | O     | 374 | TYR  |
| 2   | O     | 378 | ARG  |
| 2   | O     | 382 | LEU  |
| 2   | O     | 385 | VAL  |
| 3   | W     | 48  | ASN  |
| 3   | W     | 70  | THR  |
| 3   | W     | 79  | TYR  |
| 3   | W     | 121 | THR  |
| 3   | W     | 130 | MET  |
| 3   | W     | 143 | ASN  |
| 3   | W     | 150 | GLU  |
| 3   | W     | 155 | ASP  |
| 3   | W     | 166 | ARG  |
| 3   | W     | 178 | ASN  |
| 3   | W     | 186 | ASN  |
| 3   | W     | 195 | VAL  |
| 3   | W     | 198 | ASP  |
| 3   | W     | 246 | SER  |
| 3   | W     | 283 | GLN  |
| 3   | W     | 290 | GLN  |
| 3   | W     | 305 | LYS  |
| 3   | W     | 311 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | W     | 320  | PRO  |
| 3   | W     | 341  | ASP  |
| 3   | W     | 394  | LEU  |
| 3   | W     | 404  | GLU  |
| 3   | W     | 408  | LEU  |
| 3   | W     | 426  | ASP  |
| 3   | W     | 430  | ASN  |
| 3   | W     | 439  | PRO  |
| 3   | W     | 451  | ARG  |
| 3   | W     | 499  | GLN  |
| 3   | W     | 503  | TYR  |
| 3   | W     | 518  | TYR  |
| 3   | W     | 619  | HIS  |
| 3   | W     | 623  | THR  |
| 3   | W     | 628  | VAL  |
| 3   | W     | 629  | ASP  |
| 3   | W     | 663  | ASN  |
| 3   | W     | 690  | ARG  |
| 3   | W     | 709  | GLN  |
| 3   | W     | 717  | TYR  |
| 3   | W     | 721  | ARG  |
| 3   | W     | 723  | ARG  |
| 3   | W     | 734  | THR  |
| 3   | W     | 750  | LEU  |
| 3   | W     | 758  | THR  |
| 3   | W     | 782  | VAL  |
| 3   | W     | 808  | PHE  |
| 3   | W     | 820  | LEU  |
| 3   | W     | 835  | GLU  |
| 3   | W     | 886  | THR  |
| 3   | W     | 892  | LEU  |
| 3   | W     | 906  | ASN  |
| 3   | W     | 932  | ARG  |
| 3   | W     | 939  | VAL  |
| 3   | W     | 1003 | CYS  |
| 3   | W     | 1050 | SER  |
| 3   | W     | 1068 | LYS  |
| 3   | W     | 1078 | SER  |
| 3   | W     | 1084 | ASN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (253) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 119 | GLN  |
| 1   | A     | 137 | ASN  |
| 1   | A     | 168 | ASN  |
| 1   | A     | 230 | GLN  |
| 1   | A     | 246 | HIS  |
| 1   | A     | 260 | GLN  |
| 1   | A     | 309 | ASN  |
| 1   | A     | 365 | GLN  |
| 1   | A     | 428 | GLN  |
| 1   | A     | 443 | GLN  |
| 1   | A     | 453 | GLN  |
| 1   | A     | 462 | GLN  |
| 1   | A     | 473 | HIS  |
| 1   | A     | 490 | ASN  |
| 1   | A     | 496 | ASN  |
| 1   | A     | 553 | ASN  |
| 1   | A     | 605 | ASN  |
| 1   | A     | 609 | ASN  |
| 1   | A     | 613 | ASN  |
| 1   | A     | 615 | ASN  |
| 1   | A     | 661 | GLN  |
| 1   | A     | 683 | ASN  |
| 1   | A     | 701 | GLN  |
| 1   | A     | 722 | ASN  |
| 1   | A     | 726 | ASN  |
| 1   | A     | 803 | ASN  |
| 1   | A     | 807 | ASN  |
| 1   | A     | 840 | HIS  |
| 1   | A     | 873 | ASN  |
| 1   | B     | 119 | GLN  |
| 1   | B     | 168 | ASN  |
| 1   | B     | 190 | ASN  |
| 1   | B     | 230 | GLN  |
| 1   | B     | 237 | ASN  |
| 1   | B     | 240 | ASN  |
| 1   | B     | 246 | HIS  |
| 1   | B     | 287 | ASN  |
| 1   | B     | 302 | ASN  |
| 1   | B     | 305 | GLN  |
| 1   | B     | 311 | HIS  |
| 1   | B     | 347 | GLN  |
| 1   | B     | 361 | GLN  |
| 1   | B     | 371 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 449 | ASN  |
| 1   | B     | 465 | ASN  |
| 1   | B     | 473 | HIS  |
| 1   | B     | 476 | ASN  |
| 1   | B     | 477 | ASN  |
| 1   | B     | 491 | GLN  |
| 1   | B     | 517 | GLN  |
| 1   | B     | 553 | ASN  |
| 1   | B     | 564 | ASN  |
| 1   | B     | 590 | ASN  |
| 1   | B     | 602 | HIS  |
| 1   | B     | 605 | ASN  |
| 1   | B     | 609 | ASN  |
| 1   | B     | 611 | HIS  |
| 1   | B     | 615 | ASN  |
| 1   | B     | 629 | ASN  |
| 1   | B     | 635 | GLN  |
| 1   | B     | 683 | ASN  |
| 1   | B     | 746 | GLN  |
| 1   | B     | 807 | ASN  |
| 1   | B     | 814 | ASN  |
| 1   | B     | 831 | GLN  |
| 1   | B     | 840 | HIS  |
| 1   | B     | 878 | ASN  |
| 2   | C     | 26  | ASN  |
| 2   | C     | 35  | ASN  |
| 2   | C     | 53  | ASN  |
| 2   | C     | 72  | ASN  |
| 2   | C     | 128 | ASN  |
| 2   | C     | 131 | ASN  |
| 2   | C     | 143 | ASN  |
| 2   | C     | 146 | GLN  |
| 2   | C     | 167 | ASN  |
| 2   | C     | 239 | ASN  |
| 2   | C     | 274 | GLN  |
| 2   | C     | 284 | ASN  |
| 2   | C     | 345 | ASN  |
| 2   | D     | 26  | ASN  |
| 2   | D     | 128 | ASN  |
| 2   | D     | 131 | ASN  |
| 2   | D     | 142 | GLN  |
| 2   | D     | 146 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 167 | ASN  |
| 2   | D     | 239 | ASN  |
| 2   | D     | 274 | GLN  |
| 2   | D     | 284 | ASN  |
| 2   | D     | 345 | ASN  |
| 2   | E     | 26  | ASN  |
| 2   | E     | 53  | ASN  |
| 2   | E     | 94  | ASN  |
| 2   | E     | 131 | ASN  |
| 2   | E     | 142 | GLN  |
| 2   | E     | 167 | ASN  |
| 2   | E     | 239 | ASN  |
| 2   | E     | 274 | GLN  |
| 2   | E     | 284 | ASN  |
| 2   | E     | 345 | ASN  |
| 2   | F     | 32  | GLN  |
| 2   | F     | 53  | ASN  |
| 2   | F     | 72  | ASN  |
| 2   | F     | 94  | ASN  |
| 2   | F     | 128 | ASN  |
| 2   | F     | 131 | ASN  |
| 2   | F     | 142 | GLN  |
| 2   | F     | 167 | ASN  |
| 2   | F     | 239 | ASN  |
| 2   | F     | 274 | GLN  |
| 2   | F     | 284 | ASN  |
| 2   | F     | 345 | ASN  |
| 2   | G     | 26  | ASN  |
| 2   | G     | 35  | ASN  |
| 2   | G     | 53  | ASN  |
| 2   | G     | 128 | ASN  |
| 2   | G     | 131 | ASN  |
| 2   | G     | 142 | GLN  |
| 2   | G     | 167 | ASN  |
| 2   | G     | 239 | ASN  |
| 2   | G     | 274 | GLN  |
| 2   | G     | 284 | ASN  |
| 2   | G     | 345 | ASN  |
| 2   | H     | 26  | ASN  |
| 2   | H     | 53  | ASN  |
| 2   | H     | 83  | ASN  |
| 2   | H     | 94  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 107 | ASN  |
| 2   | H     | 128 | ASN  |
| 2   | H     | 131 | ASN  |
| 2   | H     | 142 | GLN  |
| 2   | H     | 167 | ASN  |
| 2   | H     | 239 | ASN  |
| 2   | H     | 274 | GLN  |
| 2   | H     | 284 | ASN  |
| 2   | H     | 345 | ASN  |
| 2   | I     | 32  | GLN  |
| 2   | I     | 53  | ASN  |
| 2   | I     | 76  | ASN  |
| 2   | I     | 94  | ASN  |
| 2   | I     | 128 | ASN  |
| 2   | I     | 131 | ASN  |
| 2   | I     | 143 | ASN  |
| 2   | I     | 146 | GLN  |
| 2   | I     | 167 | ASN  |
| 2   | I     | 239 | ASN  |
| 2   | I     | 274 | GLN  |
| 2   | I     | 284 | ASN  |
| 2   | I     | 345 | ASN  |
| 2   | J     | 26  | ASN  |
| 2   | J     | 53  | ASN  |
| 2   | J     | 94  | ASN  |
| 2   | J     | 128 | ASN  |
| 2   | J     | 131 | ASN  |
| 2   | J     | 142 | GLN  |
| 2   | J     | 146 | GLN  |
| 2   | J     | 167 | ASN  |
| 2   | J     | 239 | ASN  |
| 2   | J     | 274 | GLN  |
| 2   | J     | 284 | ASN  |
| 2   | J     | 345 | ASN  |
| 2   | K     | 26  | ASN  |
| 2   | K     | 53  | ASN  |
| 2   | K     | 72  | ASN  |
| 2   | K     | 94  | ASN  |
| 2   | K     | 131 | ASN  |
| 2   | K     | 143 | ASN  |
| 2   | K     | 167 | ASN  |
| 2   | K     | 239 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | K     | 274 | GLN  |
| 2   | K     | 284 | ASN  |
| 2   | K     | 345 | ASN  |
| 2   | L     | 53  | ASN  |
| 2   | L     | 72  | ASN  |
| 2   | L     | 131 | ASN  |
| 2   | L     | 140 | ASN  |
| 2   | L     | 143 | ASN  |
| 2   | L     | 146 | GLN  |
| 2   | L     | 167 | ASN  |
| 2   | L     | 239 | ASN  |
| 2   | L     | 274 | GLN  |
| 2   | L     | 284 | ASN  |
| 2   | L     | 345 | ASN  |
| 2   | M     | 36  | GLN  |
| 2   | M     | 53  | ASN  |
| 2   | M     | 128 | ASN  |
| 2   | M     | 131 | ASN  |
| 2   | M     | 142 | GLN  |
| 2   | M     | 143 | ASN  |
| 2   | M     | 167 | ASN  |
| 2   | M     | 239 | ASN  |
| 2   | M     | 274 | GLN  |
| 2   | M     | 284 | ASN  |
| 2   | M     | 345 | ASN  |
| 2   | N     | 26  | ASN  |
| 2   | N     | 32  | GLN  |
| 2   | N     | 53  | ASN  |
| 2   | N     | 94  | ASN  |
| 2   | N     | 128 | ASN  |
| 2   | N     | 131 | ASN  |
| 2   | N     | 140 | ASN  |
| 2   | N     | 142 | GLN  |
| 2   | N     | 146 | GLN  |
| 2   | N     | 167 | ASN  |
| 2   | N     | 239 | ASN  |
| 2   | N     | 274 | GLN  |
| 2   | N     | 284 | ASN  |
| 2   | N     | 345 | ASN  |
| 2   | O     | 35  | ASN  |
| 2   | O     | 53  | ASN  |
| 2   | O     | 131 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | O     | 140  | ASN  |
| 2   | O     | 142  | GLN  |
| 2   | O     | 143  | ASN  |
| 2   | O     | 153  | HIS  |
| 2   | O     | 167  | ASN  |
| 2   | O     | 239  | ASN  |
| 2   | O     | 274  | GLN  |
| 2   | O     | 284  | ASN  |
| 2   | O     | 345  | ASN  |
| 3   | W     | 31   | ASN  |
| 3   | W     | 36   | ASN  |
| 3   | W     | 42   | HIS  |
| 3   | W     | 48   | ASN  |
| 3   | W     | 68   | ASN  |
| 3   | W     | 143  | ASN  |
| 3   | W     | 185  | HIS  |
| 3   | W     | 186  | ASN  |
| 3   | W     | 283  | GLN  |
| 3   | W     | 290  | GLN  |
| 3   | W     | 308  | GLN  |
| 3   | W     | 423  | HIS  |
| 3   | W     | 473  | GLN  |
| 3   | W     | 499  | GLN  |
| 3   | W     | 565  | GLN  |
| 3   | W     | 585  | GLN  |
| 3   | W     | 604  | ASN  |
| 3   | W     | 653  | ASN  |
| 3   | W     | 703  | GLN  |
| 3   | W     | 706  | GLN  |
| 3   | W     | 760  | ASN  |
| 3   | W     | 794  | GLN  |
| 3   | W     | 810  | ASN  |
| 3   | W     | 818  | GLN  |
| 3   | W     | 824  | ASN  |
| 3   | W     | 853  | GLN  |
| 3   | W     | 862  | GLN  |
| 3   | W     | 906  | ASN  |
| 3   | W     | 956  | ASN  |
| 3   | W     | 1005 | GLN  |
| 3   | W     | 1010 | ASN  |
| 3   | W     | 1043 | ASN  |
| 3   | W     | 1048 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.