



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:20 PM UTC

PDB ID : 6WOY / pdb\_00006woy  
Title : Thermus thermophilus RNA polymerase initially transcribing complex with 3'dCTP  
Authors : Shin, Y.; Murakami, K.S.  
Deposited on : 2020-04-26  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

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:

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

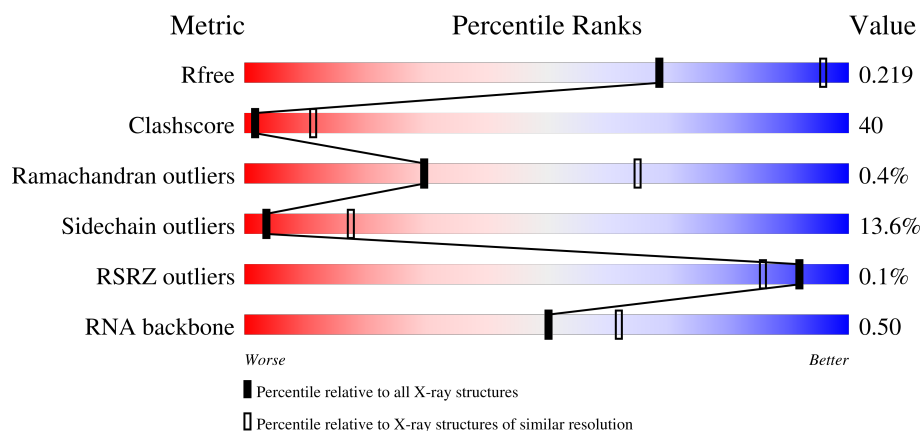
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



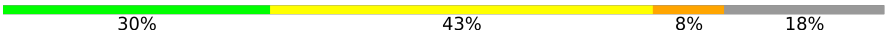
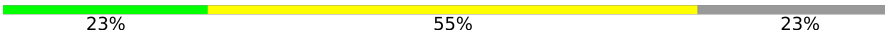
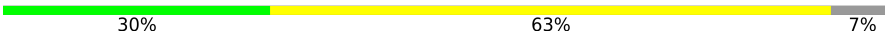
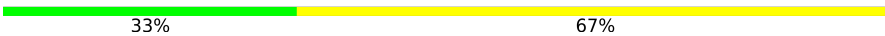
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 2672 (3.00-3.00)                                      |
| Clashscore            | 190562                      | 2977 (3.00-3.00)                                      |
| Ramachandran outliers | 187476                      | 2877 (3.00-3.00)                                      |
| Sidechain outliers    | 187428                      | 2880 (3.00-3.00)                                      |
| RSRZ outliers         | 180081                      | 2671 (3.00-3.00)                                      |
| RNA backbone          | 3983                        | 1109 (3.20-2.80)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                        |
|-----|-------|--------|-------------------------------------------------------------------------|
| 1   | A     | 315    | <div> <div>22%</div> <div>42%</div> <div>8%</div> <div>28%</div> </div> |
| 1   | B     | 315    | <div> <div>27%</div> <div>38%</div> <div>6%</div> <div>29%</div> </div> |
| 2   | C     | 1119   | <div> <div>40%</div> <div>51%</div> <div>9%</div> <div>.</div> </div>   |
| 3   | D     | 1505   | <div> <div>42%</div> <div>49%</div> <div>8%</div> <div>.</div> </div>   |

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| Mol | Chain | Length | Quality of chain                                                                                     |
|-----|-------|--------|------------------------------------------------------------------------------------------------------|
| 4   | E     | 99     | <br>41% 47% 6% 5%  |
| 5   | F     | 423    | <br>30% 43% 8% 18% |
| 6   | G     | 22     | <br>23% 55% 23%    |
| 7   | H     | 27     | <br>30% 63% 7%     |
| 8   | I     | 3      | <br>33% 67%        |

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28581 atoms, of which 12 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 226      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1782  | 1138 | 310 | 332 | 2 |         |         |       |
| 1   | B     | 224      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1767  | 1129 | 307 | 329 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | C     | 1111     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8770  | 5548 | 1564 | 1634 | 24 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3   | D     | 1485     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 11721 | 7431 | 2063 | 2192 | 35 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| D     | 86      | LYS      | ARG    | conflict | UNP Q8RQE8 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | E     | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 761   | 486 | 132 | 139 | 4 |         |         |       |

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | F     | 346      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2807  | 1770 | 509 | 524 | 4 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| F     | 46      | THR      | ALA    | conflict | UNP Q72L95 |

- Molecule 6 is a DNA chain called DNA (5'-D(P\*TP\*GP\*CP\*AP\*TP\*CP\*CP\*GP\*TP\*GP\*AP\*GP\*TP\*GP\*CP\*AP\*G)-3').

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 6   | G     | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 351   | 166 | 65 | 103 | 17 |         |         |       |

- Molecule 7 is a DNA chain called DNA (25-MER).

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 7   | H     | 25       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 516   | 246 | 99 | 147 | 24 |         |         |       |

- Molecule 8 is a RNA chain called RNA (5'-R(\*GP\*CP\*A)-3').

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 8   | I     | 3        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 62    | 29 | 13 | 18 | 2 |         |         |       |

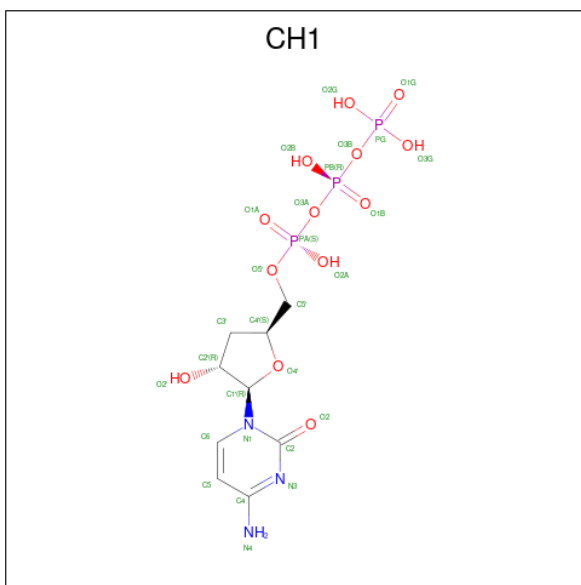
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 9   | D     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 10  | D     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 11 is 3'-DEOXY-CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CH1) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>).

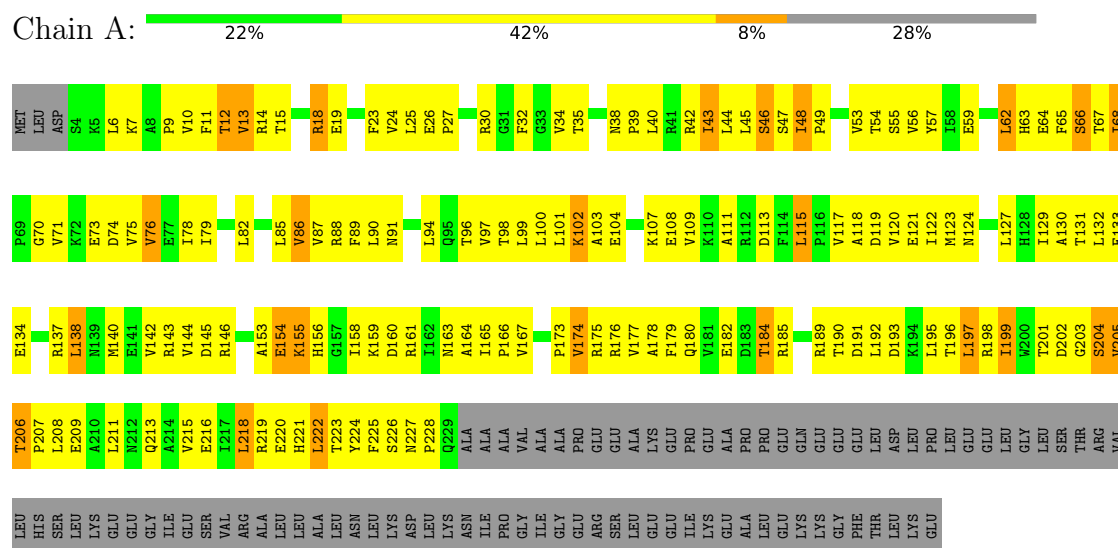


| Mol | Chain | Residues | Atoms |   |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|----|---|---------|---------|
| 11  | I     | 1        | Total | C | H  | N | O  | P | 0       | 0       |
|     |       |          | 40    | 9 | 12 | 3 | 13 | 3 |         |         |

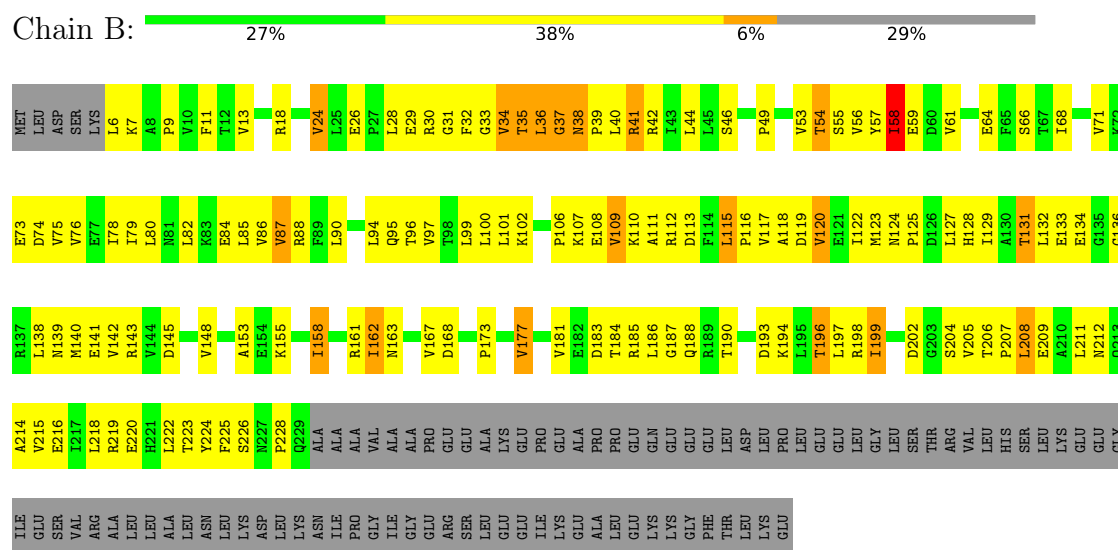
### 3 Residue-property plots

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

#### • Molecule 1: DNA-directed RNA polymerase subunit alpha

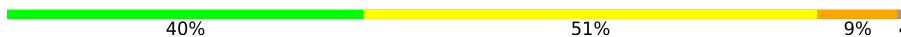


#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



#### • Molecule 2: DNA-directed RNA polymerase subunit beta

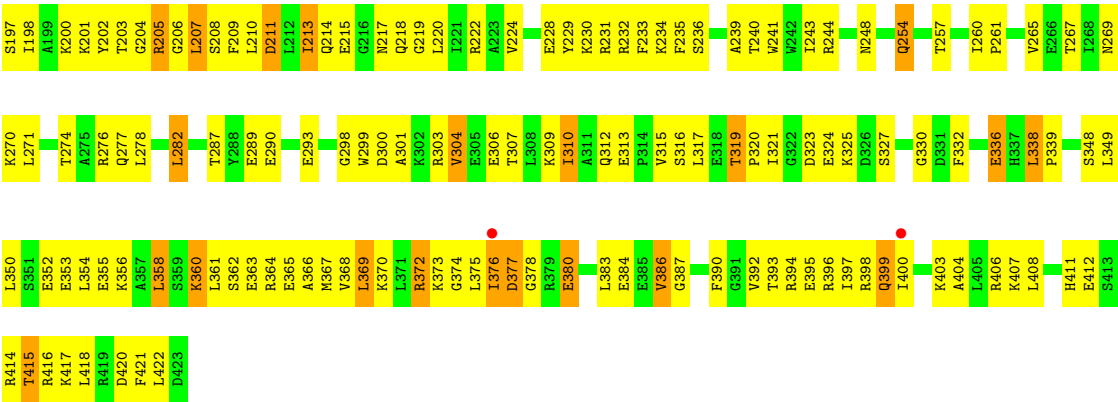
Chain C:



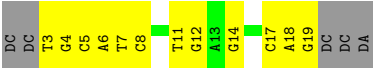
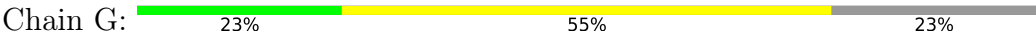
|      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| H1   | E2   | I3   | F6   | G7    | R8    | I9    | R10   | E11   | V12   | L15   | P16   | P17   | L18   | T19   | E20   | I21   | Q22   | V23   | E24   | S25   | R28   | A29   | L30   | Q31   | A32  | D33  | V34  | P35  | P36  | E37  | K38  | R39  | E40  | M41  | T44  | Q45  | A46  | R49  | E50  | T51  | P52  | P53  | M54  | E55  | E56  | GLU  | ASP  | LYS  | GLY  | LYS  | GLY  | L64  | V65  |      |
| L66  | D67  | F68  | L69  | E70   | Y71   | E72   | L73   | G74   | E75   | P76   | F79   | Q80   | R84   | E85   | K86   | D87   | L88   | Q91   | A92   | P93   | R97   | L98   | Q99   | L100  | A101 | E102 | I103 | P104 | T105 | G106 | L107 | S108 | K109 | E110 | D111 | E112 | L115 | G116 | H117 | I118 | P119 | L120 | M121 | T122 | E123 | D124 | F127 | I128 | L129 | M130 | G131 | A132 | D133 |      |
| I136 | V137 | H140 | I141 | Y142  | S143  | P144  | G145  | V146  | T149  | P150  | R154  | I162  | I163  | P164  | L165  | P166  | K167  | R168  | I172  | D173  | L174  | E175  | V176  | E177  | P178 | H179 | D180 | G181 | V182 | S183 | M184 | K185 | V186 | R189 | K190 | F191 | P192 | L193 | V194 | L195 | L196 | L197 | R198 | E199 | L200 | G201 | Y202 | D203 | Q204 | E205 | T206 |      |      |      |
| R209 | E210 | L211 | G212 | A213  | Y214  | G215  | E216  | L217  | Q219  | G220  | L221  | H222  | D223  | E224  | S225  | V226  | F227  | A228  | R229  | R230  | E233  | A234  | L235  | L236  | R237 | L238 | F239 | L240 | L241 | P244 | G245 | D246 | P247 | P248 | R249 | R250 | A253 | V254 | L260 | L261 | A262 | D263 | P264 | R265 | R266 | Y267 | D268 | L269 | E271 | K276 | A277 | E278 |      |      |
| E279 | K280 | L281 | G282 | R283  | L285  | L290  | A291  | K292  | Q2919 | F293  | E297  | F298  | K299  | D300  | E301  | V302  | F303  | L304  | P305  | T306  | L307  | R308  | Y309  | L310  | F311 | A312 | G316 | V317 | P318 | G319 | S387 | E321 | V322 | D323 | D326 | H327 | R331 | R332 | L333 | R334 | T335 | V336 | G337 | E338 | L339 | K340 | T341 | D342 | Q343 | F344 | R345 | L348 |      |      |
| L351 | A352 | R353 | G354 | V355  | R356  | R358  | K359  | L360  | K361  | G362  | S363  | E364  | D365  | S366  | L367  | T368  | P369  | A370  | K371  | L372  | R376  | P377  | L378  | E379  | A380 | A381 | L382 | R383 | E384 | F385 | F386 | S387 | R388 | S389 | Q390 | L391 | S392 | Q393 | F394 | K395 | D396 | E397 | S402 | D481 | L404 | R405 | H406 | K407 | R408 | R409 | A412 | L413 | G414 | L418 |
| T419 | R420 | E421 | R422 | V423  | A424  | F425  | D426  | Y427  | R428  | H431  | R432  | T433  | G436  | R437  | L438  | E442  | T443  | P444  | E445  | G446  | A447  | N448  | T449  | G450  | L451 | L452 | T453 | S454 | L455 | R460 | V461 | D462 | T467 | R469 | Y471 | R472 | R473 | V474 | T480 | D481 | R482 | Y485 | M486 | A488 | T489 | E490 | E491 | D492 | R493 | Y494 |      |      |      |      |
| T495 | Q498 | A499 | N500 | T501  | P502  | L503  | R507  | L508  | V513  | V514  | A515  | R516  | R517  | K518  | G519  | E520  | L521  | E522  | V524  | E528  | V529  | V534  | S535  | P536  | E537 | Q538 | V539 | F540 | S541 | V542 | N543 | T544 | N545 | L546 | L547 | E551 | H552 | D553 | D554 | R557 | A558 | L559 | M560 | M564 | Q565 | T566 | R567 | A568 | P570 | L571 |      |      |      |      |
| L572 | P577 | V578 | R579 | M580  | L583  | E584  | E585  | R586  | V587  | G588  | F589  | L590  | L592  | A593  | E594  | L595  | L596  | A597  | E598  | E599  | E602  | V603  | K605  | V606  | D607 | G608 | N609 | V613 | R614 | N615 | E616 | D617 | G618 | R619 | V623 | R626 | R627 | F628 | R630 | S631 | N632 | Q633 | Q639 | R640 | P641 | R642 | V643 | V645 |      |      |      |      |      |      |
| G646 | Q647 | R648 | V649 | K651  | L654  | L655  | A656  | G664  | F665  | L666  | A667  | G669  | Q670  | N671  | V672  | L673  | A674  | G675  | L676  | N677  | F678  | F679  | D680  | G681  | V682 | N683 | F684 | E685 | V689 | I690 | E693 | K696 | R697 | D698 | F699 | Y700 | T701 | S702 | I703 | H704 | I705 | E706 | R707 | Y708 | E709 | I710 | E711 | A712 | R713 | D714 | K716 |      |      |      |
| L717 | G718 | P719 | E720 | T721  | R722  | T723  | R724  | D725  | P726  | T727  | H728  | R729  | S730  | D736  | L737  | R738  | E739  | G740  | V742  | A743  | R744  | I745  | G746  | A747  | E748 | V749 | K750 | L751 | G752 | L753 | R754 | L755 | V756 | T759 | S760 | F761 | K762 | S765 | Q829 | V830 | R831 | L833 | Q834 | K838 | N841 | G844 | N845 | K846 | T852 | L853 | P854 |      |      |      |
| D784 | V785 | K786 | D787 | T788  | S789  | L790  | R791  | V792  | P793  | E796  | G797  | G798  | V799  | R801  | V802  | T803  | V804  | R805  | L806  | R807  | R808  | G809  | D810  | P811  | G812 | V813 | E814 | L815 | K816 | V819 | R820 | E821 | V822 | R823 | R824 | V825 | A828 | R829 | R830 | R831 | L833 | Q834 | K838 | N841 | G844 | N845 | K846 | T852 | L853 | P854 |      |      |      |      |
| V855 | E856 | M858 | L861 | P862  | D863  | G864  | P865  | G866  | V867  | G868  | V869  | L870  | R871  | N872  | P873  | L874  | G875  | V876  | S877  | R878  | R879  | M880  | N881  | L882  | G883 | Q884 | E885 | L886 | E887 | T888 | H889 | L890 | G891 | L892 | A893 | L897 | G898 | Q899 | Y901 | I902 | P904 | I905 | F906 | D907 | G908 | K910 | I914 | N915 | E916 | L917 | Y918 | E919 |      |      |
| Q920 | A921 | F926 | G927 | K928  | R929  | K930  | G931  | E932  | M933  | F934  | G935  | V936  | D937  | K938  | R939  | E940  | V941  | E942  | L944  | R945  | R946  | A947  | E948  | R949  | L950 | G951 | L952 | V953 | T954 | K957 | T958 | P959 | E960 | E961 | Q962 | L963 | K964 | L968 | Q969 | G970 | K971 | T979 | I983 | E984 | G985 | P986 | R987 | V988 | R989 | A990 | G991 | Y992 | F993 |      |
| I994 | L997 | Y998 | H999 | M1000 | V1001 | E1002 | D1003 | K1004 | M1005 | H1006 | A1007 | R1008 | S1009 | P1012 | Y1013 | S1014 | L1015 | L1016 | Q1019 | P1020 | L1021 | K1024 | G1028 | G1029 | L952 | V953 | T954 | K957 | T958 | P959 | E960 | E961 | Q962 | L963 | K964 | L968 | Q969 | G970 | K971 | T979 | I983 | E984 | G985 | P986 | R987 | V988 | R989 | A990 | G991 | Y992 | F993 |      |      |      |







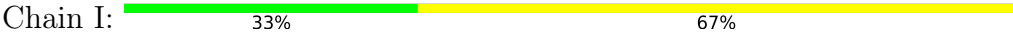
● Molecule 6: DNA (5'-D(P\*TP\*GP\*CP\*AP\*TP\*CP\*CP\*GP\*TP\*GP\*AP\*GP\*TP\*GP\*CP\*A P\*G)-3')



● Molecule 7: DNA (25-MER)



● Molecule 8: RNA (5'-R(\*GP\*CP\*A)-3')



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 185.98Å 102.47Å 296.04Å<br>90.00° 98.86° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 29.98 – 3.00<br>29.98 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.5 (29.98-3.00)<br>96.5 (29.98-3.00)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.21 (at 3.00Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.15.2_3472                                          | Depositor        |
| R, $R_{free}$                                                           | 0.206 , 0.219<br>0.206 , 0.219                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2006 reflections (1.81%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 79.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.748                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 47.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 28581                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 84.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, CH1

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     | 0.41         | 0/1814  | 0.64        | 0/2466         |
| 1   | B     | 0.41         | 0/1799  | 0.65        | 0/2447         |
| 2   | C     | 0.42         | 0/8937  | 0.62        | 0/12087        |
| 3   | D     | 0.44         | 0/11927 | 0.67        | 2/16127 (0.0%) |
| 4   | E     | 0.39         | 0/775   | 0.57        | 0/1045         |
| 5   | F     | 0.40         | 0/2852  | 0.63        | 0/3837         |
| 6   | G     | 0.51         | 0/393   | 0.63        | 0/605          |
| 7   | H     | 0.43         | 0/580   | 0.58        | 0/895          |
| 8   | I     | 0.41         | 0/69    | 0.50        | 0/106          |
| All | All   | 0.43         | 0/29146 | 0.64        | 2/39615 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | B     | 0                   | 2                   |
| 2   | C     | 0                   | 2                   |
| 3   | D     | 0                   | 6                   |
| All | All   | 0                   | 11                  |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|------|-------------|----------|
| 3   | D     | 1234 | THR  | CA-C-N | 5.92 | 132.35      | 121.70   |
| 3   | D     | 1234 | THR  | C-N-CA | 5.92 | 132.35      | 121.70   |

There are no chirality outliers.

All (11) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 46  | SER  | Peptide |
| 1   | B     | 46  | SER  | Peptide |
| 1   | B     | 58  | ILE  | Peptide |
| 2   | C     | 268 | ASP  | Peptide |
| 2   | C     | 766 | GLU  | Peptide |
| 3   | D     | 273 | ARG  | Peptide |
| 3   | D     | 275 | GLU  | Peptide |
| 3   | D     | 64  | LYS  | Peptide |
| 3   | D     | 704 | ARG  | Peptide |
| 3   | D     | 711 | LEU  | Peptide |
| 3   | D     | 782 | SER  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1782  | 0        | 1834     | 180     | 0            |
| 1   | B     | 1767  | 0        | 1816     | 194     | 0            |
| 2   | C     | 8770  | 0        | 8874     | 768     | 1            |
| 3   | D     | 11721 | 0        | 11941    | 992     | 2            |
| 4   | E     | 761   | 0        | 778      | 62      | 0            |
| 5   | F     | 2807  | 0        | 2882     | 273     | 1            |
| 6   | G     | 351   | 0        | 192      | 19      | 0            |
| 7   | H     | 516   | 0        | 283      | 29      | 0            |
| 8   | I     | 62    | 0        | 34       | 3       | 0            |
| 9   | D     | 2     | 0        | 0        | 0       | 0            |
| 10  | D     | 2     | 0        | 0        | 0       | 0            |
| 11  | I     | 28    | 12       | 11       | 2       | 0            |
| All | All   | 28569 | 12       | 28645    | 2305    | 2            |

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 40.

All (2305) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:H:15:DT:H2''    | 7:H:16:DC:H5'     | 1.22                     | 1.16              |
| 3:D:704:ARG:HB2   | 3:D:745:MET:HE2   | 1.24                     | 1.14              |
| 5:F:338:LEU:HD23  | 5:F:339:PRO:HD2   | 1.21                     | 1.13              |
| 1:A:206:THR:HG22  | 1:A:209:GLU:HG3   | 1.24                     | 1.11              |
| 3:D:203:ALA:HB1   | 3:D:393:ILE:HD11  | 1.31                     | 1.10              |
| 2:C:1012:PRO:HB2  | 2:C:1021:LEU:HD13 | 1.32                     | 1.08              |
| 5:F:367:MET:HE3   | 5:F:368:VAL:HG13  | 1.35                     | 1.08              |
| 2:C:200:LEU:HD22  | 2:C:300:ASP:HB2   | 1.24                     | 1.06              |
| 3:D:65:ARG:HB3    | 5:F:377:ASP:HA    | 1.37                     | 1.05              |
| 2:C:1052:MET:HG3  | 3:D:623:VAL:HG11  | 1.30                     | 1.05              |
| 1:A:215:VAL:HG13  | 1:B:222:LEU:HD22  | 1.37                     | 1.04              |
| 3:D:1060:SER:HB3  | 3:D:1063:GLU:HG3  | 1.39                     | 1.04              |
| 2:C:853:LEU:HB2   | 2:C:858:MET:HE1   | 1.38                     | 1.04              |
| 3:D:97:THR:HG21   | 3:D:571:LYS:HD3   | 1.36                     | 1.04              |
| 5:F:160:ASP:HA    | 5:F:163:LEU:HD12  | 1.38                     | 1.03              |
| 5:F:361:LEU:HD11  | 5:F:411:HIS:HB2   | 1.39                     | 1.03              |
| 1:A:88:ARG:HB3    | 1:A:123:MET:HE3   | 1.41                     | 1.02              |
| 3:D:767:HIS:HA    | 3:D:924:MET:HE3   | 1.38                     | 1.01              |
| 3:D:170:PRO:HA    | 3:D:392:SER:HB2   | 1.40                     | 1.01              |
| 2:C:343:GLN:HG3   | 2:C:385:PHE:HB2   | 1.43                     | 1.01              |
| 3:D:1234:THR:HB   | 3:D:1235:GLN:HB2  | 1.41                     | 1.00              |
| 3:D:705:ALA:HB3   | 3:D:706:PRO:HD3   | 1.44                     | 0.99              |
| 2:C:683:ASN:HB3   | 2:C:872:ASN:HB2   | 1.44                     | 0.99              |
| 3:D:216:VAL:HA    | 3:D:340:THR:HG22  | 1.41                     | 0.99              |
| 1:B:86:VAL:HG13   | 1:B:123:MET:HB2   | 1.46                     | 0.98              |
| 1:B:107:LYS:NZ    | 1:B:113:ASP:OD2   | 1.97                     | 0.97              |
| 3:D:473:LEU:HD21  | 3:D:495:ARG:HH21  | 1.26                     | 0.97              |
| 3:D:582:LEU:O     | 3:D:604:THR:HG23  | 1.65                     | 0.97              |
| 3:D:1047:LYS:HG2  | 3:D:1048:PRO:HD2  | 1.46                     | 0.97              |
| 1:B:128:HIS:HE1   | 1:B:131:THR:HG22  | 1.28                     | 0.96              |
| 5:F:338:LEU:HD23  | 5:F:339:PRO:CD    | 1.94                     | 0.96              |
| 2:C:1070:ILE:HG21 | 3:D:655:PRO:HB2   | 1.47                     | 0.95              |
| 2:C:880:MET:HE3   | 3:D:1037:GLN:HB2  | 1.48                     | 0.95              |
| 5:F:362:SER:HB3   | 5:F:365:GLU:HG2   | 1.44                     | 0.95              |
| 3:D:646:LYS:HB3   | 3:D:720:LEU:HD23  | 1.47                     | 0.95              |
| 2:C:150:PRO:HD3   | 2:C:322:VAL:HG11  | 1.47                     | 0.95              |
| 3:D:116:LEU:HB2   | 3:D:118:LEU:HD12  | 1.48                     | 0.95              |
| 3:D:181:ASP:HB2   | 3:D:205:TYR:CD1   | 2.02                     | 0.94              |
| 2:C:888:THR:HG22  | 2:C:990:GLY:HA3   | 1.49                     | 0.94              |
| 3:D:1236:LEU:HD22 | 3:D:1359:GLN:HG3  | 1.48                     | 0.94              |
| 5:F:358:LEU:HB3   | 5:F:366:ALA:HB1   | 1.49                     | 0.94              |
| 2:C:755:LEU:HD11  | 2:C:792:VAL:HG12  | 1.47                     | 0.94              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:853:LEU:HB2  | 2:C:858:MET:CE    | 1.96                     | 0.94              |
| 1:A:222:LEU:HD23 | 1:B:215:VAL:HG13  | 1.50                     | 0.94              |
| 3:D:1042:ARG:HB3 | 3:D:1057:VAL:HG13 | 1.50                     | 0.93              |
| 2:C:197:LEU:HA   | 2:C:200:LEU:HD12  | 1.51                     | 0.93              |
| 2:C:109:LYS:HG2  | 2:C:368:THR:HG22  | 1.51                     | 0.93              |
| 2:C:3:ILE:HD12   | 2:C:900:ARG:HB2   | 1.48                     | 0.92              |
| 3:D:643:GLY:HA3  | 3:D:727:GLN:HB2   | 1.49                     | 0.92              |
| 1:A:198:ARG:O    | 1:A:199:ILE:HG12  | 1.69                     | 0.92              |
| 3:D:949:ILE:HD11 | 3:D:1023:MET:HE1  | 1.53                     | 0.91              |
| 3:D:1234:THR:CB  | 3:D:1235:GLN:HB2  | 2.00                     | 0.91              |
| 3:D:236:TYR:H    | 3:D:319:ALA:HB3   | 1.36                     | 0.91              |
| 3:D:558:LEU:HD23 | 3:D:567:ILE:CD1   | 2.01                     | 0.90              |
| 3:D:986:ARG:HH11 | 3:D:986:ARG:HB2   | 1.36                     | 0.90              |
| 5:F:109:GLY:O    | 5:F:113:ILE:HG13  | 1.68                     | 0.90              |
| 2:C:177:GLU:HG3  | 2:C:178:PRO:HD2   | 1.54                     | 0.90              |
| 5:F:319:THR:HG22 | 5:F:320:PRO:HD2   | 1.52                     | 0.90              |
| 3:D:798:GLU:HG3  | 3:D:824:ASN:HB2   | 1.53                     | 0.90              |
| 3:D:97:THR:HG21  | 3:D:571:LYS:CD    | 2.02                     | 0.90              |
| 3:D:650:LEU:HD12 | 3:D:657:LEU:HD23  | 1.53                     | 0.90              |
| 1:A:159:LYS:HB3  | 1:A:164:ALA:HB3   | 1.54                     | 0.89              |
| 3:D:413:ASP:O    | 3:D:435:VAL:HG12  | 1.72                     | 0.89              |
| 2:C:211:LEU:HD23 | 2:C:218:VAL:HG22  | 1.55                     | 0.89              |
| 1:A:222:LEU:HD11 | 1:B:218:LEU:HD23  | 1.54                     | 0.88              |
| 2:C:234:ALA:HA   | 2:C:237:ARG:HB2   | 1.55                     | 0.88              |
| 3:D:203:ALA:HB1  | 3:D:393:ILE:CD1   | 2.03                     | 0.88              |
| 3:D:254:GLU:O    | 3:D:255:GLU:HG2   | 1.73                     | 0.88              |
| 3:D:284:LEU:HD23 | 3:D:290:PRO:HG3   | 1.53                     | 0.88              |
| 2:C:102:HIS:HB2  | 2:C:107:LEU:HB3   | 1.54                     | 0.88              |
| 2:C:666:LEU:HD11 | 2:C:668:LEU:HD21  | 1.53                     | 0.88              |
| 3:D:411:THR:HG22 | 5:F:178:ARG:HB3   | 1.53                     | 0.88              |
| 1:A:99:LEU:O     | 1:A:100:LEU:HD23  | 1.72                     | 0.88              |
| 2:C:260:LEU:HB3  | 2:C:261:ILE:HD12  | 1.54                     | 0.88              |
| 2:C:1012:PRO:HB2 | 2:C:1021:LEU:CD1  | 2.02                     | 0.87              |
| 3:D:807:ALA:O    | 3:D:830:ALA:HB2   | 1.74                     | 0.87              |
| 3:D:374:GLU:O    | 3:D:375:GLU:HG2   | 1.75                     | 0.87              |
| 3:D:401:TYR:OH   | 3:D:430:ASP:HB2   | 1.74                     | 0.87              |
| 4:E:83:ASP:HA    | 4:E:86:GLN:HG2    | 1.57                     | 0.87              |
| 7:H:20:DG:H2''   | 7:H:21:DA:H5'     | 1.57                     | 0.87              |
| 3:D:65:ARG:HD3   | 5:F:377:ASP:H     | 1.39                     | 0.87              |
| 3:D:260:GLU:OE1  | 3:D:273:ARG:NH1   | 2.08                     | 0.86              |
| 3:D:764:LEU:HD23 | 3:D:767:HIS:CD2   | 2.09                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:86:VAL:HG12   | 1:B:124:ASN:OD1   | 1.76                     | 0.86              |
| 1:A:193:ASP:OD1   | 2:C:938:LYS:NZ    | 2.09                     | 0.86              |
| 5:F:289:GLU:HG3   | 5:F:301:ALA:HB2   | 1.58                     | 0.86              |
| 3:D:407:VAL:HG13  | 3:D:422:ALA:HB2   | 1.57                     | 0.85              |
| 5:F:95:THR:HG22   | 5:F:98:GLU:CG     | 2.06                     | 0.85              |
| 3:D:558:LEU:HD23  | 3:D:567:ILE:HD12  | 1.55                     | 0.85              |
| 2:C:948:GLU:HG3   | 2:C:953:VAL:HG23  | 1.55                     | 0.85              |
| 2:C:905:ILE:HG23  | 2:C:906:PHE:HD1   | 1.41                     | 0.85              |
| 3:D:885:ILE:HD13  | 3:D:937:TYR:CD1   | 2.12                     | 0.85              |
| 3:D:204:LEU:O     | 3:D:393:ILE:HG13  | 1.76                     | 0.84              |
| 1:A:206:THR:CG2   | 1:A:209:GLU:HG3   | 2.06                     | 0.84              |
| 2:C:760:SER:HB2   | 2:C:788:THR:HG21  | 1.58                     | 0.84              |
| 3:D:65:ARG:CB     | 5:F:377:ASP:HA    | 2.06                     | 0.84              |
| 3:D:434:ARG:O     | 3:D:447:VAL:HG23  | 1.78                     | 0.84              |
| 2:C:195:LEU:HD11  | 2:C:237:ARG:HB3   | 1.59                     | 0.84              |
| 3:D:658:LEU:HA    | 3:D:661:MET:HE3   | 1.59                     | 0.84              |
| 2:C:474:VAL:HG11  | 2:C:529:VAL:HG12  | 1.58                     | 0.84              |
| 3:D:1172:HIS:HA   | 3:D:1175:ILE:HD12 | 1.60                     | 0.84              |
| 5:F:163:LEU:HB3   | 5:F:174:LEU:HD13  | 1.60                     | 0.83              |
| 3:D:657:LEU:HG    | 3:D:661:MET:HE2   | 1.60                     | 0.83              |
| 5:F:153:PRO:HA    | 5:F:156:VAL:HG12  | 1.59                     | 0.83              |
| 1:B:124:ASN:ND2   | 1:B:127:LEU:HD12  | 1.93                     | 0.83              |
| 2:C:1021:LEU:H    | 2:C:1021:LEU:HD12 | 1.41                     | 0.83              |
| 3:D:93:ILE:HD11   | 3:D:548:ILE:HD11  | 1.59                     | 0.83              |
| 2:C:317:VAL:HB    | 2:C:320:HIS:CD2   | 2.14                     | 0.83              |
| 3:D:520:LEU:O     | 3:D:525:ARG:NH1   | 2.10                     | 0.83              |
| 3:D:185:VAL:HG13  | 3:D:189:GLN:OE1   | 1.78                     | 0.83              |
| 3:D:705:ALA:CB    | 3:D:706:PRO:HD3   | 2.08                     | 0.83              |
| 3:D:956:ILE:HD13  | 3:D:1039:CYS:O    | 1.79                     | 0.83              |
| 3:D:473:LEU:HD21  | 3:D:495:ARG:NH2   | 1.94                     | 0.82              |
| 3:D:1232:PRO:O    | 3:D:1235:GLN:HB3  | 1.78                     | 0.82              |
| 2:C:181:VAL:HG23  | 2:C:221:LEU:HA    | 1.61                     | 0.82              |
| 2:C:815:LEU:HD12  | 2:C:819:VAL:HG23  | 1.60                     | 0.82              |
| 3:D:209:ARG:HH21  | 3:D:391:ALA:HA    | 1.44                     | 0.82              |
| 3:D:1065:LEU:HD23 | 3:D:1069:GLU:HB3  | 1.62                     | 0.82              |
| 5:F:95:THR:H      | 5:F:98:GLU:HG3    | 1.45                     | 0.82              |
| 1:B:36:LEU:O      | 1:B:38:ASN:N      | 2.13                     | 0.82              |
| 2:C:150:PRO:HD3   | 2:C:322:VAL:CG1   | 2.10                     | 0.82              |
| 3:D:275:GLU:O     | 3:D:277:GLU:N     | 2.12                     | 0.82              |
| 5:F:267:THR:O     | 5:F:270:LYS:HB2   | 1.80                     | 0.82              |
| 1:A:30:ARG:HB2    | 1:A:191:ASP:O     | 1.80                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:585:GLU:O    | 2:C:588:VAL:HG12 | 1.79                     | 0.82              |
| 4:E:9:LEU:HD23   | 4:E:12:MET:HE3   | 1.62                     | 0.82              |
| 5:F:392:VAL:HG21 | 5:F:396:ARG:HG2  | 1.62                     | 0.81              |
| 3:D:367:ILE:HB   | 3:D:377:VAL:HG23 | 1.62                     | 0.81              |
| 3:D:683:ILE:CG2  | 3:D:687:VAL:HG11 | 2.10                     | 0.81              |
| 3:D:1045:MET:HA  | 3:D:1045:MET:HE3 | 1.61                     | 0.81              |
| 3:D:180:LYS:O    | 3:D:183:GLU:HB2  | 1.80                     | 0.81              |
| 3:D:1234:THR:CA  | 3:D:1235:GLN:HB2 | 2.10                     | 0.81              |
| 1:A:39:PRO:O     | 1:A:43:ILE:HG13  | 1.81                     | 0.81              |
| 5:F:383:LEU:HD12 | 5:F:384:GLU:HG3  | 1.61                     | 0.81              |
| 1:B:108:GLU:HG2  | 1:B:131:THR:HB   | 1.60                     | 0.81              |
| 2:C:206:THR:HA   | 2:C:209:ARG:HB3  | 1.60                     | 0.81              |
| 3:D:1479:ASP:OD1 | 3:D:1482:ARG:NH1 | 2.13                     | 0.81              |
| 3:D:217:LYS:NZ   | 3:D:341:GLU:HG3  | 1.95                     | 0.81              |
| 2:C:597:ALA:HB2  | 2:C:655:LEU:HD11 | 1.64                     | 0.80              |
| 3:D:1485:GLN:NE2 | 4:E:82:GLU:OE1   | 2.13                     | 0.80              |
| 7:H:21:DA:H1'    | 7:H:22:DT:H5'    | 1.63                     | 0.80              |
| 2:C:704:HIS:CD2  | 2:C:831:ARG:HD2  | 2.16                     | 0.80              |
| 2:C:808:ARG:HD3  | 2:C:814:GLU:HG3  | 1.64                     | 0.80              |
| 3:D:843:PHE:HE2  | 3:D:864:VAL:HG11 | 1.46                     | 0.80              |
| 2:C:3:ILE:CD1    | 2:C:900:ARG:HB2  | 2.12                     | 0.80              |
| 2:C:194:VAL:HA   | 2:C:197:LEU:HD13 | 1.62                     | 0.80              |
| 5:F:260:ILE:HG13 | 5:F:265:VAL:CG2  | 2.12                     | 0.80              |
| 5:F:96:LEU:O     | 5:F:100:VAL:HG23 | 1.80                     | 0.80              |
| 1:A:206:THR:HB   | 1:A:209:GLU:OE1  | 1.81                     | 0.80              |
| 3:D:986:ARG:HB2  | 3:D:986:ARG:NH1  | 1.96                     | 0.79              |
| 5:F:104:ARG:O    | 5:F:108:GLU:HG3  | 1.83                     | 0.79              |
| 2:C:829:GLN:OE1  | 2:C:831:ARG:NH2  | 2.14                     | 0.79              |
| 2:C:180:GLY:O    | 2:C:217:LEU:HD22 | 1.81                     | 0.79              |
| 5:F:171:LYS:HD3  | 5:F:175:HIS:HE1  | 1.47                     | 0.79              |
| 7:H:15:DT:C2'    | 7:H:16:DC:H5'    | 2.11                     | 0.79              |
| 3:D:103:TRP:HE1  | 3:D:604:THR:HG21 | 1.44                     | 0.79              |
| 2:C:755:LEU:HD11 | 2:C:792:VAL:CG1  | 2.12                     | 0.79              |
| 2:C:136:ILE:HG21 | 2:C:336:VAL:HG23 | 1.65                     | 0.79              |
| 5:F:112:ALA:O    | 5:F:116:LEU:HB2  | 1.83                     | 0.79              |
| 2:C:540:PHE:HB3  | 2:C:544:THR:CG2  | 2.12                     | 0.79              |
| 1:A:155:LYS:O    | 1:A:155:LYS:NZ   | 2.13                     | 0.79              |
| 3:D:1236:LEU:CD2 | 3:D:1359:GLN:HG3 | 2.13                     | 0.79              |
| 6:G:6:DA:H2''    | 6:G:7:DT:O5'     | 1.83                     | 0.79              |
| 5:F:129:GLU:HG2  | 5:F:144:ILE:HG13 | 1.65                     | 0.78              |
| 5:F:166:LEU:HB2  | 5:F:171:LYS:HB2  | 1.65                     | 0.78              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:560:MET:O    | 2:C:564:MET:HG3   | 1.83                     | 0.78              |
| 4:E:50:THR:HG22  | 4:E:53:GLY:O      | 1.84                     | 0.78              |
| 2:C:674:VAL:HG23 | 2:C:869:VAL:HB    | 1.64                     | 0.78              |
| 3:D:709:HIS:O    | 3:D:711:LEU:N     | 2.16                     | 0.78              |
| 2:C:938:LYS:O    | 2:C:941:VAL:HG22  | 1.84                     | 0.78              |
| 2:C:367:LEU:HD12 | 2:C:371:LYS:NZ    | 1.98                     | 0.78              |
| 2:C:904:PRO:HD2  | 2:C:908:GLY:HA2   | 1.65                     | 0.78              |
| 3:D:693:GLU:HA   | 4:E:48:MET:HE1    | 1.64                     | 0.78              |
| 5:F:120:THR:HG21 | 5:F:122:LEU:HD22  | 1.65                     | 0.78              |
| 2:C:337:GLY:O    | 2:C:341:THR:HG23  | 1.84                     | 0.77              |
| 2:C:428:ARG:NH2  | 2:C:447:ALA:O     | 2.16                     | 0.77              |
| 3:D:1213:ARG:HG3 | 3:D:1214:PRO:HD2  | 1.65                     | 0.77              |
| 3:D:697:GLY:O    | 3:D:760:ARG:NH1   | 2.17                     | 0.77              |
| 1:A:222:LEU:HD21 | 1:B:218:LEU:CD2   | 2.13                     | 0.77              |
| 1:B:36:LEU:O     | 1:B:39:PRO:HD2    | 1.84                     | 0.77              |
| 2:C:317:VAL:HG13 | 2:C:318:PRO:HD2   | 1.66                     | 0.77              |
| 3:D:348:GLN:HB2  | 3:D:351:MET:HE2   | 1.67                     | 0.77              |
| 5:F:299:TRP:CZ3  | 5:F:303:ARG:HG2   | 2.19                     | 0.77              |
| 1:A:206:THR:HG22 | 1:A:209:GLU:H     | 1.47                     | 0.77              |
| 1:B:71:VAL:HG22  | 1:B:132:LEU:CD1   | 2.14                     | 0.77              |
| 2:C:25:SER:OG    | 2:C:335:THR:OG1   | 2.00                     | 0.77              |
| 2:C:195:LEU:HD12 | 2:C:234:ALA:HB1   | 1.66                     | 0.77              |
| 3:D:122:GLU:HG2  | 3:D:152:LEU:HD11  | 1.65                     | 0.77              |
| 3:D:796:ARG:NH2  | 3:D:859:ASP:OD2   | 2.17                     | 0.77              |
| 3:D:1100:ASP:OD1 | 3:D:1463:LYS:NZ   | 2.15                     | 0.77              |
| 3:D:1389:LEU:C   | 3:D:1390:LEU:HD23 | 2.09                     | 0.77              |
| 3:D:650:LEU:HD12 | 3:D:657:LEU:CD2   | 2.14                     | 0.77              |
| 2:C:65:VAL:HG22  | 2:C:101:ILE:HG23  | 1.65                     | 0.77              |
| 3:D:566:ILE:HD11 | 5:F:192:LEU:HD21  | 1.66                     | 0.77              |
| 2:C:425:PHE:HE2  | 3:D:1086:LEU:HD12 | 1.50                     | 0.77              |
| 2:C:751:PRO:HA   | 2:C:792:VAL:CG2   | 2.14                     | 0.77              |
| 3:D:110:SER:O    | 3:D:114:THR:HG23  | 1.84                     | 0.77              |
| 5:F:260:ILE:HG13 | 5:F:265:VAL:HG22  | 1.67                     | 0.77              |
| 5:F:364:ARG:HA   | 5:F:367:MET:HG2   | 1.66                     | 0.77              |
| 1:B:73:GLU:OE1   | 1:B:73:GLU:N      | 2.18                     | 0.76              |
| 2:C:833:LEU:HD12 | 2:C:834:GLN:H     | 1.51                     | 0.76              |
| 3:D:767:HIS:HA   | 3:D:924:MET:CE    | 2.15                     | 0.76              |
| 2:C:880:MET:HE2  | 3:D:1061:PHE:HE2  | 1.50                     | 0.76              |
| 3:D:684:LYS:O    | 3:D:687:VAL:HG12  | 1.84                     | 0.76              |
| 1:A:222:LEU:HD21 | 1:B:218:LEU:HD23  | 1.68                     | 0.76              |
| 1:B:128:HIS:CE1  | 1:B:131:THR:HG22  | 2.16                     | 0.76              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:193:LEU:HG   | 2:C:197:LEU:HD11  | 1.68                     | 0.76              |
| 3:D:245:LEU:HD13 | 3:D:307:ALA:HB1   | 1.68                     | 0.76              |
| 2:C:535:SER:OG   | 2:C:537:LYS:HG3   | 1.84                     | 0.76              |
| 3:D:701:LEU:HD13 | 3:D:763:MET:HE1   | 1.67                     | 0.76              |
| 3:D:1112:CYS:SG  | 3:D:1114:THR:HG22 | 2.26                     | 0.76              |
| 3:D:1263:PHE:HA  | 3:D:1375:MET:HE1  | 1.68                     | 0.76              |
| 6:G:3:DT:H2"     | 6:G:4:DG:C8       | 2.21                     | 0.76              |
| 2:C:808:ARG:NH2  | 2:C:808:ARG:HB3   | 2.00                     | 0.76              |
| 3:D:572:ARG:NH1  | 5:F:83:GLN:HG2    | 2.01                     | 0.76              |
| 2:C:751:PRO:HA   | 2:C:792:VAL:HG23  | 1.67                     | 0.75              |
| 3:D:171:LEU:HD12 | 3:D:171:LEU:O     | 1.86                     | 0.75              |
| 3:D:661:MET:HE1  | 3:D:677:LEU:HD11  | 1.67                     | 0.75              |
| 3:D:26:VAL:HG12  | 3:D:548:ILE:HD13  | 1.67                     | 0.75              |
| 3:D:1042:ARG:HB3 | 3:D:1057:VAL:CG1  | 2.17                     | 0.75              |
| 2:C:140:ILE:HD13 | 2:C:331:ARG:HH11  | 1.51                     | 0.75              |
| 2:C:260:LEU:C    | 2:C:261:ILE:HD12  | 2.10                     | 0.75              |
| 3:D:828:LYS:HE2  | 3:D:831:GLY:H     | 1.52                     | 0.75              |
| 2:C:715:THR:HG22 | 2:C:717:LEU:H     | 1.50                     | 0.75              |
| 2:C:805:ARG:HG3  | 2:C:823:VAL:HG23  | 1.69                     | 0.75              |
| 3:D:496:LEU:HD23 | 3:D:1390:LEU:HD13 | 1.68                     | 0.75              |
| 2:C:51:THR:HG21  | 2:C:348:LEU:HB3   | 1.67                     | 0.75              |
| 1:B:30:ARG:NH2   | 2:C:854:PRO:HB3   | 2.02                     | 0.75              |
| 1:B:86:VAL:CG1   | 1:B:123:MET:HB2   | 2.17                     | 0.75              |
| 2:C:196:LEU:HD13 | 2:C:200:LEU:HD11  | 1.68                     | 0.75              |
| 2:C:751:PRO:HD3  | 2:C:796:GLU:O     | 1.87                     | 0.75              |
| 2:C:460:ARG:HD2  | 2:C:485:TYR:CE1   | 2.22                     | 0.74              |
| 2:C:874:LEU:HD13 | 3:D:783:ARG:HB3   | 1.68                     | 0.74              |
| 3:D:1422:MET:HE3 | 3:D:1426:LYS:CG   | 2.18                     | 0.74              |
| 2:C:880:MET:HE2  | 3:D:1061:PHE:CE2  | 2.21                     | 0.74              |
| 3:D:7:LYS:HD3    | 3:D:1456:LYS:NZ   | 2.01                     | 0.74              |
| 3:D:217:LYS:HZ2  | 3:D:341:GLU:HG3   | 1.50                     | 0.74              |
| 2:C:11:GLU:HG2   | 2:C:535:SER:HB2   | 1.70                     | 0.74              |
| 2:C:498:GLN:HE21 | 3:D:1068:LEU:HD12 | 1.53                     | 0.74              |
| 3:D:95:LEU:HD22  | 3:D:574:LEU:HD21  | 1.69                     | 0.74              |
| 3:D:411:THR:HG22 | 5:F:178:ARG:CB    | 2.17                     | 0.74              |
| 2:C:766:GLU:HG2  | 2:C:767:PRO:HD2   | 1.70                     | 0.74              |
| 2:C:811:PRO:O    | 2:C:813:VAL:HG12  | 1.88                     | 0.74              |
| 2:C:815:LEU:HB2  | 2:C:819:VAL:CG2   | 2.17                     | 0.74              |
| 3:D:952:ASP:HA   | 3:D:1062:ARG:HH21 | 1.53                     | 0.74              |
| 5:F:95:THR:HG22  | 5:F:98:GLU:HG2    | 1.69                     | 0.74              |
| 1:A:201:THR:HG22 | 1:A:203:GLY:H     | 1.53                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:298:VAL:HG12  | 3:D:302:GLN:CD    | 2.12                     | 0.74              |
| 3:D:645:PRO:HG2   | 3:D:724:GLN:O     | 1.86                     | 0.74              |
| 5:F:265:VAL:O     | 5:F:269:ASN:ND2   | 2.20                     | 0.74              |
| 3:D:680:GLN:HA    | 3:D:683:ILE:CD1   | 2.18                     | 0.73              |
| 2:C:564:MET:HE1   | 2:C:846:LYS:CG    | 2.18                     | 0.73              |
| 2:C:710:ILE:HG22  | 2:C:823:VAL:HG12  | 1.70                     | 0.73              |
| 2:C:861:LEU:H     | 2:C:861:LEU:HD12  | 1.53                     | 0.73              |
| 2:C:880:MET:HE1   | 3:D:1037:GLN:CD   | 2.13                     | 0.73              |
| 3:D:236:TYR:N     | 3:D:319:ALA:HB3   | 2.02                     | 0.73              |
| 3:D:566:ILE:HD11  | 5:F:192:LEU:CD2   | 2.17                     | 0.73              |
| 2:C:84:ARG:HD3    | 2:C:629:TYR:OH    | 1.89                     | 0.73              |
| 3:D:646:LYS:CB    | 3:D:720:LEU:HD23  | 2.17                     | 0.73              |
| 5:F:123:ASP:OD1   | 5:F:126:LEU:N     | 2.19                     | 0.73              |
| 1:A:222:LEU:CD1   | 1:B:218:LEU:HD23  | 2.18                     | 0.73              |
| 3:D:982:PHE:O     | 3:D:983:LEU:HG    | 1.88                     | 0.73              |
| 3:D:1271:LYS:HD2  | 3:D:1331:ASP:HB2  | 1.69                     | 0.73              |
| 2:C:626:ARG:HD3   | 2:C:629:TYR:HD2   | 1.54                     | 0.73              |
| 3:D:348:GLN:CB    | 3:D:351:MET:HE2   | 2.18                     | 0.73              |
| 3:D:348:GLN:CG    | 3:D:351:MET:HE2   | 2.18                     | 0.73              |
| 3:D:474:GLU:OE2   | 3:D:1388:ARG:NH2  | 2.21                     | 0.73              |
| 3:D:1197:ARG:HB2  | 3:D:1398:TRP:CH2  | 2.24                     | 0.73              |
| 3:D:1312:LEU:HD21 | 3:D:1327:ARG:HE   | 1.52                     | 0.73              |
| 3:D:1444:THR:O    | 3:D:1448:THR:HG23 | 1.87                     | 0.73              |
| 2:C:425:PHE:CE2   | 3:D:1086:LEU:HD12 | 2.22                     | 0.73              |
| 2:C:551:GLU:N     | 2:C:551:GLU:OE2   | 2.19                     | 0.73              |
| 2:C:888:THR:HG22  | 2:C:990:GLY:CA    | 2.19                     | 0.73              |
| 2:C:937:ASP:HB3   | 2:C:940:GLU:HG3   | 1.71                     | 0.73              |
| 1:B:38:ASN:HB3    | 1:B:39:PRO:HD3    | 1.70                     | 0.73              |
| 5:F:393:THR:HG22  | 5:F:394:ARG:H     | 1.53                     | 0.73              |
| 2:C:312:ALA:HB1   | 2:C:317:VAL:HG21  | 1.69                     | 0.72              |
| 3:D:939:PHE:O     | 3:D:942:SER:OG    | 2.06                     | 0.72              |
| 2:C:498:GLN:NE2   | 3:D:1068:LEU:HD12 | 2.04                     | 0.72              |
| 2:C:603:VAL:HG23  | 2:C:647:GLN:O     | 1.90                     | 0.72              |
| 3:D:421:LEU:HD13  | 3:D:428:LYS:HA    | 1.71                     | 0.72              |
| 3:D:1234:THR:H    | 3:D:1235:GLN:CB   | 2.02                     | 0.72              |
| 1:A:196:THR:HG21  | 2:C:934:PHE:CE1   | 2.25                     | 0.72              |
| 3:D:185:VAL:HG13  | 3:D:189:GLN:CD    | 2.13                     | 0.72              |
| 3:D:1422:MET:HE3  | 3:D:1426:LYS:HG2  | 1.72                     | 0.72              |
| 1:A:94:LEU:O      | 1:A:146:ARG:NH1   | 2.22                     | 0.72              |
| 3:D:1141:GLU:HG2  | 3:D:1168:MET:HE1  | 1.70                     | 0.72              |
| 2:C:28:ARG:O      | 2:C:28:ARG:HG2    | 1.90                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:748:GLU:HG3   | 2:C:799:ILE:HD11  | 1.72                     | 0.72              |
| 3:D:705:ALA:HB3   | 3:D:706:PRO:CD    | 2.18                     | 0.72              |
| 3:D:1127:GLU:HB3  | 3:D:1130:ARG:HH12 | 1.55                     | 0.72              |
| 5:F:392:VAL:CG2   | 5:F:396:ARG:HG2   | 2.20                     | 0.72              |
| 2:C:211:LEU:HB3   | 2:C:218:VAL:HG22  | 1.72                     | 0.72              |
| 2:C:988:VAL:HG23  | 3:D:948:THR:CG2   | 2.20                     | 0.72              |
| 2:C:673:LEU:HD23  | 2:C:867:VAL:HA    | 1.71                     | 0.72              |
| 7:H:16:DC:H2''    | 7:H:17:DA:C8      | 2.24                     | 0.71              |
| 1:B:53:VAL:HG12   | 1:B:167:VAL:HG11  | 1.72                     | 0.71              |
| 2:C:211:LEU:HB3   | 2:C:218:VAL:CG2   | 2.20                     | 0.71              |
| 3:D:209:ARG:NH2   | 3:D:391:ALA:HA    | 2.05                     | 0.71              |
| 2:C:727:PRO:HB2   | 2:C:728:HIS:CD2   | 2.26                     | 0.71              |
| 5:F:386:VAL:HA    | 5:F:390:PHE:CE1   | 2.24                     | 0.71              |
| 5:F:408:LEU:HA    | 5:F:411:HIS:HB3   | 1.72                     | 0.71              |
| 2:C:946:ARG:HH21  | 2:C:946:ARG:HG3   | 1.54                     | 0.71              |
| 3:D:1283:ILE:HG13 | 3:D:1315:ASP:OD2  | 1.87                     | 0.71              |
| 3:D:1234:THR:N    | 3:D:1235:GLN:HB2  | 2.05                     | 0.71              |
| 2:C:727:PRO:HB2   | 2:C:728:HIS:HD2   | 1.55                     | 0.71              |
| 3:D:96:ALA:HB3    | 3:D:554:LEU:HD23  | 1.72                     | 0.71              |
| 1:B:26:GLU:OE2    | 1:B:194:LYS:HE3   | 1.90                     | 0.71              |
| 2:C:236:ILE:HG23  | 2:C:248:PRO:HB2   | 1.73                     | 0.71              |
| 5:F:126:LEU:HD12  | 5:F:126:LEU:O     | 1.90                     | 0.71              |
| 1:A:18:ARG:HH11   | 1:A:18:ARG:HG3    | 1.54                     | 0.71              |
| 1:B:26:GLU:HB3    | 1:B:194:LYS:HG3   | 1.73                     | 0.71              |
| 3:D:1295:GLU:OE1  | 3:D:1300:SER:HB3  | 1.89                     | 0.71              |
| 3:D:348:GLN:H     | 3:D:351:MET:HG3   | 1.55                     | 0.71              |
| 1:B:80:LEU:HD21   | 3:D:842:VAL:HG12  | 1.72                     | 0.70              |
| 2:C:367:LEU:HD12  | 2:C:371:LYS:HZ2   | 1.54                     | 0.70              |
| 3:D:809:PRO:O     | 3:D:813:LEU:HD12  | 1.92                     | 0.70              |
| 5:F:193:ARG:HB3   | 7:H:7:DG:H5''     | 1.72                     | 0.70              |
| 2:C:681:GLY:HA2   | 3:D:939:PHE:CE1   | 2.25                     | 0.70              |
| 3:D:314:PRO:HB2   | 3:D:317:VAL:HG12  | 1.71                     | 0.70              |
| 5:F:369:LEU:CD2   | 5:F:372:ARG:HB2   | 2.21                     | 0.70              |
| 1:B:58:ILE:HB     | 1:B:61:VAL:HG21   | 1.73                     | 0.70              |
| 1:B:38:ASN:OD1    | 2:C:979:THR:HG22  | 1.92                     | 0.70              |
| 2:C:35:PRO:HG2    | 2:C:38:LYS:HD3    | 1.73                     | 0.70              |
| 1:A:73:GLU:OE2    | 1:A:130:ALA:HA    | 1.92                     | 0.70              |
| 2:C:317:VAL:CG1   | 2:C:318:PRO:HD2   | 2.21                     | 0.70              |
| 3:D:413:ASP:HB2   | 3:D:435:VAL:HG11  | 1.73                     | 0.70              |
| 1:A:101:LEU:HD23  | 1:A:102:LYS:N     | 2.06                     | 0.70              |
| 1:A:198:ARG:C     | 1:A:199:ILE:HG12  | 2.15                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:206:THR:HG23 | 1:A:208:LEU:H    | 1.56                     | 0.70              |
| 5:F:338:LEU:CD2  | 5:F:339:PRO:HD2  | 2.12                     | 0.70              |
| 5:F:362:SER:HB3  | 5:F:365:GLU:CG   | 2.19                     | 0.70              |
| 3:D:1060:SER:CB  | 3:D:1063:GLU:HG3 | 2.21                     | 0.70              |
| 2:C:520:GLU:HG3  | 2:C:521:PRO:HD2  | 1.72                     | 0.69              |
| 3:D:658:LEU:HD23 | 3:D:661:MET:HE1  | 1.74                     | 0.69              |
| 6:G:6:DA:H5"     | 6:G:6:DA:C8      | 2.27                     | 0.69              |
| 2:C:197:LEU:HB3  | 2:C:202:TYR:HD2  | 1.57                     | 0.69              |
| 3:D:175:VAL:CG1  | 3:D:193:PRO:HG2  | 2.22                     | 0.69              |
| 3:D:581:LEU:HD23 | 3:D:582:LEU:CD2  | 2.22                     | 0.69              |
| 5:F:153:PRO:HA   | 5:F:156:VAL:CG1  | 2.21                     | 0.69              |
| 2:C:102:HIS:HB2  | 2:C:107:LEU:CB   | 2.22                     | 0.69              |
| 5:F:163:LEU:HB3  | 5:F:174:LEU:CD1  | 2.22                     | 0.69              |
| 2:C:569:VAL:HG21 | 2:C:1000:MET:CE  | 2.23                     | 0.69              |
| 2:C:680:ASP:OD2  | 3:D:943:THR:HG21 | 1.92                     | 0.69              |
| 3:D:729:HIS:ND1  | 3:D:730:PRO:HD2  | 2.07                     | 0.69              |
| 5:F:287:THR:OG1  | 5:F:290:GLU:HG3  | 1.92                     | 0.69              |
| 2:C:689:VAL:HG11 | 2:C:870:ILE:HD12 | 1.74                     | 0.69              |
| 3:D:348:GLN:HG2  | 3:D:351:MET:HE2  | 1.75                     | 0.69              |
| 3:D:689:ASP:HB3  | 4:E:51:LEU:HD13  | 1.72                     | 0.69              |
| 3:D:970:LYS:HA   | 3:D:973:GLN:HB3  | 1.75                     | 0.69              |
| 2:C:237:ARG:O    | 2:C:240:THR:OG1  | 2.11                     | 0.69              |
| 2:C:808:ARG:HG3  | 2:C:814:GLU:HA   | 1.74                     | 0.69              |
| 3:D:65:ARG:HD3   | 5:F:377:ASP:N    | 2.07                     | 0.69              |
| 1:B:106:PRO:HD3  | 1:B:134:GLU:HG2  | 1.75                     | 0.69              |
| 1:B:185:ARG:NH1  | 1:B:187:GLY:O    | 2.26                     | 0.69              |
| 2:C:564:MET:HE1  | 2:C:846:LYS:CD   | 2.22                     | 0.69              |
| 2:C:587:VAL:HG11 | 2:C:666:LEU:HD22 | 1.74                     | 0.69              |
| 2:C:971:LYS:HA   | 2:C:987:ILE:O    | 1.92                     | 0.69              |
| 2:C:1035:MET:HG2 | 2:C:1038:TRP:CZ3 | 2.28                     | 0.69              |
| 3:D:201:GLY:HA3  | 3:D:396:VAL:O    | 1.92                     | 0.69              |
| 3:D:659:LYS:NZ   | 3:D:663:GLU:OE1  | 2.25                     | 0.69              |
| 2:C:262:ALA:O    | 2:C:264:PRO:HD3  | 1.93                     | 0.69              |
| 2:C:906:PHE:CE2  | 3:D:1067:VAL:HA  | 2.28                     | 0.69              |
| 2:C:958:THR:HG23 | 2:C:961:GLU:CD   | 2.18                     | 0.69              |
| 3:D:835:SER:HB3  | 3:D:838:ARG:HE   | 1.58                     | 0.69              |
| 1:A:117:VAL:O    | 1:A:120:VAL:HG22 | 1.93                     | 0.69              |
| 2:C:54:ILE:HG21  | 2:C:355:VAL:HG23 | 1.75                     | 0.69              |
| 2:C:513:VAL:HG21 | 2:C:529:VAL:HG21 | 1.74                     | 0.69              |
| 3:D:134:VAL:CG1  | 3:D:153:LEU:HD11 | 2.23                     | 0.69              |
| 1:B:37:GLY:HA2   | 1:B:40:LEU:HG    | 1.75                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:7:LYS:HD3     | 3:D:1456:LYS:HZ3  | 1.57                     | 0.68              |
| 3:D:486:ARG:HG3   | 3:D:489:ARG:NH2   | 2.08                     | 0.68              |
| 5:F:367:MET:CE    | 5:F:368:VAL:HG13  | 2.18                     | 0.68              |
| 1:A:184:THR:HG22  | 1:A:192:LEU:HB2   | 1.74                     | 0.68              |
| 2:C:683:ASN:CB    | 2:C:872:ASN:HB2   | 2.21                     | 0.68              |
| 5:F:316:SER:O     | 5:F:319:THR:OG1   | 2.11                     | 0.68              |
| 1:A:115:LEU:O     | 1:A:115:LEU:HD23  | 1.93                     | 0.68              |
| 1:A:201:THR:HG21  | 1:A:205:VAL:O     | 1.94                     | 0.68              |
| 1:B:162:ILE:HG13  | 1:B:163:ASN:HD22  | 1.58                     | 0.68              |
| 2:C:540:PHE:HB3   | 2:C:544:THR:HG21  | 1.74                     | 0.68              |
| 3:D:1394:VAL:HG22 | 3:D:1420:LEU:CD2  | 2.24                     | 0.68              |
| 1:A:62:LEU:HA     | 1:A:163:ASN:HB3   | 1.74                     | 0.68              |
| 2:C:926:PHE:O     | 2:C:929:ARG:HB3   | 1.93                     | 0.68              |
| 1:A:138:LEU:HD11  | 1:A:140:MET:HE3   | 1.75                     | 0.68              |
| 5:F:234:LYS:HD3   | 7:H:5:DA:OP2      | 1.94                     | 0.68              |
| 5:F:354:LEU:HD12  | 5:F:355:GLU:N     | 2.09                     | 0.68              |
| 2:C:376:ARG:HD3   | 5:F:276:ARG:HD2   | 1.76                     | 0.68              |
| 2:C:690:ILE:HG13  | 2:C:852:ILE:HG23  | 1.75                     | 0.68              |
| 4:E:39:VAL:HG21   | 4:E:72:ARG:HB3    | 1.74                     | 0.68              |
| 6:G:6:DA:H2'      | 6:G:7:DT:C7       | 2.24                     | 0.68              |
| 1:B:143:ARG:HD3   | 1:B:158:ILE:HD11  | 1.76                     | 0.68              |
| 2:C:260:LEU:CB    | 2:C:261:ILE:HD12  | 2.23                     | 0.68              |
| 3:D:93:ILE:HD13   | 3:D:548:ILE:HG12  | 1.75                     | 0.68              |
| 1:A:88:ARG:CB     | 1:A:123:MET:HE3   | 2.21                     | 0.68              |
| 1:B:38:ASN:HB3    | 1:B:39:PRO:CD     | 2.23                     | 0.68              |
| 3:D:437:VAL:HG11  | 5:F:175:HIS:CD2   | 2.29                     | 0.68              |
| 1:A:9:PRO:HB3     | 1:A:27:PRO:O      | 1.94                     | 0.67              |
| 1:A:67:THR:HG21   | 2:C:609:ASN:OD1   | 1.94                     | 0.67              |
| 1:A:180:GLN:HG3   | 2:C:934:PHE:CD1   | 2.28                     | 0.67              |
| 1:B:197:LEU:HD12  | 1:B:198:ARG:N     | 2.07                     | 0.67              |
| 5:F:390:PHE:CD2   | 5:F:397:ILE:HG12  | 2.30                     | 0.67              |
| 2:C:424:GLY:O     | 2:C:428:ARG:HD2   | 1.94                     | 0.67              |
| 3:D:1273:VAL:H    | 3:D:1326:THR:CG2  | 2.06                     | 0.67              |
| 1:A:222:LEU:HD11  | 1:B:218:LEU:CD2   | 2.24                     | 0.67              |
| 2:C:49:ARG:O      | 2:C:49:ARG:HD3    | 1.94                     | 0.67              |
| 3:D:701:LEU:CD1   | 3:D:763:MET:HE1   | 2.23                     | 0.67              |
| 3:D:1057:VAL:HG21 | 3:D:1065:LEU:HD21 | 1.75                     | 0.67              |
| 3:D:1376:MET:HE1  | 3:D:1421:LEU:HD13 | 1.76                     | 0.67              |
| 3:D:1057:VAL:HG23 | 3:D:1069:GLU:CD   | 2.19                     | 0.67              |
| 2:C:709:GLU:OE2   | 2:C:824:ARG:NH1   | 2.24                     | 0.67              |
| 2:C:878:SER:HA    | 3:D:1034:GLN:NE2  | 2.10                     | 0.67              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:65:ARG:CD     | 5:F:377:ASP:HA   | 2.24                     | 0.67              |
| 5:F:206:GLY:O     | 5:F:207:LEU:HD23 | 1.95                     | 0.67              |
| 3:D:977:ALA:O     | 3:D:982:PHE:HB3  | 1.94                     | 0.67              |
| 3:D:1047:LYS:HG3  | 3:D:1053:PHE:CZ  | 2.30                     | 0.67              |
| 1:B:87:VAL:HG12   | 1:B:122:ILE:HD13 | 1.77                     | 0.67              |
| 3:D:236:TYR:HB3   | 3:D:313:MET:HG3  | 1.76                     | 0.67              |
| 3:D:335:LEU:H     | 3:D:335:LEU:HD12 | 1.58                     | 0.67              |
| 3:D:140:ALA:HA    | 3:D:450:TYR:CD1  | 2.30                     | 0.67              |
| 6:G:6:DA:H5''     | 6:G:6:DA:H8      | 1.59                     | 0.67              |
| 1:B:74:ASP:O      | 1:B:78:ILE:HG13  | 1.95                     | 0.67              |
| 2:C:689:VAL:CG1   | 2:C:870:ILE:HD12 | 2.25                     | 0.67              |
| 3:D:998:GLU:O     | 3:D:1002:LYS:HG3 | 1.95                     | 0.67              |
| 6:G:11:DT:H2''    | 6:G:12:DG:H5''   | 1.77                     | 0.67              |
| 1:B:66:SER:O      | 1:B:75:VAL:HG23  | 1.94                     | 0.66              |
| 3:D:704:ARG:CB    | 3:D:745:MET:HE2  | 2.15                     | 0.66              |
| 3:D:645:PRO:CG    | 3:D:724:GLN:O    | 2.42                     | 0.66              |
| 2:C:149:THR:HA    | 2:C:322:VAL:HG13 | 1.78                     | 0.66              |
| 2:C:716:LYS:HE2   | 3:D:37:LEU:HD11  | 1.77                     | 0.66              |
| 2:C:197:LEU:HA    | 2:C:200:LEU:CD1  | 2.25                     | 0.66              |
| 2:C:431:HIS:ND1   | 2:C:433:THR:OG1  | 2.29                     | 0.66              |
| 3:D:972:LEU:HA    | 3:D:975:GLU:HB3  | 1.77                     | 0.66              |
| 1:B:49:PRO:HA     | 1:B:148:VAL:HG12 | 1.77                     | 0.66              |
| 3:D:904:VAL:HG22  | 3:D:905:PRO:HD2  | 1.77                     | 0.66              |
| 1:B:106:PRO:CD    | 1:B:134:GLU:HG2  | 2.26                     | 0.66              |
| 3:D:59:ALA:HB2    | 3:D:78:VAL:HG21  | 1.77                     | 0.66              |
| 1:A:10:VAL:HG12   | 1:A:26:GLU:O     | 1.96                     | 0.66              |
| 2:C:425:PHE:HE2   | 3:D:1086:LEU:CD1 | 2.09                     | 0.66              |
| 2:C:892:LEU:HD13  | 2:C:989:VAL:O    | 1.96                     | 0.66              |
| 3:D:1282:ARG:HA   | 3:D:1315:ASP:OD1 | 1.95                     | 0.66              |
| 1:A:164:ALA:O     | 1:A:166:PRO:HD3  | 1.96                     | 0.66              |
| 1:B:80:LEU:HB3    | 3:D:844:ALA:HB2  | 1.76                     | 0.66              |
| 2:C:1070:ILE:HG21 | 3:D:655:PRO:CB   | 2.25                     | 0.66              |
| 3:D:558:LEU:CD2   | 3:D:567:ILE:HD12 | 2.25                     | 0.66              |
| 3:D:885:ILE:HG23  | 3:D:937:TYR:CD1  | 2.31                     | 0.66              |
| 5:F:369:LEU:HD22  | 5:F:372:ARG:HB2  | 1.76                     | 0.66              |
| 2:C:564:MET:HE1   | 2:C:846:LYS:HG2  | 1.77                     | 0.65              |
| 2:C:596:TYR:C     | 2:C:655:LEU:HD13 | 2.21                     | 0.65              |
| 2:C:719:PRO:HD2   | 2:C:761:PHE:CE1  | 2.31                     | 0.65              |
| 3:D:1433:SER:OG   | 3:D:1464:GLU:HG2 | 1.96                     | 0.65              |
| 5:F:321:ILE:HG21  | 5:F:332:PHE:HE1  | 1.61                     | 0.65              |
| 6:G:3:DT:H2''     | 6:G:4:DG:H8      | 1.62                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:24:VAL:HG13   | 1:B:196:THR:OG1   | 1.96                     | 0.65              |
| 1:B:220:GLU:O     | 1:B:223:THR:OG1   | 2.14                     | 0.65              |
| 2:C:578:VAL:HA    | 2:C:900:ARG:HD2   | 1.78                     | 0.65              |
| 2:C:756:VAL:HG21  | 2:C:823:VAL:HG11  | 1.78                     | 0.65              |
| 2:C:875:GLY:O     | 2:C:879:ARG:HD3   | 1.97                     | 0.65              |
| 3:D:356:PRO:HG2   | 3:D:359:ALA:HB2   | 1.78                     | 0.65              |
| 3:D:367:ILE:HB    | 3:D:377:VAL:CG2   | 2.26                     | 0.65              |
| 3:D:879:ARG:HB3   | 3:D:902:LEU:HD11  | 1.78                     | 0.65              |
| 3:D:904:VAL:HG22  | 3:D:905:PRO:CD    | 2.27                     | 0.65              |
| 5:F:412:GLU:CG    | 5:F:418:LEU:HD13  | 2.27                     | 0.65              |
| 1:A:107:LYS:NZ    | 1:A:113:ASP:OD2   | 2.28                     | 0.65              |
| 1:B:211:LEU:O     | 1:B:215:VAL:HG23  | 1.96                     | 0.65              |
| 3:D:46:ASP:OD1    | 3:D:48:ARG:HG2    | 1.97                     | 0.65              |
| 1:A:86:VAL:HG21   | 1:A:202:ASP:HB2   | 1.78                     | 0.65              |
| 2:C:446:GLY:O     | 2:C:449:ILE:HG22  | 1.96                     | 0.65              |
| 3:D:203:ALA:CB    | 3:D:393:ILE:HD11  | 2.19                     | 0.65              |
| 3:D:618:LEU:HD12  | 3:D:1467:ILE:HG23 | 1.77                     | 0.65              |
| 3:D:1065:LEU:HD23 | 3:D:1069:GLU:CB   | 2.26                     | 0.65              |
| 1:B:33:GLY:C      | 1:B:181:VAL:HG21  | 2.22                     | 0.65              |
| 2:C:203:ASP:HB3   | 2:C:206:THR:HG22  | 1.79                     | 0.65              |
| 2:C:250:ARG:HD2   | 2:C:250:ARG:O     | 1.95                     | 0.65              |
| 2:C:1072:LYS:HD2  | 2:C:1074:GLU:OE2  | 1.97                     | 0.65              |
| 3:D:266:GLU:OE2   | 3:D:315:ARG:NE    | 2.30                     | 0.65              |
| 3:D:298:VAL:HG12  | 3:D:302:GLN:NE2   | 2.11                     | 0.65              |
| 2:C:905:ILE:CG2   | 2:C:906:PHE:HD1   | 2.10                     | 0.65              |
| 3:D:639:LEU:HA    | 3:D:729:HIS:CD2   | 2.32                     | 0.65              |
| 1:B:109:VAL:C     | 1:B:110:LYS:HD2   | 2.21                     | 0.64              |
| 1:B:226:SER:O     | 1:B:228:PRO:HD3   | 1.97                     | 0.64              |
| 2:C:768:THR:HG23  | 2:C:771:GLU:OE1   | 1.97                     | 0.64              |
| 2:C:861:LEU:HB3   | 2:C:862:PRO:HD2   | 1.78                     | 0.64              |
| 2:C:405:ARG:HD2   | 2:C:442:GLU:OE2   | 1.97                     | 0.64              |
| 2:C:513:VAL:HG22  | 2:C:524:VAL:O     | 1.97                     | 0.64              |
| 2:C:571:LEU:HD22  | 2:C:700:TYR:HA    | 1.79                     | 0.64              |
| 3:D:112:ILE:HG23  | 3:D:465:LEU:HD11  | 1.78                     | 0.64              |
| 3:D:776:GLU:OE2   | 3:D:1362:LYS:HD3  | 1.98                     | 0.64              |
| 4:E:26:ARG:HE     | 4:E:30:LEU:HD11   | 1.63                     | 0.64              |
| 4:E:61:VAL:O      | 4:E:65:MET:HG3    | 1.98                     | 0.64              |
| 7:H:21:DA:H1'     | 7:H:22:DT:C5'     | 2.27                     | 0.64              |
| 3:D:431:VAL:HG21  | 3:D:448:GLU:OE1   | 1.97                     | 0.64              |
| 3:D:864:VAL:HG12  | 3:D:865:THR:N     | 2.13                     | 0.64              |
| 2:C:109:LYS:HD2   | 2:C:110:GLU:H     | 1.63                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:65:ARG:HB3   | 5:F:377:ASP:CA    | 2.22                     | 0.64              |
| 3:D:351:MET:HB3  | 3:D:369:ALA:O     | 1.97                     | 0.64              |
| 3:D:411:THR:O    | 5:F:178:ARG:HD2   | 1.97                     | 0.64              |
| 3:D:703:ASN:HA   | 3:D:712:GLY:O     | 1.98                     | 0.64              |
| 5:F:271:LEU:H    | 5:F:271:LEU:HD12  | 1.63                     | 0.64              |
| 2:C:1062:GLY:HA2 | 2:C:1065:ALA:HB3  | 1.77                     | 0.64              |
| 3:D:170:PRO:HA   | 3:D:392:SER:CB    | 2.22                     | 0.64              |
| 3:D:1141:GLU:CG  | 3:D:1168:MET:HE1  | 2.28                     | 0.64              |
| 3:D:1489:GLN:NE2 | 3:D:1492:LEU:HD12 | 2.12                     | 0.64              |
| 5:F:398:ARG:NH2  | 5:F:399:GLN:HG3   | 2.13                     | 0.64              |
| 1:A:32:PHE:HA    | 1:A:35:THR:HB     | 1.78                     | 0.64              |
| 1:B:40:LEU:O     | 1:B:44:LEU:HD12   | 1.97                     | 0.64              |
| 2:C:112:GLU:HG3  | 2:C:112:GLU:O     | 1.96                     | 0.64              |
| 2:C:436:GLY:HA2  | 2:C:538:GLN:O     | 1.98                     | 0.64              |
| 3:D:1293:PHE:CE1 | 3:D:1302:GLU:HB2  | 2.32                     | 0.64              |
| 2:C:22:GLN:O     | 2:C:121:MET:HE1   | 1.98                     | 0.64              |
| 2:C:988:VAL:HG23 | 3:D:948:THR:HG21  | 1.80                     | 0.64              |
| 2:C:1066:ALA:O   | 2:C:1069:ALA:N    | 2.31                     | 0.64              |
| 3:D:1499:ARG:NH1 | 4:E:84:ARG:HG2    | 2.13                     | 0.64              |
| 1:A:79:ILE:HD12  | 1:A:167:VAL:HG22  | 1.78                     | 0.64              |
| 3:D:209:ARG:O    | 3:D:346:ARG:HD3   | 1.96                     | 0.64              |
| 3:D:975:GLU:O    | 3:D:979:GLU:HB2   | 1.98                     | 0.64              |
| 3:D:1087:ARG:NH1 | 3:D:1236:LEU:O    | 2.31                     | 0.64              |
| 2:C:260:LEU:HB3  | 2:C:261:ILE:CD1   | 2.26                     | 0.64              |
| 2:C:367:LEU:HA   | 2:C:371:LYS:HZ2   | 1.61                     | 0.64              |
| 3:D:259:VAL:HG13 | 3:D:270:LEU:HD21  | 1.78                     | 0.64              |
| 3:D:343:LYS:NZ   | 3:D:380:GLU:OE2   | 2.31                     | 0.64              |
| 4:E:42:PRO:HA    | 4:E:45:ARG:HG3    | 1.80                     | 0.64              |
| 5:F:368:VAL:HG11 | 5:F:397:ILE:HD11  | 1.80                     | 0.64              |
| 1:A:97:VAL:HG12  | 1:A:98:THR:H      | 1.63                     | 0.63              |
| 1:B:96:THR:HG22  | 1:B:97:VAL:N      | 2.13                     | 0.63              |
| 2:C:890:LEU:HB2  | 2:C:914:ILE:HD12  | 1.80                     | 0.63              |
| 3:D:187:LYS:HD2  | 3:D:200:ASP:OD2   | 1.98                     | 0.63              |
| 3:D:311:LEU:O    | 3:D:311:LEU:HD12  | 1.99                     | 0.63              |
| 3:D:1376:MET:CE  | 3:D:1421:LEU:HD13 | 2.28                     | 0.63              |
| 2:C:64:LEU:HD22  | 2:C:100:LEU:HD11  | 1.80                     | 0.63              |
| 2:C:1006:HIS:HB2 | 2:C:1024:LYS:HG3  | 1.80                     | 0.63              |
| 3:D:1191:PRO:HD2 | 3:D:1369:GLU:OE1  | 1.98                     | 0.63              |
| 3:D:1493:LYS:HA  | 3:D:1493:LYS:CE   | 2.29                     | 0.63              |
| 5:F:362:SER:CB   | 5:F:365:GLU:HG2   | 2.22                     | 0.63              |
| 2:C:474:VAL:HG11 | 2:C:529:VAL:CG1   | 2.28                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:861:LEU:HD12  | 2:C:865:THR:O     | 1.97                     | 0.63              |
| 3:D:135:LEU:HD23  | 3:D:135:LEU:O     | 1.97                     | 0.63              |
| 1:B:216:GLU:OE1   | 1:B:219:ARG:NH2   | 2.30                     | 0.63              |
| 2:C:948:GLU:HG3   | 2:C:953:VAL:CG2   | 2.28                     | 0.63              |
| 5:F:364:ARG:HA    | 5:F:367:MET:CG    | 2.27                     | 0.63              |
| 5:F:398:ARG:HH21  | 5:F:399:GLN:HG3   | 1.64                     | 0.63              |
| 7:H:21:DA:H2"     | 7:H:22:DT:OP2     | 1.98                     | 0.63              |
| 1:A:222:LEU:CD2   | 1:B:218:LEU:HD23  | 2.29                     | 0.63              |
| 1:B:64:GLU:O      | 1:B:75:VAL:HB     | 1.99                     | 0.63              |
| 3:D:879:ARG:HB3   | 3:D:902:LEU:CD1   | 2.28                     | 0.63              |
| 3:D:996:TRP:CD2   | 3:D:1056:PRO:HG3  | 2.33                     | 0.63              |
| 5:F:219:GLY:O     | 5:F:222:ARG:HB2   | 1.96                     | 0.63              |
| 1:B:71:VAL:HG22   | 1:B:132:LEU:HD12  | 1.80                     | 0.63              |
| 2:C:54:ILE:HG21   | 2:C:355:VAL:CG2   | 2.29                     | 0.63              |
| 3:D:24:GLY:HA3    | 3:D:49:ILE:HG23   | 1.79                     | 0.63              |
| 3:D:1028:ALA:O    | 3:D:1029:ARG:HG2  | 1.97                     | 0.63              |
| 4:E:95:VAL:O      | 4:E:95:VAL:HG12   | 1.98                     | 0.63              |
| 2:C:910:LYS:O     | 2:C:914:ILE:HG22  | 1.99                     | 0.63              |
| 3:D:50:PHE:O      | 3:D:89:ARG:HD2    | 1.97                     | 0.63              |
| 3:D:1114:THR:HG23 | 3:D:1189:ARG:HH21 | 1.62                     | 0.63              |
| 3:D:70:GLY:H      | 3:D:80:VAL:HG23   | 1.63                     | 0.63              |
| 3:D:134:VAL:HG22  | 3:D:151:GLN:H     | 1.63                     | 0.63              |
| 3:D:1489:GLN:HE22 | 3:D:1492:LEU:HD12 | 1.62                     | 0.63              |
| 5:F:372:ARG:HA    | 5:F:372:ARG:HE    | 1.64                     | 0.63              |
| 2:C:12:VAL:HG21   | 2:C:472:ARG:NE    | 2.14                     | 0.63              |
| 2:C:474:VAL:CG1   | 2:C:529:VAL:HG12  | 2.28                     | 0.63              |
| 3:D:544:TYR:O     | 3:D:547:LEU:N     | 2.31                     | 0.63              |
| 3:D:827:ILE:HG13  | 3:D:829:VAL:HG23  | 1.81                     | 0.63              |
| 3:D:1234:THR:N    | 3:D:1235:GLN:CB   | 2.62                     | 0.63              |
| 5:F:93:LEU:HD21   | 5:F:193:ARG:HD3   | 1.80                     | 0.63              |
| 1:A:216:GLU:OE1   | 1:A:219:ARG:NH2   | 2.32                     | 0.62              |
| 2:C:128:ILE:C     | 2:C:129:ILE:HD12  | 2.24                     | 0.62              |
| 3:D:371:ILE:HG13  | 3:D:372:ASP:N     | 2.13                     | 0.62              |
| 3:D:709:HIS:C     | 3:D:711:LEU:H     | 2.07                     | 0.62              |
| 3:D:916:TYR:CE1   | 3:D:920:LEU:HD21  | 2.34                     | 0.62              |
| 3:D:952:ASP:HA    | 3:D:1062:ARG:NH2  | 2.14                     | 0.62              |
| 3:D:1003:VAL:O    | 3:D:1007:VAL:HG23 | 1.98                     | 0.62              |
| 3:D:123:LEU:O     | 3:D:127:LEU:HB2   | 1.99                     | 0.62              |
| 3:D:134:VAL:HG13  | 3:D:153:LEU:HD11  | 1.80                     | 0.62              |
| 3:D:202:VAL:O     | 3:D:202:VAL:HG22  | 1.98                     | 0.62              |
| 3:D:245:LEU:CD1   | 3:D:307:ALA:HB1   | 2.28                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:643:GLY:CA    | 3:D:727:GLN:HB2   | 2.25                     | 0.62              |
| 3:D:1273:VAL:H    | 3:D:1326:THR:HG22 | 1.64                     | 0.62              |
| 5:F:301:ALA:O     | 5:F:304:VAL:HG13  | 1.98                     | 0.62              |
| 2:C:460:ARG:HD2   | 2:C:485:TYR:CZ    | 2.34                     | 0.62              |
| 2:C:675:ALA:HB2   | 2:C:867:VAL:HG11  | 1.80                     | 0.62              |
| 3:D:586:ARG:HG2   | 3:D:586:ARG:HH11  | 1.63                     | 0.62              |
| 3:D:1394:VAL:HG22 | 3:D:1420:LEU:HD21 | 1.81                     | 0.62              |
| 5:F:88:ILE:HG23   | 5:F:193:ARG:HG2   | 1.81                     | 0.62              |
| 1:A:89:PHE:HB2    | 1:A:146:ARG:HH22  | 1.63                     | 0.62              |
| 2:C:740:GLU:HB3   | 2:C:805:ARG:HH12  | 1.65                     | 0.62              |
| 4:E:33:HIS:NE2    | 4:E:89:MET:HE3    | 2.15                     | 0.62              |
| 2:C:773:LEU:O     | 2:C:777:ILE:HD12  | 1.99                     | 0.62              |
| 3:D:658:LEU:HD23  | 3:D:661:MET:CE    | 2.29                     | 0.62              |
| 1:A:153:ALA:C     | 1:A:155:LYS:H     | 2.07                     | 0.62              |
| 2:C:140:ILE:CD1   | 2:C:331:ARG:HH11  | 2.11                     | 0.62              |
| 3:D:558:LEU:HD23  | 3:D:567:ILE:HD11  | 1.81                     | 0.62              |
| 3:D:844:ALA:HB1   | 3:D:867:ARG:NH1   | 2.14                     | 0.62              |
| 5:F:372:ARG:O     | 5:F:373:LYS:HG2   | 2.00                     | 0.62              |
| 5:F:373:LYS:HD3   | 5:F:380:GLU:OE1   | 2.00                     | 0.62              |
| 2:C:619:ARG:HH21  | 2:C:619:ARG:HB2   | 1.64                     | 0.62              |
| 2:C:683:ASN:HB3   | 2:C:872:ASN:CB    | 2.25                     | 0.62              |
| 2:C:929:ARG:NH2   | 2:C:940:GLU:OE2   | 2.26                     | 0.62              |
| 3:D:169:TYR:O     | 3:D:392:SER:HB2   | 1.98                     | 0.62              |
| 3:D:314:PRO:HB2   | 3:D:317:VAL:CG1   | 2.30                     | 0.62              |
| 3:D:557:LEU:HD13  | 3:D:566:ILE:CG2   | 2.30                     | 0.62              |
| 3:D:1047:LYS:CG   | 3:D:1048:PRO:HD2  | 2.27                     | 0.62              |
| 3:D:1198:TYR:CE2  | 3:D:1460:ILE:HD13 | 2.35                     | 0.62              |
| 1:A:220:GLU:O     | 1:A:223:THR:OG1   | 2.10                     | 0.62              |
| 2:C:654:LEU:C     | 2:C:655:LEU:HD12  | 2.24                     | 0.62              |
| 3:D:97:THR:CG2    | 3:D:571:LYS:HD3   | 2.20                     | 0.62              |
| 3:D:206:ARG:HG2   | 3:D:392:SER:O     | 2.00                     | 0.62              |
| 3:D:1108:ARG:NH2  | 3:D:1198:TYR:O    | 2.31                     | 0.62              |
| 3:D:1442:ASN:O    | 3:D:1446:VAL:HG23 | 2.00                     | 0.62              |
| 3:D:242:LEU:HD21  | 3:D:311:LEU:HD13  | 1.82                     | 0.62              |
| 3:D:955:VAL:HG23  | 3:D:955:VAL:O     | 1.98                     | 0.62              |
| 3:D:1127:GLU:HA   | 3:D:1130:ARG:HB3  | 1.81                     | 0.62              |
| 1:A:89:PHE:HB2    | 1:A:146:ARG:NH2   | 2.14                     | 0.62              |
| 1:B:117:VAL:HG12  | 1:B:118:ALA:N     | 2.15                     | 0.62              |
| 2:C:577:PRO:HG2   | 2:C:580:MET:HG2   | 1.82                     | 0.62              |
| 3:D:174:GLY:HA2   | 3:D:389:GLU:CD    | 2.24                     | 0.62              |
| 5:F:300:ASP:O     | 5:F:304:VAL:HG12  | 2.00                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:605:LYS:O    | 2:C:606:VAL:HG23  | 2.00                     | 0.61              |
| 3:D:378:ILE:H    | 3:D:378:ILE:HD12  | 1.64                     | 0.61              |
| 2:C:230:ARG:H    | 2:C:233:GLU:HG3   | 1.65                     | 0.61              |
| 2:C:267:TYR:OH   | 2:C:290:LEU:HD21  | 2.00                     | 0.61              |
| 3:D:97:THR:HG22  | 3:D:554:LEU:HD21  | 1.82                     | 0.61              |
| 3:D:175:VAL:HG11 | 3:D:193:PRO:HG2   | 1.80                     | 0.61              |
| 3:D:216:VAL:HA   | 3:D:340:THR:CG2   | 2.23                     | 0.61              |
| 5:F:260:ILE:CG1  | 5:F:265:VAL:HG22  | 2.30                     | 0.61              |
| 3:D:291:LEU:HB2  | 3:D:304:LEU:O     | 1.99                     | 0.61              |
| 3:D:1225:ALA:O   | 3:D:1229:ILE:HG13 | 2.00                     | 0.61              |
| 4:E:80:VAL:HG12  | 4:E:81:PRO:O      | 2.00                     | 0.61              |
| 1:B:94:LEU:HD21  | 1:B:96:THR:O      | 2.01                     | 0.61              |
| 2:C:355:VAL:HG12 | 2:C:372:LEU:O     | 2.01                     | 0.61              |
| 2:C:413:LEU:HD21 | 2:C:451:LEU:HD13  | 1.81                     | 0.61              |
| 2:C:564:MET:HE1  | 2:C:846:LYS:HD3   | 1.80                     | 0.61              |
| 2:C:666:LEU:HD11 | 2:C:668:LEU:CD2   | 2.27                     | 0.61              |
| 3:D:23:TYR:CE2   | 3:D:89:ARG:HD3    | 2.36                     | 0.61              |
| 3:D:672:ALA:HB2  | 5:F:420:ASP:OD1   | 2.00                     | 0.61              |
| 1:B:31:GLY:N     | 1:B:193:ASP:OD1   | 2.30                     | 0.61              |
| 2:C:1085:PHE:CE1 | 3:D:1468:LEU:HD22 | 2.35                     | 0.61              |
| 3:D:574:LEU:O    | 3:D:578:VAL:HG12  | 2.00                     | 0.61              |
| 1:A:64:GLU:HA    | 1:A:165:ILE:HD13  | 1.82                     | 0.61              |
| 2:C:281:LEU:HD22 | 2:C:308:ARG:HH22  | 1.65                     | 0.61              |
| 2:C:559:LEU:C    | 2:C:559:LEU:HD23  | 2.25                     | 0.61              |
| 2:C:743:VAL:HG23 | 2:C:800:VAL:HG11  | 1.83                     | 0.61              |
| 1:B:94:LEU:HD23  | 1:B:95:GLN:N      | 2.15                     | 0.61              |
| 2:C:221:LEU:O    | 2:C:221:LEU:HD22  | 2.00                     | 0.61              |
| 2:C:879:ARG:N    | 2:C:879:ARG:HD2   | 2.16                     | 0.61              |
| 3:D:613:ARG:O    | 3:D:618:LEU:HD23  | 2.00                     | 0.61              |
| 5:F:309:LYS:O    | 5:F:312:GLN:HB2   | 2.01                     | 0.61              |
| 2:C:700:TYR:OH   | 2:C:994:ILE:O     | 2.13                     | 0.61              |
| 3:D:371:ILE:HG13 | 3:D:372:ASP:H     | 1.64                     | 0.61              |
| 2:C:1043:TYR:CD2 | 3:D:763:MET:HG2   | 2.35                     | 0.61              |
| 1:A:211:LEU:O    | 1:A:215:VAL:HG23  | 2.01                     | 0.61              |
| 2:C:211:LEU:CD2  | 2:C:218:VAL:HG22  | 2.31                     | 0.61              |
| 3:D:1389:LEU:O   | 3:D:1390:LEU:HD23 | 2.01                     | 0.61              |
| 3:D:93:ILE:HD11  | 3:D:548:ILE:CD1   | 2.31                     | 0.60              |
| 2:C:143:SER:HB2  | 2:C:332:ARG:HD2   | 1.83                     | 0.60              |
| 3:D:1165:TYR:CZ  | 3:D:1214:PRO:HB3  | 2.37                     | 0.60              |
| 1:B:117:VAL:HG12 | 1:B:118:ALA:H     | 1.65                     | 0.60              |
| 2:C:578:VAL:HG13 | 2:C:671:ASN:CG    | 2.26                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:905:ILE:HG23  | 2:C:906:PHE:CD1   | 2.31                     | 0.60              |
| 3:D:116:LEU:HD23  | 3:D:468:LEU:HD11  | 1.82                     | 0.60              |
| 3:D:394:LEU:HG    | 3:D:396:VAL:HG23  | 1.82                     | 0.60              |
| 1:A:121:GLU:HB3   | 1:A:123:MET:HE2   | 1.83                     | 0.60              |
| 3:D:284:LEU:CD2   | 3:D:290:PRO:HG3   | 2.29                     | 0.60              |
| 3:D:581:LEU:HD23  | 3:D:582:LEU:HD23  | 1.84                     | 0.60              |
| 1:A:68:ILE:O      | 1:A:71:VAL:HG22   | 2.01                     | 0.60              |
| 1:B:108:GLU:HG2   | 1:B:131:THR:CB    | 2.31                     | 0.60              |
| 2:C:390:GLN:NE2   | 2:C:414:GLY:HA2   | 2.16                     | 0.60              |
| 3:D:230:TRP:HA    | 3:D:243:ALA:CB    | 2.31                     | 0.60              |
| 3:D:575:GLN:O     | 3:D:578:VAL:HG13  | 2.02                     | 0.60              |
| 2:C:226:VAL:O     | 2:C:229:MET:HG3   | 2.01                     | 0.60              |
| 2:C:807:ARG:HB2   | 2:C:810:ASP:OD2   | 2.01                     | 0.60              |
| 2:C:880:MET:CE    | 3:D:1037:GLN:HB2  | 2.27                     | 0.60              |
| 3:D:172:PRO:HB2   | 3:D:175:VAL:CG2   | 2.32                     | 0.60              |
| 3:D:417:PRO:HB3   | 3:D:430:ASP:O     | 2.01                     | 0.60              |
| 3:D:1305:LEU:HD13 | 3:D:1309:ALA:HB3  | 1.84                     | 0.60              |
| 1:A:44:LEU:HD13   | 1:A:199:ILE:HD13  | 1.83                     | 0.60              |
| 2:C:626:ARG:H     | 2:C:639:GLN:NE2   | 1.99                     | 0.60              |
| 2:C:736:ASP:O     | 2:C:744:ARG:HG2   | 2.02                     | 0.60              |
| 2:C:944:LEU:HD11  | 2:C:963:LEU:HD21  | 1.82                     | 0.60              |
| 3:D:478:LEU:HD12  | 3:D:479:GLU:H     | 1.67                     | 0.60              |
| 3:D:662:GLU:OE2   | 3:D:669:ASN:HA    | 2.02                     | 0.60              |
| 3:D:808:THR:O     | 3:D:811:GLU:HG2   | 2.02                     | 0.60              |
| 1:A:63:HIS:HB2    | 2:C:799:ILE:HG21  | 1.84                     | 0.60              |
| 2:C:223:ASP:O     | 2:C:226:VAL:HG23  | 2.01                     | 0.60              |
| 3:D:315:ARG:H     | 3:D:315:ARG:HD2   | 1.66                     | 0.60              |
| 3:D:860:LEU:HD22  | 3:D:878:GLY:HA2   | 1.83                     | 0.60              |
| 3:D:1336:LEU:HD12 | 3:D:1336:LEU:O    | 2.02                     | 0.60              |
| 5:F:102:LEU:HD23  | 5:F:183:ALA:HB1   | 1.83                     | 0.60              |
| 1:B:40:LEU:C      | 1:B:44:LEU:HD12   | 2.27                     | 0.59              |
| 2:C:41:ASN:OD1    | 2:C:46:ALA:HA     | 2.01                     | 0.59              |
| 3:D:500:ARG:NH1   | 3:D:1390:LEU:HD21 | 2.17                     | 0.59              |
| 3:D:840:LYS:HE3   | 3:D:841:TYR:OH    | 2.02                     | 0.59              |
| 5:F:368:VAL:CG1   | 5:F:397:ILE:HD11  | 2.32                     | 0.59              |
| 2:C:654:LEU:HD11  | 2:C:656:ALA:O     | 2.02                     | 0.59              |
| 2:C:745:ILE:HD11  | 2:C:802:ARG:HA    | 1.84                     | 0.59              |
| 3:D:1486:VAL:HA   | 4:E:74:VAL:O      | 2.03                     | 0.59              |
| 5:F:120:THR:CG2   | 5:F:122:LEU:HD22  | 2.31                     | 0.59              |
| 5:F:282:LEU:N     | 5:F:282:LEU:HD23  | 2.15                     | 0.59              |
| 2:C:397:GLU:HG3   | 2:C:631:SER:HB2   | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:626:ARG:H     | 2:C:639:GLN:HE21  | 1.50                     | 0.59              |
| 2:C:897:LEU:HD21  | 2:C:921:ALA:HB2   | 1.84                     | 0.59              |
| 3:D:696:HIS:ND1   | 4:E:57:ASP:OD1    | 2.36                     | 0.59              |
| 3:D:1350:GLU:O    | 3:D:1354:LYS:HG3  | 2.01                     | 0.59              |
| 1:A:44:LEU:O      | 1:A:174:VAL:HG21  | 2.02                     | 0.59              |
| 1:A:111:ALA:HB2   | 1:A:127:LEU:HB3   | 1.84                     | 0.59              |
| 1:A:117:VAL:HB    | 1:A:120:VAL:HG21  | 1.85                     | 0.59              |
| 2:C:740:GLU:OE1   | 2:C:805:ARG:NH1   | 2.34                     | 0.59              |
| 3:D:134:VAL:CG2   | 3:D:151:GLN:H     | 2.16                     | 0.59              |
| 3:D:1111:ASP:OD2  | 3:D:1203:LYS:HE2  | 2.02                     | 0.59              |
| 2:C:841:ASN:HD22  | 2:C:992:MET:HE2   | 1.67                     | 0.59              |
| 3:D:216:VAL:CA    | 3:D:340:THR:HG22  | 2.24                     | 0.59              |
| 3:D:366:LYS:C     | 3:D:367:ILE:HD13  | 2.28                     | 0.59              |
| 5:F:173:TYR:HA    | 5:F:176:ILE:HG12  | 1.85                     | 0.59              |
| 1:A:97:VAL:HG12   | 1:A:98:THR:N      | 2.17                     | 0.59              |
| 1:A:159:LYS:HG2   | 1:A:166:PRO:HD3   | 1.85                     | 0.59              |
| 2:C:197:LEU:CA    | 2:C:200:LEU:HD12  | 2.31                     | 0.59              |
| 2:C:724:ARG:HD2   | 2:C:739:GLU:HA    | 1.85                     | 0.59              |
| 2:C:1019:GLN:NE2  | 3:D:621:LYS:HE3   | 2.17                     | 0.59              |
| 3:D:1126:ASP:C    | 3:D:1130:ARG:HA   | 2.27                     | 0.59              |
| 2:C:284:ARG:O     | 2:C:285:LEU:HD22  | 2.03                     | 0.59              |
| 3:D:178:LEU:HD12  | 3:D:190:GLU:O     | 2.02                     | 0.59              |
| 3:D:1190:SER:OG   | 3:D:1191:PRO:HD2  | 2.03                     | 0.59              |
| 3:D:1281:VAL:HG22 | 3:D:1316:GLY:N    | 2.18                     | 0.59              |
| 2:C:136:ILE:CG2   | 2:C:336:VAL:HG23  | 2.32                     | 0.59              |
| 2:C:229:MET:HB3   | 2:C:233:GLU:HB2   | 1.85                     | 0.59              |
| 3:D:1379:VAL:HG21 | 3:D:1400:VAL:HG11 | 1.84                     | 0.59              |
| 5:F:131:VAL:HG11  | 5:F:177:ALA:HB1   | 1.83                     | 0.59              |
| 2:C:367:LEU:HA    | 2:C:371:LYS:NZ    | 2.18                     | 0.59              |
| 2:C:547:ILE:O     | 2:C:905:ILE:HD11  | 2.01                     | 0.59              |
| 3:D:116:LEU:HD12  | 3:D:118:LEU:CD1   | 2.33                     | 0.59              |
| 3:D:816:HIS:HB2   | 3:D:836:VAL:HG11  | 1.85                     | 0.59              |
| 3:D:1233:GLY:HA2  | 3:D:1236:LEU:HG   | 1.85                     | 0.59              |
| 3:D:1394:VAL:CG2  | 3:D:1420:LEU:HD21 | 2.33                     | 0.59              |
| 1:A:6:LEU:HD23    | 1:A:7:LYS:N       | 2.17                     | 0.59              |
| 1:A:196:THR:HG21  | 2:C:934:PHE:HE1   | 1.67                     | 0.59              |
| 3:D:1281:VAL:HG22 | 3:D:1316:GLY:H    | 1.66                     | 0.59              |
| 5:F:200:LYS:CG    | 5:F:201:LYS:HG3   | 2.32                     | 0.59              |
| 2:C:644:VAL:HG22  | 2:C:645:VAL:N     | 2.18                     | 0.58              |
| 2:C:958:THR:HG23  | 2:C:961:GLU:CG    | 2.33                     | 0.58              |
| 5:F:361:LEU:CD1   | 5:F:411:HIS:HB2   | 2.26                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:290:LEU:O    | 2:C:301:GLU:HB2   | 2.03                     | 0.58              |
| 2:C:1031:ARG:HB2 | 3:D:622:ARG:NH1   | 2.18                     | 0.58              |
| 1:B:117:VAL:CG1  | 1:B:118:ALA:H     | 2.16                     | 0.58              |
| 1:B:185:ARG:HB2  | 1:B:190:THR:OG1   | 2.03                     | 0.58              |
| 3:D:122:GLU:HG2  | 3:D:152:LEU:CD1   | 2.32                     | 0.58              |
| 3:D:475:LYS:O    | 3:D:478:LEU:HD12  | 2.03                     | 0.58              |
| 4:E:26:ARG:NE    | 4:E:30:LEU:HD11   | 2.19                     | 0.58              |
| 1:A:216:GLU:CD   | 1:A:219:ARG:HH22  | 2.11                     | 0.58              |
| 2:C:154:ARG:NH1  | 2:C:175:GLU:OE2   | 2.36                     | 0.58              |
| 1:B:58:ILE:HB    | 1:B:61:VAL:CG2    | 2.33                     | 0.58              |
| 2:C:35:PRO:CG    | 2:C:38:LYS:HD3    | 2.34                     | 0.58              |
| 2:C:339:LEU:HD13 | 2:C:391:LEU:HD12  | 1.86                     | 0.58              |
| 2:C:571:LEU:CD2  | 2:C:700:TYR:HA    | 2.34                     | 0.58              |
| 3:D:192:ALA:HB3  | 3:D:195:VAL:HB    | 1.84                     | 0.58              |
| 3:D:496:LEU:HG   | 3:D:500:ARG:HD2   | 1.85                     | 0.58              |
| 3:D:573:MET:SD   | 5:F:210:LEU:HB3   | 2.43                     | 0.58              |
| 3:D:1041:LEU:O   | 3:D:1041:LEU:HD23 | 2.03                     | 0.58              |
| 3:D:1198:TYR:CZ  | 3:D:1460:ILE:HD13 | 2.38                     | 0.58              |
| 5:F:374:GLY:HA3  | 5:F:378:GLY:H     | 1.68                     | 0.58              |
| 2:C:395:LYS:HE2  | 2:C:403:SER:HB2   | 1.85                     | 0.58              |
| 2:C:433:THR:CG2  | 2:C:488:ALA:HB1   | 2.34                     | 0.58              |
| 2:C:706:GLU:HB3  | 2:C:708:TYR:CE1   | 2.38                     | 0.58              |
| 3:D:683:ILE:HG22 | 3:D:687:VAL:HG11  | 1.84                     | 0.58              |
| 3:D:699:VAL:CG1  | 3:D:760:ARG:HG3   | 2.32                     | 0.58              |
| 4:E:45:ARG:NH1   | 4:E:56:ASP:OD2    | 2.34                     | 0.58              |
| 1:A:101:LEU:O    | 1:A:102:LYS:HG2   | 2.03                     | 0.58              |
| 2:C:167:LYS:HG2  | 7:H:12:DC:C5      | 2.39                     | 0.58              |
| 3:D:144:GLY:O    | 3:D:145:VAL:HG23  | 2.03                     | 0.58              |
| 3:D:266:GLU:HG3  | 3:D:314:PRO:HB3   | 1.86                     | 0.58              |
| 3:D:270:LEU:HD13 | 3:D:304:LEU:HD13  | 1.86                     | 0.58              |
| 5:F:364:ARG:O    | 5:F:367:MET:HG3   | 2.04                     | 0.58              |
| 5:F:412:GLU:HG3  | 5:F:418:LEU:HD13  | 1.84                     | 0.58              |
| 1:A:39:PRO:HG3   | 1:B:39:PRO:HG3    | 1.85                     | 0.58              |
| 1:A:79:ILE:HD12  | 1:A:167:VAL:CG2   | 2.34                     | 0.58              |
| 2:C:767:PRO:HB2  | 2:C:772:ARG:HG3   | 1.86                     | 0.58              |
| 3:D:1147:ARG:HB3 | 3:D:1188:VAL:HG22 | 1.86                     | 0.58              |
| 2:C:214:TYR:CD2  | 2:C:218:VAL:HG23  | 2.39                     | 0.58              |
| 2:C:767:PRO:HB2  | 2:C:772:ARG:CG    | 2.34                     | 0.58              |
| 3:D:204:LEU:HD11 | 3:D:445:ARG:HE    | 1.69                     | 0.58              |
| 3:D:1486:VAL:HB  | 4:E:22:VAL:HG13   | 1.86                     | 0.58              |
| 3:D:297:ILE:HD12 | 3:D:297:ILE:N     | 2.19                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:586:ARG:HG2  | 3:D:586:ARG:NH1   | 2.19                     | 0.57              |
| 3:D:676:MET:HE3  | 3:D:683:ILE:HA    | 1.86                     | 0.57              |
| 5:F:383:LEU:C    | 5:F:386:VAL:HG22  | 2.29                     | 0.57              |
| 1:A:6:LEU:HD23   | 1:A:7:LYS:O       | 2.04                     | 0.57              |
| 3:D:360:ARG:HA   | 3:D:384:VAL:HG12  | 1.86                     | 0.57              |
| 5:F:203:THR:O    | 5:F:205:ARG:HG2   | 2.04                     | 0.57              |
| 2:C:214:TYR:HD2  | 2:C:218:VAL:HG23  | 1.69                     | 0.57              |
| 3:D:618:LEU:HB3  | 3:D:1467:ILE:HG23 | 1.87                     | 0.57              |
| 3:D:1205:TYR:CZ  | 3:D:1366:LYS:HE2  | 2.39                     | 0.57              |
| 3:D:1426:LYS:HE3 | 7:H:20:DG:OP1     | 2.04                     | 0.57              |
| 2:C:713:ARG:HG2  | 2:C:720:GLU:OE1   | 2.05                     | 0.57              |
| 3:D:842:VAL:HG22 | 3:D:865:THR:HB    | 1.87                     | 0.57              |
| 3:D:970:LYS:HA   | 3:D:973:GLN:CB    | 2.33                     | 0.57              |
| 3:D:1208:ASP:OD2 | 3:D:1211:MET:HE2  | 2.04                     | 0.57              |
| 3:D:1271:LYS:CD  | 3:D:1331:ASP:HB2  | 2.33                     | 0.57              |
| 1:A:63:HIS:O     | 1:A:66:SER:OG     | 2.23                     | 0.57              |
| 1:A:222:LEU:HD21 | 1:B:218:LEU:HD22  | 1.84                     | 0.57              |
| 1:B:127:LEU:HD23 | 1:B:127:LEU:C     | 2.29                     | 0.57              |
| 2:C:127:PHE:O    | 2:C:133:ASP:HA    | 2.03                     | 0.57              |
| 2:C:197:LEU:H    | 2:C:197:LEU:HD12  | 1.69                     | 0.57              |
| 2:C:630:ARG:HB2  | 2:C:705:ILE:HD12  | 1.86                     | 0.57              |
| 3:D:132:TYR:OH   | 3:D:568:ARG:NH2   | 2.38                     | 0.57              |
| 3:D:324:ALA:HB1  | 3:D:331:VAL:HG21  | 1.86                     | 0.57              |
| 3:D:361:VAL:HG21 | 3:D:379:ALA:CB    | 2.34                     | 0.57              |
| 3:D:1314:LYS:HE2 | 3:D:1317:ASP:OD2  | 2.04                     | 0.57              |
| 5:F:95:THR:HG22  | 5:F:98:GLU:OE2    | 2.04                     | 0.57              |
| 1:A:143:ARG:NH1  | 1:A:160:ASP:OD1   | 2.37                     | 0.57              |
| 2:C:128:ILE:O    | 2:C:129:ILE:HD12  | 2.03                     | 0.57              |
| 2:C:545:ASN:HB3  | 2:C:583:LEU:HD22  | 1.85                     | 0.57              |
| 2:C:679:PHE:N    | 2:C:683:ASN:OD1   | 2.38                     | 0.57              |
| 2:C:712:ALA:HB3  | 2:C:821:GLU:HG2   | 1.85                     | 0.57              |
| 2:C:775:ARG:HH11 | 5:F:422:LEU:HD23  | 1.70                     | 0.57              |
| 3:D:137:PRO:HB3  | 3:D:147:VAL:HG23  | 1.85                     | 0.57              |
| 3:D:352:ASN:HB3  | 5:F:104:ARG:NH1   | 2.19                     | 0.57              |
| 5:F:200:LYS:HG3  | 5:F:201:LYS:HG3   | 1.86                     | 0.57              |
| 1:A:224:TYR:CG   | 1:B:9:PRO:HG2     | 2.39                     | 0.57              |
| 2:C:557:ARG:NH1  | 2:C:844:GLY:O     | 2.38                     | 0.57              |
| 3:D:14:SER:HB3   | 3:D:511:TRP:CZ2   | 2.38                     | 0.57              |
| 3:D:378:ILE:HD12 | 3:D:378:ILE:N     | 2.20                     | 0.57              |
| 3:D:885:ILE:HG23 | 3:D:937:TYR:CE1   | 2.39                     | 0.57              |
| 3:D:1093:TYR:OH  | 3:D:1441:GLN:NE2  | 2.38                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:172:ILE:HG12  | 2:C:186:VAL:CG2  | 2.35                     | 0.57              |
| 2:C:765:SER:O     | 2:C:765:SER:OG   | 2.22                     | 0.57              |
| 2:C:438:ILE:HD11  | 2:C:467:ILE:HD12 | 1.86                     | 0.57              |
| 2:C:587:VAL:O     | 2:C:591:SER:HB3  | 2.05                     | 0.57              |
| 3:D:221:ALA:O     | 3:D:335:LEU:HD12 | 2.05                     | 0.57              |
| 3:D:291:LEU:N     | 3:D:304:LEU:O    | 2.36                     | 0.57              |
| 3:D:764:LEU:HD23  | 3:D:767:HIS:NE2  | 2.18                     | 0.57              |
| 3:D:1090:ASP:N    | 3:D:1090:ASP:OD1 | 2.37                     | 0.57              |
| 2:C:1001:VAL:HB   | 3:D:724:GLN:HB2  | 1.86                     | 0.57              |
| 3:D:135:LEU:CD1   | 3:D:463:GLN:HG2  | 2.35                     | 0.57              |
| 3:D:672:ALA:HB2   | 5:F:420:ASP:CG   | 2.30                     | 0.57              |
| 3:D:764:LEU:HB3   | 3:D:767:HIS:CD2  | 2.40                     | 0.57              |
| 3:D:823:LEU:HD11  | 3:D:837:GLY:CA   | 2.35                     | 0.57              |
| 3:D:1031:ASN:OD1  | 3:D:1034:GLN:HG3 | 2.05                     | 0.57              |
| 2:C:2:GLU:O       | 2:C:3:ILE:HD13   | 2.04                     | 0.56              |
| 2:C:1021:LEU:HD12 | 2:C:1021:LEU:N   | 2.16                     | 0.56              |
| 3:D:983:LEU:HB3   | 3:D:987:GLU:OE2  | 2.04                     | 0.56              |
| 2:C:718:GLY:HA3   | 2:C:761:PHE:CD1  | 2.39                     | 0.56              |
| 2:C:743:VAL:HG13  | 2:C:755:LEU:O    | 2.04                     | 0.56              |
| 3:D:361:VAL:HG21  | 3:D:379:ALA:HB1  | 1.86                     | 0.56              |
| 3:D:556:LYS:HD3   | 5:F:218:GLN:OE1  | 2.05                     | 0.56              |
| 3:D:993:LEU:C     | 3:D:993:LEU:HD12 | 2.30                     | 0.56              |
| 1:A:39:PRO:HG3    | 1:B:39:PRO:CG    | 2.34                     | 0.56              |
| 1:B:162:ILE:HG13  | 1:B:163:ASN:ND2  | 2.20                     | 0.56              |
| 2:C:297:GLU:HG3   | 2:C:299:LYS:NZ   | 2.20                     | 0.56              |
| 2:C:690:ILE:CD1   | 2:C:852:ILE:HG23 | 2.35                     | 0.56              |
| 2:C:747:ALA:O     | 2:C:799:ILE:HA   | 2.05                     | 0.56              |
| 2:C:756:VAL:HG21  | 2:C:823:VAL:CG1  | 2.35                     | 0.56              |
| 2:C:897:LEU:HB2   | 2:C:899:GLN:HG3  | 1.88                     | 0.56              |
| 3:D:38:LYS:HB3    | 3:D:39:PRO:HD2   | 1.87                     | 0.56              |
| 3:D:229:ALA:HB1   | 3:D:244:GLU:O    | 2.05                     | 0.56              |
| 3:D:563:PRO:HB3   | 5:F:189:GLU:HG2  | 1.87                     | 0.56              |
| 3:D:828:LYS:CE    | 3:D:831:GLY:H    | 2.16                     | 0.56              |
| 3:D:864:VAL:CG1   | 3:D:865:THR:N    | 2.68                     | 0.56              |
| 3:D:1281:VAL:CG2  | 3:D:1315:ASP:HA  | 2.36                     | 0.56              |
| 2:C:396:ASP:HA    | 2:C:633:GLN:NE2  | 2.20                     | 0.56              |
| 2:C:958:THR:HG23  | 2:C:961:GLU:OE1  | 2.05                     | 0.56              |
| 3:D:236:TYR:CE1   | 3:D:242:LEU:HB2  | 2.41                     | 0.56              |
| 2:C:193:LEU:O     | 2:C:197:LEU:HD12 | 2.06                     | 0.56              |
| 1:A:10:VAL:N      | 1:A:26:GLU:O     | 2.29                     | 0.56              |
| 2:C:874:LEU:HD12  | 3:D:784:ASP:OD1  | 2.06                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:1126:ASP:O   | 3:D:1130:ARG:HA   | 2.06                     | 0.56              |
| 3:D:1461:GLY:O   | 3:D:1465:ASN:ND2  | 2.39                     | 0.56              |
| 5:F:153:PRO:CA   | 5:F:156:VAL:HG12  | 2.33                     | 0.56              |
| 5:F:202:TYR:HE1  | 5:F:248:ASN:HD21  | 1.54                     | 0.56              |
| 5:F:240:THR:O    | 5:F:244:ARG:HG2   | 2.06                     | 0.56              |
| 5:F:350:LEU:HD13 | 5:F:421:PHE:CD2   | 2.41                     | 0.56              |
| 2:C:6:PHE:CD1    | 2:C:909:ALA:HB2   | 2.41                     | 0.56              |
| 2:C:725:ASP:N    | 2:C:726:ILE:HD12  | 2.21                     | 0.56              |
| 2:C:1004:LYS:HD3 | 3:D:744:GLN:HE22  | 1.70                     | 0.56              |
| 2:C:1092:LEU:CD1 | 2:C:1099:VAL:HG21 | 2.35                     | 0.56              |
| 3:D:437:VAL:HG11 | 5:F:175:HIS:HD2   | 1.70                     | 0.56              |
| 1:B:85:LEU:HD11  | 1:B:122:ILE:HD12  | 1.88                     | 0.56              |
| 1:B:124:ASN:HD21 | 1:B:127:LEU:HD12  | 1.68                     | 0.56              |
| 2:C:8:ARG:HB3    | 2:C:8:ARG:CZ      | 2.36                     | 0.56              |
| 2:C:23:VAL:HG23  | 2:C:24:GLU:H      | 1.71                     | 0.56              |
| 2:C:35:PRO:HG2   | 2:C:38:LYS:HB2    | 1.88                     | 0.56              |
| 2:C:719:PRO:HD2  | 2:C:761:PHE:HE1   | 1.70                     | 0.56              |
| 2:C:762:LYS:HE2  | 2:C:786:LYS:HG3   | 1.88                     | 0.56              |
| 3:D:63:TYR:OH    | 3:D:74:GLU:OE1    | 2.23                     | 0.56              |
| 3:D:618:LEU:CG   | 3:D:1467:ILE:HG23 | 2.36                     | 0.56              |
| 3:D:676:MET:HE3  | 3:D:682:ASP:O     | 2.06                     | 0.56              |
| 4:E:50:THR:HG23  | 4:E:53:GLY:H      | 1.71                     | 0.56              |
| 2:C:292:ARG:NH1  | 2:C:301:GLU:OE2   | 2.39                     | 0.56              |
| 4:E:39:VAL:O     | 4:E:72:ARG:HD2    | 2.06                     | 0.56              |
| 5:F:95:THR:HG22  | 5:F:98:GLU:CD     | 2.30                     | 0.56              |
| 2:C:715:THR:HB   | 2:C:718:GLY:O     | 2.07                     | 0.56              |
| 3:D:683:ILE:HG23 | 3:D:687:VAL:HG11  | 1.88                     | 0.55              |
| 3:D:843:PHE:CE2  | 3:D:864:VAL:HG11  | 2.34                     | 0.55              |
| 3:D:1301:LYS:HG2 | 3:D:1302:GLU:H    | 1.71                     | 0.55              |
| 1:A:184:THR:HG23 | 1:A:185:ARG:N     | 2.21                     | 0.55              |
| 2:C:143:SER:HB2  | 2:C:332:ARG:CD    | 2.36                     | 0.55              |
| 2:C:368:THR:OG1  | 2:C:371:LYS:HG2   | 2.06                     | 0.55              |
| 3:D:529:GLN:HG3  | 3:D:535:PHE:CZ    | 2.42                     | 0.55              |
| 3:D:764:LEU:HD23 | 3:D:767:HIS:HD2   | 1.69                     | 0.55              |
| 3:D:823:LEU:HD11 | 3:D:837:GLY:HA2   | 1.89                     | 0.55              |
| 3:D:1353:GLN:OE1 | 3:D:1353:GLN:HA   | 2.06                     | 0.55              |
| 5:F:101:GLU:O    | 5:F:105:LYS:HG3   | 2.06                     | 0.55              |
| 5:F:171:LYS:HD3  | 5:F:175:HIS:CE1   | 2.36                     | 0.55              |
| 5:F:274:THR:O    | 5:F:278:LEU:HG    | 2.07                     | 0.55              |
| 1:B:26:GLU:HB3   | 1:B:194:LYS:CG    | 2.36                     | 0.55              |
| 1:B:197:LEU:HD12 | 1:B:198:ARG:H     | 1.69                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1090:LYS:HE3  | 3:D:88:TYR:O      | 2.06                     | 0.55              |
| 3:D:1292:VAL:HG13 | 3:D:1303:TYR:HB2  | 1.87                     | 0.55              |
| 5:F:120:THR:HG23  | 5:F:122:LEU:HD13  | 1.88                     | 0.55              |
| 2:C:150:PRO:CD    | 2:C:322:VAL:HG11  | 2.31                     | 0.55              |
| 2:C:194:VAL:HG13  | 2:C:221:LEU:CD2   | 2.36                     | 0.55              |
| 2:C:409:ARG:HG2   | 2:C:409:ARG:HH21  | 1.72                     | 0.55              |
| 2:C:743:VAL:CG1   | 2:C:755:LEU:HA    | 2.37                     | 0.55              |
| 2:C:833:LEU:HD12  | 2:C:834:GLN:N     | 2.18                     | 0.55              |
| 2:C:1047:HIS:CE1  | 3:D:1471:LEU:HD21 | 2.42                     | 0.55              |
| 3:D:256:GLU:OE1   | 3:D:300:LYS:HE2   | 2.06                     | 0.55              |
| 3:D:367:ILE:HD11  | 3:D:379:ALA:HB2   | 1.88                     | 0.55              |
| 3:D:881:LEU:O     | 3:D:885:ILE:HG13  | 2.07                     | 0.55              |
| 2:C:425:PHE:CD1   | 3:D:1079:LYS:HE3  | 2.41                     | 0.55              |
| 2:C:567:GLN:NE2   | 2:C:999:HIS:HE2   | 2.05                     | 0.55              |
| 3:D:116:LEU:CB    | 3:D:118:LEU:HD12  | 2.31                     | 0.55              |
| 3:D:553:ARG:HG3   | 3:D:553:ARG:O     | 2.07                     | 0.55              |
| 3:D:698:LYS:HB2   | 3:D:756:GLN:OE1   | 2.07                     | 0.55              |
| 3:D:800:LYS:HB3   | 3:D:822:ALA:H     | 1.71                     | 0.55              |
| 3:D:1271:LYS:HD2  | 3:D:1331:ASP:CB   | 2.37                     | 0.55              |
| 1:A:14:ARG:NH1    | 1:A:14:ARG:HB2    | 2.22                     | 0.55              |
| 1:B:208:LEU:HD12  | 1:B:208:LEU:O     | 2.07                     | 0.55              |
| 2:C:462:ASP:HB3   | 2:C:468:ARG:HD3   | 1.87                     | 0.55              |
| 3:D:676:MET:CE    | 3:D:683:ILE:HA    | 2.36                     | 0.55              |
| 1:A:124:ASN:HD21  | 1:A:127:LEU:HD22  | 1.71                     | 0.55              |
| 2:C:352:ALA:O     | 2:C:356:ARG:HD2   | 2.07                     | 0.55              |
| 2:C:422:ARG:NH2   | 7:H:13:DT:H5'     | 2.21                     | 0.55              |
| 2:C:471:TYR:OH    | 2:C:516:ARG:NH2   | 2.39                     | 0.55              |
| 3:D:141:ILE:HG13  | 3:D:142:LEU:N     | 2.22                     | 0.55              |
| 3:D:650:LEU:CD1   | 3:D:657:LEU:HD23  | 2.33                     | 0.55              |
| 3:D:1024:ALA:HA   | 3:D:1029:ARG:O    | 2.07                     | 0.55              |
| 3:D:185:VAL:CG1   | 3:D:186:VAL:N     | 2.69                     | 0.55              |
| 3:D:407:VAL:O     | 5:F:171:LYS:HE2   | 2.06                     | 0.55              |
| 3:D:410:SER:OG    | 5:F:174:LEU:HD23  | 2.06                     | 0.55              |
| 3:D:1375:MET:HE2  | 3:D:1424:VAL:HG13 | 1.88                     | 0.55              |
| 2:C:540:PHE:HB3   | 2:C:544:THR:HG22  | 1.85                     | 0.55              |
| 2:C:805:ARG:C     | 2:C:806:LEU:HD23  | 2.32                     | 0.55              |
| 2:C:1085:PHE:O    | 2:C:1088:LEU:HB3  | 2.06                     | 0.55              |
| 3:D:6:ARG:HB3     | 3:D:6:ARG:HH11    | 1.72                     | 0.55              |
| 3:D:806:PHE:O     | 3:D:829:VAL:HA    | 2.06                     | 0.55              |
| 2:C:88:LEU:O      | 2:C:131:GLY:N     | 2.40                     | 0.55              |
| 2:C:194:VAL:HA    | 2:C:197:LEU:CD1   | 2.34                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:726:ILE:HD12  | 2:C:726:ILE:N     | 2.22                     | 0.55              |
| 2:C:846:LYS:HD2   | 3:D:741:ASP:HB2   | 1.89                     | 0.55              |
| 3:D:65:ARG:HD3    | 5:F:377:ASP:CA    | 2.36                     | 0.55              |
| 3:D:137:PRO:HA    | 3:D:452:ILE:HG13  | 1.89                     | 0.55              |
| 3:D:796:ARG:HH22  | 3:D:859:ASP:CG    | 2.15                     | 0.55              |
| 3:D:828:LYS:C     | 3:D:828:LYS:HD3   | 2.32                     | 0.55              |
| 3:D:1160:LEU:HD23 | 3:D:1164:ARG:NH1  | 2.22                     | 0.55              |
| 3:D:1263:PHE:HD2  | 3:D:1375:MET:CE   | 2.19                     | 0.55              |
| 5:F:194:LEU:HB2   | 7:H:6:DT:C2       | 2.42                     | 0.55              |
| 2:C:53:PRO:HB3    | 2:C:67:ASP:OD2    | 2.07                     | 0.54              |
| 3:D:185:VAL:HG12  | 3:D:186:VAL:N     | 2.22                     | 0.54              |
| 1:B:96:THR:O      | 1:B:97:VAL:HG23   | 2.06                     | 0.54              |
| 2:C:195:LEU:CD1   | 2:C:234:ALA:HB1   | 2.37                     | 0.54              |
| 2:C:598:GLU:O     | 2:C:599:GLU:HG2   | 2.08                     | 0.54              |
| 2:C:683:ASN:CB    | 2:C:872:ASN:HD22  | 2.20                     | 0.54              |
| 3:D:116:LEU:HD12  | 3:D:118:LEU:HD12  | 1.89                     | 0.54              |
| 3:D:212:ARG:HB2   | 3:D:344:ASP:OD1   | 2.07                     | 0.54              |
| 3:D:916:TYR:CE2   | 3:D:920:LEU:HD11  | 2.41                     | 0.54              |
| 3:D:1095:THR:O    | 3:D:1099:VAL:HG23 | 2.07                     | 0.54              |
| 2:C:396:ASP:HA    | 2:C:633:GLN:HE22  | 1.72                     | 0.54              |
| 2:C:808:ARG:HB3   | 2:C:808:ARG:HH21  | 1.70                     | 0.54              |
| 2:C:1005:MET:SD   | 3:D:648:MET:HG3   | 2.48                     | 0.54              |
| 3:D:245:LEU:HD13  | 3:D:307:ALA:CB    | 2.38                     | 0.54              |
| 3:D:781:PRO:HB2   | 3:D:786:ILE:HG22  | 1.89                     | 0.54              |
| 3:D:860:LEU:HD22  | 3:D:878:GLY:CA    | 2.38                     | 0.54              |
| 5:F:353:GLU:CD    | 5:F:417:LYS:HD2   | 2.32                     | 0.54              |
| 1:A:101:LEU:C     | 1:A:102:LYS:HG2   | 2.32                     | 0.54              |
| 2:C:498:GLN:HG2   | 2:C:514:VAL:O     | 2.07                     | 0.54              |
| 2:C:723:THR:OG1   | 2:C:724:ARG:N     | 2.41                     | 0.54              |
| 2:C:1008:ARG:NH2  | 2:C:1020:PRO:HB3  | 2.23                     | 0.54              |
| 3:D:664:LYS:HE3   | 3:D:693:GLU:OE2   | 2.06                     | 0.54              |
| 3:D:1004:THR:OG1  | 3:D:1036:ARG:HD3  | 2.08                     | 0.54              |
| 3:D:1088:THR:HG21 | 6:G:14:DG:C6      | 2.43                     | 0.54              |
| 5:F:117:SER:O     | 5:F:121:GLY:N     | 2.37                     | 0.54              |
| 1:A:133:GLU:OE2   | 2:C:605:LYS:HB3   | 2.07                     | 0.54              |
| 1:A:205:VAL:HG23  | 1:A:206:THR:N     | 2.22                     | 0.54              |
| 2:C:238:LEU:O     | 2:C:241:LEU:N     | 2.38                     | 0.54              |
| 2:C:507:ARG:HB2   | 2:C:507:ARG:NH1   | 2.23                     | 0.54              |
| 2:C:690:ILE:CG1   | 2:C:852:ILE:HG23  | 2.38                     | 0.54              |
| 2:C:1008:ARG:HD2  | 2:C:1028:GLY:O    | 2.08                     | 0.54              |
| 3:D:65:ARG:HD3    | 5:F:377:ASP:HA    | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:297:ILE:HD12 | 3:D:297:ILE:H    | 1.73                     | 0.54              |
| 3:D:367:ILE:HD13 | 3:D:367:ILE:N    | 2.22                     | 0.54              |
| 3:D:955:VAL:HG22 | 3:D:1011:PHE:CZ  | 2.43                     | 0.54              |
| 2:C:679:PHE:O    | 2:C:680:ASP:HB2  | 2.08                     | 0.54              |
| 2:C:715:THR:HG22 | 2:C:716:LYS:N    | 2.22                     | 0.54              |
| 2:C:880:MET:HE3  | 3:D:1037:GLN:CB  | 2.30                     | 0.54              |
| 3:D:18:ILE:HG21  | 3:D:516:ALA:O    | 2.08                     | 0.54              |
| 3:D:55:ASP:OD1   | 3:D:83:SER:HB3   | 2.08                     | 0.54              |
| 3:D:801:GLY:HA2  | 3:D:821:VAL:HG22 | 1.89                     | 0.54              |
| 1:B:59:GLU:OE2   | 1:B:139:ASN:ND2  | 2.32                     | 0.54              |
| 2:C:281:LEU:HD22 | 2:C:308:ARG:NH2  | 2.23                     | 0.54              |
| 2:C:312:ALA:HB1  | 2:C:317:VAL:CG2  | 2.38                     | 0.54              |
| 2:C:437:ARG:HB3  | 2:C:467:ILE:HG21 | 1.89                     | 0.54              |
| 3:D:85:VAL:C     | 3:D:87:ARG:H     | 2.16                     | 0.54              |
| 3:D:704:ARG:HG2  | 3:D:705:ALA:H    | 1.73                     | 0.54              |
| 2:C:101:ILE:HA   | 2:C:107:LEU:O    | 2.08                     | 0.54              |
| 2:C:710:ILE:HD12 | 2:C:790:LEU:HB2  | 1.90                     | 0.54              |
| 2:C:983:ILE:O    | 2:C:985:GLY:N    | 2.41                     | 0.54              |
| 2:C:1008:ARG:CZ  | 2:C:1020:PRO:HB3 | 2.38                     | 0.54              |
| 3:D:948:THR:HG23 | 3:D:949:ILE:N    | 2.23                     | 0.54              |
| 3:D:1079:LYS:O   | 3:D:1079:LYS:HG3 | 2.07                     | 0.54              |
| 5:F:376:ILE:O    | 5:F:377:ASP:HB3  | 2.08                     | 0.54              |
| 1:A:40:LEU:HD23  | 1:A:218:LEU:HD12 | 1.90                     | 0.54              |
| 2:C:189:ARG:NH2  | 2:C:244:PRO:HD2  | 2.23                     | 0.54              |
| 3:D:741:ASP:OD1  | 3:D:743:ASP:OD1  | 2.25                     | 0.54              |
| 3:D:764:LEU:HB3  | 3:D:767:HIS:HD2  | 1.73                     | 0.54              |
| 3:D:1040:GLY:O   | 3:D:1060:SER:HB2 | 2.08                     | 0.54              |
| 3:D:1496:GLU:O   | 3:D:1500:LYS:HG2 | 2.08                     | 0.54              |
| 5:F:141:VAL:HG22 | 5:F:151:LEU:O    | 2.08                     | 0.54              |
| 2:C:356:ARG:HA   | 2:C:359:MET:HB2  | 1.89                     | 0.53              |
| 2:C:418:LEU:HD21 | 2:C:427:VAL:HG11 | 1.90                     | 0.53              |
| 3:D:93:ILE:CD1   | 3:D:548:ILE:HG12 | 2.37                     | 0.53              |
| 3:D:135:LEU:HD11 | 3:D:463:GLN:HG2  | 1.89                     | 0.53              |
| 3:D:566:ILE:HG13 | 5:F:217:ASN:HD22 | 1.72                     | 0.53              |
| 3:D:581:LEU:HD23 | 3:D:582:LEU:HD21 | 1.89                     | 0.53              |
| 5:F:159:ILE:O    | 5:F:163:LEU:HG   | 2.09                     | 0.53              |
| 1:A:11:PHE:CD2   | 1:B:225:PHE:HA   | 2.44                     | 0.53              |
| 1:B:100:LEU:CD2  | 1:B:141:GLU:HG2  | 2.39                     | 0.53              |
| 1:B:124:ASN:HD22 | 1:B:127:LEU:HD12 | 1.70                     | 0.53              |
| 2:C:815:LEU:HB2  | 2:C:819:VAL:HG22 | 1.88                     | 0.53              |
| 2:C:1035:MET:HA  | 2:C:1038:TRP:CE3 | 2.43                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:496:LEU:HD23  | 3:D:1390:LEU:CD1  | 2.36                     | 0.53              |
| 3:D:1106:VAL:HG12 | 3:D:1107:VAL:N    | 2.24                     | 0.53              |
| 3:D:1254:GLN:HB2  | 3:D:1258:ARG:HB2  | 1.90                     | 0.53              |
| 4:E:34:GLY:O      | 4:E:35:PHE:HB2    | 2.07                     | 0.53              |
| 2:C:11:GLU:OE2    | 2:C:537:LYS:HE2   | 2.09                     | 0.53              |
| 3:D:135:LEU:HD11  | 3:D:463:GLN:CG    | 2.37                     | 0.53              |
| 3:D:274:ARG:O     | 3:D:275:GLU:C     | 2.50                     | 0.53              |
| 3:D:1045:MET:HA   | 3:D:1045:MET:CE   | 2.24                     | 0.53              |
| 1:A:38:ASN:HB3    | 1:A:39:PRO:CD     | 2.38                     | 0.53              |
| 1:A:227:ASN:HD22  | 1:A:227:ASN:C     | 2.15                     | 0.53              |
| 1:B:41:ARG:HA     | 1:B:177:VAL:HG11  | 1.89                     | 0.53              |
| 1:B:143:ARG:HD3   | 1:B:158:ILE:CD1   | 2.39                     | 0.53              |
| 1:B:219:ARG:O     | 1:B:222:LEU:HB2   | 2.08                     | 0.53              |
| 2:C:263:ASP:C     | 2:C:265:ARG:H     | 2.16                     | 0.53              |
| 2:C:808:ARG:HB3   | 2:C:808:ARG:CZ    | 2.39                     | 0.53              |
| 3:D:1066:THR:OG1  | 3:D:1069:GLU:HG3  | 2.09                     | 0.53              |
| 1:A:138:LEU:CD1   | 1:A:140:MET:HE3   | 2.37                     | 0.53              |
| 1:B:108:GLU:CG    | 1:B:131:THR:HB    | 2.35                     | 0.53              |
| 2:C:317:VAL:HB    | 2:C:320:HIS:HD2   | 1.70                     | 0.53              |
| 3:D:82:LYS:HB2    | 3:D:84:ILE:HG22   | 1.90                     | 0.53              |
| 3:D:1165:TYR:CE2  | 3:D:1214:PRO:HB3  | 2.43                     | 0.53              |
| 4:E:39:VAL:CG2    | 4:E:72:ARG:HB3    | 2.39                     | 0.53              |
| 2:C:283:ILE:HD13  | 2:C:305:PRO:HB3   | 1.91                     | 0.53              |
| 2:C:355:VAL:HG23  | 2:C:356:ARG:N     | 2.24                     | 0.53              |
| 2:C:905:ILE:C     | 2:C:907:ASP:H     | 2.16                     | 0.53              |
| 3:D:142:LEU:HD13  | 3:D:161:LEU:HD21  | 1.91                     | 0.53              |
| 3:D:371:ILE:HD11  | 5:F:232:ARG:NH1   | 2.24                     | 0.53              |
| 3:D:626:SER:HA    | 3:D:747:VAL:O     | 2.09                     | 0.53              |
| 3:D:1311:LEU:O    | 3:D:1312:LEU:HD23 | 2.09                     | 0.53              |
| 7:H:17:DA:H2''    | 7:H:18:DC:H5'     | 1.90                     | 0.53              |
| 1:A:88:ARG:HB2    | 1:A:204:SER:HA    | 1.90                     | 0.53              |
| 1:B:173:PRO:HB2   | 1:B:205:VAL:HG12  | 1.89                     | 0.53              |
| 1:B:202:ASP:OD1   | 1:B:204:SER:HB3   | 2.08                     | 0.53              |
| 2:C:712:ALA:HB3   | 2:C:821:GLU:CG    | 2.38                     | 0.53              |
| 2:C:888:THR:O     | 2:C:891:GLY:N     | 2.41                     | 0.53              |
| 3:D:140:ALA:HA    | 3:D:450:TYR:CE1   | 2.43                     | 0.53              |
| 3:D:1057:VAL:HG21 | 3:D:1065:LEU:CD2  | 2.39                     | 0.53              |
| 2:C:1043:TYR:CG   | 3:D:763:MET:HG2   | 2.43                     | 0.53              |
| 2:C:1109:VAL:HG11 | 3:D:5:VAL:HG22    | 1.91                     | 0.53              |
| 3:D:158:TYR:CE1   | 3:D:454:ALA:HB3   | 2.44                     | 0.53              |
| 3:D:399:ARG:O     | 3:D:446:VAL:HG12  | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:462:GLN:O     | 3:D:466:LYS:HB2   | 2.09                     | 0.53              |
| 3:D:625:TYR:CE2   | 3:D:751:LEU:HD11  | 2.43                     | 0.53              |
| 3:D:882:PHE:CE2   | 3:D:906:GLN:HG3   | 2.44                     | 0.53              |
| 3:D:1405:GLU:O    | 3:D:1408:ILE:HG13 | 2.08                     | 0.53              |
| 5:F:153:PRO:C     | 5:F:156:VAL:HG12  | 2.34                     | 0.53              |
| 5:F:198:ILE:HD12  | 5:F:243:ILE:HG21  | 1.91                     | 0.53              |
| 1:A:18:ARG:HH21   | 1:A:88:ARG:CZ     | 2.20                     | 0.53              |
| 2:C:293:PHE:HD1   | 2:C:298:PHE:CE1   | 2.27                     | 0.53              |
| 2:C:390:GLN:HG3   | 5:F:323:ASP:OD1   | 2.08                     | 0.53              |
| 2:C:468:ARG:HG3   | 2:C:485:TYR:HB3   | 1.91                     | 0.53              |
| 2:C:916:GLU:O     | 2:C:920:GLN:HG3   | 2.09                     | 0.53              |
| 3:D:170:PRO:CA    | 3:D:392:SER:HB2   | 2.26                     | 0.53              |
| 3:D:970:LYS:O     | 3:D:973:GLN:HB3   | 2.08                     | 0.53              |
| 3:D:1087:ARG:HD3  | 3:D:1234:THR:O    | 2.09                     | 0.53              |
| 5:F:197:SER:HA    | 5:F:200:LYS:HE3   | 1.90                     | 0.53              |
| 1:A:196:THR:CG2   | 2:C:934:PHE:HE1   | 2.21                     | 0.53              |
| 2:C:577:PRO:HB3   | 2:C:993:PHE:CG    | 2.44                     | 0.53              |
| 3:D:74:GLU:CD     | 3:D:74:GLU:H      | 2.17                     | 0.53              |
| 3:D:699:VAL:HG21  | 3:D:715:ALA:HB1   | 1.91                     | 0.53              |
| 3:D:1301:LYS:HG2  | 3:D:1302:GLU:N    | 2.24                     | 0.53              |
| 5:F:369:LEU:HD23  | 5:F:372:ARG:HB2   | 1.90                     | 0.53              |
| 1:A:57:TYR:CE2    | 1:A:59:GLU:HA     | 2.44                     | 0.52              |
| 1:A:67:THR:HG23   | 2:C:609:ASN:HD21  | 1.74                     | 0.52              |
| 1:B:80:LEU:HB3    | 3:D:844:ALA:CB    | 2.39                     | 0.52              |
| 2:C:723:THR:OG1   | 2:C:725:ASP:N     | 2.40                     | 0.52              |
| 3:D:534:ARG:NH2   | 5:F:313:GLU:O     | 2.43                     | 0.52              |
| 3:D:1019:PRO:O    | 3:D:1023:MET:HE2  | 2.09                     | 0.52              |
| 3:D:1111:ASP:CG   | 3:D:1203:LYS:HE2  | 2.34                     | 0.52              |
| 3:D:1130:ARG:HB3  | 3:D:1130:ARG:NH1  | 2.23                     | 0.52              |
| 5:F:132:ARG:O     | 5:F:135:ILE:HG22  | 2.09                     | 0.52              |
| 1:A:138:LEU:HD21  | 1:A:140:MET:HE2   | 1.91                     | 0.52              |
| 2:C:195:LEU:O     | 2:C:199:VAL:HG23  | 2.09                     | 0.52              |
| 2:C:598:GLU:O     | 2:C:651:LYS:HE3   | 2.09                     | 0.52              |
| 3:D:242:LEU:HD21  | 3:D:311:LEU:CD1   | 2.38                     | 0.52              |
| 3:D:400:VAL:HG23  | 3:D:443:VAL:HB    | 1.90                     | 0.52              |
| 5:F:403:LYS:HA    | 5:F:406:ARG:HB2   | 1.91                     | 0.52              |
| 1:B:32:PHE:HA     | 1:B:35:THR:HB     | 1.91                     | 0.52              |
| 1:B:205:VAL:HG22  | 1:B:206:THR:N     | 2.24                     | 0.52              |
| 2:C:361:MET:HG3   | 2:C:361:MET:O     | 2.07                     | 0.52              |
| 2:C:683:ASN:HB3   | 2:C:872:ASN:HD22  | 1.75                     | 0.52              |
| 2:C:1099:VAL:HG22 | 3:D:10:ILE:HG13   | 1.90                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:238:PRO:HB3   | 3:D:315:ARG:HA    | 1.90                     | 0.52              |
| 3:D:280:ALA:HB1   | 3:D:282:TYR:CE2   | 2.44                     | 0.52              |
| 3:D:1078:ARG:HG2  | 3:D:1078:ARG:HH11 | 1.74                     | 0.52              |
| 5:F:369:LEU:HD22  | 5:F:369:LEU:O     | 2.09                     | 0.52              |
| 1:A:79:ILE:HG23   | 1:A:167:VAL:HG22  | 1.91                     | 0.52              |
| 2:C:725:ASP:C     | 2:C:726:ILE:HD12  | 2.35                     | 0.52              |
| 3:D:284:LEU:HG    | 3:D:288:MET:CE    | 2.40                     | 0.52              |
| 3:D:729:HIS:CE1   | 3:D:730:PRO:HD2   | 2.45                     | 0.52              |
| 3:D:984:THR:N     | 3:D:987:GLU:OE2   | 2.26                     | 0.52              |
| 5:F:95:THR:N      | 5:F:98:GLU:HG3    | 2.20                     | 0.52              |
| 1:B:18:ARG:O      | 1:B:207:PRO:HD3   | 2.09                     | 0.52              |
| 1:B:37:GLY:HA2    | 1:B:40:LEU:CG     | 2.40                     | 0.52              |
| 2:C:420:ARG:HG2   | 2:C:420:ARG:HH11  | 1.74                     | 0.52              |
| 2:C:745:ILE:CD1   | 2:C:802:ARG:HA    | 2.39                     | 0.52              |
| 3:D:141:ILE:HD12  | 3:D:145:VAL:C     | 2.35                     | 0.52              |
| 3:D:615:ARG:HD2   | 3:D:1096:ARG:NH2  | 2.24                     | 0.52              |
| 3:D:618:LEU:CD1   | 3:D:1467:ILE:HG23 | 2.39                     | 0.52              |
| 3:D:1045:MET:HE3  | 3:D:1045:MET:CA   | 2.36                     | 0.52              |
| 3:D:1057:VAL:HG23 | 3:D:1069:GLU:OE2  | 2.09                     | 0.52              |
| 1:A:71:VAL:HG12   | 1:A:132:LEU:HG    | 1.90                     | 0.52              |
| 1:A:228:PRO:HB3   | 1:B:13:VAL:CG2    | 2.39                     | 0.52              |
| 1:B:188:GLN:HG2   | 3:D:685:ASP:OD2   | 2.09                     | 0.52              |
| 2:C:230:ARG:N     | 2:C:233:GLU:HG3   | 2.24                     | 0.52              |
| 2:C:334:ARG:HD2   | 2:C:338:GLU:OE2   | 2.10                     | 0.52              |
| 2:C:513:VAL:HG21  | 2:C:529:VAL:CG2   | 2.40                     | 0.52              |
| 2:C:1004:LYS:HD3  | 3:D:744:GLN:NE2   | 2.25                     | 0.52              |
| 3:D:47:GLU:HB3    | 3:D:51:GLY:O      | 2.09                     | 0.52              |
| 4:E:91:ARG:HH11   | 4:E:92:LEU:HG     | 1.73                     | 0.52              |
| 1:A:143:ARG:HG3   | 1:A:143:ARG:HH11  | 1.75                     | 0.52              |
| 1:B:29:GLU:HG3    | 1:B:30:ARG:H      | 1.74                     | 0.52              |
| 1:B:96:THR:HG22   | 1:B:97:VAL:H      | 1.74                     | 0.52              |
| 3:D:1234:THR:HB   | 3:D:1235:GLN:CB   | 2.26                     | 0.52              |
| 5:F:127:ILE:O     | 5:F:131:VAL:HG23  | 2.10                     | 0.52              |
| 5:F:213:ILE:HG22  | 5:F:214:GLN:N     | 2.24                     | 0.52              |
| 2:C:64:LEU:N      | 2:C:103:LYS:HB2   | 2.25                     | 0.52              |
| 2:C:422:ARG:HH22  | 7:H:13:DT:H3'     | 1.73                     | 0.52              |
| 2:C:963:LEU:N     | 2:C:963:LEU:HD23  | 2.24                     | 0.52              |
| 3:D:64:LYS:O      | 3:D:65:ARG:HB2    | 2.08                     | 0.52              |
| 3:D:189:GLN:C     | 3:D:196:VAL:HG13  | 2.35                     | 0.52              |
| 3:D:860:LEU:O     | 3:D:876:SER:HB2   | 2.10                     | 0.52              |
| 5:F:112:ALA:HB2   | 5:F:176:ILE:HG21  | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:40:LEU:CD2    | 1:A:218:LEU:HD12  | 2.40                     | 0.52              |
| 1:B:26:GLU:CB     | 1:B:194:LYS:HG3   | 2.40                     | 0.52              |
| 2:C:322:VAL:HG12  | 2:C:323:ASP:N     | 2.25                     | 0.52              |
| 2:C:432:ARG:O     | 2:C:432:ARG:HG2   | 2.10                     | 0.52              |
| 2:C:724:ARG:O     | 2:C:724:ARG:HG2   | 2.09                     | 0.52              |
| 2:C:825:VAL:CG2   | 2:C:825:VAL:O     | 2.58                     | 0.52              |
| 2:C:928:LYS:O     | 2:C:932:GLU:HG3   | 2.10                     | 0.52              |
| 3:D:124:GLU:OE2   | 3:D:587:ARG:NH1   | 2.43                     | 0.52              |
| 2:C:196:LEU:CD1   | 2:C:200:LEU:HD11  | 2.37                     | 0.52              |
| 2:C:366:SER:O     | 2:C:366:SER:OG    | 2.25                     | 0.52              |
| 2:C:468:ARG:HB2   | 2:C:486:MET:O     | 2.10                     | 0.52              |
| 2:C:838:LYS:HD3   | 2:C:997:LEU:HD12  | 1.92                     | 0.52              |
| 2:C:926:PHE:HE1   | 2:C:929:ARG:HH11  | 1.58                     | 0.52              |
| 3:D:171:LEU:HD11  | 3:D:390:PRO:O     | 2.10                     | 0.52              |
| 3:D:975:GLU:O     | 3:D:975:GLU:HG3   | 2.10                     | 0.52              |
| 5:F:412:GLU:HG2   | 5:F:418:LEU:HD13  | 1.91                     | 0.52              |
| 1:A:218:LEU:O     | 1:A:222:LEU:HD12  | 2.11                     | 0.51              |
| 2:C:29:ALA:O      | 2:C:44:ILE:HB     | 2.11                     | 0.51              |
| 2:C:91:GLN:HA     | 2:C:119:PRO:HA    | 1.91                     | 0.51              |
| 2:C:206:THR:CA    | 2:C:209:ARG:HB3   | 2.38                     | 0.51              |
| 2:C:697:ARG:HG3   | 2:C:699:PHE:CD1   | 2.45                     | 0.51              |
| 3:D:446:VAL:O     | 3:D:446:VAL:HG13  | 2.09                     | 0.51              |
| 3:D:815:ALA:O     | 3:D:818:ARG:HB2   | 2.10                     | 0.51              |
| 3:D:832:ARG:HD3   | 3:D:832:ARG:N     | 2.25                     | 0.51              |
| 1:A:74:ASP:OD1    | 1:A:76:VAL:HB     | 2.11                     | 0.51              |
| 1:A:138:LEU:HD11  | 1:A:140:MET:CE    | 2.39                     | 0.51              |
| 1:A:176:ARG:HG2   | 1:A:177:VAL:N     | 2.25                     | 0.51              |
| 1:A:201:THR:HG22  | 1:A:203:GLY:N     | 2.22                     | 0.51              |
| 2:C:754:ILE:HG12  | 2:C:791:ARG:HD3   | 1.92                     | 0.51              |
| 3:D:584:ASN:H     | 3:D:602:SER:HB3   | 1.76                     | 0.51              |
| 3:D:1235:GLN:O    | 3:D:1236:LEU:HD23 | 2.10                     | 0.51              |
| 5:F:186:HIS:ND1   | 5:F:186:HIS:O     | 2.43                     | 0.51              |
| 5:F:271:LEU:HD12  | 5:F:271:LEU:N     | 2.23                     | 0.51              |
| 1:A:9:PRO:HB2     | 1:A:26:GLU:C      | 2.36                     | 0.51              |
| 1:A:9:PRO:CD      | 1:B:224:TYR:CD2   | 2.93                     | 0.51              |
| 1:B:90:LEU:HD12   | 1:B:119:ASP:C     | 2.35                     | 0.51              |
| 2:C:1092:LEU:HD13 | 2:C:1099:VAL:HG21 | 1.92                     | 0.51              |
| 3:D:398:ALA:HB1   | 3:D:446:VAL:O     | 2.10                     | 0.51              |
| 3:D:477:LEU:O     | 3:D:481:MET:N     | 2.43                     | 0.51              |
| 5:F:240:THR:O     | 5:F:240:THR:HG22  | 2.11                     | 0.51              |
| 1:A:34:VAL:CG2    | 1:B:42:ARG:CZ     | 2.88                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:425:PHE:CE2   | 3:D:1086:LEU:CD1  | 2.89                     | 0.51              |
| 2:C:433:THR:HG22  | 2:C:488:ALA:HB1   | 1.93                     | 0.51              |
| 3:D:479:GLU:OE2   | 3:D:482:LYS:NZ    | 2.38                     | 0.51              |
| 2:C:97:ARG:HG2    | 2:C:112:GLU:HB3   | 1.93                     | 0.51              |
| 2:C:595:LEU:HD23  | 2:C:596:TYR:N     | 2.25                     | 0.51              |
| 3:D:806:PHE:HD2   | 3:D:812:ALA:HA    | 1.75                     | 0.51              |
| 3:D:1413:THR:HG22 | 3:D:1414:PRO:HD2  | 1.93                     | 0.51              |
| 5:F:206:GLY:C     | 5:F:207:LEU:HD23  | 2.34                     | 0.51              |
| 5:F:298:GLY:O     | 5:F:303:ARG:NH1   | 2.43                     | 0.51              |
| 5:F:358:LEU:N     | 5:F:358:LEU:HD23  | 2.24                     | 0.51              |
| 1:A:42:ARG:NH2    | 1:B:34:VAL:HG22   | 2.25                     | 0.51              |
| 1:B:33:GLY:O      | 1:B:181:VAL:HG21  | 2.11                     | 0.51              |
| 1:B:80:LEU:HD22   | 3:D:844:ALA:N     | 2.25                     | 0.51              |
| 1:B:117:VAL:CG1   | 1:B:118:ALA:N     | 2.73                     | 0.51              |
| 3:D:575:GLN:HA    | 3:D:578:VAL:CG1   | 2.41                     | 0.51              |
| 3:D:845:ASN:HB2   | 3:D:846:PRO:HD2   | 1.93                     | 0.51              |
| 3:D:1300:SER:OG   | 3:D:1301:LYS:N    | 2.42                     | 0.51              |
| 1:A:9:PRO:HB2     | 1:A:26:GLU:O      | 2.10                     | 0.51              |
| 1:B:86:VAL:HG13   | 1:B:86:VAL:O      | 2.10                     | 0.51              |
| 3:D:116:LEU:HB2   | 3:D:118:LEU:CD1   | 2.31                     | 0.51              |
| 3:D:1114:THR:CG2  | 3:D:1189:ARG:HH21 | 2.24                     | 0.51              |
| 3:D:1493:LYS:HA   | 3:D:1493:LYS:HE2  | 1.92                     | 0.51              |
| 1:B:49:PRO:CA     | 1:B:148:VAL:HG12  | 2.40                     | 0.51              |
| 5:F:90:GLN:HA     | 5:F:90:GLN:NE2    | 2.26                     | 0.51              |
| 5:F:235:PHE:O     | 5:F:236:SER:C     | 2.54                     | 0.51              |
| 1:B:82:LEU:HD11   | 1:B:140:MET:HE1   | 1.93                     | 0.51              |
| 2:C:627:ARG:HH21  | 2:C:641:PRO:HD3   | 1.76                     | 0.51              |
| 3:D:180:LYS:HG3   | 3:D:181:ASP:N     | 2.24                     | 0.51              |
| 3:D:415:VAL:HG22  | 3:D:419:ASP:OD2   | 2.11                     | 0.51              |
| 3:D:478:LEU:HD12  | 3:D:479:GLU:N     | 2.25                     | 0.51              |
| 3:D:699:VAL:HG11  | 3:D:760:ARG:HG3   | 1.92                     | 0.51              |
| 3:D:955:VAL:O     | 3:D:957:PRO:HD3   | 2.10                     | 0.51              |
| 3:D:1259:VAL:CG2  | 3:D:1355:VAL:HG11 | 2.40                     | 0.51              |
| 5:F:135:ILE:HD11  | 5:F:182:ALA:HB2   | 1.93                     | 0.51              |
| 1:A:47:SER:O      | 1:A:49:PRO:HD3    | 2.11                     | 0.51              |
| 1:A:226:SER:O     | 1:A:228:PRO:HD3   | 2.10                     | 0.51              |
| 2:C:815:LEU:CD1   | 2:C:819:VAL:HG23  | 2.36                     | 0.51              |
| 2:C:952:LEU:HD12  | 2:C:969:GLN:OE1   | 2.11                     | 0.51              |
| 4:E:8:LYS:HE3     | 4:E:8:LYS:O       | 2.10                     | 0.51              |
| 1:B:102:LYS:HG3   | 1:B:139:ASN:HB2   | 1.92                     | 0.50              |
| 2:C:36:PRO:HA     | 2:C:39:ARG:HG3    | 1.92                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:723:THR:O     | 2:C:741:GLY:HA3   | 2.11                     | 0.50              |
| 2:C:766:GLU:CG    | 2:C:767:PRO:HD2   | 2.40                     | 0.50              |
| 3:D:231:VAL:O     | 3:D:236:TYR:OH    | 2.29                     | 0.50              |
| 3:D:748:HIS:O     | 3:D:750:PRO:HD3   | 2.10                     | 0.50              |
| 5:F:358:LEU:HD12  | 5:F:370:LYS:HE3   | 1.92                     | 0.50              |
| 2:C:685:GLU:OE1   | 2:C:685:GLU:HA    | 2.10                     | 0.50              |
| 2:C:879:ARG:HD2   | 2:C:879:ARG:H     | 1.76                     | 0.50              |
| 3:D:973:GLN:HG3   | 3:D:973:GLN:O     | 2.10                     | 0.50              |
| 3:D:1335:LEU:HD12 | 3:D:1335:LEU:O    | 2.11                     | 0.50              |
| 5:F:102:LEU:HD23  | 5:F:183:ALA:CB    | 2.40                     | 0.50              |
| 6:G:7:DT:H2"      | 6:G:8:DC:OP2      | 2.10                     | 0.50              |
| 2:C:881:ASN:O     | 2:C:884:GLN:HG2   | 2.12                     | 0.50              |
| 3:D:411:THR:CG2   | 5:F:178:ARG:HB3   | 2.34                     | 0.50              |
| 3:D:1389:LEU:HD12 | 3:D:1389:LEU:N    | 2.26                     | 0.50              |
| 4:E:13:VAL:HG11   | 4:E:19:LEU:N      | 2.26                     | 0.50              |
| 1:B:41:ARG:HG2    | 1:B:177:VAL:CG1   | 2.41                     | 0.50              |
| 1:B:120:VAL:O     | 1:B:120:VAL:HG12  | 2.10                     | 0.50              |
| 2:C:217:LEU:C     | 2:C:220:GLY:H     | 2.19                     | 0.50              |
| 2:C:366:SER:O     | 2:C:371:LYS:NZ    | 2.42                     | 0.50              |
| 2:C:936:VAL:HG11  | 2:C:959:PRO:HB2   | 1.93                     | 0.50              |
| 3:D:172:PRO:HB2   | 3:D:175:VAL:HG21  | 1.94                     | 0.50              |
| 3:D:767:HIS:CE1   | 4:E:3:GLU:HB2     | 2.45                     | 0.50              |
| 3:D:1208:ASP:O    | 3:D:1209:LEU:C    | 2.55                     | 0.50              |
| 1:B:101:LEU:HD11  | 1:B:109:VAL:CG1   | 2.42                     | 0.50              |
| 1:B:143:ARG:CZ    | 1:B:158:ILE:HD12  | 2.42                     | 0.50              |
| 2:C:793:PRO:HG2   | 2:C:796:GLU:OE1   | 2.12                     | 0.50              |
| 2:C:807:ARG:O     | 2:C:813:VAL:HG21  | 2.12                     | 0.50              |
| 3:D:478:LEU:HA    | 3:D:481:MET:HB2   | 1.92                     | 0.50              |
| 3:D:544:TYR:O     | 3:D:545:ARG:C     | 2.54                     | 0.50              |
| 3:D:1109:GLU:C    | 3:D:1217:ILE:HD11 | 2.36                     | 0.50              |
| 1:A:221:HIS:HA    | 1:A:224:TYR:CE2   | 2.46                     | 0.50              |
| 2:C:54:ILE:HD12   | 2:C:352:ALA:HB1   | 1.93                     | 0.50              |
| 2:C:124:ASP:HA    | 2:C:592:LEU:CD1   | 2.41                     | 0.50              |
| 2:C:263:ASP:O     | 2:C:265:ARG:N     | 2.41                     | 0.50              |
| 2:C:937:ASP:OD1   | 2:C:939:ARG:HG2   | 2.12                     | 0.50              |
| 3:D:691:LEU:O     | 3:D:694:VAL:N     | 2.45                     | 0.50              |
| 3:D:978:TYR:HD1   | 3:D:983:LEU:O     | 1.94                     | 0.50              |
| 3:D:1213:ARG:HG3  | 3:D:1214:PRO:CD   | 2.39                     | 0.50              |
| 3:D:1272:ALA:HA   | 3:D:1326:THR:HG23 | 1.94                     | 0.50              |
| 1:B:101:LEU:CD2   | 1:B:138:LEU:HD23  | 2.42                     | 0.50              |
| 2:C:109:LYS:CG    | 2:C:368:THR:HG22  | 2.33                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:537:LYS:HB3  | 2:C:545:ASN:OD1  | 2.12                     | 0.50              |
| 3:D:218:LYS:O    | 3:D:219:GLU:HG2  | 2.12                     | 0.50              |
| 3:D:529:GLN:HA   | 3:D:534:ARG:O    | 2.12                     | 0.50              |
| 3:D:687:VAL:O    | 3:D:690:ALA:HB3  | 2.12                     | 0.50              |
| 3:D:916:TYR:CZ   | 3:D:920:LEU:HD11 | 2.47                     | 0.50              |
| 3:D:1122:LEU:O   | 3:D:1135:ARG:HG3 | 2.12                     | 0.50              |
| 2:C:30:LEU:O     | 2:C:31:GLN:HB2   | 2.11                     | 0.50              |
| 3:D:85:VAL:C     | 3:D:87:ARG:N     | 2.69                     | 0.50              |
| 3:D:1263:PHE:O   | 3:D:1375:MET:HE2 | 2.11                     | 0.50              |
| 5:F:94:LEU:HD22  | 5:F:98:GLU:HB2   | 1.94                     | 0.50              |
| 1:B:112:ARG:HG3  | 1:B:113:ASP:OD1  | 2.11                     | 0.49              |
| 2:C:717:LEU:HD12 | 2:C:717:LEU:N    | 2.27                     | 0.49              |
| 2:C:721:ARG:HB2  | 2:C:759:THR:OG1  | 2.11                     | 0.49              |
| 2:C:880:MET:HE1  | 3:D:1037:GLN:NE2 | 2.27                     | 0.49              |
| 3:D:691:LEU:O    | 3:D:694:VAL:HB   | 2.11                     | 0.49              |
| 3:D:729:HIS:ND1  | 3:D:730:PRO:CD   | 2.75                     | 0.49              |
| 1:A:153:ALA:O    | 1:A:155:LYS:N    | 2.44                     | 0.49              |
| 2:C:380:ALA:O    | 2:C:384:GLU:HB2  | 2.12                     | 0.49              |
| 3:D:792:ILE:HG13 | 3:D:793:THR:HG23 | 1.93                     | 0.49              |
| 3:D:916:TYR:CZ   | 3:D:920:LEU:HD21 | 2.47                     | 0.49              |
| 1:A:122:ILE:O    | 1:A:122:ILE:HG22 | 2.11                     | 0.49              |
| 1:B:100:LEU:HD23 | 1:B:141:GLU:HG2  | 1.94                     | 0.49              |
| 2:C:283:ILE:HD13 | 2:C:305:PRO:CB   | 2.42                     | 0.49              |
| 2:C:890:LEU:N    | 2:C:914:ILE:HD11 | 2.28                     | 0.49              |
| 2:C:1070:ILE:CG2 | 3:D:655:PRO:HB2  | 2.31                     | 0.49              |
| 3:D:95:LEU:HB2   | 3:D:515:GLU:O    | 2.12                     | 0.49              |
| 3:D:399:ARG:HD2  | 3:D:431:VAL:CG2  | 2.42                     | 0.49              |
| 3:D:1256:LEU:N   | 3:D:1257:PRO:HD2 | 2.28                     | 0.49              |
| 3:D:1479:ASP:HA  | 3:D:1482:ARG:HD3 | 1.93                     | 0.49              |
| 5:F:321:ILE:HG21 | 5:F:332:PHE:CE1  | 2.44                     | 0.49              |
| 1:A:34:VAL:HG21  | 1:B:42:ARG:CZ    | 2.42                     | 0.49              |
| 2:C:422:ARG:CZ   | 7:H:13:DT:H5'    | 2.42                     | 0.49              |
| 2:C:841:ASN:ND2  | 2:C:992:MET:HE2  | 2.27                     | 0.49              |
| 3:D:500:ARG:NH2  | 3:D:1388:ARG:HG3 | 2.27                     | 0.49              |
| 3:D:618:LEU:HD12 | 3:D:1467:ILE:CG2 | 2.41                     | 0.49              |
| 3:D:806:PHE:CD2  | 3:D:812:ALA:HA   | 2.47                     | 0.49              |
| 3:D:1129:THR:C   | 3:D:1131:SER:H   | 2.21                     | 0.49              |
| 1:B:111:ALA:HB3  | 1:B:125:PRO:HA   | 1.95                     | 0.49              |
| 2:C:22:GLN:HG3   | 2:C:407:LYS:HB3  | 1.93                     | 0.49              |
| 2:C:267:TYR:HE1  | 2:C:269:LEU:HD13 | 1.76                     | 0.49              |
| 2:C:278:GLU:HG2  | 2:C:283:ILE:O    | 2.12                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:351:LEU:O    | 2:C:355:VAL:HG13  | 2.13                     | 0.49              |
| 2:C:728:HIS:HE1  | 2:C:775:ARG:NH1   | 2.11                     | 0.49              |
| 2:C:878:SER:HA   | 3:D:1034:GLN:HE22 | 1.77                     | 0.49              |
| 2:C:897:LEU:HD21 | 2:C:921:ALA:CA    | 2.43                     | 0.49              |
| 3:D:346:ARG:HG3  | 3:D:348:GLN:HE21  | 1.77                     | 0.49              |
| 3:D:421:LEU:HD13 | 3:D:428:LYS:CA    | 2.40                     | 0.49              |
| 3:D:814:ALA:O    | 3:D:818:ARG:N     | 2.44                     | 0.49              |
| 3:D:1164:ARG:NH2 | 3:D:1170:ASP:OD1  | 2.45                     | 0.49              |
| 3:D:1213:ARG:CG  | 3:D:1214:PRO:HD2  | 2.40                     | 0.49              |
| 1:B:41:ARG:HG2   | 1:B:177:VAL:HG12  | 1.95                     | 0.49              |
| 1:B:173:PRO:CB   | 1:B:205:VAL:HG12  | 2.43                     | 0.49              |
| 2:C:141:HIS:CE1  | 2:C:334:ARG:HD3   | 2.47                     | 0.49              |
| 2:C:177:GLU:CG   | 2:C:178:PRO:HD2   | 2.37                     | 0.49              |
| 2:C:413:LEU:HD11 | 2:C:448:ASN:OD1   | 2.13                     | 0.49              |
| 2:C:588:VAL:HG11 | 2:C:664:GLY:O     | 2.12                     | 0.49              |
| 2:C:798:GLY:HA3  | 2:C:828:ALA:O     | 2.12                     | 0.49              |
| 2:C:1063:ARG:HG2 | 2:C:1064:ASN:N    | 2.27                     | 0.49              |
| 3:D:483:HIS:ND1  | 3:D:484:PRO:O     | 2.46                     | 0.49              |
| 3:D:845:ASN:C    | 3:D:845:ASN:OD1   | 2.56                     | 0.49              |
| 1:A:103:ALA:HB1  | 1:A:107:LYS:HD2   | 1.93                     | 0.49              |
| 2:C:103:LYS:O    | 2:C:103:LYS:HD3   | 2.12                     | 0.49              |
| 2:C:184:MET:HG2  | 2:C:191:PHE:CE1   | 2.47                     | 0.49              |
| 3:D:44:LEU:HB3   | 3:D:525:ARG:HH21  | 1.77                     | 0.49              |
| 3:D:65:ARG:CD    | 5:F:377:ASP:CA    | 2.90                     | 0.49              |
| 3:D:508:ARG:NE   | 3:D:510:GLU:OE2   | 2.44                     | 0.49              |
| 3:D:586:ARG:HD2  | 3:D:586:ARG:C     | 2.38                     | 0.49              |
| 3:D:835:SER:HB3  | 3:D:838:ARG:NE    | 2.25                     | 0.49              |
| 3:D:1216:SER:HB3 | 4:E:15:SER:HB2    | 1.94                     | 0.49              |
| 4:E:18:ARG:HA    | 4:E:21:VAL:HG12   | 1.95                     | 0.49              |
| 1:A:142:VAL:HG12 | 1:A:143:ARG:N     | 2.28                     | 0.49              |
| 2:C:197:LEU:HB3  | 2:C:202:TYR:CD2   | 2.42                     | 0.49              |
| 2:C:198:ARG:NH1  | 2:C:229:MET:O     | 2.45                     | 0.49              |
| 2:C:234:ALA:HA   | 2:C:237:ARG:CB    | 2.34                     | 0.49              |
| 2:C:409:ARG:HD3  | 2:C:452:ILE:CG2   | 2.42                     | 0.49              |
| 5:F:194:LEU:HD12 | 7:H:6:DT:H5'      | 1.94                     | 0.49              |
| 1:A:57:TYR:CD1   | 1:A:161:ARG:HD2   | 2.47                     | 0.49              |
| 2:C:204:GLN:HB2  | 2:C:227:PHE:CE1   | 2.47                     | 0.49              |
| 2:C:340:MET:SD   | 2:C:340:MET:C     | 2.96                     | 0.49              |
| 2:C:486:MET:HE1  | 2:C:494:TYR:CE2   | 2.47                     | 0.49              |
| 2:C:616:GLU:O    | 2:C:616:GLU:HG2   | 2.12                     | 0.49              |
| 2:C:760:SER:HB2  | 2:C:788:THR:CG2   | 2.37                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:172:PRO:HB2   | 3:D:175:VAL:HG23 | 1.95                     | 0.49              |
| 3:D:372:ASP:HB3   | 3:D:374:GLU:OE1  | 2.13                     | 0.49              |
| 5:F:102:LEU:O     | 5:F:106:VAL:HG23 | 2.13                     | 0.49              |
| 1:B:86:VAL:HG12   | 1:B:124:ASN:CG   | 2.37                     | 0.49              |
| 1:B:107:LYS:HG2   | 1:B:108:GLU:N    | 2.27                     | 0.49              |
| 2:C:144:PRO:CG    | 2:C:165:LEU:HD23 | 2.43                     | 0.49              |
| 2:C:214:TYR:CD2   | 2:C:218:VAL:CG2  | 2.96                     | 0.49              |
| 2:C:486:MET:HE1   | 2:C:494:TYR:CD2  | 2.47                     | 0.49              |
| 2:C:772:ARG:HG2   | 2:C:772:ARG:HH11 | 1.77                     | 0.49              |
| 2:C:878:SER:OG    | 3:D:1029:ARG:HD2 | 2.13                     | 0.49              |
| 2:C:1016:ILE:O    | 3:D:87:ARG:NH2   | 2.46                     | 0.49              |
| 2:C:1070:ILE:CG2  | 3:D:655:PRO:CB   | 2.90                     | 0.49              |
| 3:D:674:ARG:O     | 3:D:678:GLU:HG2  | 2.12                     | 0.49              |
| 3:D:1291:SER:OG   | 3:D:1302:GLU:HG3 | 2.13                     | 0.49              |
| 3:D:1364:HIS:CD2  | 3:D:1366:LYS:HD2 | 2.47                     | 0.49              |
| 4:E:67:GLU:HB3    | 4:E:73:LEU:HD11  | 1.94                     | 0.49              |
| 4:E:75:PHE:H      | 4:E:75:PHE:HD2   | 1.61                     | 0.49              |
| 2:C:572:ILE:HG23  | 2:C:701:THR:O    | 2.13                     | 0.48              |
| 4:E:43:GLU:HG2    | 4:E:44:GLU:N     | 2.28                     | 0.48              |
| 1:B:102:LYS:HA    | 1:B:138:LEU:O    | 2.14                     | 0.48              |
| 2:C:124:ASP:HA    | 2:C:592:LEU:HD13 | 1.94                     | 0.48              |
| 2:C:196:LEU:O     | 2:C:196:LEU:HD22 | 2.13                     | 0.48              |
| 2:C:266:ARG:O     | 2:C:266:ARG:HG3  | 2.13                     | 0.48              |
| 2:C:362:GLY:O     | 2:C:363:SER:HB3  | 2.13                     | 0.48              |
| 2:C:443:THR:OG1   | 2:C:444:PRO:CD   | 2.61                     | 0.48              |
| 2:C:937:ASP:OD2   | 2:C:939:ARG:NH1  | 2.47                     | 0.48              |
| 2:C:1019:GLN:CD   | 3:D:621:LYS:HB3  | 2.38                     | 0.48              |
| 2:C:1067:TYR:O    | 2:C:1067:TYR:CD1 | 2.66                     | 0.48              |
| 3:D:248:PRO:HA    | 3:D:307:ALA:O    | 2.14                     | 0.48              |
| 3:D:371:ILE:HD13  | 5:F:232:ARG:HD3  | 1.95                     | 0.48              |
| 3:D:572:ARG:HH12  | 5:F:83:GLN:HG2   | 1.78                     | 0.48              |
| 3:D:890:VAL:HB    | 3:D:922:LEU:HD13 | 1.95                     | 0.48              |
| 3:D:1495:ILE:HG12 | 4:E:88:GLU:HB3   | 1.95                     | 0.48              |
| 5:F:231:ARG:HB3   | 5:F:233:PHE:CE2  | 2.48                     | 0.48              |
| 5:F:360:LYS:O     | 5:F:361:LEU:HD23 | 2.13                     | 0.48              |
| 1:B:6:LEU:HD13    | 1:B:6:LEU:C      | 2.39                     | 0.48              |
| 2:C:64:LEU:HD23   | 2:C:102:HIS:HA   | 1.95                     | 0.48              |
| 2:C:1019:GLN:HE21 | 3:D:621:LYS:HE3  | 1.76                     | 0.48              |
| 3:D:167:GLU:OE2   | 3:D:198:ARG:HD3  | 2.14                     | 0.48              |
| 3:D:584:ASN:H     | 3:D:602:SER:CB   | 2.26                     | 0.48              |
| 3:D:1054:GLU:O    | 3:D:1056:PRO:HD3 | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1140:ILE:HG22 | 3:D:1144:LEU:HD12 | 1.95                     | 0.48              |
| 5:F:368:VAL:HB    | 5:F:397:ILE:HD11  | 1.94                     | 0.48              |
| 5:F:404:ALA:O     | 5:F:408:LEU:HG    | 2.13                     | 0.48              |
| 2:C:235:LEU:HD21  | 2:C:254:VAL:HG22  | 1.94                     | 0.48              |
| 3:D:7:LYS:HD3     | 3:D:1456:LYS:HZ1  | 1.77                     | 0.48              |
| 3:D:62:LYS:HD2    | 3:D:63:TYR:CZ     | 2.49                     | 0.48              |
| 3:D:569:ASN:ND2   | 5:F:84:TYR:CD2    | 2.81                     | 0.48              |
| 3:D:708:LEU:N     | 3:D:708:LEU:HD23  | 2.27                     | 0.48              |
| 3:D:709:HIS:C     | 3:D:711:LEU:N     | 2.66                     | 0.48              |
| 3:D:832:ARG:HD3   | 3:D:832:ARG:H     | 1.78                     | 0.48              |
| 3:D:1019:PRO:C    | 3:D:1023:MET:HE2  | 2.38                     | 0.48              |
| 3:D:1342:GLU:CD   | 3:D:1342:GLU:H    | 2.21                     | 0.48              |
| 4:E:14:ASP:OD1    | 4:E:18:ARG:NH1    | 2.47                     | 0.48              |
| 1:A:216:GLU:CD    | 1:A:219:ARG:NH2   | 2.72                     | 0.48              |
| 1:B:56:VAL:HG23   | 1:B:142:VAL:HG22  | 1.95                     | 0.48              |
| 2:C:215:GLY:HA2   | 2:C:219:GLN:HG3   | 1.95                     | 0.48              |
| 2:C:615:TYR:HH    | 2:C:623:TYR:HH    | 1.49                     | 0.48              |
| 3:D:284:LEU:HG    | 3:D:288:MET:HE2   | 1.95                     | 0.48              |
| 5:F:172:ARG:HH11  | 5:F:172:ARG:HG3   | 1.78                     | 0.48              |
| 5:F:361:LEU:HD11  | 5:F:411:HIS:CB    | 2.28                     | 0.48              |
| 1:A:137:ARG:HG2   | 1:A:138:LEU:H     | 1.79                     | 0.48              |
| 2:C:516:ARG:HA    | 2:C:520:GLU:O     | 2.14                     | 0.48              |
| 2:C:807:ARG:HB2   | 2:C:807:ARG:HE    | 1.58                     | 0.48              |
| 3:D:63:TYR:CE2    | 3:D:73:CYS:HB2    | 2.48                     | 0.48              |
| 3:D:483:HIS:CD2   | 3:D:484:PRO:HD2   | 2.48                     | 0.48              |
| 3:D:699:VAL:HG13  | 3:D:760:ARG:HG3   | 1.95                     | 0.48              |
| 3:D:864:VAL:CG1   | 3:D:865:THR:H     | 2.26                     | 0.48              |
| 4:E:26:ARG:O      | 4:E:30:LEU:HD12   | 2.14                     | 0.48              |
| 5:F:274:THR:O     | 5:F:277:GLN:HG2   | 2.13                     | 0.48              |
| 7:H:3:DT:H2''     | 7:H:4:DA:H5'      | 1.96                     | 0.48              |
| 1:A:91:ASN:HB2    | 1:A:119:ASP:OD2   | 2.14                     | 0.48              |
| 1:B:205:VAL:CG2   | 1:B:209:GLU:HB3   | 2.44                     | 0.48              |
| 2:C:958:THR:HG23  | 2:C:961:GLU:HG3   | 1.95                     | 0.48              |
| 3:D:42:ASP:N      | 3:D:46:ASP:OD2    | 2.33                     | 0.48              |
| 3:D:134:VAL:HG12  | 3:D:454:ALA:HB2   | 1.95                     | 0.48              |
| 3:D:179:VAL:HG11  | 3:D:191:LEU:HD22  | 1.96                     | 0.48              |
| 3:D:1434:TRP:NE1  | 3:D:1457:ASP:HB2  | 2.29                     | 0.48              |
| 5:F:204:GLY:C     | 5:F:205:ARG:HG2   | 2.38                     | 0.48              |
| 5:F:392:VAL:HG21  | 5:F:396:ARG:CG    | 2.37                     | 0.48              |
| 1:B:87:VAL:CG1    | 1:B:122:ILE:HD13  | 2.43                     | 0.48              |
| 2:C:86:LYS:O      | 2:C:88:LEU:HD23   | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:480:THR:HG22 | 2:C:481:ASP:N    | 2.28                     | 0.48              |
| 3:D:208:PRO:CG   | 3:D:353:VAL:HG11 | 2.43                     | 0.48              |
| 3:D:625:TYR:CD2  | 3:D:751:LEU:HD21 | 2.48                     | 0.48              |
| 1:B:118:ALA:O    | 1:B:119:ASP:HB2  | 2.13                     | 0.48              |
| 3:D:368:VAL:HG23 | 3:D:377:VAL:CG2  | 2.44                     | 0.48              |
| 3:D:408:GLU:OE1  | 3:D:408:GLU:HA   | 2.13                     | 0.48              |
| 3:D:486:ARG:HG3  | 3:D:489:ARG:CZ   | 2.44                     | 0.48              |
| 5:F:368:VAL:CB   | 5:F:397:ILE:HD11 | 2.43                     | 0.48              |
| 2:C:177:GLU:CD   | 2:C:190:LYS:HZ2  | 2.21                     | 0.48              |
| 2:C:554:ASP:HA   | 3:D:1061:PHE:CZ  | 2.49                     | 0.48              |
| 2:C:755:LEU:HD23 | 2:C:825:VAL:HG21 | 1.96                     | 0.48              |
| 3:D:63:TYR:HE2   | 3:D:73:CYS:HB2   | 1.79                     | 0.48              |
| 3:D:82:LYS:O     | 3:D:85:VAL:HG22  | 2.14                     | 0.48              |
| 3:D:1310:ARG:H   | 3:D:1310:ARG:HD2 | 1.79                     | 0.48              |
| 3:D:1495:ILE:CG2 | 4:E:88:GLU:HG3   | 2.44                     | 0.48              |
| 5:F:260:ILE:HG13 | 5:F:265:VAL:HG23 | 1.95                     | 0.48              |
| 1:A:224:TYR:CD1  | 1:B:9:PRO:HG2    | 2.48                     | 0.47              |
| 2:C:403:SER:O    | 2:C:407:LYS:HG3  | 2.13                     | 0.47              |
| 3:D:34:TYR:CZ    | 3:D:35:ARG:HG3   | 2.49                     | 0.47              |
| 3:D:704:ARG:CG   | 3:D:705:ALA:H    | 2.27                     | 0.47              |
| 4:E:57:ASP:O     | 4:E:63:TRP:NE1   | 2.39                     | 0.47              |
| 5:F:372:ARG:HA   | 5:F:372:ARG:NE   | 2.29                     | 0.47              |
| 1:A:42:ARG:NE    | 1:B:35:THR:OG1   | 2.46                     | 0.47              |
| 2:C:230:ARG:H    | 2:C:233:GLU:CG   | 2.26                     | 0.47              |
| 2:C:565:GLN:O    | 2:C:567:GLN:N    | 2.48                     | 0.47              |
| 3:D:169:TYR:O    | 3:D:392:SER:CB   | 2.63                     | 0.47              |
| 3:D:1047:LYS:HG3 | 3:D:1053:PHE:CE2 | 2.49                     | 0.47              |
| 3:D:1271:LYS:HG2 | 3:D:1272:ALA:O   | 2.14                     | 0.47              |
| 5:F:112:ALA:HB2  | 5:F:176:ILE:CG2  | 2.45                     | 0.47              |
| 5:F:161:GLN:C    | 5:F:163:LEU:H    | 2.21                     | 0.47              |
| 5:F:325:LYS:N    | 5:F:325:LYS:HD2  | 2.29                     | 0.47              |
| 1:A:18:ARG:HG3   | 1:A:18:ARG:NH1   | 2.24                     | 0.47              |
| 1:A:64:GLU:O     | 1:A:75:VAL:HB    | 2.13                     | 0.47              |
| 1:B:80:LEU:CB    | 3:D:844:ALA:HB2  | 2.45                     | 0.47              |
| 1:B:97:VAL:HG12  | 1:B:99:LEU:HD12  | 1.94                     | 0.47              |
| 1:B:205:VAL:HG22 | 1:B:206:THR:H    | 1.80                     | 0.47              |
| 2:C:195:LEU:CD1  | 2:C:237:ARG:HB3  | 2.39                     | 0.47              |
| 2:C:524:VAL:HG22 | 2:C:528:GLU:CD   | 2.39                     | 0.47              |
| 2:C:882:LEU:HA   | 2:C:882:LEU:HD23 | 1.62                     | 0.47              |
| 3:D:258:VAL:HA   | 3:D:296:GLU:O    | 2.13                     | 0.47              |
| 3:D:810:GLU:OE2  | 3:D:810:GLU:N    | 2.21                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:868:TYR:CE2   | 3:D:869:MET:HG3  | 2.49                     | 0.47              |
| 3:D:1057:VAL:HG23 | 3:D:1069:GLU:HB3 | 1.97                     | 0.47              |
| 5:F:217:ASN:O     | 5:F:218:GLN:C    | 2.58                     | 0.47              |
| 5:F:229:TYR:CE1   | 5:F:230:LYS:HG3  | 2.48                     | 0.47              |
| 1:A:23:PHE:HE2    | 1:A:208:LEU:HD13 | 1.79                     | 0.47              |
| 1:A:38:ASN:HB3    | 1:A:39:PRO:HD3   | 1.96                     | 0.47              |
| 1:A:121:GLU:CD    | 1:A:123:MET:HE2  | 2.40                     | 0.47              |
| 1:A:138:LEU:HD21  | 1:A:140:MET:CE   | 2.44                     | 0.47              |
| 1:A:222:LEU:CD2   | 1:B:215:VAL:HG13 | 2.33                     | 0.47              |
| 1:B:88:ARG:HB2    | 1:B:88:ARG:HH11  | 1.79                     | 0.47              |
| 3:D:62:LYS:HB3    | 3:D:63:TYR:CD2   | 2.50                     | 0.47              |
| 3:D:970:LYS:CA    | 3:D:973:GLN:HB3  | 2.42                     | 0.47              |
| 5:F:374:GLY:HA3   | 5:F:378:GLY:N    | 2.29                     | 0.47              |
| 1:A:225:PHE:HA    | 1:B:11:PHE:CD2   | 2.50                     | 0.47              |
| 1:B:54:THR:HG21   | 1:B:145:ASP:OD1  | 2.14                     | 0.47              |
| 2:C:144:PRO:HB3   | 2:C:270:GLY:H    | 1.80                     | 0.47              |
| 2:C:271:GLU:OE1   | 2:C:271:GLU:O    | 2.33                     | 0.47              |
| 3:D:659:LYS:O     | 3:D:660:LYS:C    | 2.58                     | 0.47              |
| 3:D:860:LEU:HD23  | 3:D:877:PRO:HB2  | 1.95                     | 0.47              |
| 5:F:184:ARG:O     | 5:F:188:ILE:HG13 | 2.14                     | 0.47              |
| 1:A:201:THR:CG2   | 1:A:203:GLY:H    | 2.23                     | 0.47              |
| 1:B:44:LEU:HD22   | 1:B:199:ILE:HD13 | 1.96                     | 0.47              |
| 3:D:1492:LEU:HD13 | 3:D:1492:LEU:C   | 2.39                     | 0.47              |
| 1:A:70:GLY:H      | 2:C:607:ASP:CG   | 2.20                     | 0.47              |
| 1:A:71:VAL:HG12   | 1:A:132:LEU:CD1  | 2.44                     | 0.47              |
| 1:A:179:PHE:HB3   | 1:A:197:LEU:HD23 | 1.96                     | 0.47              |
| 1:B:30:ARG:HH21   | 2:C:854:PRO:HB3  | 1.78                     | 0.47              |
| 1:B:58:ILE:CB     | 1:B:61:VAL:HG21  | 2.43                     | 0.47              |
| 1:B:162:ILE:O     | 1:B:163:ASN:HB2  | 2.15                     | 0.47              |
| 2:C:425:PHE:HD1   | 3:D:1079:LYS:HE3 | 1.79                     | 0.47              |
| 2:C:615:TYR:OH    | 2:C:623:TYR:OH   | 2.23                     | 0.47              |
| 2:C:893:ALA:O     | 2:C:897:LEU:HG   | 2.14                     | 0.47              |
| 2:C:987:ILE:CG2   | 2:C:988:VAL:N    | 2.78                     | 0.47              |
| 3:D:103:TRP:HE1   | 3:D:604:THR:CG2  | 2.21                     | 0.47              |
| 3:D:137:PRO:HG2   | 3:D:147:VAL:O    | 2.14                     | 0.47              |
| 3:D:284:LEU:HD12  | 3:D:288:MET:HE1  | 1.96                     | 0.47              |
| 3:D:363:ALA:HB2   | 3:D:381:ALA:HA   | 1.95                     | 0.47              |
| 3:D:485:SER:O     | 3:D:487:ALA:N    | 2.48                     | 0.47              |
| 3:D:557:LEU:HD13  | 3:D:566:ILE:HG21 | 1.95                     | 0.47              |
| 3:D:654:LYS:HB3   | 3:D:655:PRO:HD3  | 1.95                     | 0.47              |
| 3:D:885:ILE:CG2   | 3:D:937:TYR:HD1  | 2.27                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:932:ASP:O     | 3:D:935:LYS:HB3   | 2.15                     | 0.47              |
| 3:D:1282:ARG:HD2  | 3:D:1283:ILE:O    | 2.14                     | 0.47              |
| 3:D:1405:GLU:HA   | 3:D:1408:ILE:HG12 | 1.96                     | 0.47              |
| 3:D:1410:GLU:OE1  | 3:D:1412:LYS:HE3  | 2.15                     | 0.47              |
| 5:F:299:TRP:CE3   | 5:F:303:ARG:HG2   | 2.49                     | 0.47              |
| 2:C:21:ILE:HD11   | 2:C:461:VAL:HG11  | 1.96                     | 0.47              |
| 2:C:701:THR:HA    | 2:C:831:ARG:O     | 2.15                     | 0.47              |
| 3:D:689:ASP:HB3   | 4:E:51:LEU:CD1    | 2.42                     | 0.47              |
| 3:D:235:ALA:HB1   | 3:D:319:ALA:O     | 2.15                     | 0.47              |
| 3:D:800:LYS:NZ    | 3:D:819:GLY:O     | 2.48                     | 0.47              |
| 3:D:885:ILE:HG23  | 3:D:937:TYR:HD1   | 1.79                     | 0.47              |
| 5:F:278:LEU:O     | 5:F:282:LEU:HG    | 2.15                     | 0.47              |
| 5:F:315:VAL:HG22  | 5:F:316:SER:N     | 2.30                     | 0.47              |
| 6:G:6:DA:H2'      | 6:G:7:DT:H73      | 1.97                     | 0.47              |
| 1:A:78:ILE:O      | 1:A:82:LEU:HG     | 2.14                     | 0.47              |
| 2:C:502:PRO:O     | 2:C:503:LEU:HD23  | 2.14                     | 0.47              |
| 3:D:15:PRO:O      | 3:D:19:ARG:HG3    | 2.15                     | 0.47              |
| 3:D:217:LYS:CE    | 3:D:341:GLU:HG3   | 2.45                     | 0.47              |
| 3:D:274:ARG:O     | 3:D:275:GLU:O     | 2.32                     | 0.47              |
| 3:D:1110:ALA:N    | 3:D:1217:ILE:HD11 | 2.30                     | 0.47              |
| 3:D:1148:VAL:HG22 | 3:D:1165:TYR:CD1  | 2.50                     | 0.47              |
| 3:D:1347:TYR:CZ   | 3:D:1351:GLU:HG3  | 2.50                     | 0.47              |
| 1:B:44:LEU:HD21   | 1:B:211:LEU:HA    | 1.97                     | 0.46              |
| 2:C:64:LEU:HD23   | 2:C:64:LEU:HA     | 1.72                     | 0.46              |
| 2:C:1005:MET:HE3  | 2:C:1005:MET:HB3  | 1.64                     | 0.46              |
| 2:C:1036:GLU:CD   | 2:C:1036:GLU:H    | 2.23                     | 0.46              |
| 3:D:185:VAL:CG1   | 3:D:186:VAL:H     | 2.27                     | 0.46              |
| 3:D:709:HIS:O     | 3:D:709:HIS:CD2   | 2.68                     | 0.46              |
| 3:D:1057:VAL:HG13 | 3:D:1057:VAL:O    | 2.15                     | 0.46              |
| 3:D:1353:GLN:O    | 3:D:1357:ARG:HG3  | 2.14                     | 0.46              |
| 5:F:260:ILE:CD1   | 5:F:265:VAL:HG22  | 2.45                     | 0.46              |
| 1:A:9:PRO:HD3     | 1:B:224:TYR:CD2   | 2.49                     | 0.46              |
| 2:C:44:ILE:HD12   | 2:C:344:PHE:CE1   | 2.51                     | 0.46              |
| 2:C:167:LYS:CE    | 7:H:12:DC:H5      | 2.28                     | 0.46              |
| 2:C:182:VAL:HG23  | 2:C:193:LEU:HB2   | 1.96                     | 0.46              |
| 2:C:983:ILE:C     | 2:C:985:GLY:N     | 2.73                     | 0.46              |
| 3:D:67:ARG:NH2    | 5:F:377:ASP:OD2   | 2.48                     | 0.46              |
| 3:D:800:LYS:HB3   | 3:D:822:ALA:CB    | 2.46                     | 0.46              |
| 5:F:89:GLY:HA3    | 7:H:7:DG:C6       | 2.50                     | 0.46              |
| 1:A:138:LEU:HD22  | 1:A:140:MET:HG3   | 1.95                     | 0.46              |
| 1:B:96:THR:CG2    | 1:B:97:VAL:N      | 2.79                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:153:ALA:C     | 1:B:155:LYS:H    | 2.23                     | 0.46              |
| 2:C:267:TYR:CE1   | 2:C:269:LEU:HD13 | 2.49                     | 0.46              |
| 2:C:939:ARG:HH11  | 2:C:939:ARG:CG   | 2.28                     | 0.46              |
| 2:C:942:GLU:HG2   | 2:C:945:ARG:HH21 | 1.80                     | 0.46              |
| 2:C:954:THR:HB    | 2:C:957:LYS:HD2  | 1.96                     | 0.46              |
| 3:D:192:ALA:O     | 3:D:193:PRO:C    | 2.58                     | 0.46              |
| 3:D:401:TYR:HE1   | 3:D:446:VAL:CG1  | 2.29                     | 0.46              |
| 3:D:1395:LEU:HD23 | 3:D:1395:LEU:N   | 2.29                     | 0.46              |
| 3:D:1489:GLN:OE1  | 3:D:1493:LYS:HB2 | 2.16                     | 0.46              |
| 3:D:1495:ILE:HG23 | 4:E:88:GLU:HG3   | 1.98                     | 0.46              |
| 4:E:26:ARG:NE     | 4:E:67:GLU:OE1   | 2.47                     | 0.46              |
| 5:F:197:SER:HA    | 5:F:200:LYS:CE   | 2.46                     | 0.46              |
| 5:F:310:ILE:C     | 5:F:312:GLN:H    | 2.24                     | 0.46              |
| 7:H:24:DC:H2"     | 7:H:25:DA:OP2    | 2.14                     | 0.46              |
| 2:C:540:PHE:CD1   | 2:C:544:THR:HG21 | 2.51                     | 0.46              |
| 2:C:577:PRO:HB3   | 2:C:993:PHE:CD1  | 2.51                     | 0.46              |
| 2:C:602:GLU:HG2   | 2:C:603:VAL:N    | 2.28                     | 0.46              |
| 2:C:1019:GLN:NE2  | 3:D:621:LYS:HB3  | 2.30                     | 0.46              |
| 3:D:403:PHE:CZ    | 3:D:442:ASN:HA   | 2.51                     | 0.46              |
| 3:D:930:LEU:O     | 3:D:933:ALA:HB3  | 2.15                     | 0.46              |
| 5:F:354:LEU:HD12  | 5:F:354:LEU:C    | 2.40                     | 0.46              |
| 1:A:86:VAL:HG13   | 1:A:124:ASN:OD1  | 2.16                     | 0.46              |
| 2:C:165:LEU:HD11  | 2:C:270:GLY:HA2  | 1.97                     | 0.46              |
| 2:C:567:GLN:HE22  | 2:C:999:HIS:HE2  | 1.64                     | 0.46              |
| 2:C:1031:ARG:HA   | 3:D:622:ARG:HA   | 1.97                     | 0.46              |
| 3:D:171:LEU:HD21  | 3:D:390:PRO:HG2  | 1.96                     | 0.46              |
| 3:D:207:PHE:CZ    | 5:F:101:GLU:OE2  | 2.68                     | 0.46              |
| 3:D:1267:ARG:NE   | 3:D:1331:ASP:OD2 | 2.49                     | 0.46              |
| 1:B:26:GLU:CD     | 1:B:194:LYS:HG3  | 2.40                     | 0.46              |
| 1:B:123:MET:O     | 1:B:125:PRO:HD3  | 2.16                     | 0.46              |
| 2:C:56:GLU:O      | 2:C:360:LEU:HD21 | 2.14                     | 0.46              |
| 2:C:167:LYS:HE3   | 7:H:12:DC:C5     | 2.51                     | 0.46              |
| 2:C:281:LEU:HD13  | 2:C:305:PRO:HB2  | 1.97                     | 0.46              |
| 2:C:312:ALA:O     | 2:C:317:VAL:HG23 | 2.14                     | 0.46              |
| 2:C:322:VAL:HG12  | 2:C:323:ASP:H    | 1.80                     | 0.46              |
| 2:C:918:LEU:HD23  | 2:C:918:LEU:HA   | 1.44                     | 0.46              |
| 3:D:41:ARG:HA     | 3:D:46:ASP:CG    | 2.41                     | 0.46              |
| 3:D:227:LEU:HD21  | 3:D:326:GLU:HG2  | 1.97                     | 0.46              |
| 3:D:586:ARG:HD2   | 3:D:586:ARG:O    | 2.16                     | 0.46              |
| 3:D:699:VAL:N     | 3:D:756:GLN:OE1  | 2.45                     | 0.46              |
| 5:F:122:LEU:HB2   | 5:F:127:ILE:HD11 | 1.98                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:F:383:LEU:HD12  | 5:F:384:GLU:CG   | 2.39                     | 0.46              |
| 1:A:216:GLU:OE2   | 1:A:219:ARG:NH2  | 2.45                     | 0.46              |
| 1:B:115:LEU:HA    | 1:B:115:LEU:HD22 | 1.57                     | 0.46              |
| 2:C:74:GLY:O      | 2:C:93:PRO:HD2   | 2.16                     | 0.46              |
| 2:C:577:PRO:HG2   | 2:C:580:MET:CG   | 2.45                     | 0.46              |
| 2:C:884:GLN:HB2   | 2:C:992:MET:CE   | 2.46                     | 0.46              |
| 3:D:387:LEU:HD22  | 3:D:387:LEU:N    | 2.31                     | 0.46              |
| 5:F:123:ASP:OD1   | 5:F:125:ASP:N    | 2.49                     | 0.46              |
| 2:C:35:PRO:O      | 2:C:38:LYS:N     | 2.44                     | 0.46              |
| 2:C:396:ASP:CG    | 2:C:402:SER:HB2  | 2.41                     | 0.46              |
| 2:C:750:LYS:C     | 2:C:792:VAL:HG21 | 2.39                     | 0.46              |
| 3:D:12:LEU:HB2    | 3:D:507:ASN:OD1  | 2.16                     | 0.46              |
| 3:D:245:LEU:HD22  | 3:D:249:TYR:HB3  | 1.97                     | 0.46              |
| 3:D:357:GLU:HB2   | 3:D:387:LEU:HD23 | 1.98                     | 0.46              |
| 3:D:838:ARG:HD2   | 3:D:874:GLU:OE1  | 2.16                     | 0.46              |
| 3:D:936:TYR:C     | 3:D:936:TYR:CD2  | 2.94                     | 0.46              |
| 3:D:955:VAL:HG22  | 3:D:1011:PHE:CE1 | 2.50                     | 0.46              |
| 1:A:55:SER:HB2    | 1:A:158:ILE:O    | 2.16                     | 0.46              |
| 2:C:235:LEU:HD12  | 2:C:235:LEU:O    | 2.15                     | 0.46              |
| 2:C:557:ARG:HA    | 2:C:560:MET:HG3  | 1.98                     | 0.46              |
| 3:D:702:LEU:O     | 3:D:713:ILE:HA   | 2.15                     | 0.46              |
| 5:F:375:LEU:HD23  | 5:F:375:LEU:O    | 2.15                     | 0.46              |
| 5:F:395:GLU:HB3   | 5:F:398:ARG:HH12 | 1.80                     | 0.46              |
| 2:C:217:LEU:O     | 2:C:220:GLY:N    | 2.48                     | 0.46              |
| 2:C:409:ARG:HG2   | 2:C:409:ARG:NH2  | 2.30                     | 0.46              |
| 2:C:626:ARG:HD3   | 2:C:629:TYR:CD2  | 2.43                     | 0.46              |
| 2:C:897:LEU:HD21  | 2:C:921:ALA:CB   | 2.46                     | 0.46              |
| 2:C:1097:LEU:HD23 | 2:C:1097:LEU:HA  | 1.54                     | 0.46              |
| 3:D:58:CYS:SG     | 3:D:62:LYS:HB2   | 2.55                     | 0.46              |
| 3:D:832:ARG:H     | 3:D:832:ARG:CD   | 2.29                     | 0.46              |
| 3:D:970:LYS:C     | 3:D:973:GLN:HB3  | 2.41                     | 0.46              |
| 3:D:1305:LEU:HD12 | 3:D:1305:LEU:O   | 2.16                     | 0.46              |
| 5:F:387:GLY:CA    | 5:F:394:ARG:HG2  | 2.46                     | 0.46              |
| 2:C:92:ALA:O      | 2:C:117:HIS:HA   | 2.16                     | 0.45              |
| 2:C:304:LEU:HD12  | 2:C:307:LEU:HD12 | 1.98                     | 0.45              |
| 2:C:693:GLU:HA    | 2:C:696:LYS:HD2  | 1.98                     | 0.45              |
| 2:C:813:VAL:CG2   | 2:C:815:LEU:HD21 | 2.46                     | 0.45              |
| 2:C:853:LEU:CB    | 2:C:858:MET:HE1  | 2.28                     | 0.45              |
| 2:C:1083:GLU:OE1  | 2:C:1086:ARG:HD2 | 2.16                     | 0.45              |
| 3:D:53:ILE:HG12   | 3:D:86:LYS:HD2   | 1.97                     | 0.45              |
| 3:D:62:LYS:HD2    | 3:D:63:TYR:CE2   | 2.50                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:632:VAL:O    | 3:D:727:GLN:HA   | 2.15                     | 0.45              |
| 3:D:767:HIS:HE1  | 4:E:6:ILE:HD13   | 1.81                     | 0.45              |
| 3:D:838:ARG:CD   | 3:D:874:GLU:OE1  | 2.64                     | 0.45              |
| 1:A:154:GLU:H    | 1:A:154:GLU:CD   | 2.23                     | 0.45              |
| 2:C:11:GLU:CD    | 2:C:537:LYS:HE2  | 2.41                     | 0.45              |
| 2:C:23:VAL:HG23  | 2:C:24:GLU:N     | 2.31                     | 0.45              |
| 2:C:297:GLU:HG3  | 2:C:299:LYS:HZ2  | 1.80                     | 0.45              |
| 2:C:752:GLY:HA3  | 3:D:679:ARG:HA   | 1.99                     | 0.45              |
| 2:C:834:GLN:NE2  | 3:D:724:GLN:HG2  | 2.31                     | 0.45              |
| 2:C:984:GLU:HB2  | 3:D:944:THR:O    | 2.16                     | 0.45              |
| 2:C:1065:ALA:CB  | 2:C:1077:PRO:HG3 | 2.46                     | 0.45              |
| 3:D:186:VAL:HA   | 3:D:200:ASP:HA   | 1.97                     | 0.45              |
| 3:D:236:TYR:CE1  | 3:D:242:LEU:CB   | 3.00                     | 0.45              |
| 3:D:704:ARG:O    | 3:D:705:ALA:C    | 2.58                     | 0.45              |
| 3:D:886:VAL:HG12 | 3:D:896:ALA:HB1  | 1.98                     | 0.45              |
| 5:F:317:LEU:HD23 | 5:F:317:LEU:HA   | 1.56                     | 0.45              |
| 5:F:353:GLU:HA   | 5:F:356:LYS:HB3  | 1.97                     | 0.45              |
| 5:F:392:VAL:HG22 | 5:F:393:THR:H    | 1.80                     | 0.45              |
| 1:A:65:PHE:HE2   | 2:C:703:ILE:HG23 | 1.82                     | 0.45              |
| 2:C:65:VAL:O     | 2:C:65:VAL:CG2   | 2.65                     | 0.45              |
| 2:C:214:TYR:O    | 2:C:218:VAL:HB   | 2.17                     | 0.45              |
| 2:C:443:THR:HG21 | 3:D:1078:ARG:HE  | 1.81                     | 0.45              |
| 2:C:495:THR:HG23 | 2:C:517:ARG:HG3  | 1.97                     | 0.45              |
| 2:C:633:GLN:OE1  | 2:C:633:GLN:N    | 2.48                     | 0.45              |
| 2:C:902:ILE:O    | 2:C:902:ILE:HG22 | 2.15                     | 0.45              |
| 3:D:437:VAL:O    | 3:D:437:VAL:HG12 | 2.15                     | 0.45              |
| 3:D:616:GLN:HG3  | 3:D:616:GLN:O    | 2.16                     | 0.45              |
| 3:D:796:ARG:NH1  | 3:D:862:ASP:OD1  | 2.49                     | 0.45              |
| 5:F:79:ASP:C     | 5:F:79:ASP:OD1   | 2.59                     | 0.45              |
| 5:F:135:ILE:HG23 | 5:F:136:LEU:N    | 2.32                     | 0.45              |
| 5:F:210:LEU:O    | 5:F:211:ASP:C    | 2.59                     | 0.45              |
| 1:B:101:LEU:HD11 | 1:B:109:VAL:HG11 | 1.98                     | 0.45              |
| 2:C:831:ARG:NE   | 2:C:1002:GLU:OE1 | 2.49                     | 0.45              |
| 2:C:1078:GLU:HG3 | 2:C:1079:PRO:HD2 | 1.98                     | 0.45              |
| 3:D:70:GLY:N     | 3:D:80:VAL:HG23  | 2.30                     | 0.45              |
| 3:D:314:PRO:HD2  | 3:D:317:VAL:HG11 | 1.97                     | 0.45              |
| 3:D:324:ALA:HB1  | 3:D:331:VAL:CG2  | 2.46                     | 0.45              |
| 3:D:377:VAL:HG23 | 3:D:377:VAL:O    | 2.17                     | 0.45              |
| 3:D:563:PRO:HB3  | 5:F:189:GLU:CG   | 2.46                     | 0.45              |
| 3:D:640:HIS:CD2  | 3:D:641:GLN:HG3  | 2.51                     | 0.45              |
| 3:D:775:GLY:CA   | 3:D:1209:LEU:HB3 | 2.46                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:786:ILE:HD11  | 3:D:1027:GLY:C    | 2.41                     | 0.45              |
| 1:A:107:LYS:CE    | 1:A:113:ASP:OD2   | 2.65                     | 0.45              |
| 1:A:132:LEU:HD21  | 1:A:138:LEU:HB2   | 1.98                     | 0.45              |
| 1:B:26:GLU:CD     | 1:B:194:LYS:HE3   | 2.41                     | 0.45              |
| 2:C:182:VAL:HG22  | 2:C:221:LEU:HD23  | 1.98                     | 0.45              |
| 2:C:268:ASP:OD1   | 2:C:269:LEU:O     | 2.34                     | 0.45              |
| 2:C:281:LEU:CD2   | 2:C:308:ARG:HH22  | 2.27                     | 0.45              |
| 2:C:700:TYR:HB3   | 2:C:833:LEU:HD22  | 1.99                     | 0.45              |
| 2:C:1001:VAL:HB   | 3:D:724:GLN:CB    | 2.46                     | 0.45              |
| 3:D:371:ILE:CD1   | 5:F:232:ARG:NH1   | 2.79                     | 0.45              |
| 3:D:1136:LYS:O    | 3:D:1140:ILE:HG13 | 2.17                     | 0.45              |
| 3:D:1464:GLU:H    | 3:D:1464:GLU:HG3  | 1.60                     | 0.45              |
| 5:F:156:VAL:O     | 5:F:160:ASP:HB2   | 2.16                     | 0.45              |
| 5:F:395:GLU:HB3   | 5:F:398:ARG:NH1   | 2.31                     | 0.45              |
| 5:F:414:ARG:HA    | 5:F:414:ARG:HH11  | 1.81                     | 0.45              |
| 1:A:19:GLU:O      | 1:A:207:PRO:HG3   | 2.17                     | 0.45              |
| 3:D:93:ILE:CD1    | 3:D:548:ILE:CG1   | 2.94                     | 0.45              |
| 3:D:286:VAL:CG2   | 3:D:314:PRO:HG3   | 2.46                     | 0.45              |
| 3:D:397:LYS:HD2   | 3:D:397:LYS:HA    | 1.81                     | 0.45              |
| 3:D:474:GLU:O     | 3:D:478:LEU:HG    | 2.16                     | 0.45              |
| 3:D:653:PHE:O     | 3:D:656:PHE:N     | 2.49                     | 0.45              |
| 3:D:1434:TRP:CD1  | 3:D:1457:ASP:HB2  | 2.51                     | 0.45              |
| 5:F:215:GLU:O     | 5:F:218:GLN:HB3   | 2.17                     | 0.45              |
| 5:F:412:GLU:OE1   | 5:F:416:ARG:HA    | 2.17                     | 0.45              |
| 1:B:127:LEU:C     | 1:B:127:LEU:CD2   | 2.90                     | 0.45              |
| 2:C:834:GLN:HE22  | 3:D:724:GLN:HG2   | 1.82                     | 0.45              |
| 3:D:8:VAL:HG12    | 3:D:1434:TRP:HZ2  | 1.81                     | 0.45              |
| 3:D:225:LEU:HD21  | 3:D:311:LEU:HD21  | 1.97                     | 0.45              |
| 3:D:242:LEU:CD2   | 3:D:311:LEU:CD1   | 2.95                     | 0.45              |
| 3:D:327:GLU:O     | 3:D:327:GLU:HG3   | 2.17                     | 0.45              |
| 3:D:407:VAL:HA    | 3:D:422:ALA:CB    | 2.47                     | 0.45              |
| 3:D:422:ALA:O     | 3:D:427:VAL:HG12  | 2.15                     | 0.45              |
| 3:D:1305:LEU:HD12 | 3:D:1305:LEU:C    | 2.42                     | 0.45              |
| 3:D:1403:LEU:HD12 | 3:D:1403:LEU:C    | 2.41                     | 0.45              |
| 3:D:1422:MET:HE3  | 3:D:1426:LYS:CD   | 2.46                     | 0.45              |
| 4:E:19:LEU:HD12   | 4:E:23:VAL:HG23   | 1.98                     | 0.45              |
| 6:G:17:DC:H2'     | 6:G:18:DA:C8      | 2.51                     | 0.45              |
| 1:A:118:ALA:O     | 1:A:119:ASP:HB2   | 2.17                     | 0.45              |
| 2:C:16:PRO:O      | 2:C:18:LEU:HD23   | 2.16                     | 0.45              |
| 2:C:607:ASP:OD1   | 2:C:608:GLY:N     | 2.49                     | 0.45              |
| 3:D:131:LYS:N     | 3:D:456:MET:HE2   | 2.30                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:709:HIS:O     | 3:D:709:HIS:CG   | 2.69                     | 0.45              |
| 3:D:1057:VAL:HG23 | 3:D:1069:GLU:CG  | 2.47                     | 0.45              |
| 3:D:1087:ARG:O    | 3:D:1088:THR:C   | 2.60                     | 0.45              |
| 3:D:1205:TYR:CE2  | 3:D:1366:LYS:HE2 | 2.50                     | 0.45              |
| 3:D:1208:ASP:C    | 3:D:1208:ASP:OD1 | 2.59                     | 0.45              |
| 3:D:1263:PHE:HD2  | 3:D:1375:MET:HE3 | 1.81                     | 0.45              |
| 3:D:1402:ALA:O    | 3:D:1405:GLU:HB3 | 2.17                     | 0.45              |
| 5:F:324:GLU:OE2   | 6:G:19:DG:N2     | 2.50                     | 0.45              |
| 1:A:34:VAL:O      | 1:A:35:THR:C     | 2.59                     | 0.45              |
| 1:A:89:PHE:CZ     | 1:A:97:VAL:HG23  | 2.52                     | 0.45              |
| 1:B:110:LYS:C     | 1:B:129:ILE:HD13 | 2.42                     | 0.45              |
| 2:C:9:ILE:HD11    | 2:C:500:ASN:HB3  | 1.99                     | 0.45              |
| 2:C:137:VAL:HG21  | 2:C:393:GLN:NE2  | 2.32                     | 0.45              |
| 2:C:172:ILE:HG12  | 2:C:186:VAL:HG22 | 1.98                     | 0.45              |
| 2:C:214:TYR:HD2   | 2:C:218:VAL:CG2  | 2.30                     | 0.45              |
| 2:C:539:VAL:O     | 2:C:539:VAL:CG1  | 2.65                     | 0.45              |
| 2:C:720:GLU:HG2   | 2:C:760:SER:OG   | 2.17                     | 0.45              |
| 2:C:742:VAL:CG1   | 2:C:803:THR:HG21 | 2.47                     | 0.45              |
| 2:C:775:ARG:HB3   | 2:C:780:GLU:O    | 2.17                     | 0.45              |
| 2:C:1036:GLU:CD   | 2:C:1036:GLU:N   | 2.75                     | 0.45              |
| 3:D:126:VAL:O     | 3:D:457:GLY:N    | 2.42                     | 0.45              |
| 3:D:218:LYS:HB3   | 3:D:338:GLU:HG2  | 1.99                     | 0.45              |
| 3:D:394:LEU:HD21  | 3:D:396:VAL:CG2  | 2.47                     | 0.45              |
| 3:D:553:ARG:NH2   | 5:F:211:ASP:HA   | 2.31                     | 0.45              |
| 3:D:650:LEU:CD1   | 3:D:657:LEU:CD2  | 2.91                     | 0.45              |
| 3:D:658:LEU:HA    | 3:D:661:MET:CE   | 2.38                     | 0.45              |
| 3:D:876:SER:OG    | 3:D:879:ARG:HG3  | 2.17                     | 0.45              |
| 3:D:1264:GLU:OE1  | 3:D:1264:GLU:HA  | 2.17                     | 0.45              |
| 3:D:1405:GLU:HA   | 3:D:1408:ILE:CG1 | 2.47                     | 0.45              |
| 4:E:37:ASN:OD1    | 4:E:37:ASN:N     | 2.38                     | 0.45              |
| 4:E:79:LEU:C      | 4:E:80:VAL:HG23  | 2.42                     | 0.45              |
| 5:F:88:ILE:HG13   | 5:F:192:LEU:HB2  | 1.98                     | 0.45              |
| 1:B:68:ILE:HG21   | 1:B:71:VAL:HG21  | 1.98                     | 0.45              |
| 2:C:21:ILE:HD12   | 2:C:455:LEU:HD22 | 1.99                     | 0.45              |
| 2:C:239:PHE:CD1   | 2:C:253:ALA:HA   | 2.52                     | 0.45              |
| 2:C:480:THR:HG22  | 2:C:481:ASP:H    | 1.82                     | 0.45              |
| 2:C:718:GLY:HA3   | 2:C:761:PHE:CE1  | 2.51                     | 0.45              |
| 3:D:127:LEU:HD23  | 3:D:127:LEU:HA   | 1.74                     | 0.45              |
| 3:D:131:LYS:H     | 3:D:456:MET:HE2  | 1.82                     | 0.45              |
| 3:D:446:VAL:O     | 3:D:446:VAL:CG1  | 2.65                     | 0.45              |
| 3:D:528:VAL:O     | 3:D:535:PHE:HA   | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:749:VAL:HG12  | 3:D:750:PRO:O     | 2.17                     | 0.45              |
| 3:D:960:LYS:NZ    | 3:D:1063:GLU:OE2  | 2.47                     | 0.45              |
| 3:D:972:LEU:C     | 3:D:972:LEU:HD12  | 2.42                     | 0.45              |
| 2:C:99:GLN:O      | 2:C:99:GLN:HG2    | 2.17                     | 0.44              |
| 2:C:213:ALA:HB3   | 2:C:214:TYR:CE1   | 2.51                     | 0.44              |
| 2:C:490:GLU:O     | 2:C:493:ARG:HB2   | 2.17                     | 0.44              |
| 2:C:936:VAL:HG11  | 2:C:959:PRO:CB    | 2.47                     | 0.44              |
| 3:D:26:VAL:HG12   | 3:D:548:ILE:CD1   | 2.44                     | 0.44              |
| 3:D:180:LYS:HA    | 3:D:205:TYR:OH    | 2.17                     | 0.44              |
| 3:D:230:TRP:HA    | 3:D:243:ALA:HB2   | 1.98                     | 0.44              |
| 3:D:368:VAL:HB    | 3:D:377:VAL:HG22  | 1.98                     | 0.44              |
| 3:D:625:TYR:CD2   | 3:D:751:LEU:HD11  | 2.51                     | 0.44              |
| 3:D:924:MET:HB2   | 3:D:924:MET:HE2   | 1.66                     | 0.44              |
| 3:D:1012:GLU:HB2  | 3:D:1021:TYR:OH   | 2.17                     | 0.44              |
| 3:D:1487:VAL:O    | 4:E:74:VAL:HG23   | 2.15                     | 0.44              |
| 5:F:114:LYS:HA    | 5:F:117:SER:HB3   | 1.99                     | 0.44              |
| 5:F:161:GLN:C     | 5:F:163:LEU:N     | 2.75                     | 0.44              |
| 5:F:360:LYS:HB3   | 5:F:411:HIS:CD2   | 2.52                     | 0.44              |
| 1:A:49:PRO:O      | 1:A:173:PRO:HG3   | 2.17                     | 0.44              |
| 2:C:565:GLN:C     | 2:C:567:GLN:N     | 2.75                     | 0.44              |
| 2:C:598:GLU:N     | 2:C:615:TYR:OH    | 2.46                     | 0.44              |
| 3:D:645:PRO:HG3   | 3:D:724:GLN:O     | 2.17                     | 0.44              |
| 3:D:851:LEU:HD11  | 3:D:855:HIS:HE1   | 1.82                     | 0.44              |
| 3:D:885:ILE:CG2   | 3:D:937:TYR:CD1   | 2.99                     | 0.44              |
| 3:D:1045:MET:O    | 3:D:1052:THR:HG23 | 2.17                     | 0.44              |
| 3:D:1108:ARG:NH2  | 3:D:1198:TYR:HB3  | 2.32                     | 0.44              |
| 4:E:84:ARG:HD3    | 4:E:84:ARG:HA     | 1.41                     | 0.44              |
| 5:F:287:THR:HG23  | 5:F:290:GLU:OE2   | 2.16                     | 0.44              |
| 1:A:201:THR:CG2   | 1:A:205:VAL:O     | 2.64                     | 0.44              |
| 2:C:224:GLU:C     | 2:C:226:VAL:N     | 2.74                     | 0.44              |
| 2:C:586:ARG:O     | 2:C:589:ARG:HB2   | 2.17                     | 0.44              |
| 2:C:769:PRO:HD2   | 3:D:65:ARG:NH2    | 2.33                     | 0.44              |
| 2:C:880:MET:CE    | 3:D:1037:GLN:CB   | 2.93                     | 0.44              |
| 2:C:983:ILE:HG22  | 2:C:985:GLY:H     | 1.83                     | 0.44              |
| 2:C:1008:ARG:CD   | 2:C:1028:GLY:O    | 2.65                     | 0.44              |
| 2:C:1060:ILE:HD11 | 2:C:1083:GLU:HB2  | 2.00                     | 0.44              |
| 3:D:25:GLU:HG3    | 3:D:92:HIS:NE2    | 2.32                     | 0.44              |
| 3:D:181:ASP:OD1   | 3:D:205:TYR:HB2   | 2.18                     | 0.44              |
| 3:D:1189:ARG:HH11 | 3:D:1203:LYS:HD2  | 1.83                     | 0.44              |
| 1:B:36:LEU:HB3    | 1:B:37:GLY:H      | 1.57                     | 0.44              |
| 1:B:100:LEU:HD23  | 1:B:141:GLU:CG    | 2.47                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:495:THR:OG1  | 2:C:517:ARG:NE    | 2.50                     | 0.44              |
| 2:C:507:ARG:HB2  | 2:C:507:ARG:HH11  | 1.82                     | 0.44              |
| 2:C:565:GLN:C    | 2:C:567:GLN:H     | 2.25                     | 0.44              |
| 2:C:613:VAL:O    | 2:C:613:VAL:HG23  | 2.16                     | 0.44              |
| 2:C:950:LEU:HB2  | 2:C:952:LEU:HD22  | 1.99                     | 0.44              |
| 2:C:1008:ARG:NE  | 3:D:624:ASP:OD1   | 2.50                     | 0.44              |
| 3:D:808:THR:HB   | 3:D:810:GLU:OE2   | 2.17                     | 0.44              |
| 5:F:148:LYS:HD3  | 5:F:148:LYS:HA    | 1.48                     | 0.44              |
| 1:A:117:VAL:HB   | 1:A:120:VAL:CG2   | 2.47                     | 0.44              |
| 1:A:201:THR:CG2  | 1:A:202:ASP:N     | 2.81                     | 0.44              |
| 1:B:108:GLU:HB2  | 1:B:110:LYS:NZ    | 2.33                     | 0.44              |
| 1:B:208:LEU:HD12 | 1:B:208:LEU:C     | 2.42                     | 0.44              |
| 2:C:17:PRO:O     | 2:C:20:GLU:HG2    | 2.17                     | 0.44              |
| 2:C:388:ARG:HG3  | 2:C:388:ARG:HH11  | 1.81                     | 0.44              |
| 2:C:617:ASP:HB2  | 2:C:619:ARG:HH22  | 1.83                     | 0.44              |
| 2:C:987:ILE:HG22 | 2:C:988:VAL:N     | 2.32                     | 0.44              |
| 2:C:1012:PRO:C   | 2:C:1021:LEU:CD1  | 2.91                     | 0.44              |
| 2:C:1067:TYR:O   | 2:C:1071:ILE:HD13 | 2.17                     | 0.44              |
| 4:E:14:ASP:OD2   | 4:E:14:ASP:N      | 2.50                     | 0.44              |
| 5:F:362:SER:O    | 5:F:366:ALA:CB    | 2.66                     | 0.44              |
| 1:B:94:LEU:HD23  | 1:B:95:GLN:H      | 1.80                     | 0.44              |
| 2:C:193:LEU:HG   | 2:C:197:LEU:CD1   | 2.42                     | 0.44              |
| 2:C:358:ARG:HE   | 2:C:358:ARG:HB2   | 1.51                     | 0.44              |
| 2:C:578:VAL:HG13 | 2:C:671:ASN:OD1   | 2.17                     | 0.44              |
| 3:D:1374:GLN:OE1 | 3:D:1374:GLN:HA   | 2.16                     | 0.44              |
| 8:I:2:C:H2'      | 8:I:3:A:C8        | 2.53                     | 0.44              |
| 1:A:48:ILE:O     | 1:A:173:PRO:HD3   | 2.17                     | 0.44              |
| 1:B:208:LEU:HD12 | 1:B:212:ASN:OD1   | 2.18                     | 0.44              |
| 2:C:182:VAL:HG11 | 2:C:311:PHE:CZ    | 2.53                     | 0.44              |
| 2:C:382:ILE:O    | 2:C:383:ARG:C     | 2.61                     | 0.44              |
| 2:C:717:LEU:N    | 2:C:717:LEU:CD1   | 2.81                     | 0.44              |
| 2:C:751:PRO:CA   | 2:C:792:VAL:CG2   | 2.92                     | 0.44              |
| 3:D:132:TYR:HE2  | 3:D:155:ASP:OD2   | 2.01                     | 0.44              |
| 3:D:275:GLU:C    | 3:D:277:GLU:H     | 2.24                     | 0.44              |
| 3:D:1097:LYS:HD3 | 3:D:1425:THR:OG1  | 2.18                     | 0.44              |
| 3:D:1294:VAL:O   | 3:D:1294:VAL:HG22 | 2.18                     | 0.44              |
| 5:F:317:LEU:HD22 | 5:F:330:GLY:HA2   | 1.99                     | 0.44              |
| 1:B:84:GLU:OE2   | 3:D:867:ARG:NH1   | 2.50                     | 0.44              |
| 2:C:44:ILE:HD13  | 2:C:44:ILE:HA     | 1.58                     | 0.44              |
| 2:C:701:THR:HG23 | 2:C:831:ARG:O     | 2.18                     | 0.44              |
| 2:C:905:ILE:O    | 2:C:907:ASP:N     | 2.51                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:236:TYR:HB2  | 3:D:319:ALA:CB   | 2.47                     | 0.44              |
| 3:D:396:VAL:HG12 | 3:D:397:LYS:N    | 2.31                     | 0.44              |
| 3:D:422:ALA:H    | 3:D:427:VAL:HG13 | 1.83                     | 0.44              |
| 3:D:699:VAL:CG1  | 3:D:760:ARG:CG   | 2.96                     | 0.44              |
| 3:D:919:PHE:CE2  | 3:D:924:MET:HG2  | 2.53                     | 0.44              |
| 3:D:1379:VAL:CG1 | 3:D:1397:LYS:HB2 | 2.47                     | 0.44              |
| 3:D:1485:GLN:O   | 4:E:75:PHE:HA    | 2.18                     | 0.44              |
| 7:H:2:DA:H2'     | 7:H:2:DA:O5'     | 2.18                     | 0.44              |
| 1:A:180:GLN:HG3  | 2:C:934:PHE:HD1  | 1.78                     | 0.44              |
| 1:B:216:GLU:CD   | 1:B:219:ARG:HH21 | 2.26                     | 0.44              |
| 2:C:97:ARG:HG3   | 2:C:112:GLU:HB2  | 1.98                     | 0.44              |
| 2:C:102:HIS:CB   | 2:C:107:LEU:HB3  | 2.37                     | 0.44              |
| 2:C:619:ARG:HB2  | 2:C:619:ARG:NH2  | 2.30                     | 0.44              |
| 3:D:236:TYR:CZ   | 3:D:242:LEU:HB2  | 2.53                     | 0.44              |
| 3:D:237:LYS:HB3  | 3:D:237:LYS:HE2  | 1.82                     | 0.44              |
| 3:D:644:LEU:HD12 | 3:D:645:PRO:HD2  | 2.00                     | 0.44              |
| 4:E:8:LYS:HA     | 4:E:8:LYS:HD2    | 1.69                     | 0.44              |
| 5:F:231:ARG:C    | 5:F:232:ARG:HG2  | 2.42                     | 0.44              |
| 6:G:6:DA:H2'     | 6:G:7:DT:H72     | 1.99                     | 0.44              |
| 1:A:206:THR:O    | 1:A:207:PRO:C    | 2.61                     | 0.43              |
| 2:C:140:ILE:HG22 | 2:C:412:ALA:HA   | 1.99                     | 0.43              |
| 2:C:182:VAL:HG23 | 2:C:193:LEU:CB   | 2.48                     | 0.43              |
| 2:C:841:ASN:OD1  | 2:C:841:ASN:C    | 2.60                     | 0.43              |
| 3:D:566:ILE:HG22 | 3:D:567:ILE:N    | 2.33                     | 0.43              |
| 3:D:686:GLU:H    | 3:D:686:GLU:CD   | 2.26                     | 0.43              |
| 4:E:30:LEU:HD23  | 4:E:35:PHE:HD1   | 1.83                     | 0.43              |
| 1:A:121:GLU:HB3  | 1:A:123:MET:CE   | 2.47                     | 0.43              |
| 2:C:211:LEU:HB3  | 2:C:218:VAL:HG21 | 1.99                     | 0.43              |
| 2:C:277:ALA:HA   | 2:C:280:LYS:HB3  | 1.99                     | 0.43              |
| 2:C:503:LEU:HD22 | 2:C:508:ILE:HA   | 1.99                     | 0.43              |
| 2:C:679:PHE:CE1  | 2:C:853:LEU:HD11 | 2.53                     | 0.43              |
| 2:C:841:ASN:HD22 | 2:C:992:MET:CE   | 2.29                     | 0.43              |
| 2:C:874:LEU:HD23 | 3:D:1023:MET:SD  | 2.58                     | 0.43              |
| 3:D:373:PRO:O    | 3:D:376:GLU:HG3  | 2.17                     | 0.43              |
| 3:D:982:PHE:O    | 3:D:983:LEU:CG   | 2.64                     | 0.43              |
| 3:D:1275:SER:O   | 3:D:1322:GLY:N   | 2.48                     | 0.43              |
| 5:F:201:LYS:HB2  | 5:F:201:LYS:HE3  | 1.80                     | 0.43              |
| 2:C:69:LEU:HB2   | 2:C:97:ARG:O     | 2.18                     | 0.43              |
| 3:D:298:VAL:HA   | 3:D:302:GLN:OE1  | 2.18                     | 0.43              |
| 3:D:396:VAL:CG1  | 3:D:397:LYS:N    | 2.82                     | 0.43              |
| 3:D:701:LEU:HB2  | 3:D:748:HIS:HB2  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:126:LEU:HD12  | 5:F:126:LEU:C     | 2.42                     | 0.43              |
| 5:F:129:GLU:O     | 5:F:132:ARG:HB3   | 2.18                     | 0.43              |
| 1:A:54:THR:HG22   | 1:A:158:ILE:HB    | 2.00                     | 0.43              |
| 1:B:133:GLU:O     | 1:B:136:GLY:N     | 2.52                     | 0.43              |
| 2:C:585:GLU:HG3   | 2:C:665:PHE:CD2   | 2.53                     | 0.43              |
| 2:C:590:ASP:C     | 2:C:592:LEU:N     | 2.77                     | 0.43              |
| 3:D:485:SER:C     | 3:D:487:ALA:H     | 2.25                     | 0.43              |
| 3:D:639:LEU:HA    | 3:D:639:LEU:HD12  | 1.74                     | 0.43              |
| 3:D:646:LYS:HB3   | 3:D:646:LYS:HE2   | 1.80                     | 0.43              |
| 3:D:652:LEU:HB3   | 3:D:749:VAL:HG21  | 1.99                     | 0.43              |
| 3:D:1029:ARG:O    | 3:D:1030:GLY:O    | 2.36                     | 0.43              |
| 3:D:1057:VAL:CG2  | 3:D:1069:GLU:HB3  | 2.48                     | 0.43              |
| 5:F:161:GLN:OE1   | 5:F:164:LYS:NZ    | 2.49                     | 0.43              |
| 5:F:166:LEU:HD13  | 5:F:170:HIS:HB3   | 2.00                     | 0.43              |
| 5:F:236:SER:OG    | 7:H:5:DA:OP2      | 2.35                     | 0.43              |
| 5:F:367:MET:HE3   | 5:F:368:VAL:CG1   | 2.26                     | 0.43              |
| 5:F:374:GLY:N     | 5:F:378:GLY:HA2   | 2.34                     | 0.43              |
| 1:A:65:PHE:CE2    | 2:C:703:ILE:HG23  | 2.53                     | 0.43              |
| 1:A:115:LEU:HD21  | 1:A:117:VAL:HG23  | 2.00                     | 0.43              |
| 1:A:176:ARG:CG    | 1:A:177:VAL:N     | 2.82                     | 0.43              |
| 2:C:91:GLN:HB2    | 2:C:117:HIS:HB3   | 2.01                     | 0.43              |
| 2:C:109:LYS:HG3   | 2:C:369:PRO:HD2   | 2.00                     | 0.43              |
| 3:D:508:ARG:HD2   | 3:D:508:ARG:HA    | 1.84                     | 0.43              |
| 3:D:677:LEU:H     | 3:D:677:LEU:HG    | 1.65                     | 0.43              |
| 3:D:1273:VAL:N    | 3:D:1326:THR:CG2  | 2.80                     | 0.43              |
| 5:F:383:LEU:HG    | 5:F:384:GLU:OE2   | 2.19                     | 0.43              |
| 1:A:23:PHE:CD2    | 1:A:211:LEU:CD2   | 3.02                     | 0.43              |
| 1:B:106:PRO:HB3   | 1:B:134:GLU:CG    | 2.49                     | 0.43              |
| 1:B:124:ASN:ND2   | 1:B:127:LEU:CD1   | 2.74                     | 0.43              |
| 2:C:149:THR:HA    | 2:C:322:VAL:CG1   | 2.47                     | 0.43              |
| 3:D:659:LYS:O     | 3:D:662:GLU:N     | 2.45                     | 0.43              |
| 3:D:828:LYS:HB2   | 3:D:833:GLU:OE2   | 2.18                     | 0.43              |
| 3:D:1099:VAL:HG13 | 3:D:1223:ILE:HD13 | 2.00                     | 0.43              |
| 1:B:28:LEU:HD23   | 1:B:32:PHE:HB3    | 2.01                     | 0.43              |
| 1:B:222:LEU:HA    | 1:B:222:LEU:HD23  | 1.80                     | 0.43              |
| 2:C:292:ARG:HD3   | 2:C:299:LYS:HB2   | 2.00                     | 0.43              |
| 2:C:502:PRO:C     | 2:C:503:LEU:HD23  | 2.44                     | 0.43              |
| 2:C:858:MET:HG2   | 2:C:867:VAL:O     | 2.19                     | 0.43              |
| 2:C:983:ILE:C     | 2:C:985:GLY:H     | 2.25                     | 0.43              |
| 2:C:1085:PHE:CE1  | 3:D:1468:LEU:CD2  | 3.00                     | 0.43              |
| 3:D:374:GLU:C     | 3:D:376:GLU:H     | 2.26                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:828:LYS:HE2  | 3:D:831:GLY:N    | 2.27                     | 0.43              |
| 3:D:870:GLY:O    | 3:D:871:LYS:C    | 2.62                     | 0.43              |
| 5:F:228:GLU:OE2  | 5:F:231:ARG:NE   | 2.37                     | 0.43              |
| 1:B:7:LYS:NZ     | 1:B:186:LEU:HD13 | 2.34                     | 0.43              |
| 1:B:29:GLU:HG3   | 1:B:30:ARG:N     | 2.33                     | 0.43              |
| 1:B:115:LEU:C    | 1:B:115:LEU:HD13 | 2.43                     | 0.43              |
| 2:C:31:GLN:C     | 2:C:33:ASP:H     | 2.26                     | 0.43              |
| 2:C:309:TYR:CE2  | 2:C:320:HIS:HA   | 2.53                     | 0.43              |
| 2:C:580:MET:HE2  | 2:C:580:MET:HB2  | 1.83                     | 0.43              |
| 2:C:715:THR:CG2  | 2:C:717:LEU:HD13 | 2.49                     | 0.43              |
| 2:C:743:VAL:HG13 | 2:C:755:LEU:HA   | 2.00                     | 0.43              |
| 2:C:1045:ALA:HB1 | 3:D:758:GLU:OE2  | 2.19                     | 0.43              |
| 3:D:133:ILE:O    | 3:D:133:ILE:CG2  | 2.67                     | 0.43              |
| 3:D:401:TYR:HE1  | 3:D:446:VAL:HG12 | 1.82                     | 0.43              |
| 3:D:564:GLU:O    | 3:D:565:ILE:C    | 2.62                     | 0.43              |
| 3:D:958:GLU:C    | 3:D:960:LYS:H    | 2.27                     | 0.43              |
| 3:D:1268:PRO:HG3 | 3:D:1329:ALA:HB3 | 2.00                     | 0.43              |
| 5:F:239:ALA:C    | 5:F:241:TRP:H    | 2.27                     | 0.43              |
| 1:A:82:LEU:HD23  | 1:A:129:ILE:HD12 | 1.99                     | 0.43              |
| 2:C:422:ARG:HH22 | 7:H:13:DT:C3'    | 2.31                     | 0.43              |
| 2:C:438:ILE:HD11 | 2:C:467:ILE:CD1  | 2.49                     | 0.43              |
| 2:C:723:THR:CG2  | 2:C:759:THR:HG23 | 2.49                     | 0.43              |
| 3:D:343:LYS:HG2  | 3:D:345:TYR:HE2  | 1.84                     | 0.43              |
| 3:D:357:GLU:OE2  | 3:D:387:LEU:HD23 | 2.18                     | 0.43              |
| 3:D:658:LEU:HD21 | 3:D:674:ARG:HA   | 2.01                     | 0.43              |
| 3:D:659:LYS:NZ   | 3:D:663:GLU:HB2  | 2.34                     | 0.43              |
| 3:D:767:HIS:HE1  | 4:E:3:GLU:HB2    | 1.84                     | 0.43              |
| 3:D:935:LYS:HB3  | 3:D:935:LYS:HE3  | 1.59                     | 0.43              |
| 8:I:2:C:H2'      | 8:I:3:A:H8       | 1.83                     | 0.43              |
| 1:A:131:THR:C    | 1:A:132:LEU:HD12 | 2.43                     | 0.43              |
| 2:C:343:GLN:HG3  | 2:C:385:PHE:CB   | 2.31                     | 0.43              |
| 2:C:632:ASN:HB2  | 2:C:633:GLN:OE1  | 2.19                     | 0.43              |
| 2:C:755:LEU:N    | 2:C:755:LEU:HD12 | 2.34                     | 0.43              |
| 2:C:1072:LYS:O   | 2:C:1072:LYS:HD3 | 2.19                     | 0.43              |
| 3:D:211:VAL:HG23 | 3:D:347:VAL:CG2  | 2.49                     | 0.43              |
| 3:D:694:VAL:HG12 | 3:D:695:ILE:N    | 2.33                     | 0.43              |
| 3:D:921:ARG:O    | 3:D:921:ARG:HG2  | 2.19                     | 0.43              |
| 5:F:363:GLU:HG3  | 5:F:363:GLU:O    | 2.19                     | 0.43              |
| 1:B:80:LEU:HD22  | 3:D:844:ALA:CA   | 2.49                     | 0.42              |
| 1:B:108:GLU:HA   | 1:B:131:THR:HA   | 2.00                     | 0.42              |
| 2:C:65:VAL:CG2   | 2:C:101:ILE:HG23 | 2.41                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:767:PRO:HB2   | 2:C:772:ARG:HG2  | 2.00                     | 0.42              |
| 2:C:769:PRO:HD2   | 3:D:65:ARG:CZ    | 2.49                     | 0.42              |
| 2:C:906:PHE:CE2   | 3:D:1067:VAL:CA  | 3.01                     | 0.42              |
| 2:C:997:LEU:N     | 2:C:997:LEU:HD23 | 2.33                     | 0.42              |
| 2:C:1031:ARG:HH21 | 2:C:1031:ARG:HG3 | 1.84                     | 0.42              |
| 2:C:1102:LEU:HD23 | 2:C:1108:PRO:HA  | 2.01                     | 0.42              |
| 5:F:159:ILE:HD13  | 5:F:159:ILE:HA   | 1.82                     | 0.42              |
| 2:C:1067:TYR:O    | 2:C:1067:TYR:CG  | 2.71                     | 0.42              |
| 2:C:1109:VAL:HG11 | 3:D:5:VAL:CG2    | 2.49                     | 0.42              |
| 3:D:597:ASP:O     | 3:D:599:PRO:HD3  | 2.19                     | 0.42              |
| 5:F:177:ALA:O     | 5:F:180:GLY:N    | 2.52                     | 0.42              |
| 5:F:366:ALA:O     | 5:F:370:LYS:HB2  | 2.18                     | 0.42              |
| 2:C:722:ILE:HD13  | 2:C:722:ILE:HA   | 1.85                     | 0.42              |
| 2:C:940:GLU:OE1   | 2:C:963:LEU:HD11 | 2.20                     | 0.42              |
| 2:C:1090:LYS:HE2  | 2:C:1112:PHE:CE2 | 2.54                     | 0.42              |
| 3:D:413:ASP:N     | 3:D:435:VAL:CG1  | 2.82                     | 0.42              |
| 3:D:417:PRO:HG3   | 3:D:430:ASP:O    | 2.19                     | 0.42              |
| 3:D:775:GLY:HA2   | 3:D:1209:LEU:HB3 | 2.00                     | 0.42              |
| 4:E:3:GLU:OE2     | 4:E:4:PRO:HD2    | 2.19                     | 0.42              |
| 5:F:194:LEU:HA    | 7:H:6:DT:O4'     | 2.19                     | 0.42              |
| 5:F:390:PHE:HB3   | 5:F:397:ILE:HD13 | 2.00                     | 0.42              |
| 1:B:94:LEU:O      | 1:B:95:GLN:HG3   | 2.18                     | 0.42              |
| 2:C:9:ILE:HG13    | 2:C:907:ASP:CG   | 2.43                     | 0.42              |
| 2:C:683:ASN:CG    | 2:C:872:ASN:HB2  | 2.44                     | 0.42              |
| 2:C:876:VAL:O     | 2:C:877:PRO:C    | 2.62                     | 0.42              |
| 3:D:57:GLU:HG3    | 3:D:64:LYS:HG2   | 2.01                     | 0.42              |
| 3:D:984:THR:HG23  | 3:D:987:GLU:OE2  | 2.20                     | 0.42              |
| 3:D:1264:GLU:O    | 3:D:1265:ALA:HB3 | 2.20                     | 0.42              |
| 5:F:170:HIS:C     | 5:F:172:ARG:H    | 2.27                     | 0.42              |
| 5:F:260:ILE:HG13  | 5:F:260:ILE:O    | 2.20                     | 0.42              |
| 1:B:109:VAL:O     | 1:B:110:LYS:HD2  | 2.19                     | 0.42              |
| 1:B:206:THR:OG1   | 1:B:209:GLU:HB2  | 2.19                     | 0.42              |
| 2:C:461:VAL:O     | 2:C:461:VAL:HG23 | 2.18                     | 0.42              |
| 2:C:724:ARG:HD2   | 2:C:738:ASP:O    | 2.19                     | 0.42              |
| 2:C:889:HIS:HE1   | 2:C:988:VAL:HG13 | 1.84                     | 0.42              |
| 2:C:1055:LEU:HD21 | 2:C:1079:PRO:HB3 | 2.00                     | 0.42              |
| 2:C:1058:ASP:OD2  | 2:C:1084:SER:HB2 | 2.20                     | 0.42              |
| 3:D:237:LYS:O     | 3:D:240:GLU:HB2  | 2.20                     | 0.42              |
| 6:G:4:DG:H2''     | 6:G:5:DC:O5'     | 2.20                     | 0.42              |
| 2:C:97:ARG:HA     | 2:C:112:GLU:HA   | 2.02                     | 0.42              |
| 2:C:205:GLU:O     | 2:C:209:ARG:HB3  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:206:THR:HA   | 2:C:209:ARG:CB   | 2.41                     | 0.42              |
| 2:C:480:THR:HG22 | 2:C:482:GLU:H    | 1.85                     | 0.42              |
| 2:C:946:ARG:HH21 | 2:C:946:ARG:CG   | 2.29                     | 0.42              |
| 2:C:988:VAL:HG23 | 3:D:948:THR:HG23 | 1.98                     | 0.42              |
| 3:D:111:LYS:HD2  | 3:D:1452:ILE:CD1 | 2.50                     | 0.42              |
| 3:D:144:GLY:O    | 3:D:145:VAL:CG2  | 2.67                     | 0.42              |
| 3:D:417:PRO:CB   | 3:D:430:ASP:O    | 2.67                     | 0.42              |
| 3:D:465:LEU:HD23 | 3:D:510:GLU:HA   | 2.00                     | 0.42              |
| 3:D:1041:LEU:H   | 3:D:1041:LEU:CD2 | 2.32                     | 0.42              |
| 3:D:1045:MET:HG3 | 3:D:1073:SER:HA  | 2.01                     | 0.42              |
| 3:D:1281:VAL:CG2 | 3:D:1316:GLY:H   | 2.33                     | 0.42              |
| 4:E:30:LEU:CD2   | 4:E:35:PHE:HD1   | 2.31                     | 0.42              |
| 5:F:208:SER:O    | 5:F:209:PHE:C    | 2.62                     | 0.42              |
| 1:A:104:GLU:HG3  | 1:A:137:ARG:HA   | 2.02                     | 0.42              |
| 2:C:6:PHE:CE1    | 2:C:909:ALA:HB2  | 2.54                     | 0.42              |
| 2:C:168:ARG:HE   | 2:C:345:ARG:NH1  | 2.18                     | 0.42              |
| 2:C:310:LEU:HD12 | 2:C:310:LEU:O    | 2.19                     | 0.42              |
| 2:C:336:VAL:HG13 | 2:C:337:GLY:N    | 2.34                     | 0.42              |
| 2:C:744:ARG:NH1  | 2:C:746:GLY:O    | 2.53                     | 0.42              |
| 2:C:890:LEU:HD12 | 2:C:890:LEU:O    | 2.19                     | 0.42              |
| 2:C:940:GLU:O    | 2:C:944:LEU:HD12 | 2.19                     | 0.42              |
| 2:C:1009:SER:HA  | 3:D:625:TYR:HD1  | 1.84                     | 0.42              |
| 3:D:368:VAL:HG23 | 3:D:377:VAL:HG21 | 2.02                     | 0.42              |
| 1:A:222:LEU:HD23 | 1:B:215:VAL:CG1  | 2.34                     | 0.42              |
| 1:B:74:ASP:OD2   | 3:D:872:ARG:NH1  | 2.52                     | 0.42              |
| 2:C:348:LEU:CD1  | 2:C:378:LEU:HD22 | 2.50                     | 0.42              |
| 2:C:552:HIS:CD2  | 2:C:886:LEU:HD22 | 2.55                     | 0.42              |
| 2:C:569:VAL:HG21 | 2:C:1000:MET:HE2 | 1.99                     | 0.42              |
| 3:D:26:VAL:CG1   | 3:D:548:ILE:HD13 | 2.43                     | 0.42              |
| 3:D:477:LEU:HD22 | 3:D:492:ALA:HA   | 2.01                     | 0.42              |
| 3:D:524:LEU:HD23 | 3:D:524:LEU:N    | 2.33                     | 0.42              |
| 3:D:545:ARG:NH1  | 5:F:254:GLN:O    | 2.52                     | 0.42              |
| 3:D:704:ARG:HG2  | 3:D:705:ALA:N    | 2.35                     | 0.42              |
| 3:D:757:ALA:O    | 3:D:761:ILE:HG13 | 2.19                     | 0.42              |
| 3:D:1129:THR:C   | 3:D:1131:SER:N   | 2.77                     | 0.42              |
| 3:D:1365:ASP:O   | 3:D:1366:LYS:C   | 2.61                     | 0.42              |
| 5:F:94:LEU:HD13  | 5:F:99:GLU:HA    | 2.02                     | 0.42              |
| 5:F:161:GLN:CD   | 5:F:164:LYS:HZ3  | 2.28                     | 0.42              |
| 5:F:234:LYS:HD3  | 7:H:5:DA:P       | 2.59                     | 0.42              |
| 5:F:336:GLU:H    | 5:F:336:GLU:HG2  | 1.49                     | 0.42              |
| 2:C:728:HIS:O    | 2:C:729:LEU:HD12 | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:808:ARG:CG    | 2:C:814:GLU:HA    | 2.46                     | 0.42              |
| 2:C:897:LEU:N     | 2:C:897:LEU:HD23  | 2.34                     | 0.42              |
| 2:C:946:ARG:HG3   | 2:C:946:ARG:NH2   | 2.27                     | 0.42              |
| 3:D:147:VAL:HG12  | 3:D:151:GLN:HE22  | 1.85                     | 0.42              |
| 3:D:180:LYS:HB2   | 3:D:205:TYR:OH    | 2.19                     | 0.42              |
| 3:D:325:GLU:O     | 3:D:325:GLU:CG    | 2.68                     | 0.42              |
| 3:D:394:LEU:CG    | 3:D:396:VAL:HG23  | 2.49                     | 0.42              |
| 3:D:416:ALA:HB2   | 3:D:432:TYR:CE1   | 2.55                     | 0.42              |
| 3:D:598:ARG:O     | 3:D:599:PRO:C     | 2.63                     | 0.42              |
| 3:D:618:LEU:CB    | 3:D:1467:ILE:HG23 | 2.50                     | 0.42              |
| 3:D:803:GLY:HA2   | 3:D:826:PRO:O     | 2.19                     | 0.42              |
| 3:D:1194:CYS:SG   | 3:D:1200:VAL:HA   | 2.60                     | 0.42              |
| 5:F:88:ILE:CG2    | 5:F:193:ARG:HG2   | 2.49                     | 0.42              |
| 5:F:170:HIS:C     | 5:F:172:ARG:N     | 2.77                     | 0.42              |
| 2:C:99:GLN:O      | 2:C:99:GLN:CG     | 2.68                     | 0.42              |
| 2:C:378:LEU:HD12  | 2:C:378:LEU:O     | 2.20                     | 0.42              |
| 2:C:590:ASP:C     | 2:C:592:LEU:H     | 2.25                     | 0.42              |
| 2:C:929:ARG:C     | 2:C:931:GLY:H     | 2.28                     | 0.42              |
| 3:D:247:GLU:HB2   | 3:D:248:PRO:CD    | 2.50                     | 0.42              |
| 3:D:704:ARG:HB2   | 3:D:745:MET:CE    | 2.18                     | 0.42              |
| 3:D:1234:THR:H    | 3:D:1235:GLN:HB3  | 1.80                     | 0.42              |
| 5:F:421:PHE:N     | 5:F:421:PHE:CD1   | 2.88                     | 0.42              |
| 1:A:12:THR:HG22   | 1:A:13:VAL:H      | 1.85                     | 0.41              |
| 1:A:129:ILE:HD13  | 1:A:129:ILE:HA    | 1.87                     | 0.41              |
| 1:A:173:PRO:HD2   | 1:A:174:VAL:HG23  | 2.01                     | 0.41              |
| 1:B:127:LEU:HD23  | 1:B:128:HIS:O     | 2.20                     | 0.41              |
| 2:C:194:VAL:HG13  | 2:C:221:LEU:HD21  | 2.02                     | 0.41              |
| 2:C:263:ASP:C     | 2:C:265:ARG:N     | 2.78                     | 0.41              |
| 2:C:742:VAL:HG12  | 2:C:743:VAL:O     | 2.20                     | 0.41              |
| 3:D:65:ARG:CG     | 5:F:377:ASP:HA    | 2.48                     | 0.41              |
| 3:D:206:ARG:CG    | 3:D:392:SER:O     | 2.68                     | 0.41              |
| 3:D:676:MET:O     | 3:D:682:ASP:HB2   | 2.20                     | 0.41              |
| 3:D:1171:VAL:HG12 | 3:D:1175:ILE:HD11 | 2.02                     | 0.41              |
| 4:E:30:LEU:HD23   | 4:E:35:PHE:CD1    | 2.54                     | 0.41              |
| 5:F:321:ILE:HB    | 5:F:327:SER:OG    | 2.20                     | 0.41              |
| 5:F:372:ARG:HE    | 5:F:372:ARG:CA    | 2.31                     | 0.41              |
| 1:A:45:LEU:HD23   | 1:A:45:LEU:HA     | 1.82                     | 0.41              |
| 1:A:54:THR:O      | 1:A:156:HIS:HE1   | 2.02                     | 0.41              |
| 1:A:55:SER:C      | 1:A:56:VAL:HG23   | 2.45                     | 0.41              |
| 1:A:108:GLU:O     | 1:A:109:VAL:C     | 2.63                     | 0.41              |
| 1:B:161:ARG:O     | 1:B:162:ILE:C     | 2.63                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:185:ARG:NH2  | 3:D:689:ASP:OD1   | 2.45                     | 0.41              |
| 1:B:211:LEU:O    | 1:B:214:ALA:HB3   | 2.19                     | 0.41              |
| 2:C:1006:HIS:CB  | 2:C:1024:LYS:HG3  | 2.48                     | 0.41              |
| 2:C:1065:ALA:HB1 | 2:C:1077:PRO:HG3  | 2.03                     | 0.41              |
| 3:D:1130:ARG:HB3 | 3:D:1130:ARG:HH11 | 1.85                     | 0.41              |
| 3:D:1341:PRO:O   | 3:D:1345:GLU:HG3  | 2.20                     | 0.41              |
| 5:F:271:LEU:H    | 5:F:271:LEU:CD1   | 2.29                     | 0.41              |
| 1:A:143:ARG:NH1  | 1:A:143:ARG:HG3   | 2.35                     | 0.41              |
| 1:B:58:ILE:CG2   | 1:B:61:VAL:HG21   | 2.50                     | 0.41              |
| 2:C:111:ASP:OD1  | 2:C:112:GLU:N     | 2.52                     | 0.41              |
| 2:C:644:VAL:CG2  | 2:C:645:VAL:N     | 2.83                     | 0.41              |
| 2:C:806:LEU:HD23 | 2:C:806:LEU:N     | 2.34                     | 0.41              |
| 2:C:1047:HIS:CE1 | 3:D:1471:LEU:HD11 | 2.55                     | 0.41              |
| 2:C:1068:GLU:HA  | 2:C:1071:ILE:HD11 | 2.02                     | 0.41              |
| 3:D:407:VAL:HA   | 3:D:422:ALA:HB1   | 2.03                     | 0.41              |
| 3:D:450:TYR:CD2  | 3:D:450:TYR:N     | 2.88                     | 0.41              |
| 3:D:484:PRO:C    | 3:D:486:ARG:H     | 2.28                     | 0.41              |
| 3:D:840:LYS:HE3  | 3:D:841:TYR:CZ    | 2.55                     | 0.41              |
| 3:D:976:GLN:HA   | 3:D:979:GLU:HB3   | 2.02                     | 0.41              |
| 5:F:167:PRO:HD2  | 5:F:170:HIS:HB2   | 2.01                     | 0.41              |
| 5:F:239:ALA:C    | 5:F:241:TRP:N     | 2.78                     | 0.41              |
| 1:B:96:THR:CG2   | 1:B:97:VAL:H      | 2.33                     | 0.41              |
| 2:C:115:LEU:HD23 | 2:C:115:LEU:HA    | 1.83                     | 0.41              |
| 2:C:546:LEU:HA   | 2:C:546:LEU:HD23  | 1.78                     | 0.41              |
| 2:C:675:ALA:O    | 2:C:870:ILE:HA    | 2.20                     | 0.41              |
| 2:C:987:ILE:HD13 | 2:C:987:ILE:HA    | 1.86                     | 0.41              |
| 2:C:1030:GLN:HB2 | 3:D:626:SER:OG    | 2.20                     | 0.41              |
| 3:D:101:HIS:HB3  | 3:D:104:PHE:HD2   | 1.83                     | 0.41              |
| 3:D:132:TYR:HD1  | 3:D:454:ALA:O     | 2.03                     | 0.41              |
| 3:D:162:ARG:O    | 3:D:414:ARG:NH2   | 2.44                     | 0.41              |
| 3:D:254:GLU:C    | 3:D:255:GLU:HG2   | 2.41                     | 0.41              |
| 3:D:511:TRP:C    | 3:D:513:ILE:H     | 2.29                     | 0.41              |
| 3:D:1071:PHE:O   | 3:D:1072:ILE:C    | 2.63                     | 0.41              |
| 3:D:1197:ARG:O   | 3:D:1198:TYR:HB2  | 2.20                     | 0.41              |
| 3:D:1293:PHE:CZ  | 3:D:1302:GLU:HB2  | 2.54                     | 0.41              |
| 5:F:171:LYS:CD   | 5:F:175:HIS:HE1   | 2.24                     | 0.41              |
| 6:G:18:DA:H2'    | 6:G:19:DG:O5'     | 2.20                     | 0.41              |
| 1:A:9:PRO:HD2    | 1:B:224:TYR:CD2   | 2.56                     | 0.41              |
| 1:B:86:VAL:CG1   | 1:B:86:VAL:O      | 2.68                     | 0.41              |
| 1:B:112:ARG:NH2  | 1:B:112:ARG:HB3   | 2.36                     | 0.41              |
| 1:B:115:LEU:HD13 | 1:B:116:PRO:N     | 2.35                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:118:ILE:HD13  | 2:C:340:MET:CE    | 2.50                     | 0.41              |
| 2:C:144:PRO:HD2   | 2:C:332:ARG:HD3   | 2.01                     | 0.41              |
| 2:C:438:ILE:CD1   | 2:C:467:ILE:HD12  | 2.49                     | 0.41              |
| 2:C:1009:SER:HA   | 3:D:625:TYR:CD1   | 2.56                     | 0.41              |
| 3:D:18:ILE:HD13   | 3:D:516:ALA:O     | 2.20                     | 0.41              |
| 3:D:64:LYS:O      | 3:D:65:ARG:CB     | 2.68                     | 0.41              |
| 3:D:206:ARG:HD2   | 3:D:206:ARG:HA    | 1.80                     | 0.41              |
| 3:D:767:HIS:CE1   | 4:E:6:ILE:HD13    | 2.54                     | 0.41              |
| 3:D:767:HIS:CE1   | 4:E:6:ILE:HG12    | 2.55                     | 0.41              |
| 3:D:794:GLN:OE1   | 3:D:794:GLN:HA    | 2.21                     | 0.41              |
| 5:F:157:GLU:OE1   | 5:F:157:GLU:HA    | 2.20                     | 0.41              |
| 1:B:101:LEU:HD21  | 1:B:109:VAL:HG11  | 2.01                     | 0.41              |
| 2:C:360:LEU:N     | 2:C:360:LEU:HD22  | 2.36                     | 0.41              |
| 2:C:492:ASP:HB3   | 2:C:518:LYS:HG3   | 2.02                     | 0.41              |
| 2:C:743:VAL:CG2   | 2:C:800:VAL:HG11  | 2.49                     | 0.41              |
| 2:C:890:LEU:HD11  | 2:C:901:TYR:CD2   | 2.55                     | 0.41              |
| 2:C:961:GLU:O     | 2:C:964:LYS:HB3   | 2.20                     | 0.41              |
| 3:D:12:LEU:HD21   | 3:D:104:PHE:CZ    | 2.55                     | 0.41              |
| 3:D:111:LYS:HE2   | 3:D:1449:GLU:HG2  | 2.03                     | 0.41              |
| 3:D:125:GLN:HA    | 3:D:130:SER:HB3   | 2.02                     | 0.41              |
| 3:D:637:LEU:HD13  | 3:D:642:CYS:HA    | 2.03                     | 0.41              |
| 3:D:1262:LEU:HD11 | 3:D:1351:GLU:HB3  | 2.02                     | 0.41              |
| 3:D:1280:VAL:HG12 | 3:D:1318:TYR:HA   | 2.01                     | 0.41              |
| 3:D:1482:ARG:NH1  | 3:D:1483:PHE:CZ   | 2.89                     | 0.41              |
| 4:E:9:LEU:HD23    | 4:E:9:LEU:HA      | 1.81                     | 0.41              |
| 6:G:6:DA:C2       | 6:G:7:DT:C2       | 3.08                     | 0.41              |
| 1:B:64:GLU:HG3    | 1:B:79:ILE:HD12   | 2.02                     | 0.41              |
| 2:C:185:LYS:O     | 2:C:186:VAL:HG23  | 2.19                     | 0.41              |
| 2:C:304:LEU:HB3   | 2:C:305:PRO:HD3   | 2.03                     | 0.41              |
| 2:C:882:LEU:HD11  | 3:D:1038:LEU:HD22 | 2.03                     | 0.41              |
| 2:C:939:ARG:HG2   | 2:C:939:ARG:H     | 1.53                     | 0.41              |
| 3:D:44:LEU:HB3    | 3:D:525:ARG:NH2   | 2.35                     | 0.41              |
| 3:D:135:LEU:O     | 3:D:149:LYS:HE3   | 2.20                     | 0.41              |
| 3:D:464:LEU:HA    | 3:D:464:LEU:HD12  | 1.81                     | 0.41              |
| 3:D:492:ALA:O     | 3:D:496:LEU:HB2   | 2.20                     | 0.41              |
| 3:D:800:LYS:HB3   | 3:D:822:ALA:HB2   | 2.03                     | 0.41              |
| 3:D:1031:ASN:ND2  | 3:D:1034:GLN:OE1  | 2.54                     | 0.41              |
| 3:D:1376:MET:HB2  | 3:D:1376:MET:HE3  | 1.85                     | 0.41              |
| 1:B:57:TYR:O      | 1:B:140:MET:HB2   | 2.21                     | 0.41              |
| 1:B:96:THR:O      | 1:B:97:VAL:CG2    | 2.68                     | 0.41              |
| 2:C:35:PRO:O      | 2:C:36:PRO:C      | 2.62                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:76:PRO:HG3    | 2:C:120:LEU:CD1   | 2.50                     | 0.41              |
| 2:C:85:GLU:OE2    | 2:C:802:ARG:NH2   | 2.53                     | 0.41              |
| 2:C:626:ARG:N     | 2:C:639:GLN:HE21  | 2.17                     | 0.41              |
| 2:C:641:PRO:O     | 2:C:642:ARG:HD3   | 2.21                     | 0.41              |
| 2:C:781:LYS:HB2   | 2:C:781:LYS:HE3   | 1.85                     | 0.41              |
| 3:D:706:PRO:CG    | 11:I:101:CH1:O2   | 2.68                     | 0.41              |
| 3:D:720:LEU:C     | 3:D:721:VAL:HG13  | 2.46                     | 0.41              |
| 3:D:961:LYS:HE3   | 3:D:961:LYS:HB2   | 1.65                     | 0.41              |
| 3:D:1041:LEU:HD23 | 3:D:1041:LEU:C    | 2.46                     | 0.41              |
| 3:D:1259:VAL:HG23 | 3:D:1355:VAL:HG11 | 2.03                     | 0.41              |
| 3:D:1495:ILE:HG12 | 4:E:88:GLU:CB     | 2.51                     | 0.41              |
| 4:E:9:LEU:CD2     | 4:E:12:MET:HE3    | 2.42                     | 0.41              |
| 5:F:387:GLY:HA2   | 5:F:394:ARG:HG2   | 2.03                     | 0.41              |
| 6:G:12:DG:H5"     | 6:G:12:DG:H8      | 1.86                     | 0.41              |
| 1:A:221:HIS:ND1   | 1:A:224:TYR:HE2   | 2.19                     | 0.41              |
| 1:B:31:GLY:O      | 1:B:34:VAL:HG22   | 2.21                     | 0.41              |
| 1:B:40:LEU:N      | 1:B:40:LEU:HD23   | 2.35                     | 0.41              |
| 1:B:181:VAL:HG11  | 1:B:193:ASP:OD2   | 2.21                     | 0.41              |
| 2:C:45:GLN:OE1    | 2:C:71:TYR:HE2    | 2.04                     | 0.41              |
| 2:C:107:LEU:O     | 2:C:108:ILE:HD13  | 2.21                     | 0.41              |
| 2:C:355:VAL:CG2   | 2:C:356:ARG:N     | 2.84                     | 0.41              |
| 2:C:385:PHE:O     | 2:C:389:SER:HB2   | 2.21                     | 0.41              |
| 2:C:468:ARG:HB2   | 2:C:486:MET:C     | 2.45                     | 0.41              |
| 2:C:492:ASP:HB3   | 2:C:518:LYS:CG    | 2.51                     | 0.41              |
| 2:C:588:VAL:HG13  | 2:C:596:TYR:OH    | 2.20                     | 0.41              |
| 2:C:1067:TYR:CD2  | 3:D:655:PRO:HG3   | 2.56                     | 0.41              |
| 3:D:24:GLY:HA3    | 3:D:49:ILE:CG2    | 2.49                     | 0.41              |
| 3:D:128:TYR:CE2   | 3:D:587:ARG:HD2   | 2.56                     | 0.41              |
| 3:D:174:GLY:HA2   | 3:D:389:GLU:OE2   | 2.20                     | 0.41              |
| 3:D:351:MET:CB    | 3:D:369:ALA:O     | 2.66                     | 0.41              |
| 3:D:764:LEU:CD2   | 3:D:767:HIS:CD2   | 2.94                     | 0.41              |
| 3:D:1015:TYR:CD2  | 3:D:1015:TYR:N    | 2.89                     | 0.41              |
| 3:D:1106:VAL:CG1  | 3:D:1107:VAL:N    | 2.84                     | 0.41              |
| 3:D:1285:GLU:HG3  | 3:D:1290:LEU:HD22 | 2.01                     | 0.41              |
| 5:F:115:LYS:HA    | 5:F:115:LYS:HD3   | 1.89                     | 0.41              |
| 5:F:415:THR:C     | 5:F:417:LYS:H     | 2.28                     | 0.41              |
| 6:G:8:DC:H42      | 7:H:20:DG:H1      | 1.69                     | 0.41              |
| 1:A:39:PRO:HG3    | 1:B:39:PRO:HG2    | 2.01                     | 0.41              |
| 1:B:153:ALA:HB2   | 1:B:168:ASP:N     | 2.35                     | 0.41              |
| 2:C:261:ILE:HG22  | 2:C:291:ALA:HB3   | 2.03                     | 0.41              |
| 2:C:599:GLU:HA    | 2:C:651:LYS:HG3   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:433:GLY:HA2   | 3:D:449:SER:O     | 2.20                     | 0.41              |
| 3:D:498:VAL:O     | 3:D:501:ALA:HB3   | 2.21                     | 0.41              |
| 3:D:706:PRO:HG2   | 11:I:101:CH1:O2   | 2.19                     | 0.41              |
| 3:D:1066:THR:O    | 3:D:1067:VAL:C    | 2.63                     | 0.41              |
| 3:D:1263:PHE:O    | 3:D:1375:MET:CE   | 2.69                     | 0.41              |
| 3:D:1404:ASN:O    | 3:D:1408:ILE:HG12 | 2.21                     | 0.41              |
| 3:D:1491:THR:HG21 | 4:E:89:MET:HG2    | 2.03                     | 0.41              |
| 5:F:372:ARG:NE    | 5:F:372:ARG:CA    | 2.84                     | 0.41              |
| 5:F:393:THR:HG22  | 5:F:394:ARG:N     | 2.28                     | 0.41              |
| 2:C:326:ASP:OD2   | 2:C:426:ASP:HB3   | 2.22                     | 0.40              |
| 2:C:431:HIS:CE1   | 2:C:433:THR:HG1   | 2.34                     | 0.40              |
| 2:C:740:GLU:HB3   | 2:C:805:ARG:NH1   | 2.34                     | 0.40              |
| 2:C:767:PRO:HG2   | 2:C:782:ALA:CB    | 2.51                     | 0.40              |
| 2:C:910:LYS:HD2   | 2:C:910:LYS:N     | 2.35                     | 0.40              |
| 3:D:534:ARG:HE    | 3:D:534:ARG:HB3   | 1.33                     | 0.40              |
| 3:D:563:PRO:CB    | 5:F:189:GLU:HG2   | 2.51                     | 0.40              |
| 3:D:585:GLY:O     | 3:D:586:ARG:C     | 2.64                     | 0.40              |
| 3:D:866:VAL:HG11  | 3:D:880:ILE:HG13  | 2.03                     | 0.40              |
| 3:D:989:TYR:CE1   | 3:D:993:LEU:HD23  | 2.56                     | 0.40              |
| 3:D:1086:LEU:O    | 3:D:1087:ARG:C    | 2.64                     | 0.40              |
| 5:F:152:ASP:OD1   | 5:F:154:LYS:HB3   | 2.21                     | 0.40              |
| 5:F:321:ILE:HD13  | 5:F:321:ILE:HA    | 1.80                     | 0.40              |
| 5:F:415:THR:O     | 5:F:415:THR:OG1   | 2.35                     | 0.40              |
| 1:A:38:ASN:O      | 1:A:39:PRO:C      | 2.64                     | 0.40              |
| 2:C:230:ARG:HB2   | 2:C:233:GLU:HG3   | 2.02                     | 0.40              |
| 2:C:378:LEU:HD12  | 2:C:378:LEU:C     | 2.43                     | 0.40              |
| 2:C:759:THR:HA    | 2:C:786:LYS:O     | 2.21                     | 0.40              |
| 2:C:854:PRO:HB2   | 2:C:856:GLU:OE1   | 2.21                     | 0.40              |
| 3:D:66:GLN:HB3    | 5:F:376:ILE:HG12  | 2.03                     | 0.40              |
| 3:D:704:ARG:NH2   | 8:I:3:A:O2'       | 2.39                     | 0.40              |
| 3:D:1148:VAL:CG2  | 3:D:1165:TYR:CE1  | 3.04                     | 0.40              |
| 4:E:83:ASP:OD2    | 4:E:83:ASP:N      | 2.43                     | 0.40              |
| 5:F:299:TRP:CD2   | 5:F:303:ARG:NH1   | 2.89                     | 0.40              |
| 5:F:392:VAL:HG12  | 5:F:397:ILE:HD13  | 2.03                     | 0.40              |
| 1:A:71:VAL:HA     | 1:A:131:THR:O     | 2.22                     | 0.40              |
| 1:A:221:HIS:CD2   | 1:B:32:PHE:CD2    | 3.09                     | 0.40              |
| 2:C:18:LEU:HD13   | 2:C:542:VAL:HG21  | 2.03                     | 0.40              |
| 2:C:79:PRO:O      | 2:C:80:GLN:C      | 2.63                     | 0.40              |
| 2:C:146:VAL:HG12  | 2:C:277:ALA:CB    | 2.51                     | 0.40              |
| 2:C:302:VAL:C     | 2:C:305:PRO:HD2   | 2.46                     | 0.40              |
| 2:C:309:TYR:O     | 2:C:310:LEU:C     | 2.64                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:545:ASN:HB3  | 2:C:583:LEU:CD2  | 2.51                     | 0.40              |
| 2:C:591:SER:O    | 2:C:592:LEU:C    | 2.64                     | 0.40              |
| 2:C:655:LEU:HD12 | 2:C:655:LEU:N    | 2.36                     | 0.40              |
| 2:C:1054:THR:OG1 | 2:C:1055:LEU:N   | 2.55                     | 0.40              |
| 3:D:211:VAL:HG23 | 3:D:347:VAL:HG23 | 2.03                     | 0.40              |
| 3:D:325:GLU:O    | 3:D:325:GLU:HG2  | 2.21                     | 0.40              |
| 3:D:462:GLN:O    | 3:D:462:GLN:HG2  | 2.20                     | 0.40              |
| 3:D:520:LEU:HD12 | 3:D:521:PRO:HD2  | 2.03                     | 0.40              |
| 3:D:884:ARG:HD2  | 3:D:888:GLU:OE1  | 2.20                     | 0.40              |
| 3:D:899:LEU:HD22 | 3:D:917:GLN:HB3  | 2.02                     | 0.40              |
| 3:D:1018:ASN:HA  | 3:D:1019:PRO:HD3 | 1.95                     | 0.40              |
| 3:D:1332:PRO:O   | 3:D:1335:LEU:HB3 | 2.21                     | 0.40              |
| 4:E:14:ASP:OD2   | 4:E:18:ARG:HD2   | 2.21                     | 0.40              |
| 5:F:193:ARG:HB3  | 7:H:7:DG:C5'     | 2.46                     | 0.40              |
| 5:F:363:GLU:HA   | 5:F:366:ALA:HB3  | 2.03                     | 0.40              |
| 1:A:57:TYR:HE2   | 1:A:59:GLU:HA    | 1.86                     | 0.40              |
| 1:B:74:ASP:CG    | 3:D:872:ARG:HH12 | 2.29                     | 0.40              |
| 2:C:196:LEU:HD22 | 2:C:196:LEU:C    | 2.46                     | 0.40              |
| 2:C:200:LEU:HD22 | 2:C:300:ASP:CB   | 2.18                     | 0.40              |
| 2:C:327:HIS:CE1  | 2:C:433:THR:HG21 | 2.57                     | 0.40              |
| 2:C:617:ASP:OD1  | 2:C:617:ASP:N    | 2.54                     | 0.40              |
| 2:C:874:LEU:HD23 | 2:C:874:LEU:HA   | 1.84                     | 0.40              |
| 3:D:17:LYS:O     | 3:D:20:SER:N     | 2.55                     | 0.40              |
| 3:D:116:LEU:CD2  | 3:D:468:LEU:HD11 | 2.51                     | 0.40              |
| 3:D:566:ILE:O    | 3:D:567:ILE:C    | 2.62                     | 0.40              |
| 3:D:983:LEU:HB3  | 3:D:987:GLU:CD   | 2.46                     | 0.40              |
| 3:D:1281:VAL:HA  | 3:D:1293:PHE:O   | 2.22                     | 0.40              |
| 3:D:1290:LEU:CB  | 3:D:1307:LYS:HG2 | 2.52                     | 0.40              |
| 5:F:193:ARG:H    | 5:F:193:ARG:HG3  | 1.66                     | 0.40              |
| 5:F:349:LEU:HD22 | 5:F:349:LEU:O    | 2.21                     | 0.40              |
| 1:A:178:ALA:HB2  | 2:C:864:GLY:HA3  | 2.03                     | 0.40              |
| 1:A:195:LEU:HD12 | 1:A:195:LEU:HA   | 1.75                     | 0.40              |
| 1:B:40:LEU:O     | 1:B:41:ARG:C     | 2.64                     | 0.40              |
| 2:C:339:LEU:CD1  | 2:C:391:LEU:HD12 | 2.51                     | 0.40              |
| 2:C:405:ARG:HG3  | 2:C:543:ASN:OD1  | 2.22                     | 0.40              |
| 2:C:588:VAL:HG22 | 2:C:594:ALA:HB2  | 2.02                     | 0.40              |
| 2:C:727:PRO:HB3  | 2:C:783:ARG:NH1  | 2.37                     | 0.40              |
| 3:D:237:LYS:O    | 3:D:240:GLU:CB   | 2.70                     | 0.40              |
| 3:D:284:LEU:N    | 3:D:284:LEU:CD1  | 2.84                     | 0.40              |
| 3:D:416:ALA:CB   | 3:D:432:TYR:CE1  | 3.04                     | 0.40              |
| 3:D:480:GLU:C    | 3:D:482:LYS:N    | 2.79                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:680:GLN:O     | 3:D:683:ILE:HD12 | 2.22                     | 0.40              |
| 3:D:703:ASN:HB3   | 3:D:746:ALA:HB3  | 2.03                     | 0.40              |
| 3:D:882:PHE:CZ    | 3:D:906:GLN:HG3  | 2.56                     | 0.40              |
| 3:D:1088:THR:CG2  | 6:G:14:DG:C5     | 3.04                     | 0.40              |
| 3:D:1281:VAL:HG23 | 3:D:1315:ASP:HA  | 2.03                     | 0.40              |
| 3:D:1347:TYR:CE2  | 3:D:1351:GLU:HG3 | 2.57                     | 0.40              |
| 5:F:217:ASN:O     | 5:F:220:LEU:N    | 2.55                     | 0.40              |
| 5:F:260:ILE:HA    | 5:F:261:PRO:HD2  | 1.93                     | 0.40              |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------------|--------------------------|-------------------|
| 2:C:70:GLU:OE2  | 3:D:1151:ARG:NH1[3_545] | 2.04                     | 0.16              |
| 3:D:296:GLU:OE2 | 5:F:222:ARG:NH1[4_1149] | 2.12                     | 0.08              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 224/315 (71%)   | 183 (82%)  | 40 (18%)  | 1 (0%)   | 30          | 65  |
| 1   | B     | 222/315 (70%)   | 187 (84%)  | 33 (15%)  | 2 (1%)   | 14          | 48  |
| 2   | C     | 1107/1119 (99%) | 971 (88%)  | 133 (12%) | 3 (0%)   | 36          | 70  |
| 3   | D     | 1481/1505 (98%) | 1302 (88%) | 172 (12%) | 7 (0%)   | 24          | 60  |
| 4   | E     | 92/99 (93%)     | 81 (88%)   | 11 (12%)  | 0        | 100         | 100 |
| 5   | F     | 344/423 (81%)   | 293 (85%)  | 51 (15%)  | 0        | 100         | 100 |
| All | All   | 3470/3776 (92%) | 3017 (87%) | 440 (13%) | 13 (0%)  | 30          | 65  |

All (13) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 37   | GLY  |
| 3   | D     | 276  | ASP  |
| 1   | A     | 154  | GLU  |
| 1   | B     | 36   | LEU  |
| 3   | D     | 275  | GLU  |
| 3   | D     | 705  | ALA  |
| 3   | D     | 486  | ARG  |
| 3   | D     | 710  | ARG  |
| 2   | C     | 984  | GLU  |
| 3   | D     | 783  | ARG  |
| 3   | D     | 1130 | ARG  |
| 2   | C     | 316  | GLY  |
| 2   | C     | 212  | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 199/273 (73%)   | 159 (80%)  | 40 (20%)  | 1           | 7  |
| 1   | B     | 197/273 (72%)   | 175 (89%)  | 22 (11%)  | 6           | 24 |
| 2   | C     | 936/941 (100%)  | 809 (86%)  | 127 (14%) | 3           | 17 |
| 3   | D     | 1249/1265 (99%) | 1091 (87%) | 158 (13%) | 4           | 20 |
| 4   | E     | 83/88 (94%)     | 75 (90%)   | 8 (10%)   | 8           | 31 |
| 5   | F     | 301/371 (81%)   | 254 (84%)  | 47 (16%)  | 2           | 13 |
| All | All   | 2965/3211 (92%) | 2563 (86%) | 402 (14%) | 3           | 17 |

All (402) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | THR  |
| 1   | A     | 13  | VAL  |
| 1   | A     | 15  | THR  |
| 1   | A     | 18  | ARG  |
| 1   | A     | 24  | VAL  |
| 1   | A     | 25  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 43  | ILE  |
| 1   | A     | 46  | SER  |
| 1   | A     | 48  | ILE  |
| 1   | A     | 53  | VAL  |
| 1   | A     | 62  | LEU  |
| 1   | A     | 66  | SER  |
| 1   | A     | 68  | ILE  |
| 1   | A     | 76  | VAL  |
| 1   | A     | 85  | LEU  |
| 1   | A     | 86  | VAL  |
| 1   | A     | 87  | VAL  |
| 1   | A     | 90  | LEU  |
| 1   | A     | 96  | THR  |
| 1   | A     | 102 | LYS  |
| 1   | A     | 115 | LEU  |
| 1   | A     | 134 | GLU  |
| 1   | A     | 138 | LEU  |
| 1   | A     | 144 | VAL  |
| 1   | A     | 145 | ASP  |
| 1   | A     | 155 | LYS  |
| 1   | A     | 174 | VAL  |
| 1   | A     | 175 | ARG  |
| 1   | A     | 182 | GLU  |
| 1   | A     | 184 | THR  |
| 1   | A     | 189 | ARG  |
| 1   | A     | 190 | THR  |
| 1   | A     | 197 | LEU  |
| 1   | A     | 199 | ILE  |
| 1   | A     | 204 | SER  |
| 1   | A     | 205 | VAL  |
| 1   | A     | 206 | THR  |
| 1   | A     | 213 | GLN  |
| 1   | A     | 218 | LEU  |
| 1   | A     | 222 | LEU  |
| 1   | B     | 24  | VAL  |
| 1   | B     | 34  | VAL  |
| 1   | B     | 35  | THR  |
| 1   | B     | 38  | ASN  |
| 1   | B     | 41  | ARG  |
| 1   | B     | 54  | THR  |
| 1   | B     | 55  | SER  |
| 1   | B     | 58  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 76  | VAL  |
| 1   | B     | 87  | VAL  |
| 1   | B     | 109 | VAL  |
| 1   | B     | 115 | LEU  |
| 1   | B     | 120 | VAL  |
| 1   | B     | 131 | THR  |
| 1   | B     | 158 | ILE  |
| 1   | B     | 162 | ILE  |
| 1   | B     | 177 | VAL  |
| 1   | B     | 183 | ASP  |
| 1   | B     | 184 | THR  |
| 1   | B     | 196 | THR  |
| 1   | B     | 199 | ILE  |
| 1   | B     | 208 | LEU  |
| 2   | C     | 2   | GLU  |
| 2   | C     | 8   | ARG  |
| 2   | C     | 15  | LEU  |
| 2   | C     | 21  | ILE  |
| 2   | C     | 37  | GLU  |
| 2   | C     | 44  | ILE  |
| 2   | C     | 49  | ARG  |
| 2   | C     | 64  | LEU  |
| 2   | C     | 65  | VAL  |
| 2   | C     | 73  | LEU  |
| 2   | C     | 75  | GLU  |
| 2   | C     | 101 | ILE  |
| 2   | C     | 105 | THR  |
| 2   | C     | 118 | ILE  |
| 2   | C     | 123 | GLU  |
| 2   | C     | 149 | THR  |
| 2   | C     | 162 | ILE  |
| 2   | C     | 163 | ILE  |
| 2   | C     | 174 | LEU  |
| 2   | C     | 177 | GLU  |
| 2   | C     | 182 | VAL  |
| 2   | C     | 183 | SER  |
| 2   | C     | 184 | MET  |
| 2   | C     | 194 | VAL  |
| 2   | C     | 196 | LEU  |
| 2   | C     | 200 | LEU  |
| 2   | C     | 214 | TYR  |
| 2   | C     | 221 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 224 | GLU  |
| 2   | C     | 226 | VAL  |
| 2   | C     | 235 | LEU  |
| 2   | C     | 246 | ASP  |
| 2   | C     | 269 | LEU  |
| 2   | C     | 276 | LYS  |
| 2   | C     | 279 | GLU  |
| 2   | C     | 285 | LEU  |
| 2   | C     | 308 | ARG  |
| 2   | C     | 311 | PHE  |
| 2   | C     | 335 | THR  |
| 2   | C     | 342 | ASP  |
| 2   | C     | 351 | LEU  |
| 2   | C     | 353 | ARG  |
| 2   | C     | 364 | GLU  |
| 2   | C     | 366 | SER  |
| 2   | C     | 367 | LEU  |
| 2   | C     | 368 | THR  |
| 2   | C     | 387 | SER  |
| 2   | C     | 390 | GLN  |
| 2   | C     | 403 | SER  |
| 2   | C     | 404 | LEU  |
| 2   | C     | 409 | ARG  |
| 2   | C     | 427 | VAL  |
| 2   | C     | 432 | ARG  |
| 2   | C     | 433 | THR  |
| 2   | C     | 454 | SER  |
| 2   | C     | 460 | ARG  |
| 2   | C     | 474 | VAL  |
| 2   | C     | 490 | GLU  |
| 2   | C     | 493 | ARG  |
| 2   | C     | 514 | VAL  |
| 2   | C     | 516 | ARG  |
| 2   | C     | 524 | VAL  |
| 2   | C     | 534 | VAL  |
| 2   | C     | 537 | LYS  |
| 2   | C     | 538 | GLN  |
| 2   | C     | 542 | VAL  |
| 2   | C     | 544 | THR  |
| 2   | C     | 560 | MET  |
| 2   | C     | 572 | ILE  |
| 2   | C     | 598 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 605 | LYS  |
| 2   | C     | 616 | GLU  |
| 2   | C     | 617 | ASP  |
| 2   | C     | 649 | VAL  |
| 2   | C     | 670 | GLN  |
| 2   | C     | 672 | VAL  |
| 2   | C     | 674 | VAL  |
| 2   | C     | 677 | MET  |
| 2   | C     | 680 | ASP  |
| 2   | C     | 705 | ILE  |
| 2   | C     | 706 | GLU  |
| 2   | C     | 707 | ARG  |
| 2   | C     | 717 | LEU  |
| 2   | C     | 723 | THR  |
| 2   | C     | 729 | LEU  |
| 2   | C     | 730 | SER  |
| 2   | C     | 744 | ARG  |
| 2   | C     | 745 | ILE  |
| 2   | C     | 748 | GLU  |
| 2   | C     | 750 | LYS  |
| 2   | C     | 751 | PRO  |
| 2   | C     | 768 | THR  |
| 2   | C     | 780 | GLU  |
| 2   | C     | 784 | ASP  |
| 2   | C     | 785 | VAL  |
| 2   | C     | 808 | ARG  |
| 2   | C     | 813 | VAL  |
| 2   | C     | 815 | LEU  |
| 2   | C     | 816 | LYS  |
| 2   | C     | 819 | VAL  |
| 2   | C     | 823 | VAL  |
| 2   | C     | 825 | VAL  |
| 2   | C     | 829 | GLN  |
| 2   | C     | 834 | GLN  |
| 2   | C     | 846 | LYS  |
| 2   | C     | 858 | MET  |
| 2   | C     | 861 | LEU  |
| 2   | C     | 888 | THR  |
| 2   | C     | 897 | LEU  |
| 2   | C     | 900 | ARG  |
| 2   | C     | 914 | ILE  |
| 2   | C     | 939 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 946  | ARG  |
| 2   | C     | 952  | LEU  |
| 2   | C     | 954  | THR  |
| 2   | C     | 958  | THR  |
| 2   | C     | 968  | LEU  |
| 2   | C     | 1001 | VAL  |
| 2   | C     | 1005 | MET  |
| 2   | C     | 1014 | SER  |
| 2   | C     | 1052 | MET  |
| 2   | C     | 1060 | ILE  |
| 2   | C     | 1063 | ARG  |
| 2   | C     | 1078 | GLU  |
| 2   | C     | 1080 | SER  |
| 2   | C     | 1084 | SER  |
| 2   | C     | 1115 | LEU  |
| 3   | D     | 6    | ARG  |
| 3   | D     | 10   | ILE  |
| 3   | D     | 25   | GLU  |
| 3   | D     | 40   | GLU  |
| 3   | D     | 48   | ARG  |
| 3   | D     | 53   | ILE  |
| 3   | D     | 73   | CYS  |
| 3   | D     | 74   | GLU  |
| 3   | D     | 80   | VAL  |
| 3   | D     | 81   | THR  |
| 3   | D     | 97   | THR  |
| 3   | D     | 106  | LYS  |
| 3   | D     | 115  | LEU  |
| 3   | D     | 123  | LEU  |
| 3   | D     | 133  | ILE  |
| 3   | D     | 141  | ILE  |
| 3   | D     | 143  | ASN  |
| 3   | D     | 153  | LEU  |
| 3   | D     | 161  | LEU  |
| 3   | D     | 176  | ASP  |
| 3   | D     | 179  | VAL  |
| 3   | D     | 180  | LYS  |
| 3   | D     | 187  | LYS  |
| 3   | D     | 202  | VAL  |
| 3   | D     | 212  | ARG  |
| 3   | D     | 231  | VAL  |
| 3   | D     | 249  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 270 | LEU  |
| 3   | D     | 271 | VAL  |
| 3   | D     | 275 | GLU  |
| 3   | D     | 284 | LEU  |
| 3   | D     | 289 | THR  |
| 3   | D     | 316 | GLN  |
| 3   | D     | 325 | GLU  |
| 3   | D     | 327 | GLU  |
| 3   | D     | 333 | LEU  |
| 3   | D     | 335 | LEU  |
| 3   | D     | 351 | MET  |
| 3   | D     | 353 | VAL  |
| 3   | D     | 361 | VAL  |
| 3   | D     | 371 | ILE  |
| 3   | D     | 378 | ILE  |
| 3   | D     | 380 | GLU  |
| 3   | D     | 387 | LEU  |
| 3   | D     | 389 | GLU  |
| 3   | D     | 392 | SER  |
| 3   | D     | 410 | SER  |
| 3   | D     | 411 | THR  |
| 3   | D     | 415 | VAL  |
| 3   | D     | 434 | ARG  |
| 3   | D     | 437 | VAL  |
| 3   | D     | 439 | LEU  |
| 3   | D     | 440 | VAL  |
| 3   | D     | 445 | ARG  |
| 3   | D     | 447 | VAL  |
| 3   | D     | 448 | GLU  |
| 3   | D     | 459 | GLU  |
| 3   | D     | 475 | LYS  |
| 3   | D     | 478 | LEU  |
| 3   | D     | 485 | SER  |
| 3   | D     | 486 | ARG  |
| 3   | D     | 514 | LEU  |
| 3   | D     | 525 | ARG  |
| 3   | D     | 527 | MET  |
| 3   | D     | 528 | VAL  |
| 3   | D     | 534 | ARG  |
| 3   | D     | 538 | SER  |
| 3   | D     | 553 | ARG  |
| 3   | D     | 557 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 566 | ILE  |
| 3   | D     | 574 | LEU  |
| 3   | D     | 578 | VAL  |
| 3   | D     | 582 | LEU  |
| 3   | D     | 586 | ARG  |
| 3   | D     | 592 | THR  |
| 3   | D     | 600 | LEU  |
| 3   | D     | 602 | SER  |
| 3   | D     | 603 | LEU  |
| 3   | D     | 608 | SER  |
| 3   | D     | 621 | LYS  |
| 3   | D     | 623 | VAL  |
| 3   | D     | 632 | VAL  |
| 3   | D     | 660 | LYS  |
| 3   | D     | 677 | LEU  |
| 3   | D     | 679 | ARG  |
| 3   | D     | 686 | GLU  |
| 3   | D     | 693 | GLU  |
| 3   | D     | 699 | VAL  |
| 3   | D     | 719 | VAL  |
| 3   | D     | 722 | GLU  |
| 3   | D     | 754 | PHE  |
| 3   | D     | 761 | ILE  |
| 3   | D     | 771 | SER  |
| 3   | D     | 778 | LEU  |
| 3   | D     | 786 | ILE  |
| 3   | D     | 797 | LYS  |
| 3   | D     | 835 | SER  |
| 3   | D     | 836 | VAL  |
| 3   | D     | 857 | ILE  |
| 3   | D     | 863 | VAL  |
| 3   | D     | 885 | ILE  |
| 3   | D     | 901 | GLN  |
| 3   | D     | 912 | LYS  |
| 3   | D     | 943 | THR  |
| 3   | D     | 948 | THR  |
| 3   | D     | 949 | ILE  |
| 3   | D     | 956 | ILE  |
| 3   | D     | 961 | LYS  |
| 3   | D     | 966 | GLU  |
| 3   | D     | 973 | GLN  |
| 3   | D     | 974 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 986  | ARG  |
| 3   | D     | 993  | LEU  |
| 3   | D     | 997  | THR  |
| 3   | D     | 1001 | GLU  |
| 3   | D     | 1003 | VAL  |
| 3   | D     | 1015 | TYR  |
| 3   | D     | 1026 | SER  |
| 3   | D     | 1034 | GLN  |
| 3   | D     | 1041 | LEU  |
| 3   | D     | 1042 | ARG  |
| 3   | D     | 1065 | LEU  |
| 3   | D     | 1083 | ASP  |
| 3   | D     | 1090 | ASP  |
| 3   | D     | 1100 | ASP  |
| 3   | D     | 1114 | THR  |
| 3   | D     | 1124 | GLN  |
| 3   | D     | 1126 | ASP  |
| 3   | D     | 1131 | SER  |
| 3   | D     | 1154 | GLU  |
| 3   | D     | 1186 | VAL  |
| 3   | D     | 1188 | VAL  |
| 3   | D     | 1196 | THR  |
| 3   | D     | 1208 | ASP  |
| 3   | D     | 1210 | SER  |
| 3   | D     | 1235 | GLN  |
| 3   | D     | 1280 | VAL  |
| 3   | D     | 1281 | VAL  |
| 3   | D     | 1290 | LEU  |
| 3   | D     | 1294 | VAL  |
| 3   | D     | 1304 | LYS  |
| 3   | D     | 1310 | ARG  |
| 3   | D     | 1370 | ILE  |
| 3   | D     | 1376 | MET  |
| 3   | D     | 1379 | VAL  |
| 3   | D     | 1390 | LEU  |
| 3   | D     | 1394 | VAL  |
| 3   | D     | 1400 | VAL  |
| 3   | D     | 1403 | LEU  |
| 3   | D     | 1413 | THR  |
| 3   | D     | 1420 | LEU  |
| 3   | D     | 1424 | VAL  |
| 3   | D     | 1426 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1431 | THR  |
| 3   | D     | 1456 | LYS  |
| 3   | D     | 1468 | LEU  |
| 3   | D     | 1489 | GLN  |
| 3   | D     | 1493 | LYS  |
| 4   | E     | 8    | LYS  |
| 4   | E     | 15   | SER  |
| 4   | E     | 37   | ASN  |
| 4   | E     | 70   | THR  |
| 4   | E     | 74   | VAL  |
| 4   | E     | 75   | PHE  |
| 4   | E     | 84   | ARG  |
| 4   | E     | 87   | LYS  |
| 5   | F     | 82   | ARG  |
| 5   | F     | 83   | GLN  |
| 5   | F     | 88   | ILE  |
| 5   | F     | 98   | GLU  |
| 5   | F     | 107  | GLU  |
| 5   | F     | 116  | LEU  |
| 5   | F     | 122  | LEU  |
| 5   | F     | 123  | ASP  |
| 5   | F     | 126  | LEU  |
| 5   | F     | 130  | VAL  |
| 5   | F     | 144  | ILE  |
| 5   | F     | 148  | LYS  |
| 5   | F     | 149  | GLU  |
| 5   | F     | 151  | LEU  |
| 5   | F     | 164  | LYS  |
| 5   | F     | 170  | HIS  |
| 5   | F     | 174  | LEU  |
| 5   | F     | 205  | ARG  |
| 5   | F     | 207  | LEU  |
| 5   | F     | 211  | ASP  |
| 5   | F     | 213  | ILE  |
| 5   | F     | 224  | VAL  |
| 5   | F     | 254  | GLN  |
| 5   | F     | 257  | THR  |
| 5   | F     | 282  | LEU  |
| 5   | F     | 293  | GLU  |
| 5   | F     | 304  | VAL  |
| 5   | F     | 306  | GLU  |
| 5   | F     | 307  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 310 | ILE  |
| 5   | F     | 319 | THR  |
| 5   | F     | 336 | GLU  |
| 5   | F     | 338 | LEU  |
| 5   | F     | 348 | SER  |
| 5   | F     | 352 | GLU  |
| 5   | F     | 358 | LEU  |
| 5   | F     | 360 | LYS  |
| 5   | F     | 369 | LEU  |
| 5   | F     | 372 | ARG  |
| 5   | F     | 376 | ILE  |
| 5   | F     | 377 | ASP  |
| 5   | F     | 380 | GLU  |
| 5   | F     | 386 | VAL  |
| 5   | F     | 399 | GLN  |
| 5   | F     | 400 | ILE  |
| 5   | F     | 407 | LYS  |
| 5   | F     | 415 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 227  | ASN  |
| 1   | A     | 229  | GLN  |
| 1   | B     | 63   | HIS  |
| 1   | B     | 81   | ASN  |
| 1   | B     | 128  | HIS  |
| 1   | B     | 163  | ASN  |
| 2   | C     | 22   | GLN  |
| 2   | C     | 130  | ASN  |
| 2   | C     | 187  | ASN  |
| 2   | C     | 390  | GLN  |
| 2   | C     | 552  | HIS  |
| 2   | C     | 556  | ASN  |
| 2   | C     | 565  | GLN  |
| 2   | C     | 567  | GLN  |
| 2   | C     | 639  | GLN  |
| 2   | C     | 704  | HIS  |
| 2   | C     | 728  | HIS  |
| 2   | C     | 834  | GLN  |
| 2   | C     | 991  | GLN  |
| 2   | C     | 1030 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 1050 | GLN  |
| 3   | D     | 294  | HIS  |
| 3   | D     | 348  | GLN  |
| 3   | D     | 560  | GLN  |
| 3   | D     | 640  | HIS  |
| 3   | D     | 680  | GLN  |
| 3   | D     | 709  | HIS  |
| 3   | D     | 714  | GLN  |
| 3   | D     | 737  | ASN  |
| 3   | D     | 767  | HIS  |
| 3   | D     | 816  | HIS  |
| 3   | D     | 824  | ASN  |
| 3   | D     | 909  | ASN  |
| 3   | D     | 1031 | ASN  |
| 3   | D     | 1034 | GLN  |
| 3   | D     | 1075 | HIS  |
| 3   | D     | 1195 | GLN  |
| 3   | D     | 1235 | GLN  |
| 3   | D     | 1333 | HIS  |
| 3   | D     | 1359 | GLN  |
| 3   | D     | 1441 | GLN  |
| 3   | D     | 1442 | ASN  |
| 4   | E     | 86   | GLN  |
| 5   | F     | 175  | HIS  |
| 5   | F     | 248  | ASN  |
| 5   | F     | 381  | HIS  |
| 5   | F     | 399  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed  | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------|-------------------|-----------------|
| 8   | I     | 2/3 (66%) | 0                 | 0               |

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 11  | CH1  | I     | 101 | 9    | 27,29,29     | 2.98 | 9 (33%)     | 37,45,45    | 1.36 | 5 (13%)     |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 11  | CH1  | I     | 101 | 9    | -       | 4/22/34/34 | 0/2/2/2 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 11  | I     | 101 | CH1  | C3'-C2' | -11.10 | 1.24        | 1.52     |
| 11  | I     | 101 | CH1  | O4'-C1' | -6.06  | 1.28        | 1.42     |
| 11  | I     | 101 | CH1  | O2-C2   | -3.57  | 1.17        | 1.23     |
| 11  | I     | 101 | CH1  | C2-N1   | -3.49  | 1.32        | 1.40     |
| 11  | I     | 101 | CH1  | C4-N4   | 3.16   | 1.41        | 1.33     |
| 11  | I     | 101 | CH1  | C5-C4   | -3.00  | 1.35        | 1.42     |
| 11  | I     | 101 | CH1  | C5'-C4' | -2.68  | 1.42        | 1.50     |
| 11  | I     | 101 | CH1  | C2-N3   | -2.59  | 1.31        | 1.36     |
| 11  | I     | 101 | CH1  | O4'-C4' | 2.38   | 1.49        | 1.44     |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | I     | 101 | CH1  | O4'-C4'-C3' | -3.94 | 100.08      | 105.07   |
| 11  | I     | 101 | CH1  | O4'-C1'-N1  | 3.54  | 116.38      | 108.36   |
| 11  | I     | 101 | CH1  | C2'-C3'-C4' | 2.13  | 106.82      | 102.97   |
| 11  | I     | 101 | CH1  | O2A-PA-O5'  | 2.07  | 116.96      | 107.57   |
| 11  | I     | 101 | CH1  | O4'-C1'-C2' | -2.00 | 104.63      | 106.51   |

There are no chirality outliers.

All (4) torsion outliers are listed below:

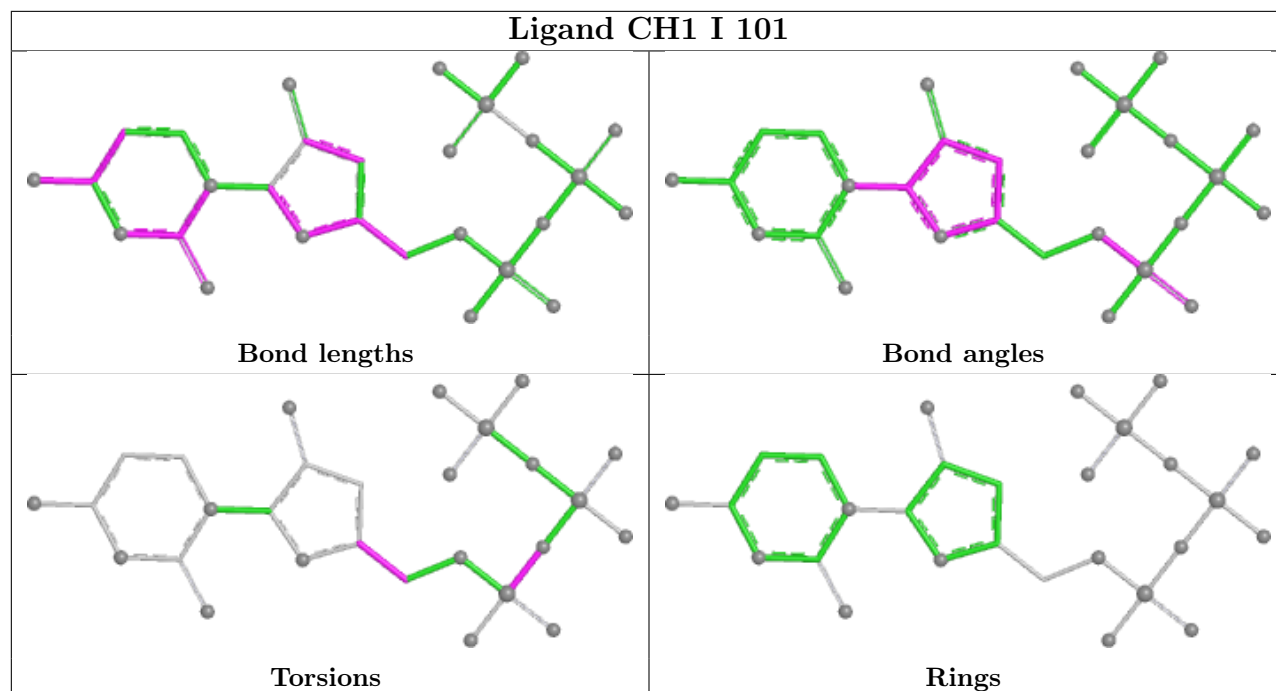
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | I     | 101 | CH1  | C3'-C4'-C5'-O5' |
| 11  | I     | 101 | CH1  | O4'-C4'-C5'-O5' |
| 11  | I     | 101 | CH1  | PB-O3A-PA-O1A   |
| 11  | I     | 101 | CH1  | PB-O3A-PA-O2A   |

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 11  | I     | 101 | CH1  | 2       | 0            |

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|--------------|-----------------------|-------|
| 1   | A     | 226/315 (71%)   | -0.52  | 0 100 100    | 58, 79, 98, 110       | 0     |
| 1   | B     | 224/315 (71%)   | -0.44  | 0 100 100    | 59, 85, 110, 122      | 0     |
| 2   | C     | 1111/1119 (99%) | -0.49  | 0 100 100    | 47, 81, 125, 144      | 0     |
| 3   | D     | 1485/1505 (98%) | -0.50  | 1 (0%) 92 86 | 40, 75, 122, 141      | 0     |
| 4   | E     | 94/99 (94%)     | -0.29  | 0 100 100    | 57, 90, 116, 121      | 0     |
| 5   | F     | 346/423 (81%)   | -0.34  | 2 (0%) 85 69 | 57, 88, 138, 150      | 0     |
| 6   | G     | 17/22 (77%)     | -0.43  | 0 100 100    | 64, 92, 152, 155      | 0     |
| 7   | H     | 25/27 (92%)     | -0.31  | 0 100 100    | 77, 106, 149, 157     | 0     |
| 8   | I     | 3/3 (100%)      | -1.01  | 0 100 100    | 72, 72, 73, 75        | 0     |
| All | All   | 3531/3828 (92%) | -0.47  | 3 (0%) 92 86 | 40, 81, 126, 157      | 0     |

All (3) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | F     | 376 | ILE  | 3.3  |
| 5   | F     | 400 | ILE  | 2.8  |
| 3   | D     | 409 | VAL  | 2.3  |

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

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

### 6.3 Carbohydrates [i](#)

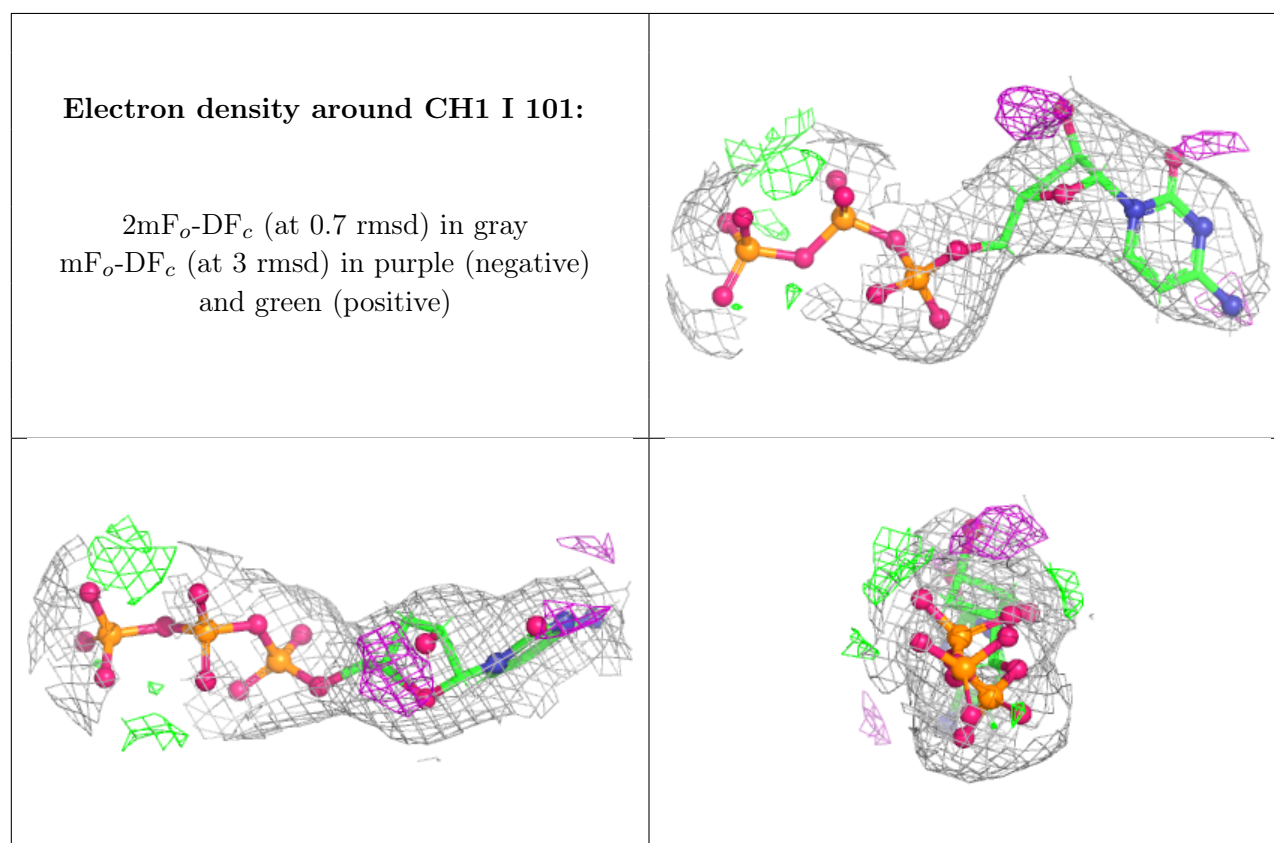
There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 9   | MG   | D     | 2002 | 1/1   | 0.91 | 0.10 | 64,64,64,64                 | 0     |
| 11  | CH1  | I     | 101  | 28/28 | 0.92 | 0.07 | 59,77,94,100                | 0     |
| 9   | MG   | D     | 2001 | 1/1   | 0.97 | 0.07 | 47,47,47,47                 | 0     |
| 10  | ZN   | D     | 2004 | 1/1   | 0.99 | 0.06 | 76,76,76,76                 | 0     |
| 10  | ZN   | D     | 2003 | 1/1   | 0.99 | 0.04 | 96,96,96,96                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.