



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:55 AM UTC

PDB ID : 9NWD / pdb\_00009nwd  
EMDB ID : EMD-46688  
Title : Human E3 ligase UBR4-KCMF1-calmodulin complex (N-terminal)  
Authors : Yang, Z.; Haakonsen, D.L.; Heider, M.; Witus, S.R.; Zelter, A.; Beschauner, T.; MacCoss, M.J.; Rape, M.  
Deposited on : 2025-03-22  
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

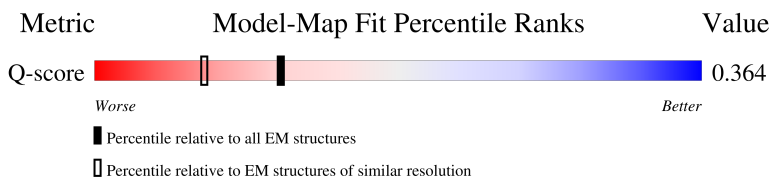
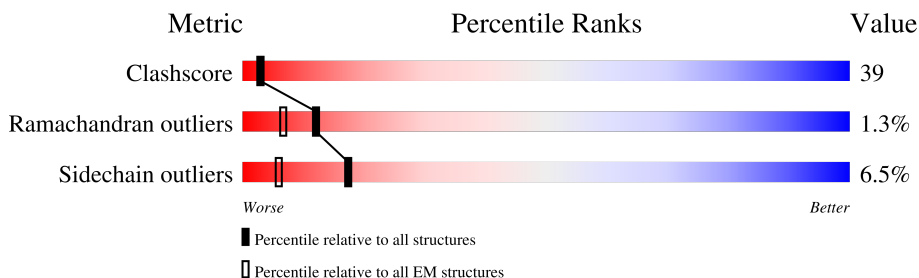
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14717 ( 2.90 - 3.90 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 5183   |                  |
| 1   | B     | 5183   |                  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21667 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called E3 ubiquitin-protein ligase UBR4.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 1396     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10853 | 6909 | 1833 | 2049 | 62 |         |       |
| 1   | B     | 1387     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10814 | 6883 | 1831 | 2038 | 62 |         |       |

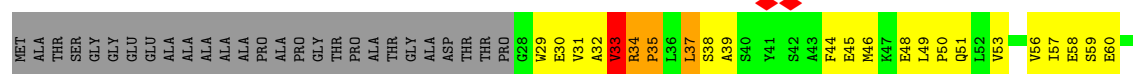






WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

- Molecule 1: E3 ubiquitin-protein ligase UBR4



|       |       |      |      |      |     |     |      |      |     |      |      |      |      |      |
|-------|-------|------|------|------|-----|-----|------|------|-----|------|------|------|------|------|
| D1125 | H1057 | L973 | ASN  | LEU  | GLU | THR | ASP  | PRO  | ASP | V352 | N280 | GLU  | A158 | I63  |
| A1126 | L1058 | D981 | SER  | ALA  | GLU | ASP | GLY  | LEU  | GLY | G353 | S281 | GLY  | K159 | H66  |
| A1127 | I1059 | D981 | ARG  | ALA  | ASP | GLY | GLY  | ALA  | ASN | S354 | F282 | ASN  | P161 |      |
| K1128 | K1060 | R985 | ARG  | R641 | SER | SER | IS11 | A441 | GLN | ALA  | F283 | GLN  | THR  | Y70  |
| S1129 | Q1061 | R985 | A903 | R646 | GLN | ASP | IS12 | L442 | GLN | VAL  | M285 | GLN  | VAL  | E71  |
| K1130 | G1062 | R985 | T904 | F647 | ASP | ASP | IS18 | R443 | VAL | VAL  | F286 | GLN  | THR  | P72  |
| Y1131 | H1063 | R985 | T905 | L648 | ASP | ASP | IS18 | R444 | ARG | ARG  | P286 | SER  | LYS  | F73  |
| Q1132 | K1064 | T992 | P906 | G649 | ASP | ASP | Q519 | R445 | THR | THR  | A287 | GLY  | THR  | Y74  |
| Y1133 | A1065 | A993 | L907 | L650 | GLU | GLU | Q520 | D446 | SER | SER  | T288 | THR  | LEU  |      |
| S1134 | E1066 | E995 | H909 | P746 | SER | SER | IS21 | L447 | GLY | GLY  |      |      |      |      |
| L1135 | H1067 | A996 | Q910 | L747 | PRO | PRO | Q522 | L448 | SER | SER  | D281 | THR  | SER  | T82  |
|       | A1068 |      | F911 | L655 | ILE | ILE | R523 |      | SER | SER  | A294 | ASP  | ASP  | H83  |
|       |       |      | E916 | L659 | LEU | LEU | R524 |      | SER | SER  | V295 | VAL  | VAL  | Y84  |
|       |       |      | L935 | L754 | GLY | GLY | IS25 |      | GLY | GLY  | S231 | GLU  | GLU  | I85  |
|       |       |      | L836 | S755 | GLN | GLN | D526 |      | GLY | GLY  | A232 | ASP  | ASP  | T86  |
|       |       |      | L840 | R759 | THR | THR | S527 |      | VAL | VAL  | K234 | LYS  | LYS  | T87  |
|       |       |      | R644 | L760 | GLU | GLU | V528 |      | GLY | GLY  | K235 | GLY  | GLY  | V88  |
|       |       |      | M948 | L761 | GLU | GLU | P529 |      | SER | SER  | K236 | LEU  | LEU  | C89  |
|       |       |      | R949 | L762 | THR | THR | L530 |      | PRO | PRO  | N237 | ALA  | ALA  | L91  |
|       |       |      | R949 | L763 | ILE | ILE | M531 |      | LYS | LYS  | F239 | SER  | SER  | I92  |
|       |       |      | V851 | L764 | ALA | ALA | L535 |      | GLY | GLY  | T240 | VAL  | VAL  | P93  |
|       |       |      | P852 | L674 | ALA | ALA | L537 |      | PRO | PRO  |      |      |      |      |
|       |       |      | R853 | S677 | PRO | PRO | T536 |      | GLY | GLY  | N243 | SER  | SER  | Q96  |
|       |       |      | L855 | L678 | GLY | GLY | L537 |      | GLY | GLY  | V244 | P182 | P182 | L97  |
|       |       |      | A856 | S679 | ALA | ALA | L538 |      | GLY | GLY  | A245 | E183 | E183 | Q98  |
|       |       |      | R857 | E680 | ALA | ALA | S539 |      | GLY | GLY  | S246 | R184 | R184 | C104 |
|       |       |      | L858 | L683 | PRO | PRO | Y542 |      | LYS | LYS  | L247 | Q186 | Q186 |      |
|       |       |      | L859 | L686 | PRO | PRO | R544 |      | LYS | LYS  | Q248 | K187 | K187 | L112 |
|       |       |      | L860 | L689 | PRO | PRO | K544 |      | PRO | PRO  | E249 | E188 | E188 | L113 |
|       |       |      | L861 | L694 | PRO | PRO | L548 |      | PRO | PRO  | L250 | V189 | V189 | R114 |
|       |       |      | L862 | L698 | PRO | PRO | Q549 |      | PRO | PRO  | G251 | Q190 | Q190 | L115 |
|       |       |      | L863 | L703 | PRO | PRO | K553 |      | PRO | PRO  | G252 | M191 | M191 | E120 |
|       |       |      | L864 | S702 | PRO | PRO | V474 |      | PRO | PRO  | S253 | N192 | N192 | A121 |
|       |       |      | L865 | E704 | PRO | PRO | I475 |      | PRO | PRO  | E254 | F193 | F193 | C122 |
|       |       |      | L866 | L699 | PRO | PRO | L478 |      | PRO | PRO  | K255 | L194 | L194 | A123 |
|       |       |      | L867 | L703 | PRO | PRO | N478 |      | PRO | PRO  | L256 | Q196 | Q196 | A123 |
|       |       |      | L868 | S703 | PRO | PRO | H479 |      | PRO | PRO  | L257 | L197 | L197 | V124 |
|       |       |      | L869 | S702 | PRO | PRO | A480 |      | PRO | PRO  | V259 | T198 | T198 | L129 |
|       |       |      | L870 | E704 | PRO | PRO | L483 |      | PRO | PRO  | C260 | S199 | S199 | I130 |
|       |       |      | L871 | L704 | PRO | PRO | L484 |      | PRO | PRO  | L261 | V200 | V200 | L131 |
|       |       |      | L872 | L704 | PRO | PRO | T485 |      | PRO | PRO  | K262 | F201 | F201 | L132 |
|       |       |      | L873 | L704 | PRO | PRO | L485 |      | PRO | PRO  | L263 | N202 | N202 | I133 |
|       |       |      | L874 | L704 | PRO | PRO | F488 |      | PRO | PRO  | P264 | P203 | P203 | L136 |
|       |       |      | L875 | L704 | PRO | PRO | Q489 |      | PRO | PRO  | F266 | R204 | R204 | R142 |
|       |       |      | L876 | L704 | PRO | PRO | L491 |      | PRO | PRO  | L267 | ALA  | ALA  | L143 |
|       |       |      | L877 | L704 | PRO | PRO | Q492 |      | PRO | PRO  | R268 | SER  | SER  | D144 |
|       |       |      | L878 | L704 | PRO | PRO | V493 |      | PRO | PRO  | Y269 | GLN  | GLN  | E147 |
|       |       |      | L879 | L704 | PRO | PRO | E494 |      | PRO | PRO  | N271 | ILE  | ILE  | F151 |
|       |       |      | L880 | L704 | PRO | PRO | L496 |      | PRO | PRO  | R272 | SER  | SER  | F151 |
|       |       |      | L881 | L704 | PRO | PRO | H497 |      | PRO | PRO  | Q274 | THR  | THR  | M164 |
|       |       |      | L882 | L704 | PRO | PRO | K498 |      | PRO | PRO  | V277 | GLN  | GLN  | M164 |
|       |       |      | L883 | L704 | PRO | PRO | G499 |      | PRO | PRO  | L278 | THR  | THR  | K156 |
|       |       |      | L884 | L704 | PRO | PRO | TRP  |      | PRO | PRO  | A279 | VAL  | VAL  | S157 |
|       |       |      | L885 | L704 | PRO | PRO | THR  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L886 | L704 | PRO | PRO | ILE  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L887 | L704 | PRO | PRO | GLY  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L888 | L704 | PRO | PRO | LYS  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L889 | L704 | PRO | PRO | ASP  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L890 | L704 | PRO | PRO | THR  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L891 | L704 | PRO | PRO | ASN  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L892 | L704 | PRO | PRO | THR  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L893 | L704 | PRO | PRO | TYR  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L894 | L704 | PRO | PRO | TYR  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L895 | L704 | PRO | PRO | GLU  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L896 | L704 | PRO | PRO | ASP  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L897 | L704 | PRO | PRO | PHE  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L898 | L704 | PRO | PRO | SER  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L899 | L704 | PRO | PRO | THR  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L900 | L704 | PRO | PRO | ASP  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L901 | L704 | PRO | PRO | GLY  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L902 | L704 | PRO | PRO | LYS  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L903 | L704 | PRO | PRO | ILE  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L904 | L704 | PRO | PRO | GLY  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L905 | L704 | PRO | PRO | LYS  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L906 | L704 | PRO | PRO | ASP  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L907 | L704 | PRO | PRO | PHE  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L908 | L704 | PRO | PRO | SER  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L909 | L704 | PRO | PRO | THR  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L910 | L704 | PRO | PRO | ASP  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L911 | L704 | PRO | PRO | GLY  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L912 | L704 | PRO | PRO | LYS  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L913 | L704 | PRO | PRO | ILE  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L914 | L704 | PRO | PRO | GLY  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L915 | L704 | PRO | PRO | LYS  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L916 | L704 | PRO | PRO | ASP  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L917 | L704 | PRO | PRO | THR  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L918 | L704 | PRO | PRO | ASN  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L919 | L704 | PRO | PRO | THR  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L920 | L704 | PRO | PRO | ASP  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L921 | L704 | PRO | PRO | GLY  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L922 | L704 | PRO | PRO | LYS  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L923 | L704 | PRO | PRO | ILE  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L924 | L704 | PRO | PRO | GLY  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L925 | L704 | PRO | PRO | LYS  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L926 | L704 | PRO | PRO | ASP  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L927 | L704 | PRO | PRO | THR  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L928 | L704 | PRO | PRO | ASN  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L929 | L704 | PRO | PRO | THR  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L930 | L704 | PRO | PRO | ASP  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L931 | L704 | PRO | PRO | GLY  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L932 | L704 | PRO | PRO | LYS  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L933 | L704 | PRO | PRO | ILE  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L934 | L704 | PRO | PRO | GLY  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L935 | L704 | PRO | PRO | LYS  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L936 | L704 | PRO | PRO | ASP  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L937 | L704 | PRO | PRO | THR  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L938 | L704 | PRO | PRO | ASN  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L939 | L704 | PRO | PRO | THR  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L940 | L704 | PRO | PRO | ASP  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L941 | L704 | PRO | PRO | GLY  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L942 | L704 | PRO | PRO | LYS  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L943 | L704 | PRO | PRO | ILE  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L944 | L704 | PRO | PRO | GLY  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L945 | L704 | PRO | PRO | LYS  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L946 | L704 | PRO | PRO | ASP  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L947 | L704 | PRO | PRO | THR  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L948 | L704 | PRO | PRO | ASN  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L949 | L704 | PRO | PRO | THR  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L950 | L704 | PRO | PRO | ASP  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L951 | L704 | PRO | PRO | GLY  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L952 | L704 | PRO | PRO | LYS  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L953 | L704 | PRO | PRO | ILE  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L954 | L704 | PRO | PRO | GLY  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L955 | L704 | PRO | PRO | LYS  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L956 | L704 | PRO | PRO | ASP  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L957 | L704 | PRO | PRO | THR  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L958 | L704 | PRO | PRO | ASN  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L959 | L704 | PRO | PRO | THR  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L960 | L704 | PRO | PRO | ASP  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L961 | L704 | PRO | PRO | GLY  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L962 | L704 | PRO | PRO | LYS  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L963 | L704 | PRO | PRO | ILE  |      | PRO | PRO  |      |      |      |      |
|       |       |      | L964 | L704 | PRO | PRO | GLY  |      | PRO | PRO  |      |      |      |      |









## 4 Experimental information

| Property                             | Value                         | Source    |
|--------------------------------------|-------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE               | Depositor |
| Imposed symmetry                     | POINT, Not provided           |           |
| Number of particles used             | 126259                        | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF             | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY           | Depositor |
| Microscope                           | TFS KRIOS                     | Depositor |
| Voltage (kV)                         | 300                           | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                            | Depositor |
| Minimum defocus (nm)                 | 1000                          | Depositor |
| Maximum defocus (nm)                 | 2200                          | Depositor |
| Magnification                        | Not provided                  |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value                    | 0.801                         | Depositor |
| Minimum map value                    | -0.495                        | Depositor |
| Average map value                    | 0.000                         | Depositor |
| Map value standard deviation         | 0.014                         | Depositor |
| Recommended contour level            | 0.068                         | Depositor |
| Map size ( $\text{\AA}$ )            | 432.64, 432.64, 432.64        | wwPDB     |
| Map dimensions                       | 520, 520, 520                 | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0              | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.832, 0.832, 0.832           | Depositor |

## 5 Model quality i

### 5.1 Standard geometry i

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     | 0.89         | 21/11051 (0.2%) | 1.14        | 66/15000 (0.4%)  |
| 1   | B     | 0.99         | 22/11008 (0.2%) | 1.26        | 65/14932 (0.4%)  |
| All | All   | 0.95         | 43/22059 (0.2%) | 1.20        | 131/29932 (0.4%) |

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                   | 4                   |
| 1   | B     | 0                   | 12                  |
| All | All   | 0                   | 16                  |

All (43) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 878  | GLU  | CA-C  | -8.95 | 1.41        | 1.52     |
| 1   | A     | 789  | THR  | CA-C  | -8.80 | 1.41        | 1.52     |
| 1   | A     | 855  | LEU  | CA-C  | -8.66 | 1.40        | 1.52     |
| 1   | A     | 858  | LEU  | CA-C  | -8.53 | 1.41        | 1.52     |
| 1   | A     | 782  | VAL  | CA-C  | -8.30 | 1.42        | 1.52     |
| 1   | A     | 877  | PHE  | N-CA  | -7.87 | 1.36        | 1.46     |
| 1   | A     | 78   | VAL  | C-O   | -7.66 | 1.15        | 1.24     |
| 1   | B     | 244  | VAL  | CA-C  | -7.50 | 1.43        | 1.52     |
| 1   | B     | 1441 | SER  | C-N   | 7.38  | 1.42        | 1.33     |
| 1   | A     | 877  | PHE  | CA-C  | -7.35 | 1.43        | 1.52     |
| 1   | A     | 782  | VAL  | CA-CB | -6.99 | 1.46        | 1.54     |
| 1   | A     | 789  | THR  | CA-CB | -6.89 | 1.42        | 1.53     |
| 1   | B     | 518  | ILE  | C-O   | -6.72 | 1.16        | 1.24     |
| 1   | B     | 1439 | GLU  | C-N   | -6.58 | 1.25        | 1.33     |
| 1   | B     | 248  | GLN  | N-CA  | -6.03 | 1.39        | 1.46     |
| 1   | B     | 1213 | THR  | C-O   | 5.88  | 1.32        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 850  | PHE  | C-N   | 5.86  | 1.40        | 1.33     |
| 1   | B     | 1442 | PRO  | C-N   | -5.85 | 1.25        | 1.32     |
| 1   | A     | 858  | LEU  | C-N   | -5.73 | 1.25        | 1.33     |
| 1   | A     | 789  | THR  | N-CA  | -5.73 | 1.39        | 1.46     |
| 1   | B     | 1446 | LEU  | C-O   | 5.72  | 1.30        | 1.24     |
| 1   | A     | 857  | ARG  | CA-CB | -5.70 | 1.44        | 1.53     |
| 1   | A     | 968  | ALA  | CA-C  | -5.69 | 1.45        | 1.52     |
| 1   | B     | 246  | SER  | CA-C  | -5.64 | 1.45        | 1.52     |
| 1   | A     | 856  | ALA  | CA-CB | -5.57 | 1.44        | 1.53     |
| 1   | B     | 1460 | GLU  | CA-C  | -5.47 | 1.46        | 1.52     |
| 1   | A     | 878  | GLU  | CA-CB | -5.44 | 1.44        | 1.53     |
| 1   | B     | 529  | PRO  | N-CA  | -5.43 | 1.40        | 1.47     |
| 1   | B     | 236  | LYS  | CA-C  | -5.43 | 1.45        | 1.52     |
| 1   | B     | 196  | GLN  | CA-CB | -5.40 | 1.45        | 1.53     |
| 1   | B     | 240  | ILE  | CA-C  | -5.40 | 1.46        | 1.52     |
| 1   | A     | 782  | VAL  | C-O   | -5.38 | 1.18        | 1.24     |
| 1   | B     | 519  | GLN  | C-N   | -5.33 | 1.26        | 1.33     |
| 1   | A     | 860  | LEU  | CA-CB | -5.27 | 1.45        | 1.53     |
| 1   | B     | 520  | ARG  | N-CA  | -5.20 | 1.40        | 1.46     |
| 1   | B     | 519  | GLN  | CA-C  | -5.13 | 1.45        | 1.52     |
| 1   | A     | 855  | LEU  | C-O   | -5.12 | 1.17        | 1.24     |
| 1   | B     | 1232 | SER  | C-O   | -5.12 | 1.18        | 1.24     |
| 1   | A     | 967  | TYR  | CA-CB | -5.11 | 1.45        | 1.53     |
| 1   | B     | 1233 | TRP  | CA-C  | -5.08 | 1.45        | 1.52     |
| 1   | B     | 1033 | CYS  | C-O   | 5.06  | 1.29        | 1.24     |
| 1   | B     | 519  | GLN  | N-CA  | -5.03 | 1.39        | 1.46     |
| 1   | B     | 202  | ASN  | CA-C  | -5.02 | 1.50        | 1.53     |

All (131) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 1   | A     | 855  | LEU  | N-CA-C | -13.01 | 96.76       | 112.89   |
| 1   | B     | 1451 | GLY  | N-CA-C | -12.54 | 98.98       | 114.16   |
| 1   | A     | 789  | THR  | N-CA-C | -12.48 | 97.67       | 111.28   |
| 1   | B     | 1083 | VAL  | N-CA-C | -12.02 | 96.91       | 110.62   |
| 1   | A     | 860  | LEU  | N-CA-C | -11.29 | 98.99       | 111.07   |
| 1   | A     | 34   | ARG  | CA-C-N | -10.40 | 108.17      | 119.19   |
| 1   | A     | 34   | ARG  | C-N-CA | -10.40 | 108.17      | 119.19   |
| 1   | B     | 1460 | GLU  | N-CA-C | -10.21 | 96.78       | 109.65   |
| 1   | B     | 34   | ARG  | CA-C-N | -10.04 | 108.24      | 119.28   |
| 1   | B     | 34   | ARG  | C-N-CA | -10.04 | 108.24      | 119.28   |
| 1   | A     | 851  | VAL  | CA-C-N | -9.87  | 107.51      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 851  | VAL  | C-N-CA   | -9.87 | 107.51      | 119.84   |
| 1   | A     | 930  | PRO  | CB-CA-C  | -9.71 | 103.71      | 111.87   |
| 1   | A     | 1123 | THR  | N-CA-C   | -9.26 | 101.19      | 111.28   |
| 1   | B     | 236  | LYS  | N-CA-C   | -8.79 | 101.62      | 111.82   |
| 1   | A     | 877  | PHE  | CA-C-N   | -8.66 | 108.68      | 120.28   |
| 1   | A     | 877  | PHE  | C-N-CA   | -8.66 | 108.68      | 120.28   |
| 1   | A     | 968  | ALA  | CA-C-N   | -8.58 | 108.78      | 120.28   |
| 1   | A     | 968  | ALA  | C-N-CA   | -8.58 | 108.78      | 120.28   |
| 1   | B     | 282  | PHE  | N-CA-C   | -8.45 | 96.85       | 110.20   |
| 1   | A     | 782  | VAL  | N-CA-C   | -8.15 | 102.60      | 110.42   |
| 1   | A     | 853  | LEU  | N-CA-C   | -8.14 | 102.36      | 111.07   |
| 1   | B     | 528  | VAL  | CA-C-N   | -8.09 | 109.73      | 119.84   |
| 1   | B     | 528  | VAL  | C-N-CA   | -8.09 | 109.73      | 119.84   |
| 1   | B     | 1520 | PRO  | CA-N-CD  | -7.94 | 100.89      | 112.00   |
| 1   | A     | 1282 | ALA  | N-CA-C   | -7.83 | 102.99      | 112.54   |
| 1   | B     | 248  | GLN  | N-CA-C   | -7.79 | 101.91      | 111.33   |
| 1   | A     | 1404 | SER  | N-CA-C   | 7.77  | 122.86      | 112.30   |
| 1   | B     | 1299 | ILE  | N-CA-C   | -7.55 | 103.58      | 111.58   |
| 1   | A     | 966  | LEU  | N-CA-C   | -7.48 | 103.41      | 112.54   |
| 1   | A     | 782  | VAL  | CB-CA-C  | -7.38 | 102.53      | 111.97   |
| 1   | B     | 229  | GLN  | N-CA-C   | -7.31 | 102.13      | 113.02   |
| 1   | A     | 38   | SER  | N-CA-C   | -7.24 | 103.42      | 111.82   |
| 1   | A     | 33   | VAL  | N-CA-C   | -7.23 | 101.47      | 111.89   |
| 1   | B     | 1123 | THR  | N-CA-C   | -7.18 | 103.46      | 111.28   |
| 1   | A     | 35   | PRO  | N-CA-C   | -7.17 | 104.18      | 113.57   |
| 1   | B     | 33   | VAL  | N-CA-C   | -7.13 | 101.62      | 111.89   |
| 1   | A     | 789  | THR  | CB-CA-C  | -7.12 | 98.96       | 110.79   |
| 1   | A     | 1402 | SER  | N-CA-C   | -7.09 | 103.59      | 111.82   |
| 1   | B     | 1447 | LEU  | N-CA-C   | -7.05 | 103.60      | 111.28   |
| 1   | B     | 1561 | VAL  | CB-CA-C  | -7.00 | 103.01      | 111.97   |
| 1   | B     | 1449 | LEU  | CA-C-N   | -6.89 | 109.53      | 121.66   |
| 1   | B     | 1449 | LEU  | C-N-CA   | -6.89 | 109.53      | 121.66   |
| 1   | B     | 1441 | SER  | O-C-N    | 6.85  | 126.46      | 121.12   |
| 1   | B     | 1057 | HIS  | CA-CB-CG | -6.76 | 107.04      | 113.80   |
| 1   | A     | 1303 | ASP  | CB-CA-C  | -6.63 | 108.92      | 116.54   |
| 1   | A     | 1198 | PHE  | N-CA-C   | -6.62 | 104.10      | 111.71   |
| 1   | B     | 1058 | LEU  | N-CA-C   | -6.61 | 104.00      | 111.07   |
| 1   | A     | 1244 | ILE  | N-CA-C   | 6.59  | 123.05      | 109.34   |
| 1   | A     | 29   | TRP  | N-CA-C   | -6.58 | 104.11      | 111.28   |
| 1   | A     | 967  | TYR  | N-CA-C   | -6.52 | 104.25      | 111.36   |
| 1   | A     | 47   | LYS  | N-CA-C   | -6.34 | 105.70      | 113.50   |
| 1   | A     | 81   | SER  | N-CA-C   | -6.33 | 104.30      | 111.14   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 788  | SER  | N-CA-C  | 6.33  | 120.21      | 112.23   |
| 1   | A     | 790  | MET  | N-CA-C  | 6.25  | 119.02      | 111.40   |
| 1   | A     | 40   | SER  | N-CA-C  | -6.19 | 104.53      | 111.28   |
| 1   | B     | 35   | PRO  | N-CA-C  | -6.19 | 105.30      | 113.65   |
| 1   | B     | 231  | SER  | N-CA-C  | -6.17 | 105.23      | 112.89   |
| 1   | B     | 520  | ARG  | N-CA-C  | -6.17 | 104.56      | 111.28   |
| 1   | A     | 877  | PHE  | N-CA-C  | -6.15 | 103.90      | 111.40   |
| 1   | B     | 887  | PRO  | N-CA-C  | 6.15  | 118.20      | 110.70   |
| 1   | A     | 390  | GLN  | N-CA-C  | -6.13 | 104.59      | 111.28   |
| 1   | A     | 854  | ILE  | N-CA-C  | 6.12  | 120.60      | 112.04   |
| 1   | B     | 296  | ARG  | N-CA-C  | -6.11 | 104.63      | 111.28   |
| 1   | A     | 1255 | THR  | CB-CA-C | -6.10 | 109.52      | 116.54   |
| 1   | A     | 1125 | ASP  | N-CA-C  | -6.07 | 104.67      | 111.28   |
| 1   | B     | 1227 | GLN  | N-CA-C  | -6.06 | 104.30      | 111.03   |
| 1   | A     | 1545 | ALA  | N-CA-C  | -6.05 | 105.16      | 112.54   |
| 1   | A     | 1082 | SER  | CA-C-N  | -6.05 | 112.80      | 120.60   |
| 1   | A     | 1082 | SER  | C-N-CA  | -6.05 | 112.80      | 120.60   |
| 1   | B     | 233  | ILE  | CB-CA-C | -5.98 | 104.31      | 111.97   |
| 1   | A     | 194  | LEU  | N-CA-C  | -5.95 | 105.12      | 112.38   |
| 1   | B     | 531  | MET  | N-CA-C  | -5.81 | 104.86      | 111.07   |
| 1   | B     | 1248 | ARG  | CB-CA-C | -5.81 | 109.86      | 116.54   |
| 1   | B     | 244  | VAL  | CB-CA-C | -5.77 | 104.26      | 112.22   |
| 1   | A     | 1575 | ASN  | N-CA-C  | -5.77 | 104.91      | 111.14   |
| 1   | A     | 1381 | LEU  | N-CA-C  | -5.74 | 105.02      | 111.28   |
| 1   | B     | 1446 | LEU  | N-CA-C  | -5.70 | 104.45      | 111.40   |
| 1   | B     | 352  | VAL  | CA-C-N  | -5.69 | 112.99      | 120.22   |
| 1   | B     | 352  | VAL  | C-N-CA  | -5.69 | 112.99      | 120.22   |
| 1   | B     | 1125 | ASP  | N-CA-C  | -5.69 | 105.08      | 111.28   |
| 1   | A     | 77   | PHE  | N-CA-C  | -5.65 | 104.81      | 110.97   |
| 1   | A     | 991  | VAL  | O-C-N   | -5.64 | 115.53      | 122.57   |
| 1   | A     | 968  | ALA  | N-CA-C  | 5.57  | 117.35      | 111.28   |
| 1   | B     | 1599 | ILE  | N-CA-C  | -5.54 | 105.10      | 110.42   |
| 1   | B     | 1413 | ALA  | N-CA-C  | -5.54 | 105.33      | 111.36   |
| 1   | B     | 336  | CYS  | N-CA-CB | 5.53  | 118.74      | 110.22   |
| 1   | A     | 46   | MET  | N-CA-C  | -5.53 | 106.91      | 113.38   |
| 1   | B     | 525  | ILE  | CB-CA-C | -5.53 | 103.15      | 112.16   |
| 1   | B     | 230  | ALA  | N-CA-C  | -5.52 | 105.53      | 114.09   |
| 1   | A     | 1003 | PHE  | N-CA-C  | -5.52 | 105.16      | 111.07   |
| 1   | A     | 1155 | THR  | N-CA-C  | -5.51 | 105.36      | 111.36   |
| 1   | B     | 1100 | SER  | CA-C-N  | -5.50 | 114.36      | 122.83   |
| 1   | B     | 1100 | SER  | C-N-CA  | -5.50 | 114.36      | 122.83   |
| 1   | A     | 1081 | SER  | N-CA-C  | -5.48 | 105.20      | 111.07   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 854  | ILE  | O-C-N   | -5.46 | 114.90      | 122.05   |
| 1   | B     | 965  | GLU  | N-CA-C  | -5.46 | 106.56      | 113.43   |
| 1   | B     | 519  | GLN  | CA-C-N  | -5.46 | 112.97      | 120.28   |
| 1   | B     | 519  | GLN  | C-N-CA  | -5.46 | 112.97      | 120.28   |
| 1   | B     | 1233 | TRP  | N-CA-C  | -5.40 | 106.39      | 112.87   |
| 1   | A     | 1002 | TYR  | CA-C-N  | -5.39 | 113.43      | 120.44   |
| 1   | A     | 1002 | TYR  | C-N-CA  | -5.39 | 113.43      | 120.44   |
| 1   | A     | 1547 | ALA  | N-CA-C  | -5.32 | 105.88      | 112.38   |
| 1   | B     | 1087 | VAL  | CA-C-O  | -5.32 | 115.88      | 121.41   |
| 1   | A     | 1315 | LEU  | CA-C-N  | -5.32 | 113.15      | 119.05   |
| 1   | A     | 1315 | LEU  | C-N-CA  | -5.32 | 113.15      | 119.05   |
| 1   | A     | 496  | LEU  | N-CA-C  | 5.31  | 117.57      | 110.35   |
| 1   | A     | 853  | LEU  | CA-C-O  | -5.31 | 115.25      | 120.82   |
| 1   | B     | 192  | ASN  | N-CA-C  | -5.31 | 105.91      | 112.38   |
| 1   | B     | 314  | SER  | N-CA-C  | -5.25 | 106.72      | 113.23   |
| 1   | B     | 1444 | PRO  | N-CA-C  | 5.22  | 123.22      | 112.47   |
| 1   | B     | 202  | ASN  | N-CA-C  | -5.20 | 101.64      | 112.40   |
| 1   | B     | 1065 | ALA  | N-CA-C  | 5.20  | 117.35      | 111.11   |
| 1   | B     | 1449 | LEU  | CA-C-O  | 5.19  | 125.77      | 119.38   |
| 1   | B     | 1086 | ASP  | N-CA-C  | -5.18 | 105.32      | 110.97   |
| 1   | A     | 48   | GLU  | N-CA-C  | -5.18 | 107.01      | 113.38   |
| 1   | B     | 201  | PHE  | CA-C-N  | -5.17 | 118.13      | 123.10   |
| 1   | B     | 201  | PHE  | C-N-CA  | -5.17 | 118.13      | 123.10   |
| 1   | B     | 268  | ARG  | CA-C-N  | -5.17 | 113.35      | 120.28   |
| 1   | B     | 268  | ARG  | C-N-CA  | -5.17 | 113.35      | 120.28   |
| 1   | A     | 83   | HIS  | CB-CA-C | -5.13 | 102.61      | 110.81   |
| 1   | A     | 782  | VAL  | CA-C-N  | -5.11 | 113.80      | 120.44   |
| 1   | A     | 782  | VAL  | C-N-CA  | -5.11 | 113.80      | 120.44   |
| 1   | B     | 1611 | SER  | N-CA-C  | -5.10 | 105.72      | 111.28   |
| 1   | B     | 1157 | ASN  | N-CA-C  | -5.09 | 105.73      | 111.28   |
| 1   | A     | 887  | PRO  | N-CA-C  | 5.08  | 116.89      | 110.70   |
| 1   | B     | 1558 | ASN  | N-CA-C  | -5.05 | 105.85      | 111.36   |
| 1   | B     | 1054 | ILE  | CA-C-O  | -5.04 | 115.82      | 121.17   |
| 1   | B     | 426  | PRO  | N-CA-C  | -5.04 | 106.52      | 113.53   |
| 1   | A     | 782  | VAL  | N-CA-CB | 5.04  | 116.45      | 110.55   |
| 1   | B     | 244  | VAL  | N-CA-C  | -5.00 | 105.67      | 110.72   |

There are no chirality outliers.

All (16) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1008 | ARG  | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1174 | ARG  | Sidechain |
| 1   | A     | 1394 | ARG  | Sidechain |
| 1   | A     | 849  | ARG  | Sidechain |
| 1   | B     | 1008 | ARG  | Sidechain |
| 1   | B     | 1096 | ARG  | Sidechain |
| 1   | B     | 1336 | ARG  | Sidechain |
| 1   | B     | 1470 | ARG  | Sidechain |
| 1   | B     | 272  | ARG  | Sidechain |
| 1   | B     | 296  | ARG  | Sidechain |
| 1   | B     | 325  | ARG  | Sidechain |
| 1   | B     | 396  | ARG  | Sidechain |
| 1   | B     | 397  | ARG  | Sidechain |
| 1   | B     | 759  | ARG  | Sidechain |
| 1   | B     | 849  | ARG  | Sidechain |
| 1   | B     | 985  | ARG  | 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     | 10853 | 0        | 10929    | 945     | 0            |
| 1   | B     | 10814 | 0        | 10915    | 803     | 0            |
| All | All   | 21667 | 0        | 21844    | 1708    | 0            |

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

All (1708) 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:313:LEU:HD11 | 1:B:332:LEU:CD2  | 1.51                     | 1.36              |
| 1:B:89:CYS:SG    | 1:B:239:PHE:HD2  | 1.54                     | 1.30              |
| 1:A:1399:GLU:O   | 1:A:1403:ASP:OD1 | 1.56                     | 1.20              |
| 1:B:89:CYS:SG    | 1:B:239:PHE:CD2  | 2.32                     | 1.20              |
| 1:A:73:PHE:CD1   | 1:A:159:LYS:HA   | 1.80                     | 1.17              |
| 1:B:1205:GLY:HA3 | 1:B:1215:GLY:HA2 | 1.25                     | 1.17              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:867:HIS:O     | 1:A:949:ASP:OD1   | 1.66                     | 1.11              |
| 1:B:31:VAL:O      | 1:B:35:PRO:HD3    | 1.49                     | 1.10              |
| 1:A:908:TYR:CE2   | 1:A:930:PRO:HB3   | 1.87                     | 1.09              |
| 1:A:1450:CYS:HB2  | 1:A:1505:GLN:HB2  | 1.33                     | 1.08              |
| 1:B:313:LEU:HD11  | 1:B:332:LEU:HD23  | 1.31                     | 1.08              |
| 1:B:1205:GLY:HA3  | 1:B:1215:GLY:CA   | 1.83                     | 1.07              |
| 1:B:313:LEU:HD11  | 1:B:332:LEU:HD21  | 1.31                     | 1.05              |
| 1:B:910:GLY:HA2   | 1:B:933:TYR:HA    | 1.37                     | 1.05              |
| 1:A:808:VAL:HG11  | 1:A:908:TYR:HB3   | 1.38                     | 1.01              |
| 1:A:881:GLN:NE2   | 1:B:193:PHE:HA    | 1.75                     | 1.01              |
| 1:B:1138:HIS:CD2  | 1:B:1143:ALA:HB3  | 1.96                     | 0.99              |
| 1:A:32:ALA:O      | 1:A:35:PRO:HD2    | 1.63                     | 0.98              |
| 1:B:352:VAL:HG22  | 1:B:467:GLN:HG2   | 1.43                     | 0.98              |
| 1:A:349:ILE:HD12  | 1:A:429:LEU:HD11  | 1.42                     | 0.98              |
| 1:B:263:LEU:HB2   | 1:B:266:PHE:HB2   | 1.45                     | 0.97              |
| 1:B:313:LEU:CD1   | 1:B:332:LEU:CD2   | 2.41                     | 0.97              |
| 1:A:53:VAL:HG11   | 1:A:99:SER:HB3    | 1.47                     | 0.97              |
| 1:A:1087:VAL:HG21 | 1:A:1154:ILE:HD13 | 1.45                     | 0.97              |
| 1:B:1090:VAL:HG13 | 1:B:1127:ALA:HB1  | 1.47                     | 0.96              |
| 1:A:1500:VAL:HG22 | 1:A:1547:ALA:HB2  | 1.45                     | 0.96              |
| 1:A:1438:THR:HA   | 1:A:1446:LEU:HD13 | 1.47                     | 0.95              |
| 1:B:1159:LEU:HA   | 1:B:1298:LEU:HD13 | 1.48                     | 0.95              |
| 1:A:1314:LEU:HG   | 1:A:1333:SER:HB2  | 1.47                     | 0.94              |
| 1:B:1438:THR:OG1  | 1:B:1446:LEU:HB3  | 1.67                     | 0.94              |
| 1:A:855:LEU:HD23  | 1:A:1002:TYR:HE2  | 1.32                     | 0.94              |
| 1:A:868:GLN:HA    | 1:A:949:ASP:OD2   | 1.68                     | 0.94              |
| 1:A:690:ILE:HA    | 1:A:710:LEU:HD21  | 1.51                     | 0.92              |
| 1:A:1570:TYR:CD2  | 1:A:1592:ILE:HG21 | 2.05                     | 0.92              |
| 1:B:318:LEU:HA    | 1:B:325:ARG:HH22  | 1.35                     | 0.91              |
| 1:B:1486:GLN:HA   | 1:B:1489:ARG:HD2  | 1.52                     | 0.91              |
| 1:B:313:LEU:CD1   | 1:B:332:LEU:HD21  | 1.99                     | 0.90              |
| 1:B:1449:LEU:O    | 1:B:1452:SER:HB3  | 1.72                     | 0.90              |
| 1:A:1541:MET:HA   | 1:A:1544:LEU:HD12 | 1.53                     | 0.89              |
| 1:A:1417:GLU:HA   | 1:A:1470:ARG:HD2  | 1.54                     | 0.89              |
| 1:B:1394:ARG:HA   | 1:B:1397:MET:HE2  | 1.53                     | 0.89              |
| 1:A:1105:ASP:H    | 1:A:1110:LEU:HD21 | 1.37                     | 0.88              |
| 1:B:32:ALA:O      | 1:B:35:PRO:HD2    | 1.74                     | 0.88              |
| 1:A:193:PHE:HB2   | 1:B:881:GLN:HE21  | 1.38                     | 0.88              |
| 1:A:910:GLY:HA2   | 1:A:933:TYR:HA    | 1.55                     | 0.88              |
| 1:B:31:VAL:O      | 1:B:34:ARG:HB3    | 1.73                     | 0.88              |
| 1:A:31:VAL:O      | 1:A:35:PRO:HD3    | 1.72                     | 0.87              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:908:TYR:CZ    | 1:A:930:PRO:HB3   | 2.09                     | 0.87              |
| 1:A:329:VAL:HG12  | 1:A:388:ILE:HG23  | 1.57                     | 0.87              |
| 1:B:1205:GLY:CA   | 1:B:1215:GLY:CA   | 2.53                     | 0.87              |
| 1:A:1453:LEU:HB3  | 1:A:1506:VAL:HG13 | 1.58                     | 0.86              |
| 1:B:1493:GLN:HG2  | 1:B:1540:VAL:HG22 | 1.54                     | 0.86              |
| 1:B:1205:GLY:CA   | 1:B:1215:GLY:HA3  | 2.06                     | 0.86              |
| 1:A:1112:LEU:HD13 | 1:A:1179:GLN:HB2  | 1.57                     | 0.86              |
| 1:A:1338:LEU:HD13 | 1:A:1346:PHE:HA   | 1.56                     | 0.85              |
| 1:A:867:HIS:O     | 1:A:949:ASP:CG    | 2.18                     | 0.85              |
| 1:A:687:ALA:HB2   | 1:A:731:LEU:HD12  | 1.58                     | 0.84              |
| 1:A:1312:ARG:O    | 1:A:1316:PRO:HD2  | 1.77                     | 0.84              |
| 1:B:1603:LEU:HA   | 1:B:1606:VAL:HB   | 1.58                     | 0.84              |
| 1:A:31:VAL:O      | 1:A:34:ARG:HB3    | 1.77                     | 0.83              |
| 1:B:1173:THR:HG22 | 1:B:1284:LEU:HD13 | 1.59                     | 0.83              |
| 1:B:1414:THR:HG1  | 1:B:1423:PHE:HE2  | 1.26                     | 0.83              |
| 1:A:193:PHE:HB2   | 1:B:881:GLN:NE2   | 1.93                     | 0.82              |
| 1:B:910:GLY:CA    | 1:B:933:TYR:HA    | 2.09                     | 0.82              |
| 1:A:420:LEU:HD22  | 1:A:442:LEU:HG    | 1.61                     | 0.82              |
| 1:B:1138:HIS:NE2  | 1:B:1143:ALA:HB3  | 1.94                     | 0.82              |
| 1:A:712:HIS:HA    | 1:A:715:HIS:CD2   | 2.15                     | 0.82              |
| 1:B:1499:ILE:HG23 | 1:B:1506:VAL:HB   | 1.61                     | 0.82              |
| 1:B:1407:LEU:HB3  | 1:B:1431:PHE:CE1  | 2.15                     | 0.82              |
| 1:B:1412:MET:HB3  | 1:B:1463:ARG:NE   | 1.94                     | 0.82              |
| 1:A:1546:SER:O    | 1:A:1549:GLN:HG3  | 1.79                     | 0.81              |
| 1:A:73:PHE:HD1    | 1:A:159:LYS:HA    | 1.37                     | 0.81              |
| 1:A:802:GLU:HG2   | 1:A:931:ARG:HD2   | 1.62                     | 0.81              |
| 1:B:1407:LEU:HB3  | 1:B:1431:PHE:HE1  | 1.45                     | 0.81              |
| 1:B:1475:PRO:HD3  | 1:B:1485:ILE:HD12 | 1.61                     | 0.81              |
| 1:A:32:ALA:C      | 1:A:35:PRO:HD2    | 2.05                     | 0.81              |
| 1:A:881:GLN:HE21  | 1:B:193:PHE:HA    | 1.42                     | 0.81              |
| 1:A:124:VAL:HG12  | 1:A:129:LEU:HG    | 1.63                     | 0.81              |
| 1:A:1545:ALA:HB2  | 1:A:1556:LEU:CB   | 2.12                     | 0.80              |
| 1:A:868:GLN:CA    | 1:A:949:ASP:OD2   | 2.29                     | 0.80              |
| 1:B:1077:THR:HG23 | 1:B:1082:SER:H    | 1.45                     | 0.80              |
| 1:A:1191:SER:HB3  | 1:A:1194:LYS:HG3  | 1.62                     | 0.80              |
| 1:A:1047:ILE:HD11 | 1:A:1256:ILE:CD1  | 2.11                     | 0.79              |
| 1:A:131:LEU:HD11  | 1:A:142:ARG:HD2   | 1.64                     | 0.79              |
| 1:A:659:THR:HA    | 1:A:663:LEU:HD12  | 1.63                     | 0.79              |
| 1:A:1450:CYS:CB   | 1:A:1505:GLN:HB2  | 2.11                     | 0.78              |
| 1:A:1515:LEU:HA   | 1:A:1544:LEU:HD13 | 1.66                     | 0.78              |
| 1:A:68:LYS:HB3    | 1:A:70:TYR:HD2    | 1.48                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1451:GLY:O    | 1:B:1454:ALA:HB3  | 1.84                     | 0.77              |
| 1:A:325:ARG:HH22  | 1:B:496:LEU:HD23  | 1.48                     | 0.77              |
| 1:A:392:ILE:O     | 1:A:399:GLY:HA2   | 1.83                     | 0.77              |
| 1:B:247:LEU:O     | 1:B:248:GLN:C     | 2.21                     | 0.77              |
| 1:B:1438:THR:HA   | 1:B:1446:LEU:HD13 | 1.66                     | 0.77              |
| 1:B:1046:ARG:HH22 | 1:B:1130:LYS:HZ1  | 1.31                     | 0.77              |
| 1:A:787:LEU:HD12  | 1:A:832:LEU:HD23  | 1.67                     | 0.77              |
| 1:A:1047:ILE:HD11 | 1:A:1256:ILE:HG12 | 1.67                     | 0.77              |
| 1:B:910:GLY:HA2   | 1:B:933:TYR:CA    | 2.13                     | 0.77              |
| 1:B:1453:LEU:O    | 1:B:1456:LEU:HB3  | 1.84                     | 0.77              |
| 1:B:867:HIS:CD2   | 1:B:936:LEU:HD21  | 2.20                     | 0.76              |
| 1:A:349:ILE:HG23  | 1:A:429:LEU:HD11  | 1.68                     | 0.76              |
| 1:A:984:ARG:HH11  | 1:A:984:ARG:HB2   | 1.51                     | 0.76              |
| 1:A:1190:PRO:HG2  | 1:A:1195:LEU:HD21 | 1.67                     | 0.76              |
| 1:A:1567:CYS:SG   | 1:A:1596:THR:HG23 | 2.26                     | 0.76              |
| 1:A:415:LEU:HD11  | 1:A:484:LEU:HD21  | 1.67                     | 0.76              |
| 1:A:922:PHE:CZ    | 1:A:928:PRO:HD2   | 2.20                     | 0.76              |
| 1:B:1407:LEU:H    | 1:B:1407:LEU:HD12 | 1.50                     | 0.76              |
| 1:B:1414:THR:HG23 | 1:B:1423:PHE:HD2  | 1.50                     | 0.76              |
| 1:B:1516:GLY:O    | 1:B:1520:PRO:HD2  | 1.84                     | 0.76              |
| 1:A:909:HIS:O     | 1:A:934:CYS:HB3   | 1.85                     | 0.76              |
| 1:B:1489:ARG:NH2  | 1:B:1533:GLY:HA2  | 2.01                     | 0.75              |
| 1:B:1600:MET:HA   | 1:B:1603:LEU:HG   | 1.68                     | 0.75              |
| 1:A:1315:LEU:HD22 | 1:A:1349:ARG:HB3  | 1.69                     | 0.75              |
| 1:B:313:LEU:CD1   | 1:B:332:LEU:HD23  | 2.10                     | 0.75              |
| 1:B:1238:THR:HG21 | 1:B:1286:HIS:N    | 2.02                     | 0.75              |
| 1:A:1159:LEU:HB3  | 1:A:1160:PRO:HD3  | 1.67                     | 0.75              |
| 1:B:1218:LEU:HD22 | 1:B:1376:ILE:HG23 | 1.68                     | 0.75              |
| 1:A:1242:PRO:HB2  | 1:A:1261:TYR:CE1  | 2.21                     | 0.74              |
| 1:B:425:SER:O     | 1:B:429:LEU:HG    | 1.86                     | 0.74              |
| 1:B:860:LEU:HB2   | 1:B:1005:ILE:HD13 | 1.69                     | 0.74              |
| 1:B:1408:VAL:HA   | 1:B:1411:MET:HE2  | 1.66                     | 0.74              |
| 1:A:1548:GLY:HA3  | 1:A:1553:HIS:N    | 2.01                     | 0.74              |
| 1:B:1550:GLY:O    | 1:B:1553:HIS:HB3  | 1.88                     | 0.74              |
| 1:A:1398:GLU:HA   | 1:A:1449:LEU:HD21 | 1.67                     | 0.74              |
| 1:A:1401:PHE:HB3  | 1:A:1407:LEU:HD12 | 1.68                     | 0.74              |
| 1:B:1445:SER:HA   | 1:B:1448:HIS:ND1  | 2.03                     | 0.74              |
| 1:B:1554:LEU:HA   | 1:B:1557:HIS:CD2  | 2.22                     | 0.74              |
| 1:B:1557:HIS:O    | 1:B:1561:VAL:HG23 | 1.86                     | 0.74              |
| 1:B:272:ARG:HD3   | 1:B:285:MET:HG3   | 1.70                     | 0.74              |
| 1:A:1401:PHE:CD1  | 1:A:1407:LEU:HG   | 2.22                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1570:TYR:CG   | 1:A:1592:ILE:HG21 | 2.22                     | 0.74              |
| 1:B:112:LEU:HD12  | 1:B:250:LEU:HD12  | 1.68                     | 0.73              |
| 1:B:248:GLN:HE22  | 1:B:316:PRO:HB2   | 1.53                     | 0.73              |
| 1:B:1201:VAL:HG13 | 1:B:1218:LEU:HB3  | 1.67                     | 0.73              |
| 1:A:333:SER:HG    | 1:A:406:PHE:HZ    | 1.34                     | 0.73              |
| 1:A:326:LEU:HG    | 1:A:511:ILE:HD12  | 1.70                     | 0.73              |
| 1:A:1567:CYS:HB2  | 1:A:1596:THR:OG1  | 1.87                     | 0.73              |
| 1:A:816:LEU:HD21  | 1:B:193:PHE:CZ    | 2.23                     | 0.73              |
| 1:B:1039:LEU:HD22 | 1:B:1130:LYS:HD3  | 1.70                     | 0.73              |
| 1:A:200:VAL:HB    | 1:B:715:HIS:CE1   | 2.23                     | 0.73              |
| 1:A:1201:VAL:CG1  | 1:A:1222:LEU:HD11 | 2.17                     | 0.73              |
| 1:A:874:VAL:HG13  | 1:B:189:VAL:HG21  | 1.69                     | 0.73              |
| 1:A:284:ILE:HD12  | 1:A:442:LEU:HD23  | 1.70                     | 0.73              |
| 1:A:1047:ILE:CG1  | 1:A:1256:ILE:HG12 | 2.19                     | 0.73              |
| 1:A:945:LEU:HB3   | 1:A:1053:TRP:CD1  | 2.23                     | 0.72              |
| 1:B:1515:LEU:HD12 | 1:B:1541:MET:HG3  | 1.71                     | 0.72              |
| 1:A:73:PHE:CE1    | 1:A:159:LYS:HA    | 2.24                     | 0.72              |
| 1:B:1204:ILE:HG21 | 1:B:1357:GLY:HA3  | 1.70                     | 0.72              |
| 1:B:1299:ILE:HG13 | 1:B:1337:ILE:HD11 | 1.70                     | 0.72              |
| 1:A:1201:VAL:HG11 | 1:A:1222:LEU:HD21 | 1.72                     | 0.72              |
| 1:A:1047:ILE:HD11 | 1:A:1256:ILE:CG1  | 2.20                     | 0.72              |
| 1:A:1500:VAL:HG21 | 1:A:1543:THR:O    | 1.90                     | 0.72              |
| 1:A:420:LEU:HD21  | 1:A:444:VAL:HA    | 1.71                     | 0.72              |
| 1:A:1518:LEU:HB3  | 1:A:1537:LEU:HD11 | 1.71                     | 0.72              |
| 1:B:1415:ALA:HB2  | 1:B:1467:TRP:HB2  | 1.72                     | 0.72              |
| 1:B:272:ARG:HD3   | 1:B:285:MET:CG    | 2.20                     | 0.72              |
| 1:A:790:MET:HE3   | 1:A:858:LEU:CD2   | 2.20                     | 0.71              |
| 1:A:881:GLN:HE21  | 1:B:193:PHE:HD2   | 1.38                     | 0.71              |
| 1:A:97:LEU:HD12   | 1:A:235:THR:HG23  | 1.72                     | 0.71              |
| 1:A:471:VAL:HG21  | 1:A:641:ARG:H     | 1.55                     | 0.71              |
| 1:A:985:ARG:HH11  | 1:A:1280:LEU:HD13 | 1.54                     | 0.71              |
| 1:A:816:LEU:HD21  | 1:B:193:PHE:HZ    | 1.53                     | 0.71              |
| 1:A:869:TYR:N     | 1:A:949:ASP:OD2   | 2.23                     | 0.71              |
| 1:A:881:GLN:NE2   | 1:B:193:PHE:HD2   | 1.89                     | 0.71              |
| 1:B:97:LEU:HB3    | 1:B:201:PHE:HE2   | 1.56                     | 0.71              |
| 1:B:273:PHE:CE1   | 1:B:334:LEU:HB3   | 2.25                     | 0.71              |
| 1:A:31:VAL:O      | 1:A:35:PRO:CD     | 2.39                     | 0.71              |
| 1:B:921:HIS:CD2   | 1:B:993:ALA:HB2   | 2.25                     | 0.71              |
| 1:A:135:GLY:HA2   | 1:A:140:CYS:O     | 1.90                     | 0.71              |
| 1:A:881:GLN:NE2   | 1:B:193:PHE:CA    | 2.52                     | 0.70              |
| 1:B:1274:CYS:SG   | 1:B:1275:SER:N    | 2.64                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:244:VAL:HG22  | 1:A:316:PRO:HG2   | 1.74                     | 0.70              |
| 1:A:329:VAL:HG12  | 1:A:388:ILE:CG2   | 2.20                     | 0.70              |
| 1:A:1545:ALA:HB2  | 1:A:1556:LEU:HB3  | 1.74                     | 0.70              |
| 1:A:1025:MET:HE3  | 1:A:1028:PRO:HD3  | 1.74                     | 0.70              |
| 1:A:855:LEU:HD23  | 1:A:1002:TYR:CE2  | 2.23                     | 0.70              |
| 1:A:82:THR:HB     | 1:A:132:LEU:HD22  | 1.74                     | 0.70              |
| 1:A:926:ALA:O     | 1:A:928:PRO:HD3   | 1.92                     | 0.70              |
| 1:B:193:PHE:CE1   | 1:B:197:LEU:HD11  | 2.26                     | 0.70              |
| 1:A:92:ILE:HD12   | 1:A:97:LEU:HA     | 1.75                     | 0.69              |
| 1:A:273:PHE:HD2   | 1:A:338:TYR:HB2   | 1.57                     | 0.69              |
| 1:A:945:LEU:HD13  | 1:A:1053:TRP:HB2  | 1.73                     | 0.69              |
| 1:B:408:LEU:HD22  | 1:B:520:ARG:HG2   | 1.73                     | 0.69              |
| 1:A:1043:SER:HB3  | 1:A:1256:ILE:HG21 | 1.75                     | 0.69              |
| 1:B:1247:TRP:CD1  | 1:B:1248:ARG:H    | 2.10                     | 0.69              |
| 1:A:73:PHE:HD1    | 1:A:158:ALA:O     | 1.75                     | 0.69              |
| 1:A:1335:GLU:HA   | 1:A:1339:GLY:O    | 1.93                     | 0.69              |
| 1:A:1177:LEU:HG   | 1:A:1233:TRP:CD2  | 2.28                     | 0.69              |
| 1:A:853:LEU:O     | 1:A:856:ALA:HB3   | 1.93                     | 0.69              |
| 1:B:1338:LEU:HD13 | 1:B:1346:PHE:HA   | 1.74                     | 0.69              |
| 1:B:1515:LEU:HD11 | 1:B:1556:LEU:HD22 | 1.74                     | 0.69              |
| 1:A:200:VAL:HB    | 1:B:715:HIS:ND1   | 2.07                     | 0.69              |
| 1:A:1047:ILE:CD1  | 1:A:1256:ILE:HG12 | 2.23                     | 0.69              |
| 1:A:1245:GLY:HA2  | 1:A:1247:TRP:CE2  | 2.28                     | 0.69              |
| 1:A:1398:GLU:HG3  | 1:A:1445:SER:HA   | 1.73                     | 0.69              |
| 1:B:1159:LEU:HB3  | 1:B:1160:PRO:HD2  | 1.75                     | 0.69              |
| 1:A:1142:MET:O    | 1:A:1143:ALA:C    | 2.35                     | 0.69              |
| 1:A:800:PRO:HG3   | 1:A:854:ILE:HD11  | 1.73                     | 0.69              |
| 1:B:763:ILE:HG22  | 1:B:767:LYS:HE3   | 1.74                     | 0.69              |
| 1:A:273:PHE:CD2   | 1:A:338:TYR:HB2   | 2.28                     | 0.68              |
| 1:B:1058:LEU:HD12 | 1:B:1068:ALA:HB1  | 1.75                     | 0.68              |
| 1:A:1047:ILE:HD11 | 1:A:1256:ILE:HD11 | 1.75                     | 0.68              |
| 1:A:1121:ILE:HG23 | 1:A:1169:TYR:HE2  | 1.58                     | 0.68              |
| 1:A:1365:HIS:HB3  | 1:A:1372:LEU:HD12 | 1.75                     | 0.68              |
| 1:A:1138:HIS:O    | 1:A:1142:MET:HG2  | 1.94                     | 0.68              |
| 1:B:1214:LEU:HD22 | 1:B:1383:TYR:CZ   | 2.29                     | 0.68              |
| 1:B:1191:SER:HB3  | 1:B:1194:LYS:HG3  | 1.75                     | 0.68              |
| 1:B:834:VAL:HG13  | 1:B:966:LEU:HD13  | 1.74                     | 0.68              |
| 1:A:715:HIS:ND1   | 1:B:200:VAL:HG21  | 2.09                     | 0.68              |
| 1:A:1041:TRP:CZ3  | 1:A:1044:ARG:HD2  | 2.28                     | 0.68              |
| 1:B:1338:LEU:HB3  | 1:B:1345:GLU:HB2  | 1.76                     | 0.68              |
| 1:A:1047:ILE:HB   | 1:A:1050:TYR:HD2  | 1.59                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1545:ALA:HB1  | 1:A:1553:HIS:CG   | 2.28                     | 0.67              |
| 1:A:922:PHE:HZ    | 1:A:928:PRO:HD2   | 1.60                     | 0.67              |
| 1:B:852:PRO:HB2   | 1:B:855:LEU:HB3   | 1.76                     | 0.67              |
| 1:B:1159:LEU:HD13 | 1:B:1298:LEU:HB3  | 1.76                     | 0.67              |
| 1:B:1445:SER:HA   | 1:B:1448:HIS:CG   | 2.30                     | 0.67              |
| 1:A:1090:VAL:HG13 | 1:A:1127:ALA:HB1  | 1.74                     | 0.67              |
| 1:A:1315:LEU:HD11 | 1:A:1350:VAL:HA   | 1.76                     | 0.67              |
| 1:A:1402:SER:HB3  | 1:A:1448:HIS:HB3  | 1.74                     | 0.67              |
| 1:A:288:THR:HB    | 1:A:291:ASP:CG    | 2.19                     | 0.67              |
| 1:A:1380:CYS:O    | 1:A:1380:CYS:SG   | 2.53                     | 0.67              |
| 1:B:185:ARG:HA    | 1:B:185:ARG:HE    | 1.59                     | 0.67              |
| 1:B:1025:MET:HG2  | 1:B:1026:ASN:N    | 2.10                     | 0.67              |
| 1:B:471:VAL:HG21  | 1:B:641:ARG:HA    | 1.76                     | 0.67              |
| 1:B:97:LEU:HB3    | 1:B:201:PHE:CE2   | 2.30                     | 0.67              |
| 1:B:318:LEU:HA    | 1:B:325:ARG:NH2   | 2.08                     | 0.67              |
| 1:B:1587:GLY:O    | 1:B:1591:MET:HG3  | 1.95                     | 0.67              |
| 1:A:352:VAL:HG21  | 1:A:429:LEU:HG    | 1.77                     | 0.67              |
| 1:A:274:GLN:O     | 1:A:277:VAL:HG22  | 1.95                     | 0.66              |
| 1:A:1545:ALA:HA   | 1:A:1553:HIS:HA   | 1.77                     | 0.66              |
| 1:B:1387:GLN:HG3  | 1:B:1393:ALA:HB1  | 1.74                     | 0.66              |
| 1:A:286:PRO:HB3   | 1:A:295:VAL:HG21  | 1.76                     | 0.66              |
| 1:B:768:ALA:HA    | 1:B:773:ASP:HB2   | 1.75                     | 0.66              |
| 1:A:1401:PHE:HD1  | 1:A:1407:LEU:HG   | 1.61                     | 0.66              |
| 1:A:1499:ILE:HG23 | 1:A:1506:VAL:HB   | 1.78                     | 0.66              |
| 1:B:39:ALA:HB1    | 1:B:44:PHE:HA     | 1.76                     | 0.66              |
| 1:A:284:ILE:HG13  | 1:A:442:LEU:HB3   | 1.77                     | 0.66              |
| 1:B:793:ASN:HB2   | 1:B:854:ILE:HG21  | 1.78                     | 0.66              |
| 1:A:1361:ILE:HA   | 1:A:1365:HIS:HB2  | 1.78                     | 0.66              |
| 1:B:909:HIS:CE1   | 1:B:937:SER:H     | 2.14                     | 0.66              |
| 1:B:1094:PHE:O    | 1:B:1098:ILE:HG13 | 1.96                     | 0.66              |
| 1:A:763:ILE:HG22  | 1:A:767:LYS:HE3   | 1.75                     | 0.66              |
| 1:A:1416:ASN:O    | 1:A:1470:ARG:NH1  | 2.28                     | 0.66              |
| 1:A:325:ARG:HH12  | 1:B:496:LEU:HD22  | 1.60                     | 0.66              |
| 1:B:1214:LEU:HD21 | 1:B:1354:LEU:HD13 | 1.76                     | 0.66              |
| 1:B:1414:THR:HG23 | 1:B:1423:PHE:CD2  | 2.31                     | 0.66              |
| 1:A:1350:VAL:O    | 1:A:1354:LEU:HG   | 1.96                     | 0.66              |
| 1:A:1194:LYS:HA   | 1:A:1370:SER:C    | 2.20                     | 0.66              |
| 1:B:415:LEU:HD12  | 1:B:524:LEU:HD22  | 1.78                     | 0.66              |
| 1:A:790:MET:HE3   | 1:A:858:LEU:HD23  | 1.76                     | 0.65              |
| 1:A:1314:LEU:HD13 | 1:A:1317:LEU:HD12 | 1.79                     | 0.65              |
| 1:B:336:CYS:O     | 1:B:381:CYS:SG    | 2.54                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1300:VAL:HG13 | 1:B:1336:ARG:HD3  | 1.78                     | 0.65              |
| 1:A:1176:TYR:CD1  | 1:A:1281:ALA:HB3  | 2.32                     | 0.65              |
| 1:B:322:ASN:O     | 1:B:323:PRO:C     | 2.38                     | 0.65              |
| 1:B:382:LEU:HD12  | 1:B:475:ILE:HG22  | 1.78                     | 0.65              |
| 1:B:711:TYR:CD2   | 1:B:888:PRO:HD3   | 2.32                     | 0.65              |
| 1:B:1238:THR:CG2  | 1:B:1285:LYS:HB3  | 2.26                     | 0.65              |
| 1:B:787:LEU:HD12  | 1:B:832:LEU:HD23  | 1.78                     | 0.65              |
| 1:A:352:VAL:CG2   | 1:A:429:LEU:HG    | 2.27                     | 0.65              |
| 1:B:89:CYS:SG     | 1:B:239:PHE:HB3   | 2.36                     | 0.65              |
| 1:A:908:TYR:HB2   | 1:A:933:TYR:HB2   | 1.79                     | 0.65              |
| 1:B:97:LEU:HD22   | 1:B:201:PHE:HZ    | 1.62                     | 0.65              |
| 1:A:1104:ILE:HG21 | 1:A:1168:THR:HG23 | 1.79                     | 0.64              |
| 1:A:1415:ALA:HB2  | 1:A:1467:TRP:HB2  | 1.77                     | 0.64              |
| 1:B:1443:ASN:H    | 1:B:1446:LEU:HD12 | 1.61                     | 0.64              |
| 1:A:507:ALA:O     | 1:A:523:ARG:NE    | 2.30                     | 0.64              |
| 1:A:1428:LEU:HB3  | 1:A:1491:LEU:HB3  | 1.78                     | 0.64              |
| 1:B:1043:SER:HB3  | 1:B:1256:ILE:HD12 | 1.80                     | 0.64              |
| 1:B:1047:ILE:O    | 1:B:1051:VAL:HG23 | 1.96                     | 0.64              |
| 1:A:93:PRO:O      | 1:A:97:LEU:N      | 2.28                     | 0.64              |
| 1:A:98:GLN:HG3    | 1:A:201:PHE:CE1   | 2.32                     | 0.64              |
| 1:B:349:ILE:HG23  | 1:B:429:LEU:HD13  | 1.79                     | 0.64              |
| 1:B:1159:LEU:CA   | 1:B:1298:LEU:HD13 | 2.24                     | 0.64              |
| 1:B:1228:THR:O    | 1:B:1231:GLU:HB3  | 1.97                     | 0.64              |
| 1:B:1307:PRO:HB3  | 1:B:1337:ILE:CG2  | 2.28                     | 0.64              |
| 1:A:1054:ILE:O    | 1:A:1058:LEU:HG   | 1.98                     | 0.64              |
| 1:A:1515:LEU:CA   | 1:A:1544:LEU:HD13 | 2.26                     | 0.64              |
| 1:A:31:VAL:C      | 1:A:34:ARG:HB3    | 2.23                     | 0.63              |
| 1:A:94:ARG:O      | 1:A:97:LEU:HB3    | 1.98                     | 0.63              |
| 1:A:1030:MET:O    | 1:A:1031:SER:O    | 2.16                     | 0.63              |
| 1:B:1175:ALA:O    | 1:B:1179:GLN:HG2  | 1.98                     | 0.63              |
| 1:A:1218:LEU:HD22 | 1:A:1376:ILE:HG23 | 1.81                     | 0.63              |
| 1:B:1118:LEU:HD13 | 1:B:1273:LEU:HB2  | 1.81                     | 0.63              |
| 1:B:1318:LEU:HD21 | 1:B:1331:SER:HA   | 1.81                     | 0.63              |
| 1:A:190:GLN:O     | 1:A:194:LEU:HG    | 1.97                     | 0.63              |
| 1:B:46:MET:O      | 1:B:50:PRO:HD3    | 1.99                     | 0.63              |
| 1:A:516:THR:HB    | 1:A:519:GLN:HG3   | 1.80                     | 0.63              |
| 1:A:1201:VAL:HG11 | 1:A:1222:LEU:HD11 | 1.79                     | 0.63              |
| 1:B:1133:VAL:HG13 | 1:B:1247:TRP:CZ3  | 2.33                     | 0.63              |
| 1:A:1019:TYR:OH   | 1:A:1038:THR:HA   | 1.99                     | 0.63              |
| 1:A:1035:ILE:HG12 | 1:A:1089:ILE:HD11 | 1.81                     | 0.63              |
| 1:A:1203:ALA:O    | 1:A:1204:ILE:C    | 2.42                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1474:SER:HA   | 1:A:1485:ILE:HD12 | 1.81                     | 0.63              |
| 1:A:136:LEU:HD22  | 1:A:239:PHE:HZ    | 1.64                     | 0.63              |
| 1:A:866:LEU:HD22  | 1:A:948:LEU:HD13  | 1.81                     | 0.63              |
| 1:B:441:ALA:HB1   | 1:B:443:ARG:HH22  | 1.62                     | 0.63              |
| 1:B:1138:HIS:NE2  | 1:B:1143:ALA:CB   | 2.61                     | 0.63              |
| 1:B:1247:TRP:HD1  | 1:B:1248:ARG:H    | 1.47                     | 0.63              |
| 1:B:1588:LYS:O    | 1:B:1592:ILE:HG12 | 1.98                     | 0.63              |
| 1:B:963:TYR:OH    | 1:B:1013:LEU:HB3  | 1.99                     | 0.63              |
| 1:A:184:LEU:HD22  | 1:A:184:LEU:H     | 1.64                     | 0.62              |
| 1:A:1214:LEU:O    | 1:A:1218:LEU:HG   | 1.98                     | 0.62              |
| 1:A:1564:LEU:HB2  | 1:A:1603:LEU:HD11 | 1.81                     | 0.62              |
| 1:A:257:LEU:HD21  | 1:A:318:LEU:HD23  | 1.79                     | 0.62              |
| 1:B:1560:ALA:HA   | 1:B:1563:TRP:CE3  | 2.34                     | 0.62              |
| 1:B:708:ALA:HA    | 1:B:888:PRO:HG2   | 1.80                     | 0.62              |
| 1:B:867:HIS:HE1   | 1:B:1012:ILE:HG21 | 1.63                     | 0.62              |
| 1:B:1499:ILE:HG12 | 1:B:1506:VAL:HG21 | 1.80                     | 0.62              |
| 1:B:1138:HIS:CD2  | 1:B:1143:ALA:CB   | 2.77                     | 0.62              |
| 1:B:1166:ILE:HD11 | 1:B:1295:THR:OG1  | 2.00                     | 0.62              |
| 1:A:104:CYS:HA    | 1:A:107:LEU:HD12  | 1.81                     | 0.62              |
| 1:A:808:VAL:HG11  | 1:A:908:TYR:CB    | 2.23                     | 0.62              |
| 1:A:1244:ILE:HG12 | 1:A:1293:ARG:NH1  | 2.15                     | 0.62              |
| 1:A:787:LEU:HD21  | 1:A:833:PHE:CZ    | 2.34                     | 0.62              |
| 1:B:1204:ILE:HG12 | 1:B:1357:GLY:HA3  | 1.80                     | 0.62              |
| 1:B:1268:ALA:O    | 1:B:1272:THR:HG23 | 1.99                     | 0.62              |
| 1:A:908:TYR:CD2   | 1:A:930:PRO:HB3   | 2.33                     | 0.62              |
| 1:A:1212:ASN:O    | 1:A:1216:PRO:HD2  | 2.00                     | 0.62              |
| 1:A:1087:VAL:HG11 | 1:A:1154:ILE:HG12 | 1.82                     | 0.62              |
| 1:A:1289:LEU:HA   | 1:A:1326:VAL:HG12 | 1.82                     | 0.62              |
| 1:B:1159:LEU:HA   | 1:B:1298:LEU:CD1  | 2.28                     | 0.62              |
| 1:B:1242:PRO:HG2  | 1:B:1261:TYR:CE1  | 2.35                     | 0.62              |
| 1:B:1427:VAL:HG13 | 1:B:1431:PHE:HE2  | 1.65                     | 0.62              |
| 1:A:1576:VAL:HA   | 1:A:1579:LYS:HD2  | 1.82                     | 0.62              |
| 1:A:1104:ILE:HG23 | 1:A:1110:LEU:HD11 | 1.82                     | 0.61              |
| 1:B:1159:LEU:O    | 1:B:1160:PRO:C    | 2.42                     | 0.61              |
| 1:A:93:PRO:O      | 1:A:96:GLN:N      | 2.33                     | 0.61              |
| 1:A:790:MET:CE    | 1:A:858:LEU:HD23  | 2.30                     | 0.61              |
| 1:B:244:VAL:O     | 1:B:248:GLN:HG2   | 2.00                     | 0.61              |
| 1:A:1030:MET:C    | 1:A:1034:ASP:HB3  | 2.25                     | 0.61              |
| 1:A:1047:ILE:CG1  | 1:A:1256:ILE:CG1  | 2.77                     | 0.61              |
| 1:A:1565:SER:O    | 1:A:1569:LYS:HG2  | 2.01                     | 0.61              |
| 1:A:333:SER:OG    | 1:A:406:PHE:HZ    | 1.84                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:104:CYS:HB3   | 1:A:136:LEU:HD13  | 1.82                     | 0.61              |
| 1:A:471:VAL:O     | 1:A:475:ILE:HG12  | 1.99                     | 0.61              |
| 1:A:1203:ALA:O    | 1:A:1320:GLU:HA   | 2.00                     | 0.61              |
| 1:A:1538:MET:HA   | 1:A:1538:MET:HE3  | 1.82                     | 0.61              |
| 1:B:190:GLN:O     | 1:B:193:PHE:HB3   | 2.00                     | 0.61              |
| 1:B:1595:CYS:O    | 1:B:1599:ILE:HG13 | 2.00                     | 0.61              |
| 1:A:265:TYR:CZ    | 1:A:301:SER:HB2   | 2.36                     | 0.61              |
| 1:A:1347:LEU:HB3  | 1:A:1351:TYR:CE2  | 2.35                     | 0.61              |
| 1:A:1214:LEU:HD21 | 1:A:1380:CYS:HB2  | 1.82                     | 0.61              |
| 1:B:867:HIS:CG    | 1:B:936:LEU:HD21  | 2.35                     | 0.61              |
| 1:A:877:PHE:O     | 1:A:878:GLU:C     | 2.38                     | 0.61              |
| 1:A:1515:LEU:CD1  | 1:A:1541:MET:HG3  | 2.31                     | 0.61              |
| 1:A:35:PRO:HB2    | 1:A:48:GLU:HB3    | 1.82                     | 0.61              |
| 1:A:881:GLN:HE22  | 1:B:193:PHE:HA    | 1.63                     | 0.61              |
| 1:A:1314:LEU:HG   | 1:A:1333:SER:CB   | 2.25                     | 0.61              |
| 1:A:1534:PHE:N    | 1:A:1535:PRO:HD2  | 2.16                     | 0.61              |
| 1:B:754:LEU:HD22  | 1:B:807:ASN:HD21  | 1.65                     | 0.61              |
| 1:B:1151:SER:HB3  | 1:B:1154:ILE:HG12 | 1.83                     | 0.61              |
| 1:B:1554:LEU:HD11 | 1:B:1610:LEU:HD11 | 1.82                     | 0.61              |
| 1:A:810:HIS:O     | 1:A:813:MET:HG3   | 2.01                     | 0.61              |
| 1:A:885:LEU:HD13  | 1:B:197:LEU:HD23  | 1.80                     | 0.61              |
| 1:A:1201:VAL:HG12 | 1:A:1222:LEU:HD11 | 1.81                     | 0.61              |
| 1:A:1285:LYS:CG   | 1:A:1325:SER:HB3  | 2.31                     | 0.61              |
| 1:A:1427:VAL:HG13 | 1:A:1431:PHE:HE2  | 1.64                     | 0.61              |
| 1:B:806:LEU:HD21  | 1:B:811:LEU:HB2   | 1.82                     | 0.61              |
| 1:A:263:LEU:HB2   | 1:A:266:PHE:HB2   | 1.83                     | 0.60              |
| 1:B:273:PHE:CD2   | 1:B:338:TYR:HB2   | 2.34                     | 0.60              |
| 1:A:93:PRO:O      | 1:A:94:ARG:C      | 2.43                     | 0.60              |
| 1:A:1315:LEU:HB3  | 1:A:1316:PRO:HD2  | 1.83                     | 0.60              |
| 1:B:230:ALA:HA    | 1:B:233:ILE:HG13  | 1.83                     | 0.60              |
| 1:B:246:SER:OG    | 1:B:247:LEU:N     | 2.31                     | 0.60              |
| 1:B:1519:THR:HG23 | 1:B:1563:TRP:CZ2  | 2.35                     | 0.60              |
| 1:A:105:LYS:HG3   | 1:A:246:SER:HB2   | 1.83                     | 0.60              |
| 1:A:1307:PRO:HB2  | 1:A:1308:PRO:HD3  | 1.83                     | 0.60              |
| 1:A:1574:LYS:HA   | 1:A:1577:VAL:HB   | 1.83                     | 0.60              |
| 1:B:834:VAL:HG11  | 1:B:961:VAL:HG13  | 1.83                     | 0.60              |
| 1:A:918:TRP:O     | 1:A:922:PHE:HB2   | 2.02                     | 0.60              |
| 1:A:1545:ALA:HB2  | 1:A:1556:LEU:HB2  | 1.82                     | 0.60              |
| 1:B:1340:PRO:HD2  | 1:B:1343:SER:HB3  | 1.84                     | 0.60              |
| 1:A:1519:THR:HB   | 1:A:1520:PRO:HD3  | 1.82                     | 0.60              |
| 1:A:1052:ASN:O    | 1:A:1053:TRP:C    | 2.45                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1523:THR:HG23 | 1:A:1566:ARG:HH11 | 1.67                     | 0.60              |
| 1:A:1607:THR:HA   | 1:A:1610:LEU:HD12 | 1.82                     | 0.60              |
| 1:B:1500:VAL:HG21 | 1:B:1543:THR:O    | 2.02                     | 0.60              |
| 1:B:1579:LYS:HB3  | 1:B:1589:HIS:CE1  | 2.37                     | 0.60              |
| 1:A:49:LEU:HB3    | 1:A:50:PRO:HD3    | 1.83                     | 0.60              |
| 1:A:130:ILE:HD12  | 1:A:308:MET:HG3   | 1.84                     | 0.60              |
| 1:B:740:PHE:HD1   | 1:B:778:GLU:HG3   | 1.66                     | 0.60              |
| 1:B:1151:SER:HB3  | 1:B:1154:ILE:CD1  | 2.32                     | 0.60              |
| 1:B:1356:THR:HA   | 1:B:1400:PHE:CZ   | 2.36                     | 0.60              |
| 1:A:73:PHE:CD1    | 1:A:159:LYS:CA    | 2.70                     | 0.60              |
| 1:A:202:ASN:HB3   | 1:A:204:ARG:NE    | 2.17                     | 0.60              |
| 1:A:252:GLY:HA2   | 1:A:255:LYS:HD2   | 1.83                     | 0.60              |
| 1:A:85:ILE:HD12   | 1:A:107:LEU:HD11  | 1.83                     | 0.60              |
| 1:B:851:VAL:HG11  | 1:B:995:GLU:HG2   | 1.84                     | 0.60              |
| 1:B:1274:CYS:O    | 1:B:1275:SER:C    | 2.45                     | 0.60              |
| 1:A:1575:ASN:O    | 1:A:1579:LYS:HG3  | 2.02                     | 0.59              |
| 1:B:921:HIS:HD2   | 1:B:993:ALA:HB2   | 1.66                     | 0.59              |
| 1:B:996:ALA:HB1   | 1:B:1274:CYS:HA   | 1.84                     | 0.59              |
| 1:A:43:ALA:O      | 1:A:44:PHE:C      | 2.44                     | 0.59              |
| 1:A:58:GLU:C      | 1:A:60:GLU:H      | 2.11                     | 0.59              |
| 1:A:318:LEU:HD13  | 1:A:321:LEU:HD21  | 1.84                     | 0.59              |
| 1:A:320:PRO:HG3   | 1:B:493:VAL:HG12  | 1.85                     | 0.59              |
| 1:A:670:ILE:O     | 1:A:674:LEU:HG    | 2.02                     | 0.59              |
| 1:B:996:ALA:CB    | 1:B:1274:CYS:HA   | 2.32                     | 0.59              |
| 1:B:1468:LEU:HA   | 1:B:1471:MET:HE2  | 1.84                     | 0.59              |
| 1:A:349:ILE:HG23  | 1:A:429:LEU:CD1   | 2.32                     | 0.59              |
| 1:A:1122:TYR:HB2  | 1:A:1269:HIS:CD2  | 2.37                     | 0.59              |
| 1:A:1204:ILE:HD11 | 1:A:1357:GLY:HA3  | 1.84                     | 0.59              |
| 1:B:1305:MET:O    | 1:B:1307:PRO:HD3  | 2.03                     | 0.59              |
| 1:B:1598:HIS:O    | 1:B:1602:TYR:N    | 2.34                     | 0.59              |
| 1:A:1568:LYS:HD3  | 1:A:1569:LYS:HD3  | 1.83                     | 0.59              |
| 1:B:151:PHE:HA    | 1:B:154:MET:HE2   | 1.84                     | 0.59              |
| 1:B:1515:LEU:CD1  | 1:B:1541:MET:HG3  | 2.32                     | 0.59              |
| 1:A:1171:SER:HA   | 1:A:1174:ARG:HD2  | 1.83                     | 0.59              |
| 1:B:889:PHE:O     | 1:B:890:GLY:C     | 2.44                     | 0.59              |
| 1:B:1084:LYS:HD2  | 1:B:1151:SER:HB2  | 1.83                     | 0.59              |
| 1:A:1047:ILE:HG13 | 1:A:1256:ILE:HG12 | 1.83                     | 0.59              |
| 1:A:1548:GLY:HA3  | 1:A:1552:GLY:C    | 2.28                     | 0.59              |
| 1:B:1015:PRO:HB2  | 1:B:1020:ILE:HD11 | 1.85                     | 0.59              |
| 1:A:84:TYR:O      | 1:A:88:VAL:HG22   | 2.03                     | 0.59              |
| 1:A:1051:VAL:HG22 | 1:A:1072:LEU:HD11 | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1428:LEU:HD13 | 1:A:1491:LEU:HB2  | 1.85                     | 0.59              |
| 1:A:1542:ALA:HA   | 1:A:1556:LEU:CD2  | 2.33                     | 0.59              |
| 1:A:1560:ALA:HA   | 1:A:1563:TRP:HE3  | 1.67                     | 0.59              |
| 1:B:104:CYS:SG    | 1:B:239:PHE:HE1   | 2.26                     | 0.59              |
| 1:B:1412:MET:HB3  | 1:B:1463:ARG:HE   | 1.67                     | 0.59              |
| 1:B:1571:LEU:HA   | 1:B:1576:VAL:HG11 | 1.85                     | 0.59              |
| 1:A:30:GLU:O      | 1:A:33:VAL:HG22   | 2.03                     | 0.59              |
| 1:B:247:LEU:C     | 1:B:249:GLU:N     | 2.56                     | 0.59              |
| 1:B:937:SER:O     | 1:B:939:GLU:N     | 2.36                     | 0.59              |
| 1:B:1063:MET:HE2  | 1:B:1067:HIS:NE2  | 2.17                     | 0.59              |
| 1:B:1208:ARG:HD3  | 1:B:1328:GLU:HB2  | 1.84                     | 0.59              |
| 1:B:1429:LYS:O    | 1:B:1430:PHE:C    | 2.45                     | 0.59              |
| 1:A:1311:ILE:HG21 | 1:A:1338:LEU:HD21 | 1.85                     | 0.58              |
| 1:B:93:PRO:HB2    | 1:B:96:GLN:HB2    | 1.85                     | 0.58              |
| 1:A:888:PRO:O     | 1:A:889:PHE:C     | 2.45                     | 0.58              |
| 1:A:74:TYR:O      | 1:A:77:PHE:HB3    | 2.03                     | 0.58              |
| 1:A:857:ARG:NH2   | 1:A:931:ARG:O     | 2.36                     | 0.58              |
| 1:A:1045:LEU:HD12 | 1:A:1072:LEU:HD11 | 1.83                     | 0.58              |
| 1:A:1222:LEU:O    | 1:A:1226:VAL:HB   | 2.03                     | 0.58              |
| 1:A:1591:MET:O    | 1:A:1594:GLU:HG2  | 2.03                     | 0.58              |
| 1:B:1045:LEU:O    | 1:B:1051:VAL:HG22 | 2.04                     | 0.58              |
| 1:A:1213:THR:O    | 1:A:1217:THR:HG23 | 2.04                     | 0.58              |
| 1:B:284:ILE:HD12  | 1:B:420:LEU:HD12  | 1.86                     | 0.58              |
| 1:A:1514:LEU:O    | 1:A:1518:LEU:HG   | 2.03                     | 0.58              |
| 1:B:31:VAL:C      | 1:B:34:ARG:HB3    | 2.29                     | 0.58              |
| 1:A:906:PRO:O     | 1:A:907:LEU:HB2   | 2.03                     | 0.58              |
| 1:A:1309:GLN:HA   | 1:A:1312:ARG:HD2  | 1.85                     | 0.58              |
| 1:B:810:HIS:O     | 1:B:813:MET:HG3   | 2.04                     | 0.58              |
| 1:A:93:PRO:HB2    | 1:A:96:GLN:HB2    | 1.86                     | 0.58              |
| 1:A:396:ARG:HH21  | 1:B:404:GLN:NE2   | 2.02                     | 0.58              |
| 1:A:908:TYR:O     | 1:A:910:GLY:N     | 2.37                     | 0.58              |
| 1:A:1312:ARG:O    | 1:A:1316:PRO:CD   | 2.49                     | 0.58              |
| 1:B:527:SER:O     | 1:B:528:VAL:HG13  | 2.04                     | 0.58              |
| 1:B:1563:TRP:HA   | 1:B:1566:ARG:HD2  | 1.86                     | 0.58              |
| 1:B:680:GLU:HB3   | 1:B:730:THR:HG21  | 1.84                     | 0.58              |
| 1:B:1214:LEU:O    | 1:B:1218:LEU:HG   | 2.04                     | 0.58              |
| 1:B:1300:VAL:CG1  | 1:B:1336:ARG:HD3  | 2.33                     | 0.58              |
| 1:A:53:VAL:O      | 1:A:57:ILE:HG13   | 2.03                     | 0.58              |
| 1:A:189:VAL:HG21  | 1:B:874:VAL:HG13  | 1.85                     | 0.58              |
| 1:A:1298:LEU:HA   | 1:A:1301:TRP:NE1  | 2.19                     | 0.58              |
| 1:B:1296:GLY:O    | 1:B:1300:VAL:HG22 | 2.04                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:256:LEU:HB3   | 1:A:312:THR:CG2   | 2.34                     | 0.57              |
| 1:A:284:ILE:H     | 1:A:442:LEU:H     | 1.52                     | 0.57              |
| 1:A:1218:LEU:HD13 | 1:A:1376:ILE:HG23 | 1.85                     | 0.57              |
| 1:A:1429:LYS:O    | 1:A:1430:PHE:C    | 2.45                     | 0.57              |
| 1:A:319:GLU:HB2   | 1:A:320:PRO:HD3   | 1.85                     | 0.57              |
| 1:A:688:SER:O     | 1:A:692:GLU:HG3   | 2.04                     | 0.57              |
| 1:A:1571:LEU:HD21 | 1:A:1593:LEU:HA   | 1.86                     | 0.57              |
| 1:B:844:MET:HB3   | 1:B:848:MET:HE3   | 1.85                     | 0.57              |
| 1:B:1083:VAL:O    | 1:B:1084:LYS:C    | 2.47                     | 0.57              |
| 1:A:833:PHE:CZ    | 1:A:861:ILE:HG21  | 2.40                     | 0.57              |
| 1:A:1210:LYS:O    | 1:A:1211:ALA:C    | 2.47                     | 0.57              |
| 1:A:1576:VAL:O    | 1:A:1580:LEU:HG   | 2.04                     | 0.57              |
| 1:B:282:PHE:CZ    | 1:B:341:VAL:HG21  | 2.38                     | 0.57              |
| 1:B:1044:ARG:C    | 1:B:1046:ARG:N    | 2.60                     | 0.57              |
| 1:B:1361:ILE:HA   | 1:B:1365:HIS:HB2  | 1.85                     | 0.57              |
| 1:A:1204:ILE:HD11 | 1:A:1357:GLY:CA   | 2.35                     | 0.57              |
| 1:B:1456:LEU:C    | 1:B:1458:CYS:N    | 2.60                     | 0.57              |
| 1:B:89:CYS:SG     | 1:B:239:PHE:CB    | 2.92                     | 0.57              |
| 1:B:284:ILE:HD13  | 1:B:345:THR:OG1   | 2.03                     | 0.57              |
| 1:B:422:LEU:HD11  | 1:B:537:LEU:HG    | 1.87                     | 0.57              |
| 1:B:528:VAL:O     | 1:B:530:LEU:N     | 2.38                     | 0.57              |
| 1:B:909:HIS:CE1   | 1:B:937:SER:N     | 2.72                     | 0.57              |
| 1:A:333:SER:OG    | 1:A:385:TYR:HA    | 2.04                     | 0.57              |
| 1:A:1203:ALA:HA   | 1:A:1320:GLU:HG3  | 1.86                     | 0.57              |
| 1:A:1481:GLN:HA   | 1:A:1481:GLN:HE21 | 1.70                     | 0.57              |
| 1:B:39:ALA:CB     | 1:B:44:PHE:HA     | 2.35                     | 0.57              |
| 1:A:867:HIS:O     | 1:A:949:ASP:OD2   | 2.21                     | 0.57              |
| 1:A:1118:LEU:HD21 | 1:A:1269:HIS:HB3  | 1.86                     | 0.57              |
| 1:B:1151:SER:O    | 1:B:1154:ILE:HG12 | 2.04                     | 0.57              |
| 1:B:1545:ALA:HB2  | 1:B:1556:LEU:CD2  | 2.34                     | 0.57              |
| 1:B:1579:LYS:HB3  | 1:B:1589:HIS:NE2  | 2.19                     | 0.57              |
| 1:A:82:THR:HA     | 1:A:107:LEU:HD13  | 1.86                     | 0.57              |
| 1:A:1029:GLU:HB3  | 1:A:1096:ARG:HH12 | 1.69                     | 0.57              |
| 1:A:1517:THR:O    | 1:A:1520:PRO:HD2  | 2.04                     | 0.57              |
| 1:B:1571:LEU:HA   | 1:B:1576:VAL:CG1  | 2.35                     | 0.57              |
| 1:A:1035:ILE:O    | 1:A:1039:LEU:HG   | 2.05                     | 0.57              |
| 1:B:58:GLU:C      | 1:B:60:GLU:H      | 2.13                     | 0.57              |
| 1:B:1159:LEU:HG   | 1:B:1160:PRO:HD3  | 1.86                     | 0.57              |
| 1:A:908:TYR:CD1   | 1:A:933:TYR:HB3   | 2.39                     | 0.57              |
| 1:A:1305:MET:O    | 1:A:1307:PRO:HD3  | 2.05                     | 0.57              |
| 1:B:82:THR:HG23   | 1:B:136:LEU:HG    | 1.87                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:783:TRP:HD1   | 1:B:821:PHE:HE2   | 1.53                     | 0.57              |
| 1:B:1047:ILE:HB   | 1:B:1050:TYR:HD2  | 1.70                     | 0.57              |
| 1:B:1178:LEU:HD11 | 1:B:1199:ALA:HB2  | 1.86                     | 0.57              |
| 1:A:310:LEU:HD13  | 1:A:384:ILE:HG12  | 1.87                     | 0.56              |
| 1:A:745:TRP:HE1   | 1:A:810:HIS:CE1   | 2.22                     | 0.56              |
| 1:B:1110:LEU:H    | 1:B:1175:ALA:CB   | 2.17                     | 0.56              |
| 1:A:1543:THR:O    | 1:A:1546:SER:HB2  | 2.04                     | 0.56              |
| 1:B:1242:PRO:HG2  | 1:B:1261:TYR:HE1  | 1.70                     | 0.56              |
| 1:A:70:TYR:HD1    | 1:A:160:LEU:HA    | 1.70                     | 0.56              |
| 1:A:70:TYR:O      | 1:A:71:GLU:C      | 2.49                     | 0.56              |
| 1:A:788:SER:O     | 1:A:789:THR:C     | 2.44                     | 0.56              |
| 1:A:1101:PHE:CD2  | 1:A:1168:THR:HG21 | 2.40                     | 0.56              |
| 1:A:1215:GLY:O    | 1:A:1216:PRO:C    | 2.47                     | 0.56              |
| 1:A:1556:LEU:HD23 | 1:A:1602:TYR:OH   | 2.05                     | 0.56              |
| 1:B:683:MET:HE3   | 1:B:727:LEU:HD23  | 1.87                     | 0.56              |
| 1:B:1058:LEU:CD1  | 1:B:1068:ALA:HB1  | 2.35                     | 0.56              |
| 1:B:1295:THR:O    | 1:B:1299:ILE:HD13 | 2.05                     | 0.56              |
| 1:A:299:PHE:O     | 1:A:303:VAL:HG23  | 2.05                     | 0.56              |
| 1:A:984:ARG:HG2   | 1:A:989:LYS:C     | 2.30                     | 0.56              |
| 1:B:470:GLY:H     | 1:B:473:SER:HB2   | 1.71                     | 0.56              |
| 1:B:1401:PHE:HD2  | 1:B:1449:LEU:HD22 | 1.70                     | 0.56              |
| 1:A:60:GLU:O      | 1:A:64:LEU:HG     | 2.05                     | 0.56              |
| 1:A:948:LEU:HG    | 1:A:953:CYS:SG    | 2.46                     | 0.56              |
| 1:A:1037:HIS:CE1  | 1:A:1041:TRP:HE1  | 2.22                     | 0.56              |
| 1:A:1169:TYR:HA   | 1:A:1172:PHE:HD2  | 1.70                     | 0.56              |
| 1:B:1495:LEU:HA   | 1:B:1498:TYR:CD2  | 2.40                     | 0.56              |
| 1:A:93:PRO:HD2    | 1:A:96:GLN:HB2    | 1.86                     | 0.56              |
| 1:B:246:SER:O     | 1:B:249:GLU:HB2   | 2.05                     | 0.56              |
| 1:B:663:LEU:HD23  | 1:B:674:LEU:CD1   | 2.36                     | 0.56              |
| 1:B:1567:CYS:HB3  | 1:B:1592:ILE:CG2  | 2.36                     | 0.56              |
| 1:A:834:VAL:HG13  | 1:A:966:LEU:HD13  | 1.87                     | 0.56              |
| 1:A:1176:TYR:CZ   | 1:A:1280:LEU:HB2  | 2.41                     | 0.56              |
| 1:A:1299:ILE:HG22 | 1:A:1336:ARG:HH11 | 1.70                     | 0.56              |
| 1:B:1566:ARG:HA   | 1:B:1569:LYS:HD2  | 1.88                     | 0.56              |
| 1:B:1603:LEU:CA   | 1:B:1606:VAL:HB   | 2.34                     | 0.56              |
| 1:A:1058:LEU:HB3  | 1:A:1063:MET:SD   | 2.46                     | 0.56              |
| 1:B:1166:ILE:HG12 | 1:B:1291:LEU:HB3  | 1.86                     | 0.56              |
| 1:B:1395:LYS:O    | 1:B:1399:GLU:HG2  | 2.06                     | 0.56              |
| 1:A:317:VAL:O     | 1:A:318:LEU:HG    | 2.06                     | 0.56              |
| 1:A:1119:GLN:NE2  | 1:A:1122:TYR:OH   | 2.39                     | 0.56              |
| 1:A:1178:LEU:CD2  | 1:A:1202:LEU:HD21 | 2.36                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1138:HIS:NE2  | 1:B:1143:ALA:O    | 2.39                     | 0.56              |
| 1:A:273:PHE:O     | 1:A:277:VAL:HG13  | 2.06                     | 0.55              |
| 1:A:491:LEU:HD21  | 1:A:518:ILE:HA    | 1.88                     | 0.55              |
| 1:B:35:PRO:HB3    | 1:B:48:GLU:HB3    | 1.88                     | 0.55              |
| 1:B:1307:PRO:O    | 1:B:1311:ILE:HG13 | 2.06                     | 0.55              |
| 1:A:145:ARG:O     | 1:A:149:ILE:HG13  | 2.06                     | 0.55              |
| 1:A:183:GLU:H     | 1:A:183:GLU:CD    | 2.13                     | 0.55              |
| 1:A:329:VAL:CG1   | 1:A:388:ILE:HG23  | 2.30                     | 0.55              |
| 1:A:982:THR:OG1   | 1:A:1117:SER:HB3  | 2.05                     | 0.55              |
| 1:A:1281:ALA:HA   | 1:A:1284:LEU:HB2  | 1.87                     | 0.55              |
| 1:A:1529:GLY:HA2  | 1:A:1592:ILE:HD11 | 1.88                     | 0.55              |
| 1:B:1453:LEU:H    | 1:B:1453:LEU:HD12 | 1.71                     | 0.55              |
| 1:A:683:MET:SD    | 1:A:727:LEU:HD23  | 2.46                     | 0.55              |
| 1:A:781:LYS:HG3   | 1:A:781:LYS:O     | 2.04                     | 0.55              |
| 1:B:31:VAL:O      | 1:B:35:PRO:CD     | 2.39                     | 0.55              |
| 1:B:32:ALA:C      | 1:B:34:ARG:N      | 2.60                     | 0.55              |
| 1:A:404:GLN:HE21  | 1:B:396:ARG:HB2   | 1.72                     | 0.55              |
| 1:B:1408:VAL:O    | 1:B:1412:MET:HG2  | 2.06                     | 0.55              |
| 1:A:183:GLU:O     | 1:A:187:LYS:HD3   | 2.06                     | 0.55              |
| 1:A:193:PHE:HD2   | 1:B:881:GLN:CG    | 2.19                     | 0.55              |
| 1:A:204:ARG:O     | 1:A:205:THR:C     | 2.50                     | 0.55              |
| 1:A:352:VAL:HB    | 1:A:426:PRO:HG3   | 1.88                     | 0.55              |
| 1:A:759:ARG:HG2   | 1:A:885:LEU:HD23  | 1.89                     | 0.55              |
| 1:B:90:SER:HB3    | 1:B:232:ALA:HB1   | 1.88                     | 0.55              |
| 1:B:347:MET:HE1   | 1:B:371:GLU:HG3   | 1.88                     | 0.55              |
| 1:B:1087:VAL:HG12 | 1:B:1091:GLU:OE1  | 2.06                     | 0.55              |
| 1:A:85:ILE:CG2    | 1:A:100:VAL:HG13  | 2.36                     | 0.55              |
| 1:A:291:ASP:O     | 1:A:295:VAL:HG23  | 2.06                     | 0.55              |
| 1:A:674:LEU:O     | 1:A:678:LEU:HG    | 2.06                     | 0.55              |
| 1:B:553:LYS:O     | 1:B:554:GLY:C     | 2.48                     | 0.55              |
| 1:B:1299:ILE:HG21 | 1:B:1336:ARG:HD2  | 1.87                     | 0.55              |
| 1:A:83:HIS:O      | 1:A:87:THR:HG23   | 2.06                     | 0.55              |
| 1:A:1156:LYS:HG2  | 1:A:1304:GLU:CD   | 2.32                     | 0.55              |
| 1:B:282:PHE:CB    | 1:B:416:ASN:HB3   | 2.37                     | 0.55              |
| 1:A:1122:TYR:HD1  | 1:A:1122:TYR:C    | 2.15                     | 0.55              |
| 1:A:1292:VAL:HG11 | 1:A:1329:ILE:HB   | 1.88                     | 0.55              |
| 1:A:1306:ASN:OD1  | 1:A:1308:PRO:HD2  | 2.06                     | 0.55              |
| 1:A:1474:SER:HB2  | 1:A:1485:ILE:HG21 | 1.89                     | 0.55              |
| 1:B:193:PHE:O     | 1:B:194:LEU:C     | 2.49                     | 0.55              |
| 1:B:943:ASP:O     | 1:B:944:ASP:C     | 2.49                     | 0.55              |
| 1:B:973:LEU:HB3   | 1:B:1002:TYR:OH   | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1101:PHE:HA   | 1:B:1104:ILE:HD13 | 1.89                     | 0.55              |
| 1:A:1127:ALA:O    | 1:A:1131:VAL:HG22 | 2.07                     | 0.54              |
| 1:B:1168:THR:HG22 | 1:B:1172:PHE:CE2  | 2.42                     | 0.54              |
| 1:A:270:ILE:HG12  | 1:A:335:SER:OG    | 2.07                     | 0.54              |
| 1:A:715:HIS:NE2   | 1:B:200:VAL:HG11  | 2.22                     | 0.54              |
| 1:B:1133:VAL:HG13 | 1:B:1247:TRP:CE3  | 2.41                     | 0.54              |
| 1:A:393:SER:HA    | 1:A:399:GLY:O     | 2.06                     | 0.54              |
| 1:A:1094:PHE:HZ   | 1:A:1128:ILE:HD13 | 1.73                     | 0.54              |
| 1:A:1122:TYR:C    | 1:A:1122:TYR:CD1  | 2.85                     | 0.54              |
| 1:B:48:GLU:O      | 1:B:51:GLN:HB3    | 2.06                     | 0.54              |
| 1:B:1159:LEU:HB3  | 1:B:1160:PRO:CD   | 2.36                     | 0.54              |
| 1:B:1387:GLN:CG   | 1:B:1393:ALA:HB1  | 2.37                     | 0.54              |
| 1:A:420:LEU:HD21  | 1:A:444:VAL:CA    | 2.35                     | 0.54              |
| 1:A:881:GLN:NE2   | 1:B:193:PHE:CD2   | 2.72                     | 0.54              |
| 1:B:195:ASN:O     | 1:B:196:GLN:C     | 2.47                     | 0.54              |
| 1:B:827:ARG:HG3   | 1:B:955:VAL:HG13  | 1.88                     | 0.54              |
| 1:A:881:GLN:HA    | 1:A:885:LEU:HD12  | 1.89                     | 0.54              |
| 1:A:1159:LEU:HB3  | 1:A:1160:PRO:CD   | 2.37                     | 0.54              |
| 1:A:1177:LEU:HG   | 1:A:1233:TRP:CE3  | 2.42                     | 0.54              |
| 1:B:783:TRP:CD1   | 1:B:821:PHE:HE2   | 2.26                     | 0.54              |
| 1:B:1063:MET:SD   | 1:B:1068:ALA:HB2  | 2.48                     | 0.54              |
| 1:B:1083:VAL:HG21 | 1:B:1138:HIS:HB2  | 1.88                     | 0.54              |
| 1:B:1456:LEU:O    | 1:B:1459:VAL:HG13 | 2.08                     | 0.54              |
| 1:A:691:LYS:HD3   | 1:A:735:LEU:HA    | 1.88                     | 0.54              |
| 1:A:1209:CYS:SG   | 1:A:1318:LEU:HD11 | 2.48                     | 0.54              |
| 1:B:184:LEU:H     | 1:B:184:LEU:HD22  | 1.73                     | 0.54              |
| 1:B:827:ARG:HG2   | 1:B:960:LEU:HD12  | 1.90                     | 0.54              |
| 1:B:1570:TYR:HA   | 1:B:1573:GLN:HE21 | 1.72                     | 0.54              |
| 1:A:32:ALA:CA     | 1:A:35:PRO:HD2    | 2.38                     | 0.54              |
| 1:A:791:LYS:HD3   | 1:A:836:ILE:HG12  | 1.89                     | 0.54              |
| 1:A:968:ALA:O     | 1:A:969:ALA:C     | 2.46                     | 0.54              |
| 1:A:1132:GLN:HE22 | 1:A:1293:ARG:HH21 | 1.56                     | 0.54              |
| 1:A:1201:VAL:HG21 | 1:A:1372:LEU:HD22 | 1.89                     | 0.54              |
| 1:B:349:ILE:HD12  | 1:B:429:LEU:HD22  | 1.90                     | 0.54              |
| 1:B:1445:SER:HA   | 1:B:1448:HIS:HB2  | 1.90                     | 0.54              |
| 1:B:1570:TYR:OH   | 1:B:1588:LYS:HD2  | 2.07                     | 0.54              |
| 1:B:1572:SER:O    | 1:B:1573:GLN:C    | 2.49                     | 0.54              |
| 1:B:1603:LEU:HA   | 1:B:1606:VAL:CB   | 2.35                     | 0.54              |
| 1:B:1384:LEU:HD13 | 1:B:1397:MET:SD   | 2.48                     | 0.54              |
| 1:A:32:ALA:C      | 1:A:34:ARG:N      | 2.57                     | 0.54              |
| 1:A:881:GLN:HE22  | 1:B:193:PHE:CA    | 2.21                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1404:SER:HB2  | 1:A:1406:GLU:HG3  | 1.90                     | 0.54              |
| 1:B:49:LEU:C      | 1:B:51:GLN:N      | 2.63                     | 0.54              |
| 1:B:282:PHE:HZ    | 1:B:341:VAL:HG21  | 1.71                     | 0.54              |
| 1:B:1025:MET:HG2  | 1:B:1026:ASN:H    | 1.72                     | 0.54              |
| 1:A:322:ASN:O     | 1:A:323:PRO:C     | 2.51                     | 0.53              |
| 1:A:1552:GLY:C    | 1:A:1554:LEU:H    | 2.16                     | 0.53              |
| 1:B:1230:CYS:SG   | 1:B:1234:ASN:ND2  | 2.81                     | 0.53              |
| 1:B:1238:THR:HG22 | 1:B:1282:ALA:O    | 2.08                     | 0.53              |
| 1:A:39:ALA:HA     | 1:A:42:SER:O      | 2.08                     | 0.53              |
| 1:A:90:SER:HB3    | 1:A:232:ALA:HB1   | 1.89                     | 0.53              |
| 1:B:30:GLU:O      | 1:B:33:VAL:HG22   | 2.08                     | 0.53              |
| 1:B:44:PHE:CD1    | 1:B:84:TYR:HB3    | 2.43                     | 0.53              |
| 1:B:49:LEU:HB3    | 1:B:50:PRO:HD3    | 1.89                     | 0.53              |
| 1:B:941:SER:C     | 1:B:943:ASP:H     | 2.16                     | 0.53              |
| 1:A:1162:THR:HG23 | 1:A:1291:LEU:HD22 | 1.89                     | 0.53              |
| 1:B:1247:TRP:HA   | 1:B:1251:PHE:HB2  | 1.91                     | 0.53              |
| 1:B:1518:LEU:HD12 | 1:B:1544:LEU:HD12 | 1.90                     | 0.53              |
| 1:B:1560:ALA:HA   | 1:B:1563:TRP:HE3  | 1.71                     | 0.53              |
| 1:A:103:ALA:O     | 1:A:107:LEU:HG    | 2.09                     | 0.53              |
| 1:A:478:ASN:OD1   | 1:A:650:LEU:HD13  | 2.08                     | 0.53              |
| 1:A:1394:ARG:HH11 | 1:A:1443:ASN:HD21 | 1.56                     | 0.53              |
| 1:A:1435:PHE:CD1  | 1:A:1498:TYR:HB3  | 2.43                     | 0.53              |
| 1:B:183:GLU:O     | 1:B:187:LYS:HG2   | 2.09                     | 0.53              |
| 1:B:1554:LEU:HD11 | 1:B:1610:LEU:CD1  | 2.38                     | 0.53              |
| 1:A:715:HIS:CE1   | 1:B:200:VAL:HB    | 2.44                     | 0.53              |
| 1:A:942:GLU:HG2   | 1:A:943:ASP:N     | 2.23                     | 0.53              |
| 1:A:1015:PRO:HG3  | 1:A:1041:TRP:CD2  | 2.44                     | 0.53              |
| 1:B:1460:GLU:OE1  | 1:B:1463:ARG:HB2  | 2.09                     | 0.53              |
| 1:A:254:GLU:HA    | 1:A:257:LEU:HD12  | 1.90                     | 0.53              |
| 1:B:1110:LEU:O    | 1:B:1175:ALA:HB1  | 2.07                     | 0.53              |
| 1:B:1522:ALA:HB1  | 1:B:1534:PHE:HE1  | 1.73                     | 0.53              |
| 1:A:545:ALA:O     | 1:A:644:PRO:HB3   | 2.07                     | 0.53              |
| 1:A:552:ARG:NH2   | 1:A:643:ASP:HA    | 2.23                     | 0.53              |
| 1:A:1080:CYS:HB3  | 1:A:1084:LYS:HE3  | 1.91                     | 0.53              |
| 1:B:1394:ARG:NH2  | 1:B:1437:LEU:HD13 | 2.23                     | 0.53              |
| 1:B:1394:ARG:HD3  | 1:B:1446:LEU:HD21 | 1.89                     | 0.53              |
| 1:A:239:PHE:HA    | 1:A:242:GLN:OE1   | 2.08                     | 0.53              |
| 1:A:985:ARG:NH1   | 1:A:1280:LEU:HD22 | 2.24                     | 0.53              |
| 1:A:1155:THR:HG21 | 1:A:1301:TRP:CD1  | 2.44                     | 0.53              |
| 1:A:1210:LYS:N    | 1:A:1210:LYS:HD2  | 2.24                     | 0.53              |
| 1:A:1515:LEU:HB2  | 1:A:1544:LEU:HD13 | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:844:MET:HE2   | 1:B:844:MET:HA    | 1.90                     | 0.53              |
| 1:B:1030:MET:O    | 1:B:1096:ARG:NH1  | 2.42                     | 0.53              |
| 1:B:1191:SER:H    | 1:B:1194:LYS:HD3  | 1.73                     | 0.53              |
| 1:B:1435:PHE:CD1  | 1:B:1498:TYR:HB3  | 2.43                     | 0.53              |
| 1:A:1299:ILE:HD11 | 1:A:1310:VAL:HG11 | 1.90                     | 0.53              |
| 1:A:1545:ALA:HB1  | 1:A:1553:HIS:CD2  | 2.44                     | 0.53              |
| 1:B:144:ASP:HB2   | 1:B:147:GLU:HG3   | 1.91                     | 0.53              |
| 1:B:261:LEU:HD11  | 1:B:328:ASP:HB3   | 1.90                     | 0.53              |
| 1:B:420:LEU:HD13  | 1:B:442:LEU:HB2   | 1.91                     | 0.53              |
| 1:B:859:LEU:O     | 1:B:1009:ILE:HD11 | 2.09                     | 0.53              |
| 1:B:1464:LEU:HD23 | 1:B:1517:THR:HG21 | 1.90                     | 0.53              |
| 1:A:1525:MET:HA   | 1:A:1530:ASP:HB2  | 1.91                     | 0.52              |
| 1:B:382:LEU:CD1   | 1:B:475:ILE:HG22  | 2.39                     | 0.52              |
| 1:B:864:TYR:HD1   | 1:B:936:LEU:HD13  | 1.74                     | 0.52              |
| 1:A:885:LEU:HD13  | 1:B:197:LEU:CD2   | 2.39                     | 0.52              |
| 1:A:1000:GLN:HG3  | 1:A:1270:LEU:HD13 | 1.91                     | 0.52              |
| 1:A:1122:TYR:HD1  | 1:A:1123:THR:N    | 2.07                     | 0.52              |
| 1:A:1315:LEU:HD21 | 1:A:1353:LYS:HB2  | 1.91                     | 0.52              |
| 1:A:1383:TYR:O    | 1:A:1387:GLN:HG2  | 2.08                     | 0.52              |
| 1:B:1084:LYS:HE3  | 1:B:1151:SER:N    | 2.23                     | 0.52              |
| 1:B:1232:SER:C    | 1:B:1234:ASN:N    | 2.64                     | 0.52              |
| 1:A:95:ASN:HB3    | 1:A:192:ASN:HD21  | 1.74                     | 0.52              |
| 1:A:230:ALA:O     | 1:A:234:LYS:HG3   | 2.09                     | 0.52              |
| 1:A:1094:PHE:O    | 1:A:1098:ILE:HG13 | 2.10                     | 0.52              |
| 1:A:1315:LEU:HB3  | 1:A:1316:PRO:CD   | 2.39                     | 0.52              |
| 1:B:32:ALA:O      | 1:B:35:PRO:CD     | 2.50                     | 0.52              |
| 1:B:265:TYR:CE2   | 1:B:301:SER:HB2   | 2.44                     | 0.52              |
| 1:B:443:ARG:HB2   | 1:B:446:ASP:CG    | 2.33                     | 0.52              |
| 1:B:1489:ARG:NH2  | 1:B:1533:GLY:CA   | 2.71                     | 0.52              |
| 1:A:839:GLU:O     | 1:A:842:VAL:HG12  | 2.09                     | 0.52              |
| 1:A:1000:GLN:HA   | 1:A:1270:LEU:HD13 | 1.91                     | 0.52              |
| 1:A:1294:LEU:O    | 1:A:1298:LEU:HG   | 2.10                     | 0.52              |
| 1:B:759:ARG:HG2   | 1:B:885:LEU:CD2   | 2.40                     | 0.52              |
| 1:B:1044:ARG:C    | 1:B:1046:ARG:H    | 2.17                     | 0.52              |
| 1:A:193:PHE:HD2   | 1:B:881:GLN:HG2   | 1.75                     | 0.52              |
| 1:A:245:ALA:O     | 1:A:249:GLU:HG3   | 2.09                     | 0.52              |
| 1:A:545:ALA:HB2   | 1:A:647:PHE:HB2   | 1.92                     | 0.52              |
| 1:A:549:GLN:O     | 1:A:553:LYS:HG2   | 2.09                     | 0.52              |
| 1:A:1196:GLN:O    | 1:A:1199:ALA:HB3  | 2.09                     | 0.52              |
| 1:B:1046:ARG:HH22 | 1:B:1130:LYS:NZ   | 2.06                     | 0.52              |
| 1:A:491:LEU:HD23  | 1:A:517:SER:OG    | 2.10                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:844:MET:HA    | 1:A:844:MET:HE2   | 1.90                     | 0.52              |
| 1:A:1225:SER:O    | 1:A:1229:VAL:HG23 | 2.10                     | 0.52              |
| 1:B:272:ARG:HD3   | 1:B:285:MET:HG2   | 1.91                     | 0.52              |
| 1:B:712:HIS:HA    | 1:B:715:HIS:CD2   | 2.44                     | 0.52              |
| 1:B:1063:MET:CG   | 1:B:1068:ALA:HB2  | 2.39                     | 0.52              |
| 1:B:1163:LEU:HA   | 1:B:1166:ILE:HD12 | 1.92                     | 0.52              |
| 1:B:1412:MET:O    | 1:B:1415:ALA:HB3  | 2.09                     | 0.52              |
| 1:B:1414:THR:HG22 | 1:B:1424:CYS:SG   | 2.50                     | 0.52              |
| 1:A:786:PHE:O     | 1:A:787:LEU:C     | 2.48                     | 0.52              |
| 1:A:1010:LEU:HB3  | 1:A:1037:HIS:HE1  | 1.75                     | 0.52              |
| 1:A:1169:TYR:HA   | 1:A:1172:PHE:CD2  | 2.44                     | 0.52              |
| 1:A:1208:ARG:HG3  | 1:A:1209:CYS:N    | 2.25                     | 0.52              |
| 1:A:1546:SER:C    | 1:A:1548:GLY:N    | 2.65                     | 0.52              |
| 1:B:1010:LEU:HD22 | 1:B:1037:HIS:CE1  | 2.44                     | 0.52              |
| 1:B:1449:LEU:O    | 1:B:1453:LEU:HD12 | 2.10                     | 0.52              |
| 1:B:123:ALA:HB1   | 1:B:154:MET:SD    | 2.50                     | 0.52              |
| 1:B:712:HIS:HA    | 1:B:715:HIS:NE2   | 2.25                     | 0.52              |
| 1:B:1127:ALA:O    | 1:B:1131:VAL:HG22 | 2.10                     | 0.52              |
| 1:B:1162:THR:HG23 | 1:B:1291:LEU:HD22 | 1.91                     | 0.52              |
| 1:A:1048:SER:HA   | 1:A:1051:VAL:HB   | 1.91                     | 0.52              |
| 1:A:1571:LEU:C    | 1:A:1573:GLN:N    | 2.65                     | 0.52              |
| 1:B:187:LYS:O     | 1:B:191:MET:HG2   | 2.09                     | 0.52              |
| 1:B:1449:LEU:C    | 1:B:1452:SER:HB3  | 2.34                     | 0.52              |
| 1:A:193:PHE:HZ    | 1:B:762:LEU:HD13  | 1.74                     | 0.52              |
| 1:A:396:ARG:HH21  | 1:B:404:GLN:CD    | 2.18                     | 0.52              |
| 1:A:1010:LEU:HB3  | 1:A:1037:HIS:CE1  | 2.45                     | 0.52              |
| 1:B:531:MET:HG3   | 1:B:677:SER:HB2   | 1.92                     | 0.52              |
| 1:B:1064:LYS:HB3  | 1:B:1067:HIS:HD2  | 1.75                     | 0.52              |
| 1:A:37:LEU:O      | 1:A:40:SER:HB3    | 2.09                     | 0.51              |
| 1:A:1210:LYS:HE3  | 1:A:1342:GLU:HG2  | 1.91                     | 0.51              |
| 1:B:740:PHE:HA    | 1:B:781:LYS:HG2   | 1.91                     | 0.51              |
| 1:B:1058:LEU:HB3  | 1:B:1063:MET:SD   | 2.50                     | 0.51              |
| 1:A:73:PHE:HB2    | 1:A:161:PRO:HD3   | 1.92                     | 0.51              |
| 1:A:299:PHE:HZ    | 1:A:346:CYS:SG    | 2.34                     | 0.51              |
| 1:A:1211:ALA:HA   | 1:A:1350:VAL:CG1  | 2.41                     | 0.51              |
| 1:B:281:SER:OG    | 1:B:445:ARG:HB2   | 2.10                     | 0.51              |
| 1:B:723:GLN:HG2   | 1:B:728:GLN:HG3   | 1.92                     | 0.51              |
| 1:B:1247:TRP:HB2  | 1:B:1251:PHE:O    | 2.11                     | 0.51              |
| 1:A:302:LEU:HD23  | 1:A:377:ILE:HD13  | 1.91                     | 0.51              |
| 1:A:317:VAL:C     | 1:A:318:LEU:HG    | 2.35                     | 0.51              |
| 1:A:546:CYS:O     | 1:A:550:ARG:HG3   | 2.11                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:661:SER:O     | 1:A:665:SER:HB2   | 2.09                     | 0.51              |
| 1:A:963:TYR:HE1   | 1:A:1013:LEU:HD13 | 1.75                     | 0.51              |
| 1:B:282:PHE:HB2   | 1:B:416:ASN:OD1   | 2.10                     | 0.51              |
| 1:B:1101:PHE:HB3  | 1:B:1104:ILE:HB   | 1.91                     | 0.51              |
| 1:A:44:PHE:HD1    | 1:A:84:TYR:HB3    | 1.76                     | 0.51              |
| 1:A:723:GLN:HG2   | 1:A:728:GLN:HG3   | 1.92                     | 0.51              |
| 1:A:985:ARG:HH12  | 1:A:1280:LEU:HD22 | 1.75                     | 0.51              |
| 1:B:282:PHE:CZ    | 1:B:338:TYR:HD2   | 2.28                     | 0.51              |
| 1:B:479:HIS:O     | 1:B:483:LEU:HG    | 2.10                     | 0.51              |
| 1:B:1159:LEU:HD13 | 1:B:1298:LEU:CB   | 2.39                     | 0.51              |
| 1:A:80:LEU:HD22   | 1:A:148:ILE:HG23  | 1.92                     | 0.51              |
| 1:A:1563:TRP:CD1  | 1:A:1566:ARG:CZ   | 2.94                     | 0.51              |
| 1:B:1082:SER:C    | 1:B:1084:LYS:N    | 2.59                     | 0.51              |
| 1:B:1516:GLY:O    | 1:B:1520:PRO:CD   | 2.57                     | 0.51              |
| 1:A:159:LYS:O     | 1:A:160:LEU:C     | 2.52                     | 0.51              |
| 1:A:202:ASN:HB3   | 1:A:204:ARG:CZ    | 2.41                     | 0.51              |
| 1:A:470:GLY:O     | 1:A:474:VAL:HG23  | 2.10                     | 0.51              |
| 1:A:548:LEU:HD11  | 1:A:647:PHE:CE2   | 2.46                     | 0.51              |
| 1:A:1019:TYR:CZ   | 1:A:1023:LEU:HD21 | 2.45                     | 0.51              |
| 1:B:291:ASP:O     | 1:B:295:VAL:HG23  | 2.10                     | 0.51              |
| 1:B:1151:SER:HB3  | 1:B:1154:ILE:CG1  | 2.40                     | 0.51              |
| 1:B:1403:ASP:OD2  | 1:B:1404:SER:N    | 2.44                     | 0.51              |
| 1:B:1473:THR:O    | 1:B:1485:ILE:HD13 | 2.10                     | 0.51              |
| 1:B:1490:GLN:O    | 1:B:1494:LEU:HD13 | 2.09                     | 0.51              |
| 1:B:1558:ASN:O    | 1:B:1561:VAL:HB   | 2.10                     | 0.51              |
| 1:B:1598:HIS:HA   | 1:B:1601:SER:HB3  | 1.92                     | 0.51              |
| 1:B:1607:THR:O    | 1:B:1611:SER:N    | 2.40                     | 0.51              |
| 1:A:985:ARG:O     | 1:A:986:LYS:C     | 2.53                     | 0.51              |
| 1:A:1156:LYS:C    | 1:A:1156:LYS:HD3  | 2.36                     | 0.51              |
| 1:B:89:CYS:SG     | 1:B:239:PHE:CG    | 2.97                     | 0.51              |
| 1:B:852:PRO:CB    | 1:B:855:LEU:HB3   | 2.41                     | 0.51              |
| 1:B:1082:SER:O    | 1:B:1083:VAL:C    | 2.54                     | 0.51              |
| 1:A:943:ASP:O     | 1:A:944:ASP:C     | 2.54                     | 0.51              |
| 1:A:1204:ILE:HG22 | 1:A:1215:GLY:HA2  | 1.93                     | 0.51              |
| 1:A:1206:SER:HB2  | 1:A:1319:LEU:HA   | 1.93                     | 0.51              |
| 1:A:1417:GLU:HA   | 1:A:1470:ARG:CD   | 2.33                     | 0.51              |
| 1:A:1568:LYS:HD3  | 1:A:1569:LYS:N    | 2.26                     | 0.51              |
| 1:B:71:GLU:OE1    | 1:B:122:CYS:HA    | 2.11                     | 0.51              |
| 1:B:247:LEU:O     | 1:B:250:LEU:N     | 2.43                     | 0.51              |
| 1:A:61:SER:HA     | 1:A:64:LEU:HD12   | 1.92                     | 0.51              |
| 1:A:491:LEU:HD22  | 1:A:518:ILE:HG12  | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1306:ASN:O    | 1:A:1310:VAL:HG23 | 2.11                     | 0.51              |
| 1:B:37:LEU:HD12   | 1:B:38:SER:N      | 2.26                     | 0.51              |
| 1:B:1214:LEU:HD22 | 1:B:1383:TYR:CE2  | 2.45                     | 0.51              |
| 1:A:405:ASN:HB2   | 1:A:511:ILE:HA    | 1.92                     | 0.51              |
| 1:A:418:LEU:HD21  | 1:A:476:LEU:HB2   | 1.93                     | 0.51              |
| 1:A:1272:THR:HB   | 1:A:1282:ALA:HB3  | 1.93                     | 0.51              |
| 1:A:1400:PHE:HB3  | 1:A:1401:PHE:HD2  | 1.76                     | 0.51              |
| 1:B:539:SER:O     | 1:B:543:ARG:HD3   | 2.11                     | 0.51              |
| 1:B:1156:LYS:O    | 1:B:1156:LYS:HD3  | 2.11                     | 0.51              |
| 1:B:1414:THR:HG21 | 1:B:1424:CYS:HA   | 1.93                     | 0.51              |
| 1:B:1545:ALA:HB2  | 1:B:1556:LEU:HD22 | 1.92                     | 0.51              |
| 1:A:788:SER:C     | 1:A:790:MET:N     | 2.59                     | 0.50              |
| 1:A:1030:MET:O    | 1:A:1035:ILE:HG13 | 2.11                     | 0.50              |
| 1:A:1058:LEU:HD23 | 1:A:1061:GLN:HE22 | 1.76                     | 0.50              |
| 1:B:303:VAL:HG22  | 1:B:377:ILE:HG13  | 1.92                     | 0.50              |
| 1:B:1238:THR:HB   | 1:B:1286:HIS:HB2  | 1.93                     | 0.50              |
| 1:A:985:ARG:NH2   | 1:A:1115:ILE:O    | 2.44                     | 0.50              |
| 1:A:1022:GLN:C    | 1:A:1024:SER:N    | 2.67                     | 0.50              |
| 1:A:1468:LEU:HD22 | 1:A:1518:LEU:HD21 | 1.92                     | 0.50              |
| 1:B:341:VAL:HB    | 1:B:417:SER:HB2   | 1.94                     | 0.50              |
| 1:B:1278:LEU:HB3  | 1:B:1281:ALA:HB2  | 1.93                     | 0.50              |
| 1:A:93:PRO:CD     | 1:A:96:GLN:HB2    | 2.41                     | 0.50              |
| 1:A:491:LEU:CD1   | 1:A:670:ILE:HD11  | 2.40                     | 0.50              |
| 1:A:1162:THR:O    | 1:A:1166:ILE:HG13 | 2.11                     | 0.50              |
| 1:A:1198:PHE:O    | 1:A:1202:LEU:HG   | 2.11                     | 0.50              |
| 1:B:1254:ASP:O    | 1:B:1255:THR:C    | 2.55                     | 0.50              |
| 1:B:1318:LEU:HD11 | 1:B:1331:SER:HA   | 1.92                     | 0.50              |
| 1:B:1456:LEU:HD22 | 1:B:1510:VAL:HG13 | 1.93                     | 0.50              |
| 1:A:535:LEU:HD12  | 1:A:682:HIS:CD2   | 2.46                     | 0.50              |
| 1:A:539:SER:HB2   | 1:A:543:ARG:NH1   | 2.25                     | 0.50              |
| 1:A:547:VAL:O     | 1:A:551:GLN:HG3   | 2.11                     | 0.50              |
| 1:A:650:LEU:O     | 1:A:654:ILE:HG13  | 2.11                     | 0.50              |
| 1:A:1001:TYR:CE2  | 1:A:1005:ILE:HD11 | 2.46                     | 0.50              |
| 1:A:1233:TRP:HE3  | 1:A:1278:LEU:HD13 | 1.76                     | 0.50              |
| 1:A:1270:LEU:O    | 1:A:1273:LEU:HB2  | 2.10                     | 0.50              |
| 1:B:243:ASN:O     | 1:B:246:SER:OG    | 2.28                     | 0.50              |
| 1:B:247:LEU:O     | 1:B:249:GLU:N     | 2.44                     | 0.50              |
| 1:B:808:VAL:HG11  | 1:B:908:TYR:HB3   | 1.94                     | 0.50              |
| 1:A:1087:VAL:HG11 | 1:A:1154:ILE:HG23 | 1.93                     | 0.50              |
| 1:B:1290:SER:HA   | 1:B:1293:ARG:HD3  | 1.93                     | 0.50              |
| 1:B:1554:LEU:HD13 | 1:B:1557:HIS:CD2  | 2.47                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1388:LEU:O    | 1:A:1394:ARG:NE   | 2.44                     | 0.50              |
| 1:A:1407:LEU:HD11 | 1:A:1449:LEU:HD22 | 1.94                     | 0.50              |
| 1:A:1269:HIS:ND1  | 1:A:1283:SER:HB3  | 2.26                     | 0.50              |
| 1:A:1499:ILE:HG12 | 1:A:1506:VAL:HG21 | 1.92                     | 0.50              |
| 1:B:34:ARG:O      | 1:B:35:PRO:C      | 2.51                     | 0.50              |
| 1:B:283:PHE:HB3   | 1:B:443:ARG:HD3   | 1.94                     | 0.50              |
| 1:B:1054:ILE:O    | 1:B:1058:LEU:HG   | 2.11                     | 0.50              |
| 1:A:130:ILE:HD13  | 1:A:312:THR:OG1   | 2.12                     | 0.50              |
| 1:A:266:PHE:O     | 1:A:270:ILE:HG13  | 2.10                     | 0.50              |
| 1:A:974:LEU:HD22  | 1:A:1003:PHE:CE1  | 2.46                     | 0.50              |
| 1:A:1094:PHE:CZ   | 1:A:1128:ILE:HD13 | 2.47                     | 0.50              |
| 1:A:1399:GLU:C    | 1:A:1403:ASP:OD1  | 2.48                     | 0.50              |
| 1:B:83:HIS:O      | 1:B:87:THR:HG23   | 2.11                     | 0.50              |
| 1:B:765:GLN:NE2   | 1:B:817:ILE:HG23  | 2.25                     | 0.50              |
| 1:B:941:SER:C     | 1:B:943:ASP:N     | 2.70                     | 0.50              |
| 1:B:1315:LEU:N    | 1:B:1316:PRO:HD2  | 2.27                     | 0.50              |
| 1:B:1384:LEU:HB3  | 1:B:1430:PHE:CE1  | 2.47                     | 0.50              |
| 1:B:1427:VAL:HG13 | 1:B:1431:PHE:CE2  | 2.47                     | 0.50              |
| 1:A:289:VAL:HA    | 1:A:349:ILE:HG22  | 1.93                     | 0.50              |
| 1:A:909:HIS:CG    | 1:A:937:SER:HA    | 2.47                     | 0.50              |
| 1:A:973:LEU:HB3   | 1:A:1002:TYR:OH   | 2.12                     | 0.50              |
| 1:A:1309:GLN:O    | 1:A:1313:THR:HG23 | 2.11                     | 0.50              |
| 1:B:39:ALA:CB     | 1:B:44:PHE:CD1    | 2.95                     | 0.50              |
| 1:B:280:ASN:O     | 1:B:281:SER:O     | 2.30                     | 0.50              |
| 1:B:443:ARG:HB2   | 1:B:446:ASP:HB2   | 1.93                     | 0.50              |
| 1:A:296:ARG:HD2   | 1:A:350:LEU:HD22  | 1.94                     | 0.49              |
| 1:A:949:ASP:O     | 1:A:950:SER:C     | 2.54                     | 0.49              |
| 1:B:193:PHE:C     | 1:B:195:ASN:N     | 2.67                     | 0.49              |
| 1:B:528:VAL:O     | 1:B:529:PRO:C     | 2.51                     | 0.49              |
| 1:B:759:ARG:HG2   | 1:B:885:LEU:HD22  | 1.93                     | 0.49              |
| 1:B:1553:HIS:CD2  | 1:B:1602:TYR:OH   | 2.65                     | 0.49              |
| 1:B:1553:HIS:CG   | 1:B:1553:HIS:O    | 2.65                     | 0.49              |
| 1:A:129:LEU:HA    | 1:A:132:LEU:HD12  | 1.94                     | 0.49              |
| 1:A:303:VAL:HG22  | 1:A:377:ILE:HG13  | 1.93                     | 0.49              |
| 1:A:396:ARG:HH21  | 1:B:404:GLN:HE22  | 1.61                     | 0.49              |
| 1:A:875:TYR:CD2   | 1:A:909:HIS:HE1   | 2.31                     | 0.49              |
| 1:A:980:LEU:HD23  | 1:A:999:LEU:HD11  | 1.93                     | 0.49              |
| 1:A:1032:GLU:OE2  | 1:A:1120:SER:HA   | 2.11                     | 0.49              |
| 1:A:1302:SER:O    | 1:A:1305:MET:HG2  | 2.13                     | 0.49              |
| 1:A:1347:LEU:HD22 | 1:A:1351:TYR:OH   | 2.13                     | 0.49              |
| 1:A:1515:LEU:CB   | 1:A:1544:LEU:HD13 | 2.42                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:283:PHE:HD2   | 1:B:285:MET:HE2   | 1.75                     | 0.49              |
| 1:B:485:THR:O     | 1:B:489:GLN:HG2   | 2.12                     | 0.49              |
| 1:B:745:TRP:HE1   | 1:B:810:HIS:CE1   | 2.30                     | 0.49              |
| 1:B:1355:ILE:HD13 | 1:B:1397:MET:HG2  | 1.94                     | 0.49              |
| 1:B:1428:LEU:CD1  | 1:B:1488:ASN:HA   | 2.42                     | 0.49              |
| 1:A:531:MET:HE1   | 1:A:535:LEU:HD11  | 1.94                     | 0.49              |
| 1:A:683:MET:HE2   | 1:A:683:MET:HA    | 1.93                     | 0.49              |
| 1:A:1299:ILE:HG22 | 1:A:1336:ARG:HE   | 1.76                     | 0.49              |
| 1:A:48:GLU:O      | 1:A:51:GLN:HB3    | 2.12                     | 0.49              |
| 1:B:49:LEU:C      | 1:B:51:GLN:H      | 2.19                     | 0.49              |
| 1:B:112:LEU:HD11  | 1:B:247:LEU:CD1   | 2.42                     | 0.49              |
| 1:B:143:LEU:HD13  | 1:B:151:PHE:CE2   | 2.47                     | 0.49              |
| 1:B:201:PHE:O     | 1:B:202:ASN:C     | 2.53                     | 0.49              |
| 1:B:663:LEU:HD23  | 1:B:674:LEU:HD13  | 1.93                     | 0.49              |
| 1:B:704:GLU:HB3   | 1:B:889:PHE:CE2   | 2.47                     | 0.49              |
| 1:B:739:PRO:HB3   | 1:B:782:VAL:HG23  | 1.94                     | 0.49              |
| 1:B:1538:MET:HG2  | 1:B:1598:HIS:HD2  | 1.76                     | 0.49              |
| 1:A:73:PHE:CD1    | 1:A:158:ALA:O     | 2.60                     | 0.49              |
| 1:A:397:ARG:O     | 1:A:398:ALA:HB3   | 2.12                     | 0.49              |
| 1:A:1047:ILE:HB   | 1:A:1050:TYR:CD2  | 2.42                     | 0.49              |
| 1:A:313:LEU:HD21  | 1:A:332:LEU:HD23  | 1.94                     | 0.49              |
| 1:A:686:LEU:O     | 1:A:690:ILE:HG13  | 2.12                     | 0.49              |
| 1:A:949:ASP:O     | 1:A:952:ALA:N     | 2.45                     | 0.49              |
| 1:A:1233:TRP:CE3  | 1:A:1278:LEU:HD13 | 2.48                     | 0.49              |
| 1:A:1244:ILE:O    | 1:A:1246:SER:N    | 2.45                     | 0.49              |
| 1:B:1244:ILE:HG13 | 1:B:1248:ARG:HB2  | 1.93                     | 0.49              |
| 1:B:1251:PHE:N    | 1:B:1251:PHE:CD1  | 2.80                     | 0.49              |
| 1:B:1388:LEU:HG   | 1:B:1397:MET:HE1  | 1.95                     | 0.49              |
| 1:A:1047:ILE:CD1  | 1:A:1256:ILE:CG1  | 2.87                     | 0.49              |
| 1:A:1101:PHE:HA   | 1:A:1104:ILE:HD13 | 1.95                     | 0.49              |
| 1:A:1493:GLN:HG2  | 1:A:1540:VAL:HG22 | 1.94                     | 0.49              |
| 1:A:1515:LEU:HD12 | 1:A:1541:MET:SD   | 2.53                     | 0.49              |
| 1:A:1548:GLY:HA2  | 1:A:1552:GLY:HA3  | 1.93                     | 0.49              |
| 1:B:491:LEU:HD21  | 1:B:667:ASN:CB    | 2.43                     | 0.49              |
| 1:B:867:HIS:O     | 1:B:949:ASP:HB2   | 2.13                     | 0.49              |
| 1:B:1214:LEU:HD23 | 1:B:1214:LEU:H    | 1.77                     | 0.49              |
| 1:A:244:VAL:O     | 1:A:248:GLN:HG2   | 2.12                     | 0.49              |
| 1:A:740:PHE:CD1   | 1:A:778:GLU:HG3   | 2.48                     | 0.49              |
| 1:A:922:PHE:CG    | 1:A:923:SER:N     | 2.80                     | 0.49              |
| 1:A:1281:ALA:CA   | 1:A:1284:LEU:HB2  | 2.43                     | 0.49              |
| 1:A:1510:VAL:O    | 1:A:1514:LEU:HG   | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:478:ASN:OD1   | 1:B:650:LEU:HD13  | 2.12                     | 0.49              |
| 1:B:786:PHE:HZ    | 1:B:806:LEU:HD22  | 1.77                     | 0.49              |
| 1:B:1000:GLN:HA   | 1:B:1270:LEU:HD13 | 1.94                     | 0.49              |
| 1:A:341:VAL:HB    | 1:A:417:SER:HB2   | 1.95                     | 0.49              |
| 1:A:1382:GLN:N    | 1:A:1426:ARG:HH21 | 2.10                     | 0.49              |
| 1:A:1557:HIS:O    | 1:A:1561:VAL:HG23 | 2.12                     | 0.49              |
| 1:B:1394:ARG:HH11 | 1:B:1446:LEU:HD21 | 1.78                     | 0.49              |
| 1:A:662:MET:HB3   | 1:A:674:LEU:HD11  | 1.94                     | 0.49              |
| 1:A:802:GLU:CG    | 1:A:931:ARG:HD2   | 2.38                     | 0.49              |
| 1:B:857:ARG:O     | 1:B:861:ILE:HG13  | 2.13                     | 0.49              |
| 1:B:908:TYR:CD2   | 1:B:908:TYR:N     | 2.81                     | 0.49              |
| 1:B:942:GLU:CG    | 1:B:947:ARG:HD2   | 2.43                     | 0.49              |
| 1:B:1043:SER:HA   | 1:B:1046:ARG:NE   | 2.28                     | 0.49              |
| 1:B:1359:TYR:CD1  | 1:B:1406:GLU:HB3  | 2.47                     | 0.49              |
| 1:B:1428:LEU:HD13 | 1:B:1491:LEU:HB2  | 1.94                     | 0.49              |
| 1:B:1428:LEU:HB3  | 1:B:1491:LEU:HB3  | 1.95                     | 0.49              |
| 1:B:1485:ILE:O    | 1:B:1489:ARG:HG3  | 2.12                     | 0.49              |
| 1:A:317:VAL:HG12  | 1:A:318:LEU:N     | 2.28                     | 0.48              |
| 1:A:1030:MET:HA   | 1:A:1034:ASP:CG   | 2.38                     | 0.48              |
| 1:A:1210:LYS:HD2  | 1:A:1210:LYS:H    | 1.78                     | 0.48              |
| 1:A:1251:PHE:CD2  | 1:A:1261:TYR:HD1  | 2.31                     | 0.48              |
| 1:A:1300:VAL:HA   | 1:A:1336:ARG:NH1  | 2.28                     | 0.48              |
| 1:A:1400:PHE:HB3  | 1:A:1401:PHE:CD2  | 2.48                     | 0.48              |
| 1:B:957:PHE:CD1   | 1:B:1061:GLN:HG2  | 2.48                     | 0.48              |
| 1:B:1486:GLN:HG3  | 1:B:1489:ARG:HH11 | 1.78                     | 0.48              |
| 1:A:318:LEU:HD22  | 1:A:329:VAL:HG22  | 1.94                     | 0.48              |
| 1:A:675:SER:HB3   | 1:A:722:LEU:HD12  | 1.95                     | 0.48              |
| 1:A:1002:TYR:O    | 1:A:1003:PHE:C    | 2.53                     | 0.48              |
| 1:A:1208:ARG:CD   | 1:A:1328:GLU:HA   | 2.43                     | 0.48              |
| 1:A:1459:VAL:HG21 | 1:A:1464:LEU:HD13 | 1.95                     | 0.48              |
| 1:B:1415:ALA:O    | 1:B:1470:ARG:HD3  | 2.13                     | 0.48              |
| 1:B:1594:GLU:O    | 1:B:1598:HIS:N    | 2.42                     | 0.48              |
| 1:A:284:ILE:HG22  | 1:A:286:PRO:HD2   | 1.96                     | 0.48              |
| 1:A:422:LEU:HD11  | 1:A:537:LEU:HD23  | 1.96                     | 0.48              |
| 1:A:860:LEU:HD12  | 1:A:860:LEU:O     | 2.12                     | 0.48              |
| 1:A:1515:LEU:HB2  | 1:A:1544:LEU:HB3  | 1.94                     | 0.48              |
| 1:B:89:CYS:SG     | 1:B:236:LYS:HG3   | 2.53                     | 0.48              |
| 1:B:266:PHE:O     | 1:B:270:ILE:HG13  | 2.14                     | 0.48              |
| 1:B:1024:SER:HB3  | 1:B:1074:LEU:HD23 | 1.95                     | 0.48              |
| 1:B:1110:LEU:H    | 1:B:1175:ALA:HB2  | 1.77                     | 0.48              |
| 1:B:1586:HIS:CD2  | 1:B:1589:HIS:CE1  | 3.01                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:813:MET:HB2   | 1:B:813:MET:HE3   | 1.68                     | 0.48              |
| 1:B:946:ASN:O     | 1:B:947:ARG:C     | 2.56                     | 0.48              |
| 1:B:1032:GLU:O    | 1:B:1035:ILE:HB   | 2.13                     | 0.48              |
| 1:B:1087:VAL:O    | 1:B:1091:GLU:HG3  | 2.14                     | 0.48              |
| 1:B:1151:SER:HB3  | 1:B:1154:ILE:HD13 | 1.95                     | 0.48              |
| 1:B:1600:MET:CA   | 1:B:1603:LEU:HG   | 2.42                     | 0.48              |
| 1:A:69:GLN:O      | 1:A:72:PRO:HD2    | 2.12                     | 0.48              |
| 1:A:336:CYS:SG    | 1:A:384:ILE:HD12  | 2.53                     | 0.48              |
| 1:A:738:ALA:HB3   | 1:A:741:SER:HB3   | 1.96                     | 0.48              |
| 1:A:1460:GLU:HB2  | 1:A:1463:ARG:HB3  | 1.94                     | 0.48              |
| 1:B:1599:ILE:O    | 1:B:1603:LEU:HG   | 2.13                     | 0.48              |
| 1:A:45:GLU:C      | 1:A:47:LYS:N      | 2.70                     | 0.48              |
| 1:A:548:LEU:HD13  | 1:A:642:LYS:C     | 2.38                     | 0.48              |
| 1:A:866:LEU:HD22  | 1:A:948:LEU:CD1   | 2.44                     | 0.48              |
| 1:A:1135:LEU:O    | 1:A:1139:PHE:HD2  | 1.96                     | 0.48              |
| 1:A:1351:TYR:HA   | 1:A:1354:LEU:HD12 | 1.95                     | 0.48              |
| 1:A:1560:ALA:HA   | 1:A:1563:TRP:CE3  | 2.49                     | 0.48              |
| 1:B:32:ALA:O      | 1:B:33:VAL:C      | 2.56                     | 0.48              |
| 1:B:245:ALA:O     | 1:B:249:GLU:HG3   | 2.14                     | 0.48              |
| 1:B:1194:LYS:HA   | 1:B:1370:SER:C    | 2.38                     | 0.48              |
| 1:B:1374:GLU:O    | 1:B:1375:SER:C    | 2.56                     | 0.48              |
| 1:A:1023:LEU:HD22 | 1:A:1038:THR:HG23 | 1.96                     | 0.48              |
| 1:A:1434:LEU:CD1  | 1:A:1449:LEU:HD12 | 2.44                     | 0.48              |
| 1:A:1453:LEU:HB3  | 1:A:1506:VAL:CG1  | 2.37                     | 0.48              |
| 1:B:285:MET:O     | 1:B:287:ALA:N     | 2.46                     | 0.48              |
| 1:B:740:PHE:CD1   | 1:B:778:GLU:HG3   | 2.48                     | 0.48              |
| 1:B:863:ASP:HB2   | 1:B:1009:ILE:HG12 | 1.95                     | 0.48              |
| 1:B:1009:ILE:O    | 1:B:1013:LEU:HG   | 2.14                     | 0.48              |
| 1:B:1094:PHE:CE1  | 1:B:1162:THR:HA   | 2.49                     | 0.48              |
| 1:B:1113:HIS:H    | 1:B:1113:HIS:CD2  | 2.31                     | 0.48              |
| 1:B:1156:LYS:O    | 1:B:1160:PRO:HD2  | 2.13                     | 0.48              |
| 1:B:1500:VAL:HG13 | 1:B:1547:ALA:HA   | 1.95                     | 0.48              |
| 1:A:85:ILE:HG21   | 1:A:104:CYS:SG    | 2.54                     | 0.48              |
| 1:A:1314:LEU:HD12 | 1:A:1330:SER:CB   | 2.44                     | 0.48              |
| 1:A:1314:LEU:HB2  | 1:A:1334:LEU:HD21 | 1.96                     | 0.48              |
| 1:A:1562:ASP:HB3  | 1:A:1566:ARG:NH2  | 2.29                     | 0.48              |
| 1:B:836:ILE:O     | 1:B:840:LEU:HG    | 2.14                     | 0.48              |
| 1:A:200:VAL:CB    | 1:B:715:HIS:ND1   | 2.77                     | 0.48              |
| 1:A:1427:VAL:HG13 | 1:A:1431:PHE:CE2  | 2.47                     | 0.48              |
| 1:B:239:PHE:O     | 1:B:243:ASN:ND2   | 2.47                     | 0.48              |
| 1:B:1394:ARG:HD3  | 1:B:1446:LEU:CD2  | 2.42                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1536:GLU:O    | 1:B:1540:VAL:HG23 | 2.13                     | 0.48              |
| 1:A:45:GLU:C      | 1:A:47:LYS:H      | 2.20                     | 0.48              |
| 1:A:1497:THR:HA   | 1:A:1543:THR:HG21 | 1.95                     | 0.48              |
| 1:B:255:LYS:HG2   | 1:B:258:ARG:NH2   | 2.29                     | 0.48              |
| 1:B:274:GLN:O     | 1:B:277:VAL:HG22  | 2.13                     | 0.48              |
| 1:B:755:SER:O     | 1:B:759:ARG:HG3   | 2.14                     | 0.48              |
| 1:B:909:HIS:HB2   | 1:B:938:PRO:HD3   | 1.95                     | 0.48              |
| 1:B:1244:ILE:CG1  | 1:B:1248:ARG:HB2  | 2.44                     | 0.48              |
| 1:B:1289:LEU:HD12 | 1:B:1326:VAL:HB   | 1.96                     | 0.48              |
| 1:A:1401:PHE:CD1  | 1:A:1406:GLU:HB2  | 2.49                     | 0.47              |
| 1:B:253:SER:O     | 1:B:317:VAL:HG13  | 2.14                     | 0.47              |
| 1:B:549:GLN:O     | 1:B:553:LYS:HG2   | 2.14                     | 0.47              |
| 1:A:327:GLN:NE2   | 1:A:512:MET:SD    | 2.87                     | 0.47              |
| 1:A:735:LEU:HD13  | 1:A:753:SER:HA    | 1.96                     | 0.47              |
| 1:A:1058:LEU:HD23 | 1:A:1061:GLN:NE2  | 2.29                     | 0.47              |
| 1:A:1208:ARG:HH11 | 1:A:1327:ALA:HB3  | 1.79                     | 0.47              |
| 1:B:337:LEU:O     | 1:B:341:VAL:HG13  | 2.14                     | 0.47              |
| 1:B:418:LEU:HD13  | 1:B:537:LEU:HD11  | 1.96                     | 0.47              |
| 1:B:544:LYS:O     | 1:B:548:LEU:HG    | 2.14                     | 0.47              |
| 1:B:1169:TYR:O    | 1:B:1173:THR:HG23 | 2.14                     | 0.47              |
| 1:B:1319:LEU:HD22 | 1:B:1354:LEU:HD21 | 1.97                     | 0.47              |
| 1:B:1445:SER:O    | 1:B:1448:HIS:HB2  | 2.14                     | 0.47              |
| 1:A:327:GLN:O     | 1:A:331:VAL:HG23  | 2.14                     | 0.47              |
| 1:B:733:GLN:HA    | 1:B:738:ALA:HB2   | 1.96                     | 0.47              |
| 1:B:1121:ILE:HG22 | 1:B:1269:HIS:CE1  | 2.49                     | 0.47              |
| 1:B:1414:THR:HA   | 1:B:1423:PHE:CD2  | 2.49                     | 0.47              |
| 1:A:1002:TYR:CD1  | 1:A:1002:TYR:C    | 2.93                     | 0.47              |
| 1:A:1203:ALA:C    | 1:A:1205:GLY:N    | 2.70                     | 0.47              |
| 1:A:130:ILE:CD1   | 1:A:308:MET:HG3   | 2.43                     | 0.47              |
| 1:A:266:PHE:CE1   | 1:A:305:ASP:HB3   | 2.50                     | 0.47              |
| 1:A:506:PRO:HB2   | 1:A:523:ARG:NH2   | 2.29                     | 0.47              |
| 1:A:811:LEU:HD11  | 1:A:861:ILE:HG12  | 1.95                     | 0.47              |
| 1:A:1541:MET:O    | 1:A:1556:LEU:HD22 | 2.14                     | 0.47              |
| 1:A:1571:LEU:C    | 1:A:1573:GLN:H    | 2.23                     | 0.47              |
| 1:A:66:HIS:HE1    | 1:A:71:GLU:HA     | 1.80                     | 0.47              |
| 1:A:922:PHE:HE1   | 1:A:927:VAL:HA    | 1.80                     | 0.47              |
| 1:A:1570:TYR:CD2  | 1:A:1570:TYR:C    | 2.93                     | 0.47              |
| 1:A:1570:TYR:CE1  | 1:A:1592:ILE:HG13 | 2.50                     | 0.47              |
| 1:B:1242:PRO:HG3  | 1:B:1264:ALA:CB   | 2.45                     | 0.47              |
| 1:A:260:CYS:O     | 1:A:263:LEU:HG    | 2.15                     | 0.47              |
| 1:A:485:THR:O     | 1:A:489:GLN:HG2   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:718:VAL:HG12  | 1:A:763:ILE:HD12  | 1.97                     | 0.47              |
| 1:A:852:PRO:O     | 1:A:853:LEU:C     | 2.56                     | 0.47              |
| 1:A:942:GLU:OE2   | 1:A:947:ARG:HD3   | 2.14                     | 0.47              |
| 1:A:1046:ARG:NH1  | 1:A:1075:ALA:O    | 2.43                     | 0.47              |
| 1:A:1414:THR:OG1  | 1:A:1427:VAL:HG21 | 2.15                     | 0.47              |
| 1:A:1552:GLY:O    | 1:A:1553:HIS:HB3  | 2.14                     | 0.47              |
| 1:B:53:VAL:O      | 1:B:57:ILE:HG13   | 2.15                     | 0.47              |
| 1:B:338:TYR:O     | 1:B:341:VAL:HG22  | 2.14                     | 0.47              |
| 1:B:387:MET:O     | 1:B:390:GLN:HG2   | 2.15                     | 0.47              |
| 1:B:470:GLY:O     | 1:B:474:VAL:HG23  | 2.15                     | 0.47              |
| 1:B:519:GLN:O     | 1:B:520:ARG:C     | 2.51                     | 0.47              |
| 1:B:765:GLN:HE22  | 1:B:817:ILE:HG23  | 1.79                     | 0.47              |
| 1:B:1047:ILE:HB   | 1:B:1050:TYR:CD2  | 2.49                     | 0.47              |
| 1:B:1093:TYR:HA   | 1:B:1096:ARG:HG2  | 1.97                     | 0.47              |
| 1:A:506:PRO:HG3   | 1:A:526:ASP:OD2   | 2.14                     | 0.47              |
| 1:A:932:PHE:HD1   | 1:A:1001:TYR:CD1  | 2.33                     | 0.47              |
| 1:A:1299:ILE:CG2  | 1:A:1336:ARG:HE   | 2.28                     | 0.47              |
| 1:B:202:ASN:N     | 1:B:203:PRO:HD3   | 2.30                     | 0.47              |
| 1:B:1159:LEU:CB   | 1:B:1160:PRO:CD   | 2.92                     | 0.47              |
| 1:B:1356:THR:HA   | 1:B:1400:PHE:CE2  | 2.50                     | 0.47              |
| 1:A:191:MET:N     | 1:A:191:MET:SD    | 2.88                     | 0.47              |
| 1:A:985:ARG:NH1   | 1:A:1280:LEU:HD13 | 2.27                     | 0.47              |
| 1:B:283:PHE:HB3   | 1:B:443:ARG:CD    | 2.44                     | 0.47              |
| 1:A:137:CYS:O     | 1:A:240:ILE:HG23  | 2.13                     | 0.47              |
| 1:A:411:ALA:O     | 1:A:412:TRP:C     | 2.56                     | 0.47              |
| 1:A:1015:PRO:HG3  | 1:A:1041:TRP:CE2  | 2.50                     | 0.47              |
| 1:A:1535:PRO:O    | 1:A:1539:VAL:HG23 | 2.15                     | 0.47              |
| 1:B:45:GLU:O      | 1:B:46:MET:C      | 2.58                     | 0.47              |
| 1:B:1177:LEU:HD21 | 1:B:1233:TRP:CD2  | 2.49                     | 0.47              |
| 1:B:1411:MET:O    | 1:B:1414:THR:HB   | 2.15                     | 0.47              |
| 1:B:1551:ALA:O    | 1:B:1554:LEU:HD23 | 2.15                     | 0.47              |
| 1:B:1586:HIS:HD2  | 1:B:1589:HIS:CE1  | 2.32                     | 0.47              |
| 1:B:1592:ILE:HA   | 1:B:1595:CYS:SG   | 2.54                     | 0.47              |
| 1:A:1101:PHE:HE2  | 1:A:1165:LEU:HD22 | 1.80                     | 0.46              |
| 1:A:1548:GLY:CA   | 1:A:1552:GLY:C    | 2.89                     | 0.46              |
| 1:A:1564:LEU:HD22 | 1:A:1603:LEU:CD1  | 2.45                     | 0.46              |
| 1:B:246:SER:HA    | 1:B:249:GLU:OE2   | 2.15                     | 0.46              |
| 1:B:694:ASP:CG    | 1:B:750:HIS:HB3   | 2.40                     | 0.46              |
| 1:B:761:LEU:HB3   | 1:B:779:CYS:SG    | 2.56                     | 0.46              |
| 1:B:1266:GLN:O    | 1:B:1270:LEU:HG   | 2.14                     | 0.46              |
| 1:A:833:PHE:HZ    | 1:A:861:ILE:HG21  | 1.79                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:867:HIS:CG    | 1:A:936:LEU:HD11  | 2.50                     | 0.46              |
| 1:A:1022:GLN:C    | 1:A:1024:SER:H    | 2.22                     | 0.46              |
| 1:A:1180:ASN:O    | 1:A:1181:PHE:C    | 2.58                     | 0.46              |
| 1:B:49:LEU:O      | 1:B:51:GLN:N      | 2.48                     | 0.46              |
| 1:B:341:VAL:HB    | 1:B:417:SER:CB    | 2.45                     | 0.46              |
| 1:B:1394:ARG:NH1  | 1:B:1446:LEU:HD21 | 2.30                     | 0.46              |
| 1:B:1431:PHE:O    | 1:B:1435:PHE:HD2  | 1.98                     | 0.46              |
| 1:A:270:ILE:O     | 1:A:274:GLN:HG3   | 2.14                     | 0.46              |
| 1:A:710:LEU:HG    | 1:A:714:ASN:HD21  | 1.80                     | 0.46              |
| 1:A:808:VAL:HG22  | 1:A:933:TYR:CD2   | 2.51                     | 0.46              |
| 1:A:945:LEU:HD22  | 1:A:1053:TRP:CG   | 2.50                     | 0.46              |
| 1:A:1101:PHE:O    | 1:A:1104:ILE:HB   | 2.14                     | 0.46              |
| 1:B:1090:VAL:CG1  | 1:B:1127:ALA:HB1  | 2.33                     | 0.46              |
| 1:B:1288:LEU:HD23 | 1:B:1326:VAL:HG11 | 1.97                     | 0.46              |
| 1:B:1572:SER:O    | 1:B:1577:VAL:HG23 | 2.15                     | 0.46              |
| 1:A:325:ARG:HH12  | 1:B:496:LEU:CD2   | 2.28                     | 0.46              |
| 1:A:847:GLN:HG3   | 1:A:976:ALA:HB2   | 1.98                     | 0.46              |
| 1:A:1281:ALA:HB2  | 1:A:1284:LEU:HD12 | 1.96                     | 0.46              |
| 1:A:1381:LEU:HB3  | 1:A:1426:ARG:NH2  | 2.29                     | 0.46              |
| 1:B:658:ILE:O     | 1:B:662:MET:HB2   | 2.16                     | 0.46              |
| 1:B:858:LEU:HD23  | 1:B:858:LEU:HA    | 1.80                     | 0.46              |
| 1:B:1162:THR:O    | 1:B:1166:ILE:HG13 | 2.16                     | 0.46              |
| 1:B:1301:TRP:O    | 1:B:1302:SER:HB2  | 2.15                     | 0.46              |
| 1:B:1600:MET:HA   | 1:B:1603:LEU:CG   | 2.41                     | 0.46              |
| 1:A:283:PHE:HA    | 1:A:442:LEU:O     | 2.16                     | 0.46              |
| 1:A:471:VAL:HG21  | 1:A:641:ARG:HG2   | 1.98                     | 0.46              |
| 1:B:414:LEU:HB3   | 1:B:480:ALA:HB2   | 1.98                     | 0.46              |
| 1:B:484:LEU:HD22  | 1:B:488:PHE:HE1   | 1.81                     | 0.46              |
| 1:B:909:HIS:CB    | 1:B:938:PRO:HD3   | 2.46                     | 0.46              |
| 1:B:1121:ILE:HG22 | 1:B:1269:HIS:HE1  | 1.80                     | 0.46              |
| 1:B:1305:MET:HE1  | 1:B:1337:ILE:HG23 | 1.97                     | 0.46              |
| 1:B:1456:LEU:O    | 1:B:1458:CYS:N    | 2.48                     | 0.46              |
| 1:A:110:PHE:CZ    | 1:A:114:ARG:HD2   | 2.51                     | 0.46              |
| 1:A:135:GLY:CA    | 1:A:140:CYS:O     | 2.63                     | 0.46              |
| 1:A:271:ASN:HD22  | 1:A:271:ASN:N     | 2.13                     | 0.46              |
| 1:A:280:ASN:HD22  | 1:A:523:ARG:HH11  | 1.64                     | 0.46              |
| 1:A:1036:LEU:HD21 | 1:A:1123:THR:HA   | 1.97                     | 0.46              |
| 1:A:1412:MET:HB3  | 1:A:1463:ARG:CZ   | 2.46                     | 0.46              |
| 1:B:668:ASN:HA    | 1:B:671:ARG:HB2   | 1.98                     | 0.46              |
| 1:B:1019:TYR:OH   | 1:B:1038:THR:HA   | 2.15                     | 0.46              |
| 1:B:1118:LEU:HD23 | 1:B:1122:TYR:CD2  | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:477:ALA:O     | 1:A:481:ILE:HG12  | 2.15                     | 0.46              |
| 1:A:1039:LEU:CD2  | 1:A:1089:ILE:HD13 | 2.44                     | 0.46              |
| 1:A:1431:PHE:O    | 1:A:1435:PHE:HD2  | 1.98                     | 0.46              |
| 1:B:58:GLU:C      | 1:B:60:GLU:N      | 2.74                     | 0.46              |
| 1:B:272:ARG:HB3   | 1:B:338:TYR:CE1   | 2.51                     | 0.46              |
| 1:B:521:ILE:HA    | 1:B:521:ILE:HD13  | 1.55                     | 0.46              |
| 1:B:827:ARG:NE    | 1:B:955:VAL:HG22  | 2.31                     | 0.46              |
| 1:B:1047:ILE:C    | 1:B:1051:VAL:HG23 | 2.41                     | 0.46              |
| 1:B:1247:TRP:CD1  | 1:B:1248:ARG:N    | 2.82                     | 0.46              |
| 1:B:1318:LEU:HD21 | 1:B:1331:SER:CB   | 2.45                     | 0.46              |
| 1:A:530:LEU:O     | 1:A:534:LEU:HG    | 2.15                     | 0.46              |
| 1:A:847:GLN:HG3   | 1:A:976:ALA:CB    | 2.46                     | 0.46              |
| 1:A:1428:LEU:CD1  | 1:A:1488:ASN:HA   | 2.46                     | 0.46              |
| 1:B:255:LYS:HG2   | 1:B:258:ARG:HH21  | 1.80                     | 0.46              |
| 1:B:1105:ASP:HB3  | 1:B:1108:THR:HB   | 1.98                     | 0.46              |
| 1:A:32:ALA:O      | 1:A:33:VAL:C      | 2.54                     | 0.46              |
| 1:A:811:LEU:HD23  | 1:A:933:TYR:HE1   | 1.80                     | 0.46              |
| 1:B:257:LEU:HD23  | 1:B:257:LEU:HA    | 1.59                     | 0.46              |
| 1:B:1272:THR:OG1  | 1:B:1283:SER:OG   | 2.32                     | 0.46              |
| 1:A:285:MET:N     | 1:A:286:PRO:CD    | 2.79                     | 0.46              |
| 1:A:844:MET:HB3   | 1:A:848:MET:HE3   | 1.98                     | 0.46              |
| 1:A:1122:TYR:CD1  | 1:A:1123:THR:N    | 2.84                     | 0.46              |
| 1:A:1201:VAL:HG11 | 1:A:1222:LEU:CD2  | 2.43                     | 0.46              |
| 1:A:1220:GLN:C    | 1:A:1222:LEU:H    | 2.24                     | 0.46              |
| 1:A:1456:LEU:HD22 | 1:A:1510:VAL:HG13 | 1.98                     | 0.46              |
| 1:A:1525:MET:SD   | 1:A:1534:PHE:HA   | 2.56                     | 0.46              |
| 1:B:327:GLN:O     | 1:B:331:VAL:HG23  | 2.16                     | 0.46              |
| 1:B:348:ALA:CB    | 1:B:421:ILE:HG23  | 2.46                     | 0.46              |
| 1:B:1553:HIS:CE1  | 1:B:1606:VAL:HG22 | 2.50                     | 0.46              |
| 1:A:32:ALA:HA     | 1:A:35:PRO:HD2    | 1.98                     | 0.45              |
| 1:A:325:ARG:O     | 1:A:329:VAL:HG23  | 2.16                     | 0.45              |
| 1:A:659:THR:HA    | 1:A:663:LEU:CD1   | 2.40                     | 0.45              |
| 1:A:1213:THR:HA   | 1:A:1216:PRO:HG2  | 1.97                     | 0.45              |
| 1:A:1299:ILE:O    | 1:A:1300:VAL:C    | 2.59                     | 0.45              |
| 1:B:747:LEU:HB3   | 1:B:806:LEU:N     | 2.31                     | 0.45              |
| 1:B:1158:LEU:O    | 1:B:1159:LEU:C    | 2.57                     | 0.45              |
| 1:B:1377:LEU:HD12 | 1:B:1377:LEU:H    | 1.81                     | 0.45              |
| 1:A:310:LEU:HD13  | 1:A:384:ILE:CG1   | 2.46                     | 0.45              |
| 1:A:715:HIS:CG    | 1:B:200:VAL:HG21  | 2.50                     | 0.45              |
| 1:A:787:LEU:HA    | 1:A:787:LEU:HD23  | 1.53                     | 0.45              |
| 1:A:911:PHE:O     | 1:A:915:GLU:HB2   | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1411:MET:HE3  | 1:A:1411:MET:HB2  | 1.78                     | 0.45              |
| 1:A:1564:LEU:HA   | 1:A:1599:ILE:HG21 | 1.98                     | 0.45              |
| 1:B:1299:ILE:HG22 | 1:B:1300:VAL:HG13 | 1.99                     | 0.45              |
| 1:B:1407:LEU:H    | 1:B:1407:LEU:CD1  | 2.25                     | 0.45              |
| 1:B:1586:HIS:HD2  | 1:B:1589:HIS:HE1  | 1.64                     | 0.45              |
| 1:B:1590:VAL:HA   | 1:B:1593:LEU:HD23 | 1.97                     | 0.45              |
| 1:A:68:LYS:C      | 1:A:70:TYR:N      | 2.74                     | 0.45              |
| 1:A:948:LEU:HD21  | 1:A:956:LEU:HD12  | 1.98                     | 0.45              |
| 1:A:1039:LEU:HD22 | 1:A:1130:LYS:HE2  | 1.98                     | 0.45              |
| 1:A:1176:TYR:CD1  | 1:A:1281:ALA:CB   | 2.99                     | 0.45              |
| 1:A:1311:ILE:HG23 | 1:A:1338:LEU:HD11 | 1.99                     | 0.45              |
| 1:B:408:LEU:HD13  | 1:B:520:ARG:HB3   | 1.99                     | 0.45              |
| 1:B:535:LEU:HD23  | 1:B:535:LEU:HA    | 1.81                     | 0.45              |
| 1:B:1115:ILE:HD13 | 1:B:1176:TYR:HB2  | 1.98                     | 0.45              |
| 1:A:104:CYS:SG    | 1:A:136:LEU:HD22  | 2.56                     | 0.45              |
| 1:A:136:LEU:O     | 1:A:243:ASN:ND2   | 2.49                     | 0.45              |
| 1:A:309:ALA:O     | 1:A:313:LEU:HG    | 2.16                     | 0.45              |
| 1:A:1039:LEU:HD21 | 1:A:1089:ILE:HD13 | 1.98                     | 0.45              |
| 1:A:1087:VAL:O    | 1:A:1091:GLU:HG3  | 2.17                     | 0.45              |
| 1:A:1346:PHE:O    | 1:A:1350:VAL:HG23 | 2.17                     | 0.45              |
| 1:B:247:LEU:HD12  | 1:B:252:GLY:HA3   | 1.97                     | 0.45              |
| 1:B:1213:THR:O    | 1:B:1216:PRO:HD2  | 2.16                     | 0.45              |
| 1:B:1456:LEU:O    | 1:B:1457:ALA:C    | 2.59                     | 0.45              |
| 1:B:1489:ARG:O    | 1:B:1493:GLN:HG3  | 2.16                     | 0.45              |
| 1:B:1570:TYR:CE2  | 1:B:1592:ILE:HG13 | 2.52                     | 0.45              |
| 1:A:93:PRO:CB     | 1:A:96:GLN:HB2    | 2.45                     | 0.45              |
| 1:A:471:VAL:CG2   | 1:A:641:ARG:H     | 2.26                     | 0.45              |
| 1:A:543:ARG:O     | 1:A:547:VAL:HG23  | 2.16                     | 0.45              |
| 1:A:863:ASP:OD2   | 1:A:1008:ARG:NH2  | 2.45                     | 0.45              |
| 1:A:984:ARG:HH11  | 1:A:984:ARG:CB    | 2.24                     | 0.45              |
| 1:A:1417:GLU:CA   | 1:A:1470:ARG:HD2  | 2.35                     | 0.45              |
| 1:B:197:LEU:O     | 1:B:198:THR:C     | 2.59                     | 0.45              |
| 1:B:240:ILE:O     | 1:B:244:VAL:HG23  | 2.16                     | 0.45              |
| 1:B:1308:PRO:O    | 1:B:1309:GLN:C    | 2.57                     | 0.45              |
| 1:A:49:LEU:C      | 1:A:51:GLN:N      | 2.74                     | 0.45              |
| 1:A:144:ASP:O     | 1:A:148:ILE:HG13  | 2.17                     | 0.45              |
| 1:A:718:VAL:HG13  | 1:A:760:LEU:HD23  | 1.98                     | 0.45              |
| 1:B:114:ARG:HD3   | 1:B:114:ARG:HA    | 1.68                     | 0.45              |
| 1:A:68:LYS:HD2    | 1:A:69:GLN:HG3    | 1.98                     | 0.45              |
| 1:A:97:LEU:HD23   | 1:A:98:GLN:N      | 2.32                     | 0.45              |
| 1:A:919:SER:O     | 1:A:920:LYS:C     | 2.57                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1023:LEU:CD2  | 1:A:1038:THR:HG23 | 2.46                     | 0.45              |
| 1:A:1048:SER:O    | 1:A:1049:SER:C    | 2.55                     | 0.45              |
| 1:A:1090:VAL:HG11 | 1:A:1131:VAL:HG22 | 1.99                     | 0.45              |
| 1:B:678:LEU:HB3   | 1:B:727:LEU:CD2   | 2.46                     | 0.45              |
| 1:B:722:LEU:H     | 1:B:722:LEU:HD12  | 1.82                     | 0.45              |
| 1:B:1063:MET:HG2  | 1:B:1068:ALA:HB2  | 1.99                     | 0.45              |
| 1:B:1231:GLU:OE2  | 1:B:1232:SER:N    | 2.49                     | 0.45              |
| 1:A:85:ILE:CG2    | 1:A:104:CYS:SG    | 3.05                     | 0.45              |
| 1:A:256:LEU:HB3   | 1:A:312:THR:HG22  | 1.97                     | 0.45              |
| 1:A:485:THR:HG22  | 1:A:657:PHE:HD1   | 1.81                     | 0.45              |
| 1:A:790:MET:O     | 1:A:791:LYS:C     | 2.59                     | 0.45              |
| 1:A:862:PHE:CE1   | 1:A:866:LEU:HD21  | 2.51                     | 0.45              |
| 1:A:868:GLN:C     | 1:A:949:ASP:OD2   | 2.59                     | 0.45              |
| 1:A:1047:ILE:CD1  | 1:A:1256:ILE:HD11 | 2.44                     | 0.45              |
| 1:A:1156:LYS:O    | 1:A:1160:PRO:HD2  | 2.16                     | 0.45              |
| 1:A:1511:CYS:O    | 1:A:1544:LEU:HD22 | 2.17                     | 0.45              |
| 1:B:286:PRO:HD2   | 1:B:342:SER:HB3   | 1.97                     | 0.45              |
| 1:B:808:VAL:HG22  | 1:B:933:TYR:CD2   | 2.51                     | 0.45              |
| 1:B:830:LEU:HA    | 1:B:830:LEU:HD23  | 1.77                     | 0.45              |
| 1:B:1315:LEU:HD21 | 1:B:1353:LYS:HB2  | 1.98                     | 0.45              |
| 1:A:38:SER:O      | 1:A:41:TYR:HB3    | 2.17                     | 0.45              |
| 1:A:341:VAL:HB    | 1:A:417:SER:CB    | 2.47                     | 0.45              |
| 1:A:1046:ARG:NH2  | 1:A:1077:THR:OG1  | 2.50                     | 0.45              |
| 1:A:1268:ALA:O    | 1:A:1272:THR:HG23 | 2.17                     | 0.45              |
| 1:A:1509:GLY:O    | 1:A:1513:VAL:HG23 | 2.17                     | 0.45              |
| 1:B:56:VAL:O      | 1:B:57:ILE:C      | 2.60                     | 0.45              |
| 1:B:414:LEU:O     | 1:B:418:LEU:HG    | 2.17                     | 0.45              |
| 1:B:1345:GLU:CD   | 1:B:1345:GLU:H    | 2.24                     | 0.45              |
| 1:B:1355:ILE:HD13 | 1:B:1397:MET:CG   | 2.47                     | 0.45              |
| 1:B:1412:MET:HB3  | 1:B:1463:ARG:CZ   | 2.46                     | 0.45              |
| 1:A:1019:TYR:CE2  | 1:A:1023:LEU:HD11 | 2.52                     | 0.45              |
| 1:A:1025:MET:O    | 1:A:1026:ASN:HB2  | 2.17                     | 0.45              |
| 1:A:1563:TRP:N    | 1:A:1566:ARG:HH21 | 2.15                     | 0.45              |
| 1:B:1053:TRP:CD1  | 1:B:1053:TRP:C    | 2.95                     | 0.45              |
| 1:B:1110:LEU:H    | 1:B:1175:ALA:HB1  | 1.81                     | 0.45              |
| 1:B:1151:SER:O    | 1:B:1155:THR:HG23 | 2.16                     | 0.45              |
| 1:B:1162:THR:HG22 | 1:B:1166:ILE:HD11 | 1.98                     | 0.45              |
| 1:B:1468:LEU:O    | 1:B:1472:THR:HG23 | 2.17                     | 0.45              |
| 1:A:349:ILE:CD1   | 1:A:429:LEU:HD11  | 2.31                     | 0.44              |
| 1:A:680:GLU:HB3   | 1:A:730:THR:HG21  | 1.99                     | 0.44              |
| 1:A:1030:MET:HG2  | 1:A:1035:ILE:HG13 | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:246:SER:O     | 1:B:250:LEU:HG    | 2.17                     | 0.44              |
| 1:B:253:SER:HB2   | 1:B:317:VAL:HA    | 2.00                     | 0.44              |
| 1:B:253:SER:HB2   | 1:B:317:VAL:O     | 2.17                     | 0.44              |
| 1:B:348:ALA:HB2   | 1:B:421:ILE:HG23  | 1.99                     | 0.44              |
| 1:B:986:LYS:HG3   | 1:B:1113:HIS:CE1  | 2.51                     | 0.44              |
| 1:B:1050:TYR:O    | 1:B:1054:ILE:HG13 | 2.17                     | 0.44              |
| 1:B:1453:LEU:O    | 1:B:1456:LEU:CB   | 2.60                     | 0.44              |
| 1:A:345:THR:HG23  | 1:A:424:LEU:HD11  | 1.99                     | 0.44              |
| 1:A:773:ASP:HB3   | 1:A:774:PRO:HD2   | 1.99                     | 0.44              |
| 1:A:1208:ARG:HD3  | 1:A:1328:GLU:HA   | 1.99                     | 0.44              |
| 1:A:1284:LEU:HD23 | 1:A:1284:LEU:HA   | 1.89                     | 0.44              |
| 1:A:1398:GLU:CG   | 1:A:1445:SER:HA   | 2.43                     | 0.44              |
| 1:B:943:ASP:N     | 1:B:943:ASP:OD2   | 2.50                     | 0.44              |
| 1:B:1450:CYS:C    | 1:B:1452:SER:N    | 2.70                     | 0.44              |
| 1:B:1498:TYR:O    | 1:B:1504:SER:HB2  | 2.17                     | 0.44              |
| 1:B:1570:TYR:CZ   | 1:B:1588:LYS:HD2  | 2.52                     | 0.44              |
| 1:A:29:TRP:CG     | 1:A:160:LEU:HD21  | 2.53                     | 0.44              |
| 1:A:297:ASN:O     | 1:A:300:HIS:NE2   | 2.50                     | 0.44              |
| 1:A:859:LEU:O     | 1:A:860:LEU:C     | 2.53                     | 0.44              |
| 1:A:1468:LEU:HA   | 1:A:1471:MET:HE2  | 1.99                     | 0.44              |
| 1:B:379:GLN:HE21  | 1:B:379:GLN:HB3   | 1.52                     | 0.44              |
| 1:B:414:LEU:CD1   | 1:B:479:HIS:HB3   | 2.48                     | 0.44              |
| 1:B:443:ARG:HB2   | 1:B:446:ASP:CB    | 2.47                     | 0.44              |
| 1:A:78:VAL:HG21   | 1:A:110:PHE:CD2   | 2.52                     | 0.44              |
| 1:A:202:ASN:CG    | 1:A:204:ARG:HG3   | 2.43                     | 0.44              |
| 1:A:288:THR:HG22  | 1:A:290:ALA:H     | 1.81                     | 0.44              |
| 1:A:416:ASN:HD22  | 1:A:416:ASN:N     | 2.15                     | 0.44              |
| 1:A:765:GLN:NE2   | 1:A:817:ILE:HG23  | 2.33                     | 0.44              |
| 1:A:1030:MET:HA   | 1:A:1034:ASP:OD2  | 2.18                     | 0.44              |
| 1:A:1077:THR:O    | 1:A:1081:SER:HB2  | 2.16                     | 0.44              |
| 1:A:1118:LEU:HD23 | 1:A:1122:TYR:CD2  | 2.53                     | 0.44              |
| 1:B:154:MET:O     | 1:B:157:SER:OG    | 2.34                     | 0.44              |
| 1:B:493:VAL:O     | 1:B:496:LEU:N     | 2.50                     | 0.44              |
| 1:B:531:MET:CG    | 1:B:677:SER:HB2   | 2.47                     | 0.44              |
| 1:B:655:LEU:HD23  | 1:B:655:LEU:HA    | 1.75                     | 0.44              |
| 1:B:674:LEU:O     | 1:B:678:LEU:HG    | 2.18                     | 0.44              |
| 1:B:1055:LYS:HA   | 1:B:1058:LEU:HG   | 1.98                     | 0.44              |
| 1:B:1242:PRO:HG3  | 1:B:1264:ALA:HB3  | 2.00                     | 0.44              |
| 1:B:1306:ASN:O    | 1:B:1307:PRO:C    | 2.60                     | 0.44              |
| 1:A:196:GLN:O     | 1:B:759:ARG:NH2   | 2.50                     | 0.44              |
| 1:A:279:ALA:O     | 1:A:280:ASN:C     | 2.59                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:284:ILE:HG22  | 1:A:286:PRO:CD    | 2.47                     | 0.44              |
| 1:A:1039:LEU:HD22 | 1:A:1130:LYS:CD   | 2.48                     | 0.44              |
| 1:A:1098:ILE:HG12 | 1:A:1165:LEU:HD21 | 2.00                     | 0.44              |
| 1:A:1194:LYS:NZ   | 1:A:1198:PHE:HZ   | 2.15                     | 0.44              |
| 1:A:1212:ASN:O    | 1:A:1212:ASN:ND2  | 2.48                     | 0.44              |
| 1:A:1296:GLY:O    | 1:A:1300:VAL:HG23 | 2.18                     | 0.44              |
| 1:A:1564:LEU:HA   | 1:A:1567:CYS:SG   | 2.56                     | 0.44              |
| 1:B:1191:SER:N    | 1:B:1194:LYS:HD3  | 2.32                     | 0.44              |
| 1:B:1307:PRO:O    | 1:B:1308:PRO:C    | 2.61                     | 0.44              |
| 1:B:1538:MET:HE2  | 1:B:1602:TYR:CG   | 2.53                     | 0.44              |
| 1:A:252:GLY:O     | 1:A:256:LEU:HG    | 2.18                     | 0.44              |
| 1:A:349:ILE:CD1   | 1:A:424:LEU:HD13  | 2.47                     | 0.44              |
| 1:A:1489:ARG:O    | 1:A:1493:GLN:HG3  | 2.18                     | 0.44              |
| 1:B:115:LEU:HD13  | 1:B:130:ILE:HG13  | 2.00                     | 0.44              |
| 1:B:855:LEU:HD23  | 1:B:1002:TYR:HE2  | 1.82                     | 0.44              |
| 1:B:862:PHE:CE1   | 1:B:866:LEU:HD11  | 2.53                     | 0.44              |
| 1:B:908:TYR:O     | 1:B:908:TYR:CG    | 2.70                     | 0.44              |
| 1:B:1204:ILE:CG2  | 1:B:1357:GLY:HA3  | 2.43                     | 0.44              |
| 1:B:1445:SER:HA   | 1:B:1448:HIS:CB   | 2.47                     | 0.44              |
| 1:A:284:ILE:O     | 1:A:442:LEU:N     | 2.50                     | 0.44              |
| 1:A:511:ILE:HG13  | 1:A:512:MET:N     | 2.31                     | 0.44              |
| 1:A:539:SER:O     | 1:A:543:ARG:HD3   | 2.18                     | 0.44              |
| 1:A:715:HIS:CE1   | 1:B:200:VAL:CB    | 3.00                     | 0.44              |
| 1:A:817:ILE:HG22  | 1:A:821:PHE:CE2   | 2.53                     | 0.44              |
| 1:A:860:LEU:HD21  | 1:A:934:CYS:HA    | 2.00                     | 0.44              |
| 1:A:945:LEU:HB3   | 1:A:1053:TRP:CG   | 2.52                     | 0.44              |
| 1:A:1025:MET:HG2  | 1:A:1027:SER:H    | 1.82                     | 0.44              |
| 1:A:1515:LEU:HB2  | 1:A:1544:LEU:CB   | 2.47                     | 0.44              |
| 1:A:1545:ALA:C    | 1:A:1548:GLY:H    | 2.24                     | 0.44              |
| 1:B:115:LEU:HD12  | 1:B:133:ILE:HD12  | 1.99                     | 0.44              |
| 1:A:197:LEU:HD23  | 1:B:885:LEU:HD13  | 1.99                     | 0.44              |
| 1:A:974:LEU:HD23  | 1:A:1006:LEU:HD23 | 1.99                     | 0.44              |
| 1:A:1118:LEU:HA   | 1:A:1121:ILE:HD12 | 1.99                     | 0.44              |
| 1:A:1200:ALA:O    | 1:A:1204:ILE:HD13 | 2.18                     | 0.44              |
| 1:B:98:GLN:HE22   | 1:B:201:PHE:N     | 2.16                     | 0.44              |
| 1:B:155:MET:C     | 1:B:157:SER:N     | 2.74                     | 0.44              |
| 1:B:268:ARG:H     | 1:B:268:ARG:HG3   | 1.42                     | 0.44              |
| 1:B:811:LEU:HD23  | 1:B:933:TYR:HE1   | 1.83                     | 0.44              |
| 1:B:1109:ILE:HG23 | 1:B:1178:LEU:HD12 | 2.00                     | 0.44              |
| 1:B:1273:LEU:O    | 1:B:1274:CYS:C    | 2.61                     | 0.44              |
| 1:B:1557:HIS:C    | 1:B:1557:HIS:ND1  | 2.76                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1048:SER:O    | 1:A:1051:VAL:HB   | 2.18                     | 0.44              |
| 1:A:1313:THR:OG1  | 1:A:1314:LEU:HD22 | 2.18                     | 0.44              |
| 1:A:1429:LYS:O    | 1:A:1432:THR:N    | 2.51                     | 0.44              |
| 1:B:97:LEU:HD13   | 1:B:201:PHE:CZ    | 2.52                     | 0.44              |
| 1:B:204:ARG:O     | 1:B:205:THR:HB    | 2.17                     | 0.44              |
| 1:B:796:GLN:HB2   | 1:B:798:VAL:HG23  | 2.00                     | 0.44              |
| 1:B:1094:PHE:CZ   | 1:B:1128:ILE:HD11 | 2.52                     | 0.44              |
| 1:A:37:LEU:HA     | 1:A:40:SER:CB     | 2.47                     | 0.43              |
| 1:A:760:LEU:HD23  | 1:A:760:LEU:HA    | 1.90                     | 0.43              |
| 1:A:932:PHE:HA    | 1:A:1001:TYR:HE1  | 1.82                     | 0.43              |
| 1:A:1213:THR:O    | 1:A:1214:LEU:C    | 2.59                     | 0.43              |
| 1:A:1214:LEU:C    | 1:A:1214:LEU:HD13 | 2.43                     | 0.43              |
| 1:A:1281:ALA:HB1  | 1:A:1284:LEU:HB2  | 1.99                     | 0.43              |
| 1:A:1314:LEU:HD12 | 1:A:1330:SER:HB3  | 2.00                     | 0.43              |
| 1:B:1083:VAL:HG11 | 1:B:1135:LEU:HD23 | 1.99                     | 0.43              |
| 1:B:1205:GLY:HA2  | 1:B:1215:GLY:HA3  | 1.94                     | 0.43              |
| 1:B:1208:ARG:HD2  | 1:B:1327:ALA:HB3  | 2.00                     | 0.43              |
| 1:B:1576:VAL:HA   | 1:B:1579:LYS:HD2  | 1.99                     | 0.43              |
| 1:A:1098:ILE:HG12 | 1:A:1165:LEU:CD2  | 2.48                     | 0.43              |
| 1:B:66:HIS:NE2    | 1:B:71:GLU:HG2    | 2.33                     | 0.43              |
| 1:B:124:VAL:HG21  | 1:B:129:LEU:HD21  | 2.00                     | 0.43              |
| 1:B:527:SER:O     | 1:B:528:VAL:CG1   | 2.66                     | 0.43              |
| 1:B:648:LEU:HD23  | 1:B:648:LEU:HA    | 1.69                     | 0.43              |
| 1:B:957:PHE:HE2   | 1:B:1057:HIS:CE1  | 2.36                     | 0.43              |
| 1:B:1429:LYS:O    | 1:B:1432:THR:N    | 2.51                     | 0.43              |
| 1:A:124:VAL:HG11  | 1:A:129:LEU:CD2   | 2.48                     | 0.43              |
| 1:A:861:ILE:O     | 1:A:865:LEU:HG    | 2.17                     | 0.43              |
| 1:A:1121:ILE:HG22 | 1:A:1287:THR:OG1  | 2.18                     | 0.43              |
| 1:A:1222:LEU:O    | 1:A:1223:PRO:O    | 2.36                     | 0.43              |
| 1:A:1548:GLY:HA2  | 1:A:1551:ALA:O    | 2.18                     | 0.43              |
| 1:B:1407:LEU:HB3  | 1:B:1431:PHE:CZ   | 2.51                     | 0.43              |
| 1:B:1480:ASP:HB3  | 1:B:1483:ASP:HB2  | 2.00                     | 0.43              |
| 1:B:1534:PHE:N    | 1:B:1535:PRO:HD2  | 2.33                     | 0.43              |
| 1:A:80:LEU:HD21   | 1:A:151:PHE:HB2   | 1.99                     | 0.43              |
| 1:A:296:ARG:HA    | 1:A:299:PHE:CE2   | 2.54                     | 0.43              |
| 1:A:782:VAL:O     | 1:A:783:TRP:C     | 2.56                     | 0.43              |
| 1:A:1032:GLU:O    | 1:A:1036:LEU:HG   | 2.19                     | 0.43              |
| 1:A:1434:LEU:HD11 | 1:A:1449:LEU:HD12 | 1.99                     | 0.43              |
| 1:B:29:TRP:CE3    | 1:B:73:PHE:HZ     | 2.37                     | 0.43              |
| 1:B:30:GLU:H      | 1:B:30:GLU:HG3    | 1.66                     | 0.43              |
| 1:B:864:TYR:CD1   | 1:B:936:LEU:HD13  | 2.52                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1191:SER:O    | 1:B:1192:LYS:C    | 2.61                     | 0.43              |
| 1:B:1345:GLU:O    | 1:B:1349:ARG:HG2  | 2.18                     | 0.43              |
| 1:B:1417:GLU:HA   | 1:B:1470:ARG:HD2  | 2.00                     | 0.43              |
| 1:B:1608:ASN:O    | 1:B:1612:GLN:HG2  | 2.17                     | 0.43              |
| 1:A:272:ARG:HD2   | 1:A:338:TYR:HE1   | 1.83                     | 0.43              |
| 1:A:488:PHE:HE2   | 1:A:670:ILE:HD12  | 1.82                     | 0.43              |
| 1:A:547:VAL:HA    | 1:A:550:ARG:HH11  | 1.83                     | 0.43              |
| 1:A:874:VAL:HG22  | 1:B:186:GLN:HA    | 2.00                     | 0.43              |
| 1:A:1200:ALA:HB2  | 1:A:1365:HIS:NE2  | 2.33                     | 0.43              |
| 1:A:1317:LEU:O    | 1:A:1323:THR:HG23 | 2.19                     | 0.43              |
| 1:A:1318:LEU:HD22 | 1:A:1319:LEU:HD23 | 1.99                     | 0.43              |
| 1:B:104:CYS:SG    | 1:B:239:PHE:CE1   | 3.10                     | 0.43              |
| 1:B:112:LEU:HD11  | 1:B:247:LEU:HD12  | 1.99                     | 0.43              |
| 1:B:474:VAL:HG11  | 1:B:646:LEU:HG    | 1.99                     | 0.43              |
| 1:B:1405:GLY:O    | 1:B:1409:GLN:HG2  | 2.18                     | 0.43              |
| 1:A:405:ASN:ND2   | 1:A:513:ALA:O     | 2.51                     | 0.43              |
| 1:A:699:LYS:O     | 1:A:703:ASP:HB2   | 2.19                     | 0.43              |
| 1:B:190:GLN:OE1   | 1:B:194:LEU:HD23  | 2.17                     | 0.43              |
| 1:B:793:ASN:O     | 1:B:797:GLY:N     | 2.52                     | 0.43              |
| 1:B:1285:LYS:HE3  | 1:B:1285:LYS:HB2  | 1.88                     | 0.43              |
| 1:A:1094:PHE:CZ   | 1:A:1128:ILE:CD1  | 3.01                     | 0.43              |
| 1:A:1546:SER:C    | 1:A:1548:GLY:H    | 2.27                     | 0.43              |
| 1:B:247:LEU:CD1   | 1:B:252:GLY:HA3   | 2.48                     | 0.43              |
| 1:B:801:SER:HA    | 1:B:930:PRO:HD3   | 1.99                     | 0.43              |
| 1:B:1141:LYS:O    | 1:B:1142:MET:CB   | 2.67                     | 0.43              |
| 1:B:1238:THR:HG23 | 1:B:1285:LYS:HB3  | 1.98                     | 0.43              |
| 1:B:1456:LEU:C    | 1:B:1458:CYS:H    | 2.27                     | 0.43              |
| 1:A:98:GLN:HG3    | 1:A:201:PHE:CZ    | 2.54                     | 0.43              |
| 1:A:269:TYR:HB3   | 1:A:338:TYR:HD1   | 1.83                     | 0.43              |
| 1:A:312:THR:O     | 1:A:315:LEU:HG    | 2.19                     | 0.43              |
| 1:A:387:MET:O     | 1:A:388:ILE:C     | 2.60                     | 0.43              |
| 1:A:404:GLN:OE1   | 1:A:404:GLN:HA    | 2.17                     | 0.43              |
| 1:A:420:LEU:O     | 1:A:424:LEU:HG    | 2.19                     | 0.43              |
| 1:A:1033:CYS:HA   | 1:A:1036:LEU:HD12 | 2.01                     | 0.43              |
| 1:A:1130:LYS:O    | 1:A:1131:VAL:C    | 2.59                     | 0.43              |
| 1:A:1576:VAL:HG13 | 1:A:1589:HIS:HA   | 2.01                     | 0.43              |
| 1:B:493:VAL:O     | 1:B:494:GLU:C     | 2.62                     | 0.43              |
| 1:B:919:SER:HA    | 1:B:922:PHE:CD2   | 2.54                     | 0.43              |
| 1:B:1133:VAL:HG22 | 1:B:1246:SER:CA   | 2.49                     | 0.43              |
| 1:B:1232:SER:C    | 1:B:1234:ASN:H    | 2.25                     | 0.43              |
| 1:B:1388:LEU:C    | 1:B:1390:SER:H    | 2.27                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:93:PRO:CG     | 1:A:96:GLN:HB2    | 2.49                     | 0.43              |
| 1:A:269:TYR:CD1   | 1:A:339:ALA:HA    | 2.54                     | 0.43              |
| 1:A:1163:LEU:HA   | 1:A:1166:ILE:HD12 | 2.01                     | 0.43              |
| 1:A:1214:LEU:HD21 | 1:A:1380:CYS:CB   | 2.46                     | 0.43              |
| 1:A:1332:ASN:HA   | 1:A:1335:GLU:CD   | 2.44                     | 0.43              |
| 1:A:1345:GLU:O    | 1:A:1349:ARG:HG2  | 2.19                     | 0.43              |
| 1:A:1548:GLY:HA2  | 1:A:1552:GLY:CA   | 2.49                     | 0.43              |
| 1:A:1562:ASP:HB3  | 1:A:1566:ARG:HH21 | 1.84                     | 0.43              |
| 1:B:1057:HIS:CE1  | 1:B:1060:LYS:HD2  | 2.54                     | 0.43              |
| 1:B:1063:MET:SD   | 1:B:1068:ALA:CB   | 3.07                     | 0.43              |
| 1:B:1216:PRO:O    | 1:B:1217:THR:C    | 2.61                     | 0.43              |
| 1:B:1311:ILE:HA   | 1:B:1334:LEU:HD21 | 2.00                     | 0.43              |
| 1:A:484:LEU:O     | 1:A:488:PHE:HD1   | 2.02                     | 0.43              |
| 1:A:732:LEU:HD21  | 1:A:760:LEU:HD12  | 2.00                     | 0.43              |
| 1:A:838:GLN:NE2   | 1:A:965:GLU:OE2   | 2.51                     | 0.43              |
| 1:A:947:ARG:O     | 1:A:948:LEU:C     | 2.61                     | 0.43              |
| 1:A:1173:THR:HG22 | 1:A:1233:TRP:HZ2  | 1.84                     | 0.43              |
| 1:A:1246:SER:HB3  | 1:A:1261:TYR:CE1  | 2.54                     | 0.43              |
| 1:B:654:ILE:O     | 1:B:658:ILE:HG13  | 2.19                     | 0.43              |
| 1:A:32:ALA:C      | 1:A:34:ARG:H      | 2.25                     | 0.42              |
| 1:A:73:PHE:HD2    | 1:A:74:TYR:HD1    | 1.66                     | 0.42              |
| 1:A:110:PHE:O     | 1:A:114:ARG:HG2   | 2.18                     | 0.42              |
| 1:A:845:ASP:HB3   | 1:A:849:ARG:HH12  | 1.84                     | 0.42              |
| 1:A:1281:ALA:CB   | 1:A:1284:LEU:HB2  | 2.49                     | 0.42              |
| 1:A:1571:LEU:O    | 1:A:1573:GLN:N    | 2.51                     | 0.42              |
| 1:A:296:ARG:HA    | 1:A:299:PHE:CZ    | 2.54                     | 0.42              |
| 1:A:797:GLY:HA3   | 1:A:850:PHE:HB3   | 2.01                     | 0.42              |
| 1:A:830:LEU:HD23  | 1:A:830:LEU:HA    | 1.85                     | 0.42              |
| 1:A:1021:ASN:OD1  | 1:A:1071:LEU:HD21 | 2.17                     | 0.42              |
| 1:A:1076:SER:O    | 1:A:1077:THR:C    | 2.62                     | 0.42              |
| 1:A:1098:ILE:O    | 1:A:1101:PHE:HB2  | 2.18                     | 0.42              |
| 1:A:1474:SER:CB   | 1:A:1485:ILE:HG21 | 2.48                     | 0.42              |
| 1:B:234:LYS:HA    | 1:B:237:ASN:HD22  | 1.84                     | 0.42              |
| 1:B:303:VAL:HG22  | 1:B:377:ILE:CG1   | 2.49                     | 0.42              |
| 1:B:1038:THR:O    | 1:B:1039:LEU:C    | 2.61                     | 0.42              |
| 1:B:1130:LYS:O    | 1:B:1131:VAL:C    | 2.62                     | 0.42              |
| 1:B:1309:GLN:NE2  | 1:B:1313:THR:OG1  | 2.52                     | 0.42              |
| 1:A:338:TYR:O     | 1:A:341:VAL:HG22  | 2.20                     | 0.42              |
| 1:A:1057:HIS:HA   | 1:A:1060:LYS:HD2  | 2.01                     | 0.42              |
| 1:A:1082:SER:O    | 1:A:1083:VAL:C    | 2.60                     | 0.42              |
| 1:A:1301:TRP:HD1  | 1:A:1303:ASP:OD1  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1563:TRP:CD1  | 1:A:1566:ARG:NH2  | 2.87                     | 0.42              |
| 1:B:386:ASP:OD1   | 1:B:479:HIS:CE1   | 2.72                     | 0.42              |
| 1:B:527:SER:C     | 1:B:528:VAL:HG13  | 2.44                     | 0.42              |
| 1:B:801:SER:O     | 1:B:805:ASP:N     | 2.52                     | 0.42              |
| 1:B:1083:VAL:HG13 | 1:B:1134:SER:HB3  | 2.01                     | 0.42              |
| 1:A:58:GLU:C      | 1:A:60:GLU:N      | 2.73                     | 0.42              |
| 1:A:273:PHE:CE1   | 1:A:334:LEU:HD13  | 2.54                     | 0.42              |
| 1:A:280:ASN:HB2   | 1:A:412:TRP:HE1   | 1.84                     | 0.42              |
| 1:A:718:VAL:HG13  | 1:A:760:LEU:CD2   | 2.49                     | 0.42              |
| 1:A:768:ALA:HA    | 1:A:773:ASP:HB2   | 2.01                     | 0.42              |
| 1:A:963:TYR:O     | 1:A:964:ASP:C     | 2.62                     | 0.42              |
| 1:A:1400:PHE:O    | 1:A:1403:ASP:HB2  | 2.18                     | 0.42              |
| 1:A:1531:GLY:HA2  | 1:A:1595:CYS:SG   | 2.59                     | 0.42              |
| 1:B:184:LEU:HD22  | 1:B:184:LEU:N     | 2.33                     | 0.42              |
| 1:B:194:LEU:O     | 1:B:198:THR:HG23  | 2.20                     | 0.42              |
| 1:B:1318:LEU:HD13 | 1:B:1334:LEU:HD12 | 2.02                     | 0.42              |
| 1:B:1359:TYR:CE1  | 1:B:1406:GLU:HB3  | 2.53                     | 0.42              |
| 1:B:1434:LEU:HD13 | 1:B:1449:LEU:HD12 | 2.01                     | 0.42              |
| 1:A:37:LEU:HA     | 1:A:40:SER:HB2    | 2.01                     | 0.42              |
| 1:A:255:LYS:O     | 1:A:259:VAL:HG23  | 2.19                     | 0.42              |
| 1:A:908:TYR:CE2   | 1:A:930:PRO:CB    | 2.79                     | 0.42              |
| 1:A:1281:ALA:C    | 1:A:1283:SER:N    | 2.73                     | 0.42              |
| 1:A:1438:THR:CA   | 1:A:1446:LEU:HD13 | 2.35                     | 0.42              |
| 1:A:1538:MET:HE1  | 1:A:1563:TRP:CZ3  | 2.53                     | 0.42              |
| 1:B:63:ILE:HA     | 1:B:74:TYR:HD2    | 1.84                     | 0.42              |
| 1:B:294:ALA:O     | 1:B:297:ASN:HB3   | 2.19                     | 0.42              |
| 1:B:1412:MET:HE1  | 1:B:1467:TRP:CD2  | 2.54                     | 0.42              |
| 1:B:1571:LEU:HB3  | 1:B:1580:LEU:HD11 | 2.02                     | 0.42              |
| 1:A:124:VAL:HG11  | 1:A:129:LEU:HD23  | 2.02                     | 0.42              |
| 1:A:300:HIS:O     | 1:A:304:ILE:HG13  | 2.19                     | 0.42              |
| 1:A:666:ARG:HA    | 1:A:671:ARG:HE    | 1.84                     | 0.42              |
| 1:A:860:LEU:HD13  | 1:A:860:LEU:HA    | 1.76                     | 0.42              |
| 1:A:987:GLU:O     | 1:A:989:LYS:HG3   | 2.20                     | 0.42              |
| 1:A:1000:GLN:HA   | 1:A:1270:LEU:HD22 | 2.01                     | 0.42              |
| 1:A:1218:LEU:HD22 | 1:A:1376:ILE:HA   | 2.01                     | 0.42              |
| 1:A:1306:ASN:HB3  | 1:A:1309:GLN:HB3  | 2.01                     | 0.42              |
| 1:B:1083:VAL:HG12 | 1:B:1087:VAL:HG23 | 2.00                     | 0.42              |
| 1:B:1139:PHE:CE2  | 1:B:1301:TRP:CE2  | 3.07                     | 0.42              |
| 1:A:78:VAL:HG11   | 1:A:110:PHE:HD2   | 1.85                     | 0.42              |
| 1:A:108:ILE:O     | 1:A:112:LEU:HG    | 2.20                     | 0.42              |
| 1:A:112:LEU:HD13  | 1:A:252:GLY:HA3   | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:150:THR:O     | 1:A:154:MET:HG3   | 2.20                     | 0.42              |
| 1:A:329:VAL:CG1   | 1:A:388:ILE:HD12  | 2.50                     | 0.42              |
| 1:A:1090:VAL:HG21 | 1:A:1131:VAL:HG13 | 2.02                     | 0.42              |
| 1:A:1251:PHE:CE1  | 1:A:1261:TYR:HA   | 2.55                     | 0.42              |
| 1:A:1345:GLU:H    | 1:A:1345:GLU:CD   | 2.27                     | 0.42              |
| 1:B:255:LYS:O     | 1:B:259:VAL:HG23  | 2.20                     | 0.42              |
| 1:B:704:GLU:HB3   | 1:B:889:PHE:CD2   | 2.55                     | 0.42              |
| 1:B:1064:LYS:HE3  | 1:B:1066:GLU:H    | 1.85                     | 0.42              |
| 1:B:1233:TRP:O    | 1:B:1233:TRP:CD1  | 2.72                     | 0.42              |
| 1:B:1556:LEU:HD23 | 1:B:1602:TYR:OH   | 2.20                     | 0.42              |
| 1:A:193:PHE:CZ    | 1:B:816:LEU:HD21  | 2.54                     | 0.42              |
| 1:A:516:THR:HG22  | 1:A:518:ILE:H     | 1.84                     | 0.42              |
| 1:A:1138:HIS:HA   | 1:A:1141:LYS:HD3  | 2.02                     | 0.42              |
| 1:B:1118:LEU:HD23 | 1:B:1122:TYR:HD2  | 1.83                     | 0.42              |
| 1:B:1387:GLN:HB3  | 1:B:1397:MET:SD   | 2.59                     | 0.42              |
| 1:B:1456:LEU:C    | 1:B:1456:LEU:HD23 | 2.44                     | 0.42              |
| 1:B:1553:HIS:CD2  | 1:B:1553:HIS:O    | 2.73                     | 0.42              |
| 1:B:1598:HIS:HA   | 1:B:1601:SER:CB   | 2.49                     | 0.42              |
| 1:A:71:GLU:O      | 1:A:72:PRO:C      | 2.63                     | 0.42              |
| 1:A:191:MET:C     | 1:A:193:PHE:N     | 2.77                     | 0.42              |
| 1:A:366:LYS:HA    | 1:A:369:ASP:CG    | 2.45                     | 0.42              |
| 1:A:418:LEU:HD11  | 1:A:477:ALA:HA    | 2.01                     | 0.42              |
| 1:A:694:ASP:CB    | 1:A:750:HIS:HB3   | 2.50                     | 0.42              |
| 1:A:1046:ARG:HD2  | 1:A:1046:ARG:HA   | 1.88                     | 0.42              |
| 1:A:1453:LEU:CB   | 1:A:1506:VAL:HG13 | 2.38                     | 0.42              |
| 1:B:131:LEU:HD11  | 1:B:142:ARG:HG3   | 2.01                     | 0.42              |
| 1:B:405:ASN:O     | 1:B:409:LEU:HG    | 2.19                     | 0.42              |
| 1:B:866:LEU:HD13  | 1:B:1013:LEU:HD21 | 2.01                     | 0.42              |
| 1:B:916:GLU:O     | 1:B:920:LYS:HG3   | 2.20                     | 0.42              |
| 1:A:292:ALA:O     | 1:A:296:ARG:HG3   | 2.19                     | 0.42              |
| 1:A:548:LEU:HD22  | 1:A:642:LYS:HA    | 2.02                     | 0.42              |
| 1:A:867:HIS:C     | 1:A:949:ASP:OD2   | 2.62                     | 0.42              |
| 1:A:945:LEU:N     | 1:A:945:LEU:HD23  | 2.35                     | 0.42              |
| 1:A:1133:VAL:HG22 | 1:A:1247:TRP:CE2  | 2.54                     | 0.42              |
| 1:A:1562:ASP:C    | 1:A:1566:ARG:HE   | 2.28                     | 0.42              |
| 1:B:115:LEU:CD1   | 1:B:130:ILE:HG13  | 2.50                     | 0.42              |
| 1:B:191:MET:C     | 1:B:193:PHE:N     | 2.75                     | 0.42              |
| 1:B:296:ARG:HA    | 1:B:299:PHE:CD2   | 2.55                     | 0.42              |
| 1:B:1443:ASN:OD1  | 1:B:1446:LEU:HG   | 2.20                     | 0.42              |
| 1:B:1573:GLN:O    | 1:B:1574:LYS:C    | 2.60                     | 0.42              |
| 1:A:693:VAL:HG21  | 1:A:710:LEU:HD22  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1195:LEU:HD23 | 1:A:1198:PHE:HD2  | 1.85                     | 0.41              |
| 1:A:1219:VAL:O    | 1:A:1222:LEU:HD12 | 2.20                     | 0.41              |
| 1:A:1398:GLU:CG   | 1:A:1399:GLU:N    | 2.83                     | 0.41              |
| 1:A:1428:LEU:HD12 | 1:A:1488:ASN:HA   | 2.01                     | 0.41              |
| 1:B:1063:MET:HE2  | 1:B:1067:HIS:CE1  | 2.54                     | 0.41              |
| 1:B:1209:CYS:SG   | 1:B:1210:LYS:N    | 2.93                     | 0.41              |
| 1:B:1241:PHE:HB3  | 1:B:1242:PRO:CD   | 2.50                     | 0.41              |
| 1:B:1599:ILE:O    | 1:B:1602:TYR:HB3  | 2.19                     | 0.41              |
| 1:A:699:LYS:O     | 1:A:704:GLU:HG3   | 2.20                     | 0.41              |
| 1:A:1030:MET:SD   | 1:A:1038:THR:HG21 | 2.60                     | 0.41              |
| 1:A:1047:ILE:HG12 | 1:A:1256:ILE:HG13 | 2.02                     | 0.41              |
| 1:A:1174:ARG:NE   | 1:A:1320:GLU:OE2  | 2.53                     | 0.41              |
| 1:A:1194:LYS:NZ   | 1:A:1194:LYS:HB3  | 2.35                     | 0.41              |
| 1:A:1201:VAL:HG11 | 1:A:1222:LEU:CD1  | 2.49                     | 0.41              |
| 1:A:1536:GLU:O    | 1:A:1540:VAL:HG23 | 2.19                     | 0.41              |
| 1:A:1545:ALA:CA   | 1:A:1553:HIS:HA   | 2.45                     | 0.41              |
| 1:B:338:TYR:HA    | 1:B:341:VAL:HG22  | 2.01                     | 0.41              |
| 1:B:512:MET:H     | 1:B:512:MET:HG2   | 1.62                     | 0.41              |
| 1:B:694:ASP:OD2   | 1:B:750:HIS:HB3   | 2.21                     | 0.41              |
| 1:B:1053:TRP:CD1  | 1:B:1057:HIS:HD2  | 2.38                     | 0.41              |
| 1:B:1122:TYR:CD1  | 1:B:1122:TYR:C    | 2.99                     | 0.41              |
| 1:B:1133:VAL:HG22 | 1:B:1246:SER:HA   | 2.00                     | 0.41              |
| 1:B:1565:SER:O    | 1:B:1569:LYS:HG3  | 2.20                     | 0.41              |
| 1:A:240:ILE:O     | 1:A:244:VAL:HG23  | 2.19                     | 0.41              |
| 1:A:1315:LEU:CB   | 1:A:1316:PRO:CD   | 2.98                     | 0.41              |
| 1:B:1447:LEU:HB3  | 1:B:1505:GLN:HG3  | 2.02                     | 0.41              |
| 1:B:1473:THR:O    | 1:B:1485:ILE:HG21 | 2.19                     | 0.41              |
| 1:B:1486:GLN:O    | 1:B:1490:GLN:HG3  | 2.20                     | 0.41              |
| 1:A:834:VAL:HG11  | 1:A:961:VAL:HG13  | 2.03                     | 0.41              |
| 1:A:966:LEU:O     | 1:A:967:TYR:C     | 2.59                     | 0.41              |
| 1:A:1319:LEU:HD11 | 1:A:1350:VAL:HA   | 2.02                     | 0.41              |
| 1:A:1388:LEU:HD23 | 1:A:1388:LEU:HA   | 1.92                     | 0.41              |
| 1:A:1568:LYS:CD   | 1:A:1569:LYS:HD3  | 2.49                     | 0.41              |
| 1:B:248:GLN:O     | 1:B:249:GLU:C     | 2.61                     | 0.41              |
| 1:B:426:PRO:HD3   | 1:B:467:GLN:NE2   | 2.35                     | 0.41              |
| 1:B:496:LEU:C     | 1:B:499:GLY:H     | 2.28                     | 0.41              |
| 1:B:808:VAL:HG11  | 1:B:908:TYR:CB    | 2.50                     | 0.41              |
| 1:B:860:LEU:HB2   | 1:B:1005:ILE:CD1  | 2.47                     | 0.41              |
| 1:B:1414:THR:CG2  | 1:B:1424:CYS:HA   | 2.50                     | 0.41              |
| 1:B:1449:LEU:N    | 1:B:1449:LEU:HD23 | 2.35                     | 0.41              |
| 1:B:1519:THR:HB   | 1:B:1520:PRO:HD2  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:852:PRO:HD2   | 1:A:999:LEU:HD23  | 2.01                     | 0.41              |
| 1:A:963:TYR:OH    | 1:A:1013:LEU:HB3  | 2.20                     | 0.41              |
| 1:A:1060:LYS:O    | 1:A:1061:GLN:C    | 2.63                     | 0.41              |
| 1:A:1292:VAL:HG12 | 1:A:1329:ILE:CG2  | 2.51                     | 0.41              |
| 1:B:678:LEU:HD23  | 1:B:678:LEU:HA    | 1.84                     | 0.41              |
| 1:B:1216:PRO:HA   | 1:B:1219:VAL:HG12 | 2.02                     | 0.41              |
| 1:B:1424:CYS:O    | 1:B:1428:LEU:HG   | 2.20                     | 0.41              |
| 1:A:1151:SER:N    | 1:A:1154:ILE:HD12 | 2.36                     | 0.41              |
| 1:A:1153:GLU:HA   | 1:A:1156:LYS:CB   | 2.50                     | 0.41              |
| 1:A:1244:ILE:HG12 | 1:A:1293:ARG:CZ   | 2.50                     | 0.41              |
| 1:A:1307:PRO:CB   | 1:A:1308:PRO:HD3  | 2.50                     | 0.41              |
| 1:A:1308:PRO:O    | 1:A:1312:ARG:HG3  | 2.20                     | 0.41              |
| 1:A:1312:ARG:O    | 1:A:1313:THR:C    | 2.60                     | 0.41              |
| 1:A:1499:ILE:HG22 | 1:A:1511:CYS:SG   | 2.60                     | 0.41              |
| 1:B:905:THR:HG22  | 1:B:906:PRO:O     | 2.21                     | 0.41              |
| 1:B:1124:LEU:O    | 1:B:1125:ASP:C    | 2.63                     | 0.41              |
| 1:B:1238:THR:HG21 | 1:B:1286:HIS:CA   | 2.50                     | 0.41              |
| 1:B:1475:PRO:HG2  | 1:B:1481:GLN:HB2  | 2.01                     | 0.41              |
| 1:A:73:PHE:CE1    | 1:A:155:MET:SD    | 3.14                     | 0.41              |
| 1:A:313:LEU:CD1   | 1:A:384:ILE:HG23  | 2.50                     | 0.41              |
| 1:A:418:LEU:O     | 1:A:422:LEU:HG    | 2.21                     | 0.41              |
| 1:A:793:ASN:O     | 1:A:797:GLY:N     | 2.53                     | 0.41              |
| 1:A:813:MET:HE3   | 1:A:813:MET:HB2   | 1.70                     | 0.41              |
| 1:A:1151:SER:N    | 1:A:1154:ILE:HB   | 2.35                     | 0.41              |
| 1:A:1151:SER:HB3  | 1:A:1154:ILE:HG13 | 2.01                     | 0.41              |
| 1:B:132:LEU:HD21  | 1:B:143:LEU:CD1   | 2.50                     | 0.41              |
| 1:B:1142:MET:HE3  | 1:B:1142:MET:HB2  | 1.93                     | 0.41              |
| 1:B:1318:LEU:HD21 | 1:B:1331:SER:CA   | 2.47                     | 0.41              |
| 1:A:493:VAL:HG12  | 1:B:320:PRO:HB3   | 2.03                     | 0.41              |
| 1:A:1003:PHE:O    | 1:A:1004:LEU:C    | 2.62                     | 0.41              |
| 1:A:1101:PHE:CE2  | 1:A:1165:LEU:HD22 | 2.56                     | 0.41              |
| 1:A:1105:ASP:N    | 1:A:1110:LEU:HD21 | 2.18                     | 0.41              |
| 1:A:1194:LYS:HZ3  | 1:A:1198:PHE:HZ   | 1.69                     | 0.41              |
| 1:A:1212:ASN:N    | 1:A:1212:ASN:HD22 | 2.18                     | 0.41              |
| 1:A:1245:GLY:C    | 1:A:1247:TRP:N    | 2.75                     | 0.41              |
| 1:A:1535:PRO:HG2  | 1:A:1536:GLU:OE2  | 2.21                     | 0.41              |
| 1:B:115:LEU:HD12  | 1:B:133:ILE:CD1   | 2.51                     | 0.41              |
| 1:B:120:GLU:H     | 1:B:120:GLU:HG3   | 1.59                     | 0.41              |
| 1:B:711:TYR:CD2   | 1:B:888:PRO:CD    | 3.03                     | 0.41              |
| 1:B:945:LEU:HG    | 1:B:946:ASN:OD1   | 2.21                     | 0.41              |
| 1:B:952:ALA:O     | 1:B:956:LEU:HG    | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1063:MET:HE3  | 1:B:1063:MET:HB2  | 1.78                     | 0.41              |
| 1:B:1486:GLN:HG3  | 1:B:1489:ARG:NH1  | 2.35                     | 0.41              |
| 1:B:1595:CYS:O    | 1:B:1599:ILE:N    | 2.51                     | 0.41              |
| 1:A:236:LYS:HE3   | 1:A:236:LYS:HB3   | 1.90                     | 0.41              |
| 1:A:390:GLN:O     | 1:A:391:ALA:C     | 2.61                     | 0.41              |
| 1:A:415:LEU:HD21  | 1:A:484:LEU:HD11  | 2.01                     | 0.41              |
| 1:A:478:ASN:O     | 1:A:482:LYS:HG3   | 2.20                     | 0.41              |
| 1:A:795:LEU:HD23  | 1:A:795:LEU:HA    | 1.94                     | 0.41              |
| 1:A:825:GLY:O     | 1:A:829:ILE:HG12  | 2.21                     | 0.41              |
| 1:A:981:ASP:OD2   | 1:A:1280:LEU:HG   | 2.21                     | 0.41              |
| 1:A:1166:ILE:HG13 | 1:A:1166:ILE:H    | 1.68                     | 0.41              |
| 1:A:1245:GLY:HA2  | 1:A:1247:TRP:CZ2  | 2.55                     | 0.41              |
| 1:A:1257:PRO:O    | 1:A:1258:SER:C    | 2.64                     | 0.41              |
| 1:A:1271:GLY:O    | 1:A:1274:CYS:HB3  | 2.21                     | 0.41              |
| 1:A:1493:GLN:HG2  | 1:A:1540:VAL:CG2  | 2.49                     | 0.41              |
| 1:B:159:LYS:HA    | 1:B:159:LYS:HD2   | 1.85                     | 0.41              |
| 1:B:336:CYS:O     | 1:B:337:LEU:C     | 2.62                     | 0.41              |
| 1:B:382:LEU:HD12  | 1:B:475:ILE:CG2   | 2.50                     | 0.41              |
| 1:B:512:MET:HE3   | 1:B:512:MET:HB3   | 1.83                     | 0.41              |
| 1:B:704:GLU:H     | 1:B:704:GLU:HG3   | 1.76                     | 0.41              |
| 1:B:791:LYS:HD3   | 1:B:836:ILE:HG12  | 2.03                     | 0.41              |
| 1:B:973:LEU:HD23  | 1:B:973:LEU:HA    | 1.86                     | 0.41              |
| 1:B:1233:TRP:O    | 1:B:1233:TRP:CG   | 2.73                     | 0.41              |
| 1:B:1528:ASN:HD22 | 1:B:1528:ASN:H    | 1.68                     | 0.41              |
| 1:B:1575:ASN:O    | 1:B:1579:LYS:HG3  | 2.21                     | 0.41              |
| 1:B:1593:LEU:HG   | 1:B:1594:GLU:N    | 2.34                     | 0.41              |
| 1:A:86:THR:CG2    | 1:A:141:SER:HB3   | 2.51                     | 0.41              |
| 1:A:414:LEU:HD12  | 1:A:483:LEU:HD12  | 2.01                     | 0.41              |
| 1:A:469:PHE:CZ    | 1:A:474:VAL:HG22  | 2.55                     | 0.41              |
| 1:A:659:THR:O     | 1:A:663:LEU:HB2   | 2.21                     | 0.41              |
| 1:A:1027:SER:N    | 1:A:1028:PRO:CD   | 2.84                     | 0.41              |
| 1:A:1041:TRP:HA   | 1:A:1044:ARG:HG3  | 2.03                     | 0.41              |
| 1:A:1151:SER:HB3  | 1:A:1154:ILE:CG1  | 2.51                     | 0.41              |
| 1:B:471:VAL:O     | 1:B:475:ILE:HG12  | 2.21                     | 0.41              |
| 1:B:1001:TYR:CE2  | 1:B:1005:ILE:HD11 | 2.56                     | 0.41              |
| 1:B:1445:SER:O    | 1:B:1449:LEU:HG   | 2.21                     | 0.41              |
| 1:B:1587:GLY:O    | 1:B:1588:LYS:C    | 2.61                     | 0.41              |
| 1:A:108:ILE:HD11  | 1:A:243:ASN:HB3   | 2.03                     | 0.40              |
| 1:A:422:LEU:HD11  | 1:A:537:LEU:CD2   | 2.51                     | 0.40              |
| 1:A:671:ARG:HB3   | 1:A:722:LEU:HD11  | 2.03                     | 0.40              |
| 1:A:1552:GLY:C    | 1:A:1554:LEU:N    | 2.78                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:92:ILE:O      | 1:B:93:PRO:C      | 2.64                     | 0.40              |
| 1:B:281:SER:HB3   | 1:B:444:VAL:HG12  | 2.03                     | 0.40              |
| 1:B:299:PHE:O     | 1:B:303:VAL:HG23  | 2.20                     | 0.40              |
| 1:B:441:ALA:HB1   | 1:B:443:ARG:NH2   | 2.33                     | 0.40              |
| 1:B:1104:ILE:HG23 | 1:B:1110:LEU:CD1  | 2.51                     | 0.40              |
| 1:B:1388:LEU:HD23 | 1:B:1394:ARG:HG3  | 2.02                     | 0.40              |
| 1:B:1555:GLN:HA   | 1:B:1558:ASN:HD22 | 1.85                     | 0.40              |
| 1:B:1573:GLN:HB2  | 1:B:1576:VAL:HG23 | 2.03                     | 0.40              |
| 1:B:1603:LEU:O    | 1:B:1607:THR:N    | 2.54                     | 0.40              |
| 1:A:35:PRO:CB     | 1:A:48:GLU:HB3    | 2.49                     | 0.40              |
| 1:A:184:LEU:HD22  | 1:A:184:LEU:N     | 2.32                     | 0.40              |
| 1:A:234:LYS:O     | 1:A:238:VAL:HG23  | 2.21                     | 0.40              |
| 1:A:538:LEU:HD12  | 1:A:651:ALA:HB1   | 2.02                     | 0.40              |
| 1:A:545:ALA:HB1   | 1:A:648:LEU:HG    | 2.04                     | 0.40              |
| 1:A:659:THR:HA    | 1:A:663:LEU:HB2   | 2.02                     | 0.40              |
| 1:A:866:LEU:HB3   | 1:A:948:LEU:HD13  | 2.03                     | 0.40              |
| 1:A:1051:VAL:HG13 | 1:A:1072:LEU:HG   | 2.02                     | 0.40              |
| 1:A:1077:THR:C    | 1:A:1081:SER:HB2  | 2.46                     | 0.40              |
| 1:A:1193:GLU:OE1  | 1:A:1369:ASN:HB3  | 2.21                     | 0.40              |
| 1:A:1534:PHE:N    | 1:A:1535:PRO:CD   | 2.83                     | 0.40              |
| 1:B:1493:GLN:CG   | 1:B:1540:VAL:HG22 | 2.37                     | 0.40              |
| 1:B:1605:ASP:C    | 1:B:1607:THR:N    | 2.78                     | 0.40              |
| 1:A:303:VAL:HG22  | 1:A:377:ILE:CG1   | 2.51                     | 0.40              |
| 1:A:484:LEU:HD22  | 1:A:530:LEU:HD11  | 2.03                     | 0.40              |
| 1:A:779:CYS:HB3   | 1:A:817:ILE:HG21  | 2.03                     | 0.40              |
| 1:A:1029:GLU:O    | 1:A:1096:ARG:NH1  | 2.54                     | 0.40              |
| 1:A:1063:MET:SD   | 1:A:1068:ALA:HB2  | 2.62                     | 0.40              |
| 1:A:1094:PHE:CE1  | 1:A:1128:ILE:HD11 | 2.56                     | 0.40              |
| 1:A:1255:THR:O    | 1:A:1256:ILE:C    | 2.64                     | 0.40              |
| 1:A:1292:VAL:CG1  | 1:A:1329:ILE:HB   | 2.52                     | 0.40              |
| 1:A:1447:LEU:HA   | 1:A:1505:GLN:HG3  | 2.04                     | 0.40              |
| 1:A:1559:ALA:HB1  | 1:A:1563:TRP:CH2  | 2.56                     | 0.40              |
| 1:B:855:LEU:CD2   | 1:B:1002:TYR:HE2  | 2.34                     | 0.40              |
| 1:B:1165:LEU:HD23 | 1:B:1165:LEU:HA   | 1.81                     | 0.40              |
| 1:B:1244:ILE:HG23 | 1:B:1244:ILE:O    | 2.22                     | 0.40              |
| 1:B:1392:GLN:CD   | 1:B:1392:GLN:H    | 2.28                     | 0.40              |
| 1:B:1445:SER:HA   | 1:B:1448:HIS:HD1  | 1.83                     | 0.40              |
| 1:B:1515:LEU:HD11 | 1:B:1556:LEU:CD2  | 2.46                     | 0.40              |
| 1:A:81:SER:O      | 1:A:82:THR:C      | 2.65                     | 0.40              |
| 1:A:481:ILE:O     | 1:A:485:THR:HG23  | 2.20                     | 0.40              |
| 1:A:925:ASP:OD1   | 1:A:925:ASP:N     | 2.54                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1039:LEU:HB3 | 1:A:1130:LYS:HD2  | 2.03                     | 0.40              |
| 1:A:1111:GLN:HB3 | 1:A:1113:HIS:ND1  | 2.36                     | 0.40              |
| 1:A:1564:LEU:O   | 1:A:1565:SER:C    | 2.64                     | 0.40              |
| 1:B:282:PHE:HB2  | 1:B:416:ASN:CB    | 2.52                     | 0.40              |
| 1:B:833:PHE:HE1  | 1:B:858:LEU:HD22  | 1.87                     | 0.40              |
| 1:B:1055:LYS:HB2 | 1:B:1072:LEU:HD12 | 2.03                     | 0.40              |
| 1:B:1299:ILE:CG2 | 1:B:1336:ARG:HD2  | 2.49                     | 0.40              |
| 1:B:1328:GLU:O   | 1:B:1331:SER:OG   | 2.34                     | 0.40              |
| 1:A:69:GLN:C     | 1:A:71:GLU:H      | 2.29                     | 0.40              |
| 1:A:317:VAL:CG1  | 1:A:318:LEU:N     | 2.85                     | 0.40              |
| 1:A:547:VAL:HG12 | 1:A:551:GLN:NE2   | 2.37                     | 0.40              |
| 1:A:932:PHE:HA   | 1:A:1001:TYR:CE1  | 2.56                     | 0.40              |
| 1:A:1128:ILE:O   | 1:A:1131:VAL:HG23 | 2.21                     | 0.40              |
| 1:A:1203:ALA:O   | 1:A:1205:GLY:N    | 2.54                     | 0.40              |
| 1:A:1381:LEU:HA  | 1:A:1381:LEU:HD23 | 1.88                     | 0.40              |
| 1:B:542:TYR:CE2  | 1:B:689:ILE:HG23  | 2.57                     | 0.40              |
| 1:B:747:LEU:HD11 | 1:B:793:ASN:ND2   | 2.37                     | 0.40              |
| 1:B:1194:LYS:HA  | 1:B:1370:SER:O    | 2.21                     | 0.40              |
| 1:B:1374:GLU:OE1 | 1:B:1423:PHE:HB2  | 2.21                     | 0.40              |
| 1:B:1474:SER:HA  | 1:B:1485:ILE:CD1  | 2.51                     | 0.40              |
| 1:B:1586:HIS:HB2 | 1:B:1589:HIS:CE1  | 2.57                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|----------|-------------|----|
| 1   | A     | 1372/5183 (26%)  | 1288 (94%) | 63 (5%)  | 21 (2%)  | 8           | 30 |
| 1   | B     | 1359/5183 (26%)  | 1262 (93%) | 82 (6%)  | 15 (1%)  | 11          | 38 |
| All | All   | 2731/10366 (26%) | 2550 (93%) | 145 (5%) | 36 (1%)  | 12          | 33 |

All (36) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 889  | PHE  |
| 1   | A     | 906  | PRO  |
| 1   | A     | 907  | LEU  |
| 1   | A     | 909  | HIS  |
| 1   | A     | 1031 | SER  |
| 1   | A     | 1223 | PRO  |
| 1   | A     | 1244 | ILE  |
| 1   | B     | 1159 | LEU  |
| 1   | A     | 910  | GLY  |
| 1   | A     | 1245 | GLY  |
| 1   | A     | 1549 | GLN  |
| 1   | B     | 197  | LEU  |
| 1   | B     | 1247 | TRP  |
| 1   | A     | 59   | SER  |
| 1   | A     | 94   | ARG  |
| 1   | A     | 1211 | ALA  |
| 1   | A     | 1221 | ASN  |
| 1   | A     | 1257 | PRO  |
| 1   | B     | 59   | SER  |
| 1   | B     | 324  | SER  |
| 1   | B     | 1142 | MET  |
| 1   | B     | 1274 | CYS  |
| 1   | B     | 1275 | SER  |
| 1   | B     | 323  | PRO  |
| 1   | B     | 492  | GLN  |
| 1   | A     | 1205 | GLY  |
| 1   | A     | 1258 | SER  |
| 1   | B     | 1255 | THR  |
| 1   | B     | 1308 | PRO  |
| 1   | A     | 1222 | LEU  |
| 1   | A     | 1300 | VAL  |
| 1   | B     | 286  | PRO  |
| 1   | B     | 937  | SER  |
| 1   | B     | 938  | PRO  |
| 1   | A     | 320  | PRO  |
| 1   | A     | 1204 | ILE  |

### 5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 1218/4521 (27%) | 1151 (94%) | 67 (6%)  | 19          | 46 |
| 1   | B     | 1217/4521 (27%) | 1126 (92%) | 91 (8%)  | 12          | 38 |
| All | All   | 2435/9042 (27%) | 2277 (94%) | 158 (6%) | 17          | 42 |

All (158) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 36   | LEU  |
| 1   | A     | 68   | LYS  |
| 1   | A     | 69   | GLN  |
| 1   | A     | 92   | ILE  |
| 1   | A     | 97   | LEU  |
| 1   | A     | 100  | VAL  |
| 1   | A     | 191  | MET  |
| 1   | A     | 277  | VAL  |
| 1   | A     | 284  | ILE  |
| 1   | A     | 336  | CYS  |
| 1   | A     | 401  | GLU  |
| 1   | A     | 444  | VAL  |
| 1   | A     | 530  | LEU  |
| 1   | A     | 686  | LEU  |
| 1   | A     | 722  | LEU  |
| 1   | A     | 747  | LEU  |
| 1   | A     | 771  | GLN  |
| 1   | A     | 789  | THR  |
| 1   | A     | 799  | VAL  |
| 1   | A     | 807  | ASN  |
| 1   | A     | 813  | MET  |
| 1   | A     | 830  | LEU  |
| 1   | A     | 854  | ILE  |
| 1   | A     | 860  | LEU  |
| 1   | A     | 885  | LEU  |
| 1   | A     | 905  | THR  |
| 1   | A     | 911  | PHE  |
| 1   | A     | 936  | LEU  |
| 1   | A     | 945  | LEU  |
| 1   | A     | 984  | ARG  |
| 1   | A     | 987  | GLU  |
| 1   | A     | 1002 | TYR  |
| 1   | A     | 1035 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1040 | ARG  |
| 1   | A     | 1045 | LEU  |
| 1   | A     | 1046 | ARG  |
| 1   | A     | 1061 | GLN  |
| 1   | A     | 1063 | MET  |
| 1   | A     | 1072 | LEU  |
| 1   | A     | 1122 | TYR  |
| 1   | A     | 1131 | VAL  |
| 1   | A     | 1154 | ILE  |
| 1   | A     | 1159 | LEU  |
| 1   | A     | 1165 | LEU  |
| 1   | A     | 1173 | THR  |
| 1   | A     | 1177 | LEU  |
| 1   | A     | 1202 | LEU  |
| 1   | A     | 1212 | ASN  |
| 1   | A     | 1244 | ILE  |
| 1   | A     | 1280 | LEU  |
| 1   | A     | 1301 | TRP  |
| 1   | A     | 1303 | ASP  |
| 1   | A     | 1314 | LEU  |
| 1   | A     | 1384 | LEU  |
| 1   | A     | 1392 | GLN  |
| 1   | A     | 1397 | MET  |
| 1   | A     | 1398 | GLU  |
| 1   | A     | 1411 | MET  |
| 1   | A     | 1471 | MET  |
| 1   | A     | 1481 | GLN  |
| 1   | A     | 1484 | VAL  |
| 1   | A     | 1485 | ILE  |
| 1   | A     | 1486 | GLN  |
| 1   | A     | 1496 | THR  |
| 1   | A     | 1500 | VAL  |
| 1   | A     | 1528 | ASN  |
| 1   | A     | 1607 | THR  |
| 1   | B     | 33   | VAL  |
| 1   | B     | 37   | LEU  |
| 1   | B     | 70   | TYR  |
| 1   | B     | 86   | THR  |
| 1   | B     | 92   | ILE  |
| 1   | B     | 96   | GLN  |
| 1   | B     | 97   | LEU  |
| 1   | B     | 113  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 124 | VAL  |
| 1   | B     | 130 | ILE  |
| 1   | B     | 147 | GLU  |
| 1   | B     | 154 | MET  |
| 1   | B     | 201 | PHE  |
| 1   | B     | 235 | THR  |
| 1   | B     | 268 | ARG  |
| 1   | B     | 278 | LEU  |
| 1   | B     | 288 | THR  |
| 1   | B     | 312 | THR  |
| 1   | B     | 318 | LEU  |
| 1   | B     | 322 | ASN  |
| 1   | B     | 350 | LEU  |
| 1   | B     | 367 | GLU  |
| 1   | B     | 378 | VAL  |
| 1   | B     | 379 | GLN  |
| 1   | B     | 381 | CYS  |
| 1   | B     | 408 | LEU  |
| 1   | B     | 424 | LEU  |
| 1   | B     | 448 | LEU  |
| 1   | B     | 511 | ILE  |
| 1   | B     | 512 | MET  |
| 1   | B     | 521 | ILE  |
| 1   | B     | 522 | GLN  |
| 1   | B     | 677 | SER  |
| 1   | B     | 680 | GLU  |
| 1   | B     | 686 | LEU  |
| 1   | B     | 698 | LEU  |
| 1   | B     | 703 | ASP  |
| 1   | B     | 717 | LEU  |
| 1   | B     | 727 | LEU  |
| 1   | B     | 799 | VAL  |
| 1   | B     | 813 | MET  |
| 1   | B     | 830 | LEU  |
| 1   | B     | 844 | MET  |
| 1   | B     | 867 | HIS  |
| 1   | B     | 909 | HIS  |
| 1   | B     | 911 | PHE  |
| 1   | B     | 922 | PHE  |
| 1   | B     | 939 | GLU  |
| 1   | B     | 943 | ASP  |
| 1   | B     | 948 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 981  | ASP  |
| 1   | B     | 992  | THR  |
| 1   | B     | 1033 | CYS  |
| 1   | B     | 1036 | LEU  |
| 1   | B     | 1040 | ARG  |
| 1   | B     | 1045 | LEU  |
| 1   | B     | 1063 | MET  |
| 1   | B     | 1067 | HIS  |
| 1   | B     | 1086 | ASP  |
| 1   | B     | 1089 | ILE  |
| 1   | B     | 1112 | LEU  |
| 1   | B     | 1118 | LEU  |
| 1   | B     | 1122 | TYR  |
| 1   | B     | 1131 | VAL  |
| 1   | B     | 1204 | ILE  |
| 1   | B     | 1212 | ASN  |
| 1   | B     | 1227 | GLN  |
| 1   | B     | 1228 | THR  |
| 1   | B     | 1231 | GLU  |
| 1   | B     | 1256 | ILE  |
| 1   | B     | 1274 | CYS  |
| 1   | B     | 1289 | LEU  |
| 1   | B     | 1299 | ILE  |
| 1   | B     | 1318 | LEU  |
| 1   | B     | 1326 | VAL  |
| 1   | B     | 1334 | LEU  |
| 1   | B     | 1338 | LEU  |
| 1   | B     | 1358 | CYS  |
| 1   | B     | 1387 | GLN  |
| 1   | B     | 1392 | GLN  |
| 1   | B     | 1459 | VAL  |
| 1   | B     | 1470 | ARG  |
| 1   | B     | 1474 | SER  |
| 1   | B     | 1486 | GLN  |
| 1   | B     | 1520 | PRO  |
| 1   | B     | 1528 | ASN  |
| 1   | B     | 1536 | GLU  |
| 1   | B     | 1549 | GLN  |
| 1   | B     | 1564 | LEU  |
| 1   | B     | 1593 | LEU  |
| 1   | B     | 1597 | CYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78)

such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 66   | HIS  |
| 1   | A     | 69   | GLN  |
| 1   | A     | 96   | GLN  |
| 1   | A     | 192  | ASN  |
| 1   | A     | 229  | GLN  |
| 1   | A     | 243  | ASN  |
| 1   | A     | 271  | ASN  |
| 1   | A     | 274  | GLN  |
| 1   | A     | 402  | HIS  |
| 1   | A     | 407  | GLN  |
| 1   | A     | 423  | ASN  |
| 1   | A     | 466  | HIS  |
| 1   | A     | 479  | HIS  |
| 1   | A     | 712  | HIS  |
| 1   | A     | 714  | ASN  |
| 1   | A     | 729  | ASN  |
| 1   | A     | 766  | HIS  |
| 1   | A     | 867  | HIS  |
| 1   | A     | 879  | GLN  |
| 1   | A     | 881  | GLN  |
| 1   | A     | 909  | HIS  |
| 1   | A     | 929  | HIS  |
| 1   | A     | 1026 | ASN  |
| 1   | A     | 1067 | HIS  |
| 1   | A     | 1119 | GLN  |
| 1   | A     | 1132 | GLN  |
| 1   | A     | 1182 | ASN  |
| 1   | A     | 1227 | GLN  |
| 1   | A     | 1253 | ASN  |
| 1   | A     | 1364 | ASN  |
| 1   | A     | 1387 | GLN  |
| 1   | A     | 1392 | GLN  |
| 1   | A     | 1418 | ASN  |
| 1   | A     | 1481 | GLN  |
| 1   | A     | 1493 | GLN  |
| 1   | A     | 1558 | ASN  |
| 1   | A     | 1589 | HIS  |
| 1   | B     | 69   | GLN  |
| 1   | B     | 83   | HIS  |
| 1   | B     | 96   | GLN  |
| 1   | B     | 98   | GLN  |
| 1   | B     | 192  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 229  | GLN  |
| 1   | B     | 237  | ASN  |
| 1   | B     | 243  | ASN  |
| 1   | B     | 248  | GLN  |
| 1   | B     | 262  | ASN  |
| 1   | B     | 379  | GLN  |
| 1   | B     | 423  | ASN  |
| 1   | B     | 467  | GLN  |
| 1   | B     | 656  | ASN  |
| 1   | B     | 729  | ASN  |
| 1   | B     | 867  | HIS  |
| 1   | B     | 881  | GLN  |
| 1   | B     | 882  | HIS  |
| 1   | B     | 909  | HIS  |
| 1   | B     | 921  | HIS  |
| 1   | B     | 979  | GLN  |
| 1   | B     | 1037 | HIS  |
| 1   | B     | 1057 | HIS  |
| 1   | B     | 1097 | GLN  |
| 1   | B     | 1111 | GLN  |
| 1   | B     | 1113 | HIS  |
| 1   | B     | 1227 | GLN  |
| 1   | B     | 1234 | ASN  |
| 1   | B     | 1249 | ASN  |
| 1   | B     | 1266 | GLN  |
| 1   | B     | 1364 | ASN  |
| 1   | B     | 1387 | GLN  |
| 1   | B     | 1486 | GLN  |
| 1   | B     | 1493 | GLN  |
| 1   | B     | 1528 | ASN  |
| 1   | B     | 1557 | HIS  |
| 1   | B     | 1573 | GLN  |
| 1   | B     | 1586 | HIS  |
| 1   | B     | 1589 | HIS  |
| 1   | B     | 1598 | HIS  |
| 1   | B     | 1612 | GLN  |

### 5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.

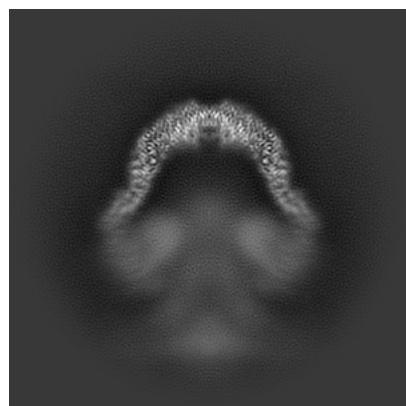
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46688. These allow visual inspection of the internal detail of the map and identification of artifacts.

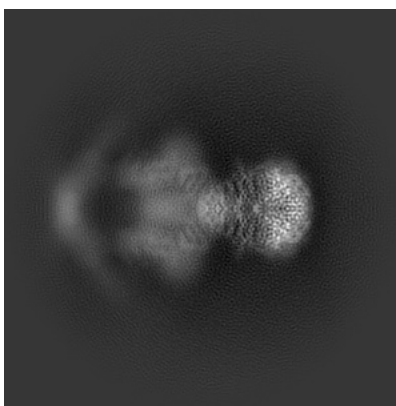
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

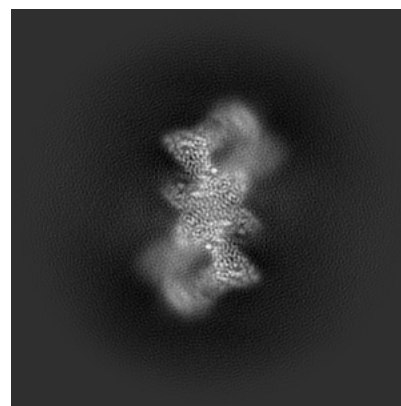
#### 6.1.1 Primary map



X

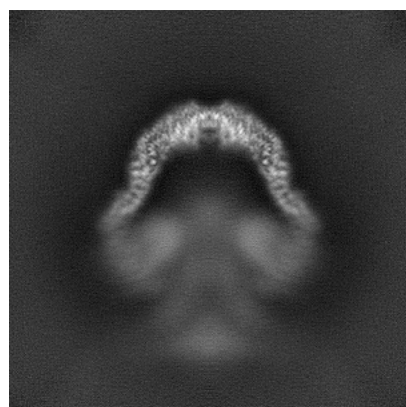


Y

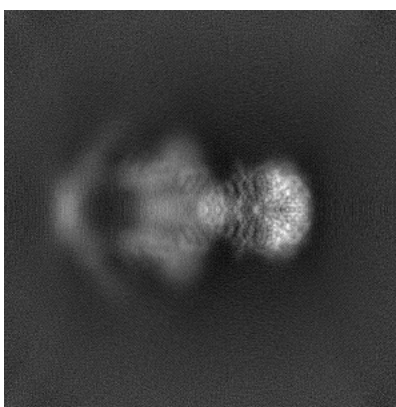


Z

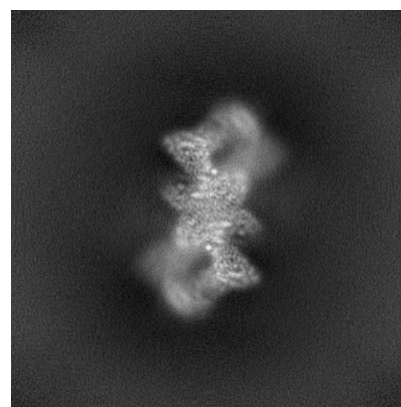
#### 6.1.2 Raw map



X



Y

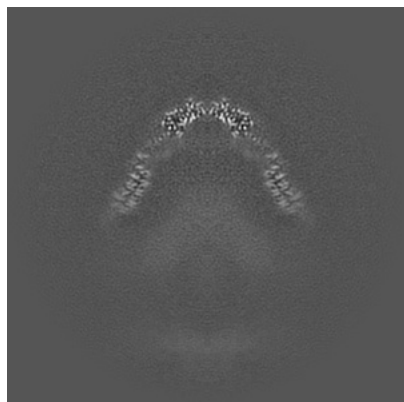


Z

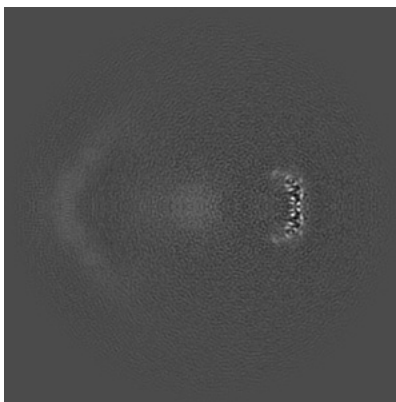
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

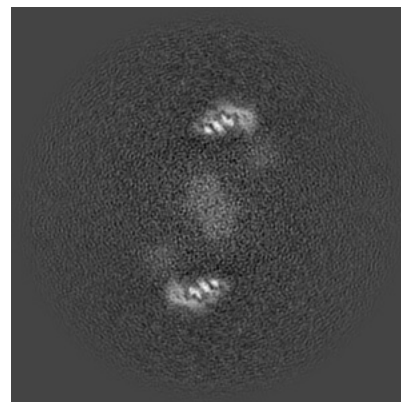
### 6.2.1 Primary map



X Index: 260

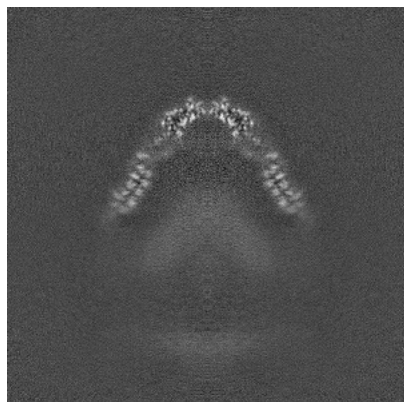


Y Index: 260

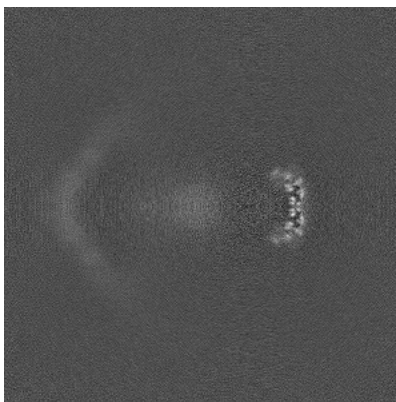


Z Index: 260

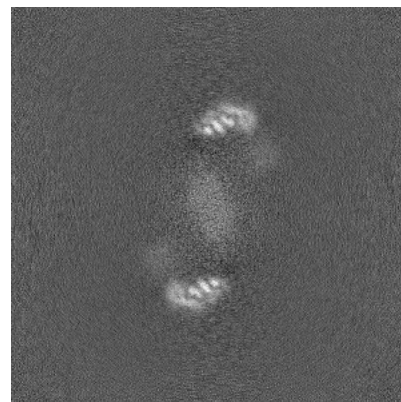
### 6.2.2 Raw map



X Index: 260



Y Index: 260

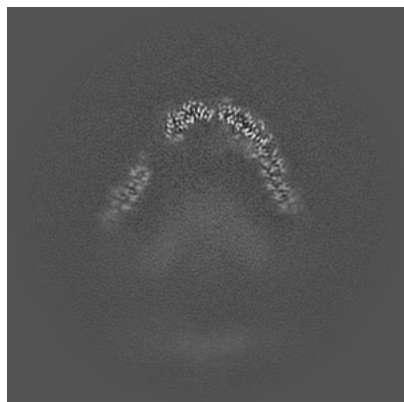


Z Index: 260

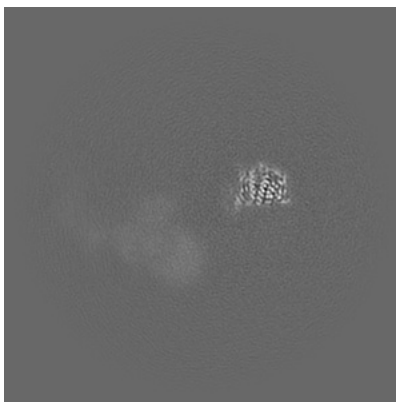
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

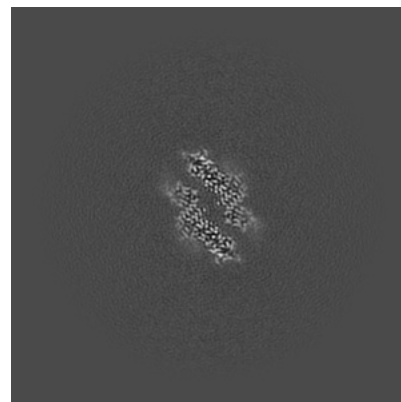
### 6.3.1 Primary map



X Index: 254

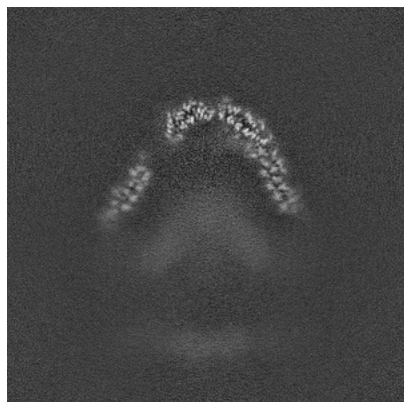


Y Index: 187

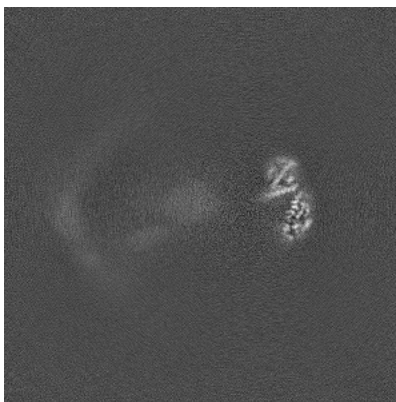


Z Index: 370

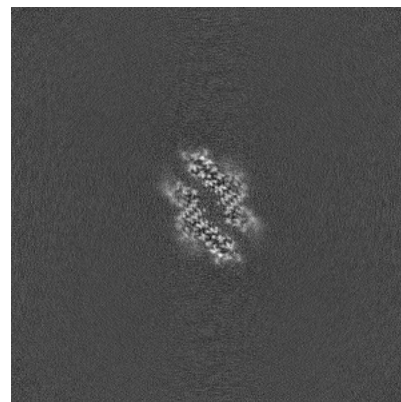
### 6.3.2 Raw map



X Index: 254



Y Index: 242

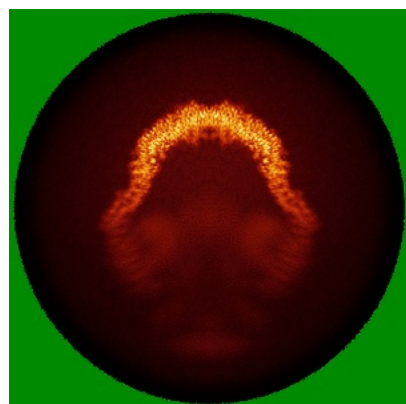


Z Index: 370

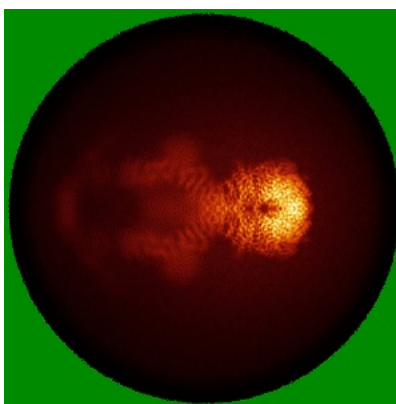
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

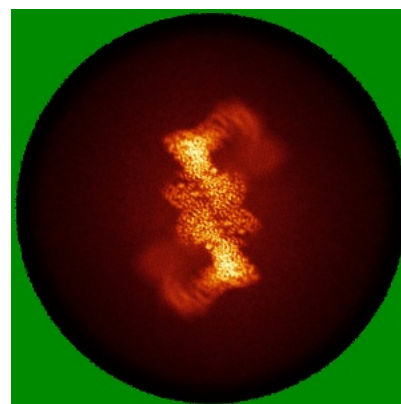
### 6.4.1 Primary map



X

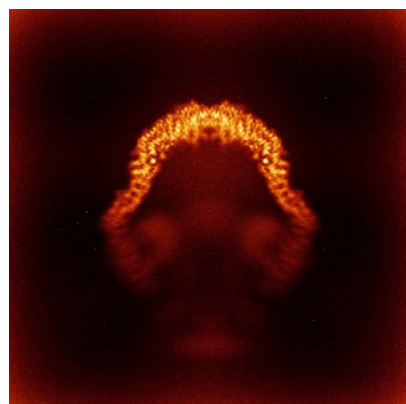


Y

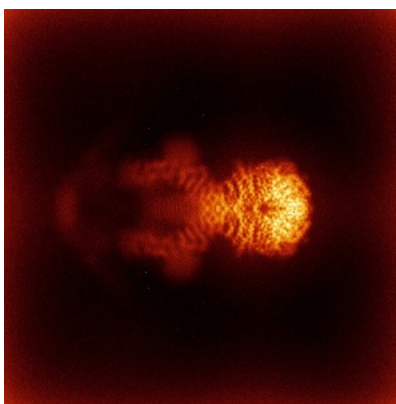


Z

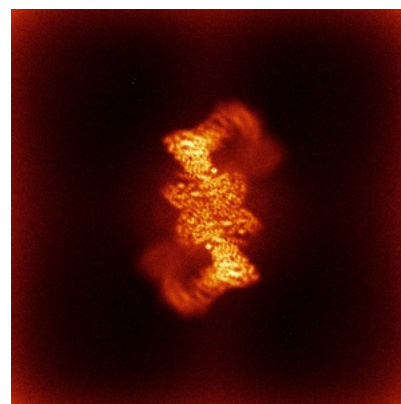
### 6.4.2 Raw map



X



Y

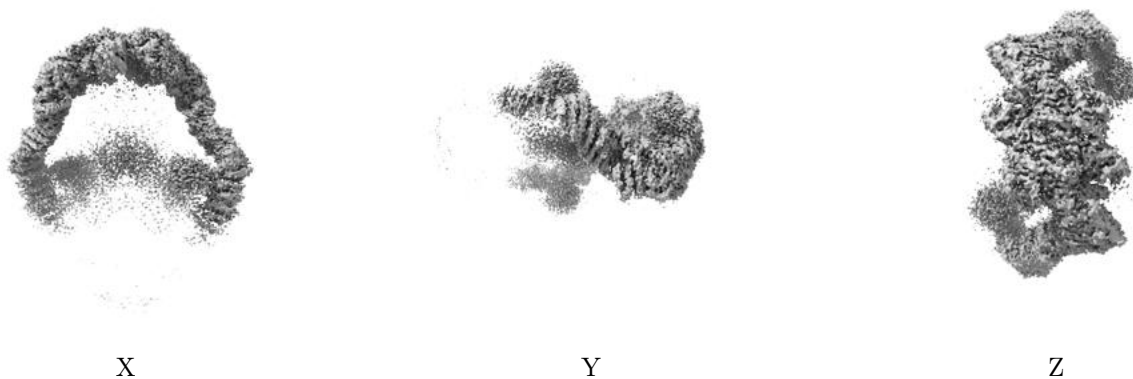


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

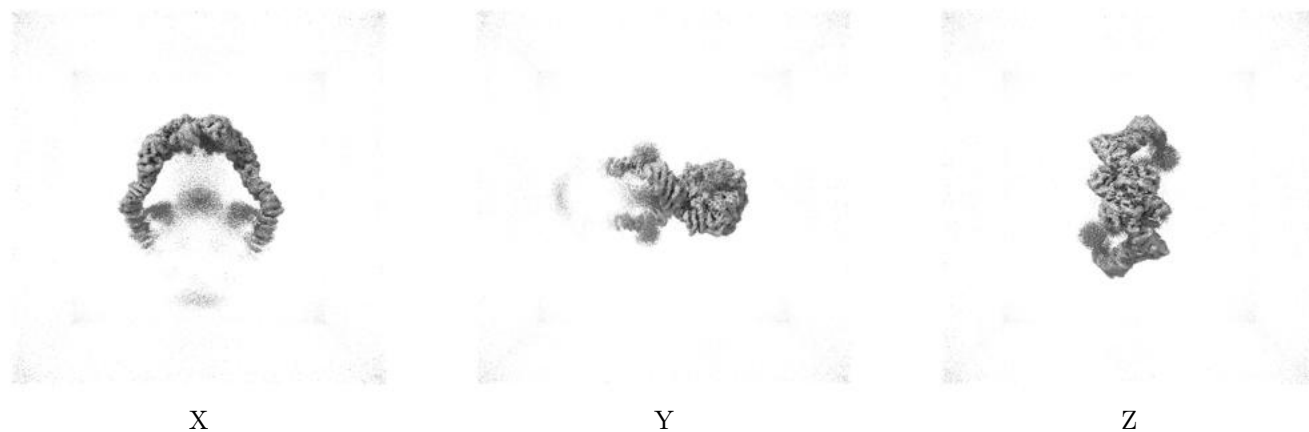
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.068. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

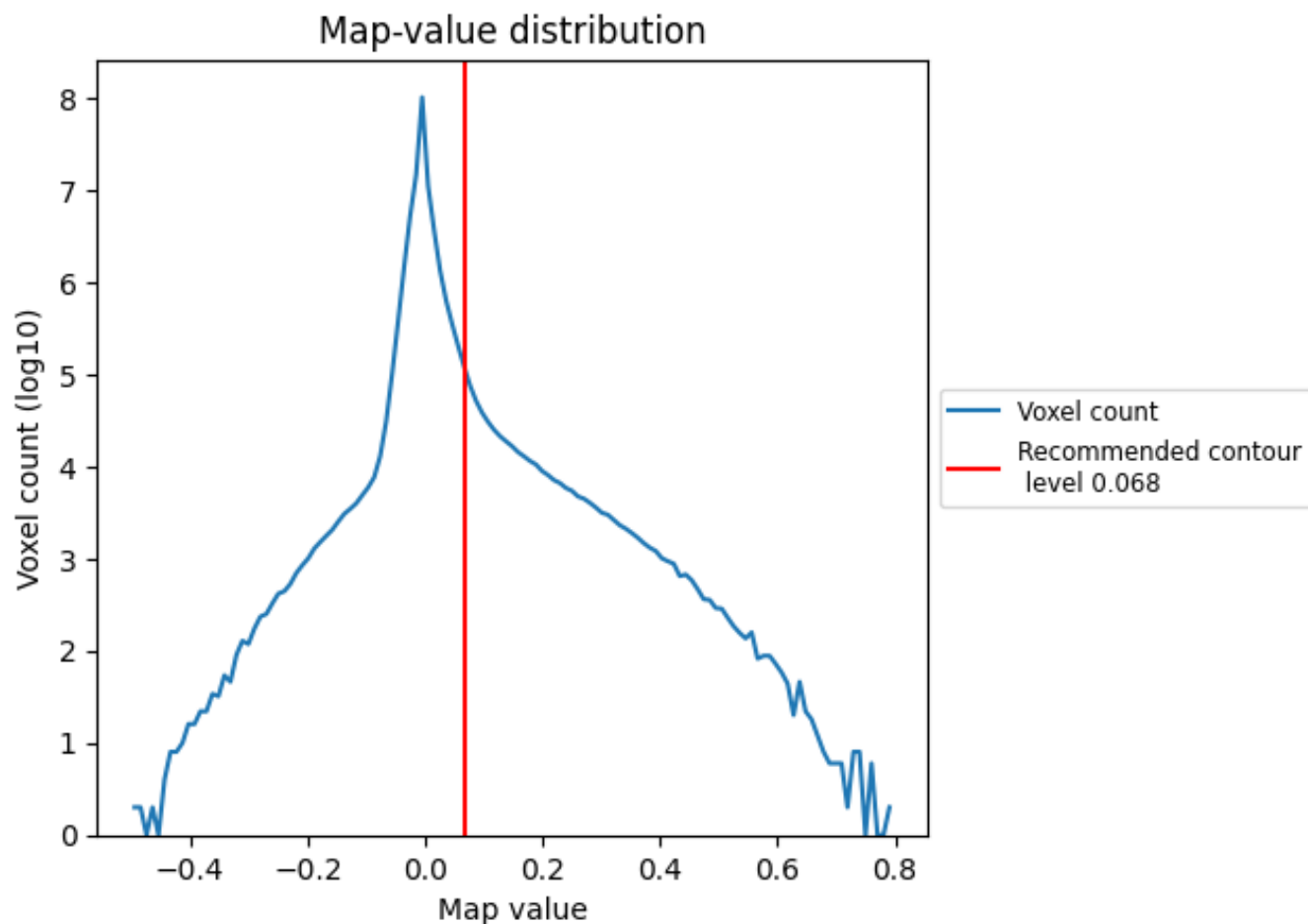
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

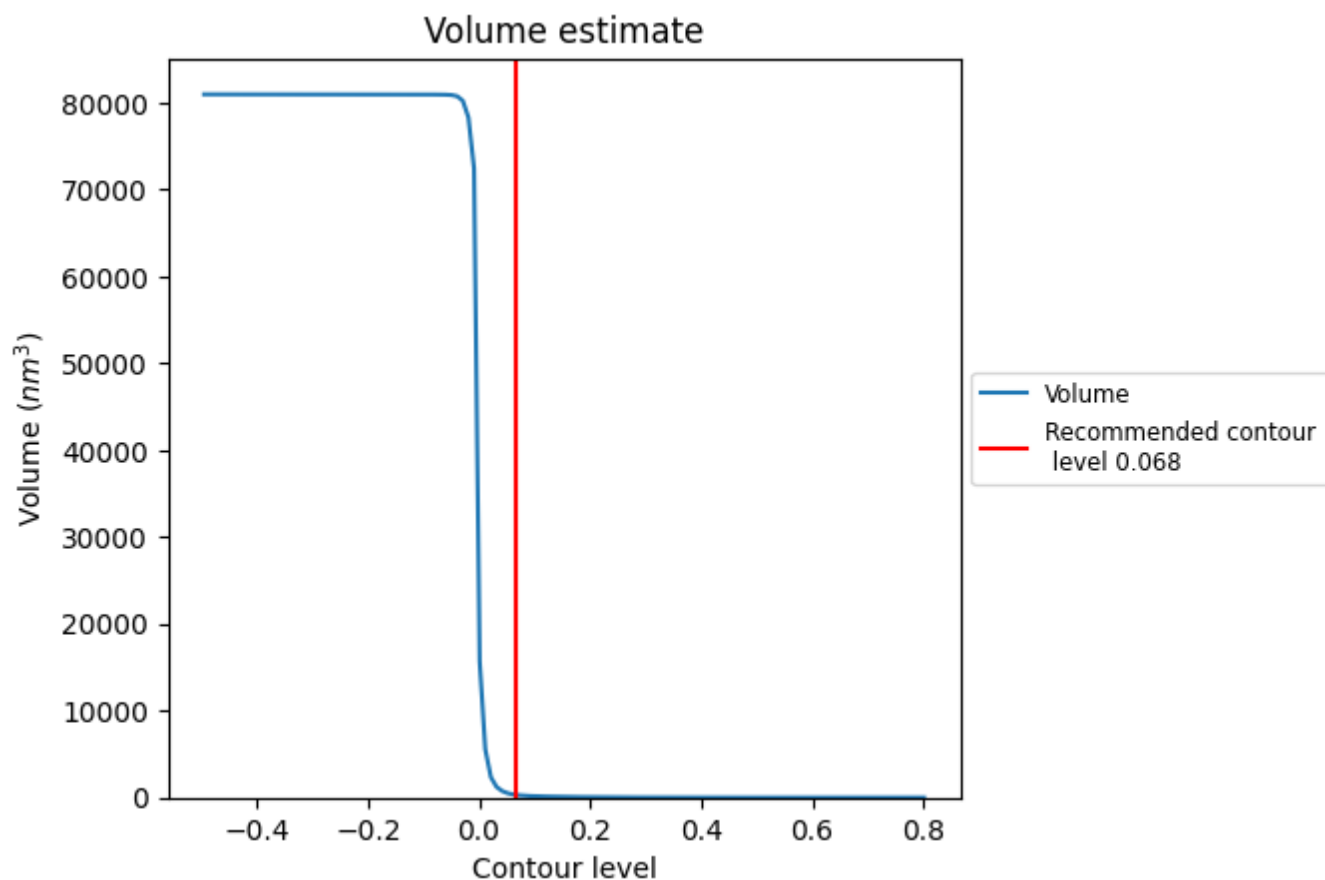
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

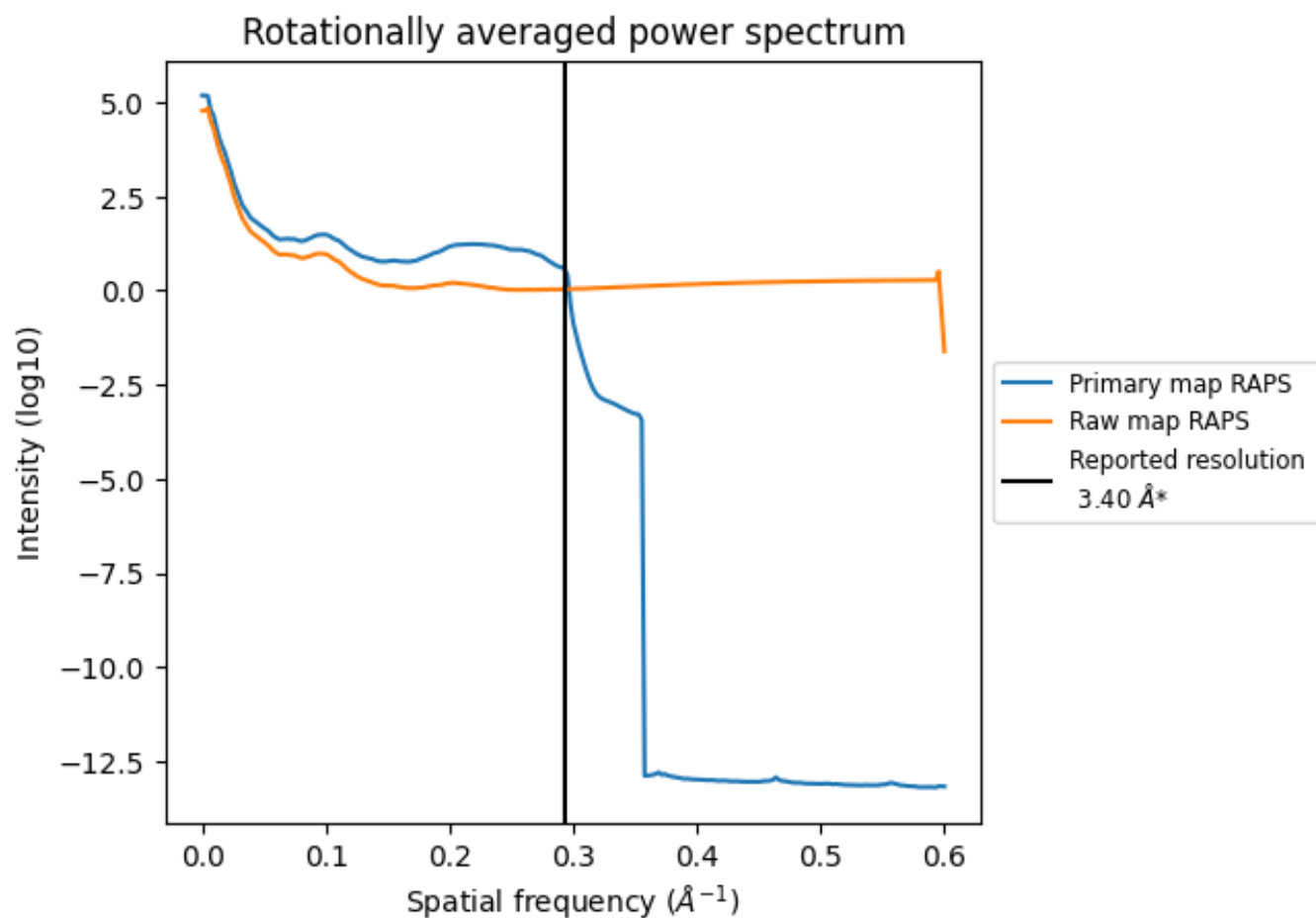
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 300 nm<sup>3</sup>; this corresponds to an approximate mass of 271 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

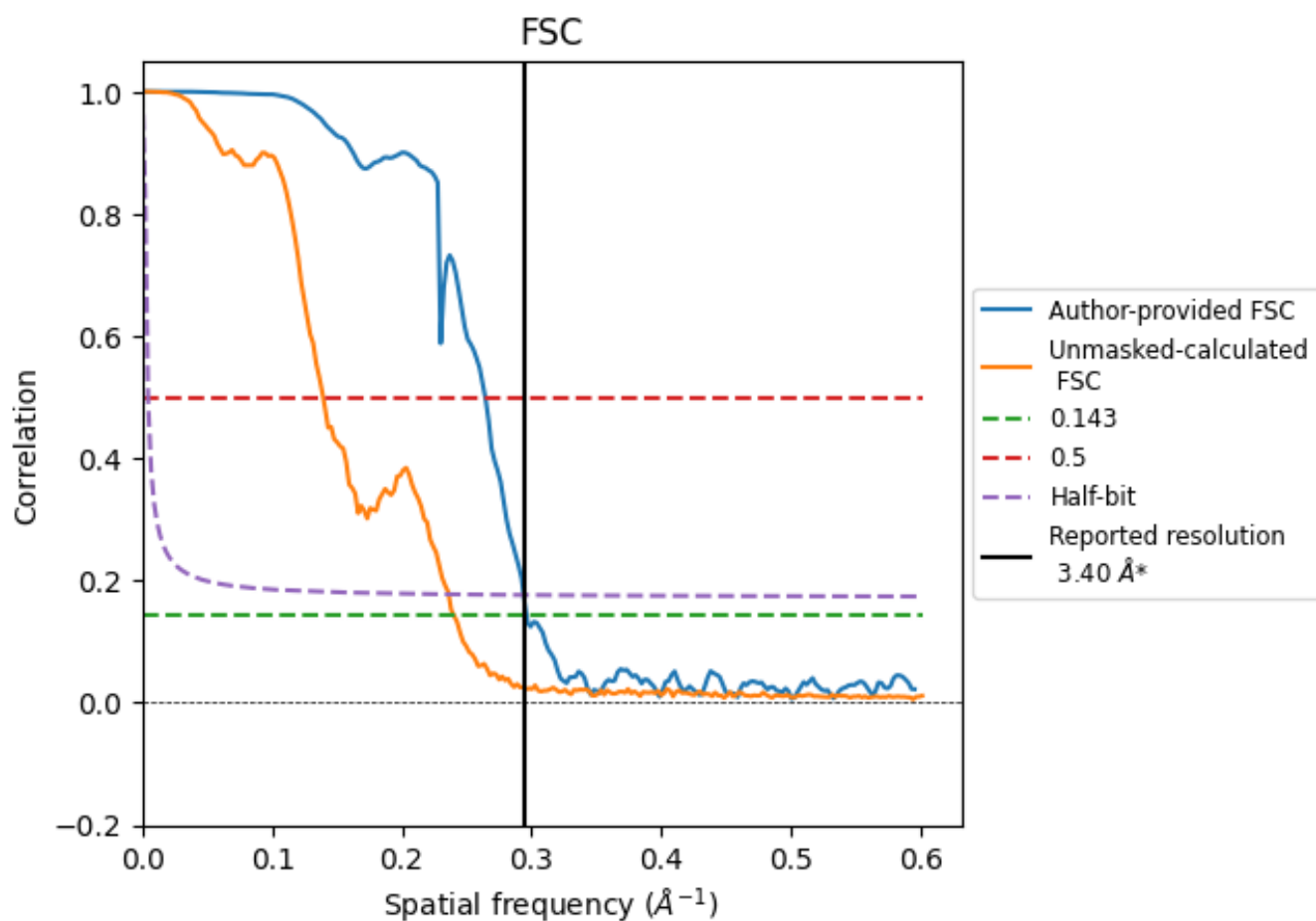


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.294  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

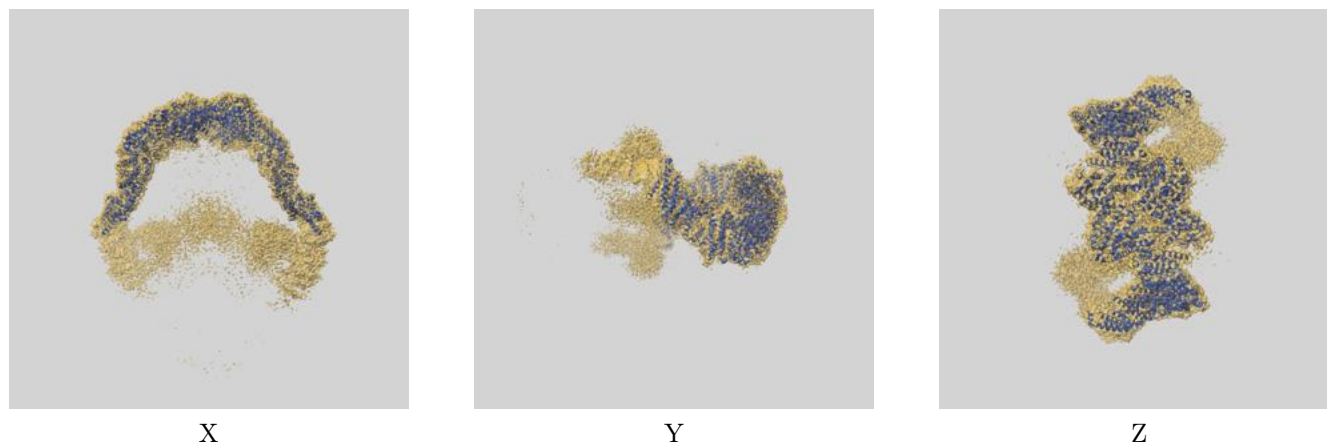
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.40                               | -    | -        |
| Author-provided FSC curve | 3.38                               | 3.78 | 3.40     |
| Unmasked-calculated*      | 4.16                               | 7.17 | 4.24     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.16 differs from the reported value 3.4 by more than 10 %

## 9 Map-model fit [i](#)

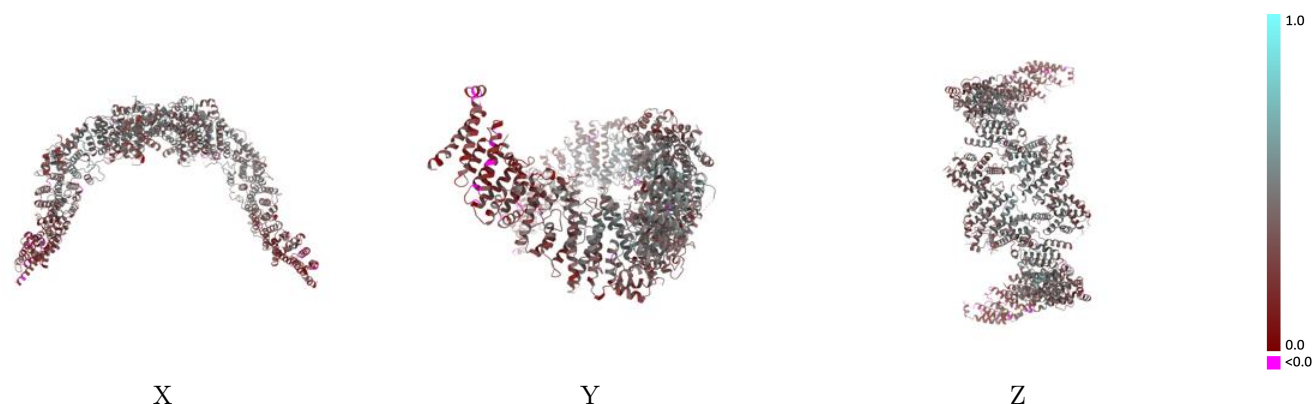
This section contains information regarding the fit between EMDB map EMD-46688 and PDB model 9NWD. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

### 9.1 Map-model overlay [i](#)



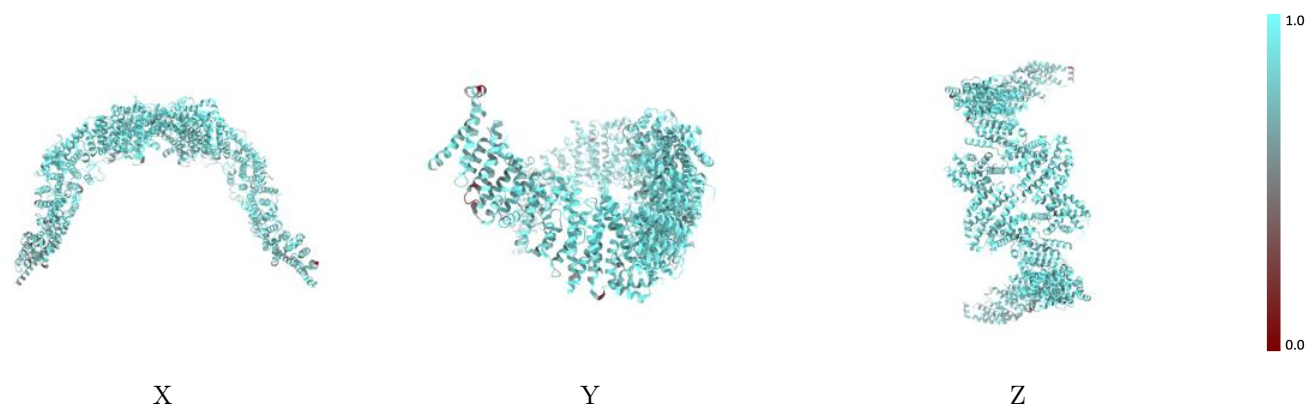
The images above show the 3D surface view of the map at the recommended contour level 0.068 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



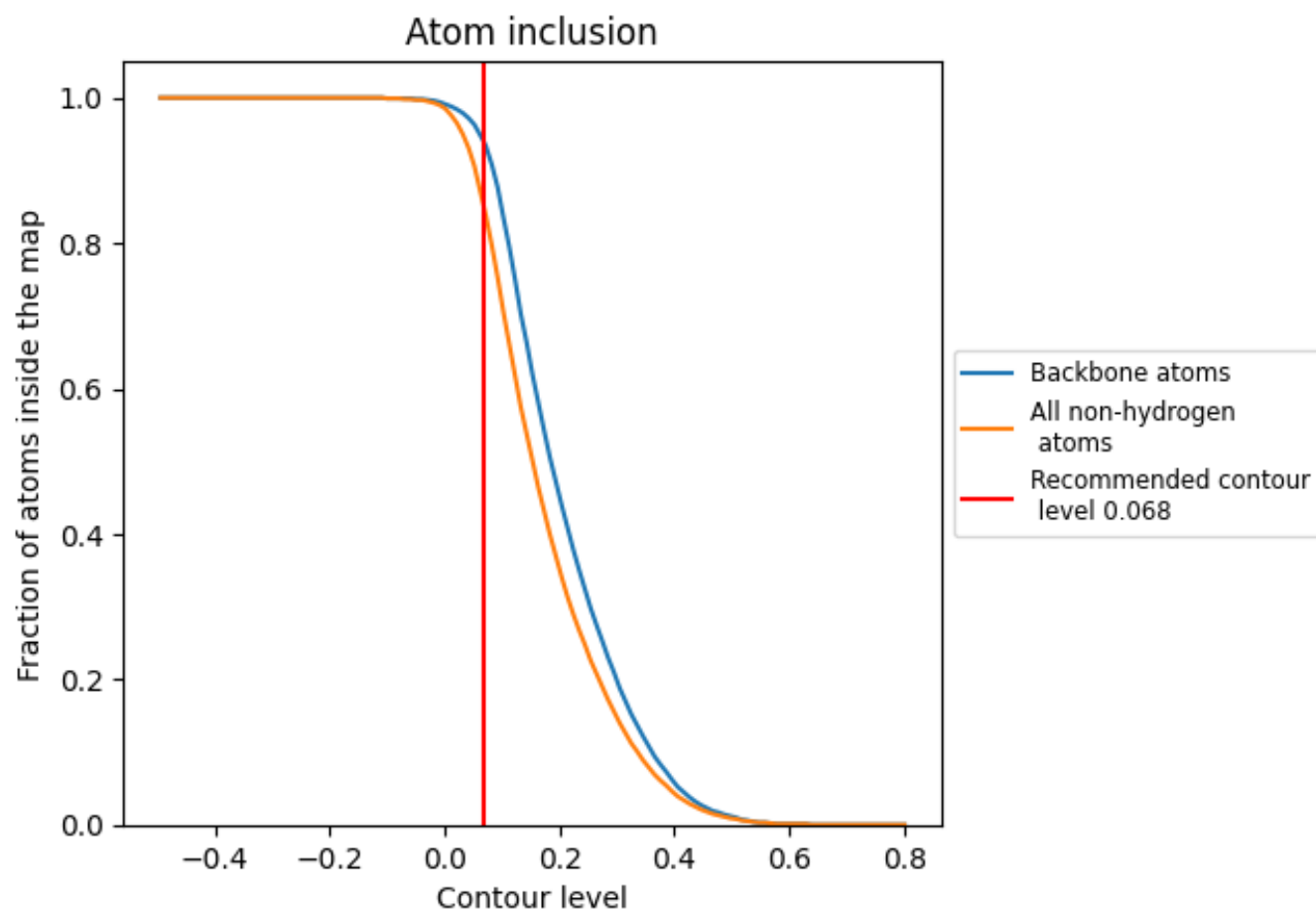
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.068).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.068) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.8510 | <div></div> 0.3640 |
| A     | <div></div> 0.8470 | <div></div> 0.3600 |
| B     | <div></div> 0.8550 | <div></div> 0.3680 |

