



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:01 PM UTC

PDB ID : 5N5Z / pdb\_00005n5z  
EMDB ID : EMD-3591  
Title : Cryo-EM structure of RNA polymerase I in complex with Rrn3 and Core Factor (Orientation II)  
Authors : Engel, C.; Gubbey, T.; Neyer, S.; Sainsbury, S.; Oberthuer, C.; Baejen, C.; Bernecky, C.; Cramer, P.  
Deposited on : 2017-02-14  
Resolution : 7.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

The types of validation reports are described at

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

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

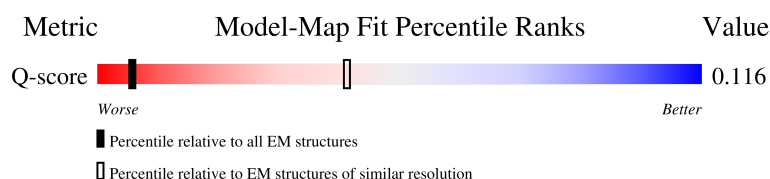
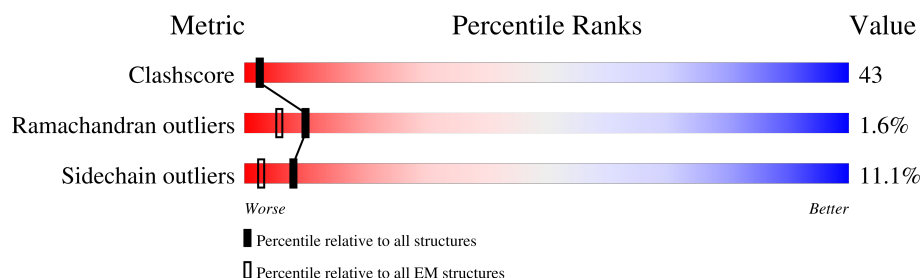
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.70 Å.

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



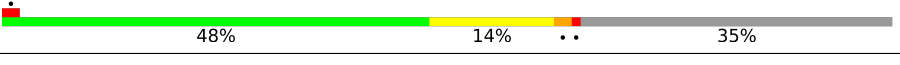
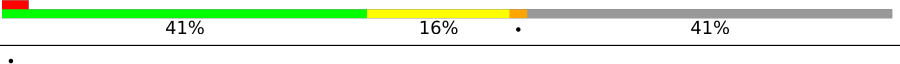
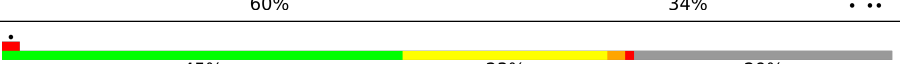
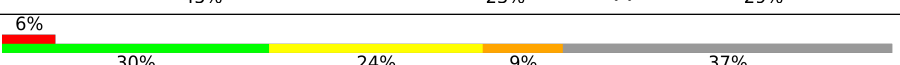
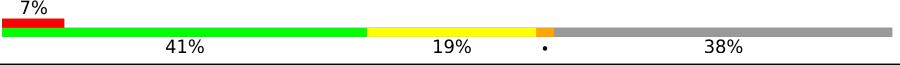
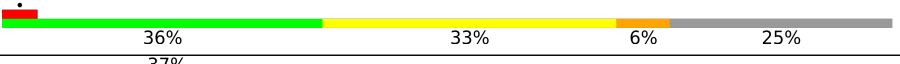
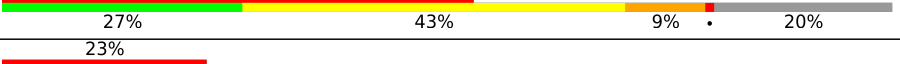
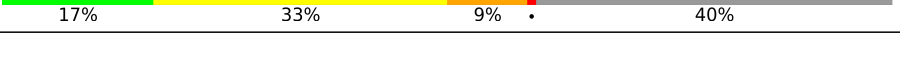
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 384 ( 7.20 - 8.20 )                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1664   |                  |
| 2   | B     | 1203   |                  |
| 3   | C     | 335    |                  |
| 4   | D     | 137    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 5   | E     | 215    |    |
| 6   | F     | 155    |    |
| 7   | G     | 326    |    |
| 8   | H     | 146    |    |
| 9   | I     | 125    |    |
| 10  | J     | 70     |    |
| 11  | K     | 142    |    |
| 12  | L     | 70     |    |
| 13  | M     | 415    |    |
| 14  | N     | 233    |    |
| 15  | O     | 627    |   |
| 16  | P     | 894    |  |
| 17  | Q     | 514    |  |
| 18  | R     | 507    |  |

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 48004 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase I subunit RPA190.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 1467     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11598 | 7327 | 2017 | 2193 | 61 |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | B     | 1172     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9312  | 5891 | 1633 | 1738 | 50 |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | C     | 305      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2423  | 1539 | 416 | 460 | 8 |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 4   | D     | 58       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 459   | 289 | 78 | 92 |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | E     | 212      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1735  | 1102 | 306 | 316 | 11 |         |       |

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 823   | 522 | 144 | 154 | 3 |         |       |

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | G     | 193      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1526  | 985 | 262 | 274 | 5 |         |       |

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1052  | 664 | 176 | 208 | 4 |         |       |

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | I     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 755   | 472 | 125 | 149 | 9 |         |       |

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | J     | 69       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 569   | 362 | 101 | 100 | 6 |         |       |

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | K     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 793   | 496 | 130 | 162 | 5 |         |       |

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12  | L     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 352   | 217 | 70 | 61 | 4 |         |       |

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 13  | M     | 108      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 856   | 543 | 142 | 171 |  |         |       |

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | N     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1151  | 735 | 188 | 224 | 4 |         |       |

- Molecule 15 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | O     | 473      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3907  | 2533 | 642 | 711 | 21 |         |       |

- Molecule 16 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 16  | P     | 583      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4729  | 3010 | 803 | 905 | 11 |         |       |

- Molecule 17 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 17  | Q     | 410      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3421  | 2219 | 579 | 603 | 20 |         |       |

- Molecule 18 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 18  | R     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2535  | 1634 | 456 | 434 | 11 |         |       |

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 19  | A     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 19  | B     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 19  | I     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 19  | J     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

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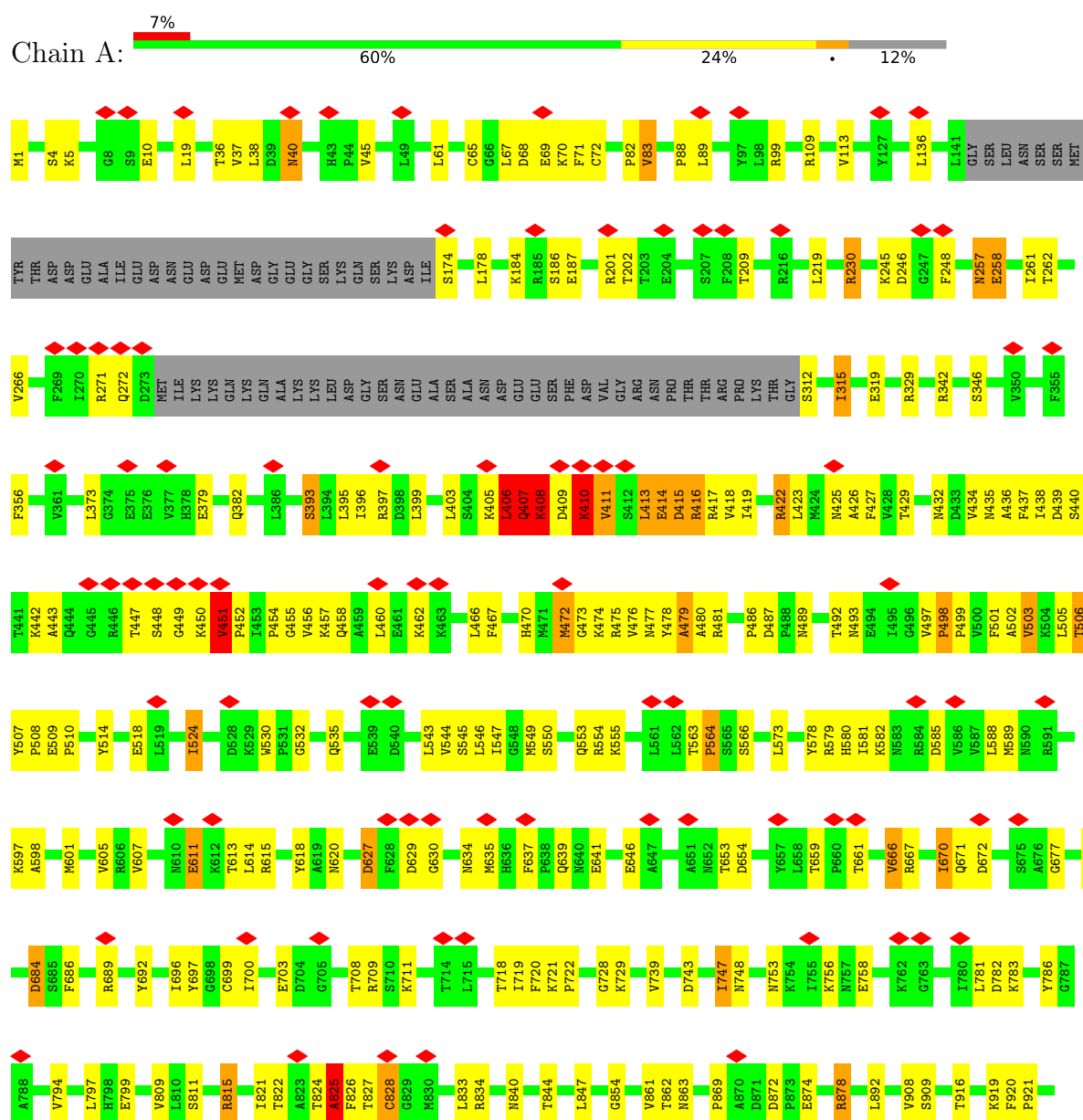
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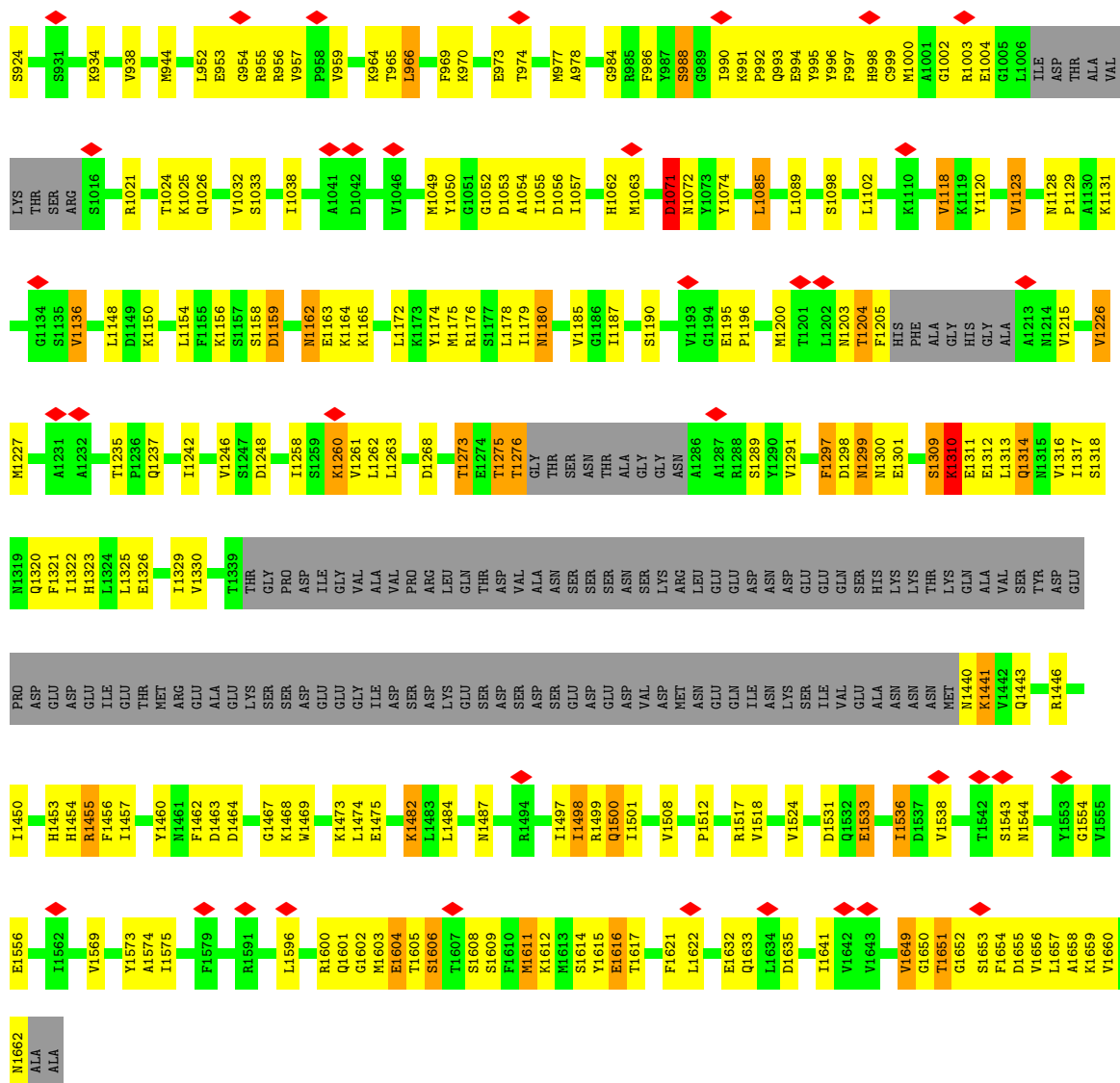
| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 19  | L     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 19  | Q     | 1        | Total<br>1 | Zn<br>1 | 0       |

### 3 Residue-property plots

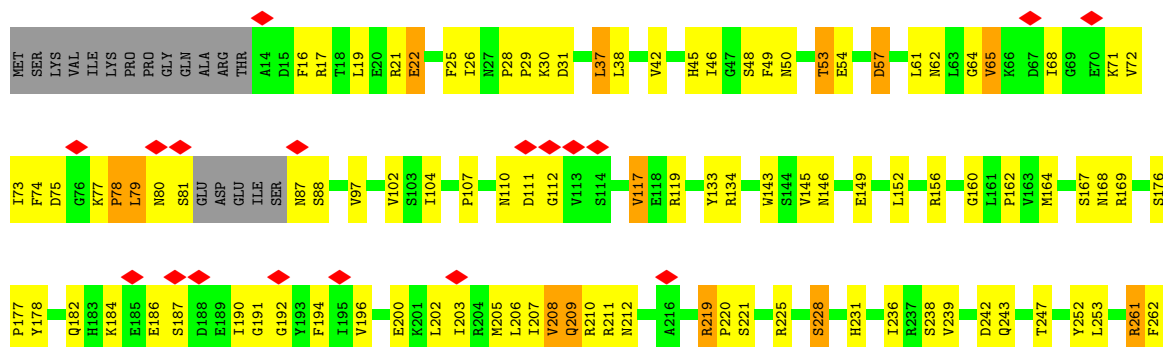
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 I subunit RPA190



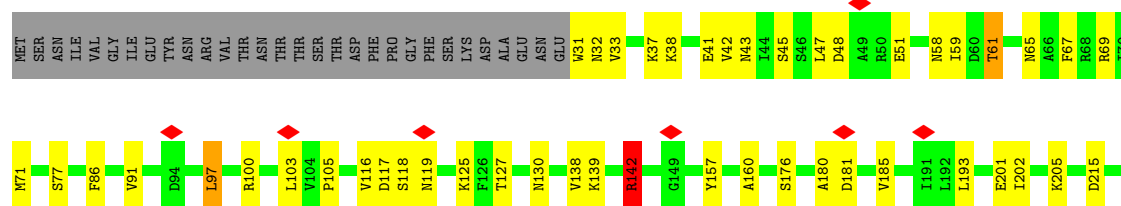


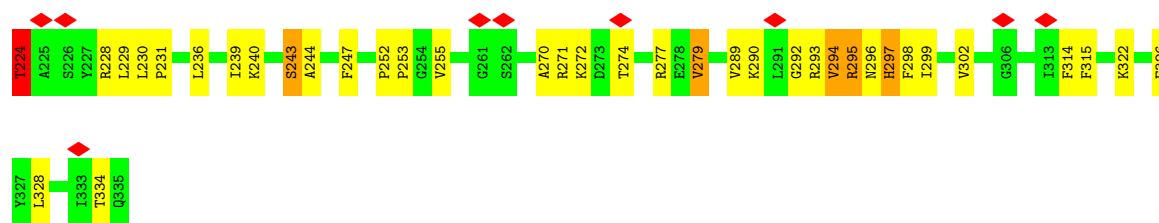
• Molecule 2: DNA-directed RNA polymerase I subunit RPA135



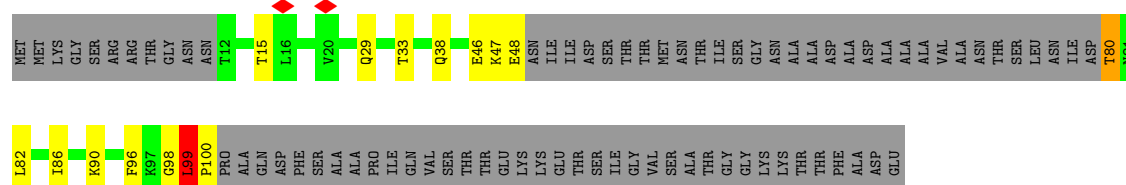


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

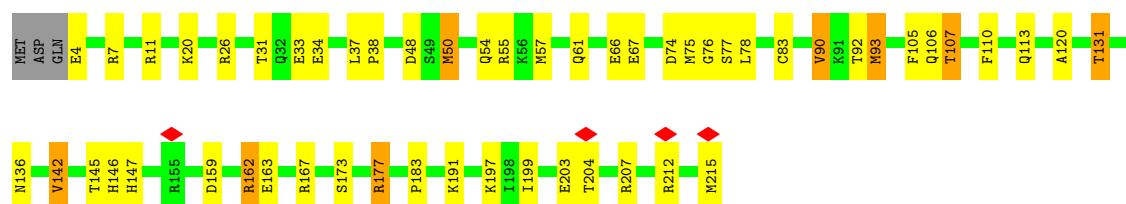




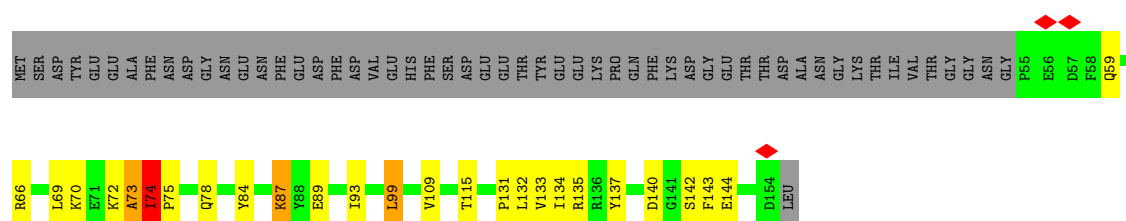
- Molecule 4: DNA-directed RNA polymerase I subunit RPA14



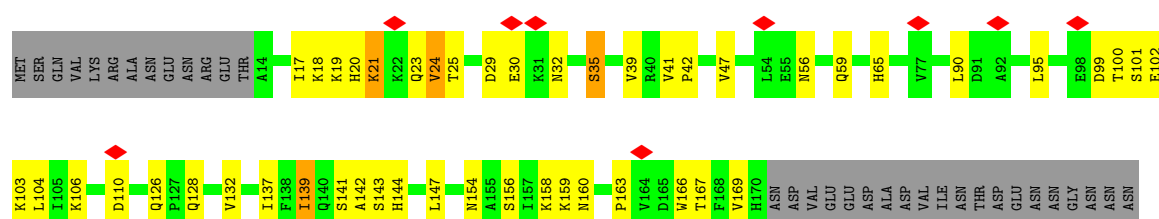
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

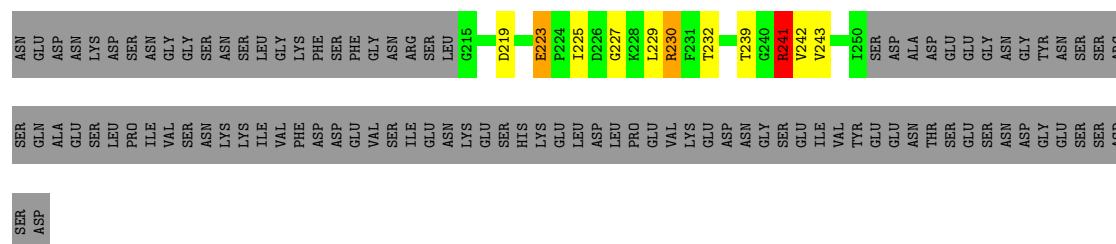


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

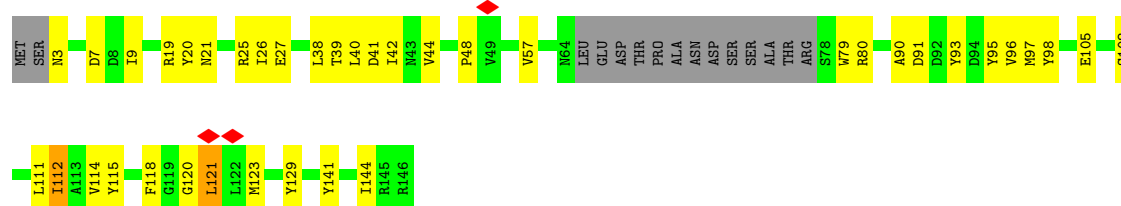


- Molecule 7: DNA-directed RNA polymerase I subunit RPA43

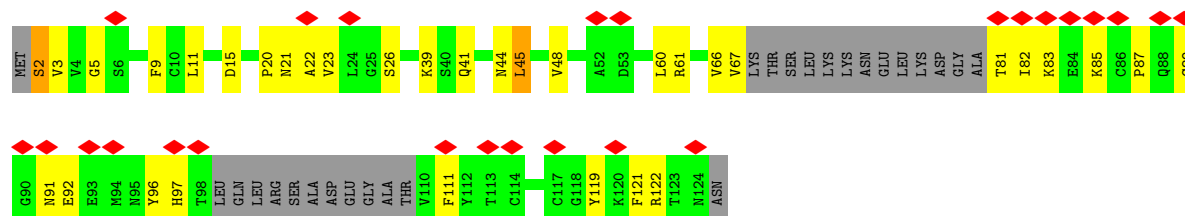




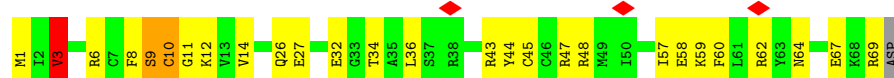
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



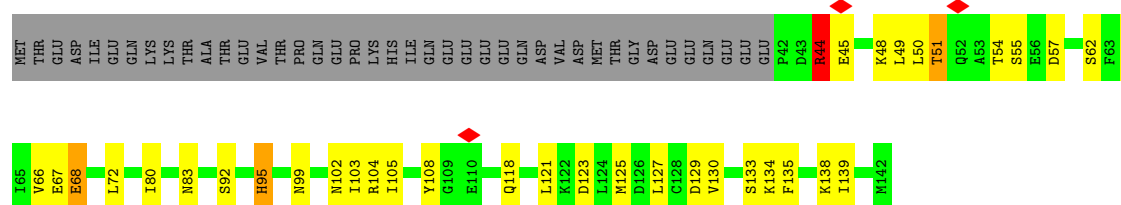
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12



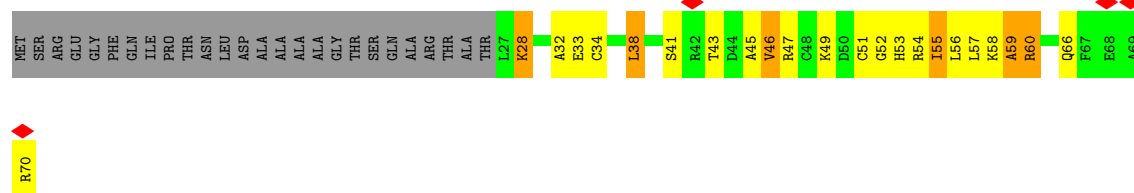
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



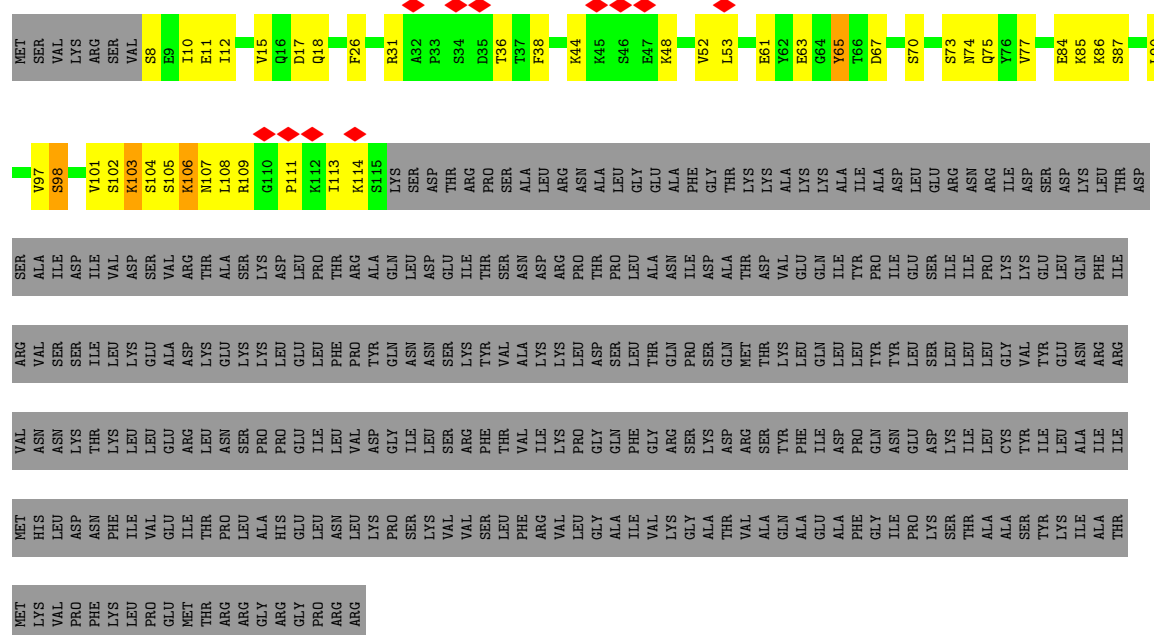
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



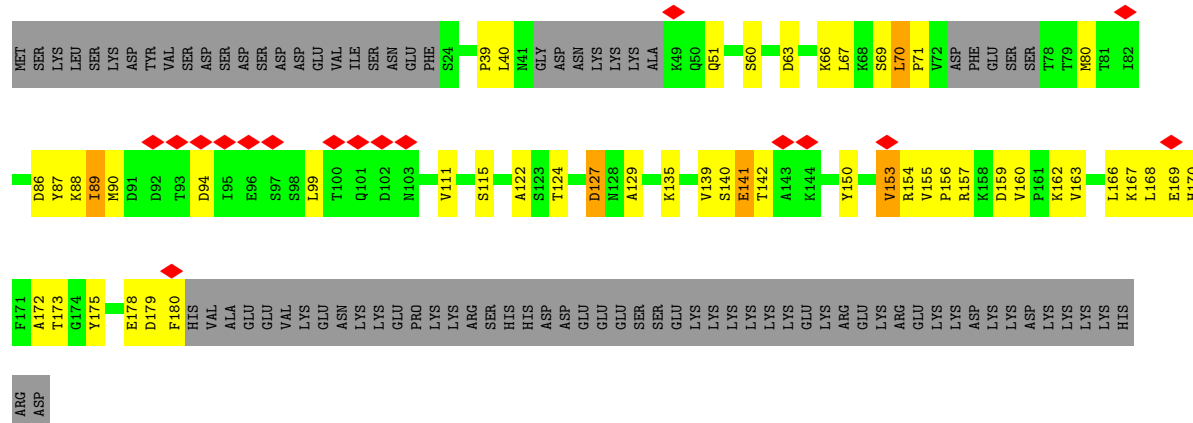
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



Chain M:  16% 9% 74%

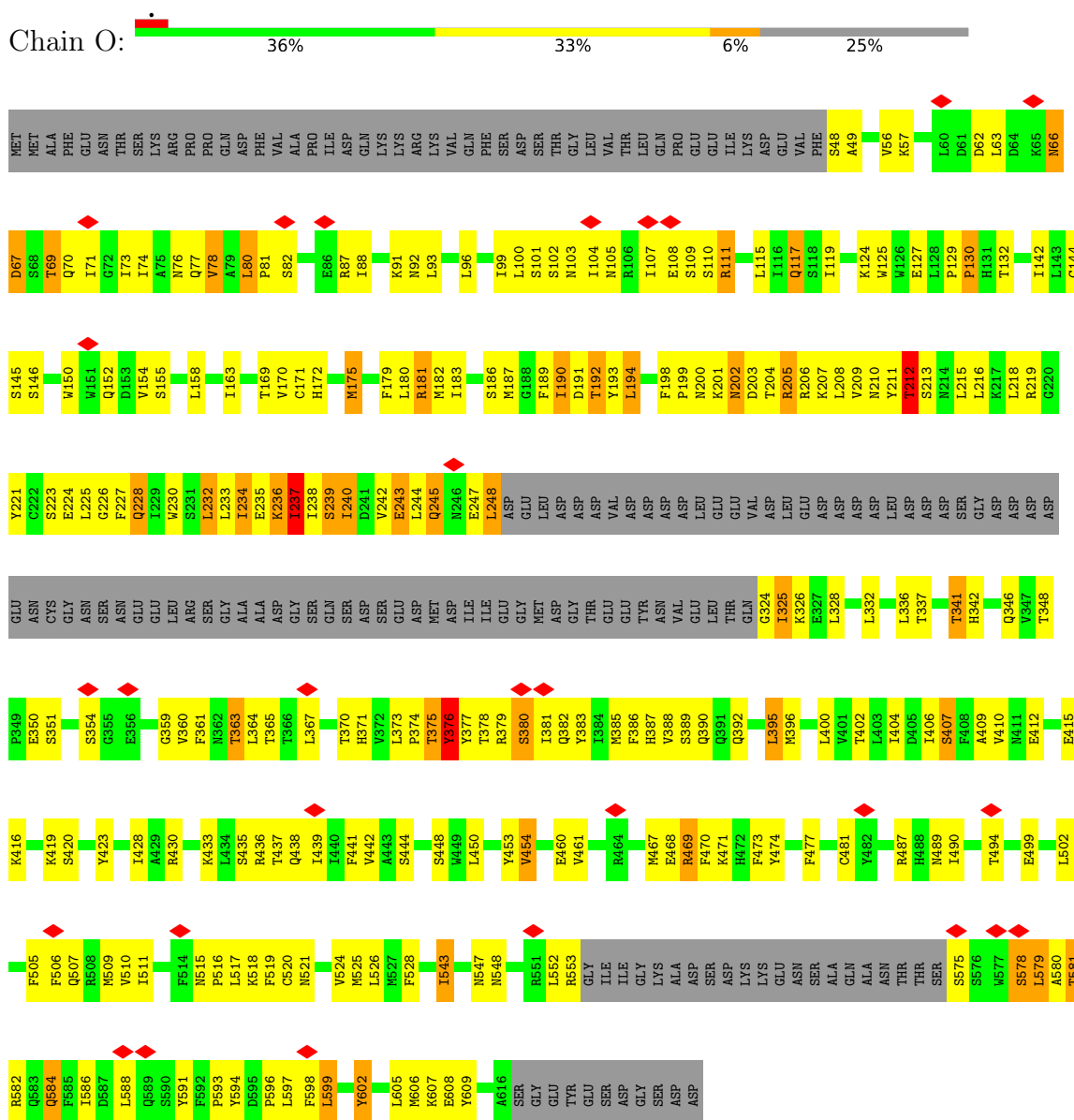


Chain N:  7% 41% 19% 33%



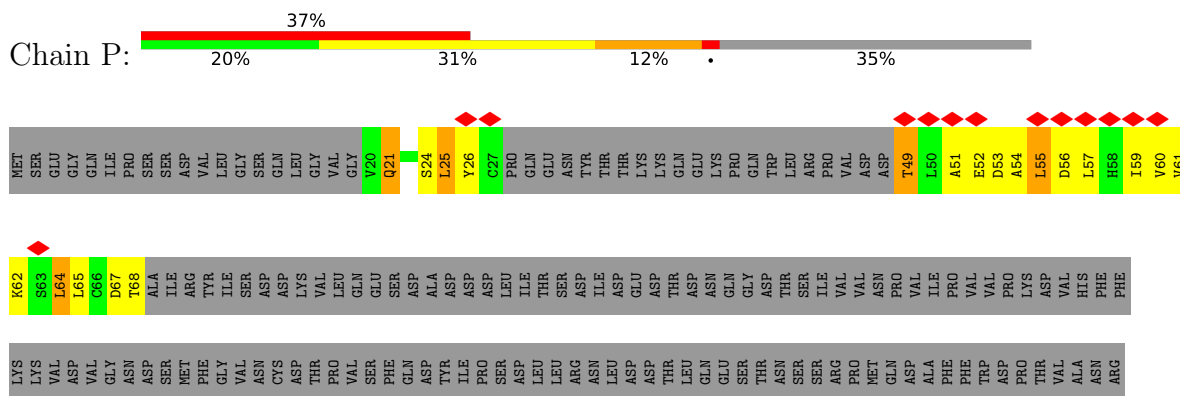
- Molecule 15: RNA polymerase I-specific transcription initiation factor RRN3

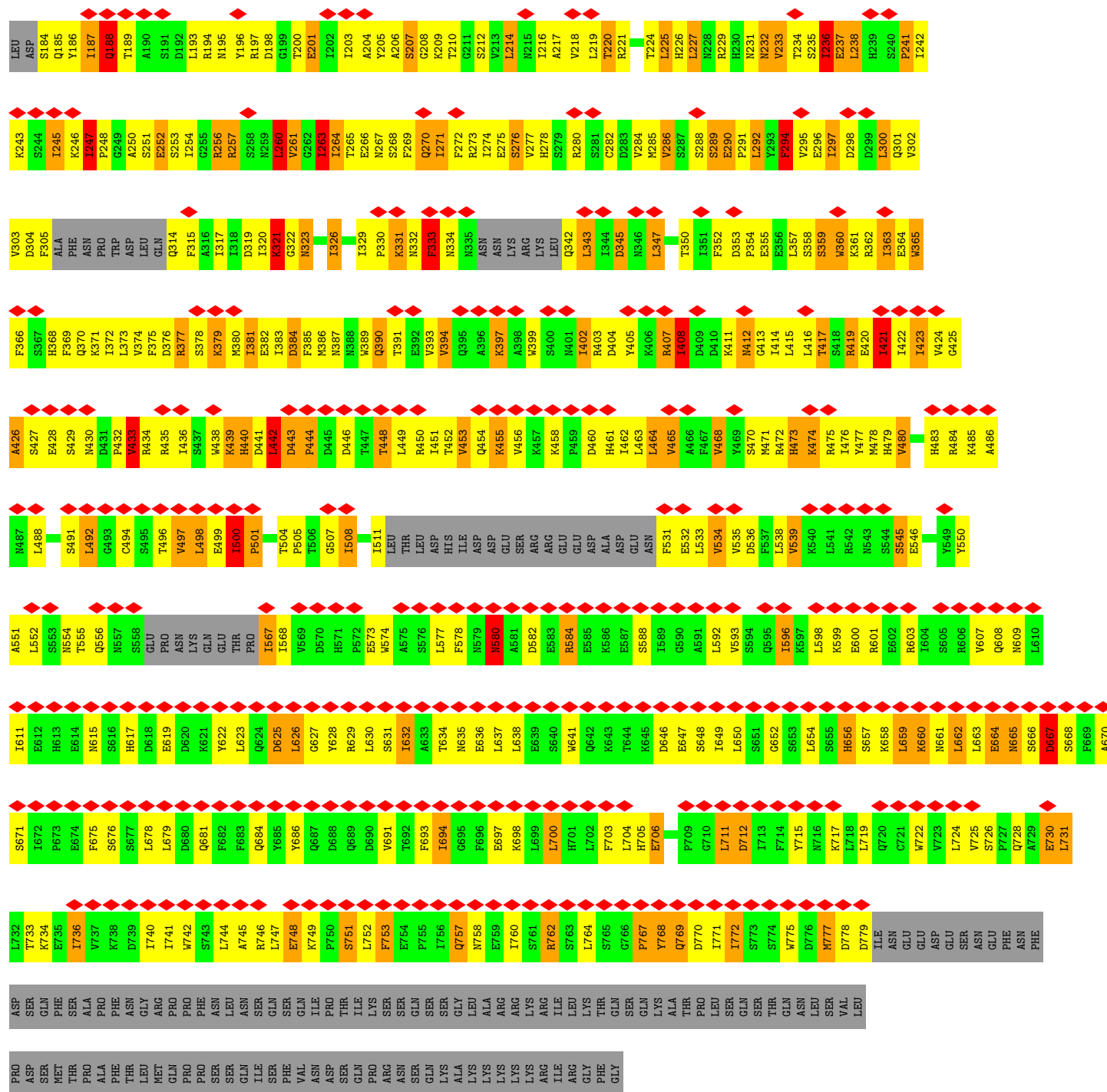
Chain 0:

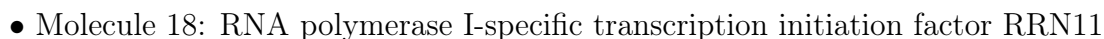


- Molecule 16: RNA polymerase I-specific transcription initiation factor RRN6

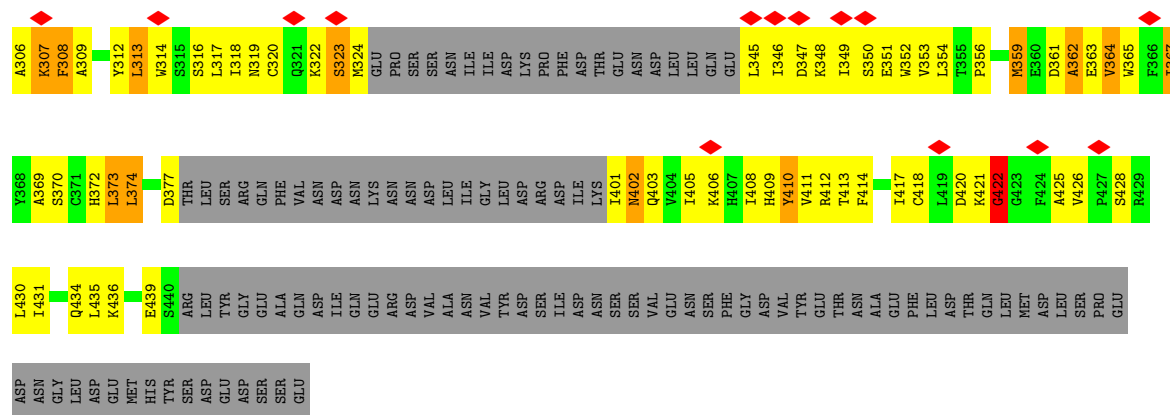
Chain P:







|  |      |      |      |     |     |
|--|------|------|------|-----|-----|
|  | V245 | T181 | SER  | GLN | M1  |
|  | Q246 | N184 | ASP  | ASN | F2  |
|  | L247 | K185 | GLU  | SER | E3  |
|  | K248 | L186 | ARG  | ALA | V4  |
|  | S249 | Y187 | LYS  | GLY | P5  |
|  | L250 | F188 | PHE  | THR | I6  |
|  | W251 | Q189 | TRP  | TYR | T7  |
|  | G252 | S190 | LYS  | ARG | L8  |
|  | I253 | I191 | LYS  | ARG | T9  |
|  | G254 |      | TYR  | SER | M0  |
|  | V255 | G194 | GLU  | VAL |     |
|  | E256 | L195 | LYS  | LEU | R11 |
|  | I257 | E196 | PRO  | Q74 | K12 |
|  | L258 | P197 | GLU  | Q75 | F13 |
|  | D259 | L198 | LYS  | K76 | A14 |
|  | M260 | K199 | S137 | K77 | Q15 |
|  | L261 | T200 | F138 | R78 | R16 |
|  | S262 | S201 | E139 | R79 | R17 |
|  | M263 | T202 | W141 | R80 | K18 |
|  | S264 | S203 | R142 | E81 | L19 |
|  | S265 | E204 | T143 | R82 | K20 |
|  | S266 | V205 | V144 | H83 | Y21 |
|  | G267 | R206 | S145 | W84 | Q22 |
|  | L268 | N207 | S146 | R85 | Y23 |
|  | D269 | Y208 | Q147 | S86 | I24 |
|  | F270 | T210 | M148 | V87 | N25 |
|  | L271 | R211 | K149 |     | Y26 |
|  | Q272 | H212 | Q150 | VAL | I27 |
|  | W273 | I213 | P151 | GLY | S28 |
|  | M274 | V214 | I152 | GLU | R29 |
|  | C275 | T215 | M153 | ILE | K30 |
|  | Q276 | L216 | K154 | TYR | F31 |
|  | I277 | T217 | Q155 | SER | D32 |
|  | S278 | D218 | X156 | THR | R33 |
|  | S280 | L219 | M157 | GLU | I34 |
|  | K281 | L220 | T158 | SER |     |
|  | S282 | H221 | Y159 | GLU | S35 |
|  | ARG  | L222 | H160 | THR | K36 |
|  | PHE  | M223 | M161 | ASP | LYS |
|  | VAL  | V224 | P162 | SER | SER |
|  | GLN  | S225 | K163 | GLN | THR |
|  | ASN  | R226 | I165 | GLU | THR |
|  | ILE  | H227 | E166 | GLU | ASP |
|  | ASN  |      | K167 | THR | LEV |
|  | TYR  | L231 | I168 | GLU | SER |
|  | R291 | A232 | P169 | GLU | PRO |
|  | V294 | K233 | L170 | GLY | THR |
|  | P295 | T234 | R171 | GLY | PRO |
|  | P296 | I235 | K172 | GLU | ASN |
|  | F297 | F236 | M173 | HIS | ASN |
|  | Q298 | A237 | E174 | ASP | SER |
|  | T299 | T238 | I175 | GLY | ALA |
|  | G300 | L239 | P176 | ILE | ALA |
|  | S301 | T240 | L177 | ASP | GLU |
|  | R302 | R241 | L178 | LYS | ASN |
|  | T303 | L242 | H179 | GLU | ASP |
|  | H304 | G244 | C180 | ASP | GLU |
|  |      |      |      |     | GLY |



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 8317                                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.071                                   | Depositor |
| Minimum map value                    | -0.035                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.005                                   | Depositor |
| Recommended contour level            | 0.018                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 324.0, 324.0, 324.0                     | wwPDB     |
| Map dimensions                       | 240, 240, 240                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.35, 1.35, 1.35                        | Depositor |

## 5 Model quality [i](#)

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

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

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

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.64         | 1/11809 (0.0%) | 0.96        | 36/15943 (0.2%)  |
| 2   | B     | 0.62         | 0/9518         | 0.98        | 35/12863 (0.3%)  |
| 3   | C     | 0.53         | 0/2475         | 0.94        | 8/3354 (0.2%)    |
| 4   | D     | 0.52         | 0/465          | 0.81        | 0/630            |
| 5   | E     | 0.49         | 0/1771         | 0.88        | 3/2383 (0.1%)    |
| 6   | F     | 0.58         | 0/838          | 0.86        | 0/1129           |
| 7   | G     | 0.50         | 0/1563         | 0.84        | 3/2124 (0.1%)    |
| 8   | H     | 0.52         | 0/1070         | 0.88        | 0/1449           |
| 9   | I     | 0.53         | 0/765          | 0.87        | 0/1030           |
| 10  | J     | 0.60         | 0/578          | 0.98        | 6/775 (0.8%)     |
| 11  | K     | 0.54         | 0/804          | 0.93        | 6/1083 (0.6%)    |
| 12  | L     | 0.50         | 0/354          | 0.91        | 2/468 (0.4%)     |
| 13  | M     | 0.49         | 0/872          | 0.87        | 0/1170           |
| 14  | N     | 0.49         | 0/1172         | 0.88        | 1/1580 (0.1%)    |
| 15  | O     | 0.45         | 1/3996 (0.0%)  | 0.82        | 2/5401 (0.0%)    |
| 16  | P     | 0.38         | 0/4822         | 0.74        | 6/6525 (0.1%)    |
| 17  | Q     | 0.36         | 1/3501 (0.0%)  | 0.67        | 2/4724 (0.0%)    |
| 18  | R     | 0.35         | 0/2592         | 0.77        | 5/3486 (0.1%)    |
| All | All   | 0.54         | 3/48965 (0.0%) | 0.89        | 115/66117 (0.2%) |

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                   | 15                  |
| 2   | B     | 0                   | 4                   |
| 3   | C     | 0                   | 1                   |
| 6   | F     | 0                   | 1                   |
| 12  | L     | 0                   | 2                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 13  | M     | 0                   | 3                   |
| 14  | N     | 0                   | 1                   |
| 15  | O     | 0                   | 4                   |
| 16  | P     | 0                   | 26                  |
| 17  | Q     | 0                   | 8                   |
| 18  | R     | 0                   | 10                  |
| All | All   | 0                   | 75                  |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | A     | 356 | PHE  | C-N   | 8.48 | 1.44        | 1.33     |
| 17  | Q     | 15  | CYS  | CA-C  | 7.48 | 1.62        | 1.52     |
| 15  | O     | 212 | THR  | CA-CB | 5.45 | 1.62        | 1.53     |

All (115) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 18  | R     | 205  | VAL  | N-CA-C  | 16.04  | 125.61      | 110.53   |
| 18  | R     | 208  | TYR  | N-CA-C  | 13.16  | 125.35      | 111.14   |
| 2   | B     | 405  | GLY  | N-CA-C  | -12.23 | 97.21       | 113.24   |
| 1   | A     | 1071 | ASP  | N-CA-C  | -9.86  | 97.51       | 110.53   |
| 3   | C     | 223  | SER  | N-CA-C  | -9.70  | 101.61      | 112.57   |
| 15  | O     | 376  | TYR  | N-CA-C  | -9.47  | 100.39      | 113.56   |
| 18  | R     | 206  | ARG  | N-CA-C  | 9.46   | 124.45      | 111.39   |
| 17  | Q     | 7    | GLY  | C-N-CD  | -9.27  | 87.00       | 125.00   |
| 1   | A     | 956  | ARG  | CA-C-O  | 8.51   | 122.87      | 117.94   |
| 1   | A     | 666  | VAL  | CB-CA-C | -8.47  | 102.35      | 110.65   |
| 2   | B     | 537  | SER  | CA-C-N  | -7.84  | 111.91      | 121.00   |
| 2   | B     | 537  | SER  | C-N-CA  | -7.84  | 111.91      | 121.00   |
| 16  | P     | 442  | LEU  | CA-C-N  | -7.76  | 113.32      | 123.34   |
| 16  | P     | 442  | LEU  | C-N-CA  | -7.76  | 113.32      | 123.34   |
| 2   | B     | 1074 | MET  | N-CA-C  | -7.66  | 102.91      | 111.71   |
| 3   | C     | 279  | VAL  | CB-CA-C | -7.41  | 102.39      | 111.88   |
| 2   | B     | 893  | ASN  | N-CA-C  | 7.38   | 120.24      | 111.02   |
| 1   | A     | 201  | ARG  | N-CA-C  | 6.95   | 120.86      | 112.38   |
| 1   | A     | 356  | PHE  | O-C-N   | -6.83  | 113.17      | 122.94   |
| 18  | R     | 207  | ASN  | N-CA-C  | 6.62   | 119.68      | 108.90   |
| 2   | B     | 1103 | VAL  | CB-CA-C | -6.57  | 100.71      | 110.82   |
| 2   | B     | 894  | LYS  | CB-CA-C | -6.56  | 108.31      | 117.23   |
| 2   | B     | 219  | ARG  | CA-C-N  | 6.54   | 128.01      | 119.84   |
| 2   | B     | 219  | ARG  | C-N-CA  | 6.54   | 128.01      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 1123 | VAL  | CB-CA-C   | -6.53 | 103.49      | 112.04   |
| 3   | C     | 51   | GLU  | N-CA-C    | 6.45  | 119.69      | 109.50   |
| 2   | B     | 1023 | ARG  | NE-CZ-NH2 | -6.42 | 113.42      | 119.20   |
| 3   | C     | 295  | ARG  | N-CA-C    | 6.40  | 118.05      | 111.14   |
| 1   | A     | 397  | ARG  | CD-NE-CZ  | 6.37  | 133.32      | 124.40   |
| 2   | B     | 261  | ARG  | CD-NE-CZ  | 6.33  | 133.26      | 124.40   |
| 2   | B     | 622  | ILE  | CB-CA-C   | -6.28 | 102.88      | 112.05   |
| 5   | E     | 203  | GLU  | N-CA-C    | -6.26 | 104.56      | 111.82   |
| 10  | J     | 64   | ASN  | CA-C-N    | 6.25  | 125.94      | 119.82   |
| 10  | J     | 64   | ASN  | C-N-CA    | 6.25  | 125.94      | 119.82   |
| 2   | B     | 452  | ARG  | NE-CZ-NH2 | -6.10 | 113.71      | 119.20   |
| 2   | B     | 72   | VAL  | N-CA-C    | 6.08  | 117.24      | 108.48   |
| 1   | A     | 329  | ARG  | NE-CZ-NH2 | -6.05 | 113.76      | 119.20   |
| 2   | B     | 452  | ARG  | CD-NE-CZ  | 6.02  | 132.83      | 124.40   |
| 2   | B     | 448  | ARG  | NE-CZ-NH2 | -5.97 | 113.82      | 119.20   |
| 16  | P     | 394  | VAL  | N-CA-C    | 5.94  | 119.37      | 111.17   |
| 1   | A     | 258  | GLU  | N-CA-C    | 5.93  | 118.23      | 111.11   |
| 2   | B     | 658  | LEU  | N-CA-C    | -5.91 | 100.92      | 109.31   |
| 2   | B     | 832  | TRP  | CA-C-N    | 5.86  | 127.16      | 119.84   |
| 2   | B     | 832  | TRP  | C-N-CA    | 5.86  | 127.16      | 119.84   |
| 1   | A     | 416  | ARG  | NE-CZ-NH2 | -5.84 | 113.95      | 119.20   |
| 2   | B     | 429  | ARG  | NE-CZ-NH2 | -5.82 | 113.96      | 119.20   |
| 1   | A     | 329  | ARG  | CD-NE-CZ  | 5.79  | 132.50      | 124.40   |
| 2   | B     | 448  | ARG  | CD-NE-CZ  | 5.77  | 132.48      | 124.40   |
| 16  | P     | 188  | GLN  | N-CA-C    | 5.76  | 123.08      | 110.80   |
| 1   | A     | 956  | ARG  | CB-CA-C   | -5.75 | 108.78      | 117.07   |
| 16  | P     | 443  | ASP  | N-CA-C    | 5.74  | 119.42      | 108.97   |
| 5   | E     | 167  | ARG  | NE-CZ-NH2 | -5.69 | 114.08      | 119.20   |
| 2   | B     | 634  | ARG  | CD-NE-CZ  | 5.68  | 132.35      | 124.40   |
| 1   | A     | 1203 | ASN  | N-CA-C    | 5.67  | 117.70      | 109.07   |
| 17  | Q     | 15   | CYS  | CA-C-O    | -5.67 | 112.39      | 120.16   |
| 1   | A     | 1261 | VAL  | N-CA-C    | 5.66  | 116.28      | 108.12   |
| 11  | K     | 44   | ARG  | CD-NE-CZ  | 5.66  | 132.33      | 124.40   |
| 1   | A     | 356  | PHE  | CA-C-N    | 5.64  | 130.73      | 122.77   |
| 1   | A     | 356  | PHE  | C-N-CA    | 5.64  | 130.73      | 122.77   |
| 11  | K     | 95   | HIS  | CA-C-N    | 5.63  | 126.88      | 119.84   |
| 11  | K     | 95   | HIS  | C-N-CA    | 5.63  | 126.88      | 119.84   |
| 1   | A     | 1498 | ILE  | N-CA-C    | 5.61  | 115.80      | 110.42   |
| 1   | A     | 416  | ARG  | CD-NE-CZ  | 5.60  | 132.23      | 124.40   |
| 1   | A     | 422  | ARG  | CD-NE-CZ  | 5.59  | 132.23      | 124.40   |
| 2   | B     | 429  | ARG  | CD-NE-CZ  | 5.59  | 132.22      | 124.40   |
| 1   | A     | 659  | THR  | CA-C-N    | -5.58 | 114.00      | 119.64   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 659  | THR  | C-N-CA    | -5.58 | 114.00      | 119.64   |
| 18  | R     | 250  | LEU  | CA-CB-CG  | 5.57  | 135.81      | 116.30   |
| 11  | K     | 44   | ARG  | NE-CZ-NH2 | -5.54 | 114.21      | 119.20   |
| 16  | P     | 333  | PHE  | N-CA-C    | 5.53  | 117.41      | 108.34   |
| 1   | A     | 549  | MET  | N-CA-C    | 5.52  | 119.10      | 110.32   |
| 12  | L     | 28   | LYS  | N-CA-C    | 5.50  | 118.04      | 111.71   |
| 10  | J     | 3    | VAL  | CA-C-N    | -5.49 | 114.31      | 119.85   |
| 10  | J     | 3    | VAL  | C-N-CA    | -5.49 | 114.31      | 119.85   |
| 1   | A     | 498  | PRO  | CA-C-N    | 5.47  | 125.30      | 119.28   |
| 1   | A     | 498  | PRO  | C-N-CA    | 5.47  | 125.30      | 119.28   |
| 1   | A     | 825  | ALA  | CB-CA-C   | -5.46 | 110.30      | 116.63   |
| 2   | B     | 1082 | HIS  | N-CA-C    | 5.46  | 117.31      | 111.36   |
| 2   | B     | 261  | ARG  | NE-CZ-NH2 | -5.46 | 114.29      | 119.20   |
| 2   | B     | 634  | ARG  | NE-CZ-NH2 | -5.46 | 114.29      | 119.20   |
| 3   | C     | 142  | ARG  | CD-NE-CZ  | 5.45  | 132.03      | 124.40   |
| 12  | L     | 52   | GLY  | N-CA-C    | -5.40 | 107.81      | 115.43   |
| 1   | A     | 397  | ARG  | NE-CZ-NH1 | 5.40  | 126.90      | 121.50   |
| 14  | N     | 127  | ASP  | N-CA-C    | -5.39 | 106.19      | 114.16   |
| 7   | G     | 241  | ARG  | CD-NE-CZ  | 5.39  | 131.94      | 124.40   |
| 7   | G     | 241  | ARG  | NE-CZ-NH2 | -5.39 | 114.35      | 119.20   |
| 5   | E     | 167  | ARG  | CD-NE-CZ  | 5.37  | 131.92      | 124.40   |
| 2   | B     | 1072 | GLY  | CA-C-N    | 5.36  | 127.91      | 120.29   |
| 2   | B     | 1072 | GLY  | C-N-CA    | 5.36  | 127.91      | 120.29   |
| 1   | A     | 825  | ALA  | N-CA-C    | 5.34  | 117.11      | 108.08   |
| 1   | A     | 245  | LYS  | N-CA-C    | 5.33  | 117.96      | 109.65   |
| 15  | O     | 580  | ALA  | N-CA-C    | -5.30 | 105.40      | 111.07   |
| 1   | A     | 397  | ARG  | NE-CZ-NH2 | -5.29 | 114.44      | 119.20   |
| 1   | A     | 1482 | LYS  | N-CA-C    | 5.29  | 117.89      | 110.23   |
| 1   | A     | 1543 | SER  | CA-C-N    | 5.29  | 127.80      | 120.29   |
| 1   | A     | 1543 | SER  | C-N-CA    | 5.29  | 127.80      | 120.29   |
| 3   | C     | 185  | VAL  | CA-C-N    | -5.28 | 114.48      | 119.76   |
| 3   | C     | 185  | VAL  | C-N-CA    | -5.28 | 114.48      | 119.76   |
| 7   | G     | 219  | ASP  | N-CA-C    | 5.26  | 116.78      | 109.31   |
| 2   | B     | 1048 | SER  | N-CA-C    | 5.25  | 116.81      | 111.14   |
| 1   | A     | 329  | ARG  | NE-CZ-NH1 | 5.25  | 126.75      | 121.50   |
| 1   | A     | 422  | ARG  | NE-CZ-NH2 | -5.20 | 114.52      | 119.20   |
| 1   | A     | 342  | ARG  | CD-NE-CZ  | 5.15  | 131.61      | 124.40   |
| 10  | J     | 9    | SER  | CA-C-N    | 5.14  | 127.43      | 120.44   |
| 10  | J     | 9    | SER  | C-N-CA    | 5.14  | 127.43      | 120.44   |
| 2   | B     | 1054 | SER  | N-CA-C    | 5.12  | 117.52      | 111.33   |
| 3   | C     | 142  | ARG  | NE-CZ-NH2 | -5.11 | 114.60      | 119.20   |
| 1   | A     | 1524 | VAL  | N-CA-C    | 5.10  | 115.47      | 108.12   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 11  | K     | 83   | ASN  | CA-C-N    | 5.09  | 124.75      | 119.56   |
| 11  | K     | 83   | ASN  | C-N-CA    | 5.09  | 124.75      | 119.56   |
| 2   | B     | 88   | SER  | N-CA-C    | 5.08  | 118.10      | 109.76   |
| 2   | B     | 511  | GLN  | N-CA-C    | -5.07 | 107.14      | 113.38   |
| 2   | B     | 1110 | ILE  | CB-CA-C   | -5.07 | 105.47      | 111.65   |
| 2   | B     | 314  | LYS  | N-CA-C    | -5.06 | 103.80      | 110.43   |
| 2   | B     | 261  | ARG  | NE-CZ-NH1 | 5.03  | 126.53      | 121.50   |

There are no chirality outliers.

All (75) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 1180 | ASN  | Peptide |
| 1   | A     | 1260 | LYS  | Peptide |
| 1   | A     | 1297 | PHE  | Peptide |
| 1   | A     | 1309 | SER  | Peptide |
| 1   | A     | 1310 | LYS  | Peptide |
| 1   | A     | 1649 | VAL  | Peptide |
| 1   | A     | 405  | LYS  | Peptide |
| 1   | A     | 406  | LEU  | Peptide |
| 1   | A     | 407  | GLN  | Peptide |
| 1   | A     | 410  | LYS  | Peptide |
| 1   | A     | 411  | VAL  | Peptide |
| 1   | A     | 506  | THR  | Peptide |
| 1   | A     | 781  | LEU  | Peptide |
| 1   | A     | 825  | ALA  | Peptide |
| 1   | A     | 828  | CYS  | Peptide |
| 2   | B     | 1049 | THR  | Peptide |
| 2   | B     | 1068 | GLY  | Peptide |
| 2   | B     | 404  | LEU  | Peptide |
| 2   | B     | 550  | ARG  | Peptide |
| 3   | C     | 294  | VAL  | Peptide |
| 6   | F     | 73   | ALA  | Peptide |
| 12  | L     | 59   | ALA  | Peptide |
| 12  | L     | 60   | ARG  | Peptide |
| 13  | M     | 103  | LYS  | Peptide |
| 13  | M     | 106  | LYS  | Peptide |
| 13  | M     | 107  | ASN  | Peptide |
| 14  | N     | 141  | GLU  | Peptide |
| 15  | O     | 236  | LYS  | Peptide |
| 15  | O     | 243  | GLU  | Peptide |
| 15  | O     | 375  | THR  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 15  | O     | 380 | SER  | Peptide |
| 16  | P     | 216 | ILE  | Peptide |
| 16  | P     | 236 | ILE  | Peptide |
| 16  | P     | 238 | LEU  | Peptide |
| 16  | P     | 247 | ILE  | Peptide |
| 16  | P     | 256 | ARG  | Peptide |
| 16  | P     | 260 | LEU  | Peptide |
| 16  | P     | 263 | ILE  | Peptide |
| 16  | P     | 270 | GLN  | Peptide |
| 16  | P     | 289 | SER  | Peptide |
| 16  | P     | 294 | PHE  | Peptide |
| 16  | P     | 295 | VAL  | Peptide |
| 16  | P     | 333 | PHE  | Peptide |
| 16  | P     | 365 | TRP  | Peptide |
| 16  | P     | 393 | VAL  | Peptide |
| 16  | P     | 408 | ILE  | Peptide |
| 16  | P     | 433 | VAL  | Peptide |
| 16  | P     | 442 | LEU  | Peptide |
| 16  | P     | 485 | LYS  | Peptide |
| 16  | P     | 500 | ILE  | Peptide |
| 16  | P     | 51  | ALA  | Peptide |
| 16  | P     | 52  | GLU  | Peptide |
| 16  | P     | 580 | ASN  | Peptide |
| 16  | P     | 661 | ASN  | Peptide |
| 16  | P     | 667 | ASP  | Peptide |
| 16  | P     | 767 | PRO  | Peptide |
| 16  | P     | 769 | GLN  | Peptide |
| 17  | Q     | 148 | PRO  | Peptide |
| 17  | Q     | 15  | CYS  | Peptide |
| 17  | Q     | 17  | SER  | Peptide |
| 17  | Q     | 221 | PRO  | Peptide |
| 17  | Q     | 25  | GLY  | Peptide |
| 17  | Q     | 29  | CYS  | Peptide |
| 17  | Q     | 290 | THR  | Peptide |
| 17  | Q     | 4   | PHE  | Peptide |
| 18  | R     | 154 | LYS  | Peptide |
| 18  | R     | 208 | TYR  | Peptide |
| 18  | R     | 247 | ILE  | Peptide |
| 18  | R     | 263 | ASN  | Peptide |
| 18  | R     | 265 | SER  | Peptide |
| 18  | R     | 303 | THR  | Peptide |
| 18  | R     | 304 | HIS  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 18  | R     | 422 | GLY  | Peptide |
| 18  | R     | 425 | ALA  | Peptide |
| 18  | R     | 9   | THR  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 11598 | 0        | 11664    | 1202    | 0            |
| 2   | B     | 9312  | 0        | 9200     | 1013    | 0            |
| 3   | C     | 2423  | 0        | 2412     | 138     | 0            |
| 4   | D     | 459   | 0        | 462      | 7       | 0            |
| 5   | E     | 1735  | 0        | 1764     | 34      | 0            |
| 6   | F     | 823   | 0        | 839      | 91      | 0            |
| 7   | G     | 1526  | 0        | 1534     | 158     | 0            |
| 8   | H     | 1052  | 0        | 1021     | 56      | 0            |
| 9   | I     | 755   | 0        | 728      | 106     | 0            |
| 10  | J     | 569   | 0        | 584      | 55      | 0            |
| 11  | K     | 793   | 0        | 790      | 54      | 0            |
| 12  | L     | 352   | 0        | 371      | 59      | 0            |
| 13  | M     | 856   | 0        | 852      | 60      | 0            |
| 14  | N     | 1151  | 0        | 1168     | 166     | 0            |
| 15  | O     | 3907  | 0        | 3902     | 417     | 0            |
| 16  | P     | 4729  | 0        | 4674     | 595     | 0            |
| 17  | Q     | 3421  | 0        | 3459     | 784     | 0            |
| 18  | R     | 2535  | 0        | 2598     | 621     | 0            |
| 19  | A     | 2     | 0        | 0        | 1       | 0            |
| 19  | B     | 1     | 0        | 0        | 0       | 0            |
| 19  | I     | 2     | 0        | 0        | 0       | 0            |
| 19  | J     | 1     | 0        | 0        | 0       | 0            |
| 19  | L     | 1     | 0        | 0        | 0       | 0            |
| 19  | Q     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 48004 | 0        | 48022    | 4131    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

All (4131) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:R:320:CYS:SG   | 18:R:374:LEU:HG   | 1.11                     | 1.67              |
| 1:A:995:TYR:CD2   | 2:B:708:ASP:HA    | 1.30                     | 1.64              |
| 17:Q:20:TRP:CZ3   | 17:Q:22:ILE:CG2   | 1.76                     | 1.64              |
| 17:Q:186:CYS:HA   | 18:R:208:TYR:CE1  | 1.31                     | 1.64              |
| 17:Q:326:TYR:CE1  | 17:Q:452:PHE:CE2  | 1.87                     | 1.63              |
| 16:P:724:LEU:HB3  | 17:Q:447:ALA:CB   | 1.28                     | 1.63              |
| 3:C:272:LYS:HA    | 14:N:175:TYR:CE1  | 1.16                     | 1.62              |
| 15:O:248:LEU:HD12 | 15:O:598:PHE:CD2  | 1.32                     | 1.61              |
| 17:Q:258:MET:HA   | 17:Q:442:LEU:CD1  | 1.23                     | 1.61              |
| 17:Q:326:TYR:CE1  | 17:Q:452:PHE:HE2  | 1.00                     | 1.60              |
| 17:Q:325:GLN:HG2  | 17:Q:452:PHE:CZ   | 1.37                     | 1.60              |
| 17:Q:12:THR:HG21  | 17:Q:33:HIS:CE1   | 1.12                     | 1.58              |
| 16:P:184:SER:CA   | 18:R:198:LEU:HD23 | 1.20                     | 1.57              |
| 1:A:545:SER:HB2   | 17:Q:34:VAL:CG2   | 1.14                     | 1.57              |
| 17:Q:258:MET:CE   | 17:Q:438:PHE:CE2  | 1.82                     | 1.57              |
| 17:Q:330:TRP:HE1  | 17:Q:449:GLN:CB   | 0.94                     | 1.57              |
| 6:F:72:LYS:HB3    | 6:F:142:SER:CA    | 1.30                     | 1.56              |
| 17:Q:258:MET:HE2  | 17:Q:438:PHE:CE2  | 1.33                     | 1.56              |
| 1:A:422:ARG:CA    | 18:R:409:HIS:HE1  | 1.10                     | 1.56              |
| 16:P:184:SER:HA   | 18:R:198:LEU:CD2  | 1.35                     | 1.56              |
| 16:P:724:LEU:CB   | 17:Q:447:ALA:HB2  | 1.09                     | 1.56              |
| 1:A:1484:LEU:HD13 | 2:B:305:ARG:CZ    | 1.24                     | 1.56              |
| 15:O:200:ASN:CG   | 17:Q:14:ASN:HB2   | 1.31                     | 1.56              |
| 7:G:143:SER:HB2   | 15:O:104:ILE:CG2  | 1.36                     | 1.55              |
| 17:Q:12:THR:CG2   | 17:Q:33:HIS:HE1   | 1.10                     | 1.55              |
| 1:A:990:ILE:CB    | 1:A:994:GLU:HB2   | 1.19                     | 1.55              |
| 1:A:1322:ILE:HG22 | 1:A:1454:HIS:CD2  | 1.37                     | 1.55              |
| 13:M:102:SER:HB3  | 13:M:105:SER:CB   | 1.28                     | 1.54              |
| 2:B:152:LEU:HB3   | 2:B:443:LYS:CE    | 1.34                     | 1.54              |
| 1:A:422:ARG:HA    | 18:R:409:HIS:CE1  | 1.04                     | 1.54              |
| 1:A:1575:ILE:CG1  | 9:I:122:ARG:NH1   | 1.68                     | 1.53              |
| 7:G:143:SER:CB    | 15:O:104:ILE:HG22 | 1.33                     | 1.53              |
| 17:Q:325:GLN:CG   | 17:Q:452:PHE:CE1  | 1.90                     | 1.53              |
| 15:O:200:ASN:CB   | 17:Q:14:ASN:HB2   | 1.07                     | 1.53              |
| 1:A:1049:MET:HG2  | 1:A:1052:GLY:C    | 1.30                     | 1.52              |
| 1:A:429:THR:CG2   | 18:R:406:LYS:HE3  | 1.37                     | 1.52              |
| 15:O:200:ASN:HB2  | 17:Q:14:ASN:CB    | 1.34                     | 1.52              |
| 1:A:547:ILE:CD1   | 17:Q:26:ARG:NH1   | 1.68                     | 1.51              |
| 1:A:990:ILE:HB    | 1:A:994:GLU:CB    | 1.06                     | 1.50              |
| 2:B:152:LEU:CB    | 2:B:443:LYS:HE3   | 1.37                     | 1.50              |
| 17:Q:352:ILE:HD11 | 17:Q:377:PHE:CD2  | 1.46                     | 1.50              |
| 15:O:248:LEU:HD12 | 15:O:598:PHE:CE2  | 0.97                     | 1.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:M:102:SER:CB   | 13:M:105:SER:HB3  | 1.13                     | 1.49              |
| 17:Q:352:ILE:CD1  | 17:Q:377:PHE:CD2  | 1.94                     | 1.49              |
| 2:B:207:ILE:HG13  | 2:B:503:VAL:CG2   | 1.41                     | 1.49              |
| 17:Q:258:MET:CA   | 17:Q:442:LEU:HD13 | 1.39                     | 1.48              |
| 3:C:253:PRO:HD2   | 14:N:180:PHE:CB   | 1.31                     | 1.48              |
| 3:C:272:LYS:CA    | 14:N:175:TYR:CE1  | 1.92                     | 1.48              |
| 15:O:248:LEU:CD1  | 15:O:598:PHE:CE2  | 1.93                     | 1.48              |
| 2:B:143:TRP:HB2   | 2:B:446:MET:CE    | 1.43                     | 1.47              |
| 15:O:248:LEU:CD1  | 15:O:598:PHE:CD2  | 1.92                     | 1.47              |
| 1:A:547:ILE:HD11  | 17:Q:26:ARG:NH1   | 1.18                     | 1.47              |
| 2:B:527:PHE:CZ    | 2:B:666:PRO:HA    | 1.49                     | 1.47              |
| 6:F:72:LYS:CD     | 6:F:142:SER:HB3   | 1.43                     | 1.47              |
| 2:B:679:GLN:CG    | 14:N:157:ARG:N    | 1.75                     | 1.46              |
| 1:A:545:SER:CB    | 17:Q:34:VAL:HG21  | 1.01                     | 1.46              |
| 2:B:1089:GLN:CG   | 2:B:1093:LEU:HD22 | 1.46                     | 1.46              |
| 2:B:527:PHE:CD1   | 2:B:666:PRO:HG3   | 1.47                     | 1.45              |
| 3:C:253:PRO:CD    | 14:N:180:PHE:HB3  | 1.09                     | 1.45              |
| 18:R:251:TRP:CE3  | 18:R:307:LYS:HE3  | 1.50                     | 1.45              |
| 1:A:878:ARG:HB3   | 9:I:67:VAL:CG1    | 1.47                     | 1.44              |
| 1:A:1297:PHE:CE2  | 1:A:1301:GLU:OE1  | 1.70                     | 1.44              |
| 7:G:141:SER:HB3   | 15:O:142:ILE:CD1  | 1.46                     | 1.43              |
| 1:A:1326:GLU:CD   | 1:A:1455:ARG:N    | 1.76                     | 1.43              |
| 2:B:679:GLN:CG    | 14:N:156:PRO:C    | 1.92                     | 1.43              |
| 2:B:68:ILE:HG21   | 2:B:71:LYS:NZ     | 1.32                     | 1.43              |
| 17:Q:325:GLN:NE2  | 17:Q:452:PHE:CE1  | 1.85                     | 1.43              |
| 1:A:597:LYS:HB2   | 2:B:1082:HIS:NE2  | 1.23                     | 1.43              |
| 2:B:848:ILE:CB    | 12:L:60:ARG:HD2   | 1.46                     | 1.43              |
| 3:C:58:ASN:HA     | 3:C:296:ASN:ND2   | 1.18                     | 1.43              |
| 1:A:756:LYS:CD    | 9:I:85:LYS:NZ     | 1.79                     | 1.43              |
| 1:A:429:THR:CG2   | 18:R:406:LYS:CE   | 1.94                     | 1.42              |
| 18:R:320:CYS:SG   | 18:R:374:LEU:CG   | 2.05                     | 1.42              |
| 1:A:629:ASP:C     | 2:B:926:VAL:HG21  | 1.42                     | 1.40              |
| 17:Q:20:TRP:HZ3   | 17:Q:22:ILE:CG2   | 1.10                     | 1.40              |
| 14:N:87:TYR:CA    | 14:N:141:GLU:HA   | 1.48                     | 1.40              |
| 15:O:240:ILE:HG22 | 15:O:380:SER:CB   | 1.48                     | 1.40              |
| 18:R:251:TRP:CE3  | 18:R:307:LYS:CE   | 2.01                     | 1.40              |
| 2:B:207:ILE:CG1   | 2:B:503:VAL:HG21  | 1.49                     | 1.40              |
| 17:Q:326:TYR:CZ   | 17:Q:452:PHE:HE2  | 1.37                     | 1.40              |
| 6:F:72:LYS:CB     | 6:F:142:SER:HA    | 1.50                     | 1.39              |
| 17:Q:325:GLN:CG   | 17:Q:452:PHE:CZ   | 2.00                     | 1.38              |
| 1:A:547:ILE:HD12  | 17:Q:26:ARG:CZ    | 1.53                     | 1.38              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1322:ILE:HD12 | 1:A:1457:ILE:CD1  | 1.53                     | 1.38              |
| 2:B:143:TRP:CE3   | 2:B:446:MET:HG3   | 1.57                     | 1.37              |
| 1:A:422:ARG:NH2   | 18:R:412:ARG:NH1  | 1.71                     | 1.37              |
| 1:A:597:LYS:HB2   | 2:B:1082:HIS:CD2  | 1.58                     | 1.37              |
| 1:A:999:CYS:HA    | 2:B:712:SER:CB    | 1.54                     | 1.37              |
| 17:Q:197:GLU:OE2  | 17:Q:387:PRO:C    | 1.68                     | 1.37              |
| 1:A:545:SER:CB    | 17:Q:34:VAL:CG2   | 1.77                     | 1.36              |
| 6:F:74:ILE:O      | 7:G:95:LEU:CD1    | 1.69                     | 1.36              |
| 2:B:322:ASN:ND2   | 13:M:108:LEU:O    | 1.57                     | 1.36              |
| 2:B:796:ARG:NE    | 10:J:8:PHE:O      | 1.58                     | 1.36              |
| 17:Q:187:THR:C    | 17:Q:380:TRP:HZ2  | 1.27                     | 1.36              |
| 1:A:1482:LYS:CE   | 2:B:304:ASP:OD1   | 1.74                     | 1.35              |
| 7:G:159:LYS:N     | 15:O:105:ASN:ND2  | 1.70                     | 1.35              |
| 3:C:272:LYS:HA    | 14:N:175:TYR:CZ   | 1.51                     | 1.35              |
| 17:Q:261:ALA:CB   | 17:Q:445:ARG:HB2  | 1.57                     | 1.35              |
| 1:A:422:ARG:HH22  | 18:R:412:ARG:CZ   | 1.13                     | 1.35              |
| 7:G:159:LYS:H     | 15:O:105:ASN:ND2  | 0.91                     | 1.35              |
| 7:G:141:SER:CB    | 15:O:142:ILE:HD12 | 1.54                     | 1.34              |
| 17:Q:351:ASN:HB3  | 17:Q:369:TRP:CH2  | 1.61                     | 1.34              |
| 1:A:1322:ILE:CG2  | 1:A:1454:HIS:CG   | 2.08                     | 1.34              |
| 2:B:143:TRP:CG    | 2:B:446:MET:SD    | 2.21                     | 1.34              |
| 7:G:24:VAL:O      | 7:G:128:GLN:HB2   | 1.17                     | 1.34              |
| 1:A:1297:PHE:CD2  | 1:A:1301:GLU:OE1  | 1.81                     | 1.34              |
| 2:B:743:ARG:NH2   | 10:J:60:PHE:CZ    | 1.96                     | 1.34              |
| 2:B:848:ILE:HB    | 12:L:60:ARG:CD    | 1.56                     | 1.34              |
| 2:B:890:ASP:O     | 12:L:54:ARG:HD3   | 1.24                     | 1.34              |
| 1:A:1322:ILE:HG22 | 1:A:1454:HIS:CG   | 1.62                     | 1.33              |
| 17:Q:326:TYR:CZ   | 17:Q:452:PHE:CE2  | 2.10                     | 1.33              |
| 17:Q:355:VAL:HG13 | 18:R:215:THR:OG1  | 1.19                     | 1.32              |
| 17:Q:194:GLN:CD   | 18:R:209:ARG:HH11 | 1.35                     | 1.32              |
| 2:B:68:ILE:CG2    | 2:B:71:LYS:NZ     | 1.91                     | 1.32              |
| 3:C:272:LYS:HA    | 14:N:175:TYR:CD1  | 1.63                     | 1.32              |
| 17:Q:367:PHE:HE1  | 18:R:1:MET:N      | 1.28                     | 1.32              |
| 7:G:159:LYS:CB    | 15:O:105:ASN:HD22 | 1.43                     | 1.31              |
| 18:R:15:GLN:OE1   | 18:R:184:ASN:ND2  | 1.63                     | 1.31              |
| 1:A:503:VAL:HA    | 1:A:580:HIS:CD2   | 1.61                     | 1.31              |
| 1:A:1276:THR:OG1  | 9:I:45:LEU:CD1    | 1.79                     | 1.31              |
| 7:G:141:SER:CB    | 15:O:142:ILE:CD1  | 2.06                     | 1.31              |
| 16:P:198:ASP:CB   | 16:P:205:TYR:O    | 1.79                     | 1.30              |
| 1:A:535:GLN:NE2   | 17:Q:26:ARG:HD3   | 1.43                     | 1.30              |
| 2:B:1072:GLY:C    | 2:B:1075:GLU:HG2  | 1.55                     | 1.30              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:337:SER:CB   | 17:Q:448:LYS:HE2  | 1.58                     | 1.30              |
| 18:R:177:LEU:O    | 18:R:185:LYS:HE2  | 1.13                     | 1.30              |
| 1:A:995:TYR:OH    | 2:B:707:SER:CB    | 1.79                     | 1.30              |
| 18:R:199:LYS:HE2  | 18:R:204:GLU:CA   | 1.62                     | 1.30              |
| 2:B:549:CYS:SG    | 2:B:649:MET:HG2   | 1.70                     | 1.30              |
| 17:Q:197:GLU:CG   | 17:Q:388:THR:O    | 1.79                     | 1.30              |
| 17:Q:325:GLN:CD   | 17:Q:452:PHE:CZ   | 2.09                     | 1.30              |
| 17:Q:413:LEU:HD21 | 18:R:273:TRP:CZ2  | 1.66                     | 1.30              |
| 1:A:756:LYS:HD3   | 9:I:85:LYS:NZ     | 0.98                     | 1.30              |
| 1:A:990:ILE:HA    | 1:A:994:GLU:OE1   | 1.30                     | 1.30              |
| 1:A:547:ILE:HD12  | 17:Q:26:ARG:NH2   | 1.45                     | 1.29              |
| 2:B:143:TRP:CD2   | 2:B:446:MET:HG3   | 1.65                     | 1.29              |
| 15:O:234:ILE:CG2  | 15:O:237:ILE:HG12 | 1.41                     | 1.29              |
| 1:A:1326:GLU:OE2  | 1:A:1455:ARG:N    | 1.60                     | 1.29              |
| 2:B:527:PHE:CZ    | 2:B:666:PRO:CA    | 2.13                     | 1.29              |
| 17:Q:20:TRP:CZ3   | 17:Q:22:ILE:HG23  | 1.48                     | 1.29              |
| 2:B:19:LEU:CD1    | 10:J:26:GLN:OE1   | 1.78                     | 1.29              |
| 2:B:679:GLN:HG2   | 14:N:157:ARG:N    | 0.96                     | 1.29              |
| 16:P:198:ASP:HB2  | 16:P:205:TYR:O    | 1.27                     | 1.29              |
| 15:O:200:ASN:CB   | 17:Q:14:ASN:CB    | 1.95                     | 1.29              |
| 1:A:990:ILE:HG13  | 1:A:995:TYR:N     | 1.47                     | 1.28              |
| 16:P:184:SER:CA   | 18:R:198:LEU:CD2  | 1.98                     | 1.28              |
| 2:B:682:GLN:C     | 14:N:154:ARG:NH2  | 1.91                     | 1.28              |
| 17:Q:26:ARG:HB3   | 17:Q:34:VAL:CG1   | 1.61                     | 1.28              |
| 2:B:75:ASP:HB3    | 2:B:440:PHE:CE2   | 1.67                     | 1.28              |
| 2:B:207:ILE:CG1   | 2:B:503:VAL:CG2   | 2.07                     | 1.28              |
| 2:B:682:GLN:C     | 14:N:154:ARG:HH21 | 1.37                     | 1.28              |
| 13:M:102:SER:O    | 13:M:106:LYS:N    | 1.66                     | 1.28              |
| 1:A:1299:ASN:OD1  | 1:A:1467:GLY:CA   | 1.70                     | 1.27              |
| 1:A:1326:GLU:CD   | 1:A:1454:HIS:HB3  | 1.57                     | 1.27              |
| 2:B:527:PHE:CE1   | 2:B:666:PRO:HG3   | 1.69                     | 1.27              |
| 1:A:429:THR:HG21  | 18:R:406:LYS:CD   | 1.62                     | 1.27              |
| 1:A:1276:THR:OG1  | 9:I:45:LEU:HD12   | 1.22                     | 1.27              |
| 2:B:1003:ALA:O    | 14:N:170:HIS:N    | 1.66                     | 1.27              |
| 14:N:86:ASP:C     | 14:N:141:GLU:HG3  | 1.58                     | 1.27              |
| 17:Q:325:GLN:HG2  | 17:Q:452:PHE:CE1  | 1.58                     | 1.27              |
| 2:B:682:GLN:CA    | 14:N:154:ARG:HH21 | 1.46                     | 1.27              |
| 3:C:253:PRO:HD2   | 14:N:180:PHE:CG   | 1.68                     | 1.27              |
| 15:O:200:ASN:CG   | 17:Q:14:ASN:CB    | 2.05                     | 1.26              |
| 18:R:199:LYS:HE2  | 18:R:204:GLU:CB   | 1.64                     | 1.26              |
| 2:B:1002:LYS:HD3  | 14:N:166:LEU:O    | 1.16                     | 1.26              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:475:ARG:NH2  | 17:Q:364:SER:OG   | 1.68                     | 1.26              |
| 16:P:436:ILE:CD1  | 18:R:143:THR:HG23 | 1.65                     | 1.26              |
| 16:P:724:LEU:CB   | 17:Q:447:ALA:CB   | 1.93                     | 1.26              |
| 1:A:1330:VAL:HG21 | 1:A:1455:ARG:CZ   | 1.66                     | 1.26              |
| 2:B:19:LEU:HD13   | 10:J:26:GLN:OE1   | 1.30                     | 1.25              |
| 2:B:683:ASN:N     | 14:N:154:ARG:NH2  | 1.84                     | 1.25              |
| 17:Q:257:VAL:CG1  | 17:Q:446:TYR:OH   | 1.84                     | 1.25              |
| 2:B:143:TRP:CB    | 2:B:446:MET:CE    | 2.13                     | 1.25              |
| 7:G:159:LYS:HD2   | 15:O:103:ASN:OD1  | 1.08                     | 1.25              |
| 15:O:376:TYR:CE2  | 15:O:377:TYR:CE2  | 2.24                     | 1.25              |
| 17:Q:187:THR:C    | 17:Q:380:TRP:CZ2  | 1.97                     | 1.25              |
| 17:Q:187:THR:HA   | 17:Q:380:TRP:CZ2  | 1.71                     | 1.25              |
| 2:B:1072:GLY:O    | 2:B:1075:GLU:HG2  | 1.26                     | 1.25              |
| 17:Q:194:GLN:NE2  | 18:R:209:ARG:HE   | 1.31                     | 1.25              |
| 1:A:435:ASN:HB3   | 1:A:442:LYS:CB    | 1.64                     | 1.25              |
| 1:A:878:ARG:CG    | 9:I:66:VAL:HG23   | 1.65                     | 1.25              |
| 18:R:199:LYS:CE   | 18:R:204:GLU:HB3  | 1.65                     | 1.24              |
| 1:A:1603:MET:HE2  | 1:A:1615:TYR:CD2  | 1.73                     | 1.24              |
| 2:B:1089:GLN:HG3  | 2:B:1093:LEU:CG   | 1.66                     | 1.24              |
| 1:A:1322:ILE:CG2  | 1:A:1454:HIS:CD2  | 2.18                     | 1.24              |
| 16:P:725:VAL:HA   | 17:Q:450:THR:CB   | 1.67                     | 1.24              |
| 17:Q:258:MET:CE   | 17:Q:438:PHE:CD2  | 2.21                     | 1.24              |
| 17:Q:325:GLN:CD   | 17:Q:452:PHE:CE1  | 2.15                     | 1.24              |
| 1:A:478:TYR:HA    | 2:B:1048:SER:O    | 1.38                     | 1.24              |
| 1:A:1180:ASN:OD1  | 6:F:87:LYS:HD3    | 1.33                     | 1.24              |
| 14:N:86:ASP:O     | 14:N:141:GLU:HG3  | 1.36                     | 1.24              |
| 16:P:184:SER:CB   | 18:R:198:LEU:CD2  | 2.15                     | 1.24              |
| 17:Q:12:THR:CG2   | 17:Q:33:HIS:CE1   | 1.95                     | 1.24              |
| 17:Q:187:THR:CA   | 17:Q:380:TRP:CZ2  | 2.21                     | 1.23              |
| 17:Q:352:ILE:CD1  | 17:Q:377:PHE:HD2  | 1.39                     | 1.23              |
| 1:A:547:ILE:CD1   | 17:Q:26:ARG:CZ    | 2.08                     | 1.23              |
| 1:A:1484:LEU:CD1  | 2:B:305:ARG:CZ    | 2.17                     | 1.23              |
| 7:G:144:HIS:CG    | 15:O:146:SER:OG   | 1.92                     | 1.23              |
| 1:A:458:GLN:O     | 1:A:462:LYS:HB2   | 1.36                     | 1.22              |
| 14:N:87:TYR:HA    | 14:N:141:GLU:CA   | 1.69                     | 1.22              |
| 17:Q:194:GLN:CG   | 18:R:209:ARG:HH11 | 1.51                     | 1.22              |
| 17:Q:351:ASN:CB   | 17:Q:369:TRP:CH2  | 2.20                     | 1.22              |
| 1:A:1326:GLU:OE2  | 1:A:1454:HIS:HB3  | 1.26                     | 1.22              |
| 18:R:201:SER:O    | 18:R:205:VAL:HG23 | 1.35                     | 1.22              |
| 1:A:403:LEU:HD11  | 1:A:419:ILE:CG2   | 1.68                     | 1.22              |
| 1:A:1575:ILE:HG13 | 9:I:122:ARG:CZ    | 1.70                     | 1.21              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:991:LYS:CB    | 1:A:993:GLN:HB2   | 1.71                     | 1.21              |
| 1:A:1329:ILE:HG21 | 1:A:1456:PHE:CE2  | 1.75                     | 1.21              |
| 2:B:1072:GLY:N    | 2:B:1075:GLU:CG   | 2.04                     | 1.21              |
| 13:M:61:GLU:OE2   | 13:M:106:LYS:CD   | 1.88                     | 1.21              |
| 14:N:86:ASP:O     | 14:N:141:GLU:CG   | 1.88                     | 1.21              |
| 15:O:374:PRO:C    | 15:O:376:TYR:HB3  | 1.64                     | 1.21              |
| 18:R:207:ASN:O    | 18:R:211:ARG:HB2  | 1.34                     | 1.21              |
| 1:A:991:LYS:N     | 1:A:994:GLU:HG3   | 1.54                     | 1.21              |
| 6:F:72:LYS:HD2    | 6:F:142:SER:CB    | 1.69                     | 1.21              |
| 1:A:1322:ILE:HG21 | 1:A:1454:HIS:ND1  | 1.54                     | 1.20              |
| 17:Q:355:VAL:CG1  | 18:R:215:THR:OG1  | 1.88                     | 1.20              |
| 18:R:199:LYS:HE3  | 18:R:203:SER:O    | 1.41                     | 1.20              |
| 1:A:474:LYS:NZ    | 2:B:1096:SER:OG   | 1.74                     | 1.20              |
| 1:A:429:THR:HG22  | 18:R:406:LYS:CE   | 1.62                     | 1.20              |
| 1:A:566:SER:CB    | 15:O:235:GLU:CD   | 2.15                     | 1.20              |
| 1:A:995:TYR:CD2   | 2:B:708:ASP:CA    | 2.23                     | 1.20              |
| 17:Q:371:GLU:HG3  | 18:R:231:LEU:CD1  | 1.71                     | 1.20              |
| 2:B:182:GLN:NE2   | 10:J:69:ARG:HB3   | 1.55                     | 1.20              |
| 2:B:683:ASN:N     | 14:N:154:ARG:HH22 | 1.37                     | 1.20              |
| 3:C:253:PRO:O     | 14:N:179:ASP:O    | 1.58                     | 1.20              |
| 16:P:498:LEU:HD21 | 17:Q:368:GLN:NE2  | 1.57                     | 1.19              |
| 1:A:545:SER:CA    | 17:Q:34:VAL:HG21  | 1.70                     | 1.19              |
| 1:A:1003:ARG:NH2  | 2:B:530:PRO:O     | 1.74                     | 1.19              |
| 2:B:679:GLN:HG3   | 14:N:156:PRO:C    | 1.55                     | 1.19              |
| 17:Q:258:MET:HE1  | 17:Q:438:PHE:CD2  | 1.74                     | 1.19              |
| 17:Q:356:VAL:HG12 | 18:R:211:ARG:CB   | 1.71                     | 1.19              |
| 1:A:474:LYS:NZ    | 2:B:1092:LEU:HD23 | 1.55                     | 1.19              |
| 2:B:943:ILE:HD12  | 10:J:44:TYR:CZ    | 1.78                     | 1.19              |
| 18:R:248:LYS:CG   | 18:R:298:GLN:HE22 | 1.54                     | 1.19              |
| 17:Q:186:CYS:CA   | 18:R:208:TYR:HE1  | 1.54                     | 1.19              |
| 17:Q:343:THR:OG1  | 17:Q:372:GLU:OE1  | 1.61                     | 1.19              |
| 1:A:1326:GLU:OE2  | 1:A:1454:HIS:CB   | 1.90                     | 1.18              |
| 2:B:566:TYR:HD2   | 13:M:73:SER:OG    | 1.23                     | 1.18              |
| 3:C:274:THR:CA    | 14:N:172:ALA:HB2  | 1.71                     | 1.18              |
| 16:P:184:SER:HB3  | 18:R:198:LEU:CG   | 1.71                     | 1.18              |
| 17:Q:188:ALA:O    | 17:Q:384:GLN:HG3  | 1.43                     | 1.18              |
| 1:A:474:LYS:CE    | 2:B:1092:LEU:HD23 | 1.73                     | 1.18              |
| 1:A:1314:GLN:NE2  | 1:A:1446:ARG:NH1  | 1.89                     | 1.18              |
| 3:C:296:ASN:O     | 3:C:298:PHE:CD1   | 1.94                     | 1.18              |
| 17:Q:337:SER:HB3  | 17:Q:448:LYS:CE   | 1.72                     | 1.18              |
| 1:A:422:ARG:CA    | 18:R:409:HIS:CE1  | 1.97                     | 1.18              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:435:ASN:O     | 1:A:439:ASP:O     | 1.61                     | 1.18              |
| 1:A:436:ALA:O     | 1:A:440:SER:N     | 1.77                     | 1.18              |
| 2:B:207:ILE:CD1   | 2:B:503:VAL:HG21  | 1.72                     | 1.18              |
| 2:B:894:LYS:HD3   | 12:L:47:ARG:CZ    | 1.74                     | 1.18              |
| 1:A:438:ILE:O     | 1:A:457:LYS:HD2   | 1.42                     | 1.18              |
| 1:A:1650:GLY:O    | 1:A:1652:GLY:N    | 1.73                     | 1.18              |
| 2:B:1120:ILE:HD12 | 15:O:117:GLN:NE2  | 1.58                     | 1.18              |
| 18:R:207:ASN:O    | 18:R:211:ARG:N    | 1.76                     | 1.18              |
| 1:A:477:ASN:O     | 2:B:1047:ARG:HD3  | 1.43                     | 1.18              |
| 1:A:1050:TYR:CZ   | 1:A:1179:ILE:HG12 | 1.79                     | 1.18              |
| 1:A:1313:LEU:HG   | 1:A:1462:PHE:CE1  | 1.79                     | 1.18              |
| 3:C:58:ASN:CA     | 3:C:296:ASN:ND2   | 2.06                     | 1.18              |
| 1:A:1322:ILE:HB   | 1:A:1454:HIS:CE1  | 1.79                     | 1.17              |
| 6:F:72:LYS:CA     | 6:F:142:SER:HB2   | 1.75                     | 1.17              |
| 7:G:24:VAL:O      | 7:G:128:GLN:CB    | 1.91                     | 1.17              |
| 7:G:241:ARG:HH11  | 15:O:189:PHE:CB   | 1.55                     | 1.17              |
| 17:Q:194:GLN:HG3  | 18:R:209:ARG:NH1  | 1.57                     | 1.17              |
| 1:A:878:ARG:CD    | 9:I:66:VAL:CG2    | 2.21                     | 1.17              |
| 1:A:1657:LEU:HD22 | 7:G:104:LEU:CD1   | 1.74                     | 1.17              |
| 1:A:1657:LEU:O    | 6:F:133:VAL:N     | 1.76                     | 1.17              |
| 2:B:145:VAL:HG11  | 2:B:441:LYS:HG2   | 1.24                     | 1.17              |
| 2:B:679:GLN:HG3   | 14:N:156:PRO:CA   | 1.75                     | 1.17              |
| 2:B:849:GLY:CA    | 12:L:60:ARG:HH22  | 1.57                     | 1.17              |
| 15:O:247:GLU:OE1  | 15:O:325:ILE:CG1  | 1.85                     | 1.17              |
| 15:O:200:ASN:HB2  | 17:Q:14:ASN:CA    | 1.73                     | 1.16              |
| 17:Q:186:CYS:HA   | 18:R:208:TYR:CZ   | 1.80                     | 1.16              |
| 1:A:422:ARG:HD3   | 18:R:409:HIS:ND1  | 1.58                     | 1.16              |
| 1:A:878:ARG:CG    | 9:I:67:VAL:HG13   | 1.73                     | 1.16              |
| 2:B:143:TRP:CD2   | 2:B:446:MET:CG    | 2.26                     | 1.16              |
| 3:C:274:THR:HA    | 14:N:172:ALA:CB   | 1.75                     | 1.16              |
| 6:F:72:LYS:HA     | 6:F:142:SER:HB2   | 1.21                     | 1.16              |
| 16:P:350:THR:HG21 | 18:R:156:LYS:H    | 1.03                     | 1.16              |
| 3:C:230:LEU:HD12  | 3:C:231:PRO:HD2   | 1.22                     | 1.16              |
| 15:O:234:ILE:HG22 | 15:O:237:ILE:HG12 | 1.25                     | 1.16              |
| 2:B:985:ILE:O     | 14:N:160:VAL:HG23 | 1.46                     | 1.16              |
| 7:G:141:SER:HB2   | 15:O:142:ILE:HD12 | 1.20                     | 1.16              |
| 17:Q:257:VAL:HG12 | 17:Q:446:TYR:OH   | 1.38                     | 1.16              |
| 1:A:953:GLU:HA    | 1:A:1205:PHE:CD2  | 1.81                     | 1.15              |
| 1:A:1049:MET:CG   | 1:A:1052:GLY:C    | 2.18                     | 1.15              |
| 1:A:422:ARG:NH2   | 18:R:412:ARG:CZ   | 1.78                     | 1.15              |
| 18:R:251:TRP:CZ3  | 18:R:307:LYS:HE2  | 1.80                     | 1.15              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:266:LYS:HE3   | 2:B:473:GLN:O     | 1.46                     | 1.15              |
| 7:G:159:LYS:HD2   | 15:O:103:ASN:CG   | 1.72                     | 1.15              |
| 1:A:991:LYS:H     | 1:A:994:GLU:CG    | 1.60                     | 1.15              |
| 2:B:1093:LEU:HG   | 2:B:1094:ASN:OD1  | 1.45                     | 1.15              |
| 17:Q:194:GLN:CG   | 18:R:209:ARG:NH1  | 2.09                     | 1.15              |
| 17:Q:198:ILE:HB   | 17:Q:390:THR:N    | 1.61                     | 1.15              |
| 17:Q:352:ILE:HD12 | 17:Q:377:PHE:CE2  | 1.80                     | 1.15              |
| 2:B:152:LEU:HD22  | 2:B:443:LYS:HD2   | 1.24                     | 1.14              |
| 17:Q:186:CYS:CA   | 18:R:208:TYR:CE1  | 2.26                     | 1.14              |
| 2:B:1089:GLN:CG   | 2:B:1093:LEU:CD2  | 2.24                     | 1.14              |
| 16:P:498:LEU:CD2  | 17:Q:368:GLN:HE21 | 1.61                     | 1.14              |
| 17:Q:22:ILE:CD1   | 17:Q:24:ASP:OD2   | 1.96                     | 1.14              |
| 1:A:403:LEU:CD1   | 1:A:419:ILE:HG21  | 1.78                     | 1.14              |
| 1:A:474:LYS:HZ2   | 2:B:1092:LEU:HA   | 1.10                     | 1.14              |
| 1:A:547:ILE:CD1   | 17:Q:26:ARG:NH2   | 2.07                     | 1.14              |
| 1:A:566:SER:CB    | 15:O:235:GLU:OE2  | 1.96                     | 1.14              |
| 1:A:1326:GLU:OE1  | 1:A:1454:HIS:HA   | 1.45                     | 1.14              |
| 2:B:1072:GLY:N    | 2:B:1075:GLU:HG3  | 1.59                     | 1.14              |
| 1:A:438:ILE:O     | 1:A:457:LYS:CD    | 1.94                     | 1.14              |
| 1:A:990:ILE:CA    | 1:A:994:GLU:HB2   | 1.78                     | 1.14              |
| 1:A:1329:ILE:CG2  | 1:A:1456:PHE:CE2  | 2.31                     | 1.14              |
| 2:B:149:GLU:OE1   | 2:B:441:LYS:NZ    | 1.80                     | 1.14              |
| 17:Q:134:LYS:O    | 17:Q:138:LEU:HB2  | 1.47                     | 1.14              |
| 17:Q:189:LYS:HA   | 17:Q:384:GLN:HE21 | 0.96                     | 1.13              |
| 17:Q:330:TRP:NE1  | 17:Q:449:GLN:HB2  | 0.82                     | 1.13              |
| 17:Q:367:PHE:CE1  | 18:R:1:MET:N      | 2.15                     | 1.13              |
| 1:A:425:ASN:ND2   | 18:R:405:ILE:HG22 | 1.62                     | 1.13              |
| 16:P:724:LEU:HB3  | 17:Q:447:ALA:HB1  | 1.18                     | 1.13              |
| 17:Q:258:MET:HA   | 17:Q:442:LEU:HD11 | 1.30                     | 1.13              |
| 2:B:894:LYS:HD3   | 12:L:47:ARG:NE    | 1.63                     | 1.13              |
| 2:B:143:TRP:HB2   | 2:B:446:MET:HE3   | 1.18                     | 1.13              |
| 3:C:334:THR:HG21  | 11:K:44:ARG:HB3   | 1.30                     | 1.13              |
| 15:O:240:ILE:CG2  | 15:O:380:SER:HB3  | 1.77                     | 1.13              |
| 17:Q:337:SER:CB   | 17:Q:448:LYS:CE   | 2.26                     | 1.13              |
| 2:B:266:LYS:HG3   | 2:B:473:GLN:O     | 1.45                     | 1.13              |
| 15:O:376:TYR:CZ   | 15:O:377:TYR:CE2  | 2.37                     | 1.13              |
| 18:R:248:LYS:CG   | 18:R:298:GLN:NE2  | 2.12                     | 1.13              |
| 1:A:1276:THR:N    | 9:I:45:LEU:O      | 1.80                     | 1.12              |
| 1:A:1556:GLU:OE2  | 5:E:212:ARG:NH1   | 1.82                     | 1.12              |
| 7:G:241:ARG:HH11  | 15:O:189:PHE:HB2  | 1.10                     | 1.12              |
| 18:R:248:LYS:HG2  | 18:R:298:GLN:NE2  | 1.62                     | 1.12              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:435:ASN:O     | 1:A:439:ASP:HB3   | 1.50                     | 1.12              |
| 1:A:506:THR:HG22  | 1:A:579:ARG:C     | 1.74                     | 1.12              |
| 1:A:878:ARG:CB    | 9:I:67:VAL:CG1    | 2.27                     | 1.12              |
| 1:A:1482:LYS:HE2  | 2:B:304:ASP:OD1   | 0.96                     | 1.12              |
| 2:B:1072:GLY:H    | 2:B:1075:GLU:CG   | 1.59                     | 1.12              |
| 17:Q:330:TRP:CD1  | 17:Q:449:GLN:HB2  | 1.84                     | 1.12              |
| 17:Q:352:ILE:CD1  | 17:Q:377:PHE:CE2  | 2.31                     | 1.12              |
| 17:Q:418:PRO:HG3  | 18:R:264:SER:OG   | 1.48                     | 1.12              |
| 1:A:1657:LEU:HD22 | 7:G:104:LEU:HD13  | 1.14                     | 1.12              |
| 14:N:87:TYR:CZ    | 14:N:141:GLU:OE1  | 2.01                     | 1.12              |
| 17:Q:258:MET:CA   | 17:Q:442:LEU:CD1  | 2.09                     | 1.12              |
| 1:A:474:LYS:NZ    | 2:B:1092:LEU:CD2  | 2.12                     | 1.12              |
| 1:A:1299:ASN:OD1  | 1:A:1467:GLY:HA3  | 1.39                     | 1.12              |
| 1:A:1600:ARG:NH2  | 1:A:1617:THR:OG1  | 1.83                     | 1.12              |
| 13:M:61:GLU:OE2   | 13:M:106:LYS:HD3  | 1.44                     | 1.12              |
| 17:Q:378:LEU:HD23 | 18:R:216:LEU:HD21 | 1.20                     | 1.12              |
| 18:R:5:PRO:HG2    | 18:R:217:THR:HG21 | 1.16                     | 1.12              |
| 16:P:354:PRO:HB2  | 18:R:27:ILE:HG22  | 1.24                     | 1.12              |
| 18:R:199:LYS:HE2  | 18:R:204:GLU:HB3  | 1.22                     | 1.12              |
| 1:A:472:MET:HB3   | 2:B:1073:GLU:CB   | 1.80                     | 1.11              |
| 1:A:954:GLY:HA3   | 1:A:1205:PHE:HB3  | 1.27                     | 1.11              |
| 1:A:1326:GLU:OE2  | 1:A:1454:HIS:C    | 1.93                     | 1.11              |
| 2:B:849:GLY:C     | 12:L:60:ARG:HH22  | 1.58                     | 1.11              |
| 3:C:272:LYS:CA    | 14:N:175:TYR:CZ   | 2.16                     | 1.11              |
| 7:G:143:SER:O     | 15:O:105:ASN:ND2  | 1.82                     | 1.11              |
| 15:O:579:LEU:HA   | 15:O:582:ARG:HB3  | 1.24                     | 1.11              |
| 18:R:317:LEU:HD12 | 18:R:367:ILE:HD13 | 1.30                     | 1.11              |
| 1:A:878:ARG:HB3   | 9:I:67:VAL:HG11   | 1.16                     | 1.11              |
| 2:B:894:LYS:CG    | 12:L:54:ARG:HH22  | 1.52                     | 1.11              |
| 16:P:724:LEU:O    | 17:Q:450:THR:CB   | 1.98                     | 1.11              |
| 17:Q:20:TRP:CZ3   | 17:Q:22:ILE:HG22  | 1.58                     | 1.11              |
| 6:F:72:LYS:CD     | 6:F:142:SER:CB    | 2.28                     | 1.11              |
| 16:P:475:ARG:HD3  | 17:Q:367:PHE:CE2  | 1.83                     | 1.11              |
| 17:Q:197:GLU:HG3  | 17:Q:388:THR:O    | 1.48                     | 1.11              |
| 18:R:5:PRO:CG     | 18:R:217:THR:HG21 | 1.79                     | 1.11              |
| 1:A:952:LEU:HD22  | 1:A:1004:GLU:HG3  | 1.15                     | 1.11              |
| 1:A:503:VAL:HG23  | 1:A:530:TRP:HB2   | 1.29                     | 1.10              |
| 2:B:143:TRP:HB2   | 2:B:446:MET:HE1   | 1.31                     | 1.10              |
| 16:P:436:ILE:HD12 | 18:R:143:THR:CG2  | 1.81                     | 1.10              |
| 1:A:474:LYS:HE3   | 2:B:1092:LEU:CD2  | 1.80                     | 1.10              |
| 1:A:474:LYS:O     | 2:B:1070:ARG:CB   | 2.00                     | 1.10              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1049:MET:HG2  | 1:A:1053:ASP:N    | 1.66                     | 1.10              |
| 1:A:1314:GLN:NE2  | 1:A:1446:ARG:HD2  | 1.67                     | 1.10              |
| 17:Q:356:VAL:HA   | 18:R:211:ARG:HG2  | 1.30                     | 1.10              |
| 2:B:1003:ALA:HA   | 14:N:169:GLU:H    | 1.04                     | 1.10              |
| 1:A:995:TYR:HD2   | 2:B:708:ASP:CA    | 1.60                     | 1.10              |
| 1:A:1310:LYS:HG2  | 1:A:1311:GLU:CD   | 1.77                     | 1.10              |
| 1:A:1482:LYS:O    | 2:B:308:LEU:HD21  | 1.50                     | 1.10              |
| 2:B:985:ILE:HB    | 14:N:160:VAL:CG2  | 1.82                     | 1.10              |
| 16:P:498:LEU:HD21 | 17:Q:368:GLN:HE21 | 0.99                     | 1.10              |
| 16:P:704:LEU:HD13 | 17:Q:439:ILE:HG12 | 1.14                     | 1.10              |
| 1:A:545:SER:H     | 17:Q:34:VAL:HG23  | 1.08                     | 1.09              |
| 1:A:999:CYS:HA    | 2:B:712:SER:HB2   | 1.32                     | 1.09              |
| 2:B:527:PHE:CE1   | 2:B:666:PRO:CG    | 2.35                     | 1.09              |
| 2:B:894:LYS:CG    | 12:L:54:ARG:NH2   | 1.92                     | 1.09              |
| 15:O:373:LEU:O    | 15:O:376:TYR:HB2  | 1.51                     | 1.09              |
| 17:Q:356:VAL:CG1  | 18:R:211:ARG:HB3  | 1.81                     | 1.09              |
| 1:A:566:SER:HB2   | 15:O:235:GLU:CD   | 1.77                     | 1.09              |
| 1:A:990:ILE:HD11  | 1:A:995:TYR:HA    | 1.24                     | 1.09              |
| 15:O:248:LEU:HD11 | 15:O:598:PHE:HD2  | 1.05                     | 1.09              |
| 2:B:1002:LYS:CD   | 14:N:166:LEU:O    | 1.99                     | 1.09              |
| 16:P:501:PRO:HB3  | 16:P:567:ILE:CG2  | 1.81                     | 1.09              |
| 17:Q:348:ILE:HD11 | 17:Q:373:GLU:HA   | 1.14                     | 1.09              |
| 1:A:476:VAL:HG22  | 2:B:1070:ARG:H    | 1.15                     | 1.09              |
| 2:B:943:ILE:HD12  | 10:J:44:TYR:CE1   | 1.88                     | 1.09              |
| 1:A:395:LEU:HD11  | 18:R:410:TYR:CE1  | 1.88                     | 1.09              |
| 1:A:475:ARG:CZ    | 2:B:1061:LYS:HB2  | 1.81                     | 1.09              |
| 1:A:824:THR:HB    | 2:B:1023:ARG:HB2  | 1.22                     | 1.09              |
| 1:A:1575:ILE:N    | 9:I:122:ARG:NH1   | 2.00                     | 1.08              |
| 2:B:1089:GLN:HG3  | 2:B:1093:LEU:CB   | 1.83                     | 1.08              |
| 1:A:564:PRO:HG2   | 15:O:370:THR:O    | 1.53                     | 1.08              |
| 2:B:551:ILE:HG21  | 2:B:647:SER:HA    | 1.29                     | 1.08              |
| 3:C:272:LYS:HG2   | 14:N:175:TYR:CD1  | 1.88                     | 1.08              |
| 16:P:436:ILE:HD12 | 18:R:143:THR:HG23 | 1.17                     | 1.08              |
| 16:P:622:TYR:O    | 16:P:626:LEU:HB2  | 1.53                     | 1.08              |
| 17:Q:418:PRO:HG2  | 18:R:233:TYR:OH   | 1.53                     | 1.08              |
| 18:R:5:PRO:HG2    | 18:R:217:THR:CG2  | 1.84                     | 1.08              |
| 1:A:1003:ARG:HH21 | 2:B:530:PRO:C     | 1.61                     | 1.08              |
| 2:B:894:LYS:HG3   | 12:L:54:ARG:NH2   | 1.41                     | 1.08              |
| 1:A:88:PRO:CG     | 1:A:438:ILE:HD12  | 1.83                     | 1.08              |
| 1:A:1322:ILE:CD1  | 1:A:1457:ILE:HD11 | 1.83                     | 1.08              |
| 6:F:74:ILE:O      | 7:G:95:LEU:HD11   | 1.43                     | 1.08              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:75:PRO:HG2    | 6:F:78:GLN:HB2    | 1.13                     | 1.08              |
| 7:G:159:LYS:CD    | 15:O:103:ASN:OD1  | 2.02                     | 1.08              |
| 15:O:374:PRO:O    | 15:O:376:TYR:HB3  | 1.53                     | 1.08              |
| 2:B:527:PHE:CE2   | 2:B:666:PRO:HA    | 1.89                     | 1.08              |
| 18:R:324:MET:SD   | 18:R:377:ASP:HA   | 1.93                     | 1.08              |
| 1:A:486:PRO:O     | 2:B:781:TYR:CD2   | 2.06                     | 1.07              |
| 1:A:597:LYS:CB    | 2:B:1082:HIS:CD2  | 2.38                     | 1.07              |
| 1:A:1049:MET:HB3  | 1:A:1052:GLY:CA   | 1.84                     | 1.07              |
| 17:Q:351:ASN:HB3  | 17:Q:369:TRP:CZ3  | 1.89                     | 1.07              |
| 1:A:1314:GLN:HE21 | 1:A:1446:ARG:NH1  | 1.46                     | 1.07              |
| 17:Q:9:ILE:HG13   | 17:Q:10:CYS:H     | 1.06                     | 1.07              |
| 17:Q:17:SER:O     | 17:Q:29:CYS:HB2   | 1.55                     | 1.07              |
| 1:A:834:ARG:NH2   | 2:B:994:ASP:OD1   | 1.87                     | 1.07              |
| 15:O:200:ASN:ND2  | 17:Q:14:ASN:O     | 1.86                     | 1.07              |
| 17:Q:26:ARG:HB3   | 17:Q:34:VAL:HG13  | 1.12                     | 1.07              |
| 1:A:429:THR:HG21  | 18:R:406:LYS:HD2  | 1.21                     | 1.07              |
| 1:A:566:SER:HB3   | 15:O:235:GLU:CD   | 1.77                     | 1.07              |
| 1:A:1313:LEU:HG   | 1:A:1462:PHE:CZ   | 1.90                     | 1.07              |
| 1:A:1326:GLU:CD   | 1:A:1454:HIS:CB   | 2.26                     | 1.07              |
| 16:P:350:THR:HG21 | 18:R:156:LYS:N    | 1.68                     | 1.07              |
| 1:A:878:ARG:HG2   | 9:I:67:VAL:HG13   | 1.09                     | 1.07              |
| 6:F:74:ILE:CG1    | 6:F:75:PRO:HD2    | 1.83                     | 1.07              |
| 16:P:185:GLN:HG3  | 18:R:190:SER:CB   | 1.84                     | 1.07              |
| 17:Q:15:CYS:HB3   | 17:Q:17:SER:N     | 1.70                     | 1.07              |
| 1:A:436:ALA:C     | 1:A:439:ASP:C     | 2.22                     | 1.06              |
| 2:B:49:PHE:HB2    | 2:B:164:MET:CE    | 1.84                     | 1.06              |
| 2:B:68:ILE:CG2    | 2:B:71:LYS:HZ3    | 1.56                     | 1.06              |
| 16:P:717:LYS:HB3  | 17:Q:439:ILE:HD13 | 1.08                     | 1.06              |
| 17:Q:188:ALA:HB3  | 17:Q:384:GLN:HB3  | 1.30                     | 1.06              |
| 1:A:597:LYS:CB    | 2:B:1082:HIS:NE2  | 2.17                     | 1.06              |
| 17:Q:414:TYR:CE1  | 18:R:240:ILE:HG21 | 1.91                     | 1.06              |
| 1:A:545:SER:N     | 17:Q:34:VAL:CG2   | 2.18                     | 1.06              |
| 1:A:1322:ILE:HB   | 1:A:1454:HIS:NE2  | 1.68                     | 1.06              |
| 1:A:1575:ILE:HG13 | 9:I:122:ARG:NH1   | 0.74                     | 1.06              |
| 3:C:253:PRO:N     | 14:N:180:PHE:CD1  | 2.19                     | 1.06              |
| 16:P:197:ARG:NE   | 16:P:261:VAL:H    | 1.54                     | 1.06              |
| 1:A:472:MET:HE2   | 1:A:472:MET:HA    | 1.31                     | 1.06              |
| 2:B:1072:GLY:H    | 2:B:1075:GLU:HG3  | 1.08                     | 1.06              |
| 1:A:474:LYS:CE    | 2:B:1092:LEU:CD2  | 2.32                     | 1.06              |
| 1:A:506:THR:HG22  | 1:A:579:ARG:O     | 1.53                     | 1.06              |
| 1:A:990:ILE:HB    | 1:A:994:GLU:HB3   | 1.17                     | 1.06              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1322:ILE:HG21 | 1:A:1454:HIS:CG   | 1.81                     | 1.06              |
| 1:A:1326:GLU:OE1  | 1:A:1454:HIS:CA   | 2.03                     | 1.06              |
| 16:P:722:TRP:CD1  | 17:Q:446:TYR:CG   | 2.29                     | 1.06              |
| 17:Q:258:MET:HE2  | 17:Q:438:PHE:CZ   | 1.91                     | 1.06              |
| 1:A:503:VAL:CA    | 1:A:580:HIS:CD2   | 2.23                     | 1.05              |
| 1:A:1660:VAL:O    | 7:G:102:GLU:HG2   | 1.54                     | 1.05              |
| 3:C:58:ASN:CA     | 3:C:296:ASN:HD21  | 1.65                     | 1.05              |
| 16:P:24:SER:HB2   | 18:R:318:ILE:HD11 | 1.35                     | 1.05              |
| 17:Q:5:ILE:O      | 17:Q:19:LEU:O     | 1.74                     | 1.05              |
| 16:P:717:LYS:HD2  | 17:Q:439:ILE:HD11 | 1.38                     | 1.05              |
| 17:Q:194:GLN:NE2  | 18:R:209:ARG:NE   | 2.05                     | 1.05              |
| 17:Q:197:GLU:OE2  | 17:Q:388:THR:N    | 1.88                     | 1.05              |
| 1:A:878:ARG:HG2   | 9:I:66:VAL:HG23   | 1.38                     | 1.05              |
| 1:A:1297:PHE:CE2  | 1:A:1301:GLU:CD   | 2.34                     | 1.05              |
| 2:B:68:ILE:CG2    | 2:B:71:LYS:HZ2    | 1.60                     | 1.05              |
| 2:B:889:GLY:HA3   | 12:L:54:ARG:O     | 1.56                     | 1.05              |
| 2:B:1092:LEU:HA   | 2:B:1096:SER:HB2  | 1.35                     | 1.05              |
| 17:Q:414:TYR:HE1  | 18:R:240:ILE:HG21 | 1.22                     | 1.05              |
| 1:A:436:ALA:HB2   | 1:A:443:ALA:HB2   | 1.15                     | 1.05              |
| 1:A:1050:TYR:CE1  | 1:A:1179:ILE:HG12 | 1.90                     | 1.05              |
| 1:A:1314:GLN:NE2  | 1:A:1446:ARG:HH11 | 1.48                     | 1.05              |
| 17:Q:189:LYS:HA   | 17:Q:384:GLN:NE2  | 1.69                     | 1.05              |
| 17:Q:325:GLN:NE2  | 17:Q:452:PHE:CZ   | 2.21                     | 1.05              |
| 1:A:1003:ARG:NH2  | 2:B:530:PRO:C     | 2.14                     | 1.04              |
| 1:A:1322:ILE:CB   | 1:A:1454:HIS:CE1  | 2.40                     | 1.04              |
| 15:O:379:ARG:HA   | 15:O:379:ARG:HH11 | 1.22                     | 1.04              |
| 1:A:1298:ASP:OD1  | 1:A:1468:LYS:NZ   | 1.90                     | 1.04              |
| 1:A:1317:ILE:CG2  | 1:A:1460:TYR:HE1  | 1.69                     | 1.04              |
| 2:B:679:GLN:HG2   | 14:N:156:PRO:C    | 1.67                     | 1.04              |
| 3:C:228:ARG:NH1   | 14:N:173:THR:O    | 1.90                     | 1.04              |
| 7:G:141:SER:HB3   | 15:O:142:ILE:HD13 | 1.35                     | 1.04              |
| 15:O:234:ILE:HG23 | 15:O:237:ILE:HG12 | 1.37                     | 1.04              |
| 16:P:184:SER:HB3  | 18:R:198:LEU:HG   | 1.05                     | 1.04              |
| 1:A:1322:ILE:CG2  | 1:A:1454:HIS:CE1  | 2.41                     | 1.04              |
| 1:A:1657:LEU:CD2  | 7:G:104:LEU:HD13  | 1.88                     | 1.04              |
| 17:Q:197:GLU:OE2  | 17:Q:387:PRO:CA   | 2.05                     | 1.04              |
| 17:Q:325:GLN:HG3  | 17:Q:452:PHE:CE1  | 1.91                     | 1.04              |
| 1:A:476:VAL:O     | 2:B:1068:GLY:HA3  | 1.57                     | 1.04              |
| 1:A:1600:ARG:CD   | 1:A:1616:GLU:OE1  | 2.05                     | 1.04              |
| 7:G:143:SER:HB3   | 15:O:104:ILE:H    | 0.90                     | 1.04              |
| 15:O:240:ILE:HG22 | 15:O:380:SER:HB3  | 1.06                     | 1.04              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:258:MET:CB   | 17:Q:442:LEU:HD13 | 1.86                     | 1.04              |
| 1:A:991:LYS:HB2   | 1:A:993:GLN:HB2   | 1.35                     | 1.04              |
| 15:O:243:GLU:OE1  | 15:O:328:LEU:HD23 | 1.58                     | 1.04              |
| 16:P:475:ARG:HH22 | 17:Q:364:SER:HA   | 1.20                     | 1.04              |
| 17:Q:198:ILE:HG21 | 17:Q:388:THR:HG23 | 1.37                     | 1.04              |
| 17:Q:258:MET:HE1  | 17:Q:438:PHE:CE2  | 1.77                     | 1.04              |
| 17:Q:261:ALA:HB1  | 17:Q:445:ARG:CB   | 1.88                     | 1.04              |
| 18:R:207:ASN:O    | 18:R:211:ARG:CB   | 2.05                     | 1.04              |
| 1:A:629:ASP:C     | 2:B:926:VAL:CG2   | 2.31                     | 1.03              |
| 1:A:721:LYS:O     | 8:H:96:VAL:N      | 1.91                     | 1.03              |
| 1:A:1049:MET:CG   | 1:A:1053:ASP:N    | 2.21                     | 1.03              |
| 1:A:1049:MET:CB   | 1:A:1052:GLY:HA2  | 1.88                     | 1.03              |
| 1:A:1317:ILE:HG21 | 1:A:1460:TYR:HE1  | 1.22                     | 1.03              |
| 2:B:527:PHE:CD1   | 2:B:666:PRO:CG    | 2.40                     | 1.03              |
| 16:P:274:ILE:O    | 16:P:289:SER:HB2  | 1.57                     | 1.03              |
| 17:Q:261:ALA:HB1  | 17:Q:445:ARG:HB2  | 1.04                     | 1.03              |
| 17:Q:263:PRO:HA   | 17:Q:446:TYR:CD1  | 1.93                     | 1.03              |
| 2:B:143:TRP:CD2   | 2:B:446:MET:SD    | 2.49                     | 1.03              |
| 2:B:1089:GLN:HG3  | 2:B:1093:LEU:CD1  | 1.87                     | 1.03              |
| 2:B:1089:GLN:HG2  | 2:B:1093:LEU:HD22 | 1.07                     | 1.03              |
| 1:A:566:SER:HB3   | 15:O:235:GLU:OE2  | 1.56                     | 1.03              |
| 2:B:566:TYR:CD2   | 13:M:73:SER:OG    | 2.11                     | 1.03              |
| 16:P:724:LEU:O    | 17:Q:450:THR:HB   | 1.57                     | 1.03              |
| 17:Q:357:TYR:O    | 18:R:206:ARG:NH1  | 1.91                     | 1.03              |
| 3:C:296:ASN:O     | 3:C:298:PHE:CE1   | 2.10                     | 1.03              |
| 17:Q:380:TRP:CZ3  | 18:R:212:HIS:CD2  | 2.46                     | 1.03              |
| 1:A:503:VAL:CG2   | 1:A:530:TRP:HB2   | 1.88                     | 1.02              |
| 1:A:615:ARG:NH1   | 2:B:929:ARG:HE    | 1.54                     | 1.02              |
| 6:F:72:LYS:HB3    | 6:F:142:SER:CB    | 1.87                     | 1.02              |
| 18:R:317:LEU:HD11 | 18:R:370:SER:CB   | 1.89                     | 1.02              |
| 2:B:551:ILE:HG23  | 2:B:648:ARG:N     | 1.73                     | 1.02              |
| 2:B:1089:GLN:HG3  | 2:B:1093:LEU:HB2  | 1.42                     | 1.02              |
| 7:G:144:HIS:CD2   | 15:O:146:SER:CA   | 2.42                     | 1.02              |
| 17:Q:337:SER:HB3  | 17:Q:448:LYS:HE2  | 1.24                     | 1.02              |
| 1:A:477:ASN:O     | 2:B:1047:ARG:CD   | 2.06                     | 1.02              |
| 1:A:684:ASP:CG    | 8:H:20:TYR:HB3    | 1.83                     | 1.02              |
| 1:A:878:ARG:CG    | 9:I:66:VAL:CG2    | 2.36                     | 1.02              |
| 1:A:991:LYS:HB3   | 1:A:993:GLN:CD    | 1.84                     | 1.02              |
| 17:Q:367:PHE:HE2  | 18:R:1:MET:HE2    | 1.24                     | 1.02              |
| 1:A:878:ARG:CD    | 9:I:66:VAL:HG23   | 1.68                     | 1.02              |
| 2:B:1092:LEU:O    | 2:B:1096:SER:HB3  | 1.59                     | 1.02              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:397:LYS:HZ1  | 18:R:85:ARG:CZ    | 1.72                     | 1.02              |
| 17:Q:414:TYR:CE1  | 18:R:240:ILE:CG2  | 2.42                     | 1.02              |
| 2:B:820:PRO:HB2   | 17:Q:412:LYS:HZ3  | 1.23                     | 1.02              |
| 7:G:159:LYS:HB2   | 15:O:105:ASN:HD22 | 1.24                     | 1.02              |
| 1:A:472:MET:CB    | 2:B:1073:GLU:HB2  | 1.89                     | 1.01              |
| 1:A:938:VAL:HG22  | 9:I:82:ILE:CD1    | 1.88                     | 1.01              |
| 2:B:182:GLN:HE22  | 10:J:69:ARG:HB3   | 1.23                     | 1.01              |
| 17:Q:337:SER:HB2  | 17:Q:448:LYS:CD   | 1.90                     | 1.01              |
| 1:A:1314:GLN:CD   | 1:A:1446:ARG:HD2  | 1.84                     | 1.01              |
| 2:B:207:ILE:CD1   | 2:B:503:VAL:CG2   | 2.34                     | 1.01              |
| 7:G:143:SER:CB    | 15:O:104:ILE:H    | 1.74                     | 1.01              |
| 18:R:177:LEU:O    | 18:R:185:LYS:CE   | 2.08                     | 1.01              |
| 1:A:998:HIS:NE2   | 2:B:711:GLN:HG3   | 1.75                     | 1.01              |
| 7:G:144:HIS:CD2   | 15:O:146:SER:HA   | 1.93                     | 1.01              |
| 1:A:954:GLY:CA    | 1:A:1205:PHE:HB3  | 1.90                     | 1.01              |
| 1:A:990:ILE:CG1   | 1:A:995:TYR:N     | 2.24                     | 1.01              |
| 7:G:159:LYS:CB    | 15:O:105:ASN:ND2  | 2.23                     | 1.01              |
| 1:A:88:PRO:HG2    | 1:A:438:ILE:CD1   | 1.91                     | 1.01              |
| 1:A:566:SER:HB2   | 15:O:235:GLU:OE1  | 1.61                     | 1.01              |
| 1:A:1276:THR:HG1  | 9:I:45:LEU:HD12   | 0.93                     | 1.01              |
| 2:B:681:ILE:HB    | 14:N:154:ARG:HG3  | 1.40                     | 1.01              |
| 7:G:143:SER:HB3   | 15:O:104:ILE:N    | 1.75                     | 1.01              |
| 17:Q:326:TYR:CD1  | 17:Q:452:PHE:HE2  | 1.78                     | 1.01              |
| 1:A:547:ILE:CD1   | 17:Q:26:ARG:HH22  | 1.71                     | 1.00              |
| 1:A:1322:ILE:HD12 | 1:A:1457:ILE:HD11 | 1.04                     | 1.00              |
| 6:F:74:ILE:HG12   | 6:F:75:PRO:CD     | 1.91                     | 1.00              |
| 17:Q:343:THR:HG21 | 17:Q:372:GLU:HB3  | 1.01                     | 1.00              |
| 18:R:199:LYS:CE   | 18:R:204:GLU:CA   | 2.37                     | 1.00              |
| 1:A:995:TYR:OH    | 2:B:707:SER:HB2   | 0.83                     | 1.00              |
| 1:A:995:TYR:CZ    | 2:B:715:ASN:ND2   | 2.29                     | 1.00              |
| 3:C:253:PRO:CD    | 14:N:180:PHE:CD1  | 2.43                     | 1.00              |
| 6:F:72:LYS:CB     | 6:F:142:SER:CB    | 2.37                     | 1.00              |
| 15:O:376:TYR:CE2  | 15:O:377:TYR:HE2  | 1.66                     | 1.00              |
| 2:B:75:ASP:HB3    | 2:B:440:PHE:CZ    | 1.96                     | 1.00              |
| 2:B:143:TRP:CZ3   | 2:B:446:MET:HG3   | 1.96                     | 1.00              |
| 17:Q:326:TYR:CD1  | 17:Q:452:PHE:CE2  | 2.49                     | 1.00              |
| 17:Q:337:SER:CB   | 17:Q:448:LYS:CD   | 2.39                     | 1.00              |
| 3:C:253:PRO:HD2   | 14:N:180:PHE:CD1  | 1.95                     | 1.00              |
| 15:O:376:TYR:CE1  | 15:O:588:LEU:CD2  | 2.45                     | 1.00              |
| 16:P:436:ILE:HB   | 18:R:143:THR:CG2  | 1.92                     | 1.00              |
| 17:Q:258:MET:CE   | 17:Q:438:PHE:HE2  | 1.66                     | 1.00              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:261:ALA:CB   | 17:Q:445:ARG:CB   | 2.40                     | 1.00              |
| 1:A:435:ASN:HB3   | 1:A:442:LYS:HB3   | 1.43                     | 1.00              |
| 1:A:545:SER:HB2   | 17:Q:34:VAL:HG22  | 1.41                     | 1.00              |
| 13:M:102:SER:O    | 13:M:105:SER:N    | 1.95                     | 1.00              |
| 17:Q:351:ASN:CA   | 17:Q:369:TRP:CH2  | 2.45                     | 1.00              |
| 1:A:909:SER:HA    | 9:I:83:LYS:NZ     | 1.75                     | 1.00              |
| 1:A:1050:TYR:CG   | 1:A:1179:ILE:HG21 | 1.96                     | 1.00              |
| 3:C:293:ARG:H     | 3:C:295:ARG:CZ    | 1.74                     | 1.00              |
| 17:Q:9:ILE:HB     | 17:Q:16:PRO:HB2   | 1.43                     | 1.00              |
| 17:Q:258:MET:HE2  | 17:Q:438:PHE:CD2  | 1.93                     | 1.00              |
| 1:A:545:SER:N     | 17:Q:34:VAL:HG23  | 1.77                     | 0.99              |
| 1:A:953:GLU:C     | 1:A:1205:PHE:CG   | 2.40                     | 0.99              |
| 14:N:86:ASP:O     | 14:N:142:THR:N    | 1.94                     | 0.99              |
| 1:A:429:THR:HG21  | 18:R:406:LYS:CE   | 1.73                     | 0.99              |
| 1:A:1317:ILE:CG2  | 1:A:1460:TYR:CE1  | 2.45                     | 0.99              |
| 2:B:682:GLN:CA    | 14:N:154:ARG:NH2  | 2.22                     | 0.99              |
| 2:B:1071:VAL:HG21 | 2:B:1091:ARG:HG3  | 1.41                     | 0.99              |
| 3:C:229:LEU:HD22  | 3:C:295:ARG:O     | 1.61                     | 0.99              |
| 17:Q:194:GLN:CD   | 18:R:209:ARG:NH1  | 2.20                     | 0.99              |
| 15:O:332:LEU:HD11 | 15:O:380:SER:OG   | 1.61                     | 0.99              |
| 18:R:320:CYS:SG   | 18:R:346:ILE:HD11 | 2.02                     | 0.99              |
| 1:A:435:ASN:HB3   | 1:A:442:LYS:HB2   | 1.40                     | 0.99              |
| 1:A:478:TYR:CA    | 2:B:1048:SER:O    | 2.10                     | 0.99              |
| 2:B:207:ILE:HD11  | 2:B:503:VAL:HG21  | 1.43                     | 0.99              |
| 16:P:725:VAL:HA   | 17:Q:450:THR:HB   | 1.42                     | 0.99              |
| 1:A:545:SER:H     | 17:Q:34:VAL:CG2   | 1.74                     | 0.99              |
| 1:A:995:TYR:CZ    | 2:B:707:SER:HB2   | 1.98                     | 0.99              |
| 16:P:21:GLN:O     | 18:R:139:GLU:OE2  | 1.79                     | 0.99              |
| 1:A:1482:LYS:HE2  | 2:B:304:ASP:CG    | 1.86                     | 0.99              |
| 2:B:143:TRP:CE2   | 2:B:446:MET:HB2   | 1.96                     | 0.99              |
| 17:Q:12:THR:CB    | 17:Q:33:HIS:CE1   | 2.44                     | 0.99              |
| 1:A:1049:MET:HB3  | 1:A:1052:GLY:HA2  | 1.42                     | 0.99              |
| 1:A:1276:THR:CB   | 9:I:45:LEU:HD12   | 1.93                     | 0.99              |
| 1:A:995:TYR:HH    | 2:B:707:SER:HB2   | 1.27                     | 0.99              |
| 1:A:995:TYR:CE2   | 2:B:708:ASP:HA    | 1.97                     | 0.99              |
| 1:A:1310:LYS:CG   | 1:A:1311:GLU:CD   | 2.26                     | 0.99              |
| 2:B:697:LEU:HB2   | 2:B:702:ASN:ND2   | 1.77                     | 0.99              |
| 18:R:15:GLN:CD    | 18:R:184:ASN:HD22 | 1.69                     | 0.99              |
| 16:P:436:ILE:HG22 | 18:R:143:THR:OG1  | 1.63                     | 0.99              |
| 17:Q:330:TRP:NE1  | 17:Q:449:GLN:CB   | 1.72                     | 0.99              |
| 17:Q:22:ILE:CD1   | 17:Q:26:ARG:NE    | 2.25                     | 0.99              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:144:HIS:NE2   | 15:O:145:SER:HB3  | 1.78                     | 0.98              |
| 2:B:1089:GLN:HG2  | 2:B:1093:LEU:CD2  | 1.90                     | 0.98              |
| 1:A:909:SER:HA    | 9:I:83:LYS:CE     | 1.93                     | 0.98              |
| 2:B:143:TRP:CE3   | 2:B:446:MET:CG    | 2.46                     | 0.98              |
| 18:R:201:SER:O    | 18:R:205:VAL:CG2  | 2.10                     | 0.98              |
| 1:A:480:ALA:CB    | 2:B:1046:VAL:HG23 | 1.93                     | 0.98              |
| 1:A:535:GLN:HE22  | 17:Q:26:ARG:CD    | 1.77                     | 0.98              |
| 2:B:1072:GLY:O    | 2:B:1075:GLU:CG   | 2.09                     | 0.98              |
| 3:C:253:PRO:CD    | 14:N:180:PHE:CB   | 1.85                     | 0.98              |
| 1:A:408:LYS:CB    | 1:A:411:VAL:HB    | 1.92                     | 0.98              |
| 7:G:24:VAL:HA     | 7:G:25:THR:HA     | 1.44                     | 0.98              |
| 17:Q:197:GLU:OE2  | 17:Q:387:PRO:HA   | 1.63                     | 0.98              |
| 17:Q:418:PRO:HG3  | 18:R:264:SER:CB   | 1.93                     | 0.98              |
| 1:A:486:PRO:HD2   | 2:B:928:SER:OG    | 1.60                     | 0.98              |
| 1:A:615:ARG:HH22  | 2:B:929:ARG:HG2   | 1.26                     | 0.98              |
| 1:A:1330:VAL:CG2  | 1:A:1455:ARG:CZ   | 2.41                     | 0.98              |
| 2:B:143:TRP:CB    | 2:B:446:MET:SD    | 2.48                     | 0.98              |
| 16:P:184:SER:CB   | 18:R:198:LEU:HD21 | 1.92                     | 0.98              |
| 13:M:102:SER:O    | 13:M:105:SER:CA   | 2.11                     | 0.98              |
| 13:M:102:SER:OG   | 13:M:105:SER:N    | 1.96                     | 0.98              |
| 2:B:1072:GLY:CA   | 2:B:1075:GLU:HG2  | 1.93                     | 0.98              |
| 1:A:1314:GLN:NE2  | 1:A:1446:ARG:CD   | 2.25                     | 0.98              |
| 2:B:943:ILE:CD1   | 10:J:44:TYR:CE1   | 2.46                     | 0.98              |
| 2:B:75:ASP:CB     | 2:B:440:PHE:CE2   | 2.47                     | 0.97              |
| 2:B:1003:ALA:HA   | 14:N:169:GLU:N    | 1.78                     | 0.97              |
| 16:P:717:LYS:CB   | 17:Q:439:ILE:HD13 | 1.93                     | 0.97              |
| 17:Q:385:PHE:CZ   | 18:R:209:ARG:HG3  | 1.99                     | 0.97              |
| 18:R:248:LYS:HG3  | 18:R:298:GLN:HE22 | 1.26                     | 0.97              |
| 1:A:953:GLU:CA    | 1:A:1205:PHE:CD2  | 2.46                     | 0.97              |
| 2:B:679:GLN:HG3   | 14:N:155:VAL:O    | 1.64                     | 0.97              |
| 16:P:436:ILE:CG2  | 18:R:143:THR:OG1  | 2.13                     | 0.97              |
| 17:Q:325:GLN:CD   | 17:Q:452:PHE:HZ   | 1.61                     | 0.97              |
| 17:Q:385:PHE:HZ   | 18:R:209:ARG:HA   | 1.29                     | 0.97              |
| 1:A:991:LYS:H     | 1:A:994:GLU:HG3   | 0.82                     | 0.97              |
| 1:A:1484:LEU:HD13 | 2:B:305:ARG:NH1   | 1.80                     | 0.97              |
| 2:B:19:LEU:HD11   | 10:J:26:GLN:OE1   | 1.61                     | 0.97              |
| 2:B:68:ILE:HG23   | 2:B:71:LYS:HZ2    | 1.21                     | 0.97              |
| 15:O:348:THR:HG22 | 15:O:351:SER:HB3  | 1.42                     | 0.97              |
| 1:A:472:MET:HB3   | 2:B:1073:GLU:HB2  | 0.99                     | 0.97              |
| 2:B:550:ARG:HB2   | 2:B:650:LEU:HB2   | 1.47                     | 0.97              |
| 1:A:953:GLU:HG2   | 1:A:1205:PHE:CE2  | 1.99                     | 0.97              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:152:LEU:HD22  | 2:B:443:LYS:CD    | 1.94                     | 0.97              |
| 1:A:438:ILE:O     | 1:A:457:LYS:CB    | 2.12                     | 0.97              |
| 1:A:474:LYS:O     | 2:B:1070:ARG:HA   | 1.65                     | 0.97              |
| 1:A:1050:TYR:CD1  | 1:A:1179:ILE:HG21 | 1.99                     | 0.97              |
| 15:O:234:ILE:CG2  | 15:O:237:ILE:CG1  | 2.31                     | 0.97              |
| 15:O:376:TYR:HE1  | 15:O:588:LEU:CD2  | 1.77                     | 0.97              |
| 1:A:721:LYS:NZ    | 8:H:90:ALA:O      | 1.97                     | 0.97              |
| 16:P:501:PRO:HB3  | 16:P:567:ILE:HG21 | 1.44                     | 0.97              |
| 2:B:202:LEU:HD22  | 2:B:488:ALA:HB2   | 1.46                     | 0.97              |
| 15:O:240:ILE:O    | 15:O:380:SER:OG   | 1.80                     | 0.97              |
| 17:Q:325:GLN:NE2  | 17:Q:452:PHE:HE1  | 1.35                     | 0.97              |
| 17:Q:348:ILE:HD12 | 17:Q:373:GLU:HG2  | 1.46                     | 0.97              |
| 1:A:991:LYS:HB3   | 1:A:993:GLN:OE1   | 1.64                     | 0.96              |
| 1:A:1326:GLU:CD   | 1:A:1454:HIS:CA   | 2.38                     | 0.96              |
| 2:B:145:VAL:HG21  | 2:B:441:LYS:HA    | 1.47                     | 0.96              |
| 17:Q:380:TRP:CZ3  | 18:R:212:HIS:HD2  | 1.84                     | 0.96              |
| 2:B:1089:GLN:HG3  | 2:B:1093:LEU:CD2  | 1.90                     | 0.96              |
| 18:R:323:SER:OG   | 18:R:374:LEU:HD11 | 1.65                     | 0.96              |
| 16:P:724:LEU:HB2  | 17:Q:447:ALA:HB2  | 0.97                     | 0.96              |
| 17:Q:257:VAL:HG11 | 17:Q:446:TYR:OH   | 1.64                     | 0.96              |
| 18:R:199:LYS:CE   | 18:R:203:SER:O    | 2.13                     | 0.96              |
| 1:A:1049:MET:HB3  | 1:A:1052:GLY:N    | 1.79                     | 0.96              |
| 1:A:1322:ILE:CD1  | 1:A:1457:ILE:CD1  | 2.43                     | 0.96              |
| 16:P:350:THR:CG2  | 18:R:156:LYS:H    | 1.79                     | 0.96              |
| 17:Q:189:LYS:CA   | 17:Q:384:GLN:HE21 | 1.78                     | 0.96              |
| 17:Q:378:LEU:CD2  | 18:R:216:LEU:HD21 | 1.95                     | 0.96              |
| 1:A:88:PRO:HG2    | 1:A:438:ILE:HD12  | 0.97                     | 0.96              |
| 1:A:862:THR:CB    | 9:I:67:VAL:HG12   | 1.95                     | 0.96              |
| 2:B:152:LEU:CA    | 2:B:443:LYS:HE3   | 1.96                     | 0.96              |
| 1:A:474:LYS:NZ    | 2:B:1092:LEU:HA   | 1.80                     | 0.95              |
| 1:A:756:LYS:HD3   | 9:I:85:LYS:HZ3    | 1.18                     | 0.95              |
| 16:P:704:LEU:O    | 17:Q:438:PHE:HB3  | 1.65                     | 0.95              |
| 1:A:999:CYS:CA    | 2:B:712:SER:CB    | 2.43                     | 0.95              |
| 15:O:233:LEU:O    | 15:O:237:ILE:HD12 | 1.65                     | 0.95              |
| 1:A:756:LYS:CD    | 9:I:85:LYS:HZ1    | 1.53                     | 0.95              |
| 2:B:71:LYS:HD3    | 2:B:421:LEU:HD13  | 1.46                     | 0.95              |
| 2:B:796:ARG:CZ    | 10:J:8:PHE:O      | 2.14                     | 0.95              |
| 16:P:184:SER:C    | 18:R:198:LEU:HD23 | 1.91                     | 0.95              |
| 2:B:207:ILE:HG13  | 2:B:503:VAL:HG23  | 1.48                     | 0.95              |
| 2:B:824:HIS:ND1   | 2:B:897:GLU:OE1   | 1.90                     | 0.95              |
| 17:Q:261:ALA:HB2  | 17:Q:445:ARG:HD3  | 1.49                     | 0.95              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:74:ILE:HG12   | 6:F:75:PRO:HD2    | 0.95                     | 0.95              |
| 17:Q:15:CYS:SG    | 17:Q:17:SER:HB2   | 2.05                     | 0.95              |
| 6:F:75:PRO:CG     | 6:F:78:GLN:HB2    | 1.96                     | 0.95              |
| 1:A:506:THR:CG2   | 1:A:579:ARG:O     | 2.15                     | 0.95              |
| 1:A:1317:ILE:HG21 | 1:A:1460:TYR:CE1  | 2.01                     | 0.95              |
| 2:B:890:ASP:O     | 12:L:54:ARG:CD    | 2.15                     | 0.95              |
| 3:C:41:GLU:OE2    | 11:K:138:LYS:HE3  | 1.64                     | 0.95              |
| 1:A:990:ILE:HD12  | 1:A:994:GLU:C     | 1.92                     | 0.95              |
| 17:Q:343:THR:CG2  | 17:Q:372:GLU:HB3  | 1.96                     | 0.95              |
| 1:A:545:SER:CA    | 17:Q:34:VAL:CG2   | 2.36                     | 0.95              |
| 1:A:1314:GLN:HE22 | 1:A:1446:ARG:HD2  | 1.28                     | 0.95              |
| 2:B:49:PHE:HB2    | 2:B:164:MET:HE3   | 1.47                     | 0.95              |
| 2:B:1003:ALA:CA   | 14:N:169:GLU:H    | 1.80                     | 0.95              |
| 6:F:66:ARG:NH2    | 7:G:90:LEU:CD1    | 2.29                     | 0.95              |
| 15:O:202:ASN:HB3  | 17:Q:31:TYR:OH    | 1.62                     | 0.95              |
| 16:P:405:TYR:HE1  | 16:P:414:ILE:HG23 | 1.31                     | 0.95              |
| 1:A:474:LYS:O     | 2:B:1070:ARG:CA   | 2.14                     | 0.95              |
| 15:O:63:LEU:HD12  | 15:O:71:ILE:HG13  | 1.47                     | 0.95              |
| 15:O:376:TYR:CD1  | 15:O:419:LYS:HE2  | 2.02                     | 0.94              |
| 17:Q:22:ILE:HD11  | 17:Q:26:ARG:NE    | 1.81                     | 0.94              |
| 1:A:672:ASP:OD2   | 2:B:777:SER:HB3   | 1.67                     | 0.94              |
| 2:B:207:ILE:HG13  | 2:B:503:VAL:HG22  | 1.47                     | 0.94              |
| 15:O:200:ASN:CG   | 17:Q:14:ASN:CG    | 2.34                     | 0.94              |
| 16:P:25:LEU:HB2   | 18:R:139:GLU:OE2  | 1.68                     | 0.94              |
| 16:P:185:GLN:OE1  | 18:R:197:PRO:HA   | 1.66                     | 0.94              |
| 2:B:1089:GLN:CG   | 2:B:1093:LEU:HD13 | 1.96                     | 0.94              |
| 2:B:1089:GLN:HG3  | 2:B:1093:LEU:HD13 | 1.49                     | 0.94              |
| 15:O:243:GLU:HB3  | 15:O:332:LEU:HD13 | 1.48                     | 0.94              |
| 16:P:473:HIS:CD2  | 18:R:1:MET:HB2    | 2.01                     | 0.94              |
| 18:R:4:VAL:HG21   | 18:R:214:VAL:HG22 | 1.47                     | 0.94              |
| 1:A:543:LEU:HB2   | 17:Q:34:VAL:O     | 1.67                     | 0.94              |
| 1:A:1484:LEU:HD13 | 2:B:305:ARG:NE    | 1.80                     | 0.94              |
| 1:A:506:THR:HA    | 1:A:579:ARG:O     | 1.67                     | 0.94              |
| 1:A:545:SER:HB3   | 17:Q:34:VAL:CG2   | 1.96                     | 0.94              |
| 1:A:990:ILE:CD1   | 1:A:995:TYR:HA    | 1.96                     | 0.94              |
| 1:A:1322:ILE:CB   | 1:A:1454:HIS:NE2  | 2.30                     | 0.94              |
| 16:P:706:GLU:HG2  | 17:Q:437:THR:HB   | 1.46                     | 0.94              |
| 17:Q:367:PHE:HE1  | 18:R:1:MET:CA     | 1.62                     | 0.94              |
| 1:A:436:ALA:O     | 1:A:439:ASP:C     | 2.11                     | 0.94              |
| 2:B:1093:LEU:O    | 2:B:1098:TYR:HB2  | 1.67                     | 0.94              |
| 15:O:247:GLU:OE1  | 15:O:325:ILE:HG12 | 1.10                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:395:LEU:HD11  | 18:R:410:TYR:HE1  | 1.20                     | 0.94              |
| 1:A:474:LYS:HZ1   | 2:B:1092:LEU:HD22 | 1.32                     | 0.93              |
| 1:A:588:LEU:HD21  | 2:B:1087:LEU:HD13 | 1.48                     | 0.93              |
| 1:A:991:LYS:HB3   | 1:A:993:GLN:HB2   | 1.50                     | 0.93              |
| 16:P:475:ARG:HH22 | 17:Q:364:SER:CA   | 1.81                     | 0.93              |
| 16:P:717:LYS:HD2  | 17:Q:439:ILE:CD1  | 1.98                     | 0.93              |
| 17:Q:341:ARG:NH1  | 17:Q:369:TRP:HE1  | 1.65                     | 0.93              |
| 17:Q:351:ASN:CG   | 17:Q:369:TRP:CZ2  | 2.45                     | 0.93              |
| 1:A:436:ALA:HA    | 1:A:439:ASP:O     | 1.68                     | 0.93              |
| 15:O:376:TYR:OH   | 15:O:588:LEU:HD21 | 1.65                     | 0.93              |
| 1:A:1049:MET:CB   | 1:A:1052:GLY:CA   | 2.44                     | 0.93              |
| 17:Q:9:ILE:HG13   | 17:Q:10:CYS:N     | 1.77                     | 0.93              |
| 1:A:407:GLN:HE21  | 1:A:407:GLN:H     | 0.94                     | 0.93              |
| 2:B:152:LEU:HB3   | 2:B:443:LYS:HE2   | 1.50                     | 0.93              |
| 17:Q:343:THR:HG21 | 17:Q:372:GLU:CB   | 1.97                     | 0.93              |
| 2:B:75:ASP:N      | 2:B:440:PHE:HE2   | 1.65                     | 0.93              |
| 17:Q:15:CYS:CB    | 17:Q:16:PRO:HA    | 1.99                     | 0.93              |
| 18:R:199:LYS:HE2  | 18:R:204:GLU:N    | 1.82                     | 0.93              |
| 2:B:1002:LYS:HD3  | 14:N:166:LEU:C    | 1.93                     | 0.93              |
| 16:P:185:GLN:OE1  | 18:R:197:PRO:CA   | 2.16                     | 0.93              |
| 18:R:5:PRO:CG     | 18:R:217:THR:CG2  | 2.42                     | 0.93              |
| 1:A:506:THR:CB    | 1:A:579:ARG:O     | 2.16                     | 0.93              |
| 1:A:990:ILE:CB    | 1:A:994:GLU:CB    | 1.98                     | 0.93              |
| 1:A:1484:LEU:HD13 | 2:B:305:ARG:NH2   | 1.82                     | 0.93              |
| 2:B:209:GLN:HG2   | 2:B:210:ARG:H     | 1.32                     | 0.93              |
| 2:B:548:LYS:HE3   | 2:B:695:ASN:CG    | 1.92                     | 0.93              |
| 16:P:488:LEU:CD2  | 18:R:138:PHE:CE2  | 2.51                     | 0.93              |
| 1:A:630:GLY:N     | 2:B:926:VAL:HG21  | 1.84                     | 0.93              |
| 1:A:938:VAL:HG22  | 9:I:82:ILE:HD13   | 1.49                     | 0.93              |
| 16:P:355:GLU:CB   | 18:R:24:ILE:HG23  | 1.99                     | 0.93              |
| 2:B:182:GLN:NE2   | 10:J:69:ARG:CB    | 2.32                     | 0.92              |
| 16:P:717:LYS:HB3  | 17:Q:439:ILE:CD1  | 1.98                     | 0.92              |
| 17:Q:9:ILE:CG1    | 17:Q:10:CYS:H     | 1.79                     | 0.92              |
| 1:A:1322:ILE:CG2  | 1:A:1454:HIS:ND1  | 2.24                     | 0.92              |
| 15:O:376:TYR:CZ   | 15:O:588:LEU:HD21 | 2.03                     | 0.92              |
| 17:Q:263:PRO:CA   | 17:Q:446:TYR:CE1  | 2.51                     | 0.92              |
| 1:A:613:THR:HG21  | 2:B:913:ILE:CG2   | 1.98                     | 0.92              |
| 1:A:953:GLU:C     | 1:A:1205:PHE:CB   | 2.42                     | 0.92              |
| 17:Q:189:LYS:HG3  | 17:Q:384:GLN:NE2  | 1.83                     | 0.92              |
| 17:Q:341:ARG:NH1  | 17:Q:369:TRP:NE1  | 2.16                     | 0.92              |
| 1:A:720:PHE:CE2   | 8:H:141:TYR:HE2   | 1.86                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1600:ARG:HD2  | 1:A:1616:GLU:OE1  | 1.66                     | 0.92              |
| 17:Q:15:CYS:HB3   | 17:Q:16:PRO:CA    | 2.00                     | 0.92              |
| 17:Q:413:LEU:HD21 | 18:R:273:TRP:HZ2  | 0.98                     | 0.92              |
| 1:A:634:ASN:ND2   | 2:B:1069:ILE:HG21 | 1.85                     | 0.92              |
| 1:A:474:LYS:O     | 2:B:1070:ARG:HB2  | 1.66                     | 0.92              |
| 17:Q:26:ARG:CB    | 17:Q:34:VAL:HG13  | 1.99                     | 0.92              |
| 18:R:199:LYS:CD   | 18:R:204:GLU:HB3  | 2.00                     | 0.92              |
| 16:P:399:TRP:HH2  | 18:R:291:ARG:O    | 1.52                     | 0.92              |
| 17:Q:263:PRO:HA   | 17:Q:446:TYR:CE1  | 2.04                     | 0.92              |
| 3:C:294:VAL:O     | 3:C:297:HIS:HB3   | 1.70                     | 0.92              |
| 17:Q:413:LEU:CD2  | 18:R:273:TRP:CZ2  | 2.53                     | 0.92              |
| 17:Q:326:TYR:CZ   | 17:Q:452:PHE:CZ   | 2.58                     | 0.92              |
| 1:A:1326:GLU:OE1  | 1:A:1455:ARG:N    | 2.03                     | 0.91              |
| 2:B:202:LEU:HD23  | 2:B:202:LEU:H     | 1.33                     | 0.91              |
| 3:C:272:LYS:HG2   | 14:N:175:TYR:HD1  | 1.28                     | 0.91              |
| 2:B:266:LYS:CG    | 2:B:473:GLN:O     | 2.18                     | 0.91              |
| 17:Q:22:ILE:HD12  | 17:Q:24:ASP:OD2   | 1.68                     | 0.91              |
| 17:Q:352:ILE:HD12 | 17:Q:377:PHE:CD2  | 1.95                     | 0.91              |
| 17:Q:414:TYR:CZ   | 18:R:240:ILE:HG23 | 2.05                     | 0.91              |
| 1:A:995:TYR:OH    | 2:B:715:ASN:ND2   | 2.04                     | 0.91              |
| 2:B:549:CYS:SG    | 2:B:649:MET:CG    | 2.57                     | 0.91              |
| 17:Q:3:THR:HG22   | 17:Q:20:TRP:HB2   | 1.53                     | 0.91              |
| 17:Q:348:ILE:CD1  | 17:Q:373:GLU:HA   | 2.00                     | 0.91              |
| 1:A:1650:GLY:C    | 1:A:1652:GLY:H    | 1.79                     | 0.91              |
| 16:P:474:LYS:NZ   | 17:Q:364:SER:OG   | 2.03                     | 0.91              |
| 16:P:488:LEU:HD23 | 18:R:138:PHE:CE2  | 2.05                     | 0.91              |
| 2:B:266:LYS:CE    | 2:B:473:GLN:O     | 2.19                     | 0.91              |
| 17:Q:348:ILE:HD11 | 17:Q:373:GLU:CA   | 2.01                     | 0.91              |
| 17:Q:371:GLU:HG3  | 18:R:231:LEU:HD12 | 1.50                     | 0.91              |
| 1:A:425:ASN:HD22  | 18:R:405:ILE:CG2  | 1.84                     | 0.91              |
| 1:A:878:ARG:CD    | 9:I:66:VAL:HG21   | 2.00                     | 0.91              |
| 2:B:64:GLY:HA2    | 2:B:242:ASP:CB    | 2.00                     | 0.91              |
| 17:Q:197:GLU:HG2  | 17:Q:388:THR:O    | 1.70                     | 0.91              |
| 18:R:173:MET:HG3  | 18:R:188:PHE:HZ   | 1.36                     | 0.91              |
| 1:A:507:TYR:CE1   | 1:A:508:PRO:O     | 2.24                     | 0.91              |
| 1:A:684:ASP:OD2   | 8:H:20:TYR:HB3    | 1.69                     | 0.91              |
| 6:F:66:ARG:NH2    | 7:G:90:LEU:HD12   | 1.85                     | 0.91              |
| 15:O:240:ILE:CG2  | 15:O:380:SER:CB   | 2.42                     | 0.91              |
| 16:P:438:TRP:HD1  | 18:R:141:TRP:HZ2  | 1.12                     | 0.91              |
| 18:R:324:MET:HE1  | 18:R:377:ASP:C    | 1.96                     | 0.91              |
| 1:A:435:ASN:CB    | 1:A:442:LYS:CB    | 2.49                     | 0.90              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:704:LEU:CD1  | 17:Q:439:ILE:HG12 | 1.99                     | 0.90              |
| 17:Q:382:GLU:HB2  | 18:R:241:ARG:NH1  | 1.85                     | 0.90              |
| 18:R:251:TRP:CE3  | 18:R:307:LYS:HE2  | 1.86                     | 0.90              |
| 1:A:403:LEU:O     | 1:A:406:LEU:HG    | 1.70                     | 0.90              |
| 1:A:436:ALA:CB    | 1:A:443:ALA:HB2   | 2.00                     | 0.90              |
| 1:A:1313:LEU:CG   | 1:A:1462:PHE:CZ   | 2.54                     | 0.90              |
| 1:A:1314:GLN:HE22 | 1:A:1446:ARG:CD   | 1.83                     | 0.90              |
| 6:F:70:LYS:CD     | 7:G:95:LEU:HD23   | 2.01                     | 0.90              |
| 1:A:581:ILE:HG13  | 1:A:585:ASP:OD2   | 1.71                     | 0.90              |
| 7:G:241:ARG:NH1   | 15:O:189:PHE:CB   | 2.35                     | 0.90              |
| 16:P:197:ARG:HE   | 16:P:261:VAL:H    | 1.16                     | 0.90              |
| 17:Q:193:PHE:HB2  | 18:R:209:ARG:NE   | 1.87                     | 0.90              |
| 17:Q:385:PHE:CZ   | 18:R:209:ARG:HA   | 2.07                     | 0.90              |
| 18:R:199:LYS:CE   | 18:R:204:GLU:CB   | 2.32                     | 0.90              |
| 1:A:486:PRO:O     | 2:B:781:TYR:CE2   | 2.25                     | 0.90              |
| 6:F:70:LYS:HD3    | 7:G:95:LEU:HD23   | 1.53                     | 0.90              |
| 14:N:86:ASP:O     | 14:N:141:GLU:HG2  | 1.71                     | 0.90              |
| 1:A:408:LYS:CA    | 1:A:411:VAL:HB    | 2.02                     | 0.90              |
| 1:A:579:ARG:HH12  | 1:A:581:ILE:HA    | 1.34                     | 0.90              |
| 1:A:1263:LEU:HA   | 1:A:1498:ILE:HD11 | 1.54                     | 0.90              |
| 2:B:1002:LYS:HD2  | 14:N:166:LEU:HB2  | 1.51                     | 0.90              |
| 7:G:159:LYS:HB3   | 15:O:105:ASN:HD22 | 1.34                     | 0.90              |
| 1:A:862:THR:HB    | 9:I:67:VAL:HG12   | 1.50                     | 0.90              |
| 17:Q:188:ALA:C    | 17:Q:384:GLN:CG   | 2.43                     | 0.90              |
| 2:B:64:GLY:HA2    | 2:B:242:ASP:HB3   | 1.54                     | 0.90              |
| 16:P:475:ARG:HH11 | 18:R:1:MET:HB3    | 1.34                     | 0.90              |
| 1:A:470:HIS:HD2   | 2:B:1058:GLN:OE1  | 1.54                     | 0.90              |
| 1:A:1276:THR:HG1  | 9:I:45:LEU:CD1    | 1.69                     | 0.90              |
| 17:Q:337:SER:CB   | 17:Q:448:LYS:HD3  | 2.02                     | 0.90              |
| 17:Q:355:VAL:HG13 | 18:R:215:THR:HG1  | 1.35                     | 0.90              |
| 18:R:324:MET:HE1  | 18:R:377:ASP:O    | 1.70                     | 0.90              |
| 1:A:422:ARG:NH2   | 18:R:412:ARG:HH11 | 1.68                     | 0.90              |
| 1:A:1604:GLU:O    | 1:A:1612:LYS:HE2  | 1.70                     | 0.90              |
| 2:B:548:LYS:HE3   | 2:B:695:ASN:OD1   | 1.70                     | 0.90              |
| 2:B:679:GLN:CG    | 14:N:156:PRO:CA   | 2.43                     | 0.90              |
| 2:B:1072:GLY:N    | 2:B:1075:GLU:HG2  | 1.81                     | 0.90              |
| 3:C:272:LYS:CG    | 14:N:175:TYR:CE1  | 2.54                     | 0.90              |
| 17:Q:352:ILE:HG23 | 18:R:212:HIS:NE2  | 1.86                     | 0.90              |
| 1:A:670:ILE:HG12  | 2:B:783:MET:CE    | 2.01                     | 0.89              |
| 1:A:1484:LEU:CD1  | 2:B:305:ARG:NE    | 2.35                     | 0.89              |
| 1:A:878:ARG:HD2   | 9:I:66:VAL:HG21   | 1.54                     | 0.89              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:849:GLY:CA    | 12:L:60:ARG:NH2   | 2.17                     | 0.89              |
| 7:G:144:HIS:NE2   | 15:O:145:SER:CB   | 2.34                     | 0.89              |
| 15:O:247:GLU:OE1  | 15:O:325:ILE:HA   | 1.71                     | 0.89              |
| 16:P:722:TRP:HD1  | 17:Q:446:TYR:CG   | 1.59                     | 0.89              |
| 17:Q:356:VAL:HG12 | 18:R:211:ARG:HB3  | 0.90                     | 0.89              |
| 18:R:251:TRP:HE3  | 18:R:307:LYS:CE   | 1.69                     | 0.89              |
| 1:A:1314:GLN:OE1  | 1:A:1446:ARG:HD2  | 1.73                     | 0.89              |
| 2:B:1092:LEU:CA   | 2:B:1096:SER:HB2  | 2.02                     | 0.89              |
| 17:Q:20:TRP:CZ3   | 17:Q:22:ILE:HG21  | 2.07                     | 0.89              |
| 17:Q:380:TRP:HZ3  | 18:R:212:HIS:CD2  | 1.87                     | 0.89              |
| 1:A:1049:MET:HB3  | 1:A:1052:GLY:H    | 1.35                     | 0.89              |
| 14:N:87:TYR:CB    | 14:N:141:GLU:HA   | 1.93                     | 0.89              |
| 16:P:297:ILE:O    | 18:R:159:TYR:CD1  | 2.25                     | 0.89              |
| 1:A:634:ASN:HD21  | 2:B:1069:ILE:HG21 | 1.37                     | 0.89              |
| 1:A:826:PHE:CD1   | 2:B:777:SER:HB2   | 2.07                     | 0.89              |
| 17:Q:418:PRO:CD   | 18:R:264:SER:HB3  | 2.03                     | 0.89              |
| 1:A:435:ASN:O     | 1:A:439:ASP:CB    | 2.21                     | 0.89              |
| 1:A:579:ARG:NH1   | 1:A:581:ILE:HA    | 1.88                     | 0.89              |
| 1:A:627:ASP:O     | 2:B:784:ASP:HB3   | 1.73                     | 0.89              |
| 2:B:894:LYS:HG3   | 12:L:54:ARG:HH22  | 0.74                     | 0.89              |
| 3:C:272:LYS:CG    | 14:N:175:TYR:CD1  | 2.56                     | 0.89              |
| 16:P:184:SER:OG   | 18:R:198:LEU:HD21 | 1.72                     | 0.89              |
| 1:A:413:LEU:O     | 1:A:416:ARG:HG2   | 1.73                     | 0.88              |
| 15:O:243:GLU:OE1  | 15:O:328:LEU:CD2  | 2.08                     | 0.88              |
| 17:Q:330:TRP:CE2  | 17:Q:449:GLN:HB2  | 2.05                     | 0.88              |
| 1:A:429:THR:CG2   | 18:R:406:LYS:NZ   | 2.36                     | 0.88              |
| 1:A:1326:GLU:CD   | 1:A:1454:HIS:C    | 2.39                     | 0.88              |
| 16:P:186:TYR:CD1  | 18:R:196:GLU:O    | 2.26                     | 0.88              |
| 1:A:474:LYS:HZ2   | 2:B:1092:LEU:HD23 | 1.36                     | 0.88              |
| 1:A:966:LEU:HD21  | 1:A:997:PHE:CE1   | 2.09                     | 0.88              |
| 2:B:26:ILE:O      | 10:J:62:ARG:NH1   | 2.05                     | 0.88              |
| 2:B:551:ILE:CG2   | 2:B:647:SER:HA    | 2.02                     | 0.88              |
| 15:O:373:LEU:O    | 15:O:376:TYR:CB   | 2.21                     | 0.88              |
| 16:P:323:ASN:ND2  | 18:R:157:MET:O    | 2.05                     | 0.88              |
| 17:Q:20:TRP:CH2   | 17:Q:22:ILE:CG2   | 2.56                     | 0.88              |
| 2:B:800:TYR:OH    | 2:B:908:ARG:NH2   | 2.07                     | 0.88              |
| 17:Q:418:PRO:O    | 18:R:233:TYR:OH   | 1.90                     | 0.88              |
| 1:A:408:LYS:HA    | 1:A:411:VAL:HB    | 1.55                     | 0.88              |
| 1:A:436:ALA:HB2   | 1:A:443:ALA:CB    | 2.01                     | 0.88              |
| 1:A:474:LYS:HZ1   | 2:B:1092:LEU:CD2  | 1.79                     | 0.88              |
| 1:A:535:GLN:HE22  | 17:Q:26:ARG:HD3   | 1.05                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1276:THR:C    | 9:I:44:ASN:HA     | 1.99                     | 0.88              |
| 17:Q:15:CYS:HB3   | 17:Q:16:PRO:C     | 1.98                     | 0.88              |
| 17:Q:341:ARG:CZ   | 17:Q:369:TRP:HE1  | 1.85                     | 0.88              |
| 1:A:756:LYS:CD    | 9:I:85:LYS:HZ3    | 1.69                     | 0.88              |
| 1:A:954:GLY:N     | 1:A:1205:PHE:CB   | 2.37                     | 0.88              |
| 1:A:1313:LEU:HD23 | 1:A:1462:PHE:HZ   | 1.38                     | 0.88              |
| 3:C:230:LEU:HD12  | 3:C:231:PRO:CD    | 2.04                     | 0.88              |
| 17:Q:352:ILE:CG2  | 18:R:212:HIS:NE2  | 2.37                     | 0.88              |
| 2:B:1151:ILE:HG12 | 7:G:21:LYS:NZ     | 1.88                     | 0.88              |
| 6:F:74:ILE:O      | 7:G:95:LEU:HD13   | 1.72                     | 0.88              |
| 16:P:248:PRO:HD2  | 16:P:267:ASN:HB3  | 1.54                     | 0.88              |
| 2:B:743:ARG:NH2   | 10:J:60:PHE:HZ    | 1.72                     | 0.88              |
| 15:O:376:TYR:CE1  | 15:O:588:LEU:HD21 | 2.07                     | 0.88              |
| 18:R:199:LYS:CE   | 18:R:204:GLU:HA   | 2.03                     | 0.88              |
| 1:A:438:ILE:O     | 1:A:457:LYS:HB2   | 1.72                     | 0.87              |
| 15:O:517:LEU:HD23 | 15:O:525:MET:HE3  | 1.56                     | 0.87              |
| 17:Q:409:ALA:O    | 17:Q:413:LEU:HB2  | 1.74                     | 0.87              |
| 1:A:756:LYS:CG    | 9:I:85:LYS:HZ2    | 1.87                     | 0.87              |
| 1:A:1053:ASP:O    | 1:A:1055:ILE:HG12 | 1.73                     | 0.87              |
| 1:A:1603:MET:HE2  | 1:A:1615:TYR:HD2  | 1.39                     | 0.87              |
| 17:Q:19:LEU:HD11  | 17:Q:27:ARG:HB3   | 1.54                     | 0.87              |
| 18:R:199:LYS:HZ1  | 18:R:204:GLU:HA   | 1.38                     | 0.87              |
| 16:P:694:ILE:HB   | 16:P:746:ARG:HD3  | 1.54                     | 0.87              |
| 1:A:998:HIS:O     | 2:B:712:SER:OG    | 1.92                     | 0.87              |
| 16:P:472:ARG:NH1  | 18:R:203:SER:HB2  | 1.88                     | 0.87              |
| 1:A:1322:ILE:CG2  | 1:A:1454:HIS:NE2  | 2.37                     | 0.87              |
| 1:A:1484:LEU:HD23 | 2:B:304:ASP:HB3   | 1.56                     | 0.87              |
| 2:B:679:GLN:CD    | 14:N:157:ARG:HA   | 1.99                     | 0.87              |
| 7:G:144:HIS:NE2   | 15:O:145:SER:C    | 2.31                     | 0.87              |
| 1:A:1056:ASP:HA   | 1:A:1179:ILE:HD13 | 1.57                     | 0.87              |
| 15:O:238:ILE:O    | 15:O:242:VAL:HG23 | 1.75                     | 0.87              |
| 1:A:547:ILE:CG1   | 17:Q:26:ARG:HH22  | 1.87                     | 0.87              |
| 2:B:679:GLN:CD    | 14:N:157:ARG:CA   | 2.48                     | 0.87              |
| 16:P:475:ARG:NH2  | 17:Q:364:SER:CB   | 2.36                     | 0.87              |
| 16:P:725:VAL:HA   | 17:Q:450:THR:OG1  | 1.75                     | 0.87              |
| 17:Q:193:PHE:HB3  | 18:R:209:ARG:CZ   | 2.04                     | 0.87              |
| 17:Q:380:TRP:CH2  | 18:R:212:HIS:CD2  | 2.62                     | 0.87              |
| 2:B:534:PRO:HA    | 2:B:720:GLN:OE1   | 1.73                     | 0.87              |
| 16:P:197:ARG:HD2  | 16:P:261:VAL:N    | 1.89                     | 0.87              |
| 1:A:1085:LEU:HD22 | 6:F:84:TYR:OH     | 1.74                     | 0.87              |
| 1:A:1482:LYS:CD   | 2:B:304:ASP:OD1   | 2.22                     | 0.87              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:149:GLU:OE1   | 2:B:441:LYS:CE    | 2.23                     | 0.87              |
| 7:G:159:LYS:H     | 15:O:105:ASN:CG   | 1.82                     | 0.87              |
| 17:Q:418:PRO:CG   | 18:R:264:SER:CB   | 2.52                     | 0.87              |
| 1:A:954:GLY:N     | 1:A:1205:PHE:HB2  | 1.90                     | 0.86              |
| 1:A:990:ILE:HG13  | 1:A:995:TYR:H     | 1.35                     | 0.86              |
| 2:B:75:ASP:N      | 2:B:440:PHE:CE2   | 2.41                     | 0.86              |
| 1:A:756:LYS:CG    | 9:I:85:LYS:NZ     | 2.38                     | 0.86              |
| 17:Q:198:ILE:CG2  | 17:Q:388:THR:HG23 | 2.05                     | 0.86              |
| 2:B:143:TRP:CB    | 2:B:446:MET:HE1   | 1.94                     | 0.86              |
| 2:B:266:LYS:HE3   | 2:B:473:GLN:C     | 1.99                     | 0.86              |
| 2:B:849:GLY:HA3   | 12:L:60:ARG:NH2   | 1.89                     | 0.86              |
| 17:Q:348:ILE:CD1  | 17:Q:373:GLU:HG2  | 2.03                     | 0.86              |
| 13:M:102:SER:O    | 13:M:105:SER:C    | 2.17                     | 0.86              |
| 17:Q:12:THR:CB    | 17:Q:33:HIS:ND1   | 2.37                     | 0.86              |
| 17:Q:261:ALA:HB2  | 17:Q:445:ARG:CD   | 2.05                     | 0.86              |
| 17:Q:326:TYR:CE1  | 17:Q:452:PHE:CD2  | 2.62                     | 0.86              |
| 1:A:403:LEU:CD1   | 1:A:419:ILE:CG2   | 2.45                     | 0.86              |
| 1:A:1313:LEU:CD2  | 1:A:1462:PHE:HZ   | 1.88                     | 0.86              |
| 1:A:1322:ILE:HD12 | 1:A:1457:ILE:HD12 | 1.57                     | 0.86              |
| 1:A:1660:VAL:O    | 7:G:102:GLU:HA    | 1.74                     | 0.86              |
| 3:C:229:LEU:O     | 3:C:293:ARG:NH1   | 2.07                     | 0.86              |
| 3:C:293:ARG:H     | 3:C:295:ARG:NH1   | 1.72                     | 0.86              |
| 6:F:74:ILE:C      | 7:G:95:LEU:HD11   | 2.00                     | 0.86              |
| 11:K:66:VAL:HG12  | 11:K:67:GLU:HG2   | 1.57                     | 0.86              |
| 17:Q:29:CYS:SG    | 17:Q:33:HIS:HB2   | 2.15                     | 0.86              |
| 3:C:274:THR:HA    | 14:N:172:ALA:HB2  | 0.90                     | 0.86              |
| 7:G:159:LYS:CA    | 15:O:105:ASN:ND2  | 2.38                     | 0.86              |
| 17:Q:358:PRO:HA   | 18:R:206:ARG:CD   | 2.05                     | 0.86              |
| 18:R:324:MET:SD   | 18:R:377:ASP:CA   | 2.63                     | 0.86              |
| 1:A:543:LEU:O     | 17:Q:34:VAL:O     | 1.92                     | 0.86              |
| 1:A:1330:VAL:HG21 | 1:A:1455:ARG:NE   | 1.91                     | 0.86              |
| 16:P:397:LYS:HZ3  | 18:R:85:ARG:HD3   | 1.38                     | 0.86              |
| 1:A:477:ASN:ND2   | 2:B:1049:THR:OG1  | 2.09                     | 0.86              |
| 1:A:478:TYR:CD1   | 2:B:1048:SER:O    | 2.29                     | 0.86              |
| 1:A:1606:SER:CB   | 1:A:1611:MET:HE3  | 2.06                     | 0.86              |
| 15:O:247:GLU:OE1  | 15:O:325:ILE:CB   | 2.20                     | 0.86              |
| 16:P:185:GLN:HG3  | 18:R:190:SER:HB2  | 1.58                     | 0.86              |
| 17:Q:378:LEU:HB3  | 18:R:238:THR:HG21 | 1.57                     | 0.86              |
| 1:A:1314:GLN:NE2  | 1:A:1446:ARG:CZ   | 2.38                     | 0.86              |
| 1:A:1326:GLU:OE2  | 1:A:1454:HIS:CA   | 2.24                     | 0.86              |
| 1:A:475:ARG:NH2   | 2:B:1061:LYS:HB2  | 1.91                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:143:TRP:CE2   | 2:B:446:MET:CB    | 2.58                     | 0.85              |
| 2:B:346:ASP:OD1   | 13:M:113:ILE:HG23 | 1.76                     | 0.85              |
| 3:C:293:ARG:N     | 3:C:295:ARG:NH1   | 2.23                     | 0.85              |
| 15:O:181:ARG:HB2  | 15:O:181:ARG:HH11 | 1.41                     | 0.85              |
| 1:A:1032:VAL:HG21 | 1:A:1050:TYR:CD1  | 2.11                     | 0.85              |
| 2:B:143:TRP:CE2   | 2:B:446:MET:CG    | 2.58                     | 0.85              |
| 16:P:184:SER:HB3  | 18:R:198:LEU:CD2  | 1.97                     | 0.85              |
| 17:Q:189:LYS:N    | 17:Q:384:GLN:HG2  | 1.91                     | 0.85              |
| 18:R:317:LEU:CD1  | 18:R:367:ILE:HD13 | 2.06                     | 0.85              |
| 2:B:143:TRP:CE3   | 2:B:446:MET:HE3   | 2.11                     | 0.85              |
| 16:P:436:ILE:CB   | 18:R:143:THR:HG23 | 2.06                     | 0.85              |
| 16:P:498:LEU:HD11 | 17:Q:368:GLN:HG3  | 1.56                     | 0.85              |
| 17:Q:194:GLN:HE22 | 18:R:209:ARG:HE   | 1.25                     | 0.85              |
| 17:Q:337:SER:HB2  | 17:Q:448:LYS:HE2  | 1.56                     | 0.85              |
| 1:A:477:ASN:C     | 2:B:1047:ARG:HD3  | 2.01                     | 0.85              |
| 2:B:143:TRP:CE2   | 2:B:446:MET:HG3   | 2.11                     | 0.85              |
| 18:R:168:ILE:HG23 | 18:R:169:PRO:HD3  | 1.58                     | 0.85              |
| 1:A:878:ARG:CB    | 9:I:67:VAL:HG13   | 1.97                     | 0.85              |
| 2:B:527:PHE:HZ    | 2:B:666:PRO:HA    | 1.39                     | 0.85              |
| 15:O:376:TYR:CZ   | 15:O:377:TYR:CZ   | 2.63                     | 0.85              |
| 1:A:564:PRO:CG    | 15:O:370:THR:O    | 2.25                     | 0.85              |
| 3:C:37:LYS:O      | 11:K:134:LYS:NZ   | 2.09                     | 0.85              |
| 3:C:272:LYS:N     | 14:N:175:TYR:CE1  | 2.35                     | 0.85              |
| 3:C:322:LYS:HE3   | 11:K:129:ASP:OD1  | 1.77                     | 0.85              |
| 15:O:200:ASN:HB2  | 17:Q:14:ASN:HA    | 1.58                     | 0.85              |
| 17:Q:330:TRP:CD1  | 17:Q:449:GLN:CB   | 2.52                     | 0.85              |
| 7:G:141:SER:HB3   | 15:O:142:ILE:HD11 | 1.58                     | 0.85              |
| 1:A:990:ILE:HD12  | 1:A:994:GLU:O     | 1.76                     | 0.85              |
| 1:A:1032:VAL:HG21 | 1:A:1050:TYR:CE1  | 2.12                     | 0.85              |
| 1:A:1262:LEU:CD2  | 1:A:1497:ILE:HG12 | 2.06                     | 0.85              |
| 1:A:613:THR:HG21  | 2:B:913:ILE:HG21  | 1.57                     | 0.84              |
| 2:B:894:LYS:CD    | 12:L:47:ARG:NE    | 2.40                     | 0.84              |
| 15:O:376:TYR:HE1  | 15:O:588:LEU:HD22 | 1.38                     | 0.84              |
| 16:P:360:TRP:CE3  | 18:R:196:GLU:OE2  | 2.31                     | 0.84              |
| 16:P:724:LEU:CG   | 17:Q:447:ALA:HB2  | 2.07                     | 0.84              |
| 17:Q:367:PHE:HE1  | 18:R:1:MET:H3     | 1.25                     | 0.84              |
| 17:Q:367:PHE:CE2  | 18:R:1:MET:HE2    | 2.12                     | 0.84              |
| 17:Q:385:PHE:CE1  | 18:R:209:ARG:HG3  | 2.12                     | 0.84              |
| 18:R:251:TRP:CD2  | 18:R:307:LYS:HE3  | 2.11                     | 0.84              |
| 18:R:317:LEU:HD11 | 18:R:370:SER:HB2  | 1.59                     | 0.84              |
| 1:A:422:ARG:HD3   | 18:R:409:HIS:CE1  | 2.10                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1317:ILE:HG22 | 1:A:1460:TYR:CE1  | 2.09                     | 0.84              |
| 3:C:59:ILE:O      | 3:C:296:ASN:HB2   | 1.78                     | 0.84              |
| 18:R:362:ALA:HB2  | 18:R:421:LYS:HB3  | 1.59                     | 0.84              |
| 1:A:422:ARG:HH21  | 18:R:412:ARG:NH1  | 1.70                     | 0.84              |
| 2:B:1089:GLN:CG   | 2:B:1093:LEU:HB2  | 2.06                     | 0.84              |
| 7:G:241:ARG:NH1   | 15:O:189:PHE:HB3  | 1.93                     | 0.84              |
| 17:Q:188:ALA:O    | 17:Q:384:GLN:CG   | 2.24                     | 0.84              |
| 1:A:436:ALA:CA    | 1:A:439:ASP:O     | 2.24                     | 0.84              |
| 1:A:1655:ASP:HB2  | 6:F:135:ARG:HB3   | 1.58                     | 0.84              |
| 2:B:985:ILE:HB    | 14:N:160:VAL:HG22 | 1.59                     | 0.84              |
| 15:O:248:LEU:CD1  | 15:O:598:PHE:HE2  | 1.54                     | 0.84              |
| 18:R:15:GLN:CD    | 18:R:184:ASN:ND2  | 2.29                     | 0.84              |
| 1:A:475:ARG:HB3   | 2:B:1059:PRO:HB2  | 1.57                     | 0.84              |
| 1:A:1322:ILE:HG21 | 1:A:1454:HIS:CE1  | 2.08                     | 0.84              |
| 15:O:181:ARG:HH11 | 15:O:181:ARG:CB   | 1.89                     | 0.84              |
| 17:Q:26:ARG:CB    | 17:Q:34:VAL:CG1   | 2.53                     | 0.84              |
| 17:Q:352:ILE:HD12 | 17:Q:377:PHE:HE2  | 1.34                     | 0.84              |
| 18:R:316:SER:HB3  | 18:R:349:ILE:HD13 | 1.59                     | 0.84              |
| 1:A:986:PHE:CD2   | 2:B:958:MET:HE2   | 2.13                     | 0.84              |
| 2:B:207:ILE:HD11  | 2:B:503:VAL:CG2   | 2.03                     | 0.84              |
| 2:B:848:ILE:CA    | 12:L:60:ARG:HD2   | 2.08                     | 0.84              |
| 16:P:475:ARG:NH2  | 17:Q:364:SER:HA   | 1.92                     | 0.84              |
| 17:Q:194:GLN:CG   | 17:Q:389:GLN:HB2  | 2.06                     | 0.84              |
| 1:A:425:ASN:ND2   | 18:R:405:ILE:CG2  | 2.40                     | 0.84              |
| 2:B:145:VAL:CG1   | 2:B:441:LYS:HG2   | 2.04                     | 0.84              |
| 2:B:623:ASP:O     | 2:B:648:ARG:NH1   | 2.10                     | 0.84              |
| 2:B:820:PRO:HB2   | 17:Q:412:LYS:NZ   | 1.86                     | 0.84              |
| 16:P:354:PRO:CB   | 18:R:27:ILE:HG22  | 2.04                     | 0.84              |
| 2:B:119:ARG:CZ    | 12:L:53:HIS:CE1   | 2.61                     | 0.84              |
| 15:O:247:GLU:OE1  | 15:O:325:ILE:CA   | 2.25                     | 0.84              |
| 1:A:425:ASN:HD22  | 18:R:405:ILE:HG22 | 1.37                     | 0.84              |
| 1:A:407:GLN:HB3   | 1:A:409:ASP:H     | 1.43                     | 0.83              |
| 1:A:1297:PHE:CE2  | 9:I:60:LEU:HD22   | 2.13                     | 0.83              |
| 3:C:58:ASN:HA     | 3:C:296:ASN:HD22  | 1.39                     | 0.83              |
| 17:Q:382:GLU:HB2  | 18:R:241:ARG:HH11 | 1.42                     | 0.83              |
| 1:A:435:ASN:O     | 1:A:439:ASP:C     | 2.21                     | 0.83              |
| 1:A:474:LYS:HZ3   | 2:B:1096:SER:CB   | 1.90                     | 0.83              |
| 1:A:480:ALA:HB2   | 2:B:1046:VAL:HG23 | 1.60                     | 0.83              |
| 1:A:828:CYS:HB3   | 2:B:1027:TYR:HB2  | 1.60                     | 0.83              |
| 1:A:938:VAL:CG2   | 9:I:82:ILE:HD13   | 2.07                     | 0.83              |
| 7:G:144:HIS:ND1   | 15:O:146:SER:OG   | 2.10                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:245:GLN:NE2  | 15:O:379:ARG:HB2  | 1.93                     | 0.83              |
| 1:A:399:LEU:HD21  | 1:A:423:LEU:HG    | 1.59                     | 0.83              |
| 2:B:25:PHE:CE1    | 10:J:59:LYS:HD2   | 2.13                     | 0.83              |
| 2:B:985:ILE:HB    | 14:N:160:VAL:HG21 | 1.59                     | 0.83              |
| 7:G:159:LYS:N     | 15:O:105:ASN:HD21 | 1.50                     | 0.83              |
| 17:Q:261:ALA:O    | 17:Q:449:GLN:OE1  | 1.95                     | 0.83              |
| 18:R:206:ARG:H    | 18:R:206:ARG:HE   | 1.26                     | 0.83              |
| 2:B:399:HIS:O     | 2:B:400:GLN:HG2   | 1.77                     | 0.83              |
| 2:B:894:LYS:CG    | 12:L:54:ARG:CZ    | 2.56                     | 0.83              |
| 13:M:102:SER:CB   | 13:M:105:SER:H    | 1.90                     | 0.83              |
| 2:B:697:LEU:HB2   | 2:B:702:ASN:CG    | 2.03                     | 0.83              |
| 1:A:506:THR:CA    | 1:A:579:ARG:O     | 2.26                     | 0.83              |
| 1:A:718:THR:O     | 8:H:98:TYR:N      | 2.11                     | 0.83              |
| 1:A:966:LEU:CD2   | 1:A:997:PHE:CE1   | 2.61                     | 0.83              |
| 1:A:1276:THR:OG1  | 9:I:45:LEU:HD13   | 1.78                     | 0.83              |
| 2:B:1089:GLN:CB   | 2:B:1093:LEU:HD22 | 2.09                     | 0.83              |
| 2:B:1092:LEU:HA   | 2:B:1096:SER:CB   | 2.09                     | 0.83              |
| 3:C:103:LEU:O     | 10:J:6:ARG:NE     | 2.12                     | 0.83              |
| 16:P:397:LYS:HZ1  | 18:R:85:ARG:NH1   | 1.77                     | 0.83              |
| 1:A:475:ARG:CZ    | 2:B:1061:LYS:CB   | 2.56                     | 0.83              |
| 2:B:776:ILE:HB    | 2:B:1026:ILE:HD13 | 1.60                     | 0.83              |
| 16:P:706:GLU:CG   | 17:Q:437:THR:HB   | 2.05                     | 0.83              |
| 17:Q:101:LYS:HG2  | 17:Q:152:LEU:HD11 | 1.58                     | 0.83              |
| 17:Q:188:ALA:C    | 17:Q:384:GLN:HG2  | 2.03                     | 0.83              |
| 1:A:966:LEU:CD2   | 1:A:997:PHE:CZ    | 2.62                     | 0.83              |
| 3:C:334:THR:CG2   | 11:K:44:ARG:HB3   | 2.09                     | 0.83              |
| 15:O:240:ILE:HG22 | 15:O:380:SER:HB2  | 1.58                     | 0.83              |
| 17:Q:351:ASN:CB   | 17:Q:369:TRP:CZ2  | 2.62                     | 0.83              |
| 18:R:199:LYS:CE   | 18:R:203:SER:C    | 2.52                     | 0.83              |
| 2:B:346:ASP:H     | 13:M:113:ILE:HG12 | 1.40                     | 0.82              |
| 2:B:566:TYR:HB3   | 13:M:74:ASN:OD1   | 1.79                     | 0.82              |
| 2:B:682:GLN:HA    | 14:N:154:ARG:NH2  | 1.92                     | 0.82              |
| 16:P:360:TRP:HE3  | 18:R:196:GLU:OE2  | 1.61                     | 0.82              |
| 18:R:6:ILE:HD11   | 18:R:213:ILE:CG2  | 2.09                     | 0.82              |
| 1:A:532:GLY:C     | 1:A:580:HIS:HD1   | 1.86                     | 0.82              |
| 1:A:629:ASP:OD1   | 2:B:926:VAL:HG23  | 1.79                     | 0.82              |
| 2:B:1089:GLN:CG   | 2:B:1093:LEU:CG   | 2.52                     | 0.82              |
| 1:A:535:GLN:NE2   | 17:Q:26:ARG:CD    | 2.34                     | 0.82              |
| 2:B:1002:LYS:HD2  | 14:N:166:LEU:CB   | 2.09                     | 0.82              |
| 17:Q:258:MET:HA   | 17:Q:442:LEU:HD13 | 0.84                     | 0.82              |
| 1:A:999:CYS:HA    | 2:B:712:SER:HB3   | 1.57                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1069:ILE:O    | 2:B:1070:ARG:HB3  | 1.76                     | 0.82              |
| 13:M:61:GLU:OE2   | 13:M:106:LYS:CE   | 2.13                     | 0.82              |
| 13:M:102:SER:C    | 13:M:105:SER:H    | 1.86                     | 0.82              |
| 6:F:70:LYS:HG2    | 7:G:95:LEU:HG     | 1.62                     | 0.82              |
| 7:G:24:VAL:HG11   | 7:G:126:GLN:NE2   | 1.95                     | 0.82              |
| 17:Q:351:ASN:CA   | 17:Q:369:TRP:HH2  | 1.92                     | 0.82              |
| 1:A:544:VAL:HG13  | 17:Q:32:GLY:O     | 1.79                     | 0.82              |
| 2:B:550:ARG:O     | 2:B:649:MET:HA    | 1.79                     | 0.82              |
| 7:G:241:ARG:HH11  | 15:O:189:PHE:HB3  | 1.40                     | 0.82              |
| 15:O:342:HIS:CE1  | 15:O:346:GLN:HE21 | 1.98                     | 0.82              |
| 17:Q:194:GLN:HG2  | 17:Q:389:GLN:HB2  | 1.62                     | 0.82              |
| 1:A:435:ASN:CB    | 1:A:442:LYS:HB3   | 2.08                     | 0.82              |
| 1:A:672:ASP:OD1   | 2:B:777:SER:OG    | 1.96                     | 0.82              |
| 1:A:824:THR:O     | 2:B:1023:ARG:N    | 2.12                     | 0.82              |
| 2:B:610:TYR:HE1   | 2:B:658:LEU:HD11  | 1.44                     | 0.82              |
| 16:P:475:ARG:HH21 | 17:Q:364:SER:HG   | 1.24                     | 0.82              |
| 1:A:984:GLY:N     | 1:A:994:GLU:OE2   | 2.13                     | 0.82              |
| 2:B:894:LYS:O     | 2:B:896:GLN:N     | 2.11                     | 0.82              |
| 18:R:426:VAL:HG12 | 18:R:428:SER:H    | 1.45                     | 0.82              |
| 1:A:429:THR:HG22  | 18:R:406:LYS:HE3  | 0.82                     | 0.82              |
| 1:A:477:ASN:HA    | 2:B:1047:ARG:NH1  | 1.95                     | 0.82              |
| 1:A:478:TYR:CG    | 2:B:1048:SER:O    | 2.33                     | 0.82              |
| 2:B:1049:THR:HG23 | 2:B:1050:GLY:N    | 1.93                     | 0.82              |
| 7:G:144:HIS:HD2   | 15:O:146:SER:HA   | 1.42                     | 0.82              |
| 16:P:24:SER:CB    | 18:R:318:ILE:HD11 | 2.08                     | 0.82              |
| 17:Q:418:PRO:CG   | 18:R:233:TYR:OH   | 2.28                     | 0.82              |
| 15:O:376:TYR:CE1  | 15:O:419:LYS:HE2  | 2.14                     | 0.82              |
| 1:A:756:LYS:HD3   | 9:I:85:LYS:HZ2    | 1.45                     | 0.81              |
| 1:A:1575:ILE:CA   | 9:I:122:ARG:NH1   | 2.43                     | 0.81              |
| 1:A:1657:LEU:HB2  | 6:F:133:VAL:HB    | 1.62                     | 0.81              |
| 2:B:796:ARG:HD2   | 10:J:8:PHE:HA     | 1.61                     | 0.81              |
| 17:Q:188:ALA:HB1  | 17:Q:384:GLN:O    | 1.78                     | 0.81              |
| 1:A:403:LEU:HD11  | 1:A:419:ILE:HG21  | 0.85                     | 0.81              |
| 1:A:952:LEU:CD2   | 1:A:1004:GLU:HG3  | 2.07                     | 0.81              |
| 2:B:207:ILE:HG12  | 2:B:503:VAL:HG21  | 1.61                     | 0.81              |
| 6:F:73:ALA:HA     | 6:F:143:PHE:O     | 1.80                     | 0.81              |
| 16:P:438:TRP:HD1  | 18:R:141:TRP:CZ2  | 1.97                     | 0.81              |
| 17:Q:20:TRP:HZ3   | 17:Q:22:ILE:HG22  | 0.65                     | 0.81              |
| 17:Q:188:ALA:CB   | 17:Q:384:GLN:HB3  | 2.09                     | 0.81              |
| 17:Q:193:PHE:CB   | 18:R:209:ARG:CZ   | 2.58                     | 0.81              |
| 2:B:29:PRO:HB2    | 2:B:177:PRO:HG2   | 1.62                     | 0.81              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 16:P:368:HIS:HB3  | 16:P:411:LYS:HZ2 | 1.45                     | 0.81              |
| 17:Q:15:CYS:HB3   | 17:Q:16:PRO:HA   | 1.60                     | 0.81              |
| 18:R:248:LYS:HG2  | 18:R:298:GLN:CD  | 2.05                     | 0.81              |
| 1:A:473:GLY:HA2   | 2:B:1072:GLY:HA2 | 1.60                     | 0.81              |
| 1:A:1310:LYS:HD3  | 1:A:1310:LYS:H   | 1.45                     | 0.81              |
| 16:P:321:LYS:H    | 16:P:321:LYS:HD3 | 1.46                     | 0.81              |
| 16:P:323:ASN:HA   | 16:P:350:THR:HA  | 1.61                     | 0.81              |
| 18:R:252:GLY:O    | 18:R:256:GLU:HB2 | 1.79                     | 0.81              |
| 1:A:478:TYR:O     | 1:A:479:ALA:HB2  | 1.79                     | 0.81              |
| 2:B:889:GLY:CA    | 12:L:54:ARG:O    | 2.28                     | 0.81              |
| 17:Q:261:ALA:HB2  | 17:Q:445:ARG:HB2 | 1.61                     | 0.81              |
| 1:A:615:ARG:NH2   | 2:B:929:ARG:HG2  | 1.94                     | 0.81              |
| 1:A:862:THR:HG22  | 9:I:67:VAL:CG1   | 2.10                     | 0.81              |
| 15:O:584:GLN:OE1  | 15:O:584:GLN:N   | 2.11                     | 0.81              |
| 16:P:475:ARG:NH1  | 17:Q:367:PHE:CD1 | 2.49                     | 0.81              |
| 17:Q:414:TYR:CZ   | 18:R:240:ILE:CG2 | 2.64                     | 0.81              |
| 1:A:719:ILE:HG12  | 8:H:97:MET:HG2   | 1.62                     | 0.81              |
| 2:B:49:PHE:CE2    | 2:B:194:PHE:CZ   | 2.68                     | 0.81              |
| 1:A:535:GLN:HE21  | 17:Q:26:ARG:HD3  | 1.44                     | 0.81              |
| 2:B:567:SER:O     | 14:N:140:SER:HB3 | 1.81                     | 0.81              |
| 2:B:679:GLN:CD    | 14:N:157:ARG:N   | 2.39                     | 0.81              |
| 2:B:1151:ILE:HG12 | 7:G:21:LYS:HZ2   | 1.45                     | 0.81              |
| 17:Q:378:LEU:HD22 | 18:R:238:THR:OG1 | 1.79                     | 0.81              |
| 1:A:399:LEU:HD23  | 1:A:423:LEU:HD23 | 1.63                     | 0.81              |
| 1:A:721:LYS:NZ    | 8:H:91:ASP:HA    | 1.96                     | 0.81              |
| 1:A:954:GLY:CA    | 1:A:1205:PHE:CB  | 2.59                     | 0.81              |
| 1:A:1120:TYR:O    | 5:E:207:ARG:NH2  | 2.12                     | 0.81              |
| 18:R:199:LYS:NZ   | 18:R:204:GLU:HA  | 1.93                     | 0.81              |
| 1:A:422:ARG:HD3   | 18:R:409:HIS:HD1 | 1.44                     | 0.80              |
| 1:A:503:VAL:CA    | 1:A:580:HIS:HD2  | 1.69                     | 0.80              |
| 13:M:102:SER:HB3  | 13:M:105:SER:CA  | 2.09                     | 0.80              |
| 1:A:615:ARG:NH1   | 2:B:929:ARG:NE   | 2.28                     | 0.80              |
| 2:B:145:VAL:HG11  | 2:B:441:LYS:CG   | 2.09                     | 0.80              |
| 2:B:975:HIS:ND1   | 14:N:169:GLU:HG3 | 1.96                     | 0.80              |
| 16:P:389:TRP:C    | 18:R:151:PRO:O   | 2.25                     | 0.80              |
| 18:R:347:ASP:O    | 18:R:351:GLU:HB2 | 1.81                     | 0.80              |
| 3:C:272:LYS:CB    | 14:N:175:TYR:CE1 | 2.64                     | 0.80              |
| 1:A:478:TYR:O     | 1:A:479:ALA:CB   | 2.29                     | 0.80              |
| 1:A:672:ASP:CG    | 2:B:777:SER:HB3  | 2.04                     | 0.80              |
| 3:C:272:LYS:HA    | 14:N:175:TYR:CE2 | 2.14                     | 0.80              |
| 6:F:74:ILE:O      | 7:G:95:LEU:HD12  | 1.79                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:N:87:TYR:CE2   | 14:N:141:GLU:OE1  | 2.34                     | 0.80              |
| 16:P:198:ASP:HB3  | 16:P:205:TYR:O    | 1.79                     | 0.80              |
| 16:P:390:GLN:N    | 18:R:151:PRO:O    | 2.15                     | 0.80              |
| 16:P:703:PHE:O    | 17:Q:438:PHE:CD2  | 2.34                     | 0.80              |
| 17:Q:418:PRO:CG   | 18:R:264:SER:OG   | 2.30                     | 0.80              |
| 1:A:429:THR:CG2   | 18:R:406:LYS:HD2  | 2.08                     | 0.80              |
| 1:A:1600:ARG:HH21 | 1:A:1617:THR:HG1  | 1.27                     | 0.80              |
| 15:O:235:GLU:O    | 15:O:238:ILE:HD12 | 1.81                     | 0.80              |
| 16:P:704:LEU:C    | 17:Q:438:PHE:HB3  | 2.07                     | 0.80              |
| 17:Q:355:VAL:O    | 18:R:211:ARG:HG3  | 1.81                     | 0.80              |
| 2:B:75:ASP:HB3    | 2:B:440:PHE:CD2   | 2.15                     | 0.80              |
| 2:B:681:ILE:HB    | 14:N:154:ARG:CG   | 2.12                     | 0.80              |
| 2:B:1003:ALA:O    | 14:N:170:HIS:CA   | 2.29                     | 0.80              |
| 1:A:990:ILE:O     | 1:A:992:PRO:N     | 2.14                     | 0.80              |
| 1:A:545:SER:CB    | 17:Q:34:VAL:HG23  | 2.08                     | 0.80              |
| 1:A:1329:ILE:CG2  | 1:A:1456:PHE:CZ   | 2.64                     | 0.80              |
| 2:B:850:THR:N     | 12:L:60:ARG:HH22  | 1.78                     | 0.80              |
| 16:P:775:TRP:H    | 17:Q:109:GLN:HE22 | 1.28                     | 0.80              |
| 17:Q:187:THR:CA   | 17:Q:380:TRP:HZ2  | 1.74                     | 0.80              |
| 2:B:794:ASP:OD1   | 2:B:911:PRO:HD2   | 1.81                     | 0.80              |
| 17:Q:188:ALA:N    | 17:Q:380:TRP:HZ2  | 1.80                     | 0.80              |
| 17:Q:197:GLU:CD   | 17:Q:388:THR:O    | 2.25                     | 0.80              |
| 12:L:34:CYS:HB3   | 12:L:51:CYS:SG    | 2.21                     | 0.80              |
| 17:Q:325:GLN:HE21 | 17:Q:452:PHE:HE1  | 0.90                     | 0.80              |
| 2:B:551:ILE:HA    | 2:B:648:ARG:O     | 1.82                     | 0.79              |
| 2:B:1089:GLN:CG   | 2:B:1093:LEU:CD1  | 2.59                     | 0.79              |
| 16:P:436:ILE:CG1  | 18:R:143:THR:HG23 | 2.12                     | 0.79              |
| 1:A:1330:VAL:CG2  | 1:A:1455:ARG:NE   | 2.44                     | 0.79              |
| 17:Q:371:GLU:HG3  | 18:R:231:LEU:CG   | 2.12                     | 0.79              |
| 1:A:581:ILE:HD12  | 1:A:637:PHE:CE1   | 2.17                     | 0.79              |
| 1:A:1482:LYS:HD2  | 2:B:307:GLU:OE1   | 1.81                     | 0.79              |
| 1:A:1575:ILE:CB   | 9:I:122:ARG:NH1   | 2.44                     | 0.79              |
| 2:B:208:VAL:HG23  | 2:B:401:GLU:HG2   | 1.64                     | 0.79              |
| 2:B:346:ASP:CG    | 13:M:113:ILE:HG23 | 2.07                     | 0.79              |
| 13:M:102:SER:CB   | 13:M:105:SER:CB   | 2.02                     | 0.79              |
| 1:A:472:MET:HG3   | 2:B:1073:GLU:OE1  | 1.82                     | 0.79              |
| 1:A:862:THR:HA    | 9:I:67:VAL:CB     | 2.12                     | 0.79              |
| 1:A:1049:MET:HG2  | 1:A:1052:GLY:CA   | 2.13                     | 0.79              |
| 17:Q:20:TRP:CE3   | 17:Q:22:ILE:HG23  | 2.15                     | 0.79              |
| 1:A:990:ILE:CD1   | 1:A:995:TYR:CA    | 2.60                     | 0.79              |
| 2:B:143:TRP:CZ2   | 2:B:446:MET:HA    | 2.18                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:N:87:TYR:HA    | 14:N:141:GLU:HA   | 0.81                     | 0.79              |
| 17:Q:193:PHE:CB   | 18:R:209:ARG:NE   | 2.44                     | 0.79              |
| 17:Q:414:TYR:CE1  | 18:R:240:ILE:HG12 | 2.17                     | 0.79              |
| 2:B:1089:GLN:CD   | 2:B:1093:LEU:HD13 | 2.07                     | 0.79              |
| 6:F:66:ARG:NH2    | 7:G:90:LEU:HD13   | 1.98                     | 0.79              |
| 15:O:201:LYS:HD2  | 15:O:239:SER:OG   | 1.82                     | 0.79              |
| 16:P:488:LEU:HD22 | 18:R:138:PHE:CE2  | 2.18                     | 0.79              |
| 1:A:407:GLN:HE21  | 1:A:407:GLN:N     | 1.78                     | 0.79              |
| 1:A:547:ILE:HD11  | 17:Q:26:ARG:CZ    | 1.90                     | 0.79              |
| 1:A:878:ARG:CG    | 9:I:67:VAL:CG1    | 2.55                     | 0.79              |
| 1:A:1180:ASN:OD1  | 6:F:87:LYS:CD     | 2.25                     | 0.79              |
| 16:P:21:GLN:HB3   | 18:R:139:GLU:OE1  | 1.83                     | 0.79              |
| 2:B:551:ILE:HG23  | 2:B:648:ARG:H     | 1.48                     | 0.79              |
| 15:O:396:MET:HE1  | 15:O:433:LYS:C    | 2.08                     | 0.79              |
| 17:Q:352:ILE:O    | 18:R:212:HIS:HE1  | 1.64                     | 0.79              |
| 18:R:199:LYS:HE3  | 18:R:203:SER:C    | 2.08                     | 0.79              |
| 16:P:436:ILE:CB   | 18:R:143:THR:CG2  | 2.61                     | 0.79              |
| 1:A:671:GLN:OE1   | 2:B:952:HIS:HB2   | 1.83                     | 0.78              |
| 13:M:102:SER:C    | 13:M:105:SER:N    | 2.40                     | 0.78              |
| 1:A:1038:ILE:HD11 | 1:A:1050:TYR:HA   | 1.65                     | 0.78              |
| 1:A:407:GLN:CB    | 1:A:409:ASP:H     | 1.95                     | 0.78              |
| 1:A:425:ASN:HD21  | 18:R:405:ILE:HG22 | 1.46                     | 0.78              |
| 2:B:49:PHE:CB     | 2:B:164:MET:HE3   | 2.13                     | 0.78              |
| 17:Q:330:TRP:HE1  | 17:Q:449:GLN:CG   | 1.94                     | 0.78              |
| 18:R:5:PRO:CD     | 18:R:217:THR:HG21 | 2.13                     | 0.78              |
| 18:R:6:ILE:HD11   | 18:R:213:ILE:HB   | 1.65                     | 0.78              |
| 18:R:139:GLU:HB2  | 18:R:314:TRP:HH2  | 1.48                     | 0.78              |
| 1:A:435:ASN:CB    | 1:A:442:LYS:HB2   | 2.11                     | 0.78              |
| 16:P:357:LEU:CD2  | 18:R:23:TYR:HE1   | 1.96                     | 0.78              |
| 17:Q:17:SER:O     | 17:Q:29:CYS:CB    | 2.30                     | 0.78              |
| 1:A:721:LYS:HB3   | 8:H:96:VAL:HB     | 1.64                     | 0.78              |
| 2:B:532:HIS:NE2   | 2:B:723:LYS:NZ    | 2.31                     | 0.78              |
| 2:B:679:GLN:CG    | 14:N:156:PRO:HA   | 2.14                     | 0.78              |
| 16:P:472:ARG:HH12 | 17:Q:360:LYS:HE3  | 1.49                     | 0.78              |
| 17:Q:186:CYS:CA   | 18:R:208:TYR:OH   | 2.32                     | 0.78              |
| 1:A:83:VAL:HG11   | 1:A:427:PHE:CZ    | 2.19                     | 0.78              |
| 1:A:862:THR:HA    | 9:I:67:VAL:CA     | 2.13                     | 0.78              |
| 1:A:1032:VAL:CG2  | 1:A:1050:TYR:CD1  | 2.67                     | 0.78              |
| 18:R:207:ASN:O    | 18:R:211:ARG:CA   | 2.32                     | 0.78              |
| 1:A:862:THR:HA    | 9:I:67:VAL:HA     | 1.65                     | 0.78              |
| 1:A:996:TYR:CE2   | 2:B:530:PRO:HG3   | 2.19                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1049:MET:HG3  | 1:A:1053:ASP:N    | 1.97                     | 0.78              |
| 2:B:49:PHE:CE2    | 2:B:194:PHE:HZ    | 2.01                     | 0.78              |
| 2:B:743:ARG:NH2   | 10:J:60:PHE:CE2   | 2.52                     | 0.78              |
| 15:O:234:ILE:HG23 | 15:O:237:ILE:CG1  | 2.06                     | 0.78              |
| 15:O:376:TYR:CG   | 15:O:419:LYS:HE2  | 2.19                     | 0.78              |
| 17:Q:366:TYR:OH   | 18:R:218:ASP:OD2  | 1.99                     | 0.78              |
| 1:A:458:GLN:O     | 1:A:462:LYS:CB    | 2.26                     | 0.78              |
| 1:A:1657:LEU:HD23 | 7:G:104:LEU:HB3   | 1.65                     | 0.78              |
| 2:B:49:PHE:CB     | 2:B:164:MET:CE    | 2.62                     | 0.78              |
| 2:B:207:ILE:HD11  | 2:B:503:VAL:HG11  | 1.66                     | 0.78              |
| 6:F:66:ARG:HH22   | 7:G:90:LEU:CD1    | 1.94                     | 0.78              |
| 6:F:72:LYS:HD3    | 6:F:142:SER:HB3   | 1.62                     | 0.78              |
| 16:P:704:LEU:HA   | 17:Q:438:PHE:HD2  | 1.49                     | 0.78              |
| 1:A:984:GLY:HA3   | 1:A:994:GLU:CD    | 2.09                     | 0.78              |
| 1:A:990:ILE:HG13  | 1:A:995:TYR:CA    | 2.14                     | 0.78              |
| 1:A:1049:MET:HG2  | 1:A:1052:GLY:O    | 1.84                     | 0.78              |
| 2:B:184:LYS:HB3   | 2:B:735:HIS:ND1   | 1.99                     | 0.78              |
| 17:Q:198:ILE:HB   | 17:Q:390:THR:CA   | 2.14                     | 0.78              |
| 1:A:435:ASN:C     | 1:A:439:ASP:O     | 2.27                     | 0.78              |
| 2:B:25:PHE:O      | 10:J:62:ARG:HD2   | 1.83                     | 0.78              |
| 3:C:272:LYS:CA    | 14:N:175:TYR:CD1  | 2.44                     | 0.78              |
| 17:Q:418:PRO:CG   | 18:R:264:SER:HB3  | 2.14                     | 0.78              |
| 2:B:415:GLU:OE2   | 2:B:474:SER:OG    | 2.02                     | 0.77              |
| 16:P:473:HIS:CD2  | 18:R:1:MET:CB     | 2.67                     | 0.77              |
| 17:Q:371:GLU:HG3  | 18:R:231:LEU:HD11 | 1.64                     | 0.77              |
| 1:A:422:ARG:CB    | 18:R:409:HIS:CE1  | 2.67                     | 0.77              |
| 1:A:1298:ASP:HA   | 1:A:1468:LYS:HZ3  | 1.50                     | 0.77              |
| 15:O:435:SER:OG   | 15:O:438:GLN:HG3  | 1.85                     | 0.77              |
| 16:P:200:THR:HG21 | 16:P:280:ARG:NH1  | 1.99                     | 0.77              |
| 17:Q:261:ALA:HB2  | 17:Q:445:ARG:CB   | 2.14                     | 0.77              |
| 18:R:177:LEU:HD22 | 18:R:185:LYS:HG2  | 1.66                     | 0.77              |
| 6:F:72:LYS:C      | 6:F:143:PHE:H     | 1.91                     | 0.77              |
| 7:G:159:LYS:H     | 15:O:105:ASN:HD21 | 0.80                     | 0.77              |
| 16:P:355:GLU:O    | 18:R:24:ILE:HD12  | 1.84                     | 0.77              |
| 1:A:1299:ASN:OD1  | 1:A:1467:GLY:C    | 2.28                     | 0.77              |
| 7:G:144:HIS:CD2   | 15:O:146:SER:OG   | 2.38                     | 0.77              |
| 1:A:422:ARG:CD    | 18:R:409:HIS:CE1  | 2.67                     | 0.77              |
| 2:B:527:PHE:CD2   | 2:B:666:PRO:HB3   | 2.19                     | 0.77              |
| 14:N:88:LYS:N     | 14:N:140:SER:O    | 2.15                     | 0.77              |
| 15:O:477:PHE:HE2  | 15:O:525:MET:HE1  | 1.50                     | 0.77              |
| 17:Q:258:MET:SD   | 17:Q:438:PHE:CE2  | 2.78                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1600:ARG:NE   | 1:A:1616:GLU:OE1  | 2.16                     | 0.77              |
| 2:B:1093:LEU:CG   | 2:B:1094:ASN:OD1  | 2.29                     | 0.77              |
| 15:O:155:SER:HA   | 15:O:158:LEU:HD12 | 1.67                     | 0.77              |
| 15:O:579:LEU:CA   | 15:O:582:ARG:HB3  | 2.11                     | 0.77              |
| 16:P:355:GLU:HB2  | 18:R:24:ILE:HG23  | 1.65                     | 0.77              |
| 1:A:88:PRO:HG3    | 1:A:434:VAL:HG12  | 1.65                     | 0.77              |
| 2:B:46:ILE:HA     | 2:B:164:MET:SD    | 2.25                     | 0.77              |
| 2:B:679:GLN:CG    | 14:N:155:VAL:O    | 2.32                     | 0.77              |
| 17:Q:15:CYS:CB    | 17:Q:16:PRO:CA    | 2.62                     | 0.77              |
| 2:B:1096:SER:O    | 2:B:1097:ASP:HB3  | 1.84                     | 0.77              |
| 1:A:990:ILE:CD1   | 1:A:994:GLU:C     | 2.57                     | 0.77              |
| 1:A:1314:GLN:CD   | 1:A:1446:ARG:CD   | 2.56                     | 0.77              |
| 2:B:75:ASP:CB     | 2:B:440:PHE:CZ    | 2.66                     | 0.77              |
| 2:B:119:ARG:NH2   | 12:L:53:HIS:CE1   | 2.52                     | 0.77              |
| 17:Q:352:ILE:HD11 | 17:Q:377:PHE:HD2  | 0.64                     | 0.77              |
| 17:Q:380:TRP:HZ3  | 18:R:212:HIS:HD2  | 1.26                     | 0.77              |
| 1:A:382:GLN:HE21  | 1:A:456:VAL:HG22  | 1.50                     | 0.76              |
| 1:A:1049:MET:CG   | 1:A:1052:GLY:CA   | 2.62                     | 0.76              |
| 2:B:49:PHE:HB2    | 2:B:164:MET:HE1   | 1.67                     | 0.76              |
| 2:B:143:TRP:CH2   | 2:B:446:MET:HA    | 2.19                     | 0.76              |
| 17:Q:258:MET:SD   | 17:Q:438:PHE:HE2  | 2.08                     | 0.76              |
| 1:A:407:GLN:H     | 1:A:407:GLN:NE2   | 1.79                     | 0.76              |
| 1:A:493:ASN:HB3   | 1:A:654:ASP:OD1   | 1.85                     | 0.76              |
| 1:A:995:TYR:CE2   | 2:B:708:ASP:CA    | 2.56                     | 0.76              |
| 2:B:346:ASP:N     | 13:M:113:ILE:HG12 | 1.99                     | 0.76              |
| 2:B:878:GLU:OE2   | 2:B:909:ARG:NH1   | 2.17                     | 0.76              |
| 15:O:235:GLU:O    | 15:O:238:ILE:CD1  | 2.33                     | 0.76              |
| 16:P:184:SER:O    | 18:R:198:LEU:HB3  | 1.85                     | 0.76              |
| 17:Q:414:TYR:CE1  | 18:R:240:ILE:CG1  | 2.69                     | 0.76              |
| 1:A:478:TYR:HA    | 2:B:1048:SER:C    | 2.10                     | 0.76              |
| 15:O:379:ARG:HA   | 15:O:379:ARG:NH1  | 1.99                     | 0.76              |
| 16:P:357:LEU:CD2  | 18:R:23:TYR:CE1   | 2.69                     | 0.76              |
| 16:P:357:LEU:HD22 | 18:R:23:TYR:CE1   | 2.21                     | 0.76              |
| 16:P:475:ARG:HH22 | 17:Q:364:SER:CB   | 1.94                     | 0.76              |
| 2:B:563:SER:CB    | 13:M:73:SER:HB3   | 2.16                     | 0.76              |
| 16:P:389:TRP:CA   | 18:R:151:PRO:O    | 2.33                     | 0.76              |
| 18:R:207:ASN:C    | 18:R:211:ARG:HB2  | 2.10                     | 0.76              |
| 1:A:547:ILE:HG13  | 17:Q:26:ARG:HH22  | 1.48                     | 0.76              |
| 2:B:73:ILE:HD12   | 2:B:425:ILE:HG23  | 1.67                     | 0.76              |
| 6:F:72:LYS:CB     | 6:F:142:SER:HB2   | 2.05                     | 0.76              |
| 15:O:186:SER:O    | 15:O:190:ILE:HG22 | 1.85                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:620:ASN:OD1   | 1:A:667:ARG:NH2   | 2.17                     | 0.76              |
| 1:A:1204:THR:HG21 | 9:I:97:HIS:HB3    | 1.66                     | 0.76              |
| 3:C:315:PHE:CE2   | 11:K:139:ILE:HD12 | 2.20                     | 0.76              |
| 1:A:409:ASP:OD1   | 1:A:410:LYS:N     | 2.19                     | 0.76              |
| 7:G:143:SER:CB    | 15:O:104:ILE:CG2  | 2.17                     | 0.76              |
| 7:G:241:ARG:NH1   | 15:O:189:PHE:HB2  | 1.95                     | 0.76              |
| 15:O:245:GLN:HA   | 15:O:245:GLN:HE21 | 1.51                     | 0.76              |
| 16:P:355:GLU:C    | 18:R:24:ILE:HD12  | 2.09                     | 0.76              |
| 16:P:405:TYR:CE1  | 16:P:414:ILE:HG23 | 2.19                     | 0.76              |
| 1:A:953:GLU:O     | 1:A:1205:PHE:CG   | 2.38                     | 0.76              |
| 1:A:1484:LEU:CD2  | 2:B:304:ASP:HB3   | 2.14                     | 0.76              |
| 7:G:144:HIS:CG    | 15:O:146:SER:CB   | 2.69                     | 0.76              |
| 8:H:80:ARG:HG3    | 11:K:108:TYR:CZ   | 2.21                     | 0.76              |
| 17:Q:12:THR:OG1   | 17:Q:33:HIS:ND1   | 2.17                     | 0.76              |
| 1:A:474:LYS:HE3   | 2:B:1092:LEU:HD23 | 1.50                     | 0.76              |
| 1:A:581:ILE:HD12  | 1:A:637:PHE:CZ    | 2.21                     | 0.76              |
| 1:A:1650:GLY:C    | 1:A:1652:GLY:N    | 2.38                     | 0.76              |
| 16:P:357:LEU:HD22 | 18:R:23:TYR:HE1   | 1.49                     | 0.76              |
| 16:P:472:ARG:NH1  | 17:Q:360:LYS:HE3  | 2.01                     | 0.76              |
| 17:Q:22:ILE:HD12  | 17:Q:24:ASP:CG    | 2.11                     | 0.76              |
| 1:A:474:LYS:HZ2   | 2:B:1092:LEU:CA   | 1.97                     | 0.76              |
| 1:A:999:CYS:HA    | 2:B:712:SER:OG    | 1.86                     | 0.76              |
| 1:A:1484:LEU:HD23 | 2:B:304:ASP:CB    | 2.15                     | 0.76              |
| 2:B:30:LYS:C      | 2:B:176:SER:HB2   | 2.11                     | 0.76              |
| 2:B:202:LEU:HD11  | 2:B:499:HIS:HB3   | 1.67                     | 0.76              |
| 2:B:894:LYS:HG3   | 12:L:54:ARG:CZ    | 2.15                     | 0.76              |
| 2:B:1003:ALA:O    | 14:N:170:HIS:HB3  | 1.85                     | 0.76              |
| 6:F:70:LYS:O      | 6:F:74:ILE:N      | 2.18                     | 0.76              |
| 7:G:159:LYS:HB2   | 15:O:105:ASN:ND2  | 1.95                     | 0.76              |
| 15:O:461:VAL:HG13 | 15:O:467:MET:HE1  | 1.65                     | 0.76              |
| 3:C:142:ARG:CZ    | 10:J:67:GLU:OE2   | 2.33                     | 0.75              |
| 7:G:143:SER:HB2   | 15:O:104:ILE:CB   | 2.15                     | 0.75              |
| 15:O:202:ASN:CB   | 17:Q:31:TYR:OH    | 2.34                     | 0.75              |
| 16:P:245:ILE:HG12 | 16:P:269:PHE:HB2  | 1.66                     | 0.75              |
| 16:P:436:ILE:CB   | 18:R:143:THR:OG1  | 2.33                     | 0.75              |
| 18:R:180:CYS:O    | 18:R:185:LYS:HE3  | 1.86                     | 0.75              |
| 15:O:200:ASN:HD22 | 17:Q:14:ASN:C     | 1.92                     | 0.75              |
| 15:O:376:TYR:OH   | 15:O:588:LEU:CD2  | 2.35                     | 0.75              |
| 16:P:24:SER:OG    | 18:R:318:ILE:HG13 | 1.87                     | 0.75              |
| 17:Q:351:ASN:HA   | 17:Q:369:TRP:CH2  | 2.19                     | 0.75              |
| 18:R:414:PHE:HA   | 18:R:417:ILE:HG22 | 1.66                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:475:ARG:NH2   | 2:B:1061:LYS:CG   | 2.49                     | 0.75              |
| 2:B:68:ILE:HG23   | 2:B:71:LYS:NZ     | 1.84                     | 0.75              |
| 16:P:355:GLU:CA   | 18:R:24:ILE:HD12  | 2.16                     | 0.75              |
| 1:A:474:LYS:NZ    | 2:B:1096:SER:CB   | 2.49                     | 0.75              |
| 2:B:497:ILE:HG12  | 2:B:699:ILE:HD13  | 1.69                     | 0.75              |
| 2:B:527:PHE:CZ    | 2:B:666:PRO:CB    | 2.70                     | 0.75              |
| 15:O:62:ASP:HB3   | 15:O:67:ASP:OD2   | 1.86                     | 0.75              |
| 16:P:436:ILE:HB   | 18:R:143:THR:OG1  | 1.85                     | 0.75              |
| 16:P:598:LEU:HD23 | 16:P:601:ARG:HD2  | 1.68                     | 0.75              |
| 2:B:205:MET:HE1   | 2:B:500:PHE:O     | 1.85                     | 0.75              |
| 17:Q:337:SER:CA   | 17:Q:448:LYS:HE2  | 2.16                     | 0.75              |
| 18:R:251:TRP:HE3  | 18:R:307:LYS:HE3  | 1.31                     | 0.75              |
| 18:R:323:SER:OG   | 18:R:374:LEU:CD1  | 2.35                     | 0.75              |
| 1:A:998:HIS:NE2   | 2:B:711:GLN:CG    | 2.50                     | 0.75              |
| 17:Q:22:ILE:CD1   | 17:Q:26:ARG:CZ    | 2.65                     | 0.75              |
| 17:Q:374:THR:HG23 | 18:R:219:LEU:CD1  | 2.17                     | 0.75              |
| 1:A:953:GLU:CG    | 1:A:1205:PHE:CE2  | 2.69                     | 0.74              |
| 2:B:527:PHE:CZ    | 2:B:666:PRO:N     | 2.54                     | 0.74              |
| 16:P:475:ARG:NH1  | 18:R:1:MET:HB3    | 2.02                     | 0.74              |
| 2:B:25:PHE:O      | 10:J:62:ARG:CD    | 2.35                     | 0.74              |
| 3:C:100:ARG:NH2   | 10:J:3:VAL:O      | 2.20                     | 0.74              |
| 7:G:142:ALA:CB    | 15:O:102:SER:O    | 2.35                     | 0.74              |
| 16:P:197:ARG:CD   | 16:P:261:VAL:N    | 2.49                     | 0.74              |
| 16:P:443:ASP:HB3  | 18:R:3:GLU:CB     | 2.16                     | 0.74              |
| 16:P:725:VAL:CA   | 17:Q:450:THR:OG1  | 2.34                     | 0.74              |
| 17:Q:325:GLN:CG   | 17:Q:452:PHE:HE1  | 1.80                     | 0.74              |
| 2:B:152:LEU:CB    | 2:B:443:LYS:CE    | 2.23                     | 0.74              |
| 15:O:243:GLU:CB   | 15:O:332:LEU:HD13 | 2.17                     | 0.74              |
| 16:P:399:TRP:CH2  | 18:R:291:ARG:O    | 2.38                     | 0.74              |
| 17:Q:187:THR:CA   | 17:Q:380:TRP:CE2  | 2.70                     | 0.74              |
| 6:F:75:PRO:HG3    | 6:F:78:GLN:CD     | 2.12                     | 0.74              |
| 7:G:144:HIS:CD2   | 15:O:146:SER:N    | 2.55                     | 0.74              |
| 16:P:355:GLU:HB3  | 18:R:24:ILE:HG23  | 1.68                     | 0.74              |
| 17:Q:22:ILE:HD11  | 17:Q:24:ASP:OD2   | 1.86                     | 0.74              |
| 17:Q:22:ILE:CG1   | 17:Q:24:ASP:OD2   | 2.34                     | 0.74              |
| 17:Q:113:LYS:HG3  | 17:Q:134:LYS:HZ1  | 1.53                     | 0.74              |
| 17:Q:351:ASN:C    | 17:Q:369:TRP:HH2  | 1.95                     | 0.74              |
| 1:A:406:LEU:HB3   | 1:A:408:LYS:H     | 1.53                     | 0.74              |
| 3:C:253:PRO:HD2   | 14:N:180:PHE:HB3  | 0.78                     | 0.74              |
| 16:P:698:LYS:HE2  | 17:Q:124:ARG:HH21 | 1.50                     | 0.74              |
| 16:P:724:LEU:O    | 17:Q:450:THR:CG2  | 2.35                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:R:4:VAL:CG2    | 18:R:214:VAL:HG22 | 2.17                     | 0.74              |
| 1:A:1204:THR:CG2  | 9:I:97:HIS:HB3    | 2.17                     | 0.74              |
| 2:B:1005:TYR:CE2  | 14:N:170:HIS:CG   | 2.75                     | 0.74              |
| 16:P:473:HIS:NE2  | 18:R:1:MET:HB2    | 2.02                     | 0.74              |
| 17:Q:337:SER:HB2  | 17:Q:448:LYS:CE   | 2.04                     | 0.74              |
| 1:A:403:LEU:CD1   | 1:A:419:ILE:HD13  | 2.18                     | 0.74              |
| 1:A:670:ILE:CG1   | 2:B:783:MET:HE3   | 2.18                     | 0.74              |
| 17:Q:3:THR:O      | 17:Q:20:TRP:HB3   | 1.87                     | 0.74              |
| 17:Q:186:CYS:CA   | 18:R:208:TYR:CZ   | 2.64                     | 0.74              |
| 15:O:248:LEU:HD11 | 15:O:598:PHE:CD2  | 1.86                     | 0.74              |
| 1:A:670:ILE:HG12  | 2:B:783:MET:HE3   | 1.70                     | 0.74              |
| 2:B:401:GLU:HG3   | 2:B:402:VAL:N     | 2.03                     | 0.74              |
| 2:B:518:ARG:NH2   | 2:B:537:SER:O     | 2.21                     | 0.74              |
| 2:B:1003:ALA:O    | 14:N:170:HIS:CB   | 2.36                     | 0.74              |
| 2:B:1151:ILE:HG23 | 7:G:21:LYS:HG3    | 1.70                     | 0.74              |
| 3:C:322:LYS:CE    | 11:K:129:ASP:OD1  | 2.35                     | 0.74              |
| 6:F:72:LYS:O      | 6:F:143:PHE:N     | 2.20                     | 0.74              |
| 7:G:141:SER:HB2   | 15:O:142:ILE:CD1  | 1.95                     | 0.74              |
| 16:P:384:ASP:HB3  | 16:P:389:TRP:HB3  | 1.69                     | 0.74              |
| 1:A:670:ILE:CG1   | 2:B:783:MET:CE    | 2.65                     | 0.74              |
| 1:A:862:THR:C     | 9:I:67:VAL:HA     | 2.13                     | 0.74              |
| 1:A:990:ILE:C     | 1:A:994:GLU:HB2   | 2.12                     | 0.74              |
| 16:P:475:ARG:HD3  | 17:Q:367:PHE:CD2  | 2.23                     | 0.74              |
| 18:R:199:LYS:HE2  | 18:R:203:SER:C    | 2.12                     | 0.74              |
| 1:A:474:LYS:H     | 2:B:1070:ARG:HG3  | 1.51                     | 0.73              |
| 1:A:481:ARG:O     | 2:B:1045:GLN:O    | 2.06                     | 0.73              |
| 1:A:543:LEU:C     | 17:Q:34:VAL:O     | 2.30                     | 0.73              |
| 6:F:72:LYS:HD2    | 6:F:142:SER:HB3   | 0.76                     | 0.73              |
| 17:Q:288:GLU:O    | 17:Q:290:THR:OG1  | 2.06                     | 0.73              |
| 1:A:921:PRO:HD3   | 8:H:19:ARG:HG2    | 1.68                     | 0.73              |
| 1:A:991:LYS:N     | 1:A:994:GLU:CG    | 2.30                     | 0.73              |
| 1:A:1298:ASP:O    | 1:A:1301:GLU:N    | 2.20                     | 0.73              |
| 2:B:566:TYR:HD2   | 13:M:73:SER:HG    | 1.19                     | 0.73              |
| 2:B:566:TYR:CE2   | 13:M:70:SER:HA    | 2.24                     | 0.73              |
| 13:M:102:SER:CB   | 13:M:105:SER:N    | 2.49                     | 0.73              |
| 1:A:629:ASP:O     | 2:B:926:VAL:HG21  | 1.87                     | 0.73              |
| 1:A:1050:TYR:HB3  | 1:A:1054:ALA:HA   | 1.69                     | 0.73              |
| 1:A:1329:ILE:HG22 | 1:A:1456:PHE:CZ   | 2.22                     | 0.73              |
| 1:A:1657:LEU:N    | 6:F:133:VAL:O     | 2.17                     | 0.73              |
| 17:Q:325:GLN:CD   | 17:Q:452:PHE:HE1  | 1.73                     | 0.73              |
| 17:Q:374:THR:HG23 | 18:R:219:LEU:HD13 | 1.71                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:408:LYS:HB2   | 1:A:411:VAL:HB    | 1.68                     | 0.73              |
| 1:A:1487:ASN:OD1  | 2:B:305:ARG:NH2   | 2.21                     | 0.73              |
| 16:P:397:LYS:NZ   | 18:R:85:ARG:HD3   | 2.03                     | 0.73              |
| 17:Q:410:ARG:HA   | 17:Q:413:LEU:HB3  | 1.69                     | 0.73              |
| 1:A:1298:ASP:CG   | 1:A:1468:LYS:NZ   | 2.46                     | 0.73              |
| 1:A:1658:ALA:HA   | 6:F:131:PRO:O     | 1.88                     | 0.73              |
| 2:B:399:HIS:O     | 2:B:400:GLN:CG    | 2.35                     | 0.73              |
| 2:B:1092:LEU:O    | 2:B:1096:SER:CB   | 2.36                     | 0.73              |
| 1:A:824:THR:CB    | 2:B:1023:ARG:HB2  | 2.11                     | 0.73              |
| 1:A:1329:ILE:HG21 | 1:A:1456:PHE:CZ   | 2.24                     | 0.73              |
| 2:B:345:SER:HA    | 13:M:113:ILE:CG1  | 2.17                     | 0.73              |
| 16:P:480:VAL:HB   | 16:P:492:LEU:HD21 | 1.68                     | 0.73              |
| 17:Q:189:LYS:HZ2  | 17:Q:380:TRP:CD1  | 2.06                     | 0.73              |
| 1:A:476:VAL:HG22  | 2:B:1070:ARG:N    | 1.97                     | 0.73              |
| 1:A:984:GLY:CA    | 1:A:994:GLU:OE2   | 2.36                     | 0.73              |
| 1:A:1313:LEU:HG   | 1:A:1462:PHE:HE1  | 1.49                     | 0.73              |
| 6:F:72:LYS:CA     | 6:F:142:SER:CB    | 2.59                     | 0.73              |
| 1:A:588:LEU:CD2   | 2:B:1087:LEU:HD13 | 2.18                     | 0.73              |
| 1:A:986:PHE:CE2   | 2:B:958:MET:HE2   | 2.24                     | 0.73              |
| 2:B:143:TRP:HB3   | 2:B:446:MET:SD    | 2.29                     | 0.73              |
| 16:P:498:LEU:CD1  | 17:Q:368:GLN:HG3  | 2.18                     | 0.73              |
| 16:P:724:LEU:HB2  | 17:Q:447:ALA:CB   | 1.88                     | 0.73              |
| 17:Q:417:PHE:CE2  | 18:R:270:PHE:HA   | 2.22                     | 0.73              |
| 1:A:472:MET:HE2   | 1:A:472:MET:CA    | 2.15                     | 0.73              |
| 1:A:618:TYR:CE1   | 2:B:783:MET:HB2   | 2.24                     | 0.73              |
| 1:A:990:ILE:CG1   | 1:A:994:GLU:HB2   | 2.16                     | 0.73              |
| 1:A:1310:LYS:HB3  | 1:A:1464:ASP:O    | 1.88                     | 0.73              |
| 2:B:73:ILE:HB     | 2:B:425:ILE:HD12  | 1.70                     | 0.73              |
| 7:G:143:SER:CB    | 15:O:104:ILE:CB   | 2.66                     | 0.73              |
| 16:P:197:ARG:NE   | 16:P:261:VAL:N    | 2.34                     | 0.73              |
| 16:P:200:THR:HG21 | 16:P:280:ARG:HH11 | 1.54                     | 0.73              |
| 17:Q:188:ALA:C    | 17:Q:384:GLN:HG3  | 2.05                     | 0.73              |
| 17:Q:418:PRO:HG3  | 18:R:264:SER:HB3  | 1.70                     | 0.73              |
| 15:O:373:LEU:HB3  | 15:O:374:PRO:HD3  | 1.70                     | 0.73              |
| 1:A:984:GLY:HA3   | 1:A:994:GLU:OE2   | 1.89                     | 0.72              |
| 1:A:990:ILE:CD1   | 1:A:995:TYR:N     | 2.52                     | 0.72              |
| 1:A:629:ASP:CA    | 2:B:926:VAL:HG21  | 2.19                     | 0.72              |
| 2:B:26:ILE:O      | 10:J:62:ARG:CZ    | 2.36                     | 0.72              |
| 2:B:985:ILE:C     | 14:N:160:VAL:HG23 | 2.14                     | 0.72              |
| 17:Q:12:THR:OG1   | 17:Q:33:HIS:CE1   | 2.42                     | 0.72              |
| 1:A:422:ARG:CB    | 18:R:409:HIS:HE1  | 1.98                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:953:GLU:HA    | 1:A:1205:PHE:HD2  | 1.52                     | 0.72              |
| 2:B:146:ASN:HD22  | 2:B:441:LYS:HE3   | 1.53                     | 0.72              |
| 2:B:1072:GLY:C    | 2:B:1075:GLU:CG   | 2.51                     | 0.72              |
| 1:A:999:CYS:CA    | 2:B:712:SER:HB3   | 2.15                     | 0.72              |
| 13:M:102:SER:O    | 13:M:105:SER:OG   | 2.08                     | 0.72              |
| 1:A:1262:LEU:HD21 | 1:A:1497:ILE:HG12 | 1.69                     | 0.72              |
| 8:H:40:LEU:HD13   | 8:H:123:MET:HE3   | 1.72                     | 0.72              |
| 16:P:350:THR:HG22 | 18:R:155:GLN:HA   | 1.72                     | 0.72              |
| 18:R:6:ILE:HD11   | 18:R:213:ILE:CB   | 2.19                     | 0.72              |
| 1:A:1309:SER:HB2  | 1:A:1310:LYS:HD3  | 1.71                     | 0.72              |
| 2:B:25:PHE:CD2    | 10:J:59:LYS:HG3   | 2.24                     | 0.72              |
| 2:B:404:LEU:O     | 2:B:407:PHE:N     | 2.23                     | 0.72              |
| 2:B:679:GLN:HG2   | 14:N:157:ARG:CA   | 2.14                     | 0.72              |
| 3:C:253:PRO:CD    | 14:N:180:PHE:CG   | 2.46                     | 0.72              |
| 16:P:446:ASP:OD2  | 16:P:448:THR:HG22 | 1.89                     | 0.72              |
| 18:R:373:LEU:HD12 | 18:R:411:VAL:HG21 | 1.70                     | 0.72              |
| 1:A:497:VAL:HG22  | 1:A:635:MET:HE1   | 1.70                     | 0.72              |
| 1:A:615:ARG:HH21  | 2:B:781:TYR:HD2   | 1.36                     | 0.72              |
| 1:A:991:LYS:CB    | 1:A:993:GLN:CB    | 2.62                     | 0.72              |
| 1:A:1554:GLY:HA2  | 5:E:183:PRO:HD2   | 1.72                     | 0.72              |
| 2:B:182:GLN:O     | 10:J:69:ARG:NE    | 2.23                     | 0.72              |
| 2:B:527:PHE:CE1   | 2:B:666:PRO:N     | 2.58                     | 0.72              |
| 1:A:399:LEU:CD2   | 1:A:423:LEU:CD2   | 2.67                     | 0.72              |
| 1:A:543:LEU:CB    | 17:Q:34:VAL:O     | 2.38                     | 0.72              |
| 1:A:1276:THR:CB   | 9:I:45:LEU:CD1    | 2.63                     | 0.72              |
| 3:C:231:PRO:HB2   | 3:C:270:ALA:HB1   | 1.72                     | 0.72              |
| 16:P:658:LYS:HB3  | 16:P:660:LYS:H    | 1.55                     | 0.72              |
| 2:B:143:TRP:CG    | 2:B:446:MET:CE    | 2.65                     | 0.72              |
| 2:B:152:LEU:HB3   | 2:B:443:LYS:HE3   | 0.73                     | 0.72              |
| 17:Q:330:TRP:CD1  | 17:Q:449:GLN:CA   | 2.73                     | 0.72              |
| 1:A:399:LEU:CD2   | 1:A:423:LEU:HD23  | 2.18                     | 0.72              |
| 2:B:68:ILE:HG21   | 2:B:71:LYS:HZ3    | 0.65                     | 0.72              |
| 2:B:527:PHE:CE1   | 2:B:666:PRO:CD    | 2.73                     | 0.72              |
| 17:Q:337:SER:HB3  | 17:Q:448:LYS:CD   | 2.13                     | 0.72              |
| 1:A:953:GLU:O     | 1:A:1205:PHE:CD1  | 2.43                     | 0.71              |
| 2:B:843:ASP:OD2   | 12:L:58:LYS:NZ    | 2.23                     | 0.71              |
| 1:A:436:ALA:C     | 1:A:439:ASP:N     | 2.32                     | 0.71              |
| 16:P:532:GLU:HA   | 16:P:554:ASN:HD22 | 1.55                     | 0.71              |
| 16:P:662:LEU:HB3  | 16:P:665:ASN:ND2  | 2.05                     | 0.71              |
| 17:Q:414:TYR:CE1  | 18:R:240:ILE:HG23 | 2.23                     | 0.71              |
| 1:A:83:VAL:CG1    | 1:A:427:PHE:CZ    | 2.73                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:581:ILE:HG13  | 1:A:585:ASP:CG    | 2.15                     | 0.71              |
| 2:B:898:LEU:N     | 12:L:46:VAL:HG21  | 2.06                     | 0.71              |
| 16:P:214:LEU:HB3  | 16:P:220:THR:HB   | 1.71                     | 0.71              |
| 1:A:435:ASN:O     | 1:A:439:ASP:CA    | 2.37                     | 0.71              |
| 1:A:921:PRO:HD2   | 8:H:19:ARG:HG3    | 1.73                     | 0.71              |
| 1:A:990:ILE:HA    | 1:A:994:GLU:CD    | 2.15                     | 0.71              |
| 2:B:207:ILE:HD11  | 2:B:503:VAL:CG1   | 2.20                     | 0.71              |
| 15:O:200:ASN:CB   | 17:Q:14:ASN:CA    | 2.53                     | 0.71              |
| 17:Q:367:PHE:HE2  | 18:R:1:MET:CE     | 2.02                     | 0.71              |
| 17:Q:414:TYR:CD1  | 18:R:240:ILE:HG12 | 2.26                     | 0.71              |
| 18:R:320:CYS:SG   | 18:R:374:LEU:CD1  | 2.79                     | 0.71              |
| 17:Q:288:GLU:HG3  | 17:Q:297:ARG:HH12 | 1.55                     | 0.71              |
| 1:A:566:SER:HB2   | 15:O:235:GLU:OE2  | 1.73                     | 0.71              |
| 1:A:953:GLU:HG2   | 1:A:1205:PHE:HE2  | 1.54                     | 0.71              |
| 1:A:1313:LEU:CG   | 1:A:1462:PHE:HZ   | 1.99                     | 0.71              |
| 2:B:1069:ILE:HD12 | 2:B:1069:ILE:N    | 2.06                     | 0.71              |
| 18:R:9:THR:HB     | 18:R:205:VAL:HG13 | 1.71                     | 0.71              |
| 1:A:436:ALA:O     | 1:A:440:SER:CA    | 2.37                     | 0.71              |
| 1:A:990:ILE:HD11  | 1:A:995:TYR:CA    | 2.11                     | 0.71              |
| 15:O:383:TYR:HD1  | 15:O:606:MET:HE3  | 1.54                     | 0.71              |
| 16:P:375:PHE:CE1  | 16:P:380:MET:HG3  | 2.25                     | 0.71              |
| 1:A:828:CYS:CB    | 2:B:1027:TYR:HB2  | 2.21                     | 0.71              |
| 15:O:376:TYR:CD1  | 15:O:419:LYS:CE   | 2.74                     | 0.71              |
| 16:P:197:ARG:CD   | 16:P:261:VAL:H    | 2.04                     | 0.71              |
| 16:P:475:ARG:NH2  | 17:Q:364:SER:CA   | 2.48                     | 0.71              |
| 2:B:679:GLN:HG3   | 14:N:155:VAL:C    | 2.16                     | 0.71              |
| 3:C:230:LEU:CD1   | 3:C:231:PRO:HD2   | 2.13                     | 0.71              |
| 3:C:296:ASN:OD1   | 3:C:297:HIS:N     | 2.24                     | 0.71              |
| 17:Q:183:LYS:O    | 17:Q:187:THR:OG1  | 2.08                     | 0.71              |
| 17:Q:351:ASN:HA   | 17:Q:369:TRP:CZ2  | 2.24                     | 0.71              |
| 1:A:507:TYR:HE1   | 1:A:509:GLU:HA    | 1.56                     | 0.71              |
| 1:A:524:ILE:O     | 1:A:554:ARG:NH1   | 2.24                     | 0.71              |
| 1:A:566:SER:CB    | 15:O:235:GLU:OE1  | 2.28                     | 0.71              |
| 1:A:686:PHE:HZ    | 8:H:121:LEU:HD11  | 1.56                     | 0.71              |
| 2:B:184:LYS:HD3   | 2:B:735:HIS:CD2   | 2.25                     | 0.71              |
| 2:B:184:LYS:HD3   | 2:B:735:HIS:NE2   | 2.04                     | 0.71              |
| 2:B:527:PHE:CE1   | 2:B:666:PRO:CA    | 2.72                     | 0.71              |
| 2:B:999:GLN:HG2   | 14:N:166:LEU:HD13 | 1.73                     | 0.71              |
| 2:B:1121:GLY:O    | 15:O:152:GLN:NE2  | 2.23                     | 0.71              |
| 16:P:436:ILE:CG2  | 18:R:143:THR:N    | 2.54                     | 0.71              |
| 17:Q:378:LEU:HD11 | 18:R:235:ILE:HD13 | 1.72                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:345:SER:HA    | 13:M:113:ILE:HD11 | 1.72                     | 0.70              |
| 16:P:350:THR:CG2  | 18:R:156:LYS:N    | 2.47                     | 0.70              |
| 16:P:656:HIS:H    | 16:P:656:HIS:CD2  | 2.06                     | 0.70              |
| 16:P:725:VAL:CG1  | 17:Q:449:GLN:CG   | 2.68                     | 0.70              |
| 1:A:399:LEU:HD23  | 1:A:423:LEU:CD2   | 2.21                     | 0.70              |
| 1:A:721:LYS:HZ3   | 8:H:90:ALA:C      | 1.97                     | 0.70              |
| 1:A:862:THR:CA    | 9:I:67:VAL:HA     | 2.21                     | 0.70              |
| 1:A:1329:ILE:HB   | 1:A:1456:PHE:HE2  | 1.54                     | 0.70              |
| 13:M:38:PHE:HB3   | 13:M:53:LEU:HD11  | 1.73                     | 0.70              |
| 15:O:216:LEU:HD13 | 15:O:342:HIS:CG   | 2.25                     | 0.70              |
| 16:P:389:TRP:HA   | 18:R:151:PRO:O    | 1.91                     | 0.70              |
| 1:A:921:PRO:CD    | 8:H:19:ARG:HG2    | 2.22                     | 0.70              |
| 2:B:75:ASP:CA     | 2:B:440:PHE:CE2   | 2.74                     | 0.70              |
| 2:B:894:LYS:HA    | 12:L:54:ARG:NE    | 2.06                     | 0.70              |
| 7:G:144:HIS:CD2   | 15:O:145:SER:C    | 2.69                     | 0.70              |
| 16:P:292:LEU:HD11 | 16:P:343:LEU:HG   | 1.72                     | 0.70              |
| 17:Q:194:GLN:NE2  | 18:R:209:ARG:HH11 | 1.90                     | 0.70              |
| 1:A:435:ASN:CG    | 1:A:442:LYS:HB3   | 2.16                     | 0.70              |
| 1:A:862:THR:CG2   | 9:I:67:VAL:HG12   | 2.21                     | 0.70              |
| 2:B:143:TRP:CB    | 2:B:446:MET:HE3   | 2.00                     | 0.70              |
| 2:B:346:ASP:OD2   | 13:M:114:LYS:N    | 2.22                     | 0.70              |
| 2:B:985:ILE:CB    | 14:N:160:VAL:CG2  | 2.67                     | 0.70              |
| 17:Q:22:ILE:CD1   | 17:Q:26:ARG:HE    | 2.04                     | 0.70              |
| 17:Q:414:TYR:OH   | 18:R:240:ILE:CG2  | 2.39                     | 0.70              |
| 18:R:317:LEU:HB2  | 18:R:367:ILE:CD1  | 2.22                     | 0.70              |
| 1:A:475:ARG:NE    | 2:B:1061:LYS:HB2  | 2.06                     | 0.70              |
| 16:P:345:ASP:OD1  | 16:P:345:ASP:N    | 2.23                     | 0.70              |
| 1:A:474:LYS:O     | 2:B:1070:ARG:CG   | 2.39                     | 0.70              |
| 1:A:1310:LYS:HD3  | 1:A:1310:LYS:N    | 2.05                     | 0.70              |
| 2:B:1089:GLN:NE2  | 2:B:1093:LEU:HD13 | 2.05                     | 0.70              |
| 2:B:1165:ASN:N    | 2:B:1165:ASN:OD1  | 2.24                     | 0.70              |
| 15:O:245:GLN:CD   | 15:O:379:ARG:HB2  | 2.16                     | 0.70              |
| 16:P:725:VAL:HA   | 17:Q:450:THR:CA   | 2.20                     | 0.70              |
| 1:A:475:ARG:NH2   | 2:B:1061:LYS:HG3  | 2.06                     | 0.70              |
| 1:A:629:ASP:HA    | 2:B:926:VAL:CG2   | 2.21                     | 0.70              |
| 1:A:1246:VAL:O    | 1:A:1517:ARG:NH2  | 2.24                     | 0.70              |
| 2:B:266:LYS:CD    | 2:B:473:GLN:O     | 2.40                     | 0.70              |
| 1:A:407:GLN:C     | 1:A:408:LYS:HZ3   | 1.99                     | 0.70              |
| 1:A:1660:VAL:O    | 7:G:102:GLU:CG    | 2.37                     | 0.70              |
| 16:P:659:LEU:H    | 16:P:659:LEU:HD13 | 1.55                     | 0.70              |
| 18:R:324:MET:CE   | 18:R:377:ASP:C    | 2.64                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:613:THR:CG2   | 2:B:913:ILE:HG21  | 2.21                     | 0.70              |
| 1:A:953:GLU:CB    | 1:A:1205:PHE:CE2  | 2.75                     | 0.70              |
| 2:B:143:TRP:CD1   | 2:B:446:MET:SD    | 2.84                     | 0.70              |
| 2:B:399:HIS:C     | 2:B:400:GLN:CG    | 2.65                     | 0.70              |
| 15:O:200:ASN:CA   | 17:Q:14:ASN:HB2   | 2.15                     | 0.70              |
| 15:O:517:LEU:HA   | 15:O:525:MET:HE3  | 1.72                     | 0.70              |
| 16:P:501:PRO:HB3  | 16:P:567:ILE:HG22 | 1.69                     | 0.70              |
| 1:A:395:LEU:CD1   | 18:R:410:TYR:CE1  | 2.73                     | 0.70              |
| 1:A:480:ALA:HB1   | 2:B:1046:VAL:HG23 | 1.74                     | 0.70              |
| 2:B:990:ASP:OD1   | 14:N:162:LYS:NZ   | 2.23                     | 0.70              |
| 3:C:272:LYS:HA    | 14:N:175:TYR:CG   | 2.24                     | 0.70              |
| 6:F:70:LYS:CG     | 7:G:95:LEU:HG     | 2.22                     | 0.70              |
| 16:P:364:GLU:O    | 16:P:373:LEU:HB2  | 1.91                     | 0.70              |
| 16:P:405:TYR:HB2  | 16:P:416:LEU:HD12 | 1.73                     | 0.70              |
| 1:A:507:TYR:CE1   | 1:A:509:GLU:HA    | 2.26                     | 0.69              |
| 1:A:1313:LEU:CD2  | 1:A:1462:PHE:CZ   | 2.72                     | 0.69              |
| 15:O:348:THR:CG2  | 15:O:351:SER:HB3  | 2.19                     | 0.69              |
| 17:Q:367:PHE:CE2  | 18:R:1:MET:CE     | 2.74                     | 0.69              |
| 1:A:1326:GLU:OE1  | 1:A:1454:HIS:C    | 2.34                     | 0.69              |
| 2:B:143:TRP:CZ2   | 2:B:446:MET:CB    | 2.75                     | 0.69              |
| 2:B:548:LYS:CE    | 2:B:695:ASN:OD1   | 2.40                     | 0.69              |
| 3:C:31:TRP:CH2    | 11:K:127:LEU:HD12 | 2.26                     | 0.69              |
| 3:C:230:LEU:HD13  | 3:C:299:ILE:HD11  | 1.72                     | 0.69              |
| 16:P:573:GLU:HB2  | 17:Q:499:LYS:HZ3  | 1.55                     | 0.69              |
| 18:R:186:LEU:C    | 18:R:186:LEU:HD13 | 2.17                     | 0.69              |
| 2:B:475:GLY:O     | 2:B:476:LEU:HB2   | 1.92                     | 0.69              |
| 2:B:894:LYS:HG2   | 12:L:47:ARG:NE    | 2.07                     | 0.69              |
| 2:B:1002:LYS:CD   | 14:N:166:LEU:C    | 2.60                     | 0.69              |
| 2:B:1069:ILE:HD12 | 2:B:1069:ILE:H    | 1.57                     | 0.69              |
| 17:Q:352:ILE:O    | 18:R:212:HIS:CE1  | 2.45                     | 0.69              |
| 17:Q:414:TYR:OH   | 18:R:240:ILE:HG23 | 1.91                     | 0.69              |
| 1:A:429:THR:HG23  | 18:R:406:LYS:NZ   | 2.05                     | 0.69              |
| 3:C:31:TRP:HH2    | 11:K:127:LEU:HD12 | 1.58                     | 0.69              |
| 16:P:436:ILE:HG21 | 18:R:143:THR:N    | 2.08                     | 0.69              |
| 17:Q:374:THR:CG2  | 18:R:219:LEU:HD13 | 2.22                     | 0.69              |
| 1:A:65:CYS:SG     | 19:A:2001:ZN:ZN   | 1.81                     | 0.69              |
| 1:A:466:LEU:HD11  | 2:B:1181:VAL:HG21 | 1.74                     | 0.69              |
| 1:A:489:ASN:HB2   | 11:K:95:HIS:CD2   | 2.27                     | 0.69              |
| 1:A:1032:VAL:CG2  | 1:A:1050:TYR:HD1  | 2.05                     | 0.69              |
| 1:A:1330:VAL:CG2  | 1:A:1455:ARG:NH1  | 2.56                     | 0.69              |
| 1:A:1482:LYS:HD3  | 2:B:304:ASP:OD1   | 1.90                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:142:ALA:HB3   | 15:O:102:SER:O    | 1.92                     | 0.69              |
| 9:I:2:SER:HB2     | 9:I:11:LEU:HD21   | 1.72                     | 0.69              |
| 2:B:212:ASN:HD21  | 2:B:361:HIS:HB2   | 1.56                     | 0.69              |
| 17:Q:22:ILE:HG13  | 17:Q:24:ASP:OD2   | 1.92                     | 0.69              |
| 16:P:725:VAL:HG11 | 17:Q:449:GLN:CG   | 2.23                     | 0.69              |
| 1:A:99:ARG:O      | 1:A:109:ARG:NH2   | 2.24                     | 0.69              |
| 1:A:436:ALA:CA    | 1:A:439:ASP:C     | 2.66                     | 0.69              |
| 1:A:507:TYR:CD1   | 1:A:508:PRO:C     | 2.70                     | 0.69              |
| 1:A:862:THR:O     | 9:I:66:VAL:O      | 2.10                     | 0.69              |
| 1:A:1314:GLN:HE22 | 1:A:1446:ARG:NE   | 1.91                     | 0.69              |
| 2:B:212:ASN:ND2   | 2:B:361:HIS:HB2   | 2.08                     | 0.69              |
| 2:B:887:LEU:HB2   | 12:L:56:LEU:O     | 1.93                     | 0.69              |
| 2:B:1049:THR:HG23 | 2:B:1050:GLY:H    | 1.57                     | 0.69              |
| 13:M:102:SER:CB   | 13:M:105:SER:CA   | 2.70                     | 0.69              |
| 16:P:438:TRP:CD1  | 18:R:141:TRP:HZ2  | 2.04                     | 0.69              |
| 17:Q:186:CYS:CB   | 18:R:208:TYR:HE1  | 2.05                     | 0.69              |
| 17:Q:258:MET:HE1  | 17:Q:438:PHE:HD2  | 1.54                     | 0.69              |
| 1:A:547:ILE:HD13  | 17:Q:26:ARG:NH1   | 1.98                     | 0.69              |
| 1:A:991:LYS:HB3   | 1:A:993:GLN:CB    | 2.23                     | 0.69              |
| 2:B:848:ILE:HG22  | 12:L:60:ARG:NH1   | 2.07                     | 0.69              |
| 2:B:850:THR:N     | 12:L:60:ARG:NH2   | 2.40                     | 0.69              |
| 15:O:237:ILE:HD12 | 15:O:237:ILE:N    | 2.08                     | 0.69              |
| 16:P:301:GLN:HG3  | 16:P:361:LYS:H    | 1.57                     | 0.69              |
| 16:P:412:ASN:OD1  | 16:P:412:ASN:N    | 2.24                     | 0.69              |
| 16:P:428:GLU:HB2  | 16:P:435:ARG:HH12 | 1.58                     | 0.69              |
| 16:P:473:HIS:HD2  | 18:R:1:MET:CB     | 2.04                     | 0.69              |
| 17:Q:194:GLN:HG3  | 17:Q:389:GLN:HB2  | 1.74                     | 0.69              |
| 17:Q:385:PHE:CE1  | 18:R:209:ARG:CG   | 2.75                     | 0.69              |
| 1:A:475:ARG:NH2   | 2:B:1061:LYS:CB   | 2.57                     | 0.68              |
| 4:D:99:LEU:HB3    | 4:D:100:PRO:CD    | 2.22                     | 0.68              |
| 16:P:184:SER:HA   | 18:R:198:LEU:HD23 | 0.69                     | 0.68              |
| 17:Q:330:TRP:CD1  | 17:Q:449:GLN:HA   | 2.28                     | 0.68              |
| 1:A:988:SER:HB2   | 2:B:988:GLU:HG2   | 1.75                     | 0.68              |
| 2:B:203:ILE:CG2   | 2:B:405:GLY:CA    | 2.71                     | 0.68              |
| 1:A:1660:VAL:HG22 | 7:G:103:LYS:O     | 1.93                     | 0.68              |
| 15:O:376:TYR:CD1  | 15:O:419:LYS:CD   | 2.76                     | 0.68              |
| 16:P:443:ASP:O    | 18:R:3:GLU:N      | 2.26                     | 0.68              |
| 16:P:584:ARG:O    | 16:P:588:SER:HB2  | 1.91                     | 0.68              |
| 1:A:470:HIS:CD2   | 2:B:1058:GLN:OE1  | 2.43                     | 0.68              |
| 2:B:551:ILE:CG2   | 2:B:647:SER:CA    | 2.71                     | 0.68              |
| 6:F:70:LYS:HG2    | 7:G:95:LEU:CD2    | 2.23                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:248:LEU:HD12 | 15:O:598:PHE:HE2  | 0.87                     | 0.68              |
| 16:P:232:ASN:N    | 16:P:232:ASN:OD1  | 2.27                     | 0.68              |
| 2:B:679:GLN:HG2   | 14:N:157:ARG:H    | 0.88                     | 0.68              |
| 17:Q:261:ALA:CB   | 17:Q:445:ARG:CG   | 2.72                     | 0.68              |
| 1:A:646:GLU:OE2   | 2:B:1086:PHE:HD2  | 1.75                     | 0.68              |
| 2:B:143:TRP:HE3   | 2:B:446:MET:HE3   | 1.56                     | 0.68              |
| 2:B:943:ILE:CD1   | 10:J:44:TYR:CZ    | 2.68                     | 0.68              |
| 16:P:725:VAL:CG1  | 17:Q:449:GLN:HG3  | 2.24                     | 0.68              |
| 18:R:359:MET:N    | 18:R:359:MET:SD   | 2.67                     | 0.68              |
| 2:B:62:ASN:OD1    | 2:B:102:VAL:HG23  | 1.93                     | 0.68              |
| 13:M:102:SER:O    | 13:M:105:SER:CB   | 2.42                     | 0.68              |
| 15:O:248:LEU:CG   | 15:O:598:PHE:CE2  | 2.74                     | 0.68              |
| 16:P:302:VAL:HG21 | 16:P:362:ARG:HD2  | 1.75                     | 0.68              |
| 16:P:717:LYS:O    | 17:Q:443:GLN:NE2  | 2.27                     | 0.68              |
| 2:B:152:LEU:CD2   | 2:B:443:LYS:HD2   | 2.15                     | 0.68              |
| 15:O:237:ILE:HD12 | 15:O:237:ILE:H    | 1.59                     | 0.68              |
| 17:Q:8:PRO:HG2    | 17:Q:19:LEU:HD23  | 1.74                     | 0.68              |
| 1:A:403:LEU:HD12  | 1:A:419:ILE:HD13  | 1.76                     | 0.68              |
| 1:A:671:GLN:OE1   | 2:B:952:HIS:CB    | 2.42                     | 0.68              |
| 2:B:291:GLY:HA3   | 2:B:375:LEU:HD13  | 1.74                     | 0.68              |
| 16:P:302:VAL:HG11 | 16:P:362:ARG:HH11 | 1.57                     | 0.68              |
| 2:B:65:VAL:HG23   | 2:B:417:ILE:HD12  | 1.74                     | 0.68              |
| 2:B:1072:GLY:C    | 2:B:1075:GLU:H    | 2.02                     | 0.68              |
| 16:P:197:ARG:CG   | 16:P:261:VAL:O    | 2.42                     | 0.68              |
| 16:P:353:ASP:OD1  | 16:P:379:LYS:NZ   | 2.27                     | 0.68              |
| 7:G:242:VAL:HG21  | 15:O:183:ILE:HG23 | 1.74                     | 0.67              |
| 16:P:53:ASP:OD2   | 16:P:54:ALA:N     | 2.27                     | 0.67              |
| 17:Q:218:SER:O    | 17:Q:218:SER:OG   | 2.11                     | 0.67              |
| 17:Q:341:ARG:CZ   | 17:Q:369:TRP:NE1  | 2.54                     | 0.67              |
| 1:A:472:MET:CE    | 2:B:1076:ARG:HD3  | 2.24                     | 0.67              |
| 1:A:502:ALA:O     | 1:A:580:HIS:HB3   | 1.93                     | 0.67              |
| 17:Q:261:ALA:HB2  | 17:Q:445:ARG:CG   | 2.23                     | 0.67              |
| 1:A:722:PRO:HD3   | 8:H:95:TYR:HA     | 1.76                     | 0.67              |
| 1:A:1655:ASP:OD2  | 6:F:137:TYR:OH    | 2.10                     | 0.67              |
| 15:O:233:LEU:O    | 15:O:236:LYS:HB2  | 1.94                     | 0.67              |
| 17:Q:355:VAL:O    | 18:R:211:ARG:CG   | 2.43                     | 0.67              |
| 1:A:472:MET:HA    | 1:A:472:MET:CE    | 2.16                     | 0.67              |
| 2:B:848:ILE:HB    | 12:L:60:ARG:HD2   | 0.71                     | 0.67              |
| 3:C:125:LYS:O     | 3:C:130:ASN:ND2   | 2.27                     | 0.67              |
| 16:P:193:LEU:HD12 | 16:P:251:SER:H    | 1.59                     | 0.67              |
| 16:P:218:VAL:HG13 | 16:P:246:LYS:H    | 1.57                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:429:THR:CG2   | 18:R:406:LYS:CD   | 2.42                     | 0.67              |
| 2:B:527:PHE:CE2   | 2:B:666:PRO:HB3   | 2.29                     | 0.67              |
| 15:O:373:LEU:HD12 | 15:O:423:TYR:CE2  | 2.30                     | 0.67              |
| 15:O:439:ILE:HD13 | 15:O:487:ARG:HD3  | 1.76                     | 0.67              |
| 16:P:622:TYR:CZ   | 16:P:668:SER:HB3  | 2.30                     | 0.67              |
| 18:R:161:ASN:HA   | 18:R:164:LYS:HD2  | 1.76                     | 0.67              |
| 1:A:629:ASP:CA    | 2:B:926:VAL:CG2   | 2.72                     | 0.67              |
| 2:B:143:TRP:CZ2   | 2:B:446:MET:HB2   | 2.28                     | 0.67              |
| 3:C:127:THR:H     | 3:C:130:ASN:HB2   | 1.59                     | 0.67              |
| 16:P:184:SER:CB   | 18:R:198:LEU:CG   | 2.49                     | 0.67              |
| 17:Q:352:ILE:HD13 | 17:Q:377:PHE:CD2  | 2.20                     | 0.67              |
| 1:A:1656:VAL:HA   | 6:F:133:VAL:O     | 1.95                     | 0.67              |
| 7:G:144:HIS:CD2   | 15:O:146:SER:CB   | 2.77                     | 0.67              |
| 15:O:66:ASN:HD22  | 15:O:66:ASN:N     | 1.89                     | 0.67              |
| 17:Q:325:GLN:HG2  | 17:Q:452:PHE:CE2  | 2.22                     | 0.67              |
| 1:A:477:ASN:HA    | 2:B:1047:ARG:HD3  | 1.77                     | 0.67              |
| 1:A:878:ARG:CB    | 9:I:67:VAL:HG11   | 2.05                     | 0.67              |
| 1:A:952:LEU:HD22  | 1:A:1004:GLU:CG   | 2.09                     | 0.67              |
| 2:B:683:ASN:H     | 14:N:154:ARG:NH2  | 1.86                     | 0.67              |
| 3:C:272:LYS:CB    | 14:N:175:TYR:CD1  | 2.78                     | 0.67              |
| 15:O:390:GLN:HG2  | 15:O:396:MET:HE3  | 1.77                     | 0.67              |
| 15:O:468:GLU:O    | 15:O:471:LYS:HG3  | 1.94                     | 0.67              |
| 1:A:475:ARG:CB    | 2:B:1059:PRO:HB2  | 2.24                     | 0.67              |
| 1:A:990:ILE:CG1   | 1:A:995:TYR:CA    | 2.72                     | 0.67              |
| 6:F:66:ARG:HH21   | 7:G:90:LEU:CD1    | 2.06                     | 0.67              |
| 15:O:376:TYR:CZ   | 15:O:588:LEU:CD2  | 2.76                     | 0.67              |
| 16:P:704:LEU:HB3  | 17:Q:439:ILE:HG13 | 1.76                     | 0.67              |
| 17:Q:186:CYS:HA   | 18:R:208:TYR:OH   | 1.94                     | 0.67              |
| 17:Q:330:TRP:NE1  | 17:Q:449:GLN:HB3  | 2.02                     | 0.67              |
| 18:R:186:LEU:HD13 | 18:R:186:LEU:O    | 1.95                     | 0.67              |
| 18:R:266:SER:O    | 18:R:269:ASP:N    | 2.28                     | 0.67              |
| 1:A:83:VAL:CG1    | 1:A:427:PHE:CE2   | 2.77                     | 0.66              |
| 1:A:1263:LEU:HA   | 1:A:1498:ILE:CD1  | 2.25                     | 0.66              |
| 1:A:1330:VAL:CG2  | 1:A:1455:ARG:CD   | 2.73                     | 0.66              |
| 16:P:448:THR:CG2  | 16:P:471:MET:H    | 2.08                     | 0.66              |
| 1:A:113:VAL:HG21  | 1:A:178:LEU:HD13  | 1.77                     | 0.66              |
| 1:A:406:LEU:N     | 1:A:406:LEU:HD23  | 2.10                     | 0.66              |
| 1:A:671:GLN:HB3   | 2:B:952:HIS:CD2   | 2.30                     | 0.66              |
| 2:B:531:VAL:O     | 2:B:716:MET:HG3   | 1.95                     | 0.66              |
| 3:C:229:LEU:CD2   | 3:C:295:ARG:O     | 2.42                     | 0.66              |
| 16:P:458:LYS:HD3  | 16:P:461:HIS:HE1  | 1.60                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:189:LYS:HA   | 17:Q:384:GLN:CG   | 2.25                     | 0.66              |
| 18:R:253:ILE:HA   | 18:R:256:GLU:HB3  | 1.76                     | 0.66              |
| 2:B:1090:ASP:O    | 2:B:1094:ASN:HB2  | 1.96                     | 0.66              |
| 17:Q:371:GLU:HG3  | 18:R:231:LEU:HG   | 1.76                     | 0.66              |
| 1:A:467:PHE:CE2   | 1:A:1614:SER:HB3  | 2.31                     | 0.66              |
| 1:A:799:GLU:HG3   | 1:A:1062:HIS:CE1  | 2.30                     | 0.66              |
| 2:B:207:ILE:CD1   | 2:B:503:VAL:HG22  | 2.21                     | 0.66              |
| 2:B:985:ILE:CB    | 14:N:160:VAL:HG21 | 2.24                     | 0.66              |
| 15:O:383:TYR:CD1  | 15:O:606:MET:HE3  | 2.31                     | 0.66              |
| 17:Q:208:PRO:HG2  | 17:Q:211:TYR:HD2  | 1.59                     | 0.66              |
| 2:B:209:GLN:O     | 2:B:401:GLU:N     | 2.27                     | 0.66              |
| 2:B:469:ASN:OD1   | 2:B:482:SER:HB3   | 1.95                     | 0.66              |
| 5:E:76:GLY:HA3    | 5:E:106:GLN:HB2   | 1.76                     | 0.66              |
| 17:Q:139:LYS:HG2  | 17:Q:237:ILE:HG12 | 1.76                     | 0.66              |
| 18:R:324:MET:SD   | 18:R:377:ASP:C    | 2.79                     | 0.66              |
| 2:B:399:HIS:C     | 2:B:400:GLN:HG3   | 2.20                     | 0.66              |
| 2:B:527:PHE:CE1   | 2:B:666:PRO:CB    | 2.79                     | 0.66              |
| 3:C:41:GLU:OE2    | 11:K:138:LYS:CE   | 2.41                     | 0.66              |
| 16:P:397:LYS:NZ   | 18:R:85:ARG:CZ    | 2.56                     | 0.66              |
| 16:P:488:LEU:HD22 | 18:R:138:PHE:CZ   | 2.30                     | 0.66              |
| 1:A:824:THR:O     | 2:B:1023:ARG:CB   | 2.44                     | 0.66              |
| 2:B:209:GLN:HG2   | 2:B:210:ARG:N     | 2.07                     | 0.66              |
| 2:B:796:ARG:O     | 10:J:8:PHE:CE1    | 2.48                     | 0.66              |
| 15:O:240:ILE:HG23 | 15:O:332:LEU:HG   | 1.78                     | 0.66              |
| 16:P:725:VAL:HG11 | 17:Q:449:GLN:HG2  | 1.78                     | 0.66              |
| 16:P:775:TRP:HE1  | 16:P:778:ASP:HA   | 1.61                     | 0.66              |
| 17:Q:263:PRO:CA   | 17:Q:446:TYR:HE1  | 1.93                     | 0.66              |
| 1:A:990:ILE:CG1   | 1:A:994:GLU:C     | 2.69                     | 0.66              |
| 2:B:531:VAL:HG13  | 2:B:716:MET:HA    | 1.77                     | 0.66              |
| 1:A:399:LEU:HD21  | 1:A:423:LEU:CG    | 2.25                     | 0.66              |
| 1:A:1032:VAL:CG2  | 1:A:1050:TYR:CE1  | 2.79                     | 0.66              |
| 1:A:1482:LYS:O    | 2:B:308:LEU:CD2   | 2.38                     | 0.66              |
| 2:B:1072:GLY:O    | 2:B:1075:GLU:N    | 2.29                     | 0.66              |
| 15:O:238:ILE:HD12 | 15:O:238:ILE:H    | 1.61                     | 0.66              |
| 17:Q:337:SER:HB2  | 17:Q:448:LYS:HD2  | 1.77                     | 0.66              |
| 18:R:199:LYS:HD3  | 18:R:204:GLU:HB3  | 1.76                     | 0.66              |
| 1:A:1657:LEU:HD22 | 7:G:104:LEU:HD12  | 1.70                     | 0.66              |
| 17:Q:330:TRP:HD1  | 17:Q:449:GLN:HA   | 1.60                     | 0.66              |
| 17:Q:358:PRO:HA   | 18:R:206:ARG:CG   | 2.26                     | 0.66              |
| 1:A:718:THR:HG23  | 8:H:118:PHE:HB3   | 1.78                     | 0.65              |
| 1:A:878:ARG:HG2   | 9:I:67:VAL:CG1    | 2.05                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:921:PRO:CD    | 8:H:19:ARG:CG     | 2.74                     | 0.65              |
| 1:A:1310:LYS:H    | 1:A:1310:LYS:CD   | 2.08                     | 0.65              |
| 2:B:894:LYS:HG2   | 12:L:47:ARG:HE    | 1.62                     | 0.65              |
| 6:F:70:LYS:HG2    | 7:G:95:LEU:CG     | 2.26                     | 0.65              |
| 16:P:322:GLY:O    | 16:P:350:THR:OG1  | 2.07                     | 0.65              |
| 16:P:717:LYS:CD   | 17:Q:439:ILE:CD1  | 2.74                     | 0.65              |
| 1:A:109:ARG:NH1   | 1:A:230:ARG:O     | 2.29                     | 0.65              |
| 1:A:1329:ILE:HG22 | 1:A:1456:PHE:CE2  | 2.30                     | 0.65              |
| 16:P:321:LYS:HA   | 16:P:361:LYS:HD3  | 1.78                     | 0.65              |
| 1:A:472:MET:SD    | 2:B:1073:GLU:CD   | 2.79                     | 0.65              |
| 14:N:87:TYR:CB    | 14:N:141:GLU:CA   | 2.65                     | 0.65              |
| 18:R:199:LYS:NZ   | 18:R:204:GLU:CB   | 2.60                     | 0.65              |
| 18:R:320:CYS:SG   | 18:R:374:LEU:CD2  | 2.84                     | 0.65              |
| 1:A:627:ASP:O     | 2:B:784:ASP:O     | 2.15                     | 0.65              |
| 1:A:824:THR:HB    | 2:B:1023:ARG:CB   | 2.13                     | 0.65              |
| 1:A:995:TYR:OH    | 2:B:715:ASN:CG    | 2.39                     | 0.65              |
| 2:B:711:GLN:HG2   | 2:B:713:PRO:HD2   | 1.78                     | 0.65              |
| 16:P:724:LEU:O    | 17:Q:450:THR:HG21 | 1.96                     | 0.65              |
| 17:Q:194:GLN:NE2  | 18:R:209:ARG:CZ   | 2.59                     | 0.65              |
| 1:A:1330:VAL:HG23 | 1:A:1455:ARG:NH1  | 2.10                     | 0.65              |
| 2:B:64:GLY:CA     | 2:B:242:ASP:CB    | 2.74                     | 0.65              |
| 16:P:443:ASP:HB3  | 18:R:3:GLU:HB2    | 1.77                     | 0.65              |
| 17:Q:196:SER:HB3  | 17:Q:204:ARG:HG2  | 1.76                     | 0.65              |
| 17:Q:208:PRO:HG2  | 17:Q:211:TYR:CD2  | 2.32                     | 0.65              |
| 18:R:242:ILE:HG22 | 18:R:245:VAL:HG22 | 1.77                     | 0.65              |
| 1:A:1484:LEU:CD2  | 2:B:304:ASP:CB    | 2.73                     | 0.65              |
| 2:B:212:ASN:ND2   | 2:B:361:HIS:CB    | 2.59                     | 0.65              |
| 15:O:392:GLN:HB2  | 15:O:395:LEU:HD22 | 1.79                     | 0.65              |
| 16:P:769:GLN:HA   | 16:P:772:ILE:HB   | 1.79                     | 0.65              |
| 18:R:173:MET:HG3  | 18:R:188:PHE:CZ   | 2.25                     | 0.65              |
| 1:A:475:ARG:C     | 2:B:1059:PRO:HG2  | 2.21                     | 0.65              |
| 1:A:615:ARG:NH2   | 2:B:781:TYR:CD2   | 2.64                     | 0.65              |
| 1:A:1660:VAL:C    | 7:G:102:GLU:HG2   | 2.22                     | 0.65              |
| 2:B:345:SER:HA    | 13:M:113:ILE:CD1  | 2.27                     | 0.65              |
| 7:G:144:HIS:CE1   | 15:O:145:SER:CB   | 2.79                     | 0.65              |
| 16:P:436:ILE:HB   | 18:R:143:THR:HG21 | 1.76                     | 0.65              |
| 17:Q:343:THR:OG1  | 17:Q:372:GLU:CD   | 2.38                     | 0.65              |
| 1:A:670:ILE:HD11  | 2:B:783:MET:HE2   | 1.79                     | 0.65              |
| 2:B:328:GLN:NE2   | 13:M:111:PRO:O    | 2.29                     | 0.65              |
| 3:C:328:LEU:HD23  | 11:K:121:LEU:HD21 | 1.79                     | 0.65              |
| 16:P:350:THR:CG2  | 18:R:155:GLN:HA   | 2.26                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:290:THR:HB   | 17:Q:292:GLU:H    | 1.61                     | 0.65              |
| 1:A:1273:THR:HG23 | 9:I:48:VAL:HG22   | 1.79                     | 0.65              |
| 2:B:373:MET:HG3   | 2:B:377:MET:HE3   | 1.79                     | 0.65              |
| 18:R:5:PRO:HG3    | 18:R:217:THR:HB   | 1.78                     | 0.65              |
| 1:A:998:HIS:CE1   | 2:B:711:GLN:HG3   | 2.31                     | 0.65              |
| 15:O:219:ARG:NH2  | 15:O:360:VAL:HG22 | 2.12                     | 0.65              |
| 1:A:862:THR:HA    | 9:I:67:VAL:HB     | 1.77                     | 0.64              |
| 2:B:49:PHE:CD2    | 2:B:194:PHE:HZ    | 2.14                     | 0.64              |
| 2:B:681:ILE:CB    | 14:N:154:ARG:HG3  | 2.23                     | 0.64              |
| 2:B:1072:GLY:O    | 2:B:1075:GLU:CA   | 2.45                     | 0.64              |
| 15:O:376:TYR:CG   | 15:O:419:LYS:CE   | 2.80                     | 0.64              |
| 16:P:184:SER:CB   | 18:R:198:LEU:HG   | 2.01                     | 0.64              |
| 1:A:408:LYS:HA    | 1:A:411:VAL:CB    | 2.25                     | 0.64              |
| 1:A:611:GLU:OE2   | 2:B:929:ARG:NH2   | 2.29                     | 0.64              |
| 17:Q:194:GLN:NE2  | 18:R:209:ARG:NH1  | 2.46                     | 0.64              |
| 1:A:825:ALA:O     | 2:B:1023:ARG:NH1  | 2.30                     | 0.64              |
| 2:B:923:GLN:NE2   | 2:B:953:ALA:O     | 2.30                     | 0.64              |
| 2:B:1069:ILE:O    | 2:B:1070:ARG:CB   | 2.45                     | 0.64              |
| 14:N:87:TYR:OH    | 14:N:141:GLU:OE1  | 2.16                     | 0.64              |
| 15:O:517:LEU:HA   | 15:O:525:MET:CE   | 2.27                     | 0.64              |
| 16:P:405:TYR:OH   | 16:P:414:ILE:HG12 | 1.97                     | 0.64              |
| 17:Q:358:PRO:HA   | 18:R:206:ARG:HD3  | 1.79                     | 0.64              |
| 1:A:486:PRO:HG2   | 2:B:781:TYR:HA    | 1.78                     | 0.64              |
| 17:Q:15:CYS:HB2   | 17:Q:16:PRO:HA    | 1.77                     | 0.64              |
| 17:Q:356:VAL:HA   | 18:R:211:ARG:CG   | 2.20                     | 0.64              |
| 1:A:1054:ALA:O    | 1:A:1179:ILE:HG22 | 1.96                     | 0.64              |
| 15:O:376:TYR:HB2  | 15:O:419:LYS:HD3  | 1.79                     | 0.64              |
| 16:P:454:GLN:HA   | 16:P:455:LYS:HE2  | 1.79                     | 0.64              |
| 18:R:303:THR:HG22 | 18:R:304:HIS:H    | 1.62                     | 0.64              |
| 2:B:341:SER:OG    | 2:B:343:ASP:OD1   | 2.13                     | 0.64              |
| 15:O:510:VAL:HG13 | 15:O:517:LEU:HD11 | 1.79                     | 0.64              |
| 16:P:263:ILE:HG22 | 16:P:264:ILE:HG22 | 1.79                     | 0.64              |
| 16:P:473:HIS:HD2  | 18:R:1:MET:HB3    | 1.63                     | 0.64              |
| 16:P:725:VAL:CG1  | 17:Q:449:GLN:HG2  | 2.27                     | 0.64              |
| 16:P:775:TRP:H    | 17:Q:109:GLN:NE2  | 1.95                     | 0.64              |
| 1:A:878:ARG:HB3   | 9:I:67:VAL:HG12   | 1.68                     | 0.64              |
| 16:P:625:ASP:O    | 16:P:629:ARG:CB   | 2.45                     | 0.64              |
| 16:P:724:LEU:CD1  | 17:Q:447:ALA:CB   | 2.76                     | 0.64              |
| 17:Q:8:PRO:HB2    | 17:Q:19:LEU:HD23  | 1.80                     | 0.64              |
| 17:Q:263:PRO:C    | 17:Q:446:TYR:CE1  | 2.76                     | 0.64              |
| 15:O:375:THR:C    | 15:O:377:TYR:H    | 2.03                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:184:SER:CB   | 18:R:198:LEU:HD23 | 1.95                     | 0.64              |
| 16:P:656:HIS:HB2  | 16:P:747:LEU:O    | 1.97                     | 0.64              |
| 16:P:662:LEU:O    | 16:P:665:ASN:ND2  | 2.31                     | 0.64              |
| 16:P:704:LEU:HA   | 17:Q:438:PHE:CD2  | 2.31                     | 0.64              |
| 1:A:406:LEU:HB3   | 1:A:408:LYS:HD3   | 1.80                     | 0.64              |
| 1:A:436:ALA:HA    | 1:A:440:SER:HA    | 1.80                     | 0.64              |
| 2:B:45:HIS:NE2    | 2:B:500:PHE:HB3   | 2.13                     | 0.64              |
| 3:C:293:ARG:HB2   | 3:C:295:ARG:HD3   | 1.80                     | 0.64              |
| 15:O:240:ILE:HA   | 15:O:332:LEU:HD12 | 1.79                     | 0.64              |
| 16:P:479:HIS:NE2  | 16:P:491:SER:OG   | 2.24                     | 0.64              |
| 17:Q:385:PHE:HZ   | 18:R:209:ARG:CA   | 2.09                     | 0.64              |
| 2:B:29:PRO:O      | 2:B:178:TYR:N     | 2.29                     | 0.64              |
| 2:B:1072:GLY:O    | 2:B:1076:ARG:N    | 2.31                     | 0.64              |
| 4:D:99:LEU:HB3    | 4:D:100:PRO:HD3   | 1.78                     | 0.64              |
| 6:F:72:LYS:HA     | 6:F:142:SER:CB    | 2.13                     | 0.64              |
| 15:O:428:ILE:HD11 | 15:O:442:VAL:HG21 | 1.79                     | 0.64              |
| 1:A:1659:LYS:HG2  | 7:G:102:GLU:OE1   | 1.98                     | 0.63              |
| 2:B:294:GLY:HA3   | 2:B:579:ALA:HB3   | 1.80                     | 0.63              |
| 3:C:292:GLY:HA3   | 3:C:295:ARG:NH2   | 2.12                     | 0.63              |
| 5:E:20:LYS:HE2    | 5:E:34:GLU:HG2    | 1.80                     | 0.63              |
| 16:P:24:SER:CB    | 18:R:318:ILE:CD1  | 2.76                     | 0.63              |
| 16:P:354:PRO:HB2  | 18:R:27:ILE:CG2   | 2.16                     | 0.63              |
| 16:P:700:LEU:HD12 | 16:P:703:PHE:HD2  | 1.62                     | 0.63              |
| 18:R:313:LEU:HD21 | 18:R:364:VAL:HG12 | 1.80                     | 0.63              |
| 18:R:412:ARG:NH2  | 18:R:439:GLU:OE2  | 2.31                     | 0.63              |
| 1:A:460:LEU:HD21  | 2:B:1188:GLU:HG3  | 1.80                     | 0.63              |
| 1:A:506:THR:HG21  | 1:A:578:TYR:O     | 1.98                     | 0.63              |
| 1:A:641:GLU:HB2   | 6:F:99:LEU:HD13   | 1.78                     | 0.63              |
| 6:F:75:PRO:HG2    | 6:F:78:GLN:CB     | 2.08                     | 0.63              |
| 7:G:159:LYS:CD    | 15:O:103:ASN:CG   | 2.63                     | 0.63              |
| 1:A:477:ASN:CA    | 2:B:1047:ARG:HD3  | 2.29                     | 0.63              |
| 1:A:671:GLN:HB3   | 2:B:952:HIS:CG    | 2.32                     | 0.63              |
| 2:B:527:PHE:CE2   | 2:B:666:PRO:CA    | 2.62                     | 0.63              |
| 2:B:1005:TYR:CD2  | 14:N:170:HIS:ND1  | 2.66                     | 0.63              |
| 7:G:241:ARG:CZ    | 15:O:189:PHE:HB3  | 2.29                     | 0.63              |
| 8:H:44:VAL:HG22   | 8:H:48:PRO:HA     | 1.81                     | 0.63              |
| 15:O:108:GLU:HG3  | 15:O:108:GLU:O    | 1.96                     | 0.63              |
| 16:P:197:ARG:NE   | 16:P:261:VAL:HG22 | 2.14                     | 0.63              |
| 16:P:532:GLU:HB2  | 16:P:554:ASN:HB3  | 1.81                     | 0.63              |
| 16:P:697:GLU:OE1  | 16:P:697:GLU:N    | 2.30                     | 0.63              |
| 18:R:141:TRP:H    | 18:R:141:TRP:CD1  | 2.16                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:432:ASN:OD1   | 1:A:443:ALA:HA    | 1.99                     | 0.63              |
| 1:A:1049:MET:HB2  | 1:A:1052:GLY:HA2  | 1.80                     | 0.63              |
| 5:E:197:LYS:HD3   | 5:E:199:ILE:HD11  | 1.79                     | 0.63              |
| 17:Q:6:ARG:O      | 17:Q:7:GLY:O      | 2.17                     | 0.63              |
| 17:Q:343:THR:HG1  | 17:Q:372:GLU:CD   | 1.97                     | 0.63              |
| 1:A:472:MET:CG    | 2:B:1073:GLU:OE1  | 2.46                     | 0.63              |
| 3:C:294:VAL:O     | 3:C:297:HIS:CB    | 2.44                     | 0.63              |
| 15:O:387:HIS:HB2  | 15:O:606:MET:HE1  | 1.79                     | 0.63              |
| 16:P:184:SER:CA   | 18:R:198:LEU:HD21 | 2.10                     | 0.63              |
| 17:Q:186:CYS:C    | 18:R:208:TYR:OH   | 2.40                     | 0.63              |
| 1:A:476:VAL:CA    | 2:B:1059:PRO:HG2  | 2.28                     | 0.63              |
| 1:A:921:PRO:HD2   | 8:H:19:ARG:CG     | 2.28                     | 0.63              |
| 1:A:1329:ILE:CB   | 1:A:1456:PHE:HE2  | 2.12                     | 0.63              |
| 2:B:1096:SER:O    | 2:B:1097:ASP:CB   | 2.47                     | 0.63              |
| 6:F:69:LEU:O      | 6:F:143:PHE:CE2   | 2.52                     | 0.63              |
| 15:O:227:PHE:HD1  | 15:O:363:THR:HB   | 1.62                     | 0.63              |
| 16:P:24:SER:HB2   | 18:R:318:ILE:CD1  | 2.22                     | 0.63              |
| 16:P:675:PHE:HE2  | 16:P:741:ILE:HG21 | 1.63                     | 0.63              |
| 17:Q:212:VAL:O    | 17:Q:216:GLU:HG2  | 1.98                     | 0.63              |
| 18:R:26:TYR:HB3   | 18:R:169:PRO:HB3  | 1.81                     | 0.63              |
| 1:A:998:HIS:CD2   | 2:B:711:GLN:HA    | 2.33                     | 0.63              |
| 2:B:848:ILE:CB    | 12:L:60:ARG:CD    | 2.39                     | 0.63              |
| 6:F:72:LYS:CG     | 6:F:142:SER:CB    | 2.77                     | 0.63              |
| 7:G:144:HIS:NE2   | 15:O:146:SER:N    | 2.46                     | 0.63              |
| 17:Q:15:CYS:SG    | 17:Q:17:SER:CB    | 2.83                     | 0.63              |
| 17:Q:194:GLN:HE21 | 18:R:209:ARG:NE   | 1.92                     | 0.63              |
| 18:R:248:LYS:CB   | 18:R:298:GLN:NE2  | 2.61                     | 0.63              |
| 1:A:475:ARG:O     | 2:B:1059:PRO:HG2  | 1.99                     | 0.63              |
| 1:A:966:LEU:CD2   | 1:A:997:PHE:HZ    | 2.11                     | 0.63              |
| 1:A:1606:SER:HB2  | 1:A:1611:MET:HE3  | 1.80                     | 0.63              |
| 2:B:143:TRP:CE3   | 2:B:446:MET:CE    | 2.82                     | 0.63              |
| 16:P:501:PRO:CB   | 16:P:567:ILE:HG21 | 2.24                     | 0.63              |
| 17:Q:8:PRO:O      | 17:Q:9:ILE:C      | 2.42                     | 0.63              |
| 17:Q:283:ASN:OD1  | 17:Q:284:LEU:N    | 2.27                     | 0.63              |
| 18:R:5:PRO:CG     | 18:R:217:THR:CB   | 2.77                     | 0.63              |
| 1:A:493:ASN:CB    | 1:A:654:ASP:OD1   | 2.47                     | 0.63              |
| 1:A:581:ILE:HD11  | 1:A:585:ASP:HB3   | 1.81                     | 0.63              |
| 1:A:799:GLU:HG3   | 1:A:1062:HIS:ND1  | 2.14                     | 0.63              |
| 2:B:527:PHE:CE2   | 2:B:666:PRO:CB    | 2.82                     | 0.63              |
| 2:B:1072:GLY:O    | 2:B:1075:GLU:CB   | 2.47                     | 0.63              |
| 2:B:1079:LEU:O    | 2:B:1083:GLY:N    | 2.31                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:374:PRO:O    | 15:O:376:TYR:CB   | 2.39                     | 0.63              |
| 17:Q:351:ASN:O    | 17:Q:369:TRP:HH2  | 1.82                     | 0.63              |
| 18:R:180:CYS:SG   | 18:R:185:LYS:HG2  | 2.39                     | 0.63              |
| 18:R:199:LYS:HZ1  | 18:R:204:GLU:CA   | 2.10                     | 0.63              |
| 18:R:305:THR:HB   | 18:R:308:PHE:HE1  | 1.64                     | 0.63              |
| 18:R:308:PHE:HD1  | 18:R:309:ALA:H    | 1.46                     | 0.63              |
| 1:A:684:ASP:OD1   | 8:H:20:TYR:HB3    | 1.97                     | 0.62              |
| 1:A:1329:ILE:CG2  | 1:A:1456:PHE:HE2  | 2.05                     | 0.62              |
| 1:A:1484:LEU:HD11 | 2:B:305:ARG:NE    | 2.14                     | 0.62              |
| 2:B:1089:GLN:CG   | 2:B:1093:LEU:CB   | 2.69                     | 0.62              |
| 7:G:144:HIS:CE1   | 15:O:145:SER:HB2  | 2.34                     | 0.62              |
| 15:O:181:ARG:HB2  | 15:O:181:ARG:NH1  | 2.13                     | 0.62              |
| 16:P:197:ARG:HE   | 16:P:261:VAL:HG22 | 1.62                     | 0.62              |
| 16:P:268:SER:HG   | 16:P:271:ILE:H    | 1.47                     | 0.62              |
| 16:P:278:HIS:HB2  | 16:P:285:MET:HE3  | 1.81                     | 0.62              |
| 17:Q:245:SER:HB3  | 17:Q:284:LEU:HB2  | 1.80                     | 0.62              |
| 17:Q:291:ASP:OD2  | 17:Q:291:ASP:N    | 2.32                     | 0.62              |
| 17:Q:420:ASP:O    | 18:R:234:LYS:NZ   | 2.23                     | 0.62              |
| 18:R:157:MET:HG3  | 18:R:162:PHE:HB2  | 1.81                     | 0.62              |
| 6:F:73:ALA:HA     | 6:F:143:PHE:CG    | 2.32                     | 0.62              |
| 17:Q:189:LYS:CA   | 17:Q:384:GLN:HG2  | 2.29                     | 0.62              |
| 1:A:467:PHE:CD2   | 1:A:1614:SER:HB2  | 2.34                     | 0.62              |
| 2:B:205:MET:CE    | 2:B:500:PHE:O     | 2.47                     | 0.62              |
| 2:B:897:GLU:HA    | 12:L:46:VAL:CG2   | 2.29                     | 0.62              |
| 15:O:181:ARG:HH11 | 15:O:181:ARG:CG   | 2.12                     | 0.62              |
| 15:O:376:TYR:CD1  | 15:O:419:LYS:HD3  | 2.34                     | 0.62              |
| 16:P:365:TRP:HB2  | 16:P:371:LYS:O    | 2.00                     | 0.62              |
| 17:Q:15:CYS:HB3   | 17:Q:17:SER:H     | 1.62                     | 0.62              |
| 1:A:486:PRO:HG2   | 2:B:781:TYR:CA    | 2.30                     | 0.62              |
| 2:B:30:LYS:C      | 2:B:176:SER:CB    | 2.72                     | 0.62              |
| 7:G:24:VAL:HA     | 7:G:25:THR:CA     | 2.25                     | 0.62              |
| 16:P:473:HIS:C    | 16:P:504:THR:HG23 | 2.24                     | 0.62              |
| 17:Q:104:PHE:CZ   | 17:Q:156:LEU:HB2  | 2.33                     | 0.62              |
| 17:Q:355:VAL:HG12 | 18:R:211:ARG:O    | 1.99                     | 0.62              |
| 1:A:422:ARG:N     | 18:R:409:HIS:HE1  | 1.90                     | 0.62              |
| 1:A:474:LYS:HE3   | 2:B:1092:LEU:HD21 | 1.77                     | 0.62              |
| 1:A:909:SER:HA    | 9:I:83:LYS:HZ1    | 1.65                     | 0.62              |
| 1:A:1329:ILE:CB   | 1:A:1456:PHE:CE2  | 2.82                     | 0.62              |
| 2:B:64:GLY:CA     | 2:B:242:ASP:HB3   | 2.28                     | 0.62              |
| 2:B:207:ILE:CG1   | 2:B:503:VAL:HG22  | 2.13                     | 0.62              |
| 2:B:547:HIS:HB2   | 2:B:698:SER:HA    | 1.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:775:TRP:O    | 17:Q:113:LYS:NZ   | 2.33                     | 0.62              |
| 17:Q:22:ILE:HD11  | 17:Q:26:ARG:HE    | 1.62                     | 0.62              |
| 1:A:1657:LEU:HB3  | 7:G:104:LEU:HD22  | 1.81                     | 0.62              |
| 15:O:56:VAL:HG21  | 15:O:99:ILE:HD12  | 1.82                     | 0.62              |
| 15:O:67:ASP:OD1   | 15:O:69:THR:HB    | 2.00                     | 0.62              |
| 1:A:399:LEU:HD21  | 1:A:423:LEU:CD2   | 2.30                     | 0.62              |
| 1:A:506:THR:CG2   | 1:A:579:ARG:C     | 2.59                     | 0.62              |
| 1:A:684:ASP:OD2   | 8:H:20:TYR:CB     | 2.45                     | 0.62              |
| 1:A:1055:ILE:HD13 | 1:A:1178:LEU:HD23 | 1.80                     | 0.62              |
| 1:A:1606:SER:HB3  | 1:A:1611:MET:HE3  | 1.79                     | 0.62              |
| 2:B:50:ASN:OD1    | 2:B:167:SER:HB2   | 1.99                     | 0.62              |
| 2:B:202:LEU:HD22  | 2:B:488:ALA:CB    | 2.25                     | 0.62              |
| 2:B:796:ARG:O     | 10:J:8:PHE:HE1    | 1.83                     | 0.62              |
| 16:P:197:ARG:HE   | 16:P:261:VAL:N    | 1.93                     | 0.62              |
| 16:P:736:ILE:HD11 | 17:Q:254:LEU:HD13 | 1.80                     | 0.62              |
| 17:Q:9:ILE:HB     | 17:Q:16:PRO:CB    | 2.26                     | 0.62              |
| 17:Q:378:LEU:CD2  | 18:R:235:ILE:HA   | 2.30                     | 0.62              |
| 1:A:472:MET:HB3   | 2:B:1073:GLU:CG   | 2.29                     | 0.62              |
| 1:A:825:ALA:HB3   | 2:B:1022:LEU:HB3  | 1.82                     | 0.62              |
| 1:A:878:ARG:HG3   | 9:I:66:VAL:CG2    | 2.27                     | 0.62              |
| 2:B:143:TRP:CD2   | 2:B:446:MET:HE3   | 2.34                     | 0.62              |
| 2:B:897:GLU:HA    | 12:L:46:VAL:HG23  | 1.80                     | 0.62              |
| 2:B:1072:GLY:CA   | 2:B:1075:GLU:CG   | 2.63                     | 0.62              |
| 15:O:467:MET:CG   | 15:O:575:SER:HA   | 2.30                     | 0.62              |
| 16:P:443:ASP:HB3  | 18:R:3:GLU:HB3    | 1.82                     | 0.62              |
| 17:Q:378:LEU:HD22 | 18:R:235:ILE:HA   | 1.82                     | 0.62              |
| 18:R:6:ILE:HD11   | 18:R:213:ILE:HG22 | 1.82                     | 0.62              |
| 2:B:563:SER:HB3   | 13:M:73:SER:HB3   | 1.82                     | 0.62              |
| 15:O:200:ASN:ND2  | 17:Q:14:ASN:C     | 2.53                     | 0.62              |
| 15:O:332:LEU:HD11 | 15:O:380:SER:CB   | 2.29                     | 0.62              |
| 17:Q:357:TYR:O    | 18:R:206:ARG:CZ   | 2.48                     | 0.62              |
| 17:Q:378:LEU:CD2  | 18:R:216:LEU:CD2  | 2.73                     | 0.62              |
| 18:R:75:GLN:HA    | 18:R:78:ARG:HE    | 1.64                     | 0.62              |
| 3:C:272:LYS:HG3   | 14:N:175:TYR:HE1  | 1.65                     | 0.62              |
| 1:A:83:VAL:HG13   | 1:A:427:PHE:CE2   | 2.34                     | 0.61              |
| 1:A:1050:TYR:CE1  | 1:A:1185:VAL:HG11 | 2.35                     | 0.61              |
| 2:B:697:LEU:CB    | 2:B:702:ASN:ND2   | 2.59                     | 0.61              |
| 15:O:245:GLN:NE2  | 15:O:245:GLN:HA   | 2.14                     | 0.61              |
| 1:A:438:ILE:O     | 1:A:457:LYS:HD3   | 1.96                     | 0.61              |
| 1:A:545:SER:N     | 17:Q:34:VAL:CB    | 2.63                     | 0.61              |
| 1:A:720:PHE:CE2   | 8:H:141:TYR:CE2   | 2.78                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:143:TRP:HB3   | 2:B:446:MET:CE    | 2.25                     | 0.61              |
| 2:B:894:LYS:CG    | 12:L:47:ARG:NE    | 2.62                     | 0.61              |
| 16:P:189:THR:O    | 16:P:450:ARG:NH2  | 2.33                     | 0.61              |
| 17:Q:10:CYS:CB    | 17:Q:17:SER:H     | 2.13                     | 0.61              |
| 17:Q:189:LYS:HG3  | 17:Q:384:GLN:HE21 | 1.65                     | 0.61              |
| 1:A:476:VAL:HG13  | 2:B:1070:ARG:HA   | 1.81                     | 0.61              |
| 5:E:93:MET:HG3    | 5:E:120:ALA:HB1   | 1.82                     | 0.61              |
| 6:F:70:LYS:CE     | 7:G:95:LEU:HD23   | 2.27                     | 0.61              |
| 15:O:361:PHE:O    | 15:O:365:THR:HG23 | 1.99                     | 0.61              |
| 15:O:373:LEU:CD1  | 15:O:423:TYR:CD2  | 2.84                     | 0.61              |
| 15:O:510:VAL:CG1  | 15:O:543:ILE:HD12 | 2.30                     | 0.61              |
| 17:Q:194:GLN:HB3  | 17:Q:389:GLN:HG3  | 1.83                     | 0.61              |
| 1:A:966:LEU:HD21  | 1:A:997:PHE:HE1   | 1.62                     | 0.61              |
| 2:B:679:GLN:CD    | 14:N:156:PRO:C    | 2.65                     | 0.61              |
| 16:P:297:ILE:O    | 18:R:159:TYR:HD1  | 1.80                     | 0.61              |
| 16:P:484:ARG:O    | 16:P:486:ALA:N    | 2.32                     | 0.61              |
| 18:R:1:MET:HE3    | 18:R:2:PHE:CE1    | 2.35                     | 0.61              |
| 1:A:438:ILE:O     | 1:A:457:LYS:CG    | 2.48                     | 0.61              |
| 2:B:146:ASN:ND2   | 2:B:441:LYS:HE3   | 2.15                     | 0.61              |
| 2:B:200:GLU:OE2   | 2:B:736:ARG:NH2   | 2.34                     | 0.61              |
| 2:B:1090:ASP:O    | 2:B:1094:ASN:N    | 2.33                     | 0.61              |
| 15:O:376:TYR:HE2  | 15:O:377:TYR:HE2  | 1.44                     | 0.61              |
| 15:O:581:THR:HA   | 15:O:584:GLN:NE2  | 2.15                     | 0.61              |
| 16:P:498:LEU:CD2  | 17:Q:368:GLN:NE2  | 2.37                     | 0.61              |
| 17:Q:413:LEU:HD21 | 18:R:273:TRP:CE2  | 2.32                     | 0.61              |
| 1:A:827:THR:CG2   | 1:A:924:SER:HB3   | 2.30                     | 0.61              |
| 1:A:990:ILE:CA    | 1:A:994:GLU:CB    | 2.64                     | 0.61              |
| 6:F:70:LYS:HA     | 6:F:73:ALA:HB3    | 1.82                     | 0.61              |
| 15:O:370:THR:OG1  | 15:O:371:HIS:HD2  | 1.84                     | 0.61              |
| 17:Q:19:LEU:HD11  | 17:Q:27:ARG:CB    | 2.27                     | 0.61              |
| 17:Q:197:GLU:OE2  | 17:Q:388:THR:O    | 2.19                     | 0.61              |
| 17:Q:351:ASN:CA   | 17:Q:369:TRP:CZ2  | 2.84                     | 0.61              |
| 17:Q:503:SER:O    | 17:Q:507:ASN:ND2  | 2.33                     | 0.61              |
| 1:A:991:LYS:CB    | 1:A:993:GLN:OE1   | 2.44                     | 0.61              |
| 3:C:272:LYS:HG3   | 14:N:175:TYR:CE1  | 2.36                     | 0.61              |
| 3:C:326:GLU:CB    | 11:K:125:MET:HE3  | 2.29                     | 0.61              |
| 7:G:158:LYS:HB3   | 15:O:105:ASN:OD1  | 1.99                     | 0.61              |
| 15:O:224:GLU:OE1  | 15:O:224:GLU:N    | 2.23                     | 0.61              |
| 16:P:362:ARG:HB3  | 16:P:375:PHE:HB2  | 1.82                     | 0.61              |
| 2:B:1091:ARG:O    | 2:B:1096:SER:HB2  | 2.01                     | 0.61              |
| 3:C:58:ASN:HA     | 3:C:296:ASN:HD21  | 0.78                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:25:ARG:NH1    | 8:H:27:GLU:OE2    | 2.34                     | 0.61              |
| 15:O:450:LEU:O    | 15:O:454:VAL:HG12 | 1.99                     | 0.61              |
| 17:Q:24:ASP:OD1   | 17:Q:26:ARG:NH1   | 2.31                     | 0.61              |
| 17:Q:418:PRO:HG3  | 18:R:264:SER:HG   | 1.62                     | 0.61              |
| 2:B:497:ILE:CG1   | 2:B:699:ILE:CD1   | 2.79                     | 0.61              |
| 2:B:995:TYR:OH    | 14:N:163:VAL:HG23 | 2.01                     | 0.61              |
| 2:B:1079:LEU:HD22 | 2:B:1084:THR:OG1  | 2.00                     | 0.61              |
| 15:O:515:ASN:HD21 | 15:O:547:ASN:HD21 | 1.47                     | 0.61              |
| 16:P:187:ILE:HB   | 16:P:188:GLN:CD   | 2.25                     | 0.61              |
| 16:P:422:ILE:O    | 16:P:439:LYS:HB2  | 2.01                     | 0.61              |
| 16:P:625:ASP:O    | 16:P:629:ARG:HB3  | 2.00                     | 0.61              |
| 1:A:472:MET:CG    | 2:B:1073:GLU:CD   | 2.73                     | 0.61              |
| 1:A:826:PHE:CD1   | 2:B:777:SER:CB    | 2.83                     | 0.61              |
| 2:B:923:GLN:NE2   | 2:B:957:ARG:HD2   | 2.16                     | 0.61              |
| 16:P:184:SER:HA   | 18:R:198:LEU:HD21 | 1.62                     | 0.61              |
| 16:P:436:ILE:CG2  | 18:R:143:THR:CB   | 2.79                     | 0.61              |
| 1:A:729:LYS:HD2   | 8:H:120:GLY:HA3   | 1.82                     | 0.60              |
| 1:A:862:THR:HG22  | 9:I:67:VAL:HG11   | 1.83                     | 0.60              |
| 1:A:966:LEU:CD2   | 1:A:997:PHE:HE1   | 2.09                     | 0.60              |
| 1:A:966:LEU:HD22  | 1:A:997:PHE:CE1   | 2.35                     | 0.60              |
| 1:A:1330:VAL:CG2  | 1:A:1455:ARG:HD2  | 2.31                     | 0.60              |
| 2:B:203:ILE:HB    | 2:B:405:GLY:HA3   | 1.82                     | 0.60              |
| 6:F:74:ILE:HG21   | 6:F:144:GLU:HG2   | 1.81                     | 0.60              |
| 16:P:197:ARG:HG3  | 16:P:261:VAL:O    | 2.01                     | 0.60              |
| 16:P:704:LEU:O    | 17:Q:438:PHE:CB   | 2.45                     | 0.60              |
| 17:Q:257:VAL:HG12 | 17:Q:446:TYR:CZ   | 2.35                     | 0.60              |
| 18:R:251:TRP:HE3  | 18:R:307:LYS:NZ   | 1.99                     | 0.60              |
| 1:A:467:PHE:CD2   | 1:A:1614:SER:CB   | 2.84                     | 0.60              |
| 1:A:474:LYS:O     | 2:B:1070:ARG:HG3  | 2.01                     | 0.60              |
| 1:A:824:THR:C     | 2:B:1023:ARG:H    | 2.08                     | 0.60              |
| 1:A:1657:LEU:CD2  | 7:G:104:LEU:CD1   | 2.61                     | 0.60              |
| 2:B:152:LEU:CG    | 2:B:443:LYS:HE3   | 2.27                     | 0.60              |
| 2:B:551:ILE:HG21  | 2:B:647:SER:CA    | 2.18                     | 0.60              |
| 15:O:100:LEU:HD22 | 15:O:107:ILE:HD11 | 1.82                     | 0.60              |
| 16:P:274:ILE:O    | 16:P:289:SER:CB   | 2.43                     | 0.60              |
| 16:P:436:ILE:HG21 | 18:R:143:THR:CA   | 2.31                     | 0.60              |
| 17:Q:355:VAL:CG1  | 18:R:215:THR:CB   | 2.79                     | 0.60              |
| 17:Q:355:VAL:CG1  | 18:R:211:ARG:O    | 2.49                     | 0.60              |
| 1:A:449:GLY:O     | 1:A:451:VAL:N     | 2.34                     | 0.60              |
| 1:A:1608:SER:OG   | 1:A:1632:GLU:OE2  | 2.12                     | 0.60              |
| 2:B:184:LYS:HB3   | 2:B:735:HIS:CG    | 2.35                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:326:GLU:HB2   | 11:K:125:MET:HE3  | 1.84                     | 0.60              |
| 15:O:477:PHE:CE2  | 15:O:525:MET:HE1  | 2.35                     | 0.60              |
| 16:P:185:GLN:OE1  | 18:R:197:PRO:N    | 2.33                     | 0.60              |
| 16:P:355:GLU:HA   | 18:R:24:ILE:HD12  | 1.83                     | 0.60              |
| 17:Q:193:PHE:HB3  | 18:R:209:ARG:NH2  | 2.15                     | 0.60              |
| 17:Q:326:TYR:CE2  | 17:Q:452:PHE:CE2  | 2.85                     | 0.60              |
| 18:R:5:PRO:CD     | 18:R:217:THR:CB   | 2.79                     | 0.60              |
| 1:A:1318:SER:OG   | 1:A:1450:ILE:HD11 | 2.00                     | 0.60              |
| 16:P:383:ILE:HG12 | 16:P:390:GLN:HG2  | 1.82                     | 0.60              |
| 16:P:665:ASN:OD1  | 16:P:665:ASN:N    | 2.31                     | 0.60              |
| 17:Q:414:TYR:CD1  | 18:R:240:ILE:CG1  | 2.85                     | 0.60              |
| 18:R:171:ARG:O    | 18:R:174:GLU:N    | 2.33                     | 0.60              |
| 18:R:206:ARG:HE   | 18:R:206:ARG:N    | 1.97                     | 0.60              |
| 1:A:414:GLU:O     | 1:A:417:ARG:N     | 2.33                     | 0.60              |
| 1:A:1050:TYR:CE1  | 1:A:1179:ILE:CG1  | 2.76                     | 0.60              |
| 3:C:228:ARG:HD3   | 14:N:173:THR:OG1  | 2.02                     | 0.60              |
| 3:C:272:LYS:CG    | 14:N:175:TYR:HE1  | 2.14                     | 0.60              |
| 16:P:185:GLN:HG3  | 18:R:190:SER:HB3  | 1.81                     | 0.60              |
| 16:P:473:HIS:CD2  | 16:P:475:ARG:HD2  | 2.35                     | 0.60              |
| 2:B:563:SER:HA    | 13:M:73:SER:CB    | 2.31                     | 0.60              |
| 2:B:1005:TYR:CZ   | 14:N:170:HIS:CE1  | 2.89                     | 0.60              |
| 3:C:314:PHE:CD2   | 11:K:135:PHE:CZ   | 2.89                     | 0.60              |
| 16:P:198:ASP:CG   | 16:P:205:TYR:O    | 2.44                     | 0.60              |
| 16:P:397:LYS:HZ1  | 18:R:85:ARG:NE    | 2.00                     | 0.60              |
| 16:P:667:ASP:OD1  | 16:P:667:ASP:N    | 2.33                     | 0.60              |
| 1:A:435:ASN:HB3   | 1:A:442:LYS:CA    | 2.32                     | 0.60              |
| 1:A:472:MET:HE1   | 2:B:1076:ARG:HD2  | 1.84                     | 0.60              |
| 2:B:143:TRP:CH2   | 2:B:446:MET:HG3   | 2.37                     | 0.60              |
| 15:O:375:THR:O    | 15:O:377:TYR:N    | 2.35                     | 0.60              |
| 15:O:582:ARG:O    | 15:O:586:ILE:HG13 | 2.02                     | 0.60              |
| 16:P:641:TRP:HZ2  | 16:P:656:HIS:HB3  | 1.66                     | 0.60              |
| 17:Q:187:THR:HA   | 17:Q:380:TRP:CE2  | 2.33                     | 0.60              |
| 17:Q:413:LEU:CD2  | 18:R:273:TRP:HZ2  | 1.92                     | 0.60              |
| 18:R:173:MET:CG   | 18:R:188:PHE:HZ   | 2.11                     | 0.60              |
| 1:A:478:TYR:CB    | 2:B:1048:SER:O    | 2.50                     | 0.60              |
| 1:A:1314:GLN:NE2  | 1:A:1446:ARG:NE   | 2.49                     | 0.60              |
| 15:O:602:TYR:HD2  | 15:O:605:LEU:HD23 | 1.66                     | 0.60              |
| 16:P:317:ILE:HG22 | 16:P:363:ILE:HD13 | 1.84                     | 0.60              |
| 16:P:475:ARG:CZ   | 17:Q:367:PHE:CG   | 2.85                     | 0.60              |
| 17:Q:321:ASP:O    | 17:Q:324:ARG:N    | 2.27                     | 0.60              |
| 17:Q:356:VAL:HG11 | 18:R:208:TYR:HA   | 1.84                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:953:GLU:C     | 1:A:1205:PHE:HB2  | 2.24                     | 0.60              |
| 1:A:1226:VAL:HG12 | 1:A:1227:MET:HG2  | 1.83                     | 0.60              |
| 2:B:345:SER:HA    | 13:M:113:ILE:HG12 | 1.83                     | 0.60              |
| 2:B:1090:ASP:HA   | 2:B:1094:ASN:CG   | 2.27                     | 0.60              |
| 2:B:1151:ILE:HG12 | 7:G:21:LYS:HZ3    | 1.67                     | 0.60              |
| 7:G:241:ARG:HG2   | 15:O:152:GLN:OE1  | 2.02                     | 0.60              |
| 13:M:101:VAL:HG12 | 13:M:105:SER:OG   | 2.01                     | 0.60              |
| 16:P:472:ARG:NH1  | 18:R:203:SER:CB   | 2.64                     | 0.60              |
| 1:A:246:ASP:HB3   | 1:A:248:PHE:H     | 1.67                     | 0.59              |
| 1:A:1606:SER:CB   | 1:A:1611:MET:CE   | 2.79                     | 0.59              |
| 2:B:743:ARG:CZ    | 10:J:60:PHE:CZ    | 2.84                     | 0.59              |
| 16:P:436:ILE:HB   | 18:R:143:THR:CB   | 2.32                     | 0.59              |
| 17:Q:20:TRP:CH2   | 17:Q:22:ILE:HG21  | 2.30                     | 0.59              |
| 17:Q:358:PRO:HB3  | 18:R:206:ARG:HG2  | 1.83                     | 0.59              |
| 2:B:143:TRP:CZ2   | 2:B:446:MET:CA    | 2.84                     | 0.59              |
| 3:C:45:SER:HB2    | 3:C:271:ARG:NH2   | 2.18                     | 0.59              |
| 17:Q:263:PRO:HA   | 17:Q:446:TYR:HD1  | 1.63                     | 0.59              |
| 1:A:613:THR:HG21  | 2:B:913:ILE:HG22  | 1.81                     | 0.59              |
| 1:A:699:CYS:O     | 1:A:815:ARG:NH1   | 2.35                     | 0.59              |
| 2:B:28:PRO:HD3    | 10:J:62:ARG:NE    | 2.17                     | 0.59              |
| 2:B:228:SER:HB2   | 2:B:253:LEU:HD23  | 1.84                     | 0.59              |
| 2:B:1120:ILE:HD12 | 15:O:117:GLN:HE21 | 1.61                     | 0.59              |
| 1:A:990:ILE:HB    | 1:A:994:GLU:HB2   | 0.64                     | 0.59              |
| 1:A:1655:ASP:O    | 6:F:135:ARG:N     | 2.23                     | 0.59              |
| 7:G:141:SER:CB    | 15:O:142:ILE:HD11 | 2.20                     | 0.59              |
| 16:P:352:PHE:CD1  | 18:R:157:MET:HG2  | 2.36                     | 0.59              |
| 17:Q:10:CYS:HB2   | 17:Q:17:SER:H     | 1.67                     | 0.59              |
| 17:Q:348:ILE:HG12 | 17:Q:376:GLU:HB3  | 1.84                     | 0.59              |
| 17:Q:366:TYR:OH   | 18:R:218:ASP:CG   | 2.46                     | 0.59              |
| 1:A:1003:ARG:NH2  | 2:B:530:PRO:CA    | 2.65                     | 0.59              |
| 1:A:1600:ARG:CG   | 1:A:1616:GLU:OE1  | 2.49                     | 0.59              |
| 2:B:1069:ILE:H    | 2:B:1069:ILE:CD1  | 2.16                     | 0.59              |
| 14:N:87:TYR:HA    | 14:N:141:GLU:C    | 2.27                     | 0.59              |
| 15:O:348:THR:HG23 | 15:O:351:SER:H    | 1.68                     | 0.59              |
| 17:Q:3:THR:HG22   | 17:Q:20:TRP:CB    | 2.29                     | 0.59              |
| 17:Q:380:TRP:HH2  | 18:R:212:HIS:CD2  | 2.19                     | 0.59              |
| 1:A:1187:ILE:HG13 | 2:B:1080:ILE:HG22 | 1.85                     | 0.59              |
| 15:O:200:ASN:ND2  | 17:Q:14:ASN:CG    | 2.60                     | 0.59              |
| 16:P:319:ASP:HB2  | 16:P:363:ILE:HG12 | 1.83                     | 0.59              |
| 16:P:384:ASP:OD2  | 16:P:387:ASN:HB2  | 2.03                     | 0.59              |
| 16:P:631:SER:O    | 16:P:686:TYR:OH   | 2.20                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:474:LYS:NZ    | 2:B:1092:LEU:HD22 | 1.97                     | 0.59              |
| 1:A:477:ASN:O     | 2:B:1047:ARG:CG   | 2.51                     | 0.59              |
| 2:B:65:VAL:CG2    | 2:B:417:ILE:HD12  | 2.32                     | 0.59              |
| 2:B:143:TRP:HB3   | 2:B:446:MET:HE1   | 1.84                     | 0.59              |
| 2:B:146:ASN:HD22  | 2:B:441:LYS:CE    | 2.15                     | 0.59              |
| 2:B:531:VAL:CG1   | 2:B:716:MET:HA    | 2.32                     | 0.59              |
| 2:B:551:ILE:CG2   | 2:B:648:ARG:N     | 2.58                     | 0.59              |
| 5:E:145:THR:C     | 5:E:147:HIS:H     | 2.10                     | 0.59              |
| 16:P:426:ALA:C    | 16:P:433:VAL:HG11 | 2.27                     | 0.59              |
| 17:Q:358:PRO:HA   | 18:R:206:ARG:HG3  | 1.84                     | 0.59              |
| 17:Q:418:PRO:CD   | 18:R:264:SER:CB   | 2.79                     | 0.59              |
| 18:R:250:LEU:HB2  | 18:R:270:PHE:CE2  | 2.37                     | 0.59              |
| 18:R:317:LEU:HB2  | 18:R:367:ILE:HD11 | 1.85                     | 0.59              |
| 1:A:475:ARG:HH22  | 2:B:1061:LYS:HG3  | 1.67                     | 0.59              |
| 1:A:1032:VAL:HG21 | 1:A:1050:TYR:HE1  | 1.68                     | 0.59              |
| 1:A:1298:ASP:O    | 1:A:1299:ASN:C    | 2.46                     | 0.59              |
| 2:B:75:ASP:CA     | 2:B:440:PHE:CZ    | 2.86                     | 0.59              |
| 2:B:679:GLN:CA    | 14:N:155:VAL:O    | 2.50                     | 0.59              |
| 15:O:240:ILE:HG23 | 15:O:332:LEU:CD1  | 2.33                     | 0.59              |
| 16:P:420:GLU:HA   | 16:P:442:LEU:O    | 2.03                     | 0.59              |
| 17:Q:333:SER:O    | 17:Q:448:LYS:HE3  | 2.03                     | 0.59              |
| 18:R:250:LEU:HB2  | 18:R:270:PHE:HE2  | 1.67                     | 0.59              |
| 1:A:476:VAL:HG22  | 2:B:1069:ILE:N    | 2.18                     | 0.59              |
| 1:A:629:ASP:HA    | 2:B:926:VAL:HG23  | 1.84                     | 0.59              |
| 1:A:999:CYS:CA    | 2:B:712:SER:HB2   | 2.21                     | 0.59              |
| 2:B:497:ILE:HG12  | 2:B:699:ILE:CD1   | 2.33                     | 0.59              |
| 3:C:322:LYS:NZ    | 11:K:129:ASP:OD1  | 2.35                     | 0.59              |
| 7:G:242:VAL:HG21  | 15:O:183:ILE:CG2  | 2.32                     | 0.59              |
| 16:P:397:LYS:NZ   | 18:R:85:ARG:CD    | 2.65                     | 0.59              |
| 1:A:921:PRO:HD3   | 8:H:19:ARG:CG     | 2.33                     | 0.59              |
| 1:A:1314:GLN:OE1  | 1:A:1446:ARG:CD   | 2.48                     | 0.59              |
| 2:B:203:ILE:HG21  | 2:B:405:GLY:CA    | 2.33                     | 0.59              |
| 5:E:55:ARG:NH2    | 5:E:113:GLN:OE1   | 2.36                     | 0.59              |
| 15:O:552:LEU:O    | 15:O:553:ARG:C    | 2.46                     | 0.59              |
| 15:O:607:LYS:HG3  | 15:O:608:GLU:N    | 2.17                     | 0.59              |
| 17:Q:12:THR:HB    | 17:Q:33:HIS:ND1   | 2.18                     | 0.59              |
| 17:Q:385:PHE:CZ   | 18:R:209:ARG:CG   | 2.81                     | 0.59              |
| 18:R:350:SER:O    | 18:R:354:LEU:HB2  | 2.03                     | 0.59              |
| 1:A:953:GLU:C     | 1:A:1205:PHE:HB3  | 2.27                     | 0.58              |
| 1:A:1003:ARG:NH2  | 2:B:530:PRO:HA    | 2.17                     | 0.58              |
| 1:A:1050:TYR:CB   | 1:A:1054:ALA:HA   | 2.33                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1313:LEU:HD23 | 1:A:1462:PHE:CZ   | 2.29                     | 0.58              |
| 8:H:80:ARG:HG3    | 11:K:108:TYR:OH   | 2.03                     | 0.58              |
| 16:P:626:LEU:HD11 | 16:P:665:ASN:HB2  | 1.84                     | 0.58              |
| 16:P:675:PHE:CZ   | 16:P:742:TRP:HZ3  | 2.21                     | 0.58              |
| 1:A:598:ALA:HB1   | 1:A:601:MET:HE3   | 1.85                     | 0.58              |
| 1:A:1487:ASN:CG   | 2:B:305:ARG:HH22  | 2.11                     | 0.58              |
| 1:A:1650:GLY:O    | 1:A:1653:SER:N    | 2.36                     | 0.58              |
| 2:B:110:ASN:O     | 2:B:112:GLY:N     | 2.35                     | 0.58              |
| 2:B:209:GLN:O     | 2:B:401:GLU:HG2   | 2.03                     | 0.58              |
| 2:B:538:PRO:HB2   | 2:B:542:LEU:HG    | 1.84                     | 0.58              |
| 6:F:70:LYS:CD     | 7:G:95:LEU:CD2    | 2.79                     | 0.58              |
| 6:F:72:LYS:NZ     | 6:F:140:ASP:OD2   | 2.21                     | 0.58              |
| 12:L:38:LEU:HD12  | 12:L:49:LYS:HG3   | 1.85                     | 0.58              |
| 15:O:227:PHE:CD1  | 15:O:363:THR:HB   | 2.38                     | 0.58              |
| 15:O:473:PHE:HZ   | 15:O:509:MET:HE3  | 1.69                     | 0.58              |
| 17:Q:162:ILE:HG21 | 17:Q:226:LEU:HD11 | 1.85                     | 0.58              |
| 17:Q:436:LEU:HD12 | 17:Q:436:LEU:H    | 1.67                     | 0.58              |
| 1:A:408:LYS:HE3   | 1:A:416:ARG:HH12  | 1.67                     | 0.58              |
| 1:A:489:ASN:CB    | 11:K:95:HIS:CD2   | 2.85                     | 0.58              |
| 1:A:953:GLU:CB    | 1:A:1205:PHE:CD2  | 2.86                     | 0.58              |
| 2:B:143:TRP:NE1   | 2:B:446:MET:HB2   | 2.18                     | 0.58              |
| 2:B:207:ILE:O     | 2:B:207:ILE:HG22  | 2.02                     | 0.58              |
| 11:K:68:GLU:HG2   | 11:K:72:LEU:HD23  | 1.86                     | 0.58              |
| 15:O:200:ASN:ND2  | 17:Q:14:ASN:OD1   | 2.36                     | 0.58              |
| 15:O:219:ARG:CZ   | 15:O:360:VAL:HG22 | 2.34                     | 0.58              |
| 16:P:67:ASP:OD1   | 16:P:545:SER:OG   | 2.15                     | 0.58              |
| 16:P:659:LEU:HD12 | 16:P:742:TRP:CD1  | 2.39                     | 0.58              |
| 1:A:4:SER:HB2     | 1:A:573:LEU:HD22  | 1.85                     | 0.58              |
| 1:A:408:LYS:HE3   | 1:A:416:ARG:NH1   | 2.19                     | 0.58              |
| 1:A:415:ASP:HA    | 1:A:418:VAL:HG12  | 1.84                     | 0.58              |
| 16:P:715:TYR:CE1  | 16:P:733:THR:HG23 | 2.38                     | 0.58              |
| 17:Q:441:ASP:O    | 17:Q:445:ARG:HG2  | 2.02                     | 0.58              |
| 1:A:472:MET:HE1   | 2:B:1076:ARG:CD   | 2.34                     | 0.58              |
| 1:A:615:ARG:HH12  | 2:B:929:ARG:CD    | 2.17                     | 0.58              |
| 1:A:953:GLU:HB3   | 1:A:1205:PHE:CE2  | 2.37                     | 0.58              |
| 1:A:984:GLY:HA3   | 1:A:994:GLU:OE1   | 2.02                     | 0.58              |
| 1:A:1298:ASP:CA   | 1:A:1468:LYS:HZ3  | 2.14                     | 0.58              |
| 2:B:683:ASN:CA    | 14:N:154:ARG:HH22 | 2.14                     | 0.58              |
| 7:G:143:SER:OG    | 15:O:104:ILE:CG2  | 2.51                     | 0.58              |
| 17:Q:22:ILE:HD11  | 17:Q:26:ARG:CD    | 2.33                     | 0.58              |
| 17:Q:385:PHE:HE1  | 18:R:209:ARG:HB3  | 1.69                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:R:206:ARG:HA   | 18:R:211:ARG:HD3  | 1.84                     | 0.58              |
| 1:A:470:HIS:HB3   | 2:B:1058:GLN:HE22 | 1.68                     | 0.58              |
| 1:A:1074:TYR:HE2  | 1:A:1159:ASP:HB3  | 1.69                     | 0.58              |
| 2:B:143:TRP:CD2   | 2:B:446:MET:CE    | 2.85                     | 0.58              |
| 2:B:679:GLN:CG    | 14:N:157:ARG:CA   | 2.70                     | 0.58              |
| 2:B:683:ASN:HA    | 14:N:150:TYR:CE2  | 2.39                     | 0.58              |
| 15:O:376:TYR:CZ   | 15:O:419:LYS:HE2  | 2.38                     | 0.58              |
| 16:P:301:GLN:N    | 16:P:319:ASP:O    | 2.37                     | 0.58              |
| 17:Q:194:GLN:CA   | 18:R:209:ARG:NH1  | 2.66                     | 0.58              |
| 17:Q:357:TYR:C    | 18:R:206:ARG:NH1  | 2.45                     | 0.58              |
| 1:A:535:GLN:HE22  | 17:Q:26:ARG:CG    | 2.17                     | 0.58              |
| 1:A:1330:VAL:HG22 | 1:A:1455:ARG:CD   | 2.34                     | 0.58              |
| 2:B:567:SER:O     | 14:N:140:SER:CB   | 2.52                     | 0.58              |
| 14:N:89:ILE:HG12  | 14:N:139:VAL:HG22 | 1.85                     | 0.58              |
| 16:P:599:LYS:HE3  | 17:Q:272:GLN:HE22 | 1.69                     | 0.58              |
| 1:A:581:ILE:HB    | 1:A:637:PHE:CE2   | 2.38                     | 0.58              |
| 1:A:1032:VAL:HG21 | 1:A:1050:TYR:HD1  | 1.65                     | 0.58              |
| 1:A:1298:ASP:CG   | 1:A:1468:LYS:HZ3  | 2.10                     | 0.58              |
| 15:O:219:ARG:NH2  | 15:O:360:VAL:CG2  | 2.67                     | 0.58              |
| 15:O:438:GLN:O    | 15:O:441:PHE:HB3  | 2.02                     | 0.58              |
| 17:Q:26:ARG:HB3   | 17:Q:34:VAL:HG11  | 1.75                     | 0.58              |
| 1:A:406:LEU:HB2   | 1:A:408:LYS:HZ2   | 1.68                     | 0.58              |
| 1:A:413:LEU:O     | 1:A:416:ARG:CG    | 2.49                     | 0.58              |
| 1:A:477:ASN:CG    | 2:B:1047:ARG:NH1  | 2.56                     | 0.58              |
| 1:A:1204:THR:HG21 | 9:I:97:HIS:CB     | 2.33                     | 0.58              |
| 1:A:1606:SER:HB2  | 1:A:1611:MET:CE   | 2.33                     | 0.58              |
| 2:B:923:GLN:HG2   | 2:B:949:ILE:HD11  | 1.85                     | 0.58              |
| 6:F:66:ARG:HH21   | 7:G:90:LEU:HD13   | 1.64                     | 0.58              |
| 7:G:142:ALA:HB1   | 15:O:102:SER:O    | 2.03                     | 0.58              |
| 7:G:143:SER:OG    | 15:O:104:ILE:HG22 | 2.01                     | 0.58              |
| 16:P:717:LYS:CD   | 17:Q:439:ILE:HD13 | 2.33                     | 0.58              |
| 16:P:724:LEU:O    | 17:Q:450:THR:OG1  | 2.21                     | 0.58              |
| 17:Q:355:VAL:HG11 | 18:R:215:THR:OG1  | 1.95                     | 0.58              |
| 17:Q:358:PRO:CA   | 18:R:206:ARG:HD3  | 2.34                     | 0.58              |
| 1:A:396:ILE:HD11  | 1:A:426:ALA:HB1   | 1.85                     | 0.58              |
| 1:A:718:THR:CG2   | 8:H:118:PHE:HB3   | 2.34                     | 0.58              |
| 1:A:828:CYS:SG    | 2:B:1027:TYR:CB   | 2.92                     | 0.58              |
| 1:A:998:HIS:CD2   | 2:B:712:SER:H     | 2.20                     | 0.58              |
| 7:G:30:GLU:HA     | 7:G:32:ASN:N      | 2.18                     | 0.58              |
| 16:P:317:ILE:HG13 | 16:P:326:ILE:HD13 | 1.86                     | 0.58              |
| 16:P:725:VAL:CA   | 17:Q:450:THR:HB   | 2.27                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:354:LYS:HD2  | 17:Q:369:TRP:HZ2  | 1.69                     | 0.58              |
| 17:Q:351:ASN:HD21 | 17:Q:373:GLU:CD   | 2.12                     | 0.57              |
| 17:Q:355:VAL:HG11 | 18:R:215:THR:CB   | 2.33                     | 0.57              |
| 1:A:615:ARG:CZ    | 2:B:929:ARG:HE    | 2.16                     | 0.57              |
| 1:A:1314:GLN:HE22 | 1:A:1446:ARG:CZ   | 2.11                     | 0.57              |
| 1:A:1574:ALA:C    | 9:I:122:ARG:NH1   | 2.62                     | 0.57              |
| 3:C:42:VAL:HB     | 11:K:138:LYS:HG3  | 1.86                     | 0.57              |
| 17:Q:152:LEU:HB3  | 17:Q:154:LEU:HD22 | 1.85                     | 0.57              |
| 18:R:199:LYS:NZ   | 18:R:204:GLU:CA   | 2.62                     | 0.57              |
| 1:A:1260:LYS:HE2  | 1:A:1262:LEU:CD2  | 2.33                     | 0.57              |
| 3:C:86:PHE:HE2    | 3:C:205:LYS:HG3   | 1.69                     | 0.57              |
| 12:L:33:GLU:HG3   | 12:L:53:HIS:CE1   | 2.39                     | 0.57              |
| 13:M:10:ILE:HB    | 14:N:70:LEU:HB3   | 1.86                     | 0.57              |
| 15:O:201:LYS:CD   | 15:O:239:SER:OG   | 2.49                     | 0.57              |
| 16:P:446:ASP:HA   | 18:R:200:THR:HG22 | 1.85                     | 0.57              |
| 16:P:725:VAL:CA   | 17:Q:450:THR:CB   | 2.61                     | 0.57              |
| 17:Q:222:PHE:HA   | 17:Q:492:ALA:HB1  | 1.85                     | 0.57              |
| 17:Q:362:THR:O    | 17:Q:365:ASP:HB2  | 2.04                     | 0.57              |
| 1:A:436:ALA:C     | 1:A:439:ASP:CA    | 2.76                     | 0.57              |
| 1:A:909:SER:CA    | 9:I:83:LYS:NZ     | 2.61                     | 0.57              |
| 2:B:548:LYS:O     | 2:B:549:CYS:C     | 2.47                     | 0.57              |
| 16:P:268:SER:OG   | 16:P:269:PHE:N    | 2.36                     | 0.57              |
| 16:P:407:ARG:HH22 | 16:P:411:LYS:HA   | 1.69                     | 0.57              |
| 16:P:422:ILE:HG12 | 16:P:442:LEU:CD1  | 2.34                     | 0.57              |
| 16:P:719:LEU:HD13 | 16:P:733:THR:HG21 | 1.85                     | 0.57              |
| 17:Q:194:GLN:HG2  | 17:Q:389:GLN:CB   | 2.33                     | 0.57              |
| 17:Q:410:ARG:HE   | 17:Q:413:LEU:HD13 | 1.69                     | 0.57              |
| 1:A:83:VAL:HG11   | 1:A:427:PHE:CE2   | 2.37                     | 0.57              |
| 1:A:408:LYS:HA    | 1:A:411:VAL:CG2   | 2.34                     | 0.57              |
| 1:A:545:SER:N     | 17:Q:34:VAL:HB    | 2.19                     | 0.57              |
| 1:A:1322:ILE:C    | 1:A:1454:HIS:CD2  | 2.82                     | 0.57              |
| 1:A:1657:LEU:CB   | 7:G:104:LEU:HD13  | 2.35                     | 0.57              |
| 2:B:49:PHE:CG     | 2:B:164:MET:HE3   | 2.40                     | 0.57              |
| 2:B:203:ILE:CG2   | 2:B:405:GLY:HA3   | 2.35                     | 0.57              |
| 6:F:74:ILE:C      | 7:G:95:LEU:CD1    | 2.62                     | 0.57              |
| 7:G:143:SER:CB    | 15:O:104:ILE:N    | 2.49                     | 0.57              |
| 15:O:205:ARG:O    | 15:O:209:VAL:HG12 | 2.05                     | 0.57              |
| 15:O:510:VAL:HG12 | 15:O:543:ILE:HD12 | 1.86                     | 0.57              |
| 16:P:484:ARG:HD2  | 16:P:488:LEU:HD12 | 1.85                     | 0.57              |
| 2:B:149:GLU:CD    | 2:B:441:LYS:HZ1   | 2.13                     | 0.57              |
| 2:B:551:ILE:HG23  | 2:B:647:SER:C     | 2.29                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:679:GLN:HG3   | 14:N:156:PRO:N    | 2.19                     | 0.57              |
| 7:G:144:HIS:CE1   | 15:O:145:SER:HB3  | 2.38                     | 0.57              |
| 16:P:473:HIS:ND1  | 16:P:473:HIS:O    | 2.37                     | 0.57              |
| 18:R:207:ASN:H    | 18:R:211:ARG:CD   | 2.18                     | 0.57              |
| 1:A:909:SER:HA    | 9:I:83:LYS:HE3    | 1.84                     | 0.57              |
| 2:B:1072:GLY:H    | 2:B:1075:GLU:CD   | 2.13                     | 0.57              |
| 16:P:724:LEU:CD1  | 17:Q:447:ALA:HB2  | 2.34                     | 0.57              |
| 18:R:173:MET:CG   | 18:R:188:PHE:CZ   | 2.87                     | 0.57              |
| 1:A:435:ASN:HB3   | 1:A:442:LYS:C     | 2.29                     | 0.57              |
| 1:A:1484:LEU:HD11 | 2:B:305:ARG:CD    | 2.35                     | 0.57              |
| 6:F:72:LYS:HD3    | 6:F:142:SER:CB    | 2.28                     | 0.57              |
| 15:O:376:TYR:CD2  | 15:O:419:LYS:HE2  | 2.40                     | 0.57              |
| 16:P:712:ASP:OD1  | 16:P:712:ASP:N    | 2.38                     | 0.57              |
| 18:R:317:LEU:CD1  | 18:R:370:SER:HB2  | 2.32                     | 0.57              |
| 1:A:1235:THR:O    | 1:A:1544:ASN:ND2  | 2.38                     | 0.57              |
| 2:B:833:PRO:HG2   | 2:B:836:TRP:CE2   | 2.40                     | 0.57              |
| 16:P:722:TRP:HD1  | 17:Q:446:TYR:CB   | 2.17                     | 0.57              |
| 1:A:618:TYR:HE1   | 2:B:783:MET:HB2   | 1.67                     | 0.57              |
| 1:A:991:LYS:N     | 1:A:994:GLU:CB    | 2.67                     | 0.57              |
| 2:B:30:LYS:HG2    | 2:B:178:TYR:CB    | 2.35                     | 0.57              |
| 2:B:49:PHE:CE2    | 2:B:194:PHE:CE2   | 2.93                     | 0.57              |
| 2:B:1013:MET:SD   | 2:B:1026:ILE:HG12 | 2.45                     | 0.57              |
| 15:O:190:ILE:HA   | 15:O:193:TYR:CD2  | 2.39                     | 0.57              |
| 15:O:379:ARG:HH11 | 15:O:379:ARG:CA   | 2.09                     | 0.57              |
| 16:P:462:ILE:HB   | 16:P:483:HIS:HB3  | 1.87                     | 0.57              |
| 17:Q:22:ILE:HD12  | 17:Q:24:ASP:OD1   | 2.04                     | 0.57              |
| 17:Q:189:LYS:HA   | 17:Q:384:GLN:CD   | 2.29                     | 0.57              |
| 18:R:5:PRO:CG     | 18:R:217:THR:HB   | 2.35                     | 0.57              |
| 1:A:1603:MET:HG2  | 1:A:1611:MET:HE1  | 1.85                     | 0.56              |
| 16:P:358:SER:HB3  | 16:P:377:ARG:HD3  | 1.87                     | 0.56              |
| 17:Q:20:TRP:CE2   | 17:Q:28:THR:HB    | 2.39                     | 0.56              |
| 11:K:49:LEU:HD23  | 11:K:51:THR:HG23  | 1.86                     | 0.56              |
| 1:A:721:LYS:NZ    | 8:H:90:ALA:C      | 2.60                     | 0.56              |
| 1:A:966:LEU:HD22  | 1:A:997:PHE:CZ    | 2.40                     | 0.56              |
| 2:B:119:ARG:CZ    | 12:L:53:HIS:HE1   | 2.17                     | 0.56              |
| 2:B:796:ARG:NH2   | 10:J:8:PHE:O      | 2.37                     | 0.56              |
| 5:E:90:VAL:HG13   | 5:E:120:ALA:HA    | 1.88                     | 0.56              |
| 5:E:159:ASP:OD1   | 5:E:162:ARG:NH1   | 2.38                     | 0.56              |
| 7:G:56:ASN:HB3    | 7:G:59:GLN:HB3    | 1.86                     | 0.56              |
| 15:O:109:SER:OG   | 15:O:111:ARG:HG3  | 2.05                     | 0.56              |
| 15:O:200:ASN:OD1  | 17:Q:14:ASN:CG    | 2.47                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:376:TYR:CE1  | 15:O:588:LEU:HD22 | 2.25                     | 0.56              |
| 16:P:375:PHE:HD1  | 16:P:402:ILE:HD13 | 1.69                     | 0.56              |
| 16:P:662:LEU:HB3  | 16:P:665:ASN:HD21 | 1.67                     | 0.56              |
| 17:Q:318:LEU:HB3  | 17:Q:476:ILE:HD12 | 1.87                     | 0.56              |
| 17:Q:411:ARG:O    | 17:Q:415:LYS:HB2  | 2.05                     | 0.56              |
| 1:A:436:ALA:HA    | 1:A:439:ASP:C     | 2.28                     | 0.56              |
| 1:A:506:THR:HB    | 1:A:579:ARG:O     | 2.03                     | 0.56              |
| 1:A:672:ASP:CG    | 2:B:777:SER:CB    | 2.77                     | 0.56              |
| 1:A:797:LEU:HD13  | 1:A:809:VAL:HG21  | 1.87                     | 0.56              |
| 1:A:1032:VAL:HG22 | 1:A:1050:TYR:CD1  | 2.39                     | 0.56              |
| 1:A:1482:LYS:HD3  | 2:B:304:ASP:CG    | 2.29                     | 0.56              |
| 2:B:54:GLU:HG3    | 2:B:168:ASN:HD21  | 1.71                     | 0.56              |
| 2:B:338:PHE:HZ    | 2:B:357:ILE:HD12  | 1.70                     | 0.56              |
| 2:B:681:ILE:HB    | 14:N:154:ARG:CB   | 2.34                     | 0.56              |
| 16:P:365:TRP:HB3  | 16:P:372:ILE:HG22 | 1.86                     | 0.56              |
| 17:Q:263:PRO:C    | 17:Q:446:TYR:HE1  | 2.14                     | 0.56              |
| 17:Q:367:PHE:CE1  | 18:R:1:MET:CA     | 2.45                     | 0.56              |
| 18:R:180:CYS:SG   | 18:R:185:LYS:CG   | 2.94                     | 0.56              |
| 18:R:181:THR:O    | 18:R:185:LYS:HG3  | 2.04                     | 0.56              |
| 6:F:66:ARG:HH22   | 7:G:90:LEU:CB     | 2.19                     | 0.56              |
| 7:G:24:VAL:N      | 7:G:128:GLN:CD    | 2.28                     | 0.56              |
| 15:O:234:ILE:CG1  | 15:O:367:LEU:HD13 | 2.36                     | 0.56              |
| 15:O:243:GLU:HB3  | 15:O:332:LEU:CD1  | 2.30                     | 0.56              |
| 16:P:608:GLN:HA   | 16:P:611:ILE:HD12 | 1.87                     | 0.56              |
| 16:P:703:PHE:O    | 17:Q:438:PHE:CE2  | 2.59                     | 0.56              |
| 17:Q:380:TRP:CH2  | 18:R:212:HIS:HD2  | 2.11                     | 0.56              |
| 18:R:6:ILE:CD1    | 18:R:213:ILE:HB   | 2.35                     | 0.56              |
| 18:R:83:HIS:O     | 18:R:85:ARG:N     | 2.39                     | 0.56              |
| 18:R:236:PHE:O    | 18:R:240:ILE:HG22 | 2.05                     | 0.56              |
| 1:A:672:ASP:OD1   | 2:B:777:SER:CB    | 2.53                     | 0.56              |
| 1:A:938:VAL:CG2   | 9:I:82:ILE:CD1    | 2.68                     | 0.56              |
| 1:A:1025:LYS:HZ2  | 2:B:1076:ARG:NH1  | 2.04                     | 0.56              |
| 1:A:1499:ARG:O    | 1:A:1500:GLN:HB2  | 2.05                     | 0.56              |
| 2:B:404:LEU:O     | 2:B:405:GLY:C     | 2.47                     | 0.56              |
| 2:B:1005:TYR:CE1  | 14:N:170:HIS:CE1  | 2.94                     | 0.56              |
| 3:C:223:SER:HB3   | 10:J:12:LYS:HB2   | 1.87                     | 0.56              |
| 5:E:145:THR:O     | 5:E:147:HIS:N     | 2.39                     | 0.56              |
| 15:O:578:SER:O    | 15:O:579:LEU:HB2  | 2.06                     | 0.56              |
| 2:B:829:ASN:OD1   | 2:B:829:ASN:N     | 2.36                     | 0.56              |
| 15:O:200:ASN:ND2  | 17:Q:14:ASN:CB    | 2.65                     | 0.56              |
| 16:P:362:ARG:HH22 | 16:P:364:GLU:HG3  | 1.71                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:103:LEU:HD21 | 17:Q:205:ILE:HG21 | 1.88                     | 0.56              |
| 17:Q:211:TYR:O    | 17:Q:214:ILE:HG22 | 2.05                     | 0.56              |
| 17:Q:351:ASN:CG   | 17:Q:369:TRP:CE2  | 2.83                     | 0.56              |
| 1:A:615:ARG:HH12  | 2:B:929:ARG:HD3   | 1.71                     | 0.56              |
| 1:A:878:ARG:NH2   | 9:I:66:VAL:O      | 2.37                     | 0.56              |
| 1:A:966:LEU:HD21  | 1:A:997:PHE:CZ    | 2.36                     | 0.56              |
| 1:A:1658:ALA:HA   | 6:F:132:LEU:HA    | 1.87                     | 0.56              |
| 2:B:45:HIS:O      | 2:B:164:MET:HE1   | 2.06                     | 0.56              |
| 2:B:184:LYS:CD    | 2:B:735:HIS:CD2   | 2.89                     | 0.56              |
| 16:P:233:VAL:HG12 | 16:P:234:THR:H    | 1.71                     | 0.56              |
| 18:R:4:VAL:HG21   | 18:R:214:VAL:CG2  | 2.30                     | 0.56              |
| 1:A:503:VAL:HG23  | 1:A:530:TRP:CB    | 2.19                     | 0.56              |
| 2:B:679:GLN:OE1   | 14:N:157:ARG:HB2  | 2.06                     | 0.56              |
| 14:N:69:SER:OG    | 14:N:70:LEU:N     | 2.37                     | 0.56              |
| 15:O:332:LEU:CD2  | 15:O:599:LEU:HD21 | 2.36                     | 0.56              |
| 16:P:185:GLN:HE22 | 18:R:197:PRO:HB3  | 1.71                     | 0.56              |
| 17:Q:198:ILE:HB   | 17:Q:389:GLN:C    | 2.26                     | 0.56              |
| 17:Q:380:TRP:CH2  | 18:R:212:HIS:NE2  | 2.73                     | 0.56              |
| 1:A:408:LYS:H     | 1:A:408:LYS:HD3   | 1.70                     | 0.56              |
| 1:A:995:TYR:CZ    | 2:B:707:SER:CB    | 2.72                     | 0.56              |
| 2:B:30:LYS:O      | 2:B:176:SER:CB    | 2.54                     | 0.56              |
| 2:B:563:SER:HA    | 13:M:73:SER:OG    | 2.06                     | 0.56              |
| 6:F:72:LYS:HB3    | 6:F:142:SER:HA    | 0.59                     | 0.56              |
| 15:O:191:ASP:O    | 15:O:194:LEU:HB2  | 2.06                     | 0.56              |
| 15:O:412:GLU:OE1  | 15:O:416:LYS:HD3  | 2.06                     | 0.56              |
| 16:P:185:GLN:CG   | 18:R:190:SER:CB   | 2.74                     | 0.56              |
| 16:P:397:LYS:NZ   | 18:R:85:ARG:NE    | 2.54                     | 0.56              |
| 17:Q:274:ILE:HG23 | 17:Q:282:ARG:HH22 | 1.71                     | 0.56              |
| 1:A:821:ILE:O     | 1:A:825:ALA:N     | 2.40                     | 0.55              |
| 1:A:953:GLU:HB3   | 1:A:1205:PHE:CZ   | 2.41                     | 0.55              |
| 1:A:986:PHE:CE2   | 2:B:958:MET:CE    | 2.88                     | 0.55              |
| 15:O:63:LEU:HD23  | 15:O:111:ARG:HD2  | 1.87                     | 0.55              |
| 18:R:187:TYR:O    | 18:R:191:ILE:HG23 | 2.07                     | 0.55              |
| 1:A:429:THR:HG22  | 18:R:406:LYS:NZ   | 2.13                     | 0.55              |
| 1:A:1187:ILE:HG13 | 2:B:1080:ILE:CG2  | 2.36                     | 0.55              |
| 15:O:243:GLU:CB   | 15:O:332:LEU:CD1  | 2.84                     | 0.55              |
| 16:P:186:TYR:CE1  | 18:R:196:GLU:O    | 2.58                     | 0.55              |
| 16:P:218:VAL:HG22 | 16:P:246:LYS:HB3  | 1.89                     | 0.55              |
| 17:Q:348:ILE:CD1  | 17:Q:373:GLU:CG   | 2.82                     | 0.55              |
| 2:B:1047:ARG:HG2  | 2:B:1049:THR:N    | 2.21                     | 0.55              |
| 3:C:315:PHE:CE2   | 11:K:139:ILE:CD1  | 2.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:592:LEU:O    | 16:P:596:ILE:HG22 | 2.06                     | 0.55              |
| 16:P:724:LEU:C    | 17:Q:447:ALA:HA   | 2.32                     | 0.55              |
| 17:Q:385:PHE:CE1  | 18:R:209:ARG:CB   | 2.90                     | 0.55              |
| 18:R:246:GLN:HG2  | 18:R:247:ILE:H    | 1.72                     | 0.55              |
| 18:R:317:LEU:HD11 | 18:R:370:SER:HB3  | 1.82                     | 0.55              |
| 1:A:508:PRO:CD    | 1:A:639:GLN:HG3   | 2.37                     | 0.55              |
| 1:A:721:LYS:HE2   | 8:H:93:TYR:O      | 2.06                     | 0.55              |
| 1:A:1118:VAL:HG11 | 5:E:199:ILE:HG13  | 1.87                     | 0.55              |
| 1:A:1162:ASN:HD21 | 1:A:1164:LYS:HB2  | 1.71                     | 0.55              |
| 1:A:1162:ASN:HD22 | 1:A:1165:LYS:HG3  | 1.71                     | 0.55              |
| 2:B:401:GLU:HG3   | 2:B:402:VAL:H     | 1.70                     | 0.55              |
| 2:B:985:ILE:CG1   | 14:N:160:VAL:HG21 | 2.37                     | 0.55              |
| 2:B:1071:VAL:C    | 2:B:1075:GLU:HG3  | 2.27                     | 0.55              |
| 10:J:10:CYS:HB3   | 10:J:43:ARG:NH1   | 2.21                     | 0.55              |
| 15:O:219:ARG:NE   | 15:O:230:TRP:HE1  | 2.05                     | 0.55              |
| 15:O:602:TYR:CD2  | 15:O:605:LEU:HD23 | 2.40                     | 0.55              |
| 16:P:357:LEU:HD21 | 18:R:23:TYR:CD1   | 2.41                     | 0.55              |
| 16:P:504:THR:HG22 | 16:P:505:PRO:HD2  | 1.88                     | 0.55              |
| 17:Q:227:TYR:O    | 17:Q:230:ILE:HG13 | 2.06                     | 0.55              |
| 18:R:308:PHE:HD1  | 18:R:309:ALA:N    | 2.04                     | 0.55              |
| 1:A:545:SER:CB    | 17:Q:34:VAL:HG22  | 2.10                     | 0.55              |
| 1:A:916:THR:O     | 1:A:919:LYS:NZ    | 2.40                     | 0.55              |
| 1:A:1298:ASP:HA   | 1:A:1468:LYS:NZ   | 2.20                     | 0.55              |
| 18:R:320:CYS:O    | 18:R:323:SER:N    | 2.40                     | 0.55              |
| 1:A:1655:ASP:N    | 6:F:135:ARG:O     | 2.36                     | 0.55              |
| 3:C:65:ASN:O      | 3:C:69:ARG:HG3    | 2.07                     | 0.55              |
| 7:G:144:HIS:CE1   | 15:O:146:SER:OG   | 2.60                     | 0.55              |
| 13:M:15:VAL:HG22  | 13:M:90:LEU:HB2   | 1.88                     | 0.55              |
| 15:O:375:THR:C    | 15:O:377:TYR:N    | 2.65                     | 0.55              |
| 16:P:444:PRO:HG2  | 16:P:449:LEU:HD11 | 1.89                     | 0.55              |
| 17:Q:8:PRO:HB2    | 17:Q:19:LEU:CD2   | 2.36                     | 0.55              |
| 17:Q:371:GLU:CG   | 18:R:231:LEU:HG   | 2.36                     | 0.55              |
| 17:Q:374:THR:OG1  | 18:R:219:LEU:HD13 | 2.06                     | 0.55              |
| 1:A:719:ILE:HA    | 8:H:97:MET:HA     | 1.89                     | 0.55              |
| 1:A:1275:THR:C    | 9:I:45:LEU:O      | 2.48                     | 0.55              |
| 2:B:859:CYS:HB3   | 2:B:872:LYS:HB2   | 1.88                     | 0.55              |
| 15:O:359:GLY:O    | 15:O:363:THR:CG2  | 2.53                     | 0.55              |
| 16:P:357:LEU:HD21 | 18:R:23:TYR:CE1   | 2.41                     | 0.55              |
| 16:P:468:VAL:HG22 | 16:P:477:TYR:HB3  | 1.89                     | 0.55              |
| 16:P:488:LEU:HD23 | 18:R:138:PHE:CD2  | 2.42                     | 0.55              |
| 17:Q:343:THR:HG22 | 17:Q:373:GLU:HG3  | 1.87                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:436:ALA:CA    | 1:A:440:SER:HA    | 2.37                     | 0.55              |
| 1:A:1482:LYS:CE   | 2:B:304:ASP:CG    | 2.64                     | 0.55              |
| 2:B:819:ASP:CG    | 2:B:820:PRO:HD2   | 2.31                     | 0.55              |
| 3:C:314:PHE:CE2   | 11:K:135:PHE:CE1  | 2.95                     | 0.55              |
| 6:F:72:LYS:CB     | 6:F:142:SER:CA    | 2.24                     | 0.55              |
| 15:O:169:THR:HA   | 15:O:172:HIS:ND1  | 2.22                     | 0.55              |
| 15:O:348:THR:HG22 | 15:O:351:SER:CB   | 2.26                     | 0.55              |
| 16:P:359:SER:OG   | 18:R:194:GLY:O    | 2.25                     | 0.55              |
| 16:P:436:ILE:HG22 | 18:R:143:THR:N    | 2.21                     | 0.55              |
| 17:Q:326:TYR:CE2  | 17:Q:452:PHE:CZ   | 2.95                     | 0.55              |
| 17:Q:352:ILE:HG22 | 18:R:212:HIS:NE2  | 2.21                     | 0.55              |
| 17:Q:366:TYR:HE1  | 18:R:218:ASP:HB3  | 1.71                     | 0.55              |
| 18:R:369:ALA:HB1  | 18:R:411:VAL:HG23 | 1.86                     | 0.55              |
| 1:A:425:ASN:HD21  | 18:R:406:LYS:HD3  | 1.72                     | 0.55              |
| 2:B:48:SER:HB3    | 2:B:404:LEU:HD13  | 1.88                     | 0.55              |
| 2:B:322:ASN:HB3   | 2:B:325:GLN:H     | 1.71                     | 0.55              |
| 2:B:849:GLY:C     | 12:L:60:ARG:NH2   | 2.44                     | 0.55              |
| 3:C:139:LYS:HG2   | 3:C:201:GLU:HB3   | 1.89                     | 0.55              |
| 7:G:229:LEU:HD12  | 7:G:230:ARG:H     | 1.72                     | 0.55              |
| 15:O:163:ILE:HD12 | 15:O:207:LYS:HE3  | 1.89                     | 0.55              |
| 16:P:355:GLU:HA   | 18:R:24:ILE:CD1   | 2.36                     | 0.55              |
| 16:P:534:VAL:HA   | 16:P:552:LEU:O    | 2.06                     | 0.55              |
| 1:A:502:ALA:HB1   | 1:A:530:TRP:NE1   | 2.21                     | 0.55              |
| 2:B:21:ARG:NH1    | 2:B:22:GLU:OE1    | 2.40                     | 0.55              |
| 2:B:202:LEU:HD23  | 2:B:202:LEU:N     | 2.11                     | 0.55              |
| 2:B:574:SER:O     | 13:M:97:VAL:HG22  | 2.07                     | 0.55              |
| 16:P:474:LYS:O    | 16:P:499:GLU:HB2  | 2.06                     | 0.55              |
| 17:Q:24:ASP:CG    | 17:Q:26:ARG:HE    | 2.14                     | 0.55              |
| 17:Q:196:SER:CB   | 17:Q:204:ARG:HG2  | 2.37                     | 0.55              |
| 17:Q:258:MET:C    | 17:Q:442:LEU:HD13 | 2.26                     | 0.55              |
| 17:Q:374:THR:HG23 | 18:R:219:LEU:HD12 | 1.89                     | 0.55              |
| 18:R:26:TYR:CB    | 18:R:169:PRO:HB3  | 2.37                     | 0.55              |
| 1:A:476:VAL:HA    | 2:B:1059:PRO:HG2  | 1.88                     | 0.54              |
| 1:A:477:ASN:CA    | 2:B:1047:ARG:NH1  | 2.69                     | 0.54              |
| 1:A:581:ILE:HG12  | 1:A:582:LYS:N     | 2.21                     | 0.54              |
| 1:A:671:GLN:CB    | 2:B:952:HIS:CD2   | 2.90                     | 0.54              |
| 3:C:315:PHE:HE2   | 11:K:139:ILE:HD12 | 1.70                     | 0.54              |
| 8:H:80:ARG:NH1    | 11:K:108:TYR:CD1  | 2.74                     | 0.54              |
| 13:M:11:GLU:N     | 13:M:86:LYS:O     | 2.36                     | 0.54              |
| 16:P:315:PHE:HB3  | 16:P:317:ILE:CD1  | 2.37                     | 0.54              |
| 16:P:722:TRP:CD1  | 17:Q:264:PRO:HD3  | 2.42                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:R:158:THR:HG23 | 18:R:161:ASN:H    | 1.72                     | 0.54              |
| 1:A:1260:LYS:HE2  | 1:A:1262:LEU:HG   | 1.89                     | 0.54              |
| 2:B:42:VAL:HG21   | 2:B:190:ILE:HD12  | 1.89                     | 0.54              |
| 2:B:143:TRP:CG    | 2:B:446:MET:HE3   | 2.37                     | 0.54              |
| 2:B:373:MET:O     | 2:B:377:MET:HG3   | 2.07                     | 0.54              |
| 15:O:69:THR:O     | 15:O:73:ILE:HG13  | 2.07                     | 0.54              |
| 16:P:194:ARG:HA   | 16:P:209:LYS:O    | 2.07                     | 0.54              |
| 17:Q:6:ARG:HA     | 17:Q:18:ARG:HD2   | 1.88                     | 0.54              |
| 17:Q:198:ILE:HG22 | 17:Q:389:GLN:HA   | 1.87                     | 0.54              |
| 17:Q:287:TRP:NE1  | 17:Q:289:ARG:HB3  | 2.21                     | 0.54              |
| 1:A:403:LEU:CD1   | 1:A:419:ILE:HG23  | 2.35                     | 0.54              |
| 1:A:475:ARG:HD2   | 2:B:1059:PRO:O    | 2.07                     | 0.54              |
| 1:A:827:THR:HG21  | 1:A:924:SER:HB3   | 1.89                     | 0.54              |
| 1:A:1025:LYS:NZ   | 2:B:1076:ARG:NH1  | 2.56                     | 0.54              |
| 15:O:359:GLY:O    | 15:O:363:THR:HG22 | 2.08                     | 0.54              |
| 16:P:414:ILE:HB   | 16:P:425:GLY:C    | 2.32                     | 0.54              |
| 17:Q:163:SER:HA   | 17:Q:230:ILE:HG22 | 1.88                     | 0.54              |
| 17:Q:193:PHE:HB2  | 18:R:209:ARG:CD   | 2.37                     | 0.54              |
| 18:R:353:VAL:CG1  | 18:R:364:VAL:HB   | 2.36                     | 0.54              |
| 1:A:1317:ILE:HA   | 1:A:1321:PHE:HB3  | 1.90                     | 0.54              |
| 2:B:1003:ALA:C    | 14:N:169:GLU:H    | 2.15                     | 0.54              |
| 17:Q:333:SER:HA   | 17:Q:336:GLU:HG2  | 1.89                     | 0.54              |
| 17:Q:418:PRO:CB   | 18:R:233:TYR:OH   | 2.55                     | 0.54              |
| 18:R:161:ASN:O    | 18:R:164:LYS:HB2  | 2.07                     | 0.54              |
| 18:R:213:ILE:HG12 | 18:R:242:ILE:HD13 | 1.90                     | 0.54              |
| 1:A:721:LYS:NZ    | 8:H:91:ASP:CA     | 2.68                     | 0.54              |
| 2:B:548:LYS:O     | 2:B:550:ARG:CZ    | 2.56                     | 0.54              |
| 17:Q:341:ARG:NH2  | 17:Q:369:TRP:HE1  | 2.05                     | 0.54              |
| 1:A:492:THR:HG23  | 1:A:811:SER:OG    | 2.08                     | 0.54              |
| 1:A:998:HIS:NE2   | 2:B:711:GLN:HA    | 2.22                     | 0.54              |
| 1:A:1310:LYS:HG2  | 1:A:1311:GLU:CG   | 2.38                     | 0.54              |
| 2:B:16:PHE:HD2    | 10:J:32:GLU:OE2   | 1.90                     | 0.54              |
| 2:B:625:GLU:OE1   | 2:B:667:PHE:HB3   | 2.07                     | 0.54              |
| 3:C:33:VAL:CG1    | 11:K:130:VAL:HG21 | 2.38                     | 0.54              |
| 15:O:467:MET:HG2  | 15:O:575:SER:HA   | 1.89                     | 0.54              |
| 16:P:623:LEU:HG   | 16:P:678:LEU:HD12 | 1.88                     | 0.54              |
| 17:Q:263:PRO:CA   | 17:Q:446:TYR:CD1  | 2.73                     | 0.54              |
| 17:Q:351:ASN:C    | 17:Q:369:TRP:CH2  | 2.80                     | 0.54              |
| 18:R:207:ASN:H    | 18:R:211:ARG:HD2  | 1.73                     | 0.54              |
| 18:R:324:MET:CE   | 18:R:377:ASP:HB3  | 2.38                     | 0.54              |
| 15:O:373:LEU:HD12 | 15:O:423:TYR:CD2  | 2.43                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:320:ILE:HG13 | 16:P:323:ASN:OD1  | 2.07                     | 0.54              |
| 17:Q:290:THR:HB   | 17:Q:292:GLU:N    | 2.22                     | 0.54              |
| 17:Q:335:THR:HG21 | 17:Q:478:ARG:HG3  | 1.88                     | 0.54              |
| 17:Q:381:MET:HE1  | 18:R:212:HIS:HB3  | 1.90                     | 0.54              |
| 18:R:273:TRP:O    | 18:R:277:ILE:HG22 | 2.08                     | 0.54              |
| 1:A:67:LEU:HD13   | 1:A:71:PHE:O      | 2.08                     | 0.54              |
| 1:A:408:LYS:HB2   | 1:A:411:VAL:O     | 2.08                     | 0.54              |
| 1:A:1641:ILE:HG23 | 2:B:1092:LEU:HD13 | 1.88                     | 0.54              |
| 2:B:284:SER:OG    | 2:B:287:GLU:HG3   | 2.07                     | 0.54              |
| 15:O:243:GLU:HA   | 15:O:328:LEU:HD23 | 1.90                     | 0.54              |
| 16:P:438:TRP:HB2  | 18:R:141:TRP:HE1  | 1.73                     | 0.54              |
| 16:P:448:THR:HG23 | 16:P:471:MET:H    | 1.71                     | 0.54              |
| 16:P:711:LEU:HD21 | 16:P:741:ILE:HD13 | 1.90                     | 0.54              |
| 2:B:550:ARG:O     | 2:B:648:ARG:O     | 2.26                     | 0.54              |
| 2:B:1073:GLU:HA   | 2:B:1076:ARG:CB   | 2.38                     | 0.54              |
| 3:C:230:LEU:HD22  | 3:C:297:HIS:CE1   | 2.43                     | 0.54              |
| 7:G:132:VAL:HG22  | 7:G:232:THR:HG22  | 1.90                     | 0.54              |
| 16:P:352:PHE:CE1  | 18:R:162:PHE:CD1  | 2.95                     | 0.54              |
| 16:P:659:LEU:HD12 | 16:P:742:TRP:NE1  | 2.23                     | 0.54              |
| 17:Q:375:LEU:HD21 | 18:R:231:LEU:HD23 | 1.89                     | 0.54              |
| 1:A:1262:LEU:HD23 | 1:A:1497:ILE:HA   | 1.90                     | 0.54              |
| 1:A:1297:PHE:CZ   | 1:A:1301:GLU:OE1  | 2.52                     | 0.54              |
| 2:B:38:LEU:HD11   | 2:B:493:PHE:CZ    | 2.43                     | 0.54              |
| 3:C:45:SER:CB     | 3:C:271:ARG:NH2   | 2.71                     | 0.54              |
| 3:C:292:GLY:HA3   | 3:C:295:ARG:HH22  | 1.71                     | 0.54              |
| 18:R:350:SER:HA   | 18:R:353:VAL:HB   | 1.90                     | 0.54              |
| 2:B:212:ASN:OD1   | 2:B:238:SER:HA    | 2.08                     | 0.53              |
| 2:B:679:GLN:N     | 14:N:155:VAL:O    | 2.41                     | 0.53              |
| 2:B:788:ILE:HB    | 2:B:948:ILE:HB    | 1.89                     | 0.53              |
| 16:P:265:THR:HG23 | 16:P:274:ILE:HG12 | 1.90                     | 0.53              |
| 16:P:492:LEU:HD22 | 16:P:492:LEU:H    | 1.73                     | 0.53              |
| 16:P:662:LEU:HB3  | 16:P:665:ASN:CG   | 2.33                     | 0.53              |
| 18:R:5:PRO:CD     | 18:R:217:THR:CG2  | 2.83                     | 0.53              |
| 18:R:305:THR:HB   | 18:R:308:PHE:CE1  | 2.43                     | 0.53              |
| 18:R:361:ASP:C    | 18:R:363:GLU:H    | 2.14                     | 0.53              |
| 1:A:1446:ARG:O    | 1:A:1450:ILE:HG13 | 2.08                     | 0.53              |
| 2:B:203:ILE:HG22  | 2:B:405:GLY:HA2   | 1.89                     | 0.53              |
| 2:B:894:LYS:HG2   | 12:L:47:ARG:CD    | 2.38                     | 0.53              |
| 2:B:985:ILE:C     | 14:N:160:VAL:CG2  | 2.80                     | 0.53              |
| 3:C:315:PHE:CZ    | 11:K:139:ILE:HD12 | 2.42                     | 0.53              |
| 15:O:189:PHE:CD1  | 15:O:190:ILE:N    | 2.76                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:223:SER:O    | 15:O:226:GLY:N    | 2.35                     | 0.53              |
| 16:P:197:ARG:HB3  | 16:P:261:VAL:O    | 2.08                     | 0.53              |
| 16:P:365:TRP:HE3  | 16:P:372:ILE:HG22 | 1.73                     | 0.53              |
| 18:R:168:ILE:HD11 | 18:R:172:LYS:HE2  | 1.90                     | 0.53              |
| 2:B:134:ARG:HD2   | 2:B:160:GLY:HA3   | 1.91                     | 0.53              |
| 2:B:203:ILE:CG2   | 2:B:405:GLY:HA2   | 2.37                     | 0.53              |
| 2:B:550:ARG:N     | 2:B:650:LEU:O     | 2.40                     | 0.53              |
| 13:M:12:ILE:HD12  | 14:N:67:LEU:HB2   | 1.90                     | 0.53              |
| 15:O:245:GLN:HG3  | 15:O:377:TYR:O    | 2.09                     | 0.53              |
| 17:Q:341:ARG:HH12 | 17:Q:369:TRP:NE1  | 2.05                     | 0.53              |
| 18:R:6:ILE:HG21   | 18:R:210:THR:HG22 | 1.91                     | 0.53              |
| 1:A:407:GLN:O     | 1:A:408:LYS:NZ    | 2.37                     | 0.53              |
| 1:A:862:THR:CA    | 9:I:67:VAL:HG12   | 2.39                     | 0.53              |
| 1:A:1650:GLY:O    | 1:A:1651:THR:C    | 2.41                     | 0.53              |
| 15:O:66:ASN:N     | 15:O:66:ASN:ND2   | 2.53                     | 0.53              |
| 15:O:100:LEU:HD22 | 15:O:107:ILE:CD1  | 2.38                     | 0.53              |
| 17:Q:309:TYR:O    | 17:Q:313:THR:OG1  | 2.20                     | 0.53              |
| 18:R:352:TRP:O    | 18:R:356:PRO:HD3  | 2.09                     | 0.53              |
| 2:B:497:ILE:CG1   | 2:B:699:ILE:HD13  | 2.38                     | 0.53              |
| 2:B:1091:ARG:CZ   | 2:B:1095:SER:OG   | 2.56                     | 0.53              |
| 5:E:145:THR:C     | 5:E:147:HIS:N     | 2.65                     | 0.53              |
| 16:P:221:ARG:HH12 | 16:P:266:GLU:HB3  | 1.72                     | 0.53              |
| 16:P:472:ARG:HH12 | 18:R:203:SER:HB2  | 1.73                     | 0.53              |
| 1:A:824:THR:O     | 2:B:1023:ARG:HB2  | 2.08                     | 0.53              |
| 1:A:1002:GLY:HA3  | 2:B:713:PRO:HD3   | 1.91                     | 0.53              |
| 1:A:1136:VAL:HG22 | 1:A:1174:TYR:CG   | 2.43                     | 0.53              |
| 1:A:1297:PHE:CD2  | 9:I:60:LEU:HD13   | 2.43                     | 0.53              |
| 1:A:1654:PHE:CD2  | 6:F:134:ILE:HG23  | 2.44                     | 0.53              |
| 7:G:154:ASN:HD21  | 15:O:182:MET:HE3  | 1.73                     | 0.53              |
| 15:O:468:GLU:C    | 15:O:470:PHE:N    | 2.65                     | 0.53              |
| 16:P:355:GLU:O    | 18:R:24:ILE:CD1   | 2.55                     | 0.53              |
| 16:P:472:ARG:NE   | 18:R:200:THR:HG23 | 2.23                     | 0.53              |
| 16:P:650:LEU:HD13 | 16:P:652:GLY:H    | 1.74                     | 0.53              |
| 17:Q:115:GLN:HB3  | 17:Q:190:MET:HE2  | 1.91                     | 0.53              |
| 17:Q:361:PRO:O    | 17:Q:364:SER:N    | 2.42                     | 0.53              |
| 18:R:410:TYR:O    | 18:R:413:THR:OG1  | 2.20                     | 0.53              |
| 1:A:403:LEU:HD11  | 1:A:419:ILE:HD13  | 1.88                     | 0.53              |
| 2:B:38:LEU:HD11   | 2:B:493:PHE:HZ    | 1.74                     | 0.53              |
| 2:B:317:TYR:HB3   | 2:B:320:LEU:HD12  | 1.89                     | 0.53              |
| 2:B:664:VAL:HG22  | 2:B:672:MET:HE1   | 1.91                     | 0.53              |
| 13:M:75:GLN:HB2   | 14:N:60:SER:HA    | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:63:LEU:CD2   | 15:O:111:ARG:HD2  | 2.38                     | 0.53              |
| 17:Q:162:ILE:HG22 | 17:Q:226:LEU:HD21 | 1.90                     | 0.53              |
| 18:R:5:PRO:HD3    | 18:R:217:THR:OG1  | 2.09                     | 0.53              |
| 1:A:686:PHE:CZ    | 8:H:121:LEU:HD11  | 2.40                     | 0.53              |
| 2:B:762:MET:HE2   | 2:B:762:MET:HA    | 1.91                     | 0.53              |
| 2:B:1005:TYR:HH   | 10:J:44:TYR:HD2   | 1.49                     | 0.53              |
| 2:B:1092:LEU:C    | 2:B:1096:SER:CB   | 2.82                     | 0.53              |
| 16:P:302:VAL:O    | 16:P:363:ILE:HD11 | 2.09                     | 0.53              |
| 17:Q:8:PRO:CB     | 17:Q:19:LEU:HD23  | 2.39                     | 0.53              |
| 17:Q:22:ILE:HD12  | 17:Q:26:ARG:NH1   | 2.24                     | 0.53              |
| 17:Q:358:PRO:HB3  | 18:R:206:ARG:CG   | 2.38                     | 0.53              |
| 18:R:139:GLU:HB2  | 18:R:314:TRP:CH2  | 2.37                     | 0.53              |
| 1:A:544:VAL:HA    | 17:Q:34:VAL:H     | 1.74                     | 0.53              |
| 2:B:112:GLY:HA3   | 2:B:893:ASN:HB3   | 1.91                     | 0.53              |
| 3:C:37:LYS:HG3    | 11:K:134:LYS:HZ2  | 1.74                     | 0.53              |
| 15:O:468:GLU:C    | 15:O:470:PHE:H    | 2.15                     | 0.53              |
| 17:Q:370:SER:O    | 17:Q:373:GLU:N    | 2.42                     | 0.53              |
| 1:A:507:TYR:CE1   | 1:A:508:PRO:C     | 2.87                     | 0.53              |
| 1:A:954:GLY:N     | 1:A:1205:PHE:HB3  | 2.10                     | 0.53              |
| 1:A:969:PHE:CE2   | 1:A:978:ALA:HA    | 2.44                     | 0.53              |
| 9:I:96:TYR:HA     | 9:I:111:PHE:O     | 2.09                     | 0.53              |
| 16:P:292:LEU:CD1  | 16:P:343:LEU:HG   | 2.39                     | 0.53              |
| 16:P:408:ILE:HB   | 16:P:453:VAL:HG21 | 1.91                     | 0.53              |
| 17:Q:22:ILE:HD12  | 17:Q:26:ARG:NE    | 2.18                     | 0.53              |
| 17:Q:101:LYS:O    | 17:Q:105:LEU:HG   | 2.07                     | 0.53              |
| 17:Q:337:SER:HB3  | 17:Q:448:LYS:HD3  | 1.81                     | 0.53              |
| 17:Q:417:PHE:CZ   | 18:R:270:PHE:HA   | 2.44                     | 0.53              |
| 17:Q:505:ILE:HA   | 17:Q:508:ALA:HB3  | 1.90                     | 0.53              |
| 18:R:171:ARG:O    | 18:R:174:GLU:HB3  | 2.09                     | 0.53              |
| 1:A:422:ARG:CZ    | 18:R:412:ARG:HH11 | 2.21                     | 0.52              |
| 1:A:1318:SER:HA   | 1:A:1450:ILE:CD1  | 2.39                     | 0.52              |
| 2:B:25:PHE:CZ     | 10:J:59:LYS:HD2   | 2.44                     | 0.52              |
| 2:B:64:GLY:CA     | 2:B:242:ASP:HB2   | 2.38                     | 0.52              |
| 2:B:535:ASP:CG    | 2:B:720:GLN:HE22  | 2.17                     | 0.52              |
| 3:C:33:VAL:HG12   | 11:K:130:VAL:HG21 | 1.90                     | 0.52              |
| 16:P:273:ARG:HG2  | 16:P:291:PRO:HB3  | 1.90                     | 0.52              |
| 17:Q:187:THR:HB   | 17:Q:380:TRP:NE1  | 2.23                     | 0.52              |
| 18:R:5:PRO:HD3    | 18:R:217:THR:CB   | 2.39                     | 0.52              |
| 18:R:347:ASP:O    | 18:R:351:GLU:CB   | 2.56                     | 0.52              |
| 1:A:414:GLU:C     | 1:A:416:ARG:N     | 2.67                     | 0.52              |
| 1:A:990:ILE:CB    | 1:A:994:GLU:HB3   | 2.06                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:527:PHE:CG    | 2:B:666:PRO:HB3   | 2.44                     | 0.52              |
| 3:C:67:PHE:O      | 3:C:71:MET:HG3    | 2.08                     | 0.52              |
| 3:C:272:LYS:HD3   | 14:N:179:ASP:HB3  | 1.91                     | 0.52              |
| 15:O:240:ILE:HD13 | 15:O:240:ILE:N    | 2.23                     | 0.52              |
| 15:O:376:TYR:CE2  | 15:O:377:TYR:CD2  | 2.93                     | 0.52              |
| 15:O:467:MET:HA   | 15:O:467:MET:HE2  | 1.91                     | 0.52              |
| 16:P:185:GLN:HG3  | 18:R:190:SER:OG   | 2.09                     | 0.52              |
| 1:A:615:ARG:HH12  | 2:B:929:ARG:NE    | 2.02                     | 0.52              |
| 1:A:822:THR:O     | 2:B:1015:SER:HB2  | 2.09                     | 0.52              |
| 1:A:1482:LYS:CD   | 2:B:304:ASP:CG    | 2.81                     | 0.52              |
| 1:A:1657:LEU:O    | 6:F:132:LEU:C     | 2.49                     | 0.52              |
| 2:B:49:PHE:CD2    | 2:B:194:PHE:CZ    | 2.95                     | 0.52              |
| 2:B:679:GLN:HA    | 14:N:155:VAL:O    | 2.09                     | 0.52              |
| 2:B:1065:ARG:O    | 2:B:1065:ARG:HG3  | 2.08                     | 0.52              |
| 11:K:48:LYS:HE2   | 11:K:64:GLN:NE2   | 2.23                     | 0.52              |
| 17:Q:418:PRO:O    | 18:R:233:TYR:CZ   | 2.62                     | 0.52              |
| 18:R:242:ILE:HG23 | 18:R:244:GLY:H    | 1.73                     | 0.52              |
| 1:A:1329:ILE:HG21 | 1:A:1456:PHE:CD2  | 2.40                     | 0.52              |
| 2:B:699:ILE:O     | 2:B:703:LEU:HG    | 2.08                     | 0.52              |
| 6:F:66:ARG:HH22   | 7:G:90:LEU:HD12   | 1.57                     | 0.52              |
| 16:P:394:VAL:HG22 | 16:P:434:ARG:HH11 | 1.73                     | 0.52              |
| 16:P:472:ARG:CZ   | 18:R:203:SER:HB2  | 2.38                     | 0.52              |
| 16:P:473:HIS:HD2  | 16:P:475:ARG:HH11 | 1.58                     | 0.52              |
| 1:A:1050:TYR:CE1  | 1:A:1185:VAL:CG1  | 2.93                     | 0.52              |
| 1:A:1657:LEU:CD2  | 7:G:104:LEU:HB3   | 2.38                     | 0.52              |
| 3:C:97:LEU:HD11   | 3:C:202:ILE:HD13  | 1.90                     | 0.52              |
| 3:C:293:ARG:N     | 3:C:295:ARG:CZ    | 2.55                     | 0.52              |
| 15:O:376:TYR:CG   | 15:O:419:LYS:HD3  | 2.44                     | 0.52              |
| 15:O:402:THR:O    | 15:O:406:ILE:HG13 | 2.09                     | 0.52              |
| 16:P:294:PHE:HB2  | 16:P:296:GLU:H    | 1.75                     | 0.52              |
| 16:P:354:PRO:CB   | 18:R:27:ILE:CG2   | 2.82                     | 0.52              |
| 18:R:201:SER:C    | 18:R:205:VAL:HG23 | 2.28                     | 0.52              |
| 1:A:209:THR:HG21  | 5:E:173:SER:OG    | 2.09                     | 0.52              |
| 1:A:481:ARG:HB3   | 2:B:1045:GLN:O    | 2.09                     | 0.52              |
| 1:A:990:ILE:C     | 1:A:994:GLU:CB    | 2.82                     | 0.52              |
| 1:A:1289:SER:HB3  | 1:A:1475:GLU:HG2  | 1.91                     | 0.52              |
| 2:B:156:ARG:NH2   | 2:B:455:GLU:OE1   | 2.24                     | 0.52              |
| 2:B:796:ARG:HB3   | 10:J:8:PHE:HD1    | 1.75                     | 0.52              |
| 2:B:833:PRO:O     | 2:B:834:LYS:HB3   | 2.10                     | 0.52              |
| 2:B:894:LYS:HG2   | 12:L:47:ARG:HD2   | 1.90                     | 0.52              |
| 3:C:142:ARG:NH2   | 10:J:67:GLU:OE2   | 2.42                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:80:THR:OG1    | 15:O:228:GLN:HG2  | 2.10                     | 0.52              |
| 15:O:206:ARG:HA   | 15:O:209:VAL:HG12 | 1.91                     | 0.52              |
| 16:P:452:THR:HG21 | 16:P:508:ILE:HG22 | 1.92                     | 0.52              |
| 1:A:476:VAL:CG2   | 2:B:1070:ARG:H    | 2.05                     | 0.52              |
| 1:A:1657:LEU:O    | 6:F:132:LEU:HA    | 2.09                     | 0.52              |
| 7:G:30:GLU:HA     | 7:G:32:ASN:H      | 1.75                     | 0.52              |
| 14:N:87:TYR:CE2   | 14:N:141:GLU:CD   | 2.88                     | 0.52              |
| 15:O:235:GLU:O    | 15:O:238:ILE:HD13 | 2.07                     | 0.52              |
| 15:O:337:THR:O    | 15:O:341:THR:OG1  | 2.27                     | 0.52              |
| 16:P:448:THR:HG21 | 16:P:471:MET:H    | 1.74                     | 0.52              |
| 17:Q:116:ILE:O    | 17:Q:120:ILE:HG12 | 2.09                     | 0.52              |
| 18:R:177:LEU:HD22 | 18:R:185:LYS:CG   | 2.37                     | 0.52              |
| 1:A:476:VAL:CG2   | 2:B:1069:ILE:N    | 2.73                     | 0.52              |
| 2:B:16:PHE:CD2    | 10:J:32:GLU:OE2   | 2.63                     | 0.52              |
| 3:C:215:ASP:CG    | 12:L:70:ARG:HH22  | 2.17                     | 0.52              |
| 3:C:272:LYS:HA    | 14:N:175:TYR:CD2  | 2.43                     | 0.52              |
| 15:O:499:GLU:O    | 15:O:502:LEU:HG   | 2.09                     | 0.52              |
| 17:Q:198:ILE:HG22 | 17:Q:388:THR:C    | 2.35                     | 0.52              |
| 2:B:25:PHE:O      | 10:J:62:ARG:HD3   | 2.08                     | 0.52              |
| 2:B:943:ILE:CD1   | 10:J:44:TYR:CD1   | 2.93                     | 0.52              |
| 15:O:473:PHE:HE2  | 15:O:516:PRO:HG3  | 1.73                     | 0.52              |
| 16:P:384:ASP:HB3  | 16:P:389:TRP:CD1  | 2.45                     | 0.52              |
| 17:Q:10:CYS:HB2   | 17:Q:17:SER:N     | 2.25                     | 0.52              |
| 1:A:474:LYS:CE    | 2:B:1092:LEU:HD22 | 2.33                     | 0.52              |
| 2:B:497:ILE:HG13  | 2:B:699:ILE:CD1   | 2.40                     | 0.52              |
| 16:P:426:ALA:O    | 16:P:433:VAL:HG11 | 2.10                     | 0.52              |
| 16:P:475:ARG:NH1  | 17:Q:367:PHE:CE1  | 2.78                     | 0.52              |
| 1:A:1276:THR:OG1  | 9:I:45:LEU:O      | 2.27                     | 0.51              |
| 2:B:22:GLU:O      | 2:B:26:ILE:HG13   | 2.10                     | 0.51              |
| 2:B:678:PRO:O     | 14:N:154:ARG:HA   | 2.10                     | 0.51              |
| 2:B:1005:TYR:CD2  | 14:N:170:HIS:CG   | 2.98                     | 0.51              |
| 15:O:518:LYS:HD3  | 15:O:519:PHE:CZ   | 2.45                     | 0.51              |
| 1:A:429:THR:CG2   | 18:R:406:LYS:HZ1  | 2.22                     | 0.51              |
| 1:A:1298:ASP:CB   | 1:A:1468:LYS:HZ3  | 2.23                     | 0.51              |
| 2:B:532:HIS:NE2   | 2:B:723:LYS:CE    | 2.73                     | 0.51              |
| 2:B:535:ASP:N     | 2:B:720:GLN:OE1   | 2.43                     | 0.51              |
| 7:G:20:HIS:ND1    | 7:G:20:HIS:O      | 2.38                     | 0.51              |
| 1:A:408:LYS:CD    | 1:A:408:LYS:N     | 2.73                     | 0.51              |
| 1:A:970:LYS:HG2   | 1:A:973:GLU:HG2   | 1.92                     | 0.51              |
| 1:A:1654:PHE:CZ   | 6:F:89:GLU:HA     | 2.45                     | 0.51              |
| 1:A:1662:ASN:C    | 7:G:101:SER:HB2   | 2.35                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:858:ILE:HD13  | 2:B:872:LYS:O     | 2.10                     | 0.51              |
| 16:P:193:LEU:CD1  | 16:P:251:SER:H    | 2.23                     | 0.51              |
| 17:Q:358:PRO:CA   | 18:R:206:ARG:CD   | 2.85                     | 0.51              |
| 2:B:1069:ILE:N    | 2:B:1069:ILE:CD1  | 2.73                     | 0.51              |
| 15:O:248:LEU:HD23 | 15:O:248:LEU:O    | 2.10                     | 0.51              |
| 15:O:378:THR:O    | 15:O:379:ARG:NH1  | 2.44                     | 0.51              |
| 16:P:420:GLU:HA   | 16:P:442:LEU:HD22 | 1.93                     | 0.51              |
| 17:Q:371:GLU:CG   | 18:R:231:LEU:HD12 | 2.33                     | 0.51              |
| 1:A:670:ILE:HG13  | 2:B:783:MET:HE3   | 1.92                     | 0.51              |
| 2:B:307:GLU:OE2   | 2:B:311:ARG:NH1   | 2.43                     | 0.51              |
| 2:B:743:ARG:CZ    | 10:J:60:PHE:HZ    | 2.23                     | 0.51              |
| 2:B:894:LYS:CA    | 12:L:54:ARG:HE    | 2.18                     | 0.51              |
| 3:C:326:GLU:HG3   | 11:K:125:MET:CE   | 2.40                     | 0.51              |
| 15:O:235:GLU:CA   | 15:O:237:ILE:HB   | 2.40                     | 0.51              |
| 16:P:186:TYR:O    | 18:R:195:LEU:HB3  | 2.11                     | 0.51              |
| 16:P:355:GLU:C    | 18:R:24:ILE:CD1   | 2.81                     | 0.51              |
| 16:P:472:ARG:HH12 | 17:Q:360:LYS:CE   | 2.21                     | 0.51              |
| 17:Q:8:PRO:CG     | 17:Q:19:LEU:HD23  | 2.40                     | 0.51              |
| 17:Q:189:LYS:HA   | 17:Q:384:GLN:HG2  | 1.92                     | 0.51              |
| 17:Q:414:TYR:CE2  | 17:Q:419:LEU:HB3  | 2.45                     | 0.51              |
| 1:A:475:ARG:O     | 2:B:1059:PRO:HD2  | 2.10                     | 0.51              |
| 1:A:697:TYR:CE2   | 11:K:92:SER:OG    | 2.58                     | 0.51              |
| 1:A:1297:PHE:HD2  | 9:I:60:LEU:HD13   | 1.75                     | 0.51              |
| 1:A:1450:ILE:HD12 | 1:A:1460:TYR:CD2  | 2.46                     | 0.51              |
| 2:B:721:MET:HE2   | 2:B:721:MET:HA    | 1.92                     | 0.51              |
| 5:E:131:THR:HG21  | 5:E:191:LYS:HE2   | 1.91                     | 0.51              |
| 10:J:1:MET:HG2    | 10:J:57:ILE:HB    | 1.93                     | 0.51              |
| 15:O:144:CYS:HB2  | 15:O:179:PHE:CZ   | 2.46                     | 0.51              |
| 15:O:467:MET:HG3  | 15:O:519:PHE:CZ   | 2.45                     | 0.51              |
| 17:Q:447:ALA:HA   | 17:Q:450:THR:HB   | 1.91                     | 0.51              |
| 18:R:202:THR:HA   | 18:R:205:VAL:CG2  | 2.41                     | 0.51              |
| 1:A:597:LYS:HD3   | 2:B:1081:GLY:C    | 2.36                     | 0.51              |
| 16:P:272:PHE:HE1  | 16:P:303:VAL:HB   | 1.75                     | 0.51              |
| 16:P:498:LEU:HD11 | 17:Q:368:GLN:CG   | 2.35                     | 0.51              |
| 16:P:498:LEU:HD23 | 16:P:499:GLU:H    | 1.75                     | 0.51              |
| 17:Q:22:ILE:HD12  | 17:Q:26:ARG:CZ    | 2.40                     | 0.51              |
| 18:R:5:PRO:HD2    | 18:R:217:THR:HG21 | 1.89                     | 0.51              |
| 1:A:1484:LEU:CD1  | 2:B:305:ARG:NH1   | 2.56                     | 0.51              |
| 1:A:1573:TYR:HA   | 9:I:111:PHE:HE2   | 1.76                     | 0.51              |
| 2:B:29:PRO:O      | 2:B:177:PRO:HB2   | 2.11                     | 0.51              |
| 15:O:169:THR:O    | 15:O:170:VAL:C    | 2.54                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:313:THR:O    | 17:Q:317:MET:HB2  | 2.11                     | 0.51              |
| 18:R:324:MET:HE1  | 18:R:377:ASP:HB3  | 1.93                     | 0.51              |
| 2:B:208:VAL:HG23  | 2:B:401:GLU:CG    | 2.35                     | 0.51              |
| 2:B:475:GLY:O     | 2:B:476:LEU:CB    | 2.59                     | 0.51              |
| 2:B:1010:ASN:HB3  | 2:B:1025:ASP:HB3  | 1.92                     | 0.51              |
| 3:C:47:LEU:HD23   | 3:C:48:ASP:N      | 2.25                     | 0.51              |
| 15:O:240:ILE:CG2  | 15:O:332:LEU:HD11 | 2.41                     | 0.51              |
| 15:O:374:PRO:O    | 15:O:376:TYR:CD2  | 2.63                     | 0.51              |
| 16:P:363:ILE:HG22 | 16:P:374:VAL:HG22 | 1.93                     | 0.51              |
| 16:P:382:GLU:OE2  | 16:P:432:PRO:HG2  | 2.10                     | 0.51              |
| 16:P:414:ILE:HB   | 16:P:425:GLY:O    | 2.10                     | 0.51              |
| 16:P:778:ASP:CG   | 16:P:779:ASP:H    | 2.19                     | 0.51              |
| 17:Q:189:LYS:CA   | 17:Q:384:GLN:CG   | 2.88                     | 0.51              |
| 18:R:206:ARG:H    | 18:R:206:ARG:NE   | 2.03                     | 0.51              |
| 1:A:466:LEU:HD11  | 2:B:1181:VAL:CG2  | 2.41                     | 0.51              |
| 1:A:507:TYR:HD1   | 1:A:509:GLU:HG2   | 1.76                     | 0.51              |
| 1:A:544:VAL:CG1   | 17:Q:32:GLY:O     | 2.57                     | 0.51              |
| 1:A:909:SER:HA    | 9:I:83:LYS:HZ3    | 1.68                     | 0.51              |
| 1:A:1484:LEU:HD22 | 2:B:305:ARG:HH21  | 1.76                     | 0.51              |
| 2:B:545:PHE:CE1   | 2:B:649:MET:SD    | 3.04                     | 0.51              |
| 2:B:1005:TYR:CE2  | 14:N:170:HIS:CD2  | 2.99                     | 0.51              |
| 4:D:48:GLU:OE2    | 4:D:90:LYS:NZ     | 2.43                     | 0.51              |
| 8:H:38:LEU:HD11   | 8:H:123:MET:HE2   | 1.93                     | 0.51              |
| 11:K:55:SER:OG    | 11:K:57:ASP:OD1   | 2.28                     | 0.51              |
| 15:O:216:LEU:HD13 | 15:O:342:HIS:CB   | 2.41                     | 0.51              |
| 16:P:317:ILE:HD11 | 16:P:326:ILE:HG23 | 1.92                     | 0.51              |
| 16:P:573:GLU:HB3  | 17:Q:499:LYS:HD3  | 1.94                     | 0.51              |
| 17:Q:303:GLU:O    | 17:Q:306:VAL:N    | 2.44                     | 0.51              |
| 1:A:472:MET:CE    | 2:B:1076:ARG:CD   | 2.88                     | 0.50              |
| 1:A:670:ILE:CD1   | 2:B:783:MET:HE2   | 2.42                     | 0.50              |
| 1:A:1148:LEU:HD22 | 1:A:1163:GLU:HG3  | 1.93                     | 0.50              |
| 16:P:225:LEU:HD11 | 16:P:235:SER:HB3  | 1.93                     | 0.50              |
| 16:P:389:TRP:CZ3  | 18:R:149:LYS:O    | 2.64                     | 0.50              |
| 1:A:472:MET:HG3   | 2:B:1073:GLU:CD   | 2.34                     | 0.50              |
| 1:A:827:THR:CG2   | 1:A:924:SER:CB    | 2.89                     | 0.50              |
| 1:A:840:ASN:O     | 1:A:844:THR:HG23  | 2.11                     | 0.50              |
| 1:A:1310:LYS:CG   | 1:A:1311:GLU:OE1  | 2.37                     | 0.50              |
| 15:O:240:ILE:HG23 | 15:O:332:LEU:CG   | 2.41                     | 0.50              |
| 16:P:360:TRP:CZ3  | 18:R:196:GLU:OE2  | 2.64                     | 0.50              |
| 16:P:422:ILE:HG12 | 16:P:442:LEU:HD12 | 1.93                     | 0.50              |
| 16:P:603:ARG:O    | 16:P:607:VAL:HG23 | 2.12                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:10:CYS:HB3   | 17:Q:16:PRO:HA    | 1.93                     | 0.50              |
| 17:Q:193:PHE:CZ   | 18:R:208:TYR:CE1  | 2.63                     | 0.50              |
| 1:A:438:ILE:O     | 1:A:457:LYS:HB3   | 2.04                     | 0.50              |
| 1:A:689:ARG:HD2   | 8:H:79:TRP:HZ3    | 1.76                     | 0.50              |
| 1:A:1658:ALA:CA   | 6:F:131:PRO:O     | 2.58                     | 0.50              |
| 2:B:894:LYS:HG2   | 12:L:54:ARG:CZ    | 2.38                     | 0.50              |
| 15:O:507:GLN:O    | 15:O:511:ILE:HG23 | 2.12                     | 0.50              |
| 16:P:681:GLN:HA   | 16:P:684:GLN:HB2  | 1.93                     | 0.50              |
| 16:P:725:VAL:HG13 | 17:Q:449:GLN:CG   | 2.39                     | 0.50              |
| 16:P:770:ASP:HB2  | 17:Q:145:ASN:CG   | 2.36                     | 0.50              |
| 17:Q:10:CYS:SG    | 17:Q:29:CYS:SG    | 3.07                     | 0.50              |
| 17:Q:137:TRP:O    | 17:Q:141:LEU:HB2  | 2.12                     | 0.50              |
| 17:Q:385:PHE:CZ   | 18:R:209:ARG:CA   | 2.86                     | 0.50              |
| 17:Q:414:TYR:OH   | 18:R:237:ALA:HA   | 2.11                     | 0.50              |
| 18:R:364:VAL:HA   | 18:R:367:ILE:HB   | 1.93                     | 0.50              |
| 1:A:597:LYS:HD3   | 2:B:1082:HIS:N    | 2.27                     | 0.50              |
| 1:A:497:VAL:HG21  | 1:A:605:VAL:HG13  | 1.92                     | 0.50              |
| 1:A:563:THR:HG22  | 15:O:375:THR:CG2  | 2.42                     | 0.50              |
| 1:A:597:LYS:HD2   | 2:B:1082:HIS:CE1  | 2.47                     | 0.50              |
| 2:B:531:VAL:HG13  | 2:B:716:MET:CA    | 2.41                     | 0.50              |
| 2:B:1090:ASP:OD1  | 2:B:1094:ASN:ND2  | 2.43                     | 0.50              |
| 2:B:1092:LEU:C    | 2:B:1096:SER:HB2  | 2.37                     | 0.50              |
| 8:H:26:ILE:HD12   | 8:H:42:ILE:HD12   | 1.93                     | 0.50              |
| 15:O:324:GLY:O    | 15:O:326:LYS:N    | 2.44                     | 0.50              |
| 16:P:217:ALA:O    | 16:P:219:LEU:N    | 2.43                     | 0.50              |
| 16:P:442:LEU:HD13 | 16:P:442:LEU:N    | 2.26                     | 0.50              |
| 17:Q:118:TRP:CZ2  | 17:Q:189:LYS:HB3  | 2.47                     | 0.50              |
| 17:Q:193:PHE:CB   | 18:R:209:ARG:CD   | 2.88                     | 0.50              |
| 1:A:477:ASN:HA    | 2:B:1047:ARG:CD   | 2.42                     | 0.50              |
| 1:A:1323:HIS:N    | 1:A:1454:HIS:NE2  | 2.60                     | 0.50              |
| 2:B:212:ASN:ND2   | 2:B:361:HIS:CG    | 2.79                     | 0.50              |
| 13:M:103:LYS:HA   | 13:M:106:LYS:HB2  | 1.93                     | 0.50              |
| 16:P:194:ARG:NH2  | 16:P:208:GLY:HA3  | 2.27                     | 0.50              |
| 17:Q:186:CYS:HA   | 18:R:208:TYR:HE1  | 0.78                     | 0.50              |
| 1:A:990:ILE:CA    | 1:A:994:GLU:OE1   | 2.26                     | 0.50              |
| 2:B:293:ILE:HG12  | 2:B:306:LEU:HD13  | 1.94                     | 0.50              |
| 2:B:551:ILE:CG2   | 2:B:648:ARG:H     | 2.22                     | 0.50              |
| 3:C:272:LYS:CA    | 14:N:175:TYR:CE2  | 2.83                     | 0.50              |
| 6:F:73:ALA:CA     | 6:F:143:PHE:O     | 2.56                     | 0.50              |
| 15:O:428:ILE:CD1  | 15:O:442:VAL:HG21 | 2.42                     | 0.50              |
| 16:P:436:ILE:CG2  | 18:R:143:THR:HG23 | 2.41                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:768:TYR:O    | 16:P:771:ILE:HB   | 2.12                     | 0.50              |
| 17:Q:15:CYS:CB    | 17:Q:17:SER:N     | 2.59                     | 0.50              |
| 17:Q:413:LEU:HA   | 17:Q:416:ILE:HD12 | 1.94                     | 0.50              |
| 1:A:486:PRO:CD    | 2:B:928:SER:OG    | 2.49                     | 0.50              |
| 2:B:68:ILE:HD13   | 2:B:418:ASP:OD1   | 2.12                     | 0.50              |
| 2:B:554:GLN:O     | 2:B:555:GLN:C     | 2.54                     | 0.50              |
| 3:C:58:ASN:N      | 3:C:296:ASN:ND2   | 2.58                     | 0.50              |
| 16:P:197:ARG:HD2  | 16:P:261:VAL:O    | 2.12                     | 0.50              |
| 16:P:365:TRP:CB   | 16:P:372:ILE:HA   | 2.42                     | 0.50              |
| 16:P:625:ASP:O    | 16:P:629:ARG:HB2  | 2.11                     | 0.50              |
| 16:P:767:PRO:O    | 16:P:771:ILE:HG12 | 2.11                     | 0.50              |
| 17:Q:108:PHE:CZ   | 17:Q:156:LEU:HD22 | 2.47                     | 0.50              |
| 18:R:269:ASP:N    | 18:R:269:ASP:OD2  | 2.43                     | 0.50              |
| 1:A:467:PHE:CD2   | 1:A:1614:SER:HB3  | 2.46                     | 0.50              |
| 1:A:597:LYS:HD2   | 2:B:1082:HIS:CG   | 2.46                     | 0.50              |
| 1:A:1025:LYS:NZ   | 2:B:1076:ARG:HH12 | 2.09                     | 0.50              |
| 1:A:1089:LEU:HD11 | 1:A:1175:MET:HE1  | 1.92                     | 0.50              |
| 1:A:1314:GLN:CD   | 1:A:1446:ARG:HH11 | 2.13                     | 0.50              |
| 2:B:338:PHE:CE1   | 2:B:353:VAL:HG22  | 2.47                     | 0.50              |
| 16:P:185:GLN:NE2  | 18:R:197:PRO:HB3  | 2.27                     | 0.50              |
| 16:P:253:SER:HA   | 16:P:261:VAL:HG11 | 1.94                     | 0.50              |
| 16:P:274:ILE:HD13 | 16:P:305:PHE:HZ   | 1.76                     | 0.50              |
| 1:A:514:TYR:O     | 6:F:115:THR:HG22  | 2.12                     | 0.49              |
| 1:A:719:ILE:HG12  | 8:H:97:MET:CG     | 2.40                     | 0.49              |
| 1:A:1053:ASP:C    | 1:A:1055:ILE:HG12 | 2.36                     | 0.49              |
| 1:A:1276:THR:H    | 9:I:45:LEU:C      | 2.11                     | 0.49              |
| 2:B:62:ASN:OD1    | 2:B:102:VAL:CG2   | 2.60                     | 0.49              |
| 2:B:212:ASN:HD21  | 2:B:361:HIS:CB    | 2.20                     | 0.49              |
| 2:B:841:ASP:OD1   | 2:B:842:GLU:N     | 2.40                     | 0.49              |
| 9:I:91:ASN:OD1    | 9:I:92:GLU:N      | 2.45                     | 0.49              |
| 18:R:231:LEU:O    | 18:R:235:ILE:HG12 | 2.12                     | 0.49              |
| 1:A:408:LYS:N     | 1:A:408:LYS:CE    | 2.75                     | 0.49              |
| 1:A:1657:LEU:CG   | 7:G:104:LEU:HD13  | 2.39                     | 0.49              |
| 2:B:1066:HIS:NE2  | 17:Q:23:ILE:HD13  | 2.27                     | 0.49              |
| 15:O:591:TYR:CE2  | 15:O:593:PRO:HG3  | 2.46                     | 0.49              |
| 17:Q:352:ILE:CG2  | 18:R:212:HIS:CE1  | 2.93                     | 0.49              |
| 18:R:372:HIS:CD2  | 18:R:410:TYR:HB3  | 2.47                     | 0.49              |
| 1:A:437:PHE:HA    | 1:A:455:GLY:HA3   | 1.93                     | 0.49              |
| 2:B:679:GLN:NE2   | 14:N:155:VAL:O    | 2.45                     | 0.49              |
| 13:M:65:TYR:CE1   | 13:M:97:VAL:HB    | 2.48                     | 0.49              |
| 15:O:240:ILE:HG22 | 15:O:380:SER:OG   | 2.03                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:355:VAL:HG11 | 18:R:215:THR:HB   | 1.93                     | 0.49              |
| 17:Q:366:TYR:CE1  | 18:R:218:ASP:HB3  | 2.47                     | 0.49              |
| 18:R:361:ASP:HB3  | 18:R:364:VAL:HG13 | 1.94                     | 0.49              |
| 1:A:422:ARG:CG    | 18:R:409:HIS:CE1  | 2.95                     | 0.49              |
| 1:A:435:ASN:CA    | 1:A:442:LYS:HB2   | 2.41                     | 0.49              |
| 2:B:30:LYS:O      | 2:B:176:SER:HB3   | 2.13                     | 0.49              |
| 2:B:152:LEU:HD22  | 2:B:443:LYS:CE    | 2.43                     | 0.49              |
| 2:B:203:ILE:HG22  | 2:B:405:GLY:CA    | 2.42                     | 0.49              |
| 2:B:550:ARG:HG2   | 2:B:650:LEU:O     | 2.12                     | 0.49              |
| 15:O:248:LEU:HB2  | 15:O:598:PHE:CE2  | 2.47                     | 0.49              |
| 16:P:656:HIS:CE1  | 16:P:748:GLU:HG3  | 2.47                     | 0.49              |
| 1:A:747:ILE:HD13  | 1:A:748:ASN:H     | 1.77                     | 0.49              |
| 1:A:991:LYS:CA    | 1:A:994:GLU:HG3   | 2.39                     | 0.49              |
| 2:B:202:LEU:H     | 2:B:202:LEU:CD2   | 2.13                     | 0.49              |
| 2:B:252:TYR:OH    | 2:B:305:ARG:NH1   | 2.44                     | 0.49              |
| 2:B:1005:TYR:HH   | 10:J:44:TYR:HE2   | 1.49                     | 0.49              |
| 3:C:47:LEU:HD23   | 3:C:48:ASP:H      | 1.77                     | 0.49              |
| 6:F:70:LYS:CG     | 7:G:95:LEU:CD2    | 2.90                     | 0.49              |
| 15:O:190:ILE:HD13 | 15:O:190:ILE:C    | 2.37                     | 0.49              |
| 15:O:336:LEU:HD13 | 15:O:602:TYR:CE1  | 2.48                     | 0.49              |
| 15:O:474:TYR:HB3  | 15:O:520:CYS:SG   | 2.53                     | 0.49              |
| 16:P:472:ARG:HH12 | 18:R:203:SER:CB   | 2.26                     | 0.49              |
| 17:Q:418:PRO:HD3  | 18:R:264:SER:HB3  | 1.91                     | 0.49              |
| 1:A:613:THR:CG2   | 2:B:913:ILE:CG2   | 2.79                     | 0.49              |
| 1:A:861:VAL:HG21  | 1:A:892:LEU:HA    | 1.93                     | 0.49              |
| 2:B:262:PHE:CD1   | 2:B:357:ILE:HD13  | 2.47                     | 0.49              |
| 2:B:656:LEU:HD22  | 14:N:153:VAL:CG2  | 2.42                     | 0.49              |
| 8:H:112:ILE:HD12  | 8:H:129:TYR:HB2   | 1.94                     | 0.49              |
| 15:O:199:PRO:HB2  | 15:O:208:LEU:HD23 | 1.95                     | 0.49              |
| 17:Q:152:LEU:HD12 | 17:Q:154:LEU:HD11 | 1.94                     | 0.49              |
| 1:A:477:ASN:C     | 2:B:1049:THR:HA   | 2.38                     | 0.49              |
| 1:A:671:GLN:HB3   | 2:B:952:HIS:CE1   | 2.48                     | 0.49              |
| 7:G:47:VAL:HB     | 7:G:65:HIS:CD2    | 2.47                     | 0.49              |
| 15:O:515:ASN:HD21 | 15:O:547:ASN:ND2  | 2.10                     | 0.49              |
| 15:O:518:LYS:NZ   | 15:O:575:SER:HB2  | 2.27                     | 0.49              |
| 15:O:521:ASN:O    | 15:O:525:MET:HG2  | 2.12                     | 0.49              |
| 16:P:599:LYS:HG2  | 17:Q:272:GLN:OE1  | 2.13                     | 0.49              |
| 17:Q:194:GLN:CG   | 17:Q:389:GLN:CB   | 2.85                     | 0.49              |
| 17:Q:385:PHE:HE1  | 18:R:209:ARG:CB   | 2.25                     | 0.49              |
| 1:A:999:CYS:N     | 2:B:712:SER:HB3   | 2.28                     | 0.49              |
| 3:C:37:LYS:HG3    | 11:K:134:LYS:NZ   | 2.27                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:157:TYR:HB2   | 3:C:160:ALA:HB2   | 1.94                     | 0.49              |
| 15:O:208:LEU:O    | 15:O:212:THR:HG23 | 2.12                     | 0.49              |
| 15:O:581:THR:HA   | 15:O:584:GLN:CD   | 2.38                     | 0.49              |
| 17:Q:189:LYS:HD2  | 17:Q:380:TRP:HE1  | 1.76                     | 0.49              |
| 1:A:507:TYR:HE1   | 1:A:510:PRO:HD3   | 1.77                     | 0.49              |
| 1:A:720:PHE:N     | 8:H:96:VAL:O      | 2.46                     | 0.49              |
| 2:B:28:PRO:CD     | 10:J:62:ARG:NE    | 2.76                     | 0.49              |
| 2:B:682:GLN:N     | 14:N:154:ARG:HH21 | 2.03                     | 0.49              |
| 15:O:591:TYR:HE2  | 15:O:593:PRO:HG3  | 1.77                     | 0.49              |
| 16:P:359:SER:OG   | 18:R:194:GLY:C    | 2.55                     | 0.49              |
| 18:R:273:TRP:HZ3  | 18:R:274:MET:HE2  | 1.78                     | 0.49              |
| 1:A:1200:MET:HE1  | 1:A:1569:VAL:HG12 | 1.95                     | 0.49              |
| 2:B:162:PRO:HG2   | 2:B:465:LEU:HD12  | 1.94                     | 0.49              |
| 6:F:66:ARG:HH22   | 7:G:90:LEU:HB3    | 1.77                     | 0.49              |
| 15:O:436:ARG:HG3  | 15:O:490:ILE:HG23 | 1.95                     | 0.49              |
| 16:P:68:THR:HG23  | 16:P:214:LEU:HA   | 1.95                     | 0.49              |
| 16:P:315:PHE:HB2  | 16:P:365:TRP:HH2  | 1.78                     | 0.49              |
| 16:P:420:GLU:HG2  | 16:P:441:ASP:HB2  | 1.95                     | 0.49              |
| 16:P:427:SER:HA   | 16:P:433:VAL:HB   | 1.95                     | 0.49              |
| 16:P:499:GLU:OE1  | 16:P:499:GLU:HA   | 2.13                     | 0.49              |
| 17:Q:22:ILE:HD12  | 17:Q:26:ARG:HE    | 1.78                     | 0.49              |
| 1:A:410:LYS:CB    | 1:A:411:VAL:HG23  | 2.43                     | 0.48              |
| 1:A:826:PHE:CE1   | 2:B:777:SER:OG    | 2.66                     | 0.48              |
| 5:E:54:GLN:HB2    | 5:E:57:MET:HE2    | 1.95                     | 0.48              |
| 7:G:137:ILE:HG13  | 7:G:227:GLY:O     | 2.13                     | 0.48              |
| 7:G:156:SER:OG    | 15:O:146:SER:HA   | 2.13                     | 0.48              |
| 15:O:198:PHE:CZ   | 15:O:236:LYS:HG3  | 2.48                     | 0.48              |
| 15:O:236:LYS:N    | 15:O:237:ILE:CD1  | 2.75                     | 0.48              |
| 16:P:226:HIS:CE1  | 16:P:234:THR:HG22 | 2.48                     | 0.48              |
| 16:P:488:LEU:CD2  | 18:R:138:PHE:CD2  | 2.96                     | 0.48              |
| 16:P:733:THR:HA   | 16:P:736:ILE:HG22 | 1.95                     | 0.48              |
| 16:P:757:GLN:HE21 | 16:P:758:ASN:N    | 2.10                     | 0.48              |
| 17:Q:352:ILE:HG23 | 18:R:212:HIS:CE1  | 2.45                     | 0.48              |
| 18:R:198:LEU:HD12 | 18:R:199:LYS:HB2  | 1.95                     | 0.48              |
| 1:A:509:GLU:CG    | 1:A:579:ARG:HE    | 2.26                     | 0.48              |
| 1:A:1603:MET:HE2  | 1:A:1615:TYR:CG   | 2.39                     | 0.48              |
| 2:B:25:PHE:CE2    | 10:J:59:LYS:HG3   | 2.48                     | 0.48              |
| 2:B:25:PHE:CG     | 10:J:59:LYS:CG    | 2.96                     | 0.48              |
| 2:B:68:ILE:HD13   | 2:B:71:LYS:NZ     | 2.29                     | 0.48              |
| 2:B:143:TRP:CZ2   | 2:B:446:MET:HG3   | 2.47                     | 0.48              |
| 2:B:225:ARG:NH2   | 2:B:261:ARG:HD3   | 2.27                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1089:GLN:HB3  | 2:B:1093:LEU:HD22 | 1.91                     | 0.48              |
| 7:G:158:LYS:CB    | 15:O:105:ASN:OD1  | 2.61                     | 0.48              |
| 14:N:111:VAL:HG13 | 14:N:122:ALA:HB2  | 1.96                     | 0.48              |
| 15:O:124:LYS:HD3  | 15:O:127:GLU:OE2  | 2.14                     | 0.48              |
| 16:P:197:ARG:HD2  | 16:P:260:LEU:C    | 2.38                     | 0.48              |
| 16:P:227:LEU:HD13 | 16:P:227:LEU:H    | 1.78                     | 0.48              |
| 16:P:264:ILE:HG12 | 16:P:265:THR:N    | 2.27                     | 0.48              |
| 16:P:441:ASP:HA   | 16:P:442:LEU:HD13 | 1.94                     | 0.48              |
| 17:Q:165:LEU:HD13 | 17:Q:190:MET:HE1  | 1.95                     | 0.48              |
| 17:Q:414:TYR:HE2  | 17:Q:419:LEU:HB3  | 1.78                     | 0.48              |
| 18:R:273:TRP:CZ3  | 18:R:274:MET:HE2  | 2.48                     | 0.48              |
| 1:A:720:PHE:CE1   | 8:H:98:TYR:HB2    | 2.47                     | 0.48              |
| 1:A:1055:ILE:HD11 | 1:A:1174:TYR:CE1  | 2.48                     | 0.48              |
| 2:B:182:GLN:HE22  | 10:J:69:ARG:CB    | 2.08                     | 0.48              |
| 2:B:1073:GLU:HA   | 2:B:1076:ARG:HB2  | 1.95                     | 0.48              |
| 7:G:35:SER:HG     | 7:G:132:VAL:H     | 1.59                     | 0.48              |
| 16:P:277:VAL:HG23 | 16:P:286:VAL:HG12 | 1.95                     | 0.48              |
| 16:P:458:LYS:HD3  | 16:P:461:HIS:CE1  | 2.46                     | 0.48              |
| 17:Q:197:GLU:CD   | 17:Q:387:PRO:HA   | 2.35                     | 0.48              |
| 1:A:410:LYS:CB    | 1:A:411:VAL:CG2   | 2.91                     | 0.48              |
| 1:A:991:LYS:N     | 1:A:994:GLU:N     | 2.58                     | 0.48              |
| 1:A:1317:ILE:HB   | 1:A:1460:TYR:OH   | 2.13                     | 0.48              |
| 1:A:1538:VAL:HG21 | 5:E:142:VAL:CG2   | 2.43                     | 0.48              |
| 3:C:230:LEU:HD22  | 3:C:297:HIS:NE2   | 2.28                     | 0.48              |
| 3:C:326:GLU:CG    | 11:K:125:MET:HE3  | 2.43                     | 0.48              |
| 15:O:91:LYS:HG3   | 15:O:92:ASN:N     | 2.28                     | 0.48              |
| 17:Q:193:PHE:HB3  | 18:R:209:ARG:NE   | 2.21                     | 0.48              |
| 18:R:85:ARG:HG2   | 18:R:85:ARG:HH11  | 1.77                     | 0.48              |
| 2:B:74:PHE:C      | 2:B:440:PHE:HE2   | 2.20                     | 0.48              |
| 2:B:202:LEU:CD1   | 2:B:499:HIS:HB3   | 2.40                     | 0.48              |
| 14:N:87:TYR:CA    | 14:N:141:GLU:CA   | 2.45                     | 0.48              |
| 17:Q:198:ILE:HG22 | 17:Q:389:GLN:CA   | 2.43                     | 0.48              |
| 18:R:9:THR:O      | 18:R:13:PHE:HD2   | 1.97                     | 0.48              |
| 18:R:177:LEU:CD2  | 18:R:185:LYS:HA   | 2.43                     | 0.48              |
| 1:A:68:ASP:O      | 1:A:70:LYS:N      | 2.46                     | 0.48              |
| 1:A:456:VAL:HG13  | 2:B:1188:GLU:OE1  | 2.14                     | 0.48              |
| 1:A:478:TYR:CE1   | 2:B:1049:THR:HB   | 2.49                     | 0.48              |
| 1:A:545:SER:HB2   | 17:Q:34:VAL:HG21  | 0.51                     | 0.48              |
| 1:A:629:ASP:O     | 2:B:926:VAL:CG2   | 2.55                     | 0.48              |
| 1:A:1050:TYR:CD1  | 1:A:1179:ILE:CG2  | 2.85                     | 0.48              |
| 1:A:1260:LYS:CE   | 1:A:1262:LEU:HD21 | 2.44                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:623:ASP:OD2   | 2:B:648:ARG:NH2   | 2.40                     | 0.48              |
| 2:B:679:GLN:OE1   | 14:N:157:ARG:CB   | 2.61                     | 0.48              |
| 3:C:228:ARG:HH22  | 14:N:175:TYR:HE2  | 1.62                     | 0.48              |
| 7:G:23:GLN:O      | 7:G:25:THR:N      | 2.46                     | 0.48              |
| 15:O:376:TYR:CB   | 15:O:419:LYS:HD3  | 2.43                     | 0.48              |
| 16:P:626:LEU:HD22 | 16:P:626:LEU:HA   | 1.59                     | 0.48              |
| 16:P:658:LYS:CB   | 16:P:660:LYS:H    | 2.24                     | 0.48              |
| 17:Q:161:THR:OG1  | 17:Q:162:ILE:N    | 2.46                     | 0.48              |
| 17:Q:198:ILE:H    | 17:Q:389:GLN:HA   | 1.78                     | 0.48              |
| 1:A:828:CYS:SG    | 2:B:1027:TYR:HB2  | 2.53                     | 0.48              |
| 2:B:415:GLU:OE2   | 2:B:472:SER:HB2   | 2.13                     | 0.48              |
| 2:B:1047:ARG:HD3  | 2:B:1049:THR:O    | 2.14                     | 0.48              |
| 10:J:6:ARG:HD2    | 10:J:11:GLY:O     | 2.13                     | 0.48              |
| 16:P:257:ARG:HG3  | 16:P:411:LYS:HZ1  | 1.78                     | 0.48              |
| 16:P:675:PHE:HZ   | 16:P:742:TRP:HZ3  | 1.61                     | 0.48              |
| 17:Q:258:MET:HB3  | 17:Q:442:LEU:HD13 | 1.84                     | 0.48              |
| 18:R:15:GLN:OE1   | 18:R:181:THR:HG23 | 2.14                     | 0.48              |
| 18:R:207:ASN:C    | 18:R:211:ARG:H    | 2.05                     | 0.48              |
| 1:A:1604:GLU:CD   | 1:A:1621:PHE:HE1  | 2.21                     | 0.48              |
| 2:B:53:THR:HG21   | 2:B:104:ILE:HD12  | 1.95                     | 0.48              |
| 2:B:243:GLN:CD    | 2:B:646:HIS:HE2   | 2.20                     | 0.48              |
| 15:O:234:ILE:HG21 | 15:O:367:LEU:HB3  | 1.95                     | 0.48              |
| 15:O:361:PHE:CE2  | 15:O:365:THR:HG21 | 2.48                     | 0.48              |
| 16:P:762:ARG:HG3  | 17:Q:139:LYS:HE3  | 1.95                     | 0.48              |
| 17:Q:194:GLN:CB   | 17:Q:389:GLN:HG3  | 2.42                     | 0.48              |
| 18:R:206:ARG:N    | 18:R:206:ARG:NE   | 2.60                     | 0.48              |
| 1:A:869:PRO:HG2   | 1:A:872:ASP:HB2   | 1.96                     | 0.48              |
| 1:A:1312:GLU:O    | 1:A:1316:VAL:HG23 | 2.13                     | 0.48              |
| 2:B:208:VAL:CG2   | 2:B:401:GLU:CG    | 2.92                     | 0.48              |
| 2:B:551:ILE:CG2   | 2:B:647:SER:C     | 2.87                     | 0.48              |
| 2:B:812:ALA:HA    | 2:B:815:ARG:HD3   | 1.96                     | 0.48              |
| 5:E:48:ASP:OD1    | 5:E:50:MET:HB3    | 2.13                     | 0.48              |
| 6:F:72:LYS:CG     | 6:F:142:SER:CA    | 2.91                     | 0.48              |
| 16:P:475:ARG:CD   | 17:Q:367:PHE:CD2  | 2.95                     | 0.48              |
| 16:P:476:ILE:HD12 | 16:P:508:ILE:HD11 | 1.96                     | 0.48              |
| 16:P:501:PRO:CB   | 16:P:567:ILE:CG2  | 2.72                     | 0.48              |
| 17:Q:352:ILE:HD13 | 17:Q:377:PHE:CE2  | 2.40                     | 0.48              |
| 1:A:436:ALA:HA    | 1:A:440:SER:CA    | 2.44                     | 0.48              |
| 1:A:718:THR:HG21  | 8:H:118:PHE:O     | 2.14                     | 0.48              |
| 1:A:986:PHE:HD2   | 2:B:958:MET:HE2   | 1.75                     | 0.48              |
| 1:A:1118:VAL:CG1  | 5:E:199:ILE:HG13  | 2.44                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:54:GLU:HG3    | 2:B:168:ASN:ND2   | 2.29                     | 0.48              |
| 2:B:848:ILE:CA    | 12:L:60:ARG:CD    | 2.72                     | 0.48              |
| 2:B:1005:TYR:CE2  | 14:N:170:HIS:ND1  | 2.82                     | 0.48              |
| 3:C:293:ARG:O     | 3:C:295:ARG:HD3   | 2.14                     | 0.48              |
| 15:O:66:ASN:CG    | 15:O:111:ARG:NH1  | 2.72                     | 0.48              |
| 16:P:290:GLU:HG3  | 16:P:291:PRO:O    | 2.14                     | 0.48              |
| 16:P:724:LEU:O    | 17:Q:447:ALA:HA   | 2.14                     | 0.48              |
| 1:A:382:GLN:NE2   | 1:A:456:VAL:HG22  | 2.23                     | 0.47              |
| 1:A:454:PRO:HG2   | 1:A:462:LYS:HZ2   | 1.79                     | 0.47              |
| 1:A:747:ILE:HD13  | 1:A:748:ASN:N     | 2.29                     | 0.47              |
| 1:A:959:VAL:HG22  | 1:A:965:THR:HG22  | 1.95                     | 0.47              |
| 1:A:999:CYS:SG    | 2:B:712:SER:HB3   | 2.54                     | 0.47              |
| 1:A:1162:ASN:ND2  | 1:A:1165:LYS:HG3  | 2.29                     | 0.47              |
| 2:B:211:ARG:NH2   | 2:B:646:HIS:O     | 2.47                     | 0.47              |
| 2:B:975:HIS:CE1   | 14:N:169:GLU:HG3  | 2.49                     | 0.47              |
| 3:C:58:ASN:C      | 3:C:296:ASN:ND2   | 2.72                     | 0.47              |
| 16:P:355:GLU:HB2  | 18:R:24:ILE:CG2   | 2.40                     | 0.47              |
| 16:P:577:LEU:O    | 17:Q:506:LYS:NZ   | 2.47                     | 0.47              |
| 17:Q:359:ASP:OD2  | 17:Q:359:ASP:N    | 2.47                     | 0.47              |
| 18:R:82:ARG:HD2   | 18:R:82:ARG:O     | 2.14                     | 0.47              |
| 1:A:40:ASN:N      | 1:A:40:ASN:OD1    | 2.44                     | 0.47              |
| 1:A:1055:ILE:CD1  | 1:A:1178:LEU:HD23 | 2.44                     | 0.47              |
| 1:A:1574:ALA:HB1  | 9:I:121:PHE:HA    | 1.96                     | 0.47              |
| 2:B:338:PHE:CZ    | 2:B:357:ILE:HD12  | 2.49                     | 0.47              |
| 15:O:48:SER:O     | 15:O:49:ALA:C     | 2.57                     | 0.47              |
| 16:P:185:GLN:HA   | 18:R:197:PRO:HA   | 1.96                     | 0.47              |
| 16:P:381:ILE:HA   | 16:P:391:THR:O    | 2.14                     | 0.47              |
| 18:R:361:ASP:O    | 18:R:363:GLU:N    | 2.40                     | 0.47              |
| 1:A:258:GLU:HA    | 1:A:261:ILE:HD12  | 1.96                     | 0.47              |
| 1:A:862:THR:O     | 9:I:67:VAL:HA     | 2.14                     | 0.47              |
| 1:A:1032:VAL:HG22 | 1:A:1050:TYR:HD1  | 1.75                     | 0.47              |
| 1:A:1049:MET:HG3  | 1:A:1053:ASP:H    | 1.77                     | 0.47              |
| 1:A:1298:ASP:O    | 1:A:1300:ASN:N    | 2.47                     | 0.47              |
| 2:B:212:ASN:CG    | 2:B:361:HIS:CG    | 2.92                     | 0.47              |
| 2:B:584:CYS:HB3   | 2:B:596:VAL:HG23  | 1.95                     | 0.47              |
| 7:G:144:HIS:HB3   | 15:O:146:SER:HB3  | 1.96                     | 0.47              |
| 13:M:102:SER:CA   | 13:M:105:SER:H    | 2.28                     | 0.47              |
| 15:O:245:GLN:NE2  | 15:O:379:ARG:CB   | 2.74                     | 0.47              |
| 15:O:407:SER:HB3  | 15:O:420:SER:HB2  | 1.96                     | 0.47              |
| 16:P:49:THR:HG22  | 18:R:318:ILE:HG22 | 1.96                     | 0.47              |
| 16:P:184:SER:O    | 18:R:198:LEU:HD23 | 2.13                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:22:ILE:HD11  | 17:Q:26:ARG:CG    | 2.44                     | 0.47              |
| 1:A:410:LYS:HB3   | 1:A:411:VAL:HG22  | 1.96                     | 0.47              |
| 1:A:474:LYS:NZ    | 2:B:1096:SER:HB2  | 2.30                     | 0.47              |
| 1:A:505:LEU:O     | 1:A:580:HIS:HA    | 2.14                     | 0.47              |
| 1:A:563:THR:HG22  | 15:O:375:THR:HG22 | 1.95                     | 0.47              |
| 1:A:1317:ILE:CG2  | 1:A:1460:TYR:CZ   | 2.96                     | 0.47              |
| 1:A:1603:MET:SD   | 1:A:1612:LYS:HA   | 2.54                     | 0.47              |
| 1:A:1655:ASP:CB   | 6:F:135:ARG:HB3   | 2.38                     | 0.47              |
| 2:B:894:LYS:HD3   | 12:L:47:ARG:NH2   | 2.26                     | 0.47              |
| 12:L:45:ALA:O     | 12:L:47:ARG:N     | 2.46                     | 0.47              |
| 15:O:240:ILE:HG22 | 15:O:332:LEU:HD11 | 1.96                     | 0.47              |
| 16:P:49:THR:O     | 16:P:49:THR:OG1   | 2.27                     | 0.47              |
| 16:P:59:ILE:HG22  | 16:P:60:VAL:H     | 1.78                     | 0.47              |
| 17:Q:7:GLY:HA3    | 17:Q:8:PRO:HD2    | 1.44                     | 0.47              |
| 18:R:162:PHE:HA   | 18:R:165:ILE:HD12 | 1.95                     | 0.47              |
| 1:A:498:PRO:HA    | 1:A:499:PRO:HD3   | 1.81                     | 0.47              |
| 1:A:826:PHE:CD2   | 1:A:827:THR:N     | 2.82                     | 0.47              |
| 2:B:736:ARG:HD3   | 2:B:738:ASP:OD2   | 2.15                     | 0.47              |
| 15:O:376:TYR:CD1  | 15:O:419:LYS:HG2  | 2.49                     | 0.47              |
| 16:P:56:ASP:OD1   | 16:P:554:ASN:ND2  | 2.48                     | 0.47              |
| 16:P:475:ARG:HD3  | 17:Q:367:PHE:CZ   | 2.45                     | 0.47              |
| 18:R:361:ASP:C    | 18:R:363:GLU:N    | 2.73                     | 0.47              |
| 1:A:422:ARG:CD    | 18:R:409:HIS:ND1  | 2.49                     | 0.47              |
| 2:B:209:GLN:CG    | 2:B:210:ARG:H     | 2.08                     | 0.47              |
| 2:B:679:GLN:OE1   | 14:N:157:ARG:CA   | 2.63                     | 0.47              |
| 3:C:222:VAL:C     | 3:C:224:THR:H     | 2.20                     | 0.47              |
| 3:C:292:GLY:CA    | 3:C:295:ARG:HH22  | 2.27                     | 0.47              |
| 15:O:386:PHE:HB2  | 15:O:594:TYR:CE2  | 2.49                     | 0.47              |
| 15:O:477:PHE:CE2  | 15:O:481:CYS:SG   | 3.07                     | 0.47              |
| 16:P:333:PHE:CD2  | 16:P:334:ASN:HB2  | 2.49                     | 0.47              |
| 16:P:480:VAL:HB   | 16:P:492:LEU:CD2  | 2.41                     | 0.47              |
| 1:A:508:PRO:HD2   | 1:A:639:GLN:HG3   | 1.95                     | 0.47              |
| 1:A:588:LEU:HD21  | 2:B:1087:LEU:CD1  | 2.31                     | 0.47              |
| 1:A:641:GLU:HB2   | 6:F:99:LEU:CD1    | 2.44                     | 0.47              |
| 1:A:1297:PHE:HE2  | 1:A:1301:GLU:CD   | 2.14                     | 0.47              |
| 1:A:1575:ILE:CD1  | 9:I:122:ARG:NH1   | 2.64                     | 0.47              |
| 3:C:247:PHE:HE1   | 3:C:289:VAL:HG21  | 1.80                     | 0.47              |
| 6:F:74:ILE:N      | 7:G:95:LEU:HD11   | 2.30                     | 0.47              |
| 15:O:243:GLU:HG2  | 15:O:332:LEU:HB2  | 1.97                     | 0.47              |
| 15:O:409:ALA:HB3  | 15:O:412:GLU:HG3  | 1.96                     | 0.47              |
| 17:Q:189:LYS:CG   | 17:Q:384:GLN:HE21 | 2.28                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:198:ILE:HG22 | 17:Q:388:THR:O    | 2.15                     | 0.47              |
| 17:Q:235:GLY:HA3  | 17:Q:287:TRP:CD1  | 2.50                     | 0.47              |
| 17:Q:263:PRO:HG3  | 17:Q:449:GLN:HG3  | 1.84                     | 0.47              |
| 18:R:186:LEU:C    | 18:R:186:LEU:CD1  | 2.86                     | 0.47              |
| 1:A:407:GLN:C     | 1:A:409:ASP:H     | 2.23                     | 0.47              |
| 1:A:1050:TYR:HB3  | 1:A:1054:ALA:CA   | 2.43                     | 0.47              |
| 2:B:413:LEU:O     | 2:B:417:ILE:HG13  | 2.14                     | 0.47              |
| 2:B:470:LEU:HD21  | 2:B:476:LEU:HD12  | 1.97                     | 0.47              |
| 5:E:61:GLN:HE21   | 5:E:105:PHE:HE1   | 1.62                     | 0.47              |
| 12:L:28:LYS:O     | 12:L:59:ALA:N     | 2.40                     | 0.47              |
| 15:O:383:TYR:HB3  | 15:O:606:MET:HE3  | 1.96                     | 0.47              |
| 16:P:300:LEU:HA   | 16:P:320:ILE:HG22 | 1.96                     | 0.47              |
| 16:P:422:ILE:HG12 | 16:P:442:LEU:HD11 | 1.96                     | 0.47              |
| 16:P:770:ASP:HB2  | 17:Q:145:ASN:OD1  | 2.14                     | 0.47              |
| 17:Q:250:GLN:HB3  | 17:Q:267:TYR:OH   | 2.15                     | 0.47              |
| 17:Q:258:MET:CA   | 17:Q:442:LEU:HD11 | 2.08                     | 0.47              |
| 18:R:30:ARG:NE    | 18:R:168:ILE:HD12 | 2.30                     | 0.47              |
| 1:A:934:LYS:HG2   | 2:B:955:PRO:HG2   | 1.96                     | 0.47              |
| 2:B:549:CYS:SG    | 2:B:649:MET:CB    | 3.03                     | 0.47              |
| 15:O:206:ARG:HA   | 15:O:209:VAL:CG1  | 2.45                     | 0.47              |
| 16:P:24:SER:OG    | 18:R:318:ILE:CG1  | 2.61                     | 0.47              |
| 16:P:197:ARG:CB   | 16:P:261:VAL:O    | 2.63                     | 0.47              |
| 16:P:390:GLN:HB2  | 18:R:152:ILE:HA   | 1.96                     | 0.47              |
| 17:Q:287:TRP:CE2  | 17:Q:289:ARG:HB3  | 2.50                     | 0.47              |
| 18:R:402:ASN:O    | 18:R:406:LYS:HG2  | 2.15                     | 0.47              |
| 1:A:19:LEU:HD11   | 2:B:1190:SER:HB2  | 1.96                     | 0.47              |
| 1:A:89:LEU:HD11   | 2:B:1192:MET:HB3  | 1.97                     | 0.47              |
| 1:A:476:VAL:HG11  | 2:B:1071:VAL:HG23 | 1.96                     | 0.47              |
| 2:B:407:PHE:HE2   | 2:B:647:SER:OG    | 1.98                     | 0.47              |
| 16:P:725:VAL:HA   | 17:Q:450:THR:HA   | 1.95                     | 0.47              |
| 17:Q:189:LYS:NZ   | 17:Q:380:TRP:HD1  | 2.12                     | 0.47              |
| 17:Q:351:ASN:ND2  | 17:Q:369:TRP:CE2  | 2.83                     | 0.47              |
| 17:Q:355:VAL:CG2  | 18:R:215:THR:HG21 | 2.45                     | 0.47              |
| 18:R:257:ILE:HG21 | 18:R:266:SER:HA   | 1.96                     | 0.47              |
| 1:A:466:LEU:HD21  | 2:B:1181:VAL:HG22 | 1.98                     | 0.46              |
| 1:A:991:LYS:HA    | 1:A:992:PRO:N     | 2.29                     | 0.46              |
| 1:A:1440:ASN:HA   | 1:A:1443:GLN:HB2  | 1.96                     | 0.46              |
| 2:B:1103:VAL:HG22 | 2:B:1176:VAL:HG22 | 1.97                     | 0.46              |
| 5:E:131:THR:HG21  | 5:E:191:LYS:CE    | 2.44                     | 0.46              |
| 15:O:374:PRO:C    | 15:O:376:TYR:CB   | 2.60                     | 0.46              |
| 16:P:421:ILE:CG2  | 16:P:423:ILE:HG13 | 2.44                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:444:PRO:CG   | 16:P:449:LEU:HD11 | 2.45                     | 0.46              |
| 16:P:704:LEU:HD23 | 17:Q:258:MET:HE1  | 1.96                     | 0.46              |
| 17:Q:193:PHE:HA   | 17:Q:219:ILE:HD11 | 1.97                     | 0.46              |
| 1:A:407:GLN:C     | 1:A:408:LYS:NZ    | 2.73                     | 0.46              |
| 6:F:69:LEU:HG     | 6:F:143:PHE:HE2   | 1.80                     | 0.46              |
| 7:G:139:ILE:HD13  | 15:O:145:SER:OG   | 2.14                     | 0.46              |
| 15:O:232:LEU:HD12 | 15:O:232:LEU:HA   | 1.74                     | 0.46              |
| 1:A:1258:ILE:HB   | 1:A:1501:ILE:HD12 | 1.97                     | 0.46              |
| 1:A:1482:LYS:HD3  | 2:B:304:ASP:HA    | 1.97                     | 0.46              |
| 1:A:1484:LEU:HD11 | 2:B:305:ARG:HD3   | 1.97                     | 0.46              |
| 2:B:990:ASP:OD2   | 14:N:159:ASP:HB3  | 2.16                     | 0.46              |
| 15:O:93:LEU:HD23  | 15:O:132:THR:CG2  | 2.45                     | 0.46              |
| 16:P:290:GLU:OE2  | 16:P:291:PRO:HD2  | 2.15                     | 0.46              |
| 16:P:417:THR:OG1  | 16:P:451:ILE:HB   | 2.16                     | 0.46              |
| 17:Q:250:GLN:OE1  | 17:Q:271:LYS:HD2  | 2.15                     | 0.46              |
| 18:R:295:PRO:HB3  | 18:R:296:PRO:HD2  | 1.97                     | 0.46              |
| 2:B:49:PHE:CD2    | 2:B:164:MET:HE3   | 2.51                     | 0.46              |
| 2:B:397:THR:HA    | 2:B:400:GLN:OE1   | 2.14                     | 0.46              |
| 2:B:774:ALA:HB1   | 2:B:1026:ILE:HD11 | 1.97                     | 0.46              |
| 2:B:1047:ARG:CD   | 2:B:1049:THR:O    | 2.60                     | 0.46              |
| 2:B:1047:ARG:HG2  | 2:B:1049:THR:H    | 1.81                     | 0.46              |
| 4:D:33:THR:HG23   | 4:D:96:PHE:HD1    | 1.80                     | 0.46              |
| 15:O:74:ILE:O     | 15:O:78:VAL:HG13  | 2.16                     | 0.46              |
| 15:O:379:ARG:NH1  | 15:O:379:ARG:CA   | 2.73                     | 0.46              |
| 15:O:388:VAL:HG13 | 15:O:389:SER:N    | 2.31                     | 0.46              |
| 17:Q:366:TYR:CE1  | 18:R:218:ASP:CB   | 2.98                     | 0.46              |
| 18:R:202:THR:HA   | 18:R:205:VAL:HG21 | 1.98                     | 0.46              |
| 18:R:236:PHE:CZ   | 18:R:253:ILE:HB   | 2.51                     | 0.46              |
| 1:A:407:GLN:C     | 1:A:409:ASP:N     | 2.74                     | 0.46              |
| 1:A:474:LYS:HZ2   | 2:B:1096:SER:HB2  | 1.80                     | 0.46              |
| 2:B:54:GLU:OE2    | 2:B:168:ASN:ND2   | 2.46                     | 0.46              |
| 3:C:117:ASP:OD1   | 3:C:119:ASN:ND2   | 2.44                     | 0.46              |
| 3:C:222:VAL:HB    | 3:C:224:THR:H     | 1.81                     | 0.46              |
| 16:P:366:PHE:HE2  | 16:P:433:VAL:H    | 1.64                     | 0.46              |
| 2:B:25:PHE:CG     | 10:J:59:LYS:HG2   | 2.51                     | 0.46              |
| 2:B:202:LEU:N     | 2:B:202:LEU:CD2   | 2.75                     | 0.46              |
| 2:B:448:ARG:HA    | 2:B:451:MET:HE3   | 1.97                     | 0.46              |
| 7:G:35:SER:OG     | 7:G:132:VAL:N     | 2.46                     | 0.46              |
| 9:I:23:VAL:O      | 9:I:39:LYS:NZ     | 2.49                     | 0.46              |
| 13:M:65:TYR:HE1   | 13:M:97:VAL:HB    | 1.81                     | 0.46              |
| 15:O:181:ARG:NH1  | 15:O:181:ARG:CG   | 2.77                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:61:VAL:HB    | 16:P:551:ALA:HB3  | 1.97                     | 0.46              |
| 16:P:225:LEU:H    | 16:P:225:LEU:HG   | 1.60                     | 0.46              |
| 16:P:408:ILE:HG23 | 16:P:413:GLY:C    | 2.41                     | 0.46              |
| 16:P:478:MET:HE2  | 16:P:497:VAL:HG13 | 1.97                     | 0.46              |
| 17:Q:341:ARG:HH12 | 17:Q:369:TRP:HE1  | 1.53                     | 0.46              |
| 1:A:507:TYR:CD1   | 1:A:509:GLU:HG2   | 2.50                     | 0.46              |
| 2:B:404:LEU:C     | 2:B:406:GLY:N     | 2.66                     | 0.46              |
| 3:C:230:LEU:CD1   | 3:C:299:ILE:HD11  | 2.44                     | 0.46              |
| 16:P:272:PHE:HB2  | 16:P:300:LEU:HD11 | 1.97                     | 0.46              |
| 16:P:357:LEU:CD2  | 18:R:23:TYR:CD1   | 2.98                     | 0.46              |
| 16:P:724:LEU:C    | 17:Q:450:THR:HB   | 2.36                     | 0.46              |
| 2:B:265:ARG:NH2   | 2:B:339:GLN:OE1   | 2.48                     | 0.46              |
| 2:B:293:ILE:CD1   | 2:B:302:LEU:HB3   | 2.46                     | 0.46              |
| 2:B:401:GLU:C     | 2:B:402:VAL:HG23  | 2.41                     | 0.46              |
| 2:B:890:ASP:HB3   | 2:B:896:GLN:OE1   | 2.15                     | 0.46              |
| 3:C:239:ILE:HG23  | 3:C:243:SER:HB3   | 1.96                     | 0.46              |
| 15:O:224:GLU:H    | 15:O:224:GLU:CD   | 2.17                     | 0.46              |
| 15:O:240:ILE:CG2  | 15:O:332:LEU:CD1  | 2.93                     | 0.46              |
| 16:P:596:ILE:HD12 | 16:P:596:ILE:O    | 2.16                     | 0.46              |
| 17:Q:19:LEU:CD1   | 17:Q:27:ARG:CB    | 2.94                     | 0.46              |
| 18:R:222:LEU:HD23 | 18:R:226:ARG:NH2  | 2.31                     | 0.46              |
| 1:A:476:VAL:N     | 2:B:1059:PRO:HG2  | 2.31                     | 0.46              |
| 4:D:46:GLU:OE1    | 4:D:47:LYS:HE2    | 2.15                     | 0.46              |
| 16:P:54:ALA:HA    | 16:P:55:LEU:HD12  | 1.98                     | 0.46              |
| 16:P:436:ILE:HG21 | 18:R:143:THR:CB   | 2.44                     | 0.46              |
| 1:A:489:ASN:CB    | 11:K:95:HIS:HD2   | 2.29                     | 0.46              |
| 1:A:581:ILE:CD1   | 1:A:637:PHE:CZ    | 2.97                     | 0.46              |
| 1:A:582:LYS:O     | 1:A:585:ASP:HB2   | 2.16                     | 0.46              |
| 1:A:720:PHE:HB2   | 8:H:96:VAL:HG12   | 1.97                     | 0.46              |
| 2:B:699:ILE:HG22  | 2:B:700:LEU:HD12  | 1.98                     | 0.46              |
| 2:B:894:LYS:CG    | 12:L:47:ARG:CD    | 2.94                     | 0.46              |
| 3:C:176:SER:O     | 3:C:180:ALA:HB2   | 2.16                     | 0.46              |
| 15:O:376:TYR:CE2  | 15:O:419:LYS:HE2  | 2.50                     | 0.46              |
| 16:P:326:ILE:HG21 | 16:P:385:PHE:CE1  | 2.51                     | 0.46              |
| 16:P:436:ILE:HG21 | 18:R:143:THR:HG23 | 1.98                     | 0.46              |
| 16:P:580:ASN:HB2  | 17:Q:506:LYS:HE2  | 1.98                     | 0.46              |
| 16:P:728:GLN:HB3  | 16:P:731:LEU:HB3  | 1.97                     | 0.46              |
| 16:P:770:ASP:OD2  | 17:Q:141:LEU:HG   | 2.15                     | 0.46              |
| 18:R:177:LEU:HD21 | 18:R:185:LYS:HA   | 1.98                     | 0.46              |
| 1:A:184:LYS:HA    | 1:A:187:GLU:HG2   | 1.98                     | 0.45              |
| 1:A:1323:HIS:HE1  | 1:A:1453:HIS:HB3  | 1.82                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:786:ALA:HB1   | 2:B:928:SER:HB2   | 1.98                     | 0.45              |
| 2:B:1090:ASP:O    | 2:B:1094:ASN:CB   | 2.64                     | 0.45              |
| 5:E:67:GLU:CD     | 5:E:67:GLU:H      | 2.23                     | 0.45              |
| 15:O:236:LYS:HA   | 15:O:236:LYS:HD3  | 1.73                     | 0.45              |
| 16:P:296:GLU:HB3  | 16:P:298:ASP:OD1  | 2.16                     | 0.45              |
| 16:P:498:LEU:HD23 | 16:P:499:GLU:O    | 2.16                     | 0.45              |
| 16:P:574:TRP:CH2  | 17:Q:495:LYS:HD2  | 2.51                     | 0.45              |
| 17:Q:137:TRP:CH2  | 17:Q:141:LEU:HD13 | 2.51                     | 0.45              |
| 17:Q:261:ALA:CB   | 17:Q:445:ARG:HD3  | 2.33                     | 0.45              |
| 17:Q:326:TYR:CD1  | 17:Q:452:PHE:CD2  | 2.98                     | 0.45              |
| 1:A:68:ASP:C      | 1:A:70:LYS:H      | 2.24                     | 0.45              |
| 1:A:1574:ALA:HB3  | 9:I:122:ARG:HB3   | 1.99                     | 0.45              |
| 1:A:1574:ALA:HB3  | 9:I:122:ARG:HG2   | 1.97                     | 0.45              |
| 3:C:71:MET:HE1    | 3:C:302:VAL:HG21  | 1.97                     | 0.45              |
| 13:M:26:PHE:CE1   | 13:M:98:SER:HB2   | 2.51                     | 0.45              |
| 16:P:56:ASP:O     | 16:P:57:LEU:HD13  | 2.16                     | 0.45              |
| 16:P:189:THR:HB   | 16:P:247:ILE:HG23 | 1.98                     | 0.45              |
| 16:P:198:ASP:OD1  | 16:P:204:ALA:CB   | 2.64                     | 0.45              |
| 16:P:330:PRO:HG3  | 16:P:342:GLN:CG   | 2.45                     | 0.45              |
| 16:P:384:ASP:CB   | 16:P:389:TRP:HB3  | 2.43                     | 0.45              |
| 16:P:584:ARG:O    | 16:P:588:SER:CB   | 2.62                     | 0.45              |
| 17:Q:152:LEU:HA   | 17:Q:152:LEU:HD13 | 1.67                     | 0.45              |
| 17:Q:194:GLN:CG   | 17:Q:389:GLN:HG3  | 2.47                     | 0.45              |
| 17:Q:351:ASN:OD1  | 17:Q:369:TRP:CZ2  | 2.69                     | 0.45              |
| 18:R:365:TRP:HB3  | 18:R:418:CYS:HB2  | 1.98                     | 0.45              |
| 1:A:998:HIS:C     | 2:B:712:SER:OG    | 2.59                     | 0.45              |
| 2:B:679:GLN:HG2   | 14:N:156:PRO:CA   | 2.33                     | 0.45              |
| 2:B:822:THR:HB    | 2:B:823:GLN:HG3   | 1.98                     | 0.45              |
| 2:B:1045:GLN:HB3  | 2:B:1063:ARG:HG3  | 1.97                     | 0.45              |
| 5:E:7:ARG:O       | 5:E:11:ARG:HG3    | 2.17                     | 0.45              |
| 6:F:93:ILE:HD13   | 6:F:93:ILE:HA     | 1.70                     | 0.45              |
| 15:O:175:MET:HE3  | 15:O:175:MET:HB2  | 1.81                     | 0.45              |
| 16:P:197:ARG:CD   | 16:P:261:VAL:O    | 2.64                     | 0.45              |
| 16:P:210:THR:HB   | 16:P:226:HIS:NE2  | 2.32                     | 0.45              |
| 16:P:254:ILE:HG21 | 16:P:368:HIS:CE1  | 2.51                     | 0.45              |
| 16:P:323:ASN:HB3  | 16:P:350:THR:HB   | 1.98                     | 0.45              |
| 16:P:394:VAL:HG22 | 16:P:434:ARG:NH1  | 2.32                     | 0.45              |
| 16:P:408:ILE:HD12 | 16:P:464:LEU:HD13 | 1.97                     | 0.45              |
| 16:P:704:LEU:HB3  | 17:Q:439:ILE:CG1  | 2.46                     | 0.45              |
| 17:Q:123:MET:HE2  | 17:Q:184:TRP:CZ2  | 2.51                     | 0.45              |
| 17:Q:274:ILE:HG23 | 17:Q:282:ARG:NH2  | 2.29                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:410:LYS:HB2   | 1:A:410:LYS:HE3   | 1.87                     | 0.45              |
| 1:A:514:TYR:CD1   | 6:F:115:THR:O     | 2.70                     | 0.45              |
| 1:A:996:TYR:CE1   | 2:B:525:TRP:CE3   | 3.05                     | 0.45              |
| 7:G:106:LYS:HB2   | 7:G:106:LYS:HE3   | 1.82                     | 0.45              |
| 9:I:89:CYS:SG     | 9:I:91:ASN:HB2    | 2.56                     | 0.45              |
| 15:O:521:ASN:HD22 | 15:O:524:VAL:H    | 1.64                     | 0.45              |
| 15:O:578:SER:O    | 15:O:579:LEU:CB   | 2.64                     | 0.45              |
| 16:P:446:ASP:OD2  | 16:P:448:THR:N    | 2.40                     | 0.45              |
| 17:Q:109:GLN:CD   | 17:Q:137:TRP:HE1  | 2.24                     | 0.45              |
| 17:Q:494:SER:HB2  | 17:Q:497:GLN:H    | 1.82                     | 0.45              |
| 17:Q:502:ILE:HA   | 17:Q:505:ILE:HG22 | 1.99                     | 0.45              |
| 1:A:721:LYS:HZ1   | 8:H:91:ASP:HA     | 1.75                     | 0.45              |
| 1:A:991:LYS:HB3   | 1:A:993:GLN:CG    | 2.46                     | 0.45              |
| 1:A:1600:ARG:HB2  | 1:A:1616:GLU:OE2  | 2.16                     | 0.45              |
| 2:B:152:LEU:HA    | 2:B:443:LYS:HE3   | 1.94                     | 0.45              |
| 3:C:293:ARG:O     | 3:C:295:ARG:CD    | 2.64                     | 0.45              |
| 15:O:243:GLU:OE1  | 15:O:243:GLU:HA   | 2.17                     | 0.45              |
| 15:O:390:GLN:NE2  | 15:O:433:LYS:H    | 2.13                     | 0.45              |
| 17:Q:198:ILE:HB   | 17:Q:390:THR:C    | 2.41                     | 0.45              |
| 18:R:1:MET:HG3    | 18:R:2:PHE:CD1    | 2.51                     | 0.45              |
| 18:R:323:SER:OG   | 18:R:324:MET:N    | 2.46                     | 0.45              |
| 1:A:5:LYS:HB3     | 1:A:5:LYS:HE2     | 1.68                     | 0.45              |
| 1:A:472:MET:CB    | 2:B:1073:GLU:OE1  | 2.64                     | 0.45              |
| 1:A:597:LYS:HB3   | 2:B:1082:HIS:CD2  | 2.42                     | 0.45              |
| 2:B:145:VAL:CG2   | 2:B:440:PHE:O     | 2.65                     | 0.45              |
| 2:B:292:ILE:HB    | 2:B:306:LEU:HD11  | 1.98                     | 0.45              |
| 2:B:585:CYS:HB2   | 2:B:595:TRP:CZ3   | 2.51                     | 0.45              |
| 11:K:49:LEU:HG    | 11:K:54:THR:HG21  | 1.98                     | 0.45              |
| 16:P:224:THR:HG21 | 16:P:237:GLU:HA   | 1.99                     | 0.45              |
| 16:P:724:LEU:HD13 | 17:Q:447:ALA:CB   | 2.46                     | 0.45              |
| 17:Q:310:PHE:O    | 17:Q:314:ILE:HG13 | 2.16                     | 0.45              |
| 17:Q:325:GLN:HG3  | 17:Q:452:PHE:HE1  | 1.61                     | 0.45              |
| 18:R:76:LYS:O     | 18:R:80:ARG:HG3   | 2.17                     | 0.45              |
| 18:R:252:GLY:O    | 18:R:256:GLU:CB   | 2.56                     | 0.45              |
| 1:A:403:LEU:HD12  | 1:A:403:LEU:HA    | 1.71                     | 0.45              |
| 1:A:1237:GLN:H    | 1:A:1544:ASN:HB2  | 1.81                     | 0.45              |
| 1:A:1660:VAL:HG23 | 7:G:103:LYS:H     | 1.82                     | 0.45              |
| 3:C:228:ARG:HG3   | 3:C:299:ILE:HB    | 1.98                     | 0.45              |
| 3:C:292:GLY:CA    | 3:C:295:ARG:NH2   | 2.80                     | 0.45              |
| 10:J:36:LEU:HD13  | 10:J:47:ARG:HB3   | 1.98                     | 0.45              |
| 15:O:129:PRO:O    | 15:O:130:PRO:C    | 2.59                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:263:ILE:HG21 | 16:P:276:SER:C    | 2.42                     | 0.45              |
| 1:A:219:LEU:HD23  | 1:A:219:LEU:HA    | 1.85                     | 0.45              |
| 1:A:589:MET:HE1   | 1:A:614:LEU:HD13  | 1.98                     | 0.45              |
| 1:A:1154:LEU:O    | 1:A:1158:SER:HB2  | 2.17                     | 0.45              |
| 1:A:1322:ILE:CB   | 1:A:1454:HIS:CD2  | 2.85                     | 0.45              |
| 2:B:64:GLY:HA2    | 2:B:242:ASP:HB2   | 1.90                     | 0.45              |
| 2:B:78:PRO:O      | 2:B:79:LEU:HB3    | 2.17                     | 0.45              |
| 16:P:196:TYR:HA   | 16:P:207:SER:O    | 2.16                     | 0.45              |
| 16:P:454:GLN:HE22 | 16:P:536:ASP:H    | 1.65                     | 0.45              |
| 17:Q:435:GLN:H    | 17:Q:435:GLN:HG3  | 1.38                     | 0.45              |
| 18:R:299:THR:CG2  | 18:R:305:THR:HA   | 2.46                     | 0.45              |
| 1:A:407:GLN:HB3   | 1:A:409:ASP:N     | 2.23                     | 0.45              |
| 1:A:475:ARG:HD3   | 2:B:1060:VAL:O    | 2.16                     | 0.45              |
| 1:A:921:PRO:CD    | 8:H:19:ARG:HG3    | 2.42                     | 0.45              |
| 1:A:1053:ASP:O    | 1:A:1055:ILE:CG1  | 2.55                     | 0.45              |
| 1:A:1463:ASP:HB2  | 1:A:1469:TRP:CE2  | 2.52                     | 0.45              |
| 2:B:682:GLN:HA    | 14:N:154:ARG:CZ   | 2.46                     | 0.45              |
| 5:E:78:LEU:HD13   | 5:E:107:THR:HB    | 1.98                     | 0.45              |
| 7:G:17:ILE:C      | 7:G:19:LYS:H      | 2.25                     | 0.45              |
| 7:G:159:LYS:HB3   | 15:O:105:ASN:ND2  | 2.12                     | 0.45              |
| 15:O:376:TYR:CD1  | 15:O:376:TYR:O    | 2.70                     | 0.45              |
| 15:O:468:GLU:O    | 15:O:470:PHE:N    | 2.49                     | 0.45              |
| 16:P:62:LYS:HE2   | 16:P:550:TYR:OH   | 2.17                     | 0.45              |
| 1:A:449:GLY:C     | 1:A:451:VAL:H     | 2.22                     | 0.45              |
| 1:A:629:ASP:O     | 2:B:916:LYS:HE2   | 2.17                     | 0.45              |
| 1:A:721:LYS:HD2   | 8:H:90:ALA:HB1    | 1.99                     | 0.45              |
| 2:B:49:PHE:HE2    | 2:B:194:PHE:CZ    | 2.30                     | 0.45              |
| 2:B:833:PRO:HG2   | 2:B:836:TRP:CZ2   | 2.52                     | 0.45              |
| 2:B:894:LYS:CG    | 12:L:47:ARG:HD2   | 2.47                     | 0.45              |
| 2:B:1090:ASP:CA   | 2:B:1093:LEU:HB3  | 2.36                     | 0.45              |
| 14:N:40:LEU:HD12  | 14:N:40:LEU:HA    | 1.84                     | 0.45              |
| 16:P:198:ASP:N    | 16:P:206:ALA:HA   | 2.32                     | 0.45              |
| 16:P:252:GLU:OE1  | 16:P:253:SER:N    | 2.35                     | 0.45              |
| 16:P:425:GLY:O    | 16:P:426:ALA:HB2  | 2.17                     | 0.45              |
| 16:P:753:PHE:HD1  | 16:P:753:PHE:HA   | 1.68                     | 0.45              |
| 17:Q:137:TRP:HE3  | 17:Q:140:ILE:HD11 | 1.82                     | 0.45              |
| 17:Q:484:ALA:O    | 17:Q:488:LEU:HG   | 2.17                     | 0.45              |
| 18:R:19:LEU:HB3   | 18:R:188:PHE:CD1  | 2.52                     | 0.45              |
| 1:A:721:LYS:HZ2   | 8:H:91:ASP:HA     | 1.79                     | 0.44              |
| 2:B:548:LYS:HG2   | 2:B:695:ASN:O     | 2.18                     | 0.44              |
| 5:E:93:MET:CG     | 5:E:120:ALA:HB1   | 2.46                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:321:LYS:HB2  | 16:P:321:LYS:NZ   | 2.31                     | 0.44              |
| 17:Q:234:CYS:SG   | 17:Q:284:LEU:HB3  | 2.58                     | 0.44              |
| 17:Q:262:LEU:HD23 | 17:Q:262:LEU:HA   | 1.84                     | 0.44              |
| 18:R:23:TYR:HA    | 18:R:173:MET:HE3  | 1.99                     | 0.44              |
| 18:R:187:TYR:CE2  | 18:R:191:ILE:HG21 | 2.52                     | 0.44              |
| 1:A:991:LYS:CB    | 1:A:994:GLU:HG3   | 2.48                     | 0.44              |
| 1:A:1260:LYS:HE2  | 1:A:1262:LEU:CG   | 2.47                     | 0.44              |
| 2:B:403:LEU:HD11  | 2:B:411:MET:HE3   | 1.99                     | 0.44              |
| 2:B:1158:ILE:HA   | 2:B:1167:PHE:O    | 2.17                     | 0.44              |
| 7:G:163:PRO:HG2   | 7:G:166:TRP:CD1   | 2.52                     | 0.44              |
| 16:P:193:LEU:HD12 | 16:P:250:ALA:HA   | 1.99                     | 0.44              |
| 16:P:627:GLY:C    | 16:P:628:TYR:HD1  | 2.25                     | 0.44              |
| 17:Q:197:GLU:CD   | 17:Q:387:PRO:C    | 2.72                     | 0.44              |
| 18:R:11:ARG:H     | 18:R:11:ARG:HG3   | 1.53                     | 0.44              |
| 1:A:408:LYS:HG3   | 1:A:416:ARG:HE    | 1.72                     | 0.44              |
| 1:A:535:GLN:HA    | 1:A:546:LEU:HG    | 1.99                     | 0.44              |
| 1:A:863:ASN:HB2   | 9:I:66:VAL:O      | 2.17                     | 0.44              |
| 2:B:190:ILE:HG13  | 2:B:191:GLY:N     | 2.32                     | 0.44              |
| 16:P:686:TYR:O    | 16:P:691:VAL:HG11 | 2.17                     | 0.44              |
| 17:Q:105:LEU:HD13 | 17:Q:141:LEU:HD11 | 1.99                     | 0.44              |
| 17:Q:195:ALA:O    | 17:Q:196:SER:C    | 2.60                     | 0.44              |
| 17:Q:358:PRO:CA   | 18:R:206:ARG:HG3  | 2.48                     | 0.44              |
| 17:Q:374:THR:O    | 17:Q:377:PHE:HB3  | 2.17                     | 0.44              |
| 1:A:257:ASN:OD1   | 1:A:258:GLU:N     | 2.51                     | 0.44              |
| 1:A:436:ALA:O     | 1:A:440:SER:HA    | 2.15                     | 0.44              |
| 1:A:535:GLN:HE22  | 17:Q:26:ARG:HG2   | 1.81                     | 0.44              |
| 1:A:697:TYR:OH    | 11:K:102:ASN:HB3  | 2.17                     | 0.44              |
| 1:A:1063:MET:HE1  | 1:A:1174:TYR:CD2  | 2.52                     | 0.44              |
| 1:A:1156:LYS:C    | 1:A:1158:SER:H    | 2.25                     | 0.44              |
| 1:A:1484:LEU:CD2  | 2:B:304:ASP:HB2   | 2.46                     | 0.44              |
| 11:K:80:ILE:HD13  | 11:K:105:ILE:HD11 | 1.98                     | 0.44              |
| 15:O:69:THR:HG22  | 15:O:70:GLN:N     | 2.31                     | 0.44              |
| 15:O:200:ASN:CB   | 17:Q:14:ASN:O     | 2.65                     | 0.44              |
| 16:P:350:THR:HG22 | 18:R:155:GLN:CA   | 2.45                     | 0.44              |
| 16:P:366:PHE:HZ   | 16:P:433:VAL:HG12 | 1.82                     | 0.44              |
| 17:Q:187:THR:HB   | 17:Q:380:TRP:HE1  | 1.81                     | 0.44              |
| 17:Q:204:ARG:HG3  | 17:Q:205:ILE:HG13 | 1.99                     | 0.44              |
| 17:Q:221:PRO:HA   | 17:Q:225:GLN:HB2  | 1.99                     | 0.44              |
| 17:Q:418:PRO:C    | 18:R:233:TYR:OH   | 2.60                     | 0.44              |
| 1:A:403:LEU:HD13  | 1:A:419:ILE:HG23  | 1.99                     | 0.44              |
| 1:A:487:ASP:CG    | 2:B:781:TYR:OH    | 2.61                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:545:SER:CA    | 17:Q:34:VAL:HG23  | 2.29                     | 0.44              |
| 1:A:545:SER:OG    | 17:Q:26:ARG:NH2   | 2.50                     | 0.44              |
| 1:A:920:PHE:CD1   | 1:A:921:PRO:HA    | 2.52                     | 0.44              |
| 1:A:1291:VAL:HG22 | 1:A:1473:LYS:HG3  | 1.98                     | 0.44              |
| 1:A:1575:ILE:CD1  | 9:I:122:ARG:CZ    | 2.95                     | 0.44              |
| 2:B:119:ARG:CZ    | 12:L:53:HIS:NE2   | 2.79                     | 0.44              |
| 2:B:427:GLN:HA    | 2:B:430:MET:HE3   | 1.98                     | 0.44              |
| 7:G:158:LYS:HB3   | 15:O:105:ASN:CG   | 2.42                     | 0.44              |
| 15:O:342:HIS:HE1  | 15:O:346:GLN:HE21 | 1.58                     | 0.44              |
| 16:P:198:ASP:OD1  | 16:P:204:ALA:HB1  | 2.17                     | 0.44              |
| 16:P:413:GLY:HA2  | 16:P:426:ALA:HB2  | 1.99                     | 0.44              |
| 17:Q:104:PHE:HZ   | 17:Q:156:LEU:HB2  | 1.77                     | 0.44              |
| 17:Q:137:TRP:CE3  | 17:Q:140:ILE:HD11 | 2.53                     | 0.44              |
| 17:Q:286:LEU:CD2  | 17:Q:300:ASN:HB3  | 2.47                     | 0.44              |
| 17:Q:318:LEU:HD12 | 17:Q:318:LEU:HA   | 1.77                     | 0.44              |
| 2:B:1001:ALA:O    | 14:N:168:LEU:HD23 | 2.17                     | 0.44              |
| 16:P:532:GLU:HB2  | 16:P:554:ASN:CB   | 2.46                     | 0.44              |
| 17:Q:128:GLU:O    | 17:Q:132:VAL:HG23 | 2.17                     | 0.44              |
| 17:Q:188:ALA:CB   | 17:Q:384:GLN:O    | 2.59                     | 0.44              |
| 17:Q:189:LYS:NZ   | 17:Q:380:TRP:CD1  | 2.81                     | 0.44              |
| 1:A:598:ALA:CB    | 1:A:601:MET:HE3   | 2.47                     | 0.44              |
| 1:A:1596:LEU:HD22 | 1:A:1602:GLY:HA2  | 2.00                     | 0.44              |
| 2:B:45:HIS:CE1    | 2:B:205:MET:HE2   | 2.52                     | 0.44              |
| 3:C:228:ARG:CD    | 14:N:173:THR:OG1  | 2.64                     | 0.44              |
| 3:C:326:GLU:HG3   | 11:K:125:MET:HE3  | 2.00                     | 0.44              |
| 16:P:198:ASP:HB2  | 16:P:206:ALA:HA   | 1.99                     | 0.44              |
| 16:P:428:GLU:HB2  | 16:P:435:ARG:NH1  | 2.30                     | 0.44              |
| 16:P:632:ILE:O    | 16:P:636:GLU:HG3  | 2.17                     | 0.44              |
| 16:P:725:VAL:HG13 | 17:Q:449:GLN:HG2  | 2.00                     | 0.44              |
| 17:Q:22:ILE:HD13  | 17:Q:26:ARG:CZ    | 2.45                     | 0.44              |
| 17:Q:189:LYS:CB   | 17:Q:384:GLN:HE21 | 2.27                     | 0.44              |
| 18:R:217:THR:HG22 | 18:R:239:LEU:HD21 | 2.00                     | 0.44              |
| 18:R:236:PHE:CE2  | 18:R:253:ILE:HD12 | 2.52                     | 0.44              |
| 1:A:36:THR:HG22   | 1:A:45:VAL:HG21   | 2.00                     | 0.44              |
| 1:A:413:LEU:HD22  | 1:A:413:LEU:HA    | 1.78                     | 0.44              |
| 1:A:1318:SER:HA   | 1:A:1450:ILE:HD13 | 2.00                     | 0.44              |
| 2:B:894:LYS:CG    | 12:L:54:ARG:NH1   | 2.81                     | 0.44              |
| 2:B:1002:LYS:HD2  | 14:N:166:LEU:C    | 2.42                     | 0.44              |
| 16:P:229:ARG:HG3  | 16:P:231:ASN:H    | 1.82                     | 0.44              |
| 16:P:760:ILE:O    | 16:P:764:LEU:HG   | 2.18                     | 0.44              |
| 2:B:46:ILE:HG13   | 2:B:192:GLY:HA2   | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:203:ILE:CB    | 2:B:405:GLY:HA3   | 2.46                     | 0.44              |
| 16:P:21:GLN:O     | 16:P:25:LEU:HB2   | 2.17                     | 0.44              |
| 16:P:331:LYS:HD3  | 16:P:331:LYS:HA   | 1.72                     | 0.44              |
| 16:P:362:ARG:NH2  | 16:P:364:GLU:HG3  | 2.31                     | 0.44              |
| 16:P:533:LEU:H    | 16:P:554:ASN:HB2  | 1.82                     | 0.44              |
| 16:P:675:PHE:HZ   | 16:P:742:TRP:CZ3  | 2.36                     | 0.44              |
| 16:P:717:LYS:CB   | 17:Q:439:ILE:CD1  | 2.76                     | 0.44              |
| 17:Q:160:SER:HA   | 17:Q:163:SER:HB2  | 2.00                     | 0.44              |
| 17:Q:255:LYS:O    | 17:Q:259:GLN:HB2  | 2.18                     | 0.44              |
| 17:Q:311:MET:HE3  | 17:Q:311:MET:HB3  | 1.89                     | 0.44              |
| 17:Q:355:VAL:HG21 | 18:R:215:THR:HG21 | 2.00                     | 0.44              |
| 18:R:362:ALA:CB   | 18:R:421:LYS:HB3  | 2.38                     | 0.44              |
| 1:A:677:GLY:HA3   | 1:A:786:TYR:OH    | 2.18                     | 0.43              |
| 1:A:756:LYS:HD2   | 9:I:85:LYS:HZ3    | 1.69                     | 0.43              |
| 1:A:1655:ASP:O    | 6:F:134:ILE:HA    | 2.17                     | 0.43              |
| 2:B:77:LYS:NZ     | 2:B:439:ASN:HA    | 2.33                     | 0.43              |
| 2:B:679:GLN:OE1   | 14:N:157:ARG:HA   | 2.16                     | 0.43              |
| 2:B:697:LEU:CB    | 2:B:702:ASN:CG    | 2.85                     | 0.43              |
| 5:E:177:ARG:HD3   | 5:E:215:MET:HB2   | 1.99                     | 0.43              |
| 6:F:75:PRO:CG     | 6:F:78:GLN:CB     | 2.82                     | 0.43              |
| 7:G:143:SER:CB    | 15:O:104:ILE:HB   | 2.48                     | 0.43              |
| 14:N:94:ASP:HB3   | 14:N:99:LEU:HG    | 2.00                     | 0.43              |
| 16:P:194:ARG:HG2  | 16:P:209:LYS:O    | 2.18                     | 0.43              |
| 16:P:357:LEU:HG   | 18:R:24:ILE:HD11  | 2.00                     | 0.43              |
| 16:P:399:TRP:O    | 16:P:419:ARG:NH2  | 2.51                     | 0.43              |
| 16:P:619:GLU:OE2  | 16:P:670:ALA:N    | 2.52                     | 0.43              |
| 18:R:299:THR:HG21 | 18:R:305:THR:HA   | 2.00                     | 0.43              |
| 1:A:472:MET:CA    | 1:A:472:MET:CE    | 2.86                     | 0.43              |
| 1:A:543:LEU:CA    | 17:Q:34:VAL:O     | 2.66                     | 0.43              |
| 1:A:1276:THR:HB   | 9:I:45:LEU:CD1    | 2.47                     | 0.43              |
| 1:A:1441:LYS:HE2  | 1:A:1441:LYS:HB3  | 1.76                     | 0.43              |
| 2:B:42:VAL:HG21   | 2:B:190:ILE:HB    | 2.00                     | 0.43              |
| 2:B:75:ASP:HA     | 2:B:440:PHE:CZ    | 2.53                     | 0.43              |
| 2:B:107:PRO:HG2   | 2:B:133:TYR:CZ    | 2.52                     | 0.43              |
| 2:B:563:SER:CA    | 13:M:73:SER:HB3   | 2.48                     | 0.43              |
| 15:O:515:ASN:N    | 15:O:516:PRO:HD3  | 2.33                     | 0.43              |
| 16:P:363:ILE:O    | 16:P:363:ILE:HD12 | 2.18                     | 0.43              |
| 16:P:433:VAL:HG22 | 16:P:434:ARG:O    | 2.17                     | 0.43              |
| 16:P:751:SER:O    | 16:P:753:PHE:N    | 2.51                     | 0.43              |
| 18:R:80:ARG:O     | 18:R:83:HIS:HB3   | 2.18                     | 0.43              |
| 18:R:250:LEU:HB3  | 18:R:274:MET:HE3  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:37:VAL:HG12   | 1:A:38:LEU:HG     | 2.00                     | 0.43              |
| 1:A:422:ARG:N     | 18:R:409:HIS:CE1  | 2.75                     | 0.43              |
| 1:A:478:TYR:CZ    | 2:B:1049:THR:HB   | 2.53                     | 0.43              |
| 1:A:697:TYR:CE2   | 11:K:92:SER:CB    | 3.01                     | 0.43              |
| 1:A:1484:LEU:HB3  | 2:B:305:ARG:NH2   | 2.34                     | 0.43              |
| 2:B:30:LYS:HG2    | 2:B:178:TYR:HB2   | 2.00                     | 0.43              |
| 2:B:1003:ALA:C    | 14:N:170:HIS:HB3  | 2.41                     | 0.43              |
| 2:B:1151:ILE:CG1  | 7:G:21:LYS:HZ3    | 2.31                     | 0.43              |
| 15:O:78:VAL:HA    | 15:O:88:ILE:HG22  | 2.00                     | 0.43              |
| 15:O:390:GLN:CG   | 15:O:396:MET:HE3  | 2.45                     | 0.43              |
| 15:O:433:LYS:HZ2  | 15:O:609:TYR:HE1  | 1.61                     | 0.43              |
| 16:P:265:THR:HG21 | 16:P:303:VAL:HG21 | 2.00                     | 0.43              |
| 16:P:507:GLY:O    | 16:P:539:VAL:HA   | 2.19                     | 0.43              |
| 1:A:475:ARG:NH2   | 2:B:1061:LYS:HD2  | 2.34                     | 0.43              |
| 1:A:653:THR:OG1   | 1:A:654:ASP:OD1   | 2.35                     | 0.43              |
| 2:B:548:LYS:O     | 2:B:550:ARG:NH1   | 2.50                     | 0.43              |
| 2:B:683:ASN:OD1   | 14:N:154:ARG:NH1  | 2.51                     | 0.43              |
| 2:B:954:PHE:H     | 2:B:955:PRO:HD2   | 1.83                     | 0.43              |
| 16:P:246:LYS:HB3  | 16:P:246:LYS:HE3  | 1.59                     | 0.43              |
| 16:P:290:GLU:HB3  | 16:P:342:GLN:HG2  | 1.99                     | 0.43              |
| 16:P:363:ILE:HG23 | 16:P:374:VAL:HG13 | 2.00                     | 0.43              |
| 16:P:472:ARG:N    | 16:P:504:THR:HG21 | 2.33                     | 0.43              |
| 16:P:574:TRP:HB3  | 16:P:578:PHE:CE2  | 2.53                     | 0.43              |
| 16:P:730:GLU:O    | 16:P:734:LYS:HB2  | 2.19                     | 0.43              |
| 17:Q:351:ASN:O    | 17:Q:355:VAL:HG23 | 2.19                     | 0.43              |
| 18:R:248:LYS:O    | 18:R:250:LEU:N    | 2.49                     | 0.43              |
| 18:R:348:LYS:HE2  | 18:R:352:TRP:HE1  | 1.83                     | 0.43              |
| 1:A:756:LYS:HD3   | 9:I:85:LYS:HZ1    | 0.60                     | 0.43              |
| 1:A:1003:ARG:HH22 | 2:B:530:PRO:HA    | 1.84                     | 0.43              |
| 1:A:1330:VAL:HG23 | 1:A:1455:ARG:HD2  | 2.00                     | 0.43              |
| 2:B:893:ASN:O     | 2:B:895:PHE:HD1   | 2.01                     | 0.43              |
| 9:I:26:SER:O      | 9:I:39:LYS:HB2    | 2.19                     | 0.43              |
| 16:P:361:LYS:HA   | 16:P:375:PHE:O    | 2.18                     | 0.43              |
| 1:A:414:GLU:O     | 1:A:416:ARG:N     | 2.52                     | 0.43              |
| 1:A:477:ASN:CB    | 2:B:1047:ARG:NH1  | 2.81                     | 0.43              |
| 1:A:833:LEU:C     | 1:A:944:MET:HE3   | 2.43                     | 0.43              |
| 1:A:1325:LEU:HD21 | 1:A:1474:LEU:HD11 | 2.00                     | 0.43              |
| 2:B:897:GLU:HA    | 12:L:46:VAL:HG21  | 2.01                     | 0.43              |
| 15:O:506:PHE:CG   | 15:O:528:PHE:HZ   | 2.35                     | 0.43              |
| 16:P:412:ASN:O    | 16:P:426:ALA:HB1  | 2.18                     | 0.43              |
| 17:Q:193:PHE:HD2  | 18:R:209:ARG:HD2  | 1.82                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:355:VAL:CG2  | 18:R:215:THR:OG1  | 2.67                     | 0.43              |
| 17:Q:358:PRO:CA   | 18:R:206:ARG:CG   | 2.95                     | 0.43              |
| 18:R:353:VAL:HG13 | 18:R:364:VAL:HB   | 1.98                     | 0.43              |
| 1:A:530:TRP:CZ2   | 1:A:607:VAL:HG21  | 2.53                     | 0.43              |
| 2:B:681:ILE:HB    | 14:N:154:ARG:HB2  | 2.01                     | 0.43              |
| 2:B:883:GLU:HG3   | 2:B:906:ARG:HB2   | 2.01                     | 0.43              |
| 13:M:101:VAL:CG1  | 13:M:105:SER:OG   | 2.66                     | 0.43              |
| 14:N:80:MET:HE3   | 14:N:80:MET:HB2   | 1.91                     | 0.43              |
| 15:O:198:PHE:CD2  | 15:O:199:PRO:HD2  | 2.53                     | 0.43              |
| 15:O:453:TYR:CE2  | 15:O:473:PHE:HB2  | 2.54                     | 0.43              |
| 16:P:368:HIS:CB   | 16:P:411:LYS:HZ2  | 2.24                     | 0.43              |
| 16:P:498:LEU:CD1  | 17:Q:368:GLN:CG   | 2.92                     | 0.43              |
| 17:Q:120:ILE:HA   | 17:Q:125:PHE:HB2  | 2.01                     | 0.43              |
| 18:R:171:ARG:C    | 18:R:174:GLU:H    | 2.26                     | 0.43              |
| 1:A:410:LYS:HB2   | 1:A:411:VAL:HG23  | 2.01                     | 0.43              |
| 1:A:581:ILE:CD1   | 1:A:637:PHE:CE1   | 2.98                     | 0.43              |
| 2:B:219:ARG:HA    | 2:B:220:PRO:HD2   | 1.73                     | 0.43              |
| 7:G:29:ASP:OD1    | 7:G:30:GLU:N      | 2.52                     | 0.43              |
| 16:P:391:THR:HG23 | 18:R:149:LYS:HG2  | 2.01                     | 0.43              |
| 17:Q:140:ILE:HG22 | 17:Q:236:MET:HG2  | 2.00                     | 0.43              |
| 1:A:684:ASP:OD2   | 8:H:21:ASN:N      | 2.51                     | 0.43              |
| 1:A:722:PRO:HD2   | 8:H:95:TYR:HD1    | 1.83                     | 0.43              |
| 3:C:252:PRO:HD2   | 3:C:255:VAL:HG21  | 1.99                     | 0.43              |
| 12:L:32:ALA:HB3   | 12:L:55:ILE:HG23  | 2.01                     | 0.43              |
| 16:P:330:PRO:HG3  | 16:P:342:GLN:HG3  | 2.00                     | 0.43              |
| 16:P:762:ARG:NE   | 16:P:762:ARG:HA   | 2.34                     | 0.43              |
| 17:Q:132:VAL:O    | 17:Q:136:ILE:HG13 | 2.19                     | 0.43              |
| 17:Q:375:LEU:HD23 | 17:Q:375:LEU:HA   | 1.88                     | 0.43              |
| 17:Q:410:ARG:HA   | 17:Q:413:LEU:CB   | 2.45                     | 0.43              |
| 1:A:684:ASP:OD2   | 8:H:20:TYR:CA     | 2.66                     | 0.43              |
| 2:B:61:LEU:HA     | 2:B:61:LEU:HD23   | 1.75                     | 0.43              |
| 13:M:8:SER:O      | 14:N:71:PRO:HA    | 2.19                     | 0.43              |
| 15:O:76:ASN:O     | 15:O:80:LEU:HD13  | 2.18                     | 0.43              |
| 15:O:199:PRO:HD3  | 15:O:211:TYR:CG   | 2.54                     | 0.43              |
| 15:O:444:SER:O    | 15:O:448:SER:HB3  | 2.18                     | 0.43              |
| 16:P:238:LEU:HD22 | 16:P:284:VAL:H    | 1.84                     | 0.43              |
| 16:P:722:TRP:CD1  | 17:Q:446:TYR:CD1  | 3.00                     | 0.43              |
| 17:Q:153:LYS:HE2  | 17:Q:153:LYS:HB3  | 1.57                     | 0.43              |
| 17:Q:239:PHE:CG   | 17:Q:240:LYS:N    | 2.86                     | 0.43              |
| 1:A:486:PRO:CG    | 2:B:781:TYR:O     | 2.67                     | 0.42              |
| 1:A:711:LYS:HA    | 11:K:104:ARG:HH22 | 1.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1172:LEU:O    | 1:A:1176:ARG:HG2  | 2.19                     | 0.42              |
| 1:A:1313:LEU:O    | 1:A:1317:ILE:HD12 | 2.18                     | 0.42              |
| 2:B:26:ILE:HD11   | 10:J:58:GLU:HG2   | 2.00                     | 0.42              |
| 2:B:1005:TYR:CZ   | 14:N:170:HIS:NE2  | 2.87                     | 0.42              |
| 16:P:438:TRP:HE1  | 18:R:297:PHE:HZ   | 1.67                     | 0.42              |
| 16:P:474:LYS:CD   | 16:P:474:LYS:H    | 2.30                     | 0.42              |
| 16:P:607:VAL:HB   | 16:P:731:LEU:HD13 | 2.01                     | 0.42              |
| 17:Q:106:LYS:O    | 17:Q:110:PHE:HB3  | 2.18                     | 0.42              |
| 18:R:18:LYS:HA    | 18:R:78:ARG:HD3   | 2.00                     | 0.42              |
| 1:A:475:ARG:CD    | 2:B:1059:PRO:O    | 2.67                     | 0.42              |
| 2:B:57:ASP:OD1    | 2:B:57:ASP:N      | 2.52                     | 0.42              |
| 2:B:848:ILE:N     | 12:L:60:ARG:NE    | 2.67                     | 0.42              |
| 3:C:116:VAL:HG11  | 3:C:125:LYS:HE3   | 2.01                     | 0.42              |
| 15:O:202:ASN:N    | 15:O:202:ASN:OD1  | 2.52                     | 0.42              |
| 15:O:235:GLU:C    | 15:O:237:ILE:HB   | 2.44                     | 0.42              |
| 15:O:235:GLU:HA   | 15:O:237:ILE:HB   | 2.01                     | 0.42              |
| 15:O:376:TYR:CG   | 15:O:376:TYR:O    | 2.71                     | 0.42              |
| 15:O:468:GLU:HG2  | 15:O:469:ARG:N    | 2.34                     | 0.42              |
| 16:P:300:LEU:N    | 16:P:300:LEU:HD23 | 2.34                     | 0.42              |
| 16:P:697:GLU:HG2  | 16:P:698:LYS:H    | 1.84                     | 0.42              |
| 17:Q:103:LEU:HD21 | 17:Q:205:ILE:HD13 | 2.00                     | 0.42              |
| 18:R:180:CYS:SG   | 18:R:185:LYS:HG3  | 2.59                     | 0.42              |
| 1:A:407:GLN:O     | 1:A:408:LYS:HE2   | 2.19                     | 0.42              |
| 1:A:581:ILE:CG1   | 1:A:582:LYS:N     | 2.83                     | 0.42              |
| 1:A:964:LYS:HB3   | 1:A:964:LYS:HE2   | 1.83                     | 0.42              |
| 1:A:1484:LEU:HD22 | 2:B:305:ARG:NH2   | 2.34                     | 0.42              |
| 13:M:102:SER:HB3  | 13:M:105:SER:HB3  | 0.45                     | 0.42              |
| 15:O:169:THR:O    | 15:O:172:HIS:N    | 2.52                     | 0.42              |
| 15:O:189:PHE:HA   | 15:O:192:THR:HG23 | 2.00                     | 0.42              |
| 15:O:400:LEU:O    | 15:O:404:ILE:HG13 | 2.19                     | 0.42              |
| 16:P:361:LYS:HG3  | 16:P:376:ASP:HB3  | 2.01                     | 0.42              |
| 16:P:366:PHE:CZ   | 16:P:433:VAL:HG12 | 2.54                     | 0.42              |
| 16:P:369:PHE:O    | 16:P:369:PHE:HD1  | 2.01                     | 0.42              |
| 16:P:740:ILE:O    | 16:P:744:LEU:HG   | 2.19                     | 0.42              |
| 17:Q:332:LEU:HD13 | 17:Q:332:LEU:HA   | 1.80                     | 0.42              |
| 17:Q:418:PRO:HD2  | 18:R:264:SER:HB3  | 1.95                     | 0.42              |
| 1:A:828:CYS:HG    | 2:B:1027:TYR:CB   | 2.31                     | 0.42              |
| 2:B:574:SER:HB3   | 13:M:67:ASP:OD2   | 2.20                     | 0.42              |
| 2:B:848:ILE:CG1   | 12:L:60:ARG:HD2   | 2.36                     | 0.42              |
| 7:G:223:GLU:H     | 7:G:223:GLU:HG3   | 1.71                     | 0.42              |
| 15:O:96:LEU:O     | 15:O:100:LEU:HG   | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:236:LYS:N    | 15:O:237:ILE:HD13 | 2.28                     | 0.42              |
| 16:P:274:ILE:HD13 | 16:P:305:PHE:CZ   | 2.53                     | 0.42              |
| 16:P:663:LEU:HD12 | 16:P:664:GLU:N    | 2.34                     | 0.42              |
| 17:Q:177:TYR:OH   | 17:Q:252:LEU:N    | 2.52                     | 0.42              |
| 17:Q:406:GLN:HA   | 17:Q:409:ALA:HB3  | 2.00                     | 0.42              |
| 17:Q:502:ILE:O    | 17:Q:506:LYS:HB2  | 2.20                     | 0.42              |
| 18:R:15:GLN:HE21  | 18:R:15:GLN:HB2   | 1.73                     | 0.42              |
| 18:R:25:ASN:O     | 18:R:29:ARG:HB2   | 2.19                     | 0.42              |
| 18:R:141:TRP:H    | 18:R:141:TRP:HD1  | 1.63                     | 0.42              |
| 18:R:253:ILE:HG12 | 18:R:257:ILE:HG13 | 2.01                     | 0.42              |
| 1:A:827:THR:HG21  | 1:A:924:SER:CB    | 2.49                     | 0.42              |
| 1:A:977:MET:HE1   | 1:A:991:LYS:HD2   | 2.01                     | 0.42              |
| 2:B:535:ASP:OD1   | 2:B:720:GLN:NE2   | 2.49                     | 0.42              |
| 2:B:637:TYR:HA    | 2:B:638:PRO:HD3   | 1.87                     | 0.42              |
| 15:O:218:LEU:HD12 | 15:O:221:TYR:CZ   | 2.54                     | 0.42              |
| 16:P:302:VAL:HG11 | 16:P:362:ARG:NH1  | 2.30                     | 0.42              |
| 16:P:465:VAL:HG13 | 16:P:480:VAL:HG13 | 2.01                     | 0.42              |
| 18:R:76:LYS:HA    | 18:R:79:ARG:HB2   | 2.01                     | 0.42              |
| 18:R:306:ALA:O    | 18:R:307:LYS:C    | 2.62                     | 0.42              |
| 18:R:426:VAL:C    | 18:R:428:SER:N    | 2.76                     | 0.42              |
| 1:A:88:PRO:HG3    | 1:A:434:VAL:CG1   | 2.43                     | 0.42              |
| 1:A:474:LYS:NZ    | 2:B:1092:LEU:CA   | 2.67                     | 0.42              |
| 1:A:550:SER:OG    | 1:A:553:GLN:HG3   | 2.19                     | 0.42              |
| 1:A:721:LYS:HB3   | 8:H:96:VAL:CB     | 2.40                     | 0.42              |
| 1:A:1297:PHE:CD2  | 9:I:60:LEU:HD22   | 2.52                     | 0.42              |
| 2:B:550:ARG:HA    | 2:B:550:ARG:HD3   | 1.81                     | 0.42              |
| 3:C:61:THR:HA     | 3:C:298:PHE:CZ    | 2.55                     | 0.42              |
| 7:G:41:VAL:HA     | 7:G:42:PRO:HD3    | 1.93                     | 0.42              |
| 15:O:77:GLN:HG2   | 15:O:88:ILE:HB    | 2.01                     | 0.42              |
| 16:P:241:PRO:C    | 16:P:242:ILE:HG13 | 2.45                     | 0.42              |
| 16:P:705:HIS:HB2  | 17:Q:438:PHE:HB2  | 2.00                     | 0.42              |
| 17:Q:509:CYS:O    | 17:Q:513:MET:HB2  | 2.20                     | 0.42              |
| 1:A:1053:ASP:OD2  | 5:E:204:THR:CG2   | 2.67                     | 0.42              |
| 2:B:37:LEU:HD23   | 2:B:37:LEU:HA     | 1.89                     | 0.42              |
| 2:B:679:GLN:NE2   | 14:N:156:PRO:O    | 2.53                     | 0.42              |
| 2:B:800:TYR:OH    | 2:B:908:ARG:CZ    | 2.66                     | 0.42              |
| 2:B:995:TYR:HE1   | 14:N:162:LYS:HA   | 1.85                     | 0.42              |
| 3:C:229:LEU:C     | 3:C:293:ARG:HD2   | 2.44                     | 0.42              |
| 11:K:50:LEU:O     | 11:K:54:THR:HG23  | 2.20                     | 0.42              |
| 16:P:237:GLU:H    | 16:P:237:GLU:HG2  | 1.55                     | 0.42              |
| 16:P:317:ILE:CG1  | 16:P:326:ILE:HD13 | 2.49                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:436:ILE:CD1  | 18:R:143:THR:CG2  | 2.54                     | 0.42              |
| 17:Q:4:PHE:HE1    | 17:Q:18:ARG:HH11  | 1.67                     | 0.42              |
| 17:Q:414:TYR:CE1  | 18:R:240:ILE:HG13 | 2.52                     | 0.42              |
| 1:A:475:ARG:NH2   | 2:B:1061:LYS:CD   | 2.82                     | 0.42              |
| 1:A:826:PHE:CG    | 1:A:827:THR:N     | 2.88                     | 0.42              |
| 1:A:828:CYS:SG    | 2:B:1027:TYR:CG   | 3.11                     | 0.42              |
| 1:A:1089:LEU:CD1  | 1:A:1175:MET:HE1  | 2.48                     | 0.42              |
| 1:A:1603:MET:HB3  | 1:A:1603:MET:HE3  | 1.79                     | 0.42              |
| 1:A:1657:LEU:O    | 6:F:132:LEU:CA    | 2.68                     | 0.42              |
| 2:B:145:VAL:HG21  | 2:B:440:PHE:O     | 2.20                     | 0.42              |
| 2:B:656:LEU:HD21  | 2:B:689:VAL:HG12  | 2.02                     | 0.42              |
| 15:O:66:ASN:ND2   | 15:O:111:ARG:CZ   | 2.83                     | 0.42              |
| 15:O:244:LEU:HD23 | 15:O:244:LEU:O    | 2.20                     | 0.42              |
| 16:P:64:LEU:H     | 16:P:64:LEU:CD2   | 2.33                     | 0.42              |
| 16:P:273:ARG:NH1  | 16:P:288:SER:OG   | 2.53                     | 0.42              |
| 16:P:535:VAL:HG13 | 16:P:552:LEU:HD12 | 2.01                     | 0.42              |
| 17:Q:101:LYS:H    | 17:Q:101:LYS:HG3  | 1.65                     | 0.42              |
| 17:Q:350:ARG:NH1  | 17:Q:490:ASP:OD2  | 2.40                     | 0.42              |
| 18:R:248:LYS:C    | 18:R:250:LEU:H    | 2.27                     | 0.42              |
| 1:A:67:LEU:HB2    | 1:A:72:CYS:HB2    | 2.02                     | 0.42              |
| 1:A:501:PHE:CD1   | 2:B:1046:VAL:HG21 | 2.55                     | 0.42              |
| 1:A:874:GLU:OE2   | 1:A:878:ARG:HD2   | 2.20                     | 0.42              |
| 1:A:1575:ILE:H    | 9:I:122:ARG:NH1   | 2.03                     | 0.42              |
| 2:B:45:HIS:CD2    | 2:B:500:PHE:HD1   | 2.37                     | 0.42              |
| 2:B:534:PRO:CA    | 2:B:720:GLN:OE1   | 2.57                     | 0.42              |
| 2:B:809:VAL:HG13  | 2:B:901:VAL:HB    | 2.02                     | 0.42              |
| 2:B:923:GLN:HG2   | 2:B:949:ILE:CD1   | 2.47                     | 0.42              |
| 2:B:943:ILE:HD13  | 10:J:44:TYR:CE1   | 2.47                     | 0.42              |
| 14:N:63:ASP:OD2   | 14:N:66:LYS:NZ    | 2.35                     | 0.42              |
| 16:P:265:THR:HG1  | 16:P:305:PHE:HE1  | 1.66                     | 0.42              |
| 16:P:641:TRP:CZ2  | 16:P:656:HIS:HB3  | 2.50                     | 0.42              |
| 16:P:712:ASP:O    | 16:P:715:TYR:N    | 2.53                     | 0.42              |
| 16:P:717:LYS:CG   | 17:Q:439:ILE:HD13 | 2.48                     | 0.42              |
| 18:R:421:LYS:HG3  | 18:R:422:GLY:N    | 2.34                     | 0.42              |
| 1:A:83:VAL:HG21   | 1:A:427:PHE:CZ    | 2.55                     | 0.42              |
| 1:A:878:ARG:NH2   | 9:I:66:VAL:C      | 2.75                     | 0.42              |
| 1:A:1268:ASP:OD1  | 9:I:61:ARG:NH2    | 2.52                     | 0.42              |
| 2:B:1005:TYR:CE2  | 14:N:170:HIS:CE1  | 3.08                     | 0.42              |
| 16:P:596:ILE:HD13 | 17:Q:272:GLN:OE1  | 2.20                     | 0.42              |
| 16:P:762:ARG:HG3  | 17:Q:139:LYS:NZ   | 2.35                     | 0.42              |
| 17:Q:9:ILE:CG1    | 17:Q:10:CYS:N     | 2.50                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:R:8:LEU:H      | 18:R:8:LEU:HD22   | 1.83                     | 0.42              |
| 18:R:138:PHE:CE1  | 18:R:140:ILE:HD11 | 2.53                     | 0.42              |
| 18:R:268:LEU:HD11 | 18:R:316:SER:OG   | 2.20                     | 0.42              |
| 1:A:1:MET:HE2     | 7:G:110:ASP:OD1   | 2.20                     | 0.41              |
| 1:A:408:LYS:HD3   | 1:A:408:LYS:N     | 2.33                     | 0.41              |
| 1:A:489:ASN:HB3   | 11:K:95:HIS:CD2   | 2.54                     | 0.41              |
| 1:A:680:LEU:O     | 1:A:728:GLY:HA3   | 2.20                     | 0.41              |
| 1:A:692:TYR:O     | 1:A:696:ILE:HG12  | 2.19                     | 0.41              |
| 1:A:697:TYR:CD2   | 11:K:92:SER:HB3   | 2.53                     | 0.41              |
| 1:A:1050:TYR:CE2  | 1:A:1179:ILE:HG12 | 2.46                     | 0.41              |
| 1:A:1056:ASP:OD2  | 1:A:1057:ILE:N    | 2.53                     | 0.41              |
| 1:A:1063:MET:HE2  | 1:A:1063:MET:HB3  | 1.66                     | 0.41              |
| 1:A:1554:GLY:CA   | 5:E:183:PRO:HD2   | 2.46                     | 0.41              |
| 1:A:1622:LEU:HD21 | 2:B:1189:LEU:HD22 | 2.01                     | 0.41              |
| 2:B:247:THR:OG1   | 2:B:477:ASP:OD2   | 2.35                     | 0.41              |
| 2:B:799:GLY:O     | 2:B:911:PRO:HG3   | 2.20                     | 0.41              |
| 2:B:1002:LYS:C    | 14:N:168:LEU:HD23 | 2.45                     | 0.41              |
| 2:B:1092:LEU:CA   | 2:B:1096:SER:CB   | 2.79                     | 0.41              |
| 3:C:105:PRO:HG3   | 10:J:6:ARG:CZ     | 2.50                     | 0.41              |
| 8:H:105:GLU:HG2   | 8:H:115:TYR:HE1   | 1.84                     | 0.41              |
| 16:P:319:ASP:HB2  | 16:P:363:ILE:CG1  | 2.48                     | 0.41              |
| 16:P:384:ASP:HB3  | 16:P:389:TRP:CB   | 2.46                     | 0.41              |
| 17:Q:257:VAL:HG13 | 17:Q:262:LEU:HB2  | 2.02                     | 0.41              |
| 17:Q:329:LYS:O    | 17:Q:332:LEU:N    | 2.53                     | 0.41              |
| 1:A:4:SER:HB2     | 1:A:573:LEU:CD2   | 2.49                     | 0.41              |
| 1:A:477:ASN:CG    | 2:B:1049:THR:OG1  | 2.61                     | 0.41              |
| 2:B:469:ASN:OD1   | 2:B:482:SER:CB    | 2.67                     | 0.41              |
| 5:E:26:ARG:O      | 5:E:75:MET:HE1    | 2.20                     | 0.41              |
| 15:O:125:TRP:C    | 15:O:127:GLU:N    | 2.78                     | 0.41              |
| 16:P:607:VAL:O    | 16:P:611:ILE:HG13 | 2.20                     | 0.41              |
| 17:Q:192:TYR:CD1  | 17:Q:193:PHE:CD1  | 3.08                     | 0.41              |
| 17:Q:378:LEU:HD21 | 18:R:235:ILE:HA   | 2.00                     | 0.41              |
| 18:R:75:GLN:HA    | 18:R:78:ARG:NE    | 2.33                     | 0.41              |
| 18:R:436:LYS:HA   | 18:R:439:GLU:HB2  | 2.02                     | 0.41              |
| 1:A:703:GLU:HG2   | 11:K:50:LEU:HD13  | 2.02                     | 0.41              |
| 1:A:908:VAL:C     | 9:I:83:LYS:HZ1    | 2.28                     | 0.41              |
| 1:A:986:PHE:HE2   | 2:B:958:MET:CE    | 2.31                     | 0.41              |
| 2:B:49:PHE:HB3    | 2:B:164:MET:SD    | 2.60                     | 0.41              |
| 2:B:186:GLU:OE2   | 2:B:731:VAL:HB    | 2.20                     | 0.41              |
| 2:B:196:VAL:HG21  | 2:B:465:LEU:HB3   | 2.02                     | 0.41              |
| 2:B:262:PHE:CE1   | 2:B:357:ILE:HD13  | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:345:SER:CA    | 13:M:113:ILE:HG12 | 2.48                     | 0.41              |
| 2:B:910:THR:HA    | 2:B:911:PRO:HD3   | 1.91                     | 0.41              |
| 2:B:999:GLN:HG2   | 14:N:166:LEU:CD1  | 2.48                     | 0.41              |
| 9:I:87:PRO:HG2    | 9:I:119:TYR:CE2   | 2.56                     | 0.41              |
| 13:M:61:GLU:OE2   | 13:M:106:LYS:HD2  | 2.04                     | 0.41              |
| 15:O:234:ILE:HD13 | 15:O:234:ILE:HA   | 1.74                     | 0.41              |
| 16:P:263:ILE:HB   | 16:P:275:GLU:O    | 2.21                     | 0.41              |
| 16:P:427:SER:HB2  | 16:P:429:SER:O    | 2.19                     | 0.41              |
| 16:P:473:HIS:CG   | 16:P:475:ARG:HD2  | 2.54                     | 0.41              |
| 16:P:484:ARG:HB2  | 16:P:488:LEU:HB3  | 2.02                     | 0.41              |
| 17:Q:385:PHE:CZ   | 18:R:209:ARG:CB   | 3.03                     | 0.41              |
| 18:R:5:PRO:CD     | 18:R:217:THR:OG1  | 2.67                     | 0.41              |
| 18:R:173:MET:O    | 18:R:176:PRO:HD2  | 2.20                     | 0.41              |
| 1:A:1263:LEU:HD12 | 1:A:1498:ILE:HD11 | 2.02                     | 0.41              |
| 2:B:985:ILE:HG13  | 14:N:160:VAL:HG21 | 2.02                     | 0.41              |
| 8:H:41:ASP:HB2    | 8:H:121:LEU:HB3   | 2.02                     | 0.41              |
| 14:N:90:MET:HE3   | 14:N:90:MET:HB2   | 1.86                     | 0.41              |
| 15:O:150:TRP:O    | 15:O:154:VAL:HG23 | 2.21                     | 0.41              |
| 15:O:379:ARG:NH1  | 15:O:382:GLN:HE22 | 2.17                     | 0.41              |
| 17:Q:129:PHE:HE1  | 17:Q:169:SER:N    | 2.19                     | 0.41              |
| 17:Q:348:ILE:HD11 | 17:Q:373:GLU:CG   | 2.50                     | 0.41              |
| 1:A:711:LYS:HA    | 11:K:104:ARG:NH2  | 2.35                     | 0.41              |
| 1:A:1024:THR:HG22 | 1:A:1190:SER:CB   | 2.50                     | 0.41              |
| 1:A:1242:ILE:HG22 | 1:A:1536:ILE:HG22 | 2.01                     | 0.41              |
| 1:A:1322:ILE:C    | 1:A:1454:HIS:NE2  | 2.79                     | 0.41              |
| 2:B:977:ILE:HG21  | 2:B:977:ILE:HD13  | 1.72                     | 0.41              |
| 3:C:314:PHE:HD2   | 11:K:135:PHE:CE2  | 2.38                     | 0.41              |
| 15:O:182:MET:HE2  | 15:O:183:ILE:HG13 | 2.03                     | 0.41              |
| 15:O:248:LEU:HB2  | 15:O:598:PHE:HE2  | 1.85                     | 0.41              |
| 15:O:548:ASN:O    | 15:O:552:LEU:HG   | 2.21                     | 0.41              |
| 16:P:65:LEU:HD21  | 16:P:226:HIS:CE1  | 2.55                     | 0.41              |
| 16:P:352:PHE:CE1  | 18:R:157:MET:HG2  | 2.55                     | 0.41              |
| 16:P:404:ASP:OD1  | 16:P:405:TYR:N    | 2.50                     | 0.41              |
| 16:P:421:ILE:HA   | 16:P:440:HIS:O    | 2.21                     | 0.41              |
| 16:P:428:GLU:CB   | 16:P:435:ARG:HH12 | 2.31                     | 0.41              |
| 17:Q:194:GLN:CG   | 17:Q:389:GLN:CG   | 2.99                     | 0.41              |
| 18:R:158:THR:OG1  | 18:R:159:TYR:N    | 2.53                     | 0.41              |
| 1:A:476:VAL:O     | 2:B:1068:GLY:CA   | 2.47                     | 0.41              |
| 1:A:854:GLY:HA3   | 1:A:974:THR:O     | 2.21                     | 0.41              |
| 1:A:1055:ILE:HD13 | 1:A:1178:LEU:CD2  | 2.48                     | 0.41              |
| 2:B:697:LEU:HD13  | 2:B:702:ASN:HA    | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:82:LEU:O      | 4:D:86:ILE:HG23   | 2.20                     | 0.41              |
| 9:I:20:PRO:C      | 9:I:22:ALA:H      | 2.29                     | 0.41              |
| 15:O:56:VAL:HG23  | 15:O:57:LYS:N     | 2.35                     | 0.41              |
| 15:O:460:GLU:O    | 15:O:469:ARG:NH1  | 2.51                     | 0.41              |
| 16:P:397:LYS:CE   | 18:R:85:ARG:NE    | 2.84                     | 0.41              |
| 17:Q:26:ARG:H     | 17:Q:26:ARG:HG3   | 1.57                     | 0.41              |
| 17:Q:282:ARG:HG2  | 17:Q:302:ALA:HB1  | 2.02                     | 0.41              |
| 17:Q:498:LEU:O    | 17:Q:502:ILE:HG23 | 2.19                     | 0.41              |
| 18:R:220:LEU:N    | 18:R:235:ILE:HG21 | 2.36                     | 0.41              |
| 18:R:234:LYS:O    | 18:R:238:THR:OG1  | 2.33                     | 0.41              |
| 18:R:264:SER:O    | 18:R:265:SER:C    | 2.62                     | 0.41              |
| 1:A:82:PRO:HD3    | 1:A:393:SER:OG    | 2.20                     | 0.41              |
| 1:A:514:TYR:CE1   | 6:F:115:THR:O     | 2.74                     | 0.41              |
| 1:A:1538:VAL:HG21 | 5:E:142:VAL:HG22  | 2.01                     | 0.41              |
| 2:B:436:MET:HE1   | 2:B:448:ARG:HD3   | 2.02                     | 0.41              |
| 2:B:550:ARG:H     | 2:B:650:LEU:H     | 1.66                     | 0.41              |
| 15:O:115:LEU:O    | 15:O:119:ILE:HG13 | 2.21                     | 0.41              |
| 16:P:347:LEU:HD12 | 16:P:347:LEU:N    | 2.35                     | 0.41              |
| 16:P:378:SER:HB2  | 16:P:379:LYS:HD2  | 2.03                     | 0.41              |
| 16:P:500:ILE:HB   | 16:P:501:PRO:CD   | 2.50                     | 0.41              |
| 17:Q:134:LYS:HD3  | 17:Q:134:LYS:HA   | 1.78                     | 0.41              |
| 17:Q:140:ILE:O    | 17:Q:143:THR:HG22 | 2.21                     | 0.41              |
| 17:Q:315:ASN:HB2  | 17:Q:480:LEU:HD11 | 2.03                     | 0.41              |
| 17:Q:378:LEU:HD23 | 18:R:216:LEU:CD2  | 2.13                     | 0.41              |
| 18:R:24:ILE:O     | 18:R:28:SER:OG    | 2.38                     | 0.41              |
| 1:A:501:PHE:CE1   | 2:B:1046:VAL:HB   | 2.56                     | 0.41              |
| 1:A:634:ASN:OD1   | 2:B:1069:ILE:HG12 | 2.21                     | 0.41              |
| 1:A:826:PHE:HE1   | 2:B:952:HIS:CE1   | 2.39                     | 0.41              |
| 1:A:1000:MET:HG2  | 2:B:520:LEU:HD23  | 2.02                     | 0.41              |
| 1:A:1180:ASN:N    | 1:A:1180:ASN:HD22 | 2.18                     | 0.41              |
| 1:A:1275:THR:HA   | 9:I:45:LEU:O      | 2.21                     | 0.41              |
| 1:A:1310:LYS:HG2  | 1:A:1311:GLU:OE1  | 2.07                     | 0.41              |
| 2:B:65:VAL:CG2    | 2:B:417:ILE:CD1   | 2.98                     | 0.41              |
| 2:B:152:LEU:CD2   | 2:B:443:LYS:CD    | 2.72                     | 0.41              |
| 2:B:427:GLN:OE1   | 2:B:452:ARG:NH1   | 2.54                     | 0.41              |
| 3:C:230:LEU:O     | 3:C:293:ARG:HA    | 2.20                     | 0.41              |
| 3:C:236:LEU:HD11  | 3:C:290:LYS:HG3   | 2.02                     | 0.41              |
| 7:G:18:LYS:H      | 7:G:18:LYS:HG2    | 1.61                     | 0.41              |
| 7:G:144:HIS:NE2   | 15:O:145:SER:CA   | 2.84                     | 0.41              |
| 7:G:159:LYS:HB3   | 15:O:105:ASN:HB2  | 2.03                     | 0.41              |
| 12:L:33:GLU:HG3   | 12:L:53:HIS:ND1   | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:364:LEU:HB3  | 15:O:385:MET:HE3  | 2.01                     | 0.41              |
| 15:O:396:MET:HE1  | 15:O:433:LYS:HB2  | 2.02                     | 0.41              |
| 15:O:430:ARG:NH2  | 15:O:596:PRO:HD3  | 2.36                     | 0.41              |
| 16:P:304:ASP:HB2  | 16:P:363:ILE:O    | 2.20                     | 0.41              |
| 17:Q:408:ILE:HD11 | 17:Q:412:LYS:HE3  | 2.02                     | 0.41              |
| 18:R:24:ILE:HD13  | 18:R:24:ILE:HA    | 1.91                     | 0.41              |
| 1:A:475:ARG:O     | 2:B:1059:PRO:CG   | 2.66                     | 0.41              |
| 1:A:1071:ASP:O    | 1:A:1072:ASN:HB2  | 2.21                     | 0.41              |
| 2:B:48:SER:HB3    | 2:B:404:LEU:CD1   | 2.49                     | 0.41              |
| 2:B:547:HIS:CB    | 2:B:697:LEU:O     | 2.69                     | 0.41              |
| 2:B:736:ARG:NH1   | 2:B:738:ASP:OD1   | 2.54                     | 0.41              |
| 2:B:944:GLN:HA    | 2:B:945:PRO:HD3   | 1.96                     | 0.41              |
| 3:C:314:PHE:HE2   | 11:K:135:PHE:CD1  | 2.39                     | 0.41              |
| 5:E:37:LEU:HA     | 5:E:38:PRO:HD3    | 1.87                     | 0.41              |
| 6:F:73:ALA:HA     | 6:F:143:PHE:C     | 2.44                     | 0.41              |
| 7:G:24:VAL:O      | 7:G:128:GLN:HB3   | 2.04                     | 0.41              |
| 7:G:159:LYS:N     | 15:O:105:ASN:CG   | 2.58                     | 0.41              |
| 11:K:54:THR:HG22  | 11:K:62:SER:H     | 1.86                     | 0.41              |
| 14:N:70:LEU:HA    | 14:N:71:PRO:HD3   | 1.84                     | 0.41              |
| 15:O:56:VAL:CG2   | 15:O:99:ILE:HD12  | 2.48                     | 0.41              |
| 15:O:107:ILE:CD1  | 15:O:115:LEU:HD23 | 2.51                     | 0.41              |
| 15:O:107:ILE:O    | 15:O:109:SER:N    | 2.47                     | 0.41              |
| 15:O:210:ASN:HD22 | 15:O:210:ASN:HA   | 1.67                     | 0.41              |
| 15:O:607:LYS:HE2  | 15:O:607:LYS:HB2  | 1.88                     | 0.41              |
| 16:P:56:ASP:HB2   | 16:P:554:ASN:OD1  | 2.21                     | 0.41              |
| 16:P:301:GLN:CD   | 16:P:360:TRP:HA   | 2.45                     | 0.41              |
| 16:P:436:ILE:CG2  | 18:R:143:THR:CG2  | 2.98                     | 0.41              |
| 16:P:473:HIS:CD2  | 16:P:475:ARG:HH11 | 2.38                     | 0.41              |
| 16:P:648:SER:HA   | 16:P:757:GLN:NE2  | 2.35                     | 0.41              |
| 16:P:675:PHE:CZ   | 16:P:742:TRP:CZ3  | 3.06                     | 0.41              |
| 17:Q:6:ARG:HA     | 17:Q:18:ARG:CD    | 2.50                     | 0.41              |
| 17:Q:26:ARG:HD2   | 17:Q:34:VAL:HG11  | 2.01                     | 0.41              |
| 17:Q:118:TRP:O    | 17:Q:122:GLU:HB2  | 2.21                     | 0.41              |
| 17:Q:187:THR:CB   | 17:Q:380:TRP:NE1  | 2.84                     | 0.41              |
| 17:Q:341:ARG:CZ   | 17:Q:369:TRP:CD1  | 3.04                     | 0.41              |
| 17:Q:375:LEU:HA   | 17:Q:378:LEU:HD12 | 2.01                     | 0.41              |
| 18:R:165:ILE:H    | 18:R:165:ILE:HG13 | 1.62                     | 0.41              |
| 18:R:408:ILE:HG23 | 18:R:435:LEU:HD13 | 2.03                     | 0.41              |
| 1:A:410:LYS:HB3   | 1:A:411:VAL:CG2   | 2.50                     | 0.41              |
| 1:A:481:ARG:N     | 2:B:1045:GLN:O    | 2.53                     | 0.41              |
| 1:A:581:ILE:HD11  | 1:A:585:ASP:CB    | 2.48                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1248:ASP:OD1  | 1:A:1517:ARG:NH1  | 2.49                     | 0.41              |
| 1:A:1657:LEU:CB   | 7:G:104:LEU:HD22  | 2.47                     | 0.41              |
| 2:B:25:PHE:CD2    | 10:J:59:LYS:CG    | 3.01                     | 0.41              |
| 2:B:68:ILE:HD13   | 2:B:71:LYS:HZ3    | 1.84                     | 0.41              |
| 2:B:279:ALA:HB2   | 2:B:326:VAL:HG12  | 2.03                     | 0.41              |
| 2:B:415:GLU:CD    | 2:B:472:SER:CB    | 2.94                     | 0.41              |
| 17:Q:384:GLN:C    | 17:Q:387:PRO:HD2  | 2.46                     | 0.41              |
| 18:R:402:ASN:O    | 18:R:405:ILE:HB   | 2.20                     | 0.41              |
| 1:A:83:VAL:CG2    | 1:A:427:PHE:CZ    | 3.05                     | 0.40              |
| 1:A:315:ILE:HG13  | 1:A:319:GLU:HB2   | 2.03                     | 0.40              |
| 1:A:407:GLN:CB    | 1:A:409:ASP:N     | 2.73                     | 0.40              |
| 1:A:475:ARG:NH1   | 2:B:1061:LYS:HA   | 2.36                     | 0.40              |
| 1:A:476:VAL:HG13  | 2:B:1070:ARG:CA   | 2.50                     | 0.40              |
| 1:A:753:ASN:HB2   | 1:A:782:ASP:OD2   | 2.21                     | 0.40              |
| 2:B:152:LEU:CD2   | 2:B:443:LYS:HE3   | 2.51                     | 0.40              |
| 2:B:286:ARG:HA    | 2:B:286:ARG:HD2   | 1.88                     | 0.40              |
| 2:B:1060:VAL:HG22 | 2:B:1065:ARG:NH2  | 2.36                     | 0.40              |
| 5:E:66:GLU:H      | 5:E:66:GLU:HG2    | 1.62                     | 0.40              |
| 8:H:7:ASP:HA      | 8:H:57:VAL:O      | 2.22                     | 0.40              |
| 8:H:95:TYR:HD2    | 8:H:144:ILE:HD12  | 1.86                     | 0.40              |
| 13:M:11:GLU:O     | 13:M:87:SER:HA    | 2.22                     | 0.40              |
| 15:O:80:LEU:HA    | 15:O:81:PRO:HD3   | 1.86                     | 0.40              |
| 16:P:470:SER:O    | 16:P:504:THR:HG22 | 2.21                     | 0.40              |
| 17:Q:239:PHE:HB2  | 17:Q:245:SER:OG   | 2.21                     | 0.40              |
| 18:R:219:LEU:HD23 | 18:R:219:LEU:HA   | 1.83                     | 0.40              |
| 18:R:362:ALA:O    | 18:R:365:TRP:HB2  | 2.21                     | 0.40              |
| 1:A:435:ASN:C     | 1:A:442:LYS:HB2   | 2.46                     | 0.40              |
| 1:A:487:ASP:HB2   | 1:A:615:ARG:HB3   | 2.02                     | 0.40              |
| 1:A:878:ARG:NE    | 9:I:66:VAL:C      | 2.79                     | 0.40              |
| 1:A:995:TYR:CE1   | 2:B:715:ASN:ND2   | 2.87                     | 0.40              |
| 1:A:1195:GLU:HB3  | 1:A:1196:PRO:HD3  | 2.03                     | 0.40              |
| 1:A:1260:LYS:HE2  | 1:A:1262:LEU:HD21 | 2.01                     | 0.40              |
| 1:A:1326:GLU:HB3  | 1:A:1455:ARG:NH1  | 2.36                     | 0.40              |
| 2:B:31:ASP:N      | 2:B:176:SER:HB2   | 2.36                     | 0.40              |
| 2:B:152:LEU:CG    | 2:B:443:LYS:CE    | 2.94                     | 0.40              |
| 2:B:206:LEU:HD23  | 2:B:206:LEU:HA    | 1.81                     | 0.40              |
| 2:B:491:ILE:HB    | 2:B:495:ARG:HD2   | 2.03                     | 0.40              |
| 2:B:550:ARG:HB2   | 2:B:650:LEU:CB    | 2.34                     | 0.40              |
| 5:E:83:CYS:HB2    | 5:E:110:PHE:CZ    | 2.56                     | 0.40              |
| 7:G:144:HIS:CB    | 15:O:146:SER:OG   | 2.63                     | 0.40              |
| 11:K:135:PHE:CE2  | 11:K:139:ILE:HD11 | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:245:GLN:O    | 15:O:248:LEU:N    | 2.40                     | 0.40              |
| 16:P:436:ILE:CB   | 18:R:143:THR:CB   | 2.97                     | 0.40              |
| 16:P:454:GLN:HB3  | 16:P:465:VAL:HG23 | 2.02                     | 0.40              |
| 16:P:660:LYS:HD3  | 16:P:660:LYS:HA   | 1.69                     | 0.40              |
| 16:P:711:LEU:CD2  | 16:P:741:ILE:HD13 | 2.51                     | 0.40              |
| 17:Q:351:ASN:ND2  | 17:Q:373:GLU:CD   | 2.78                     | 0.40              |
| 18:R:15:GLN:O     | 18:R:18:LYS:HB2   | 2.21                     | 0.40              |
| 18:R:199:LYS:HZ1  | 18:R:204:GLU:CB   | 2.31                     | 0.40              |
| 18:R:317:LEU:HD11 | 18:R:370:SER:OG   | 2.20                     | 0.40              |
| 18:R:317:LEU:HB2  | 18:R:367:ILE:HD13 | 2.02                     | 0.40              |
| 18:R:362:ALA:HA   | 18:R:365:TRP:HD1  | 1.86                     | 0.40              |
| 1:A:68:ASP:C      | 1:A:70:LYS:N      | 2.77                     | 0.40              |
| 1:A:413:LEU:HD13  | 1:A:416:ARG:HG3   | 2.03                     | 0.40              |
| 1:A:435:ASN:CB    | 1:A:442:LYS:O     | 2.70                     | 0.40              |
| 1:A:451:VAL:HA    | 1:A:452:PRO:HD3   | 1.95                     | 0.40              |
| 1:A:743:ASP:OD1   | 1:A:743:ASP:N     | 2.54                     | 0.40              |
| 1:A:847:LEU:HD23  | 1:A:847:LEU:HA    | 1.91                     | 0.40              |
| 1:A:862:THR:HA    | 9:I:67:VAL:CG1    | 2.52                     | 0.40              |
| 1:A:878:ARG:HH11  | 9:I:66:VAL:HG21   | 1.63                     | 0.40              |
| 1:A:1136:VAL:HG22 | 1:A:1174:TYR:CD2  | 2.57                     | 0.40              |
| 1:A:1484:LEU:CD1  | 2:B:305:ARG:CD    | 2.97                     | 0.40              |
| 1:A:1484:LEU:HD23 | 2:B:304:ASP:HB2   | 2.01                     | 0.40              |
| 1:A:1484:LEU:HD21 | 2:B:304:ASP:HB3   | 2.00                     | 0.40              |
| 1:A:1600:ARG:NH2  | 1:A:1621:PHE:CE2  | 2.89                     | 0.40              |
| 7:G:160:ASN:OD1   | 7:G:160:ASN:N     | 2.52                     | 0.40              |
| 15:O:219:ARG:CZ   | 15:O:360:VAL:CG2  | 2.98                     | 0.40              |
| 15:O:244:LEU:CD1  | 15:O:599:LEU:HD21 | 2.52                     | 0.40              |
| 15:O:505:PHE:CD2  | 15:O:505:PHE:C    | 2.99                     | 0.40              |
| 16:P:21:GLN:HA    | 18:R:314:TRP:CZ3  | 2.57                     | 0.40              |
| 16:P:377:ARG:NH2  | 16:P:378:SER:OG   | 2.38                     | 0.40              |
| 16:P:390:GLN:HB2  | 18:R:151:PRO:O    | 2.20                     | 0.40              |
| 17:Q:6:ARG:HA     | 17:Q:18:ARG:HG3   | 2.02                     | 0.40              |
| 18:R:271:LEU:HD13 | 18:R:312:TYR:CB   | 2.51                     | 0.40              |
| 18:R:428:SER:HA   | 18:R:431:ILE:HG12 | 2.03                     | 0.40              |
| 18:R:430:LEU:O    | 18:R:434:GLN:HG3  | 2.21                     | 0.40              |
| 1:A:480:ALA:HB1   | 2:B:1046:VAL:CG2  | 2.49                     | 0.40              |
| 1:A:581:ILE:CG1   | 1:A:585:ASP:OD2   | 2.56                     | 0.40              |
| 1:A:634:ASN:CG    | 2:B:1069:ILE:HG12 | 2.46                     | 0.40              |
| 1:A:756:LYS:HG3   | 9:I:85:LYS:HZ2    | 1.76                     | 0.40              |
| 1:A:826:PHE:CG    | 2:B:777:SER:HB2   | 2.51                     | 0.40              |
| 1:A:1128:ASN:HA   | 1:A:1129:PRO:HD2  | 1.96                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:326:GLU:HA    | 11:K:125:MET:SD   | 2.62                     | 0.40              |
| 7:G:24:VAL:CA     | 7:G:25:THR:HA     | 2.32                     | 0.40              |
| 7:G:144:HIS:CD2   | 15:O:145:SER:O    | 2.75                     | 0.40              |
| 14:N:127:ASP:OD2  | 14:N:129:ALA:HB2  | 2.21                     | 0.40              |
| 15:O:200:ASN:OD1  | 17:Q:14:ASN:CB    | 2.61                     | 0.40              |
| 16:P:198:ASP:OD1  | 16:P:205:TYR:O    | 2.39                     | 0.40              |
| 16:P:448:THR:HG21 | 16:P:471:MET:HB2  | 2.03                     | 0.40              |
| 17:Q:178:THR:HG21 | 17:Q:227:TYR:OH   | 2.22                     | 0.40              |
| 17:Q:245:SER:HB3  | 17:Q:284:LEU:HD13 | 2.04                     | 0.40              |
| 17:Q:309:TYR:CZ   | 17:Q:505:ILE:HD11 | 2.57                     | 0.40              |
| 17:Q:415:LYS:HD2  | 17:Q:419:LEU:HD11 | 2.03                     | 0.40              |
| 17:Q:474:GLU:HB3  | 17:Q:478:ARG:HH11 | 1.86                     | 0.40              |
| 18:R:11:ARG:HH22  | 18:R:12:LYS:HE2   | 1.86                     | 0.40              |
| 18:R:177:LEU:HD23 | 18:R:177:LEU:HA   | 1.94                     | 0.40              |
| 1:A:425:ASN:ND2   | 18:R:406:LYS:HD3  | 2.36                     | 0.40              |
| 1:A:486:PRO:O     | 2:B:781:TYR:HD2   | 1.85                     | 0.40              |
| 1:A:532:GLY:C     | 1:A:580:HIS:ND1   | 2.68                     | 0.40              |
| 1:A:564:PRO:CD    | 15:O:370:THR:O    | 2.68                     | 0.40              |
| 1:A:597:LYS:HD2   | 2:B:1082:HIS:CD2  | 2.57                     | 0.40              |
| 1:A:1317:ILE:O    | 1:A:1322:ILE:HG12 | 2.21                     | 0.40              |
| 2:B:168:ASN:O     | 2:B:169:ARG:HD3   | 2.21                     | 0.40              |
| 2:B:415:GLU:CD    | 2:B:472:SER:HB2   | 2.47                     | 0.40              |
| 2:B:1002:LYS:O    | 14:N:168:LEU:HD23 | 2.21                     | 0.40              |
| 3:C:58:ASN:C      | 3:C:296:ASN:HD22  | 2.30                     | 0.40              |
| 3:C:240:LYS:HA    | 3:C:244:ALA:HB2   | 2.03                     | 0.40              |
| 7:G:166:TRP:HZ3   | 7:G:225:ILE:HD13  | 1.86                     | 0.40              |
| 9:I:2:SER:HA      | 9:I:9:PHE:O       | 2.22                     | 0.40              |
| 16:P:57:LEU:HD11  | 18:R:227:HIS:NE2  | 2.37                     | 0.40              |
| 17:Q:100:ALA:HB3  | 17:Q:211:TYR:HE2  | 1.87                     | 0.40              |
| 18:R:304:HIS:CE1  | 18:R:306:ALA:HA   | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 1449/1664 (87%) | 1375 (95%) | 60 (4%)  | 14 (1%)  | 12          | 48  |
| 2   | B     | 1164/1203 (97%) | 1095 (94%) | 51 (4%)  | 18 (2%)  | 8           | 40  |
| 3   | C     | 303/335 (90%)   | 288 (95%)  | 12 (4%)  | 3 (1%)   | 12          | 48  |
| 4   | D     | 54/137 (39%)    | 50 (93%)   | 2 (4%)   | 2 (4%)   | 2           | 20  |
| 5   | E     | 210/215 (98%)   | 197 (94%)  | 11 (5%)  | 2 (1%)   | 12          | 48  |
| 6   | F     | 98/155 (63%)    | 95 (97%)   | 2 (2%)   | 1 (1%)   | 12          | 48  |
| 7   | G     | 187/326 (57%)   | 173 (92%)  | 12 (6%)  | 2 (1%)   | 11          | 46  |
| 8   | H     | 127/146 (87%)   | 121 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 9   | I     | 91/125 (73%)    | 80 (88%)   | 8 (9%)   | 3 (3%)   | 3           | 21  |
| 10  | J     | 67/70 (96%)     | 63 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 11  | K     | 99/142 (70%)    | 92 (93%)   | 7 (7%)   | 0        | 100         | 100 |
| 12  | L     | 42/70 (60%)     | 36 (86%)   | 4 (10%)  | 2 (5%)   | 2           | 16  |
| 13  | M     | 106/415 (26%)   | 96 (91%)   | 8 (8%)   | 2 (2%)   | 6           | 32  |
| 14  | N     | 139/233 (60%)   | 123 (88%)  | 13 (9%)  | 3 (2%)   | 5           | 29  |
| 15  | O     | 467/627 (74%)   | 426 (91%)  | 35 (8%)  | 6 (1%)   | 9           | 42  |
| 16  | P     | 569/894 (64%)   | 473 (83%)  | 76 (13%) | 20 (4%)  | 3           | 20  |
| 17  | Q     | 396/514 (77%)   | 345 (87%)  | 41 (10%) | 10 (2%)  | 4           | 26  |
| 18  | R     | 291/507 (57%)   | 245 (84%)  | 40 (14%) | 6 (2%)   | 5           | 30  |
| All | All   | 5859/7778 (75%) | 5373 (92%) | 392 (7%) | 94 (2%)  | 10          | 38  |

All (94) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 408  | LYS  |
| 1   | A     | 479  | ALA  |
| 1   | A     | 1651 | THR  |
| 2   | B     | 111  | ASP  |
| 2   | B     | 895  | PHE  |
| 2   | B     | 1097 | ASP  |
| 3   | C     | 224  | THR  |
| 4   | D     | 99   | LEU  |
| 9   | I     | 41   | GLN  |
| 15  | O     | 237  | ILE  |
| 15  | O     | 325  | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 16  | P     | 188  | GLN  |
| 16  | P     | 321  | LYS  |
| 16  | P     | 332  | ASN  |
| 16  | P     | 444  | PRO  |
| 16  | P     | 500  | ILE  |
| 16  | P     | 501  | PRO  |
| 17  | Q     | 8    | PRO  |
| 17  | Q     | 9    | ILE  |
| 17  | Q     | 15   | CYS  |
| 1   | A     | 415  | ASP  |
| 1   | A     | 448  | SER  |
| 1   | A     | 1500 | GLN  |
| 1   | A     | 1533 | GLU  |
| 1   | A     | 1606 | SER  |
| 2   | B     | 817  | ARG  |
| 2   | B     | 1049 | THR  |
| 2   | B     | 1140 | LYS  |
| 4   | D     | 98   | GLY  |
| 5   | E     | 50   | MET  |
| 9   | I     | 5    | GLY  |
| 16  | P     | 236  | ILE  |
| 16  | P     | 426  | ALA  |
| 16  | P     | 657  | SER  |
| 16  | P     | 745  | ALA  |
| 16  | P     | 752  | LEU  |
| 17  | Q     | 7    | GLY  |
| 17  | Q     | 196  | SER  |
| 18  | R     | 11   | ARG  |
| 18  | R     | 267  | GLY  |
| 18  | R     | 422  | GLY  |
| 1   | A     | 69   | GLU  |
| 1   | A     | 450  | LYS  |
| 2   | B     | 78   | PRO  |
| 2   | B     | 208  | VAL  |
| 2   | B     | 209  | GLN  |
| 2   | B     | 1070 | ARG  |
| 2   | B     | 1084 | THR  |
| 7   | G     | 99   | ASP  |
| 9   | I     | 21   | ASN  |
| 12  | L     | 46   | VAL  |
| 13  | M     | 85   | LYS  |
| 15  | O     | 82   | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 15  | O     | 469  | ARG  |
| 16  | P     | 201  | GLU  |
| 16  | P     | 241  | PRO  |
| 16  | P     | 247  | ILE  |
| 16  | P     | 666  | SER  |
| 16  | P     | 777  | MET  |
| 17  | Q     | 197  | GLU  |
| 1   | A     | 1299 | ASN  |
| 2   | B     | 834  | LYS  |
| 3   | C     | 297  | HIS  |
| 7   | G     | 100  | THR  |
| 12  | L     | 43   | THR  |
| 13  | M     | 36   | THR  |
| 14  | N     | 115  | SER  |
| 15  | O     | 130  | PRO  |
| 15  | O     | 187  | MET  |
| 16  | P     | 294  | PHE  |
| 17  | Q     | 13   | ASP  |
| 1   | A     | 451  | VAL  |
| 1   | A     | 564  | PRO  |
| 2   | B     | 80   | ASN  |
| 2   | B     | 117  | VAL  |
| 2   | B     | 1062 | GLY  |
| 3   | C     | 32   | ASN  |
| 5   | E     | 146  | HIS  |
| 17  | Q     | 16   | PRO  |
| 17  | Q     | 193  | PHE  |
| 18  | R     | 249  | SER  |
| 1   | A     | 1512 | PRO  |
| 2   | B     | 1063 | ARG  |
| 16  | P     | 568  | ILE  |
| 17  | Q     | 148  | PRO  |
| 18  | R     | 362  | ALA  |
| 6   | F     | 74   | ILE  |
| 14  | N     | 70   | LEU  |
| 16  | P     | 421  | ILE  |
| 18  | R     | 295  | PRO  |
| 14  | N     | 39   | PRO  |
| 2   | B     | 833  | PRO  |
| 2   | B     | 954  | PHE  |
| 16  | P     | 203  | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 1297/1465 (88%) | 1205 (93%) | 92 (7%)   | 13          | 35 |
| 2   | B     | 1025/1053 (97%) | 962 (94%)  | 63 (6%)   | 17          | 38 |
| 3   | C     | 269/296 (91%)   | 254 (94%)  | 15 (6%)   | 19          | 40 |
| 4   | D     | 55/116 (47%)    | 50 (91%)   | 5 (9%)    | 9           | 27 |
| 5   | E     | 194/197 (98%)   | 179 (92%)  | 15 (8%)   | 12          | 32 |
| 6   | F     | 90/137 (66%)    | 85 (94%)   | 5 (6%)    | 19          | 40 |
| 7   | G     | 171/291 (59%)   | 158 (92%)  | 13 (8%)   | 12          | 33 |
| 8   | H     | 115/128 (90%)   | 107 (93%)  | 8 (7%)    | 14          | 35 |
| 9   | I     | 89/110 (81%)    | 84 (94%)   | 5 (6%)    | 19          | 40 |
| 10  | J     | 64/65 (98%)     | 56 (88%)   | 8 (12%)   | 4           | 16 |
| 11  | K     | 91/130 (70%)    | 82 (90%)   | 9 (10%)   | 7           | 24 |
| 12  | L     | 39/57 (68%)     | 34 (87%)   | 5 (13%)   | 4           | 15 |
| 13  | M     | 98/371 (26%)    | 85 (87%)   | 13 (13%)  | 4           | 14 |
| 14  | N     | 135/220 (61%)   | 128 (95%)  | 7 (5%)    | 21          | 42 |
| 15  | O     | 439/576 (76%)   | 383 (87%)  | 56 (13%)  | 4           | 15 |
| 16  | P     | 539/828 (65%)   | 386 (72%)  | 153 (28%) | 0           | 2  |
| 17  | Q     | 383/476 (80%)   | 320 (84%)  | 63 (16%)  | 2           | 10 |
| 18  | R     | 286/474 (60%)   | 223 (78%)  | 63 (22%)  | 1           | 6  |
| All | All   | 5379/6990 (77%) | 4781 (89%) | 598 (11%) | 8           | 19 |

All (598) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | GLU  |
| 1   | A     | 40  | ASN  |
| 1   | A     | 61  | LEU  |
| 1   | A     | 83  | VAL  |
| 1   | A     | 136 | LEU  |
| 1   | A     | 174 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 186 | SER  |
| 1   | A     | 202 | THR  |
| 1   | A     | 230 | ARG  |
| 1   | A     | 257 | ASN  |
| 1   | A     | 262 | THR  |
| 1   | A     | 266 | VAL  |
| 1   | A     | 271 | ARG  |
| 1   | A     | 272 | GLN  |
| 1   | A     | 312 | SER  |
| 1   | A     | 315 | ILE  |
| 1   | A     | 346 | SER  |
| 1   | A     | 373 | LEU  |
| 1   | A     | 379 | GLU  |
| 1   | A     | 393 | SER  |
| 1   | A     | 406 | LEU  |
| 1   | A     | 407 | GLN  |
| 1   | A     | 408 | LYS  |
| 1   | A     | 410 | LYS  |
| 1   | A     | 413 | LEU  |
| 1   | A     | 414 | GLU  |
| 1   | A     | 447 | THR  |
| 1   | A     | 451 | VAL  |
| 1   | A     | 472 | MET  |
| 1   | A     | 503 | VAL  |
| 1   | A     | 518 | GLU  |
| 1   | A     | 524 | ILE  |
| 1   | A     | 555 | LYS  |
| 1   | A     | 611 | GLU  |
| 1   | A     | 627 | ASP  |
| 1   | A     | 661 | THR  |
| 1   | A     | 666 | VAL  |
| 1   | A     | 670 | ILE  |
| 1   | A     | 684 | ASP  |
| 1   | A     | 700 | ILE  |
| 1   | A     | 708 | THR  |
| 1   | A     | 709 | ARG  |
| 1   | A     | 739 | VAL  |
| 1   | A     | 747 | ILE  |
| 1   | A     | 758 | GLU  |
| 1   | A     | 783 | LYS  |
| 1   | A     | 794 | VAL  |
| 1   | A     | 815 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 878  | ARG  |
| 1   | A     | 955  | ARG  |
| 1   | A     | 957  | VAL  |
| 1   | A     | 966  | LEU  |
| 1   | A     | 988  | SER  |
| 1   | A     | 1021 | ARG  |
| 1   | A     | 1026 | GLN  |
| 1   | A     | 1033 | SER  |
| 1   | A     | 1071 | ASP  |
| 1   | A     | 1085 | LEU  |
| 1   | A     | 1098 | SER  |
| 1   | A     | 1102 | LEU  |
| 1   | A     | 1118 | VAL  |
| 1   | A     | 1123 | VAL  |
| 1   | A     | 1131 | LYS  |
| 1   | A     | 1136 | VAL  |
| 1   | A     | 1150 | LYS  |
| 1   | A     | 1159 | ASP  |
| 1   | A     | 1162 | ASN  |
| 1   | A     | 1204 | THR  |
| 1   | A     | 1215 | VAL  |
| 1   | A     | 1226 | VAL  |
| 1   | A     | 1273 | THR  |
| 1   | A     | 1275 | THR  |
| 1   | A     | 1276 | THR  |
| 1   | A     | 1310 | LYS  |
| 1   | A     | 1314 | GLN  |
| 1   | A     | 1320 | GLN  |
| 1   | A     | 1441 | LYS  |
| 1   | A     | 1455 | ARG  |
| 1   | A     | 1508 | VAL  |
| 1   | A     | 1518 | VAL  |
| 1   | A     | 1531 | ASP  |
| 1   | A     | 1533 | GLU  |
| 1   | A     | 1536 | ILE  |
| 1   | A     | 1601 | GLN  |
| 1   | A     | 1604 | GLU  |
| 1   | A     | 1605 | THR  |
| 1   | A     | 1609 | SER  |
| 1   | A     | 1611 | MET  |
| 1   | A     | 1616 | GLU  |
| 1   | A     | 1633 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1635 | ASP  |
| 1   | A     | 1649 | VAL  |
| 2   | B     | 17   | ARG  |
| 2   | B     | 22   | GLU  |
| 2   | B     | 37   | LEU  |
| 2   | B     | 53   | THR  |
| 2   | B     | 57   | ASP  |
| 2   | B     | 65   | VAL  |
| 2   | B     | 79   | LEU  |
| 2   | B     | 81   | SER  |
| 2   | B     | 87   | ASN  |
| 2   | B     | 97   | VAL  |
| 2   | B     | 117  | VAL  |
| 2   | B     | 187  | SER  |
| 2   | B     | 221  | SER  |
| 2   | B     | 228  | SER  |
| 2   | B     | 231  | HIS  |
| 2   | B     | 236  | ILE  |
| 2   | B     | 239  | VAL  |
| 2   | B     | 276  | ILE  |
| 2   | B     | 305  | ARG  |
| 2   | B     | 306  | LEU  |
| 2   | B     | 311  | ARG  |
| 2   | B     | 315  | LYS  |
| 2   | B     | 357  | ILE  |
| 2   | B     | 481  | VAL  |
| 2   | B     | 486  | VAL  |
| 2   | B     | 490  | LYS  |
| 2   | B     | 523  | GLU  |
| 2   | B     | 537  | SER  |
| 2   | B     | 583  | LEU  |
| 2   | B     | 622  | ILE  |
| 2   | B     | 658  | LEU  |
| 2   | B     | 720  | GLN  |
| 2   | B     | 725  | THR  |
| 2   | B     | 731  | VAL  |
| 2   | B     | 753  | LYS  |
| 2   | B     | 782  | ASP  |
| 2   | B     | 811  | LEU  |
| 2   | B     | 813  | LEU  |
| 2   | B     | 822  | THR  |
| 2   | B     | 829  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 833  | PRO  |
| 2   | B     | 835  | GLU  |
| 2   | B     | 858  | ILE  |
| 2   | B     | 871  | ILE  |
| 2   | B     | 883  | GLU  |
| 2   | B     | 897  | GLU  |
| 2   | B     | 977  | ILE  |
| 2   | B     | 998  | GLU  |
| 2   | B     | 1026 | ILE  |
| 2   | B     | 1038 | HIS  |
| 2   | B     | 1047 | ARG  |
| 2   | B     | 1060 | VAL  |
| 2   | B     | 1064 | LYS  |
| 2   | B     | 1069 | ILE  |
| 2   | B     | 1075 | GLU  |
| 2   | B     | 1103 | VAL  |
| 2   | B     | 1125 | THR  |
| 2   | B     | 1136 | GLU  |
| 2   | B     | 1141 | LEU  |
| 2   | B     | 1153 | ILE  |
| 2   | B     | 1163 | GLN  |
| 2   | B     | 1165 | ASN  |
| 2   | B     | 1174 | THR  |
| 3   | C     | 38   | LYS  |
| 3   | C     | 43   | ASN  |
| 3   | C     | 61   | THR  |
| 3   | C     | 77   | SER  |
| 3   | C     | 91   | VAL  |
| 3   | C     | 97   | LEU  |
| 3   | C     | 118  | SER  |
| 3   | C     | 138  | VAL  |
| 3   | C     | 142  | ARG  |
| 3   | C     | 181  | ASP  |
| 3   | C     | 193  | LEU  |
| 3   | C     | 224  | THR  |
| 3   | C     | 243  | SER  |
| 3   | C     | 277  | ARG  |
| 3   | C     | 279  | VAL  |
| 4   | D     | 15   | THR  |
| 4   | D     | 29   | GLN  |
| 4   | D     | 38   | GLN  |
| 4   | D     | 80   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 99  | LEU  |
| 5   | E     | 4   | GLU  |
| 5   | E     | 31  | THR  |
| 5   | E     | 33  | GLU  |
| 5   | E     | 74  | ASP  |
| 5   | E     | 77  | SER  |
| 5   | E     | 90  | VAL  |
| 5   | E     | 92  | THR  |
| 5   | E     | 93  | MET  |
| 5   | E     | 107 | THR  |
| 5   | E     | 131 | THR  |
| 5   | E     | 136 | ASN  |
| 5   | E     | 142 | VAL  |
| 5   | E     | 162 | ARG  |
| 5   | E     | 163 | GLU  |
| 5   | E     | 177 | ARG  |
| 6   | F     | 59  | GLN  |
| 6   | F     | 74  | ILE  |
| 6   | F     | 87  | LYS  |
| 6   | F     | 99  | LEU  |
| 6   | F     | 109 | VAL  |
| 7   | G     | 21  | LYS  |
| 7   | G     | 24  | VAL  |
| 7   | G     | 35  | SER  |
| 7   | G     | 39  | VAL  |
| 7   | G     | 139 | ILE  |
| 7   | G     | 147 | LEU  |
| 7   | G     | 167 | THR  |
| 7   | G     | 169 | VAL  |
| 7   | G     | 223 | GLU  |
| 7   | G     | 230 | ARG  |
| 7   | G     | 239 | THR  |
| 7   | G     | 241 | ARG  |
| 7   | G     | 243 | VAL  |
| 8   | H     | 3   | ASN  |
| 8   | H     | 9   | ILE  |
| 8   | H     | 39  | THR  |
| 8   | H     | 108 | SER  |
| 8   | H     | 111 | LEU  |
| 8   | H     | 112 | ILE  |
| 8   | H     | 114 | VAL  |
| 8   | H     | 121 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | I     | 2   | SER  |
| 9   | I     | 3   | VAL  |
| 9   | I     | 15  | ASP  |
| 9   | I     | 45  | LEU  |
| 9   | I     | 81  | THR  |
| 10  | J     | 3   | VAL  |
| 10  | J     | 9   | SER  |
| 10  | J     | 10  | CYS  |
| 10  | J     | 14  | VAL  |
| 10  | J     | 27  | GLU  |
| 10  | J     | 34  | THR  |
| 10  | J     | 45  | CYS  |
| 10  | J     | 48  | ARG  |
| 11  | K     | 44  | ARG  |
| 11  | K     | 45  | GLU  |
| 11  | K     | 51  | THR  |
| 11  | K     | 68  | GLU  |
| 11  | K     | 99  | ASN  |
| 11  | K     | 103 | ILE  |
| 11  | K     | 118 | GLN  |
| 11  | K     | 123 | ASP  |
| 11  | K     | 133 | SER  |
| 12  | L     | 38  | LEU  |
| 12  | L     | 41  | SER  |
| 12  | L     | 55  | ILE  |
| 12  | L     | 57  | LEU  |
| 12  | L     | 66  | GLN  |
| 13  | M     | 17  | ASP  |
| 13  | M     | 18  | GLN  |
| 13  | M     | 31  | ARG  |
| 13  | M     | 44  | LYS  |
| 13  | M     | 48  | LYS  |
| 13  | M     | 52  | VAL  |
| 13  | M     | 63  | GLU  |
| 13  | M     | 65  | TYR  |
| 13  | M     | 77  | VAL  |
| 13  | M     | 84  | GLU  |
| 13  | M     | 98  | SER  |
| 13  | M     | 104 | SER  |
| 13  | M     | 109 | ARG  |
| 14  | N     | 51  | GLN  |
| 14  | N     | 89  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | N     | 124 | THR  |
| 14  | N     | 135 | LYS  |
| 14  | N     | 153 | VAL  |
| 14  | N     | 167 | LYS  |
| 14  | N     | 178 | GLU  |
| 15  | O     | 66  | ASN  |
| 15  | O     | 67  | ASP  |
| 15  | O     | 69  | THR  |
| 15  | O     | 78  | VAL  |
| 15  | O     | 80  | LEU  |
| 15  | O     | 87  | ARG  |
| 15  | O     | 101 | SER  |
| 15  | O     | 110 | SER  |
| 15  | O     | 111 | ARG  |
| 15  | O     | 117 | GLN  |
| 15  | O     | 171 | CYS  |
| 15  | O     | 175 | MET  |
| 15  | O     | 180 | LEU  |
| 15  | O     | 181 | ARG  |
| 15  | O     | 190 | ILE  |
| 15  | O     | 192 | THR  |
| 15  | O     | 194 | LEU  |
| 15  | O     | 202 | ASN  |
| 15  | O     | 203 | ASP  |
| 15  | O     | 204 | THR  |
| 15  | O     | 205 | ARG  |
| 15  | O     | 212 | THR  |
| 15  | O     | 213 | SER  |
| 15  | O     | 215 | LEU  |
| 15  | O     | 225 | LEU  |
| 15  | O     | 228 | GLN  |
| 15  | O     | 232 | LEU  |
| 15  | O     | 234 | ILE  |
| 15  | O     | 237 | ILE  |
| 15  | O     | 239 | SER  |
| 15  | O     | 240 | ILE  |
| 15  | O     | 245 | GLN  |
| 15  | O     | 248 | LEU  |
| 15  | O     | 341 | THR  |
| 15  | O     | 350 | GLU  |
| 15  | O     | 354 | SER  |
| 15  | O     | 363 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | O     | 376 | TYR  |
| 15  | O     | 381 | ILE  |
| 15  | O     | 395 | LEU  |
| 15  | O     | 407 | SER  |
| 15  | O     | 410 | VAL  |
| 15  | O     | 415 | GLU  |
| 15  | O     | 437 | THR  |
| 15  | O     | 454 | VAL  |
| 15  | O     | 489 | ASN  |
| 15  | O     | 494 | THR  |
| 15  | O     | 526 | LEU  |
| 15  | O     | 543 | ILE  |
| 15  | O     | 578 | SER  |
| 15  | O     | 579 | LEU  |
| 15  | O     | 581 | THR  |
| 15  | O     | 584 | GLN  |
| 15  | O     | 597 | LEU  |
| 15  | O     | 599 | LEU  |
| 15  | O     | 602 | TYR  |
| 16  | P     | 21  | GLN  |
| 16  | P     | 25  | LEU  |
| 16  | P     | 26  | TYR  |
| 16  | P     | 49  | THR  |
| 16  | P     | 55  | LEU  |
| 16  | P     | 64  | LEU  |
| 16  | P     | 187 | ILE  |
| 16  | P     | 195 | ASN  |
| 16  | P     | 201 | GLU  |
| 16  | P     | 207 | SER  |
| 16  | P     | 212 | SER  |
| 16  | P     | 214 | LEU  |
| 16  | P     | 220 | THR  |
| 16  | P     | 225 | LEU  |
| 16  | P     | 227 | LEU  |
| 16  | P     | 232 | ASN  |
| 16  | P     | 233 | VAL  |
| 16  | P     | 236 | ILE  |
| 16  | P     | 237 | GLU  |
| 16  | P     | 243 | LYS  |
| 16  | P     | 245 | ILE  |
| 16  | P     | 252 | GLU  |
| 16  | P     | 256 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | P     | 257 | ARG  |
| 16  | P     | 260 | LEU  |
| 16  | P     | 261 | VAL  |
| 16  | P     | 263 | ILE  |
| 16  | P     | 264 | ILE  |
| 16  | P     | 270 | GLN  |
| 16  | P     | 271 | ILE  |
| 16  | P     | 276 | SER  |
| 16  | P     | 282 | CYS  |
| 16  | P     | 286 | VAL  |
| 16  | P     | 290 | GLU  |
| 16  | P     | 292 | LEU  |
| 16  | P     | 297 | ILE  |
| 16  | P     | 300 | LEU  |
| 16  | P     | 314 | GLN  |
| 16  | P     | 321 | LYS  |
| 16  | P     | 323 | ASN  |
| 16  | P     | 326 | ILE  |
| 16  | P     | 329 | ILE  |
| 16  | P     | 331 | LYS  |
| 16  | P     | 333 | PHE  |
| 16  | P     | 343 | LEU  |
| 16  | P     | 345 | ASP  |
| 16  | P     | 347 | LEU  |
| 16  | P     | 359 | SER  |
| 16  | P     | 360 | TRP  |
| 16  | P     | 363 | ILE  |
| 16  | P     | 370 | GLN  |
| 16  | P     | 377 | ARG  |
| 16  | P     | 379 | LYS  |
| 16  | P     | 381 | ILE  |
| 16  | P     | 384 | ASP  |
| 16  | P     | 386 | MET  |
| 16  | P     | 390 | GLN  |
| 16  | P     | 397 | LYS  |
| 16  | P     | 402 | ILE  |
| 16  | P     | 403 | ARG  |
| 16  | P     | 407 | ARG  |
| 16  | P     | 408 | ILE  |
| 16  | P     | 412 | ASN  |
| 16  | P     | 415 | LEU  |
| 16  | P     | 417 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | P     | 419 | ARG  |
| 16  | P     | 421 | ILE  |
| 16  | P     | 423 | ILE  |
| 16  | P     | 424 | VAL  |
| 16  | P     | 430 | ASN  |
| 16  | P     | 433 | VAL  |
| 16  | P     | 439 | LYS  |
| 16  | P     | 440 | HIS  |
| 16  | P     | 442 | LEU  |
| 16  | P     | 448 | THR  |
| 16  | P     | 453 | VAL  |
| 16  | P     | 455 | LYS  |
| 16  | P     | 456 | VAL  |
| 16  | P     | 460 | ASP  |
| 16  | P     | 463 | LEU  |
| 16  | P     | 464 | LEU  |
| 16  | P     | 465 | VAL  |
| 16  | P     | 468 | VAL  |
| 16  | P     | 473 | HIS  |
| 16  | P     | 474 | LYS  |
| 16  | P     | 480 | VAL  |
| 16  | P     | 492 | LEU  |
| 16  | P     | 494 | CYS  |
| 16  | P     | 496 | THR  |
| 16  | P     | 497 | VAL  |
| 16  | P     | 498 | LEU  |
| 16  | P     | 500 | ILE  |
| 16  | P     | 508 | ILE  |
| 16  | P     | 511 | ILE  |
| 16  | P     | 531 | PHE  |
| 16  | P     | 534 | VAL  |
| 16  | P     | 538 | LEU  |
| 16  | P     | 539 | VAL  |
| 16  | P     | 545 | SER  |
| 16  | P     | 546 | GLU  |
| 16  | P     | 555 | THR  |
| 16  | P     | 556 | GLN  |
| 16  | P     | 567 | ILE  |
| 16  | P     | 580 | ASN  |
| 16  | P     | 582 | ASP  |
| 16  | P     | 584 | ARG  |
| 16  | P     | 593 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | P     | 596 | ILE  |
| 16  | P     | 600 | GLU  |
| 16  | P     | 609 | ASN  |
| 16  | P     | 615 | ASN  |
| 16  | P     | 617 | HIS  |
| 16  | P     | 625 | ASP  |
| 16  | P     | 626 | LEU  |
| 16  | P     | 630 | LEU  |
| 16  | P     | 632 | ILE  |
| 16  | P     | 634 | THR  |
| 16  | P     | 635 | ASN  |
| 16  | P     | 637 | LEU  |
| 16  | P     | 638 | LEU  |
| 16  | P     | 646 | ASP  |
| 16  | P     | 647 | GLU  |
| 16  | P     | 649 | ILE  |
| 16  | P     | 654 | LEU  |
| 16  | P     | 656 | HIS  |
| 16  | P     | 659 | LEU  |
| 16  | P     | 660 | LYS  |
| 16  | P     | 662 | LEU  |
| 16  | P     | 664 | GLU  |
| 16  | P     | 665 | ASN  |
| 16  | P     | 667 | ASP  |
| 16  | P     | 671 | SER  |
| 16  | P     | 676 | SER  |
| 16  | P     | 679 | LEU  |
| 16  | P     | 693 | PHE  |
| 16  | P     | 694 | ILE  |
| 16  | P     | 700 | LEU  |
| 16  | P     | 706 | GLU  |
| 16  | P     | 711 | LEU  |
| 16  | P     | 712 | ASP  |
| 16  | P     | 726 | SER  |
| 16  | P     | 730 | GLU  |
| 16  | P     | 731 | LEU  |
| 16  | P     | 736 | ILE  |
| 16  | P     | 748 | GLU  |
| 16  | P     | 749 | LYS  |
| 16  | P     | 751 | SER  |
| 16  | P     | 753 | PHE  |
| 16  | P     | 757 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | P     | 762 | ARG  |
| 16  | P     | 768 | TYR  |
| 16  | P     | 772 | ILE  |
| 16  | P     | 777 | MET  |
| 17  | Q     | 17  | SER  |
| 17  | Q     | 26  | ARG  |
| 17  | Q     | 27  | ARG  |
| 17  | Q     | 94  | LYS  |
| 17  | Q     | 101 | LYS  |
| 17  | Q     | 103 | LEU  |
| 17  | Q     | 111 | ILE  |
| 17  | Q     | 112 | LEU  |
| 17  | Q     | 138 | LEU  |
| 17  | Q     | 139 | LYS  |
| 17  | Q     | 143 | THR  |
| 17  | Q     | 144 | ILE  |
| 17  | Q     | 145 | ASN  |
| 17  | Q     | 147 | GLN  |
| 17  | Q     | 149 | GLN  |
| 17  | Q     | 150 | GLU  |
| 17  | Q     | 154 | LEU  |
| 17  | Q     | 159 | THR  |
| 17  | Q     | 164 | ILE  |
| 17  | Q     | 167 | LEU  |
| 17  | Q     | 169 | SER  |
| 17  | Q     | 173 | SER  |
| 17  | Q     | 176 | VAL  |
| 17  | Q     | 187 | THR  |
| 17  | Q     | 204 | ARG  |
| 17  | Q     | 207 | LEU  |
| 17  | Q     | 218 | SER  |
| 17  | Q     | 226 | LEU  |
| 17  | Q     | 232 | LEU  |
| 17  | Q     | 248 | SER  |
| 17  | Q     | 273 | VAL  |
| 17  | Q     | 278 | GLU  |
| 17  | Q     | 286 | LEU  |
| 17  | Q     | 288 | GLU  |
| 17  | Q     | 290 | THR  |
| 17  | Q     | 291 | ASP  |
| 17  | Q     | 297 | ARG  |
| 17  | Q     | 301 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | Q     | 312 | LEU  |
| 17  | Q     | 318 | LEU  |
| 17  | Q     | 328 | LEU  |
| 17  | Q     | 332 | LEU  |
| 17  | Q     | 337 | SER  |
| 17  | Q     | 348 | ILE  |
| 17  | Q     | 363 | SER  |
| 17  | Q     | 367 | PHE  |
| 17  | Q     | 368 | GLN  |
| 17  | Q     | 378 | LEU  |
| 17  | Q     | 379 | LYS  |
| 17  | Q     | 384 | GLN  |
| 17  | Q     | 419 | LEU  |
| 17  | Q     | 435 | GLN  |
| 17  | Q     | 436 | LEU  |
| 17  | Q     | 439 | ILE  |
| 17  | Q     | 443 | GLN  |
| 17  | Q     | 444 | GLU  |
| 17  | Q     | 453 | PHE  |
| 17  | Q     | 494 | SER  |
| 17  | Q     | 495 | LYS  |
| 17  | Q     | 496 | GLU  |
| 17  | Q     | 498 | LEU  |
| 17  | Q     | 502 | ILE  |
| 17  | Q     | 513 | MET  |
| 18  | R     | 1   | MET  |
| 18  | R     | 4   | VAL  |
| 18  | R     | 8   | LEU  |
| 18  | R     | 10  | ASN  |
| 18  | R     | 11  | ARG  |
| 18  | R     | 28  | SER  |
| 18  | R     | 34  | ILE  |
| 18  | R     | 74  | GLN  |
| 18  | R     | 80  | ARG  |
| 18  | R     | 84  | TRP  |
| 18  | R     | 85  | ARG  |
| 18  | R     | 87  | VAL  |
| 18  | R     | 143 | THR  |
| 18  | R     | 150 | GLN  |
| 18  | R     | 155 | GLN  |
| 18  | R     | 156 | LYS  |
| 18  | R     | 165 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | R     | 167 | LYS  |
| 18  | R     | 168 | ILE  |
| 18  | R     | 175 | ILE  |
| 18  | R     | 178 | LEU  |
| 18  | R     | 181 | THR  |
| 18  | R     | 202 | THR  |
| 18  | R     | 206 | ARG  |
| 18  | R     | 209 | ARG  |
| 18  | R     | 210 | THR  |
| 18  | R     | 211 | ARG  |
| 18  | R     | 212 | HIS  |
| 18  | R     | 216 | LEU  |
| 18  | R     | 218 | ASP  |
| 18  | R     | 231 | LEU  |
| 18  | R     | 235 | ILE  |
| 18  | R     | 238 | THR  |
| 18  | R     | 242 | ILE  |
| 18  | R     | 247 | ILE  |
| 18  | R     | 248 | LYS  |
| 18  | R     | 250 | LEU  |
| 18  | R     | 255 | VAL  |
| 18  | R     | 266 | SER  |
| 18  | R     | 269 | ASP  |
| 18  | R     | 272 | GLN  |
| 18  | R     | 276 | GLN  |
| 18  | R     | 294 | VAL  |
| 18  | R     | 298 | GLN  |
| 18  | R     | 299 | THR  |
| 18  | R     | 302 | ARG  |
| 18  | R     | 307 | LYS  |
| 18  | R     | 308 | PHE  |
| 18  | R     | 313 | LEU  |
| 18  | R     | 319 | ASN  |
| 18  | R     | 322 | LYS  |
| 18  | R     | 323 | SER  |
| 18  | R     | 345 | LEU  |
| 18  | R     | 359 | MET  |
| 18  | R     | 364 | VAL  |
| 18  | R     | 367 | ILE  |
| 18  | R     | 373 | LEU  |
| 18  | R     | 374 | LEU  |
| 18  | R     | 401 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | R     | 402 | ASN  |
| 18  | R     | 403 | GLN  |
| 18  | R     | 410 | TYR  |
| 18  | R     | 420 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 126  | GLN  |
| 1   | A     | 378  | HIS  |
| 1   | A     | 382  | GLN  |
| 1   | A     | 407  | GLN  |
| 1   | A     | 425  | ASN  |
| 1   | A     | 431  | GLN  |
| 1   | A     | 470  | HIS  |
| 1   | A     | 535  | GLN  |
| 1   | A     | 590  | ASN  |
| 1   | A     | 636  | HIS  |
| 1   | A     | 693  | GLN  |
| 1   | A     | 1026 | GLN  |
| 1   | A     | 1088 | HIS  |
| 1   | A     | 1162 | ASN  |
| 1   | A     | 1314 | GLN  |
| 1   | A     | 1320 | GLN  |
| 2   | B     | 87   | ASN  |
| 2   | B     | 182  | GLN  |
| 2   | B     | 321  | GLN  |
| 2   | B     | 422  | GLN  |
| 2   | B     | 462  | GLN  |
| 2   | B     | 473  | GLN  |
| 2   | B     | 554  | GLN  |
| 2   | B     | 702  | ASN  |
| 2   | B     | 893  | ASN  |
| 2   | B     | 1163 | GLN  |
| 3   | C     | 232  | GLN  |
| 3   | C     | 323  | ASN  |
| 3   | C     | 335  | GLN  |
| 5   | E     | 5    | ASN  |
| 5   | E     | 32   | GLN  |
| 6   | F     | 59   | GLN  |
| 7   | G     | 23   | GLN  |
| 7   | G     | 59   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 126 | GLN  |
| 9   | I     | 44  | ASN  |
| 9   | I     | 97  | HIS  |
| 12  | L     | 53  | HIS  |
| 13  | M     | 18  | GLN  |
| 14  | N     | 61  | ASN  |
| 14  | N     | 132 | GLN  |
| 15  | O     | 66  | ASN  |
| 15  | O     | 70  | GLN  |
| 15  | O     | 105 | ASN  |
| 15  | O     | 210 | ASN  |
| 15  | O     | 228 | GLN  |
| 15  | O     | 245 | GLN  |
| 15  | O     | 342 | HIS  |
| 15  | O     | 362 | ASN  |
| 15  | O     | 371 | HIS  |
| 15  | O     | 390 | GLN  |
| 15  | O     | 488 | HIS  |
| 15  | O     | 497 | ASN  |
| 15  | O     | 521 | ASN  |
| 15  | O     | 533 | GLN  |
| 15  | O     | 547 | ASN  |
| 15  | O     | 549 | ASN  |
| 16  | P     | 226 | HIS  |
| 16  | P     | 228 | ASN  |
| 16  | P     | 368 | HIS  |
| 16  | P     | 388 | ASN  |
| 16  | P     | 461 | HIS  |
| 16  | P     | 635 | ASN  |
| 16  | P     | 705 | HIS  |
| 17  | Q     | 194 | GLN  |
| 17  | Q     | 351 | ASN  |
| 17  | Q     | 368 | GLN  |
| 17  | Q     | 384 | GLN  |
| 18  | R     | 160 | HIS  |
| 18  | R     | 184 | ASN  |
| 18  | R     | 212 | HIS  |
| 18  | R     | 223 | ASN  |
| 18  | R     | 228 | ASN  |
| 18  | R     | 409 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | A     | 2                |
| 7   | G     | 1                |
| 9   | I     | 1                |
| 17  | Q     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | G     | 24:VAL    | C      | 25:THR    | N      | 4.53         |
| 1     | I     | 45:LEU    | C      | 46:LYS    | N      | 3.17         |
| 1     | Q     | 369:TRP   | C      | 370:SER   | N      | 3.11         |
| 1     | A     | 438:ILE   | C      | 439:ASP   | N      | 2.97         |
| 1     | A     | 991:LYS   | C      | 992:PRO   | N      | 2.87         |

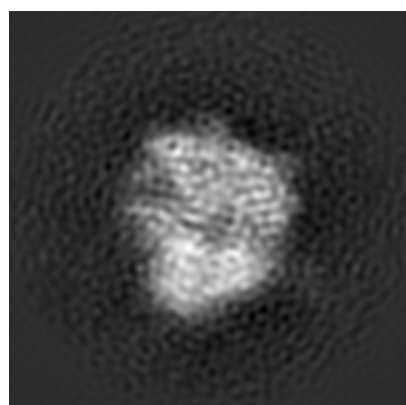
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3591. These allow visual inspection of the internal detail of the map and identification of artifacts.

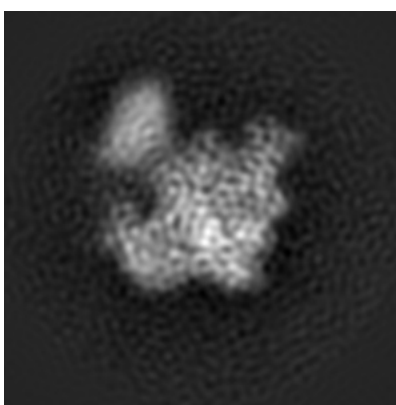
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

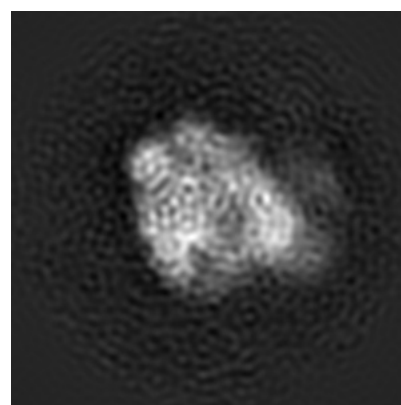
#### 6.1.1 Primary map



X



Y

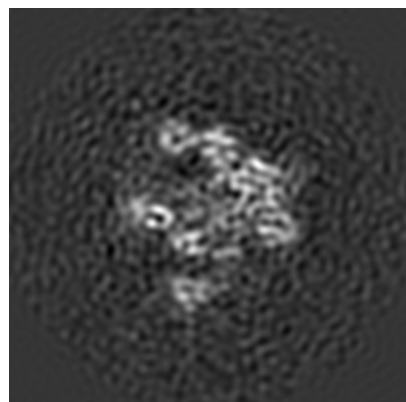


Z

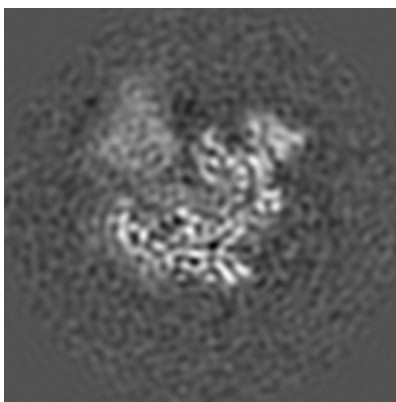
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

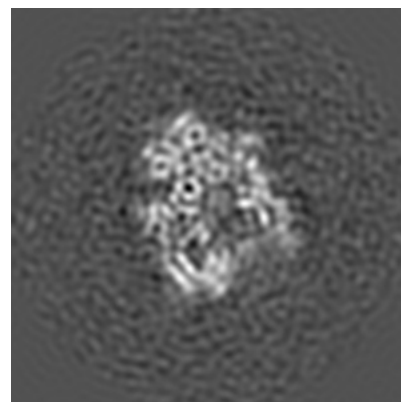
#### 6.2.1 Primary map



X Index: 120



Y Index: 120

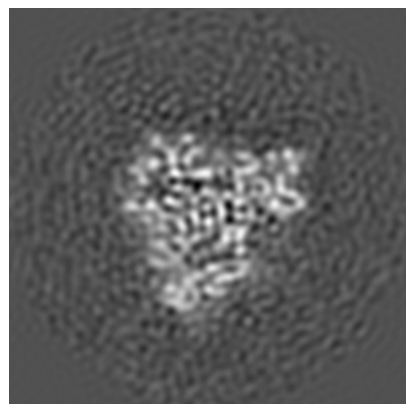


Z Index: 120

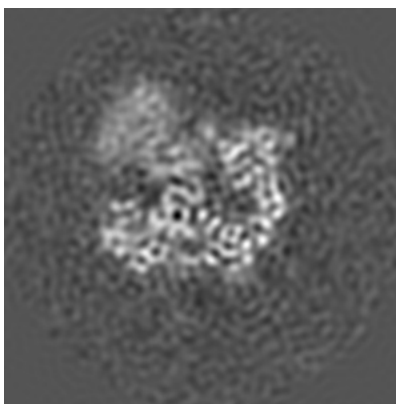
The images above show central slices of the map in three orthogonal directions.

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

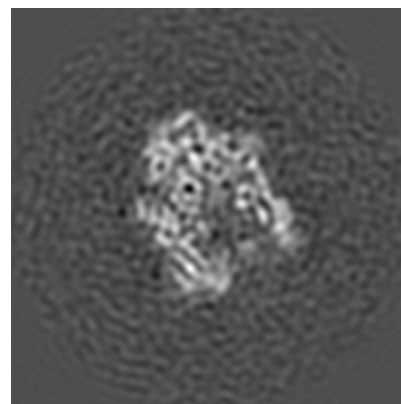
### 6.3.1 Primary map



X Index: 105



Y Index: 102

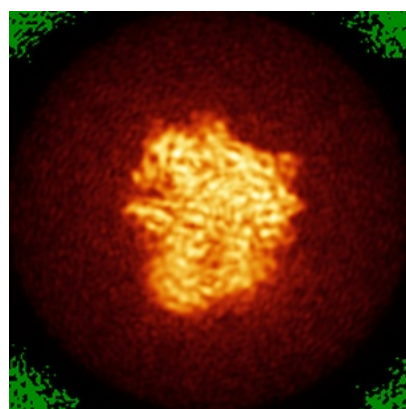


Z Index: 122

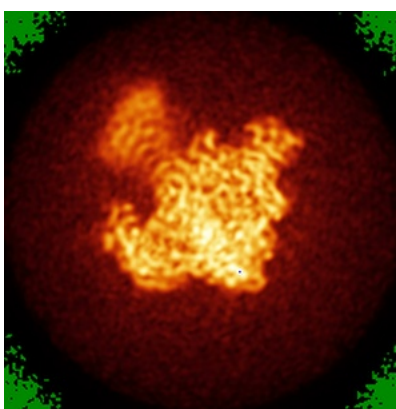
The images above show the largest variance slices of the map in three orthogonal directions.

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

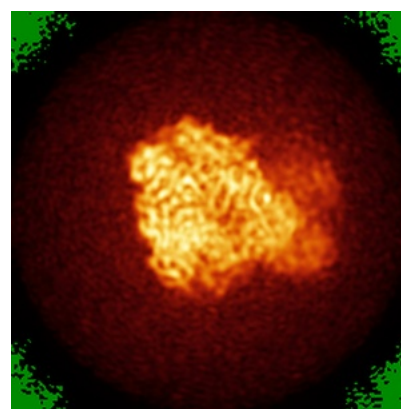
### 6.4.1 Primary map



X



Y

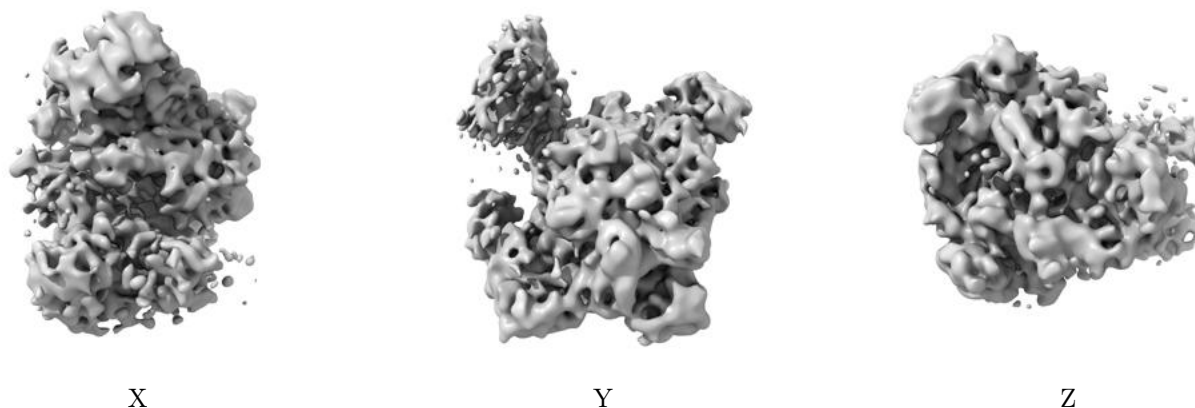


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

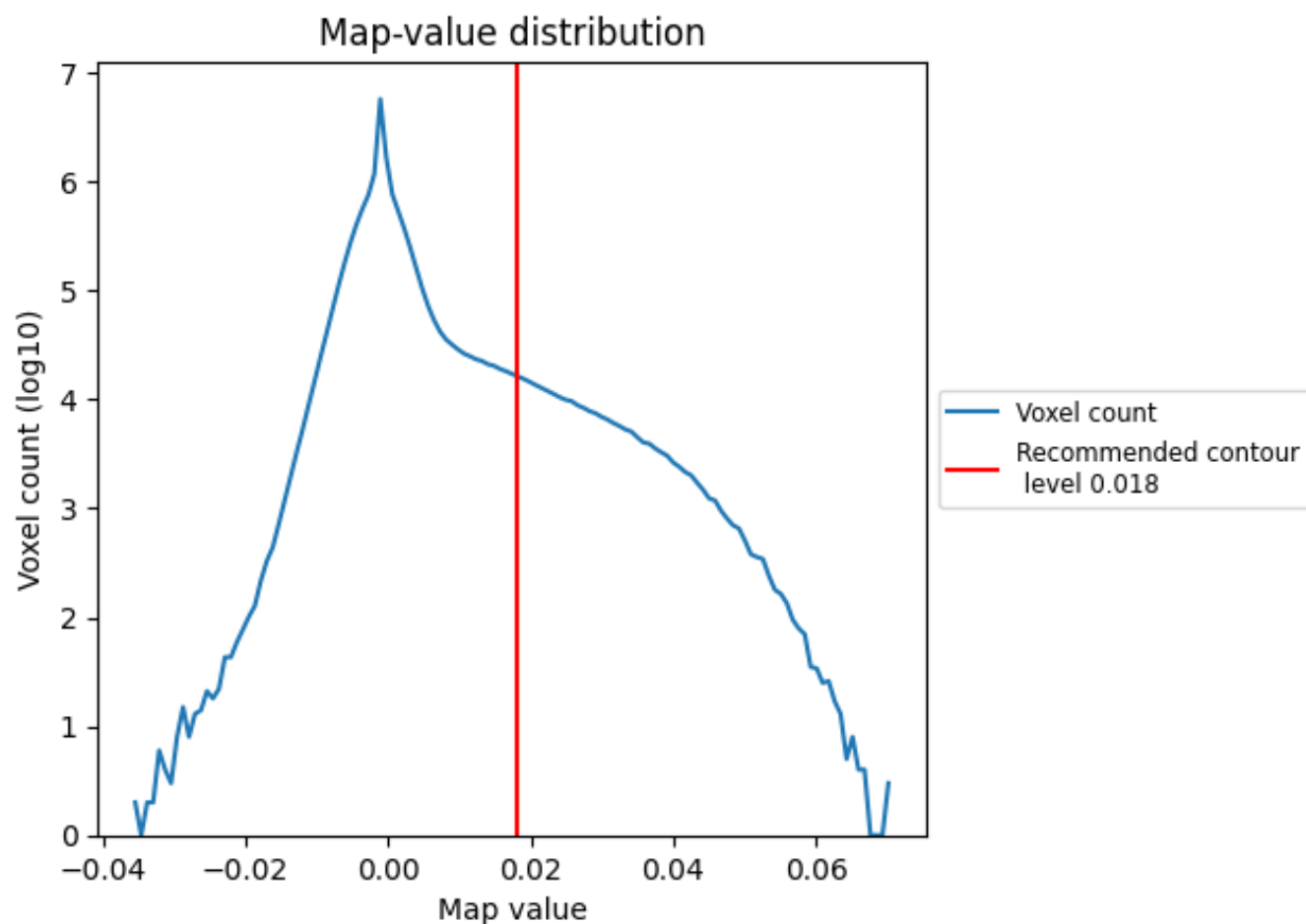
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

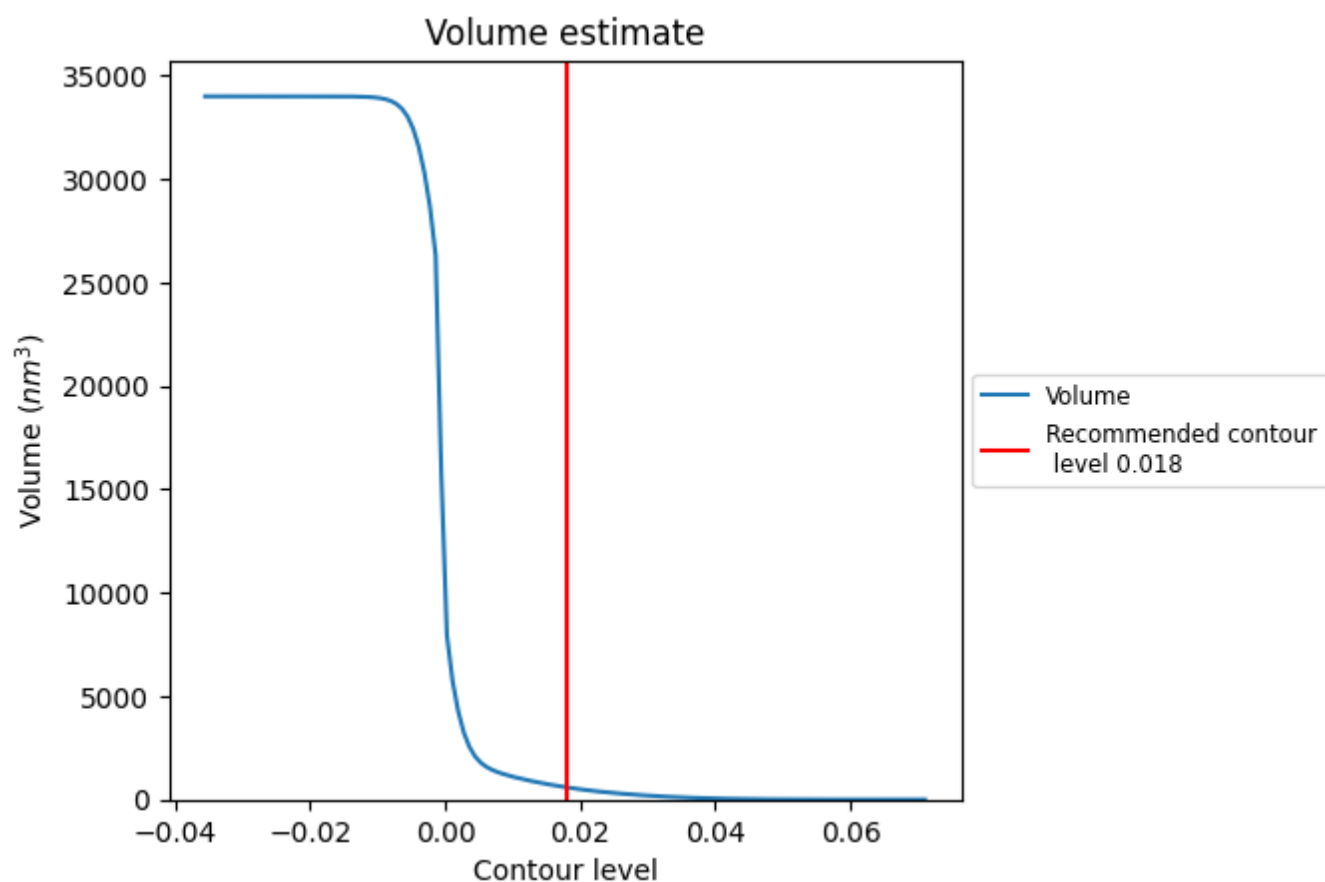
This section contains the results of statistical analysis of the map.

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



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

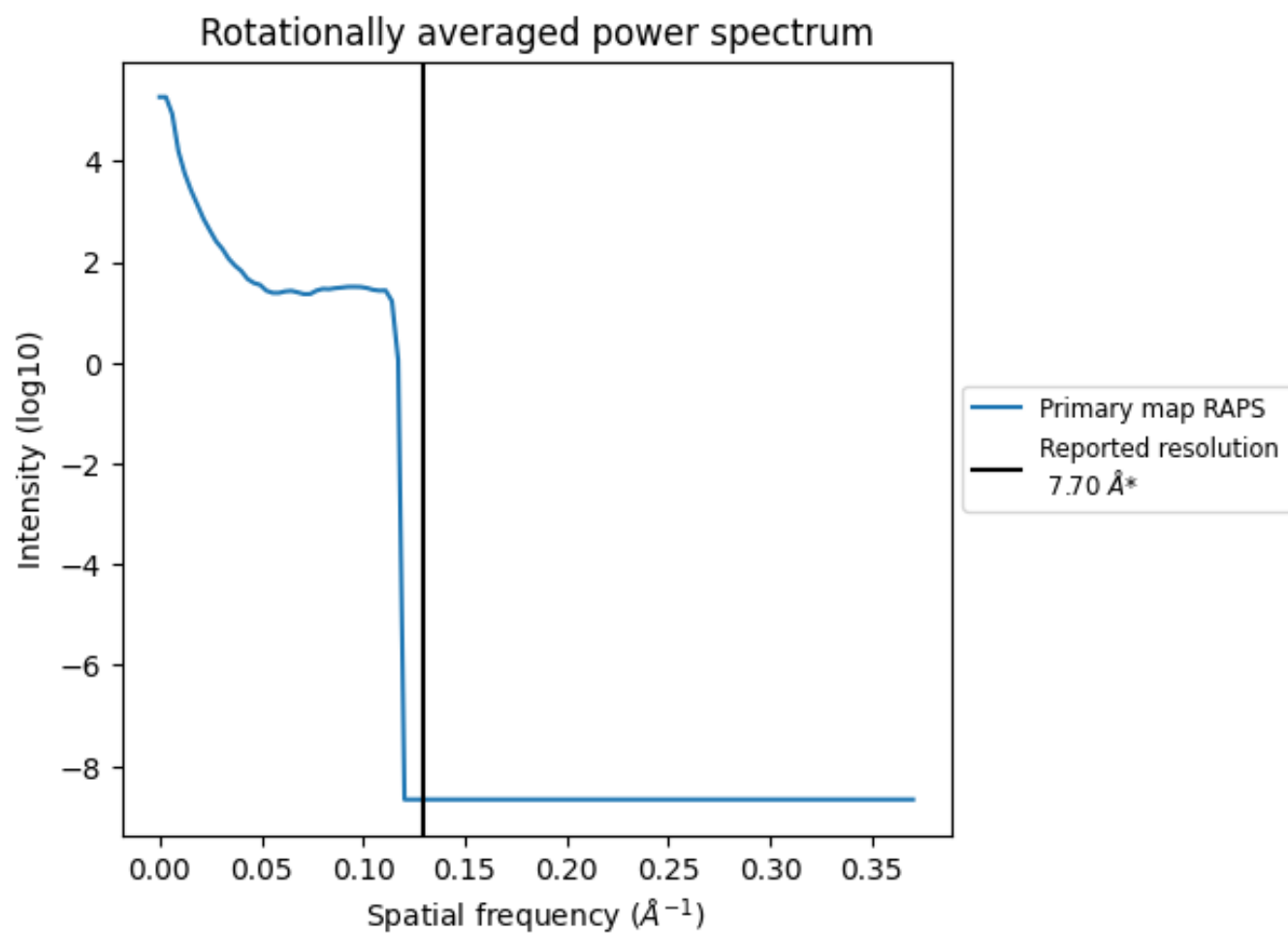
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 591  $\text{nm}^3$ ; this corresponds to an approximate mass of 534 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.130 Å<sup>-1</sup>

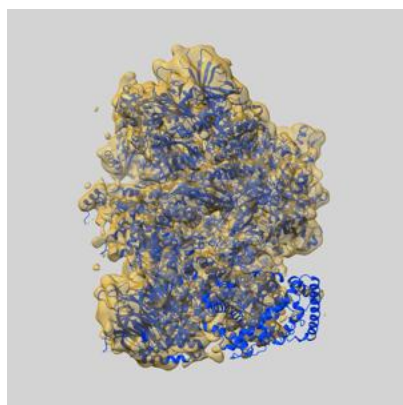
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

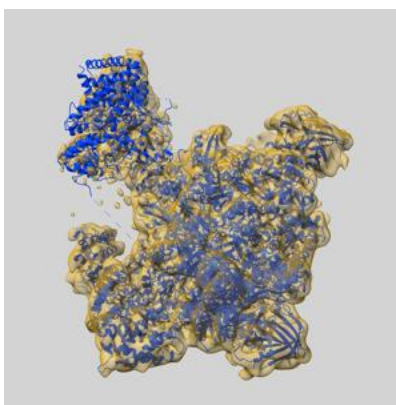
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3591 and PDB model 5N5Z. Per-residue inclusion information can be found in section [3](#) on page [8](#).

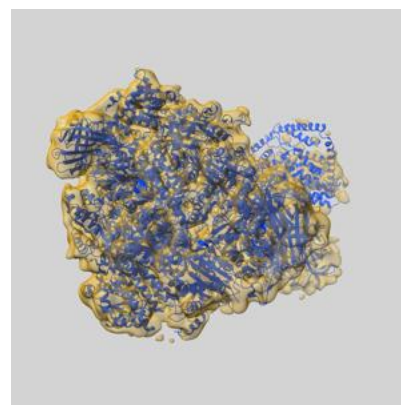
### 9.1 Map-model overlay [i](#)



X



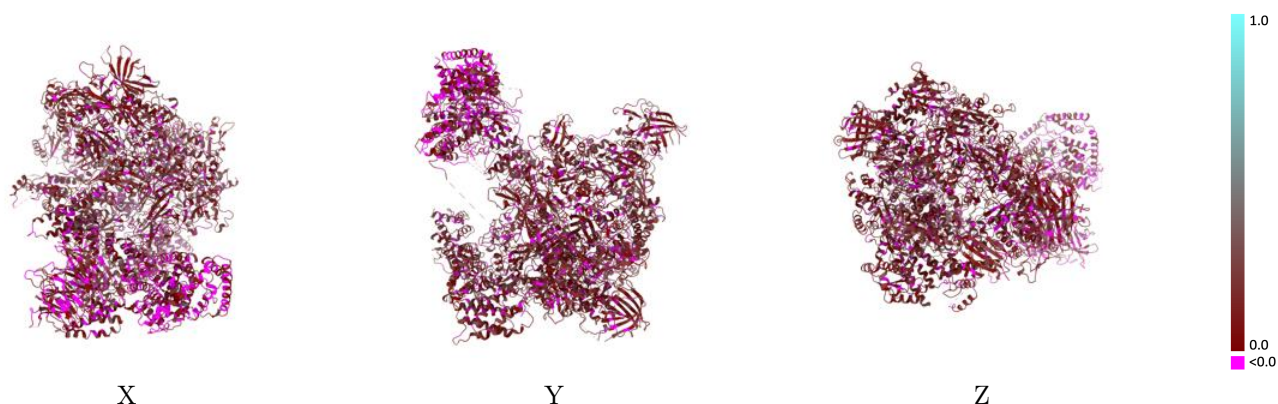
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

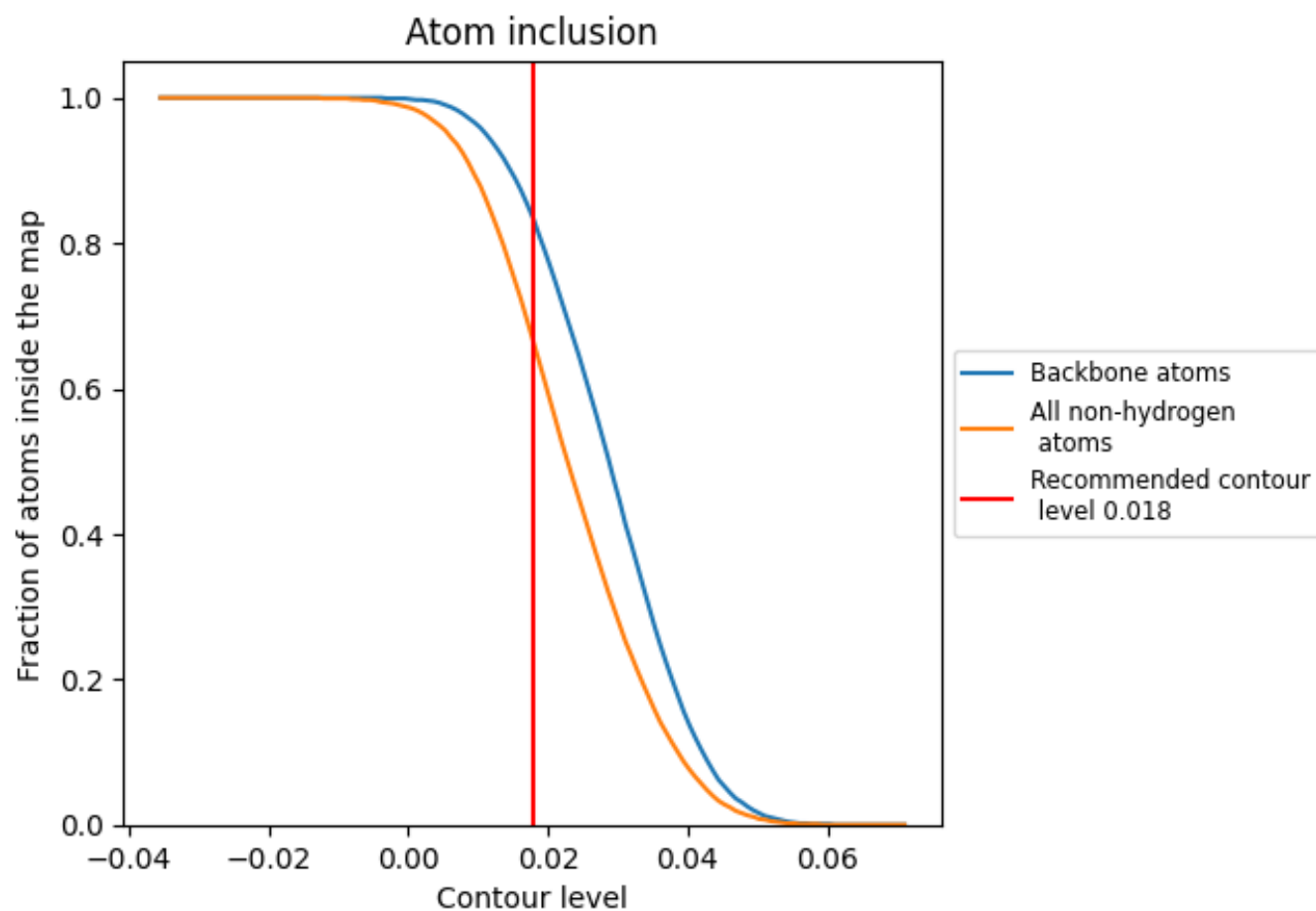


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6620   |  0.1160   |
| A     |  0.7270   |  0.1310   |
| B     |  0.7230   |  0.1220   |
| C     |  0.7900   |  0.1330   |
| D     |  0.7980   |  0.1690   |
| E     |  0.8020   |  0.1410   |
| F     |  0.7480   |  0.1420   |
| G     |  0.7940   |  0.1310   |
| H     |  0.8430   |  0.1530   |
| I     |  0.6210   |  0.1250   |
| J     |  0.7300   |  0.1190   |
| K     |  0.7930   |  0.1530   |
| L     |  0.7440   |  0.0950   |
| M     |  0.7180   |  0.1130   |
| N     |  0.7280  |  0.1420  |
| O     |  0.7620 |  0.1370 |
| P     |  0.3710 |  0.0470 |
| Q     |  0.3000 |  0.0550 |
| R     |  0.4930 |  0.1040 |

