



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:15 AM UTC

PDB ID : 7OLE / pdb\_00007ole  
EMDB ID : EMD-12979  
Title : Cryo-EM structure of the TELO2-TTI1-TTI2-RUVBL1-RUVBL2 complex  
Authors : Pal, M.; Llorca, O.; Pearl, L.  
Deposited on : 2021-05-19  
Resolution : 3.41 Å(reported)  
Based on initial model : 6FO1

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  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

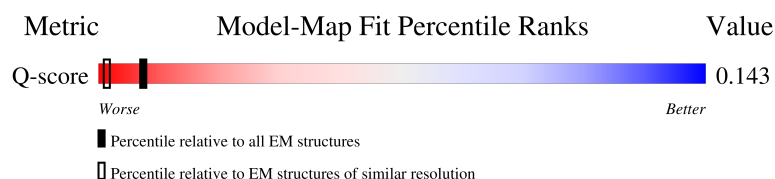
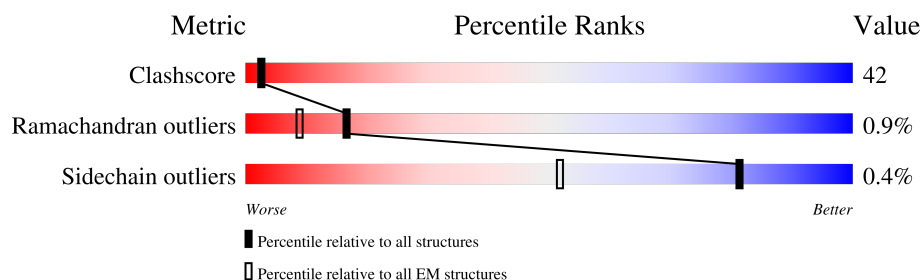
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.41 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.



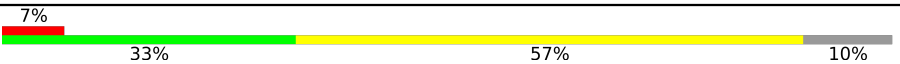
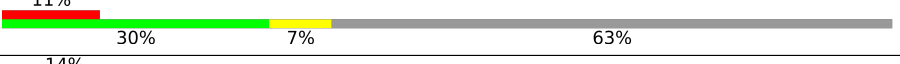
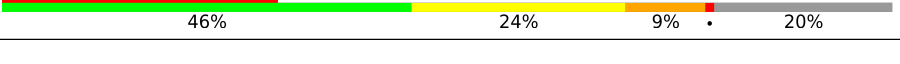
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 13997 ( 2.91 - 3.91 )                                    |

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     | 456    | <div> <div>36%</div> <div>32%</div> <div>59%</div> <div>5%</div> </div>  |
| 1   | C     | 456    | <div> <div>25%</div> <div>38%</div> <div>54%</div> <div>6%</div> </div>  |
| 1   | E     | 456    | <div> <div>42%</div> <div>48%</div> <div>9%</div> </div>                 |
| 2   | B     | 463    | <div> <div>39%</div> <div>38%</div> <div>52%</div> <div>10%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 2   | D     | 463    |  |
| 2   | F     | 463    |  |
| 3   | H     | 1733   |  |
| 4   | J     | 964    |  |
| 5   | K     | 491    |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 6   | ADP  | B     | 501 | -         | -        | X       | -                |
| 6   | ADP  | D     | 501 | -         | -        | X       | -                |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26995 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 RuvB-like 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 433      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3328  | 2095 | 568 | 651 | 14 |         |       |
| 1   | C     | 427      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3281  | 2065 | 561 | 641 | 14 |         |       |
| 1   | E     | 413      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3156  | 1988 | 538 | 618 | 12 |         |       |

- Molecule 2 is a protein called RuvB-like 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 418      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3209  | 2003 | 562 | 628 | 16 |         |       |
| 2   | D     | 419      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3224  | 2013 | 564 | 631 | 16 |         |       |
| 2   | F     | 419      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3232  | 2019 | 567 | 630 | 16 |         |       |

- Molecule 3 is a protein called TELO2-interacting protein 1 homolog,TELO2-interacting protein 1 homolog,TTI1.

| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 3   | H     | 644      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 3208  | 1922 | 644 | 642 |         |       |

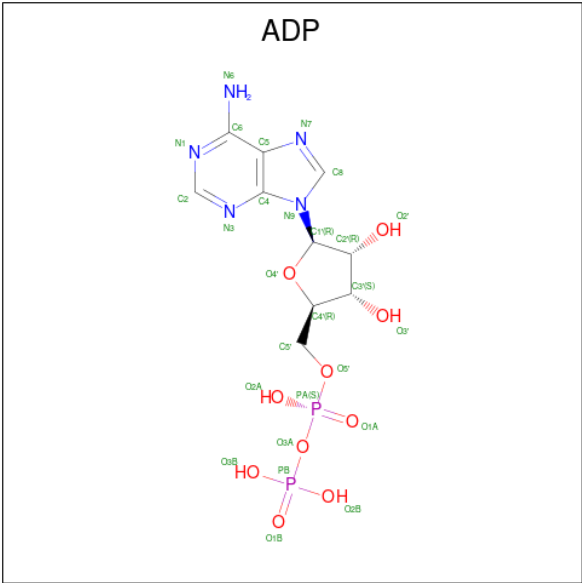
- Molecule 4 is a protein called TELO2-interacting protein 2,TELO2-interacting protein 2,TTI2.

| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 4   | J     | 456      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2273  | 1362 | 456 | 455 |         |       |

- Molecule 5 is a protein called Telomere length regulation protein TEL2 homolog.

| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 5   | K     | 394      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1949  | 1161 | 394 | 394 |         |       |

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

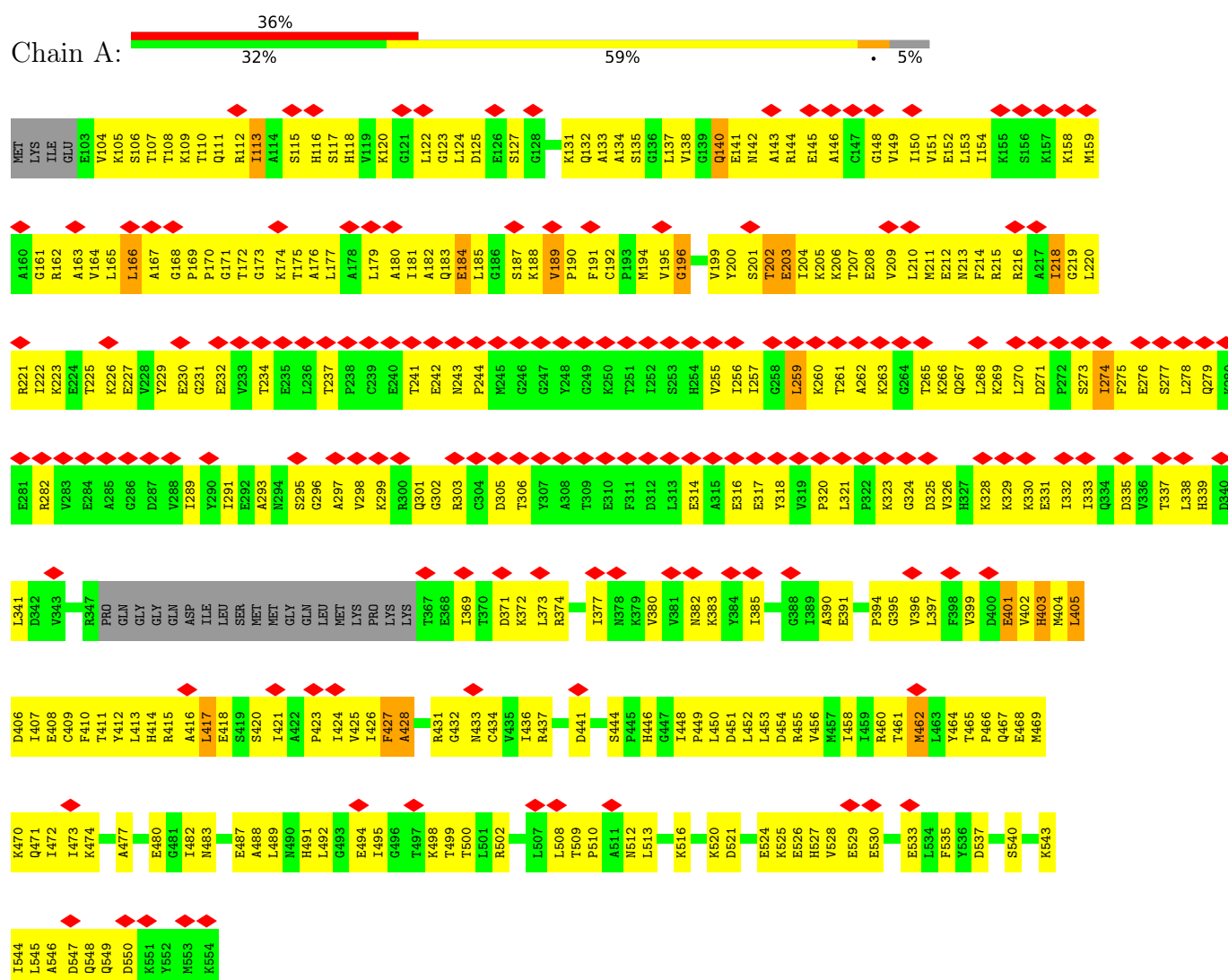


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 6   | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 6   | C     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 6   | D     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 6   | E     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 6   | F     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

### 3 Residue-property plots

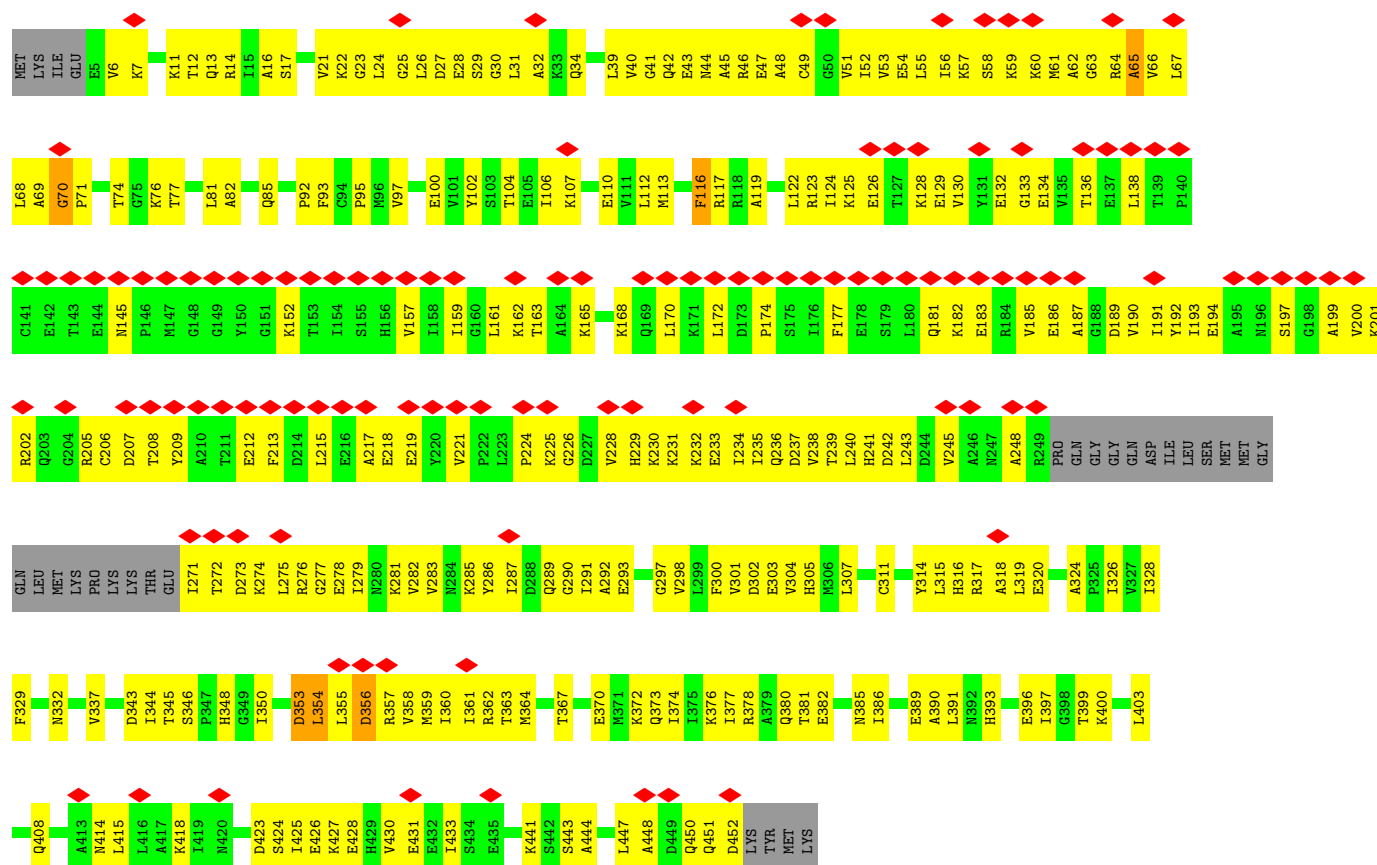
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: RuvB-like 1

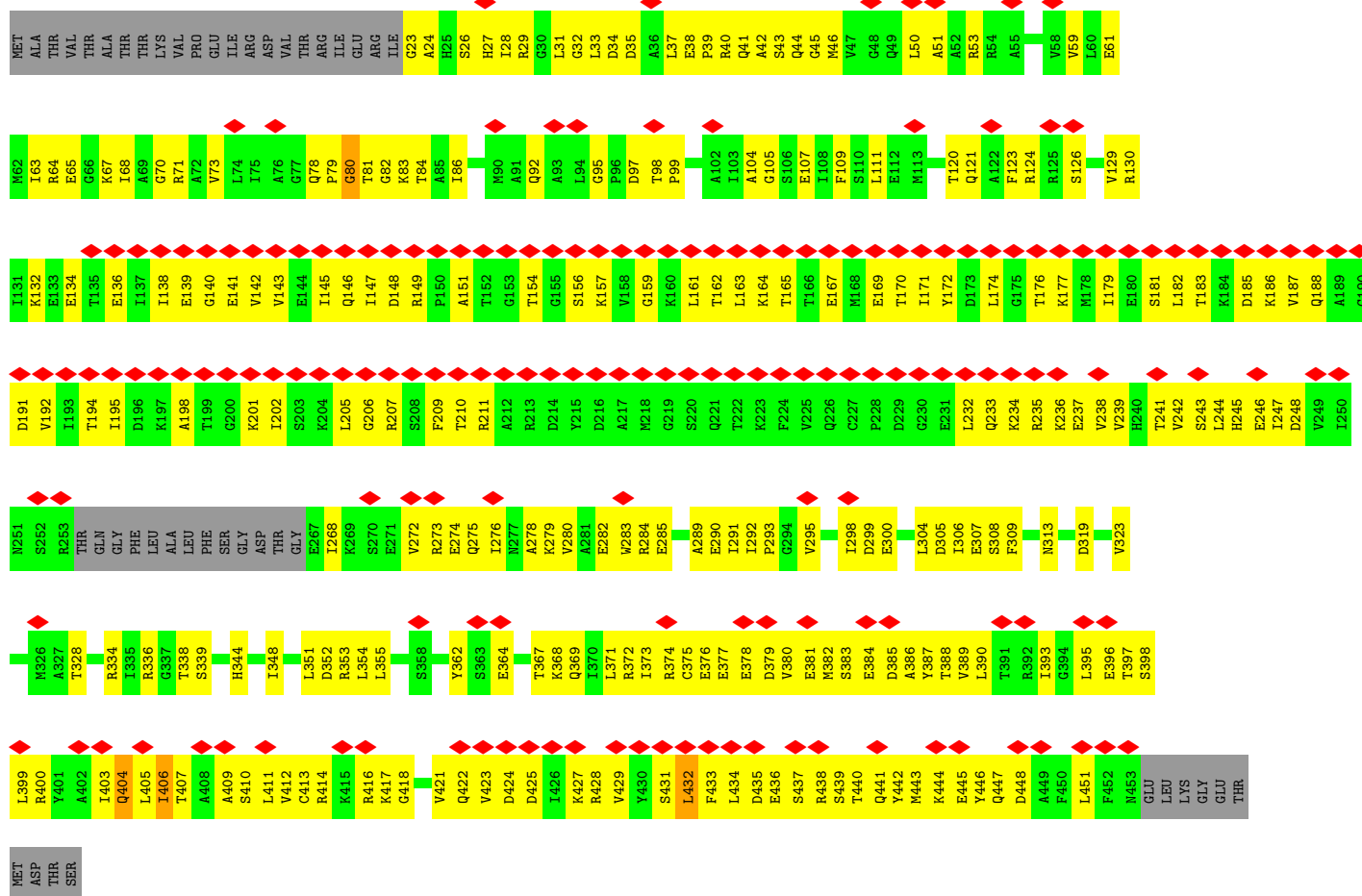


#### • Molecule 1: RuvB-like 1



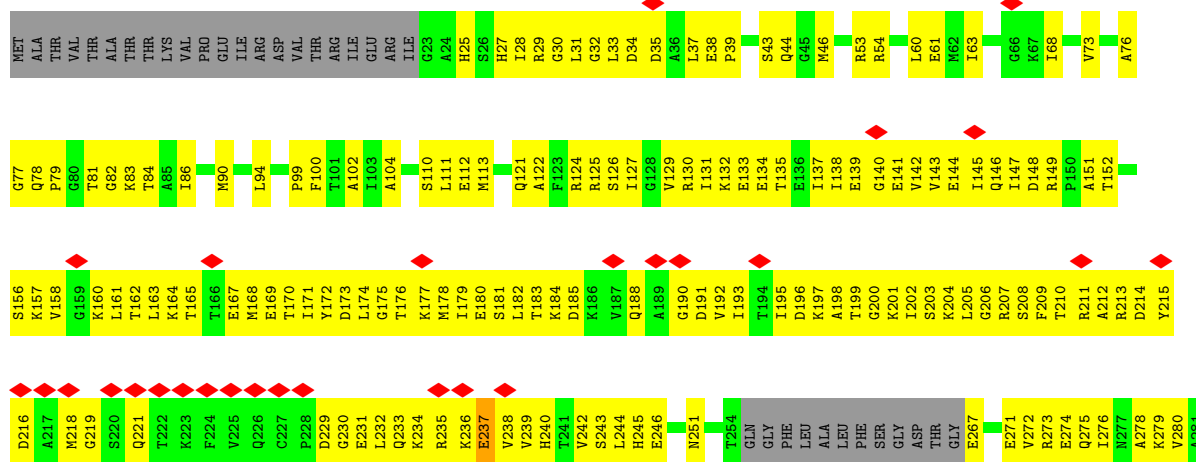


Chain B: 



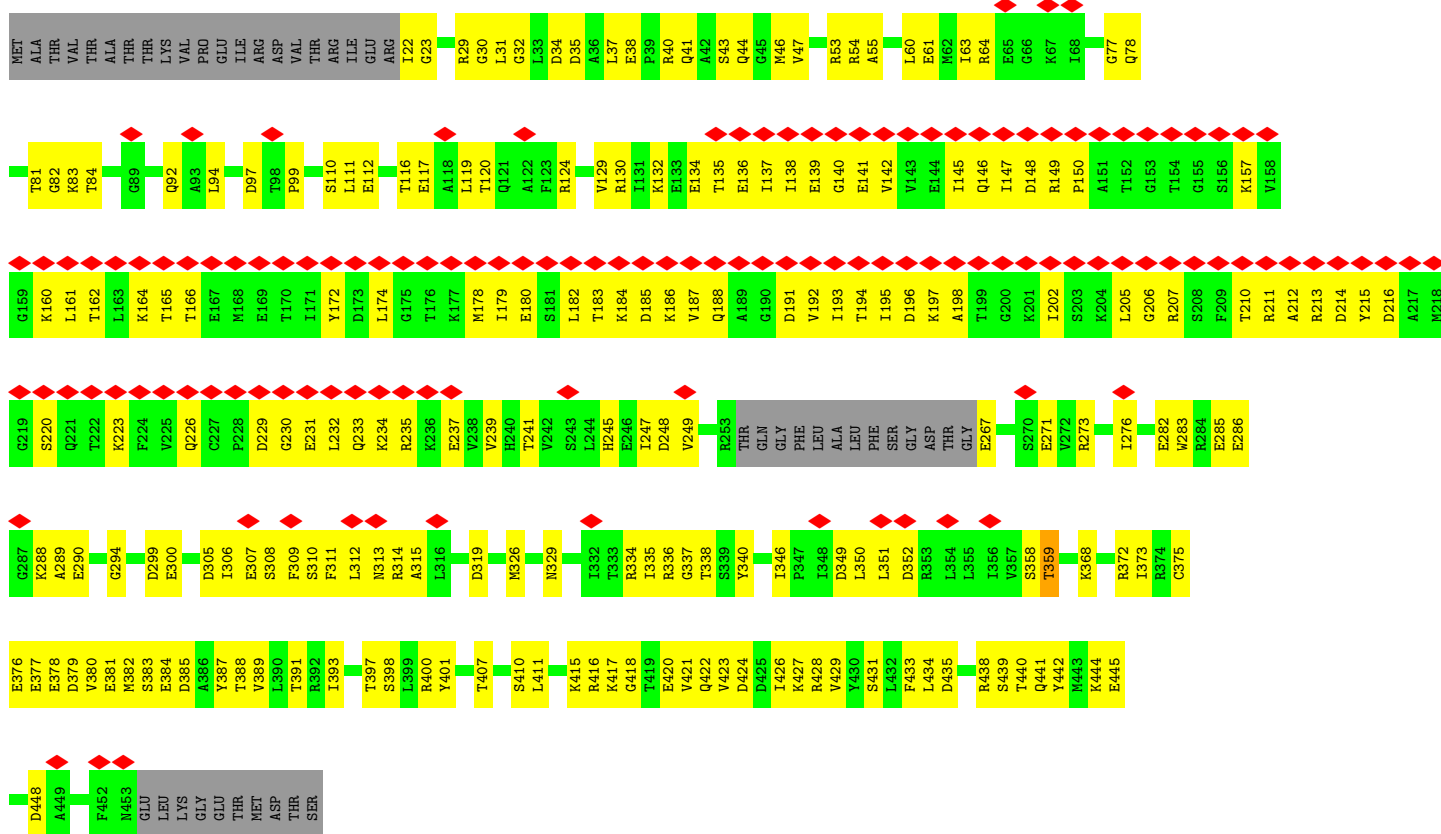
• Molecule 2: RuvB-like 2

Chain D: 

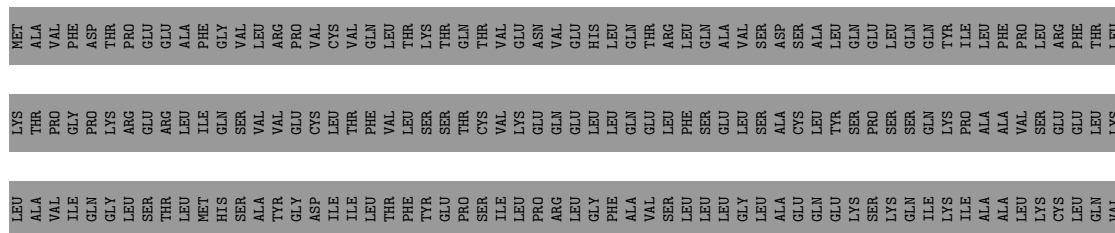




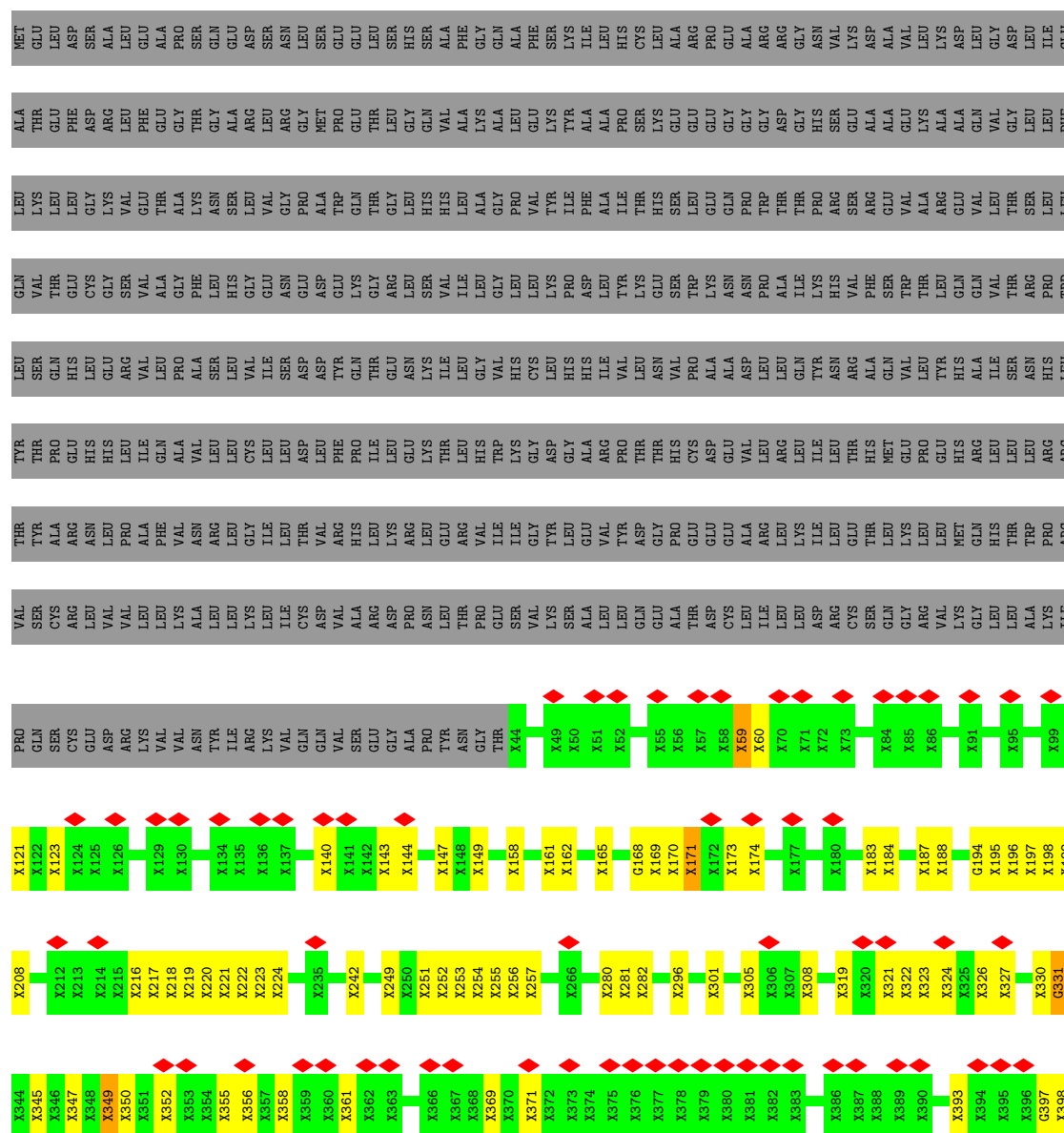
- Molecule 2: RuvB-like 2

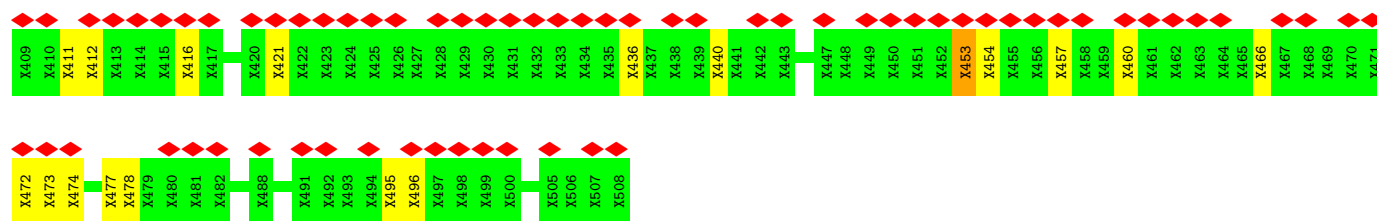


- Molecule 3: Telo2-interacting protein 1 homolog, Telo2-interacting protein 1 homolog, TTI1

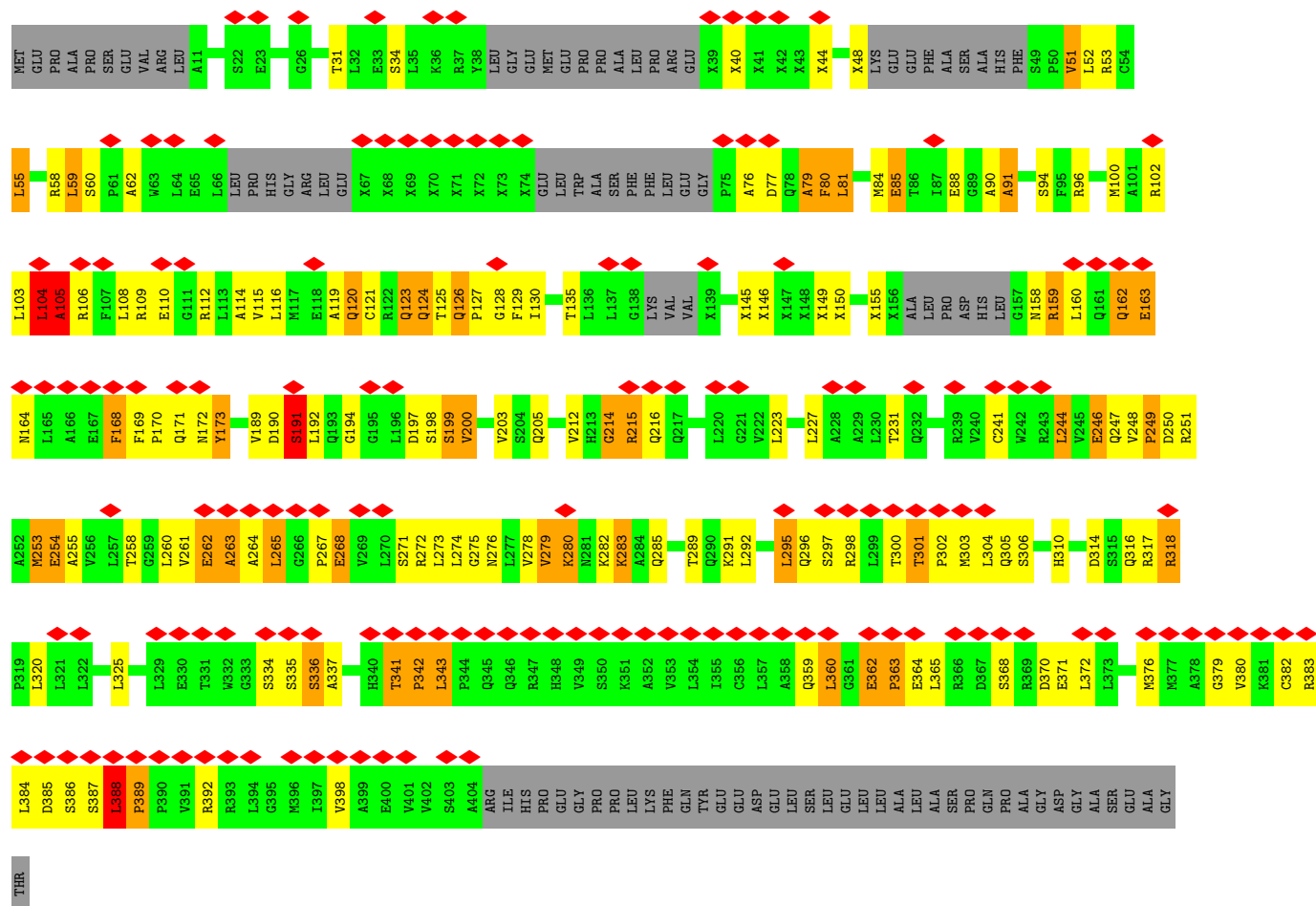








• Molecule 5: Telomere length regulation protein TEL2 homolog



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 267149                                  | 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 ( $e^-/\text{\AA}^2$ ) | 60.17                                   | Depositor |
| Minimum defocus (nm)                 | 1200                                    | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | 130000                                  | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.054                                   | Depositor |
| Minimum map value                    | -0.019                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.003                                   | Depositor |
| Recommended contour level            | 0.0106                                  | Depositor |
| Map size (Å)                         | 299.6, 299.6, 299.6                     | wwPDB     |
| Map dimensions                       | 280, 280, 280                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.07, 1.07, 1.07                        | 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: ADP

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     | 0.46         | 0/3371          | 0.82        | 6/4548 (0.1%)    |
| 1   | C     | 0.43         | 0/3323          | 0.65        | 0/4483           |
| 1   | E     | 0.44         | 0/3195          | 0.56        | 1/4313 (0.0%)    |
| 2   | B     | 0.43         | 0/3244          | 0.63        | 0/4370           |
| 2   | D     | 0.44         | 0/3260          | 0.62        | 1/4391 (0.0%)    |
| 2   | F     | 0.45         | 1/3268 (0.0%)   | 0.55        | 0/4401           |
| 3   | H     | 1.02         | 0/18            | 1.23        | 0/12             |
| 4   | J     | 1.07         | 0/18            | 1.96        | 1/12 (8.3%)      |
| 5   | K     | 2.01         | 54/1766 (3.1%)  | 2.49        | 99/2453 (4.0%)   |
| All | All   | 0.72         | 55/21463 (0.3%) | 0.95        | 108/28983 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 10                  |
| 1   | C     | 0                   | 4                   |
| 1   | E     | 0                   | 1                   |
| 2   | B     | 0                   | 3                   |
| 2   | D     | 0                   | 1                   |
| 2   | F     | 0                   | 1                   |
| 3   | H     | 0                   | 12                  |
| 4   | J     | 0                   | 8                   |
| 5   | K     | 0                   | 7                   |
| All | All   | 0                   | 47                  |

All (55) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | K     | 268 | GLU  | C-O   | -9.58 | 1.13        | 1.24     |
| 5   | K     | 120 | GLN  | C-O   | -9.13 | 1.12        | 1.24     |
| 5   | K     | 380 | VAL  | CA-C  | -8.90 | 1.42        | 1.52     |
| 5   | K     | 280 | LYS  | C-O   | 8.56  | 1.35        | 1.23     |
| 5   | K     | 380 | VAL  | C-O   | -8.48 | 1.14        | 1.24     |
| 5   | K     | 215 | ARG  | CA-C  | 8.46  | 1.64        | 1.52     |
| 5   | K     | 376 | MET  | C-O   | -8.11 | 1.14        | 1.24     |
| 5   | K     | 116 | LEU  | C-O   | -7.96 | 1.14        | 1.24     |
| 5   | K     | 372 | LEU  | C-O   | -7.95 | 1.15        | 1.24     |
| 5   | K     | 112 | ARG  | C-O   | -7.88 | 1.15        | 1.24     |
| 5   | K     | 223 | LEU  | C-O   | -7.75 | 1.15        | 1.24     |
| 5   | K     | 280 | LYS  | N-CA  | 7.27  | 1.55        | 1.46     |
| 5   | K     | 55  | LEU  | C-O   | -6.97 | 1.15        | 1.24     |
| 5   | K     | 314 | ASP  | C-O   | -6.90 | 1.16        | 1.24     |
| 5   | K     | 109 | ARG  | C-O   | -6.85 | 1.15        | 1.24     |
| 5   | K     | 203 | VAL  | C-O   | -6.62 | 1.16        | 1.24     |
| 5   | K     | 227 | LEU  | CA-C  | -6.58 | 1.44        | 1.52     |
| 5   | K     | 314 | ASP  | CA-C  | -6.56 | 1.44        | 1.52     |
| 5   | K     | 241 | CYS  | C-O   | 6.53  | 1.31        | 1.24     |
| 5   | K     | 317 | ARG  | C-O   | 6.39  | 1.30        | 1.23     |
| 5   | K     | 306 | SER  | CA-C  | -6.35 | 1.44        | 1.52     |
| 5   | K     | 58  | ARG  | C-O   | -6.14 | 1.16        | 1.24     |
| 5   | K     | 200 | VAL  | C-O   | -6.03 | 1.17        | 1.24     |
| 5   | K     | 271 | SER  | C-O   | -6.00 | 1.16        | 1.24     |
| 5   | K     | 280 | LYS  | CA-C  | 5.82  | 1.60        | 1.52     |
| 5   | K     | 310 | HIS  | CA-C  | -5.82 | 1.45        | 1.52     |
| 5   | K     | 310 | HIS  | C-O   | -5.80 | 1.17        | 1.24     |
| 5   | K     | 80  | PHE  | C-O   | -5.75 | 1.16        | 1.24     |
| 5   | K     | 301 | THR  | C-O   | -5.74 | 1.16        | 1.24     |
| 5   | K     | 371 | GLU  | C-O   | -5.73 | 1.17        | 1.24     |
| 5   | K     | 258 | THR  | C-O   | -5.66 | 1.17        | 1.24     |
| 5   | K     | 265 | LEU  | C-O   | -5.64 | 1.19        | 1.24     |
| 5   | K     | 110 | GLU  | CA-C  | -5.52 | 1.46        | 1.52     |
| 5   | K     | 59  | LEU  | C-O   | -5.52 | 1.16        | 1.24     |
| 5   | K     | 303 | MET  | CA-C  | -5.50 | 1.45        | 1.52     |
| 5   | K     | 359 | GLN  | N-CA  | 5.44  | 1.52        | 1.45     |
| 5   | K     | 126 | GLN  | C-O   | -5.36 | 1.19        | 1.24     |
| 5   | K     | 231 | THR  | CA-C  | -5.31 | 1.46        | 1.52     |
| 5   | K     | 376 | MET  | CA-C  | -5.29 | 1.46        | 1.52     |
| 5   | K     | 123 | GLN  | C-O   | -5.28 | 1.17        | 1.24     |
| 2   | F     | 359 | THR  | C-N   | -5.23 | 1.25        | 1.33     |
| 5   | K     | 304 | LEU  | N-CA  | -5.21 | 1.40        | 1.46     |
| 5   | K     | 116 | LEU  | CA-C  | -5.20 | 1.46        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | K     | 274 | LEU  | C-O   | -5.18 | 1.17        | 1.24     |
| 5   | K     | 119 | ALA  | C-O   | -5.17 | 1.18        | 1.24     |
| 5   | K     | 372 | LEU  | CA-C  | -5.16 | 1.46        | 1.52     |
| 5   | K     | 363 | PRO  | C-O   | 5.15  | 1.30        | 1.24     |
| 5   | K     | 365 | LEU  | C-O   | -5.14 | 1.17        | 1.24     |
| 5   | K     | 384 | LEU  | CA-C  | -5.11 | 1.45        | 1.52     |
| 5   | K     | 126 | GLN  | N-CA  | -5.11 | 1.41        | 1.46     |
| 5   | K     | 51  | VAL  | C-O   | -5.11 | 1.18        | 1.24     |
| 5   | K     | 254 | GLU  | C-O   | -5.11 | 1.17        | 1.24     |
| 5   | K     | 115 | VAL  | C-O   | -5.07 | 1.18        | 1.24     |
| 5   | K     | 108 | LEU  | C-O   | -5.03 | 1.18        | 1.24     |
| 5   | K     | 215 | ARG  | N-CA  | 5.02  | 1.52        | 1.46     |

All (108) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 5   | K     | 318 | ARG  | CA-C-N | 27.46  | 154.17      | 119.84   |
| 5   | K     | 318 | ARG  | C-N-CA | 27.46  | 154.17      | 119.84   |
| 5   | K     | 273 | LEU  | N-CA-C | -17.84 | 91.22       | 111.03   |
| 5   | K     | 169 | PHE  | CA-C-N | 14.89  | 134.97      | 119.19   |
| 5   | K     | 169 | PHE  | C-N-CA | 14.89  | 134.97      | 119.19   |
| 5   | K     | 279 | VAL  | N-CA-C | 14.74  | 128.46      | 108.27   |
| 5   | K     | 121 | CYS  | N-CA-C | -13.67 | 95.85       | 111.03   |
| 5   | K     | 191 | SER  | N-CA-C | -12.70 | 83.75       | 110.80   |
| 5   | K     | 387 | SER  | O-C-N  | 11.73  | 134.29      | 122.09   |
| 5   | K     | 359 | GLN  | N-CA-C | 11.47  | 126.51      | 109.07   |
| 5   | K     | 362 | GLU  | CA-C-N | 10.69  | 133.20      | 119.84   |
| 5   | K     | 362 | GLU  | C-N-CA | 10.69  | 133.20      | 119.84   |
| 5   | K     | 85  | GLU  | N-CA-C | -10.42 | 99.88       | 111.14   |
| 5   | K     | 253 | MET  | N-CA-C | -10.36 | 99.68       | 110.97   |
| 5   | K     | 214 | GLY  | O-C-N  | -10.11 | 109.55      | 122.70   |
| 5   | K     | 317 | ARG  | N-CA-C | 9.97   | 123.19      | 109.54   |
| 5   | K     | 248 | VAL  | CA-C-N | 8.99   | 131.08      | 119.84   |
| 5   | K     | 248 | VAL  | C-N-CA | 8.99   | 131.08      | 119.84   |
| 5   | K     | 249 | PRO  | N-CA-C | -8.89  | 94.15       | 112.47   |
| 5   | K     | 316 | GLN  | N-CA-C | -8.89  | 101.54      | 111.14   |
| 5   | K     | 130 | ILE  | N-CA-C | -8.87  | 101.76      | 110.72   |
| 5   | K     | 168 | PHE  | N-CA-C | -8.55  | 97.84       | 110.23   |
| 5   | K     | 246 | GLU  | N-CA-C | 8.47   | 119.11      | 108.19   |
| 5   | K     | 199 | SER  | N-CA-C | -8.31  | 101.80      | 111.03   |
| 5   | K     | 162 | GLN  | O-C-N  | 8.24   | 130.85      | 122.12   |
| 5   | K     | 389 | PRO  | N-CA-C | -8.17  | 100.73      | 110.70   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | K     | 110 | GLU  | N-CA-C   | -8.14 | 102.09      | 110.97   |
| 5   | K     | 124 | GLN  | N-CA-C   | -8.11 | 101.72      | 111.69   |
| 5   | K     | 91  | ALA  | N-CA-C   | -8.11 | 102.13      | 110.97   |
| 5   | K     | 278 | VAL  | N-CA-C   | -8.10 | 92.49       | 109.34   |
| 5   | K     | 100 | MET  | N-CA-C   | -7.99 | 102.52      | 111.07   |
| 5   | K     | 300 | THR  | N-CA-C   | -7.92 | 102.59      | 111.14   |
| 5   | K     | 289 | THR  | N-CA-C   | -7.77 | 102.75      | 111.14   |
| 5   | K     | 320 | LEU  | N-CA-C   | -7.74 | 102.54      | 110.97   |
| 5   | K     | 60  | SER  | N-CA-C   | -7.65 | 102.10      | 112.35   |
| 5   | K     | 96  | ARG  | N-CA-C   | -7.59 | 102.95      | 111.07   |
| 5   | K     | 126 | GLN  | N-CA-C   | -7.52 | 102.48      | 113.16   |
| 5   | K     | 336 | SER  | N-CA-C   | -7.50 | 103.05      | 111.07   |
| 5   | K     | 279 | VAL  | O-C-N    | -7.42 | 114.50      | 123.03   |
| 5   | K     | 53  | ARG  | N-CA-C   | -7.37 | 103.19      | 111.07   |
| 5   | K     | 267 | PRO  | N-CA-C   | -7.35 | 102.96      | 113.47   |
| 5   | K     | 295 | LEU  | CA-C-N   | 7.26  | 134.76      | 121.70   |
| 5   | K     | 295 | LEU  | C-N-CA   | 7.26  | 134.76      | 121.70   |
| 5   | K     | 280 | LYS  | CA-C-O   | 7.13  | 127.30      | 119.24   |
| 5   | K     | 343 | LEU  | CA-C-N   | 7.10  | 126.72      | 119.19   |
| 5   | K     | 343 | LEU  | C-N-CA   | 7.10  | 126.72      | 119.19   |
| 5   | K     | 282 | LYS  | N-CA-C   | 7.08  | 125.88      | 110.80   |
| 5   | K     | 171 | GLN  | N-CA-C   | -7.05 | 103.29      | 110.97   |
| 5   | K     | 205 | GLN  | N-CA-C   | -6.99 | 103.35      | 110.97   |
| 5   | K     | 265 | LEU  | N-CA-C   | 6.96  | 119.84      | 108.08   |
| 1   | A     | 166 | LEU  | CA-CB-CG | 6.94  | 140.58      | 116.30   |
| 5   | K     | 84  | MET  | N-CA-C   | -6.89 | 103.55      | 112.23   |
| 5   | K     | 262 | GLU  | N-CA-C   | -6.82 | 103.53      | 110.97   |
| 5   | K     | 260 | LEU  | N-CA-C   | -6.81 | 103.79      | 111.14   |
| 5   | K     | 173 | TYR  | N-CA-C   | -6.73 | 103.19      | 111.33   |
| 5   | K     | 102 | ARG  | N-CA-C   | 6.72  | 121.08      | 112.34   |
| 5   | K     | 79  | ALA  | N-CA-C   | -6.69 | 103.80      | 112.23   |
| 5   | K     | 388 | LEU  | N-CA-C   | -6.66 | 95.09       | 109.81   |
| 5   | K     | 125 | THR  | O-C-N    | 6.56  | 128.85      | 122.03   |
| 5   | K     | 384 | LEU  | O-C-N    | 6.45  | 131.08      | 122.43   |
| 5   | K     | 114 | ALA  | N-CA-C   | -6.45 | 103.94      | 110.97   |
| 5   | K     | 60  | SER  | CA-C-N   | -6.39 | 112.25      | 119.28   |
| 5   | K     | 60  | SER  | C-N-CA   | -6.39 | 112.25      | 119.28   |
| 5   | K     | 104 | LEU  | O-C-N    | -6.26 | 114.27      | 122.59   |
| 5   | K     | 159 | ARG  | N-CA-C   | -6.25 | 104.39      | 111.14   |
| 4   | J     | 331 | GLY  | N-CA-C   | -6.16 | 95.43       | 113.30   |
| 5   | K     | 380 | VAL  | CA-C-O   | -6.15 | 115.02      | 121.41   |
| 5   | K     | 265 | LEU  | CB-CA-C  | -6.14 | 109.50      | 116.63   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | K     | 380 | VAL  | CB-CA-C | -6.13 | 103.86      | 111.70   |
| 1   | A     | 403 | HIS  | N-CA-C  | 6.11  | 120.44      | 111.34   |
| 5   | K     | 81  | LEU  | N-CA-C  | -6.03 | 104.63      | 112.23   |
| 5   | K     | 105 | ALA  | N-CA-C  | 6.01  | 123.60      | 110.80   |
| 5   | K     | 291 | LYS  | N-CA-C  | -5.94 | 104.71      | 111.07   |
| 5   | K     | 119 | ALA  | N-CA-C  | -5.92 | 104.74      | 111.07   |
| 5   | K     | 283 | LYS  | N-CA-C  | 5.87  | 123.30      | 110.80   |
| 5   | K     | 129 | PHE  | N-CA-C  | -5.86 | 104.85      | 112.23   |
| 5   | K     | 325 | LEU  | N-CA-C  | -5.81 | 104.85      | 111.07   |
| 5   | K     | 303 | MET  | N-CA-C  | -5.79 | 98.47       | 110.80   |
| 5   | K     | 384 | LEU  | N-CA-C  | -5.74 | 105.53      | 112.54   |
| 5   | K     | 379 | GLY  | CA-C-N  | 5.71  | 128.25      | 120.77   |
| 5   | K     | 379 | GLY  | C-N-CA  | 5.71  | 128.25      | 120.77   |
| 5   | K     | 388 | LEU  | CA-C-N  | 5.68  | 126.23      | 120.38   |
| 5   | K     | 388 | LEU  | C-N-CA  | 5.68  | 126.23      | 120.38   |
| 5   | K     | 59  | LEU  | N-CA-C  | -5.66 | 105.87      | 112.89   |
| 1   | A     | 203 | GLU  | N-CA-C  | 5.51  | 122.53      | 110.80   |
| 1   | A     | 145 | GLU  | N-CA-C  | 5.49  | 117.13      | 111.03   |
| 5   | K     | 115 | VAL  | CA-C-N  | 5.46  | 128.38      | 120.79   |
| 5   | K     | 115 | VAL  | C-N-CA  | 5.46  | 128.38      | 120.79   |
| 5   | K     | 368 | SER  | O-C-N   | 5.44  | 129.72      | 122.43   |
| 5   | K     | 380 | VAL  | N-CA-CB | 5.42  | 116.31      | 110.62   |
| 5   | K     | 380 | VAL  | N-CA-C  | -5.40 | 104.61      | 110.23   |
| 5   | K     | 370 | ASP  | N-CA-C  | -5.38 | 105.11      | 110.97   |
| 5   | K     | 255 | ALA  | N-CA-C  | -5.36 | 105.33      | 111.07   |
| 5   | K     | 251 | ARG  | N-CA-C  | -5.32 | 105.18      | 110.97   |
| 1   | A     | 401 | GLU  | N-CA-C  | 5.30  | 117.11      | 110.91   |
| 5   | K     | 212 | VAL  | CB-CA-C | -5.26 | 104.97      | 111.70   |
| 5   | K     | 274 | LEU  | CA-C-N  | 5.19  | 126.88      | 120.34   |
| 5   | K     | 274 | LEU  | C-N-CA  | 5.19  | 126.88      | 120.34   |
| 5   | K     | 276 | ASN  | N-CA-C  | -5.18 | 105.71      | 112.23   |
| 5   | K     | 172 | ASN  | O-C-N   | 5.18  | 128.28      | 122.22   |
| 5   | K     | 125 | THR  | N-CA-C  | -5.15 | 105.35      | 110.97   |
| 1   | A     | 196 | GLY  | N-CA-C  | 5.12  | 118.62      | 111.19   |
| 5   | K     | 215 | ARG  | CA-C-O  | 5.11  | 127.81      | 120.51   |
| 2   | D     | 429 | VAL  | N-CA-C  | -5.10 | 106.94      | 112.80   |
| 1   | E     | 88  | GLY  | N-CA-C  | 5.08  | 118.37      | 111.72   |
| 5   | K     | 227 | LEU  | O-C-N   | 5.05  | 127.48      | 122.08   |
| 5   | K     | 215 | ARG  | N-CA-C  | 5.03  | 121.52      | 110.80   |
| 5   | K     | 398 | VAL  | CB-CA-C | -5.03 | 105.44      | 111.88   |

There are no chirality outliers.

All (47) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 140 | GLN  | Peptide   |
| 1   | A     | 184 | GLU  | Peptide   |
| 1   | A     | 187 | SER  | Peptide   |
| 1   | A     | 189 | VAL  | Peptide   |
| 1   | A     | 202 | THR  | Peptide   |
| 1   | A     | 259 | LEU  | Peptide   |
| 1   | A     | 274 | ILE  | Peptide   |
| 1   | A     | 417 | LEU  | Peptide   |
| 1   | A     | 427 | PHE  | Peptide   |
| 1   | A     | 462 | MET  | Peptide   |
| 2   | B     | 404 | GLN  | Peptide   |
| 2   | B     | 406 | ILE  | Peptide   |
| 2   | B     | 432 | LEU  | Peptide   |
| 1   | C     | 354 | LEU  | Peptide   |
| 1   | C     | 356 | ASP  | Peptide   |
| 1   | C     | 65  | ALA  | Peptide   |
| 1   | C     | 70  | GLY  | Peptide   |
| 2   | D     | 237 | GLU  | Peptide   |
| 1   | E     | 214 | ASP  | Peptide   |
| 2   | F     | 307 | GLU  | Peptide   |
| 3   | H     | 103 | UNK  | Mainchain |
| 3   | H     | 177 | UNK  | Peptide   |
| 3   | H     | 220 | UNK  | Mainchain |
| 3   | H     | 433 | UNK  | Mainchain |
| 3   | H     | 475 | UNK  | Mainchain |
| 3   | H     | 497 | UNK  | Mainchain |
| 3   | H     | 540 | UNK  | Mainchain |
| 3   | H     | 556 | UNK  | Peptide   |
| 3   | H     | 582 | UNK  | Mainchain |
| 3   | H     | 600 | UNK  | Peptide   |
| 3   | H     | 84  | UNK  | Mainchain |
| 3   | H     | 98  | UNK  | Mainchain |
| 4   | J     | 171 | UNK  | Peptide   |
| 4   | J     | 242 | UNK  | Peptide   |
| 4   | J     | 305 | UNK  | Mainchain |
| 4   | J     | 349 | UNK  | Peptide   |
| 4   | J     | 421 | UNK  | Peptide   |
| 4   | J     | 453 | UNK  | Peptide   |
| 4   | J     | 473 | UNK  | Mainchain |
| 4   | J     | 59  | UNK  | Mainchain |
| 5   | K     | 104 | LEU  | Mainchain |
| 5   | K     | 168 | PHE  | Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 5   | K     | 214 | GLY  | Mainchain |
| 5   | K     | 247 | GLN  | Mainchain |
| 5   | K     | 263 | ALA  | Mainchain |
| 5   | K     | 279 | VAL  | Mainchain |
| 5   | K     | 360 | LEU  | Peptide   |

## 5.2 Too-close contacts [i](#)

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     | 3328  | 0        | 3405     | 473     | 0            |
| 1   | C     | 3281  | 0        | 3363     | 289     | 0            |
| 1   | E     | 3156  | 0        | 3214     | 230     | 0            |
| 2   | B     | 3209  | 0        | 3254     | 368     | 0            |
| 2   | D     | 3224  | 0        | 3270     | 378     | 0            |
| 2   | F     | 3232  | 0        | 3286     | 202     | 0            |
| 3   | H     | 3208  | 0        | 680      | 117     | 0            |
| 4   | J     | 2273  | 0        | 495      | 91      | 0            |
| 5   | K     | 1949  | 0        | 858      | 94      | 0            |
| 6   | B     | 27    | 0        | 12       | 13      | 0            |
| 6   | C     | 27    | 0        | 12       | 0       | 0            |
| 6   | D     | 27    | 0        | 11       | 21      | 0            |
| 6   | E     | 27    | 0        | 12       | 5       | 0            |
| 6   | F     | 27    | 0        | 12       | 6       | 0            |
| All | All   | 26995 | 0        | 21884    | 2066    | 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 42.

All (2066) 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) |
|----------------|----------------|--------------------------|-------------------|
| 5:K:250:ASP:HA | 5:K:253:MET:CB | 1.27                     | 1.57              |
| 5:K:124:GLN:HA | 5:K:127:PRO:CB | 1.32                     | 1.56              |
| 4:J:416:UNK:HA | 4:J:466:UNK:CB | 1.36                     | 1.54              |
| 5:K:302:PRO:CA | 5:K:305:GLN:CB | 1.86                     | 1.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:H:593:UNK:CB   | 3:H:631:UNK:CB   | 1.85                     | 1.51              |
| 4:J:416:UNK:CA   | 4:J:466:UNK:CB   | 1.95                     | 1.45              |
| 5:K:91:ALA:O     | 5:K:94:SER:CB    | 1.70                     | 1.40              |
| 4:J:416:UNK:CB   | 4:J:466:UNK:CB   | 1.97                     | 1.38              |
| 5:K:302:PRO:HA   | 5:K:305:GLN:CB   | 0.90                     | 1.38              |
| 5:K:124:GLN:CA   | 5:K:127:PRO:CB   | 2.02                     | 1.36              |
| 1:A:123:GLY:N    | 2:B:410:SER:HA   | 1.38                     | 1.36              |
| 3:H:91:UNK:CB    | 3:H:141:UNK:CB   | 2.04                     | 1.35              |
| 2:B:362:TYR:OH   | 6:B:501:ADP:N7   | 1.57                     | 1.33              |
| 2:D:201:LYS:HE3  | 4:J:281:UNK:O    | 1.27                     | 1.32              |
| 4:J:350:UNK:O    | 4:J:355:UNK:CB   | 1.80                     | 1.30              |
| 3:H:273:UNK:CB   | 3:H:302:UNK:CB   | 2.12                     | 1.28              |
| 5:K:250:ASP:CA   | 5:K:253:MET:CB   | 2.18                     | 1.21              |
| 5:K:261:VAL:O    | 5:K:264:ALA:HB3  | 1.39                     | 1.20              |
| 5:K:123:GLN:O    | 5:K:127:PRO:N    | 1.79                     | 1.16              |
| 1:A:138:VAL:HG23 | 2:B:433:PHE:HD2  | 0.97                     | 1.14              |
| 1:A:138:VAL:HG23 | 2:B:433:PHE:CD2  | 1.80                     | 1.14              |
| 1:A:134:ALA:HB1  | 2:B:412:VAL:HG12 | 1.32                     | 1.11              |
| 2:D:37:LEU:HD11  | 1:E:419:ILE:HG13 | 1.32                     | 1.11              |
| 1:C:314:TYR:HB2  | 2:D:111:LEU:HD13 | 1.21                     | 1.10              |
| 4:J:350:UNK:O    | 4:J:355:UNK:CA   | 2.00                     | 1.10              |
| 5:K:200:VAL:CB   | 5:K:244:LEU:CB   | 2.31                     | 1.08              |
| 3:H:125:UNK:CB   | 3:H:163:UNK:CA   | 2.30                     | 1.08              |
| 3:H:125:UNK:CB   | 3:H:163:UNK:HA   | 1.83                     | 1.07              |
| 3:H:125:UNK:CB   | 3:H:163:UNK:CB   | 2.32                     | 1.07              |
| 1:A:144:ARG:HD2  | 2:B:407:THR:HG22 | 1.33                     | 1.06              |
| 3:H:369:UNK:O    | 3:H:373:UNK:N    | 1.89                     | 1.06              |
| 1:A:131:LYS:HE3  | 2:B:413:CYS:HB3  | 1.35                     | 1.06              |
| 2:D:201:LYS:CE   | 4:J:281:UNK:O    | 2.03                     | 1.05              |
| 3:H:204:UNK:CB   | 5:K:336:SER:CB   | 2.34                     | 1.05              |
| 1:A:132:GLN:HB3  | 2:B:425:ASP:HB3  | 1.36                     | 1.05              |
| 4:J:393:UNK:HA   | 4:J:400:GLY:CA   | 1.78                     | 1.04              |
| 1:A:138:VAL:HB   | 2:B:433:PHE:H    | 0.87                     | 1.04              |
| 2:D:81:THR:HB    | 6:D:501:ADP:H4'  | 1.36                     | 1.04              |
| 1:A:138:VAL:HB   | 2:B:433:PHE:N    | 1.73                     | 1.03              |
| 1:A:134:ALA:HB1  | 2:B:412:VAL:CG1  | 1.87                     | 1.03              |
| 2:B:46:MET:SD    | 2:B:53:ARG:NH2   | 2.32                     | 1.03              |
| 4:J:301:UNK:CB   | 4:J:308:UNK:CB   | 2.36                     | 1.03              |
| 1:A:182:ALA:HA   | 1:A:185:LEU:HB2  | 1.40                     | 1.01              |
| 4:J:350:UNK:C    | 4:J:355:UNK:CB   | 2.39                     | 0.99              |
| 1:A:124:LEU:O    | 2:B:410:SER:OG   | 1.78                     | 0.99              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 4:J:319:UNK:O    | 4:J:323:UNK:CB  | 2.10                     | 0.99              |
| 4:J:280:UNK:O    | 4:J:282:UNK:N   | 1.96                     | 0.98              |
| 4:J:352:UNK:O    | 4:J:356:UNK:N   | 1.97                     | 0.98              |
| 4:J:319:UNK:O    | 4:J:323:UNK:N   | 1.97                     | 0.97              |
| 1:A:138:VAL:CG2  | 2:B:433:PHE:HD2 | 1.77                     | 0.97              |
| 3:H:593:UNK:CA   | 3:H:631:UNK:CB  | 2.43                     | 0.96              |
| 2:B:362:TYR:OH   | 6:B:501:ADP:C5  | 2.18                     | 0.96              |
| 1:A:109:LYS:N    | 1:A:427:PHE:O   | 1.99                     | 0.95              |
| 1:A:133:ALA:HB3  | 2:B:427:LYS:H   | 1.31                     | 0.95              |
| 1:A:108:THR:HA   | 1:A:427:PHE:HB2 | 1.48                     | 0.94              |
| 1:A:123:GLY:H    | 2:B:410:SER:HA  | 0.88                     | 0.94              |
| 1:A:133:ALA:HB1  | 2:B:429:VAL:H   | 1.33                     | 0.94              |
| 1:A:170:PRO:HA   | 1:A:446:HIS:HD2 | 1.33                     | 0.94              |
| 1:A:123:GLY:HA2  | 2:B:411:LEU:N   | 1.82                     | 0.94              |
| 3:H:616:UNK:HA   | 3:H:625:UNK:CB  | 1.98                     | 0.93              |
| 2:D:430:TYR:HA   | 2:D:433:PHE:HB2 | 1.50                     | 0.93              |
| 2:B:78:GLN:NE2   | 1:C:450:GLN:OE1 | 2.01                     | 0.93              |
| 1:A:133:ALA:O    | 2:B:427:LYS:HE3 | 1.70                     | 0.92              |
| 1:C:314:TYR:HB2  | 2:D:111:LEU:CD1 | 2.00                     | 0.92              |
| 4:J:220:UNK:O    | 4:J:224:UNK:N   | 2.02                     | 0.92              |
| 1:C:65:ALA:H     | 1:C:354:LEU:H   | 1.02                     | 0.92              |
| 1:A:131:LYS:HE3  | 2:B:413:CYS:CB  | 1.98                     | 0.91              |
| 1:A:123:GLY:CA   | 2:B:410:SER:HA  | 2.00                     | 0.91              |
| 1:A:275:PHE:H    | 1:A:296:GLY:H   | 1.14                     | 0.91              |
| 4:J:208:UNK:CB   | 4:J:216:UNK:CB  | 2.47                     | 0.91              |
| 5:K:334:SER:HA   | 5:K:337:ALA:HB3 | 1.53                     | 0.91              |
| 1:E:386:ILE:HD11 | 1:E:391:LEU:HG  | 1.51                     | 0.90              |
| 1:C:42:GLN:NE2   | 1:C:362:ARG:O   | 2.03                     | 0.90              |
| 1:A:104:VAL:HB   | 1:A:188:LYS:HB2 | 1.51                     | 0.90              |
| 1:A:204:ILE:N    | 2:F:308:SER:O   | 2.03                     | 0.90              |
| 2:D:81:THR:CB    | 6:D:501:ADP:H4' | 2.02                     | 0.90              |
| 5:K:189:VAL:O    | 5:K:191:SER:N   | 2.04                     | 0.90              |
| 1:A:124:LEU:N    | 2:B:410:SER:OG  | 2.05                     | 0.89              |
| 4:J:408:UNK:O    | 4:J:412:UNK:N   | 2.05                     | 0.89              |
| 2:D:434:LEU:HB2  | 2:D:438:ARG:HD2 | 1.54                     | 0.89              |
| 1:A:470:LYS:HA   | 1:A:474:LYS:HB2 | 1.52                     | 0.89              |
| 4:J:393:UNK:HA   | 4:J:400:GLY:HA3 | 1.54                     | 0.89              |
| 1:A:123:GLY:N    | 2:B:410:SER:CA  | 2.32                     | 0.89              |
| 1:A:116:HIS:O    | 1:A:462:MET:N   | 2.06                     | 0.89              |
| 1:A:162:ARG:HH22 | 1:A:418:GLU:HB3 | 1.36                     | 0.88              |
| 2:D:81:THR:O     | 6:D:501:ADP:O2' | 1.89                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:81:THR:HB    | 6:D:501:ADP:C4'  | 2.03                     | 0.88              |
| 5:K:40:UNK:CB    | 5:K:44:UNK:CB    | 2.52                     | 0.88              |
| 3:H:125:UNK:CA   | 3:H:163:UNK:CB   | 2.52                     | 0.88              |
| 1:C:74:THR:O     | 1:C:362:ARG:NE   | 2.07                     | 0.87              |
| 1:A:133:ALA:CB   | 2:B:428:ARG:H    | 1.87                     | 0.87              |
| 5:K:124:GLN:C    | 5:K:127:PRO:CB   | 2.47                     | 0.87              |
| 5:K:76:ALA:O     | 5:K:80:PHE:N     | 2.08                     | 0.87              |
| 2:D:400:ARG:HH22 | 6:D:501:ADP:H2   | 1.22                     | 0.87              |
| 1:A:202:THR:HG22 | 2:F:306:ILE:HG22 | 1.58                     | 0.86              |
| 1:A:222:ILE:HG13 | 1:A:390:ALA:HB2  | 1.57                     | 0.86              |
| 3:H:519:UNK:O    | 3:H:523:UNK:CB   | 2.23                     | 0.86              |
| 2:B:362:TYR:CZ   | 6:B:501:ADP:N7   | 2.43                     | 0.86              |
| 5:K:123:GLN:HA   | 5:K:126:GLN:CB   | 2.06                     | 0.85              |
| 5:K:77:ASP:O     | 5:K:81:LEU:N     | 2.09                     | 0.85              |
| 1:A:399:VAL:H    | 1:A:425:VAL:HG21 | 1.41                     | 0.85              |
| 4:J:168:GLY:O    | 4:J:171:UNK:N    | 2.09                     | 0.85              |
| 3:H:238:UNK:O    | 3:H:240:UNK:N    | 2.10                     | 0.85              |
| 1:C:65:ALA:N     | 1:C:354:LEU:H    | 1.73                     | 0.85              |
| 2:B:413:CYS:SG   | 2:B:414:ARG:NH1  | 2.50                     | 0.85              |
| 3:H:125:UNK:HA   | 3:H:163:UNK:CB   | 2.07                     | 0.85              |
| 5:K:302:PRO:HA   | 5:K:305:GLN:CA   | 2.05                     | 0.85              |
| 1:A:259:LEU:O    | 1:A:266:LYS:HB3  | 1.76                     | 0.84              |
| 2:D:137:ILE:N    | 2:D:206:GLY:O    | 2.08                     | 0.84              |
| 4:J:218:UNK:O    | 4:J:222:UNK:N    | 2.10                     | 0.84              |
| 1:A:144:ARG:CD   | 2:B:407:THR:HG22 | 2.07                     | 0.84              |
| 1:A:123:GLY:H    | 2:B:410:SER:CA   | 1.82                     | 0.84              |
| 5:K:301:THR:O    | 5:K:305:GLN:N    | 2.08                     | 0.84              |
| 1:E:40:VAL:H     | 6:E:501:ADP:HN62 | 1.22                     | 0.84              |
| 2:D:435:ASP:O    | 2:D:439:SER:N    | 2.11                     | 0.83              |
| 2:F:420:GLU:O    | 2:F:422:GLN:NE2  | 2.10                     | 0.83              |
| 2:B:374:ARG:NE   | 2:B:374:ARG:O    | 2.11                     | 0.82              |
| 1:A:396:VAL:HA   | 1:A:424:ILE:HB   | 1.60                     | 0.82              |
| 2:D:37:LEU:O     | 2:D:54:ARG:NH1   | 2.13                     | 0.82              |
| 3:H:261:UNK:HA   | 3:H:265:UNK:CB   | 2.10                     | 0.82              |
| 2:D:436:GLU:O    | 2:D:440:THR:N    | 2.12                     | 0.82              |
| 2:D:359:THR:H    | 6:D:501:ADP:PB   | 2.03                     | 0.82              |
| 5:K:262:GLU:O    | 5:K:265:LEU:N    | 2.14                     | 0.81              |
| 1:A:123:GLY:CA   | 2:B:411:LEU:N    | 2.44                     | 0.81              |
| 1:A:229:TYR:HB3  | 1:A:266:LYS:HG2  | 1.62                     | 0.81              |
| 2:B:148:ASP:HB2  | 2:B:182:LEU:HD13 | 1.63                     | 0.81              |
| 1:C:165:LYS:HD3  | 1:C:225:LYS:HB3  | 1.62                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:437:SER:O    | 2:D:442:TYR:N    | 2.13                     | 0.81              |
| 2:D:445:GLU:HA   | 2:D:448:ASP:HB2  | 1.63                     | 0.81              |
| 1:A:166:LEU:HD22 | 1:A:456:VAL:HB   | 1.63                     | 0.81              |
| 1:C:161:LEU:HD22 | 1:C:191:ILE:HD11 | 1.59                     | 0.81              |
| 1:A:133:ALA:HB1  | 2:B:429:VAL:N    | 1.95                     | 0.81              |
| 1:E:134:GLU:HB2  | 1:E:187:ALA:HA   | 1.63                     | 0.81              |
| 1:C:65:ALA:HB1   | 1:C:350:ILE:HG22 | 1.62                     | 0.80              |
| 1:A:125:ASP:OD1  | 2:B:414:ARG:NH2  | 2.14                     | 0.80              |
| 1:A:122:LEU:HB3  | 2:B:409:ALA:O    | 1.81                     | 0.80              |
| 1:A:395:GLY:O    | 1:A:424:ILE:N    | 2.14                     | 0.80              |
| 2:D:139:GLU:OE1  | 2:D:234:LYS:NZ   | 2.14                     | 0.80              |
| 1:A:203:GLU:HG3  | 2:F:311:PHE:H    | 1.46                     | 0.80              |
| 5:K:170:PRO:HA   | 5:K:173:TYR:CB   | 2.12                     | 0.80              |
| 1:A:138:VAL:CB   | 2:B:433:PHE:H    | 1.83                     | 0.80              |
| 1:A:158:LYS:HG2  | 1:A:159:MET:HG3  | 1.62                     | 0.80              |
| 2:B:441:GLN:HA   | 2:B:444:LYS:HB2  | 1.62                     | 0.80              |
| 3:H:494:UNK:C    | 3:H:496:UNK:N    | 2.43                     | 0.80              |
| 2:B:375:CYS:HB2  | 2:B:380:VAL:H    | 1.46                     | 0.79              |
| 2:D:441:GLN:O    | 2:D:445:GLU:N    | 2.14                     | 0.79              |
| 3:H:637:UNK:N    | 3:H:640:UNK:CB   | 2.45                     | 0.79              |
| 1:C:389:GLU:O    | 1:C:427:LYS:NZ   | 2.14                     | 0.79              |
| 2:B:375:CYS:O    | 2:B:379:ASP:N    | 2.13                     | 0.79              |
| 2:B:400:ARG:NH2  | 6:B:501:ADP:O3A  | 2.15                     | 0.79              |
| 1:C:69:ALA:HA    | 1:C:348:HIS:NE2  | 1.98                     | 0.79              |
| 5:K:261:VAL:O    | 5:K:264:ALA:CB   | 2.27                     | 0.79              |
| 2:F:286:GLU:HG3  | 2:F:288:LYS:H    | 1.47                     | 0.79              |
| 3:H:261:UNK:O    | 3:H:265:UNK:CB   | 2.31                     | 0.78              |
| 2:F:138:ILE:HG21 | 2:F:198:ALA:HB2  | 1.64                     | 0.78              |
| 5:K:123:GLN:O    | 5:K:127:PRO:CA   | 2.31                     | 0.78              |
| 1:C:125:LYS:HE2  | 1:C:235:ILE:HB   | 1.63                     | 0.78              |
| 1:A:105:LYS:HG3  | 1:A:107:THR:HG23 | 1.64                     | 0.78              |
| 1:C:190:VAL:HG23 | 1:C:206:CYS:HA   | 1.64                     | 0.78              |
| 2:D:359:THR:OG1  | 6:D:501:ADP:O3B  | 2.00                     | 0.78              |
| 1:A:123:GLY:HA2  | 2:B:410:SER:C    | 2.08                     | 0.78              |
| 1:C:373:GLN:HA   | 1:C:376:LYS:HB3  | 1.64                     | 0.78              |
| 3:H:593:UNK:CB   | 3:H:631:UNK:CA   | 2.61                     | 0.78              |
| 3:H:657:UNK:O    | 3:H:660:UNK:CB   | 2.31                     | 0.78              |
| 4:J:350:UNK:O    | 4:J:355:UNK:N    | 2.16                     | 0.78              |
| 2:B:78:GLN:HB2   | 2:B:79:PRO:HD3   | 1.63                     | 0.78              |
| 2:D:37:LEU:CD1   | 1:E:419:ILE:HG13 | 2.12                     | 0.78              |
| 1:A:142:ASN:HB3  | 2:B:400:ARG:HB3  | 1.63                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:212:GLU:O    | 1:A:216:ARG:N    | 2.17                     | 0.77              |
| 1:E:134:GLU:OE1  | 1:E:188:GLY:N    | 2.17                     | 0.77              |
| 3:H:368:UNK:O    | 3:H:372:UNK:N    | 2.17                     | 0.77              |
| 2:D:37:LEU:HG    | 1:E:419:ILE:HG21 | 1.66                     | 0.77              |
| 1:A:170:PRO:HA   | 1:A:446:HIS:CD2  | 2.17                     | 0.77              |
| 5:K:250:ASP:O    | 5:K:254:GLU:N    | 2.15                     | 0.77              |
| 2:D:129:VAL:H    | 2:D:242:VAL:HG13 | 1.49                     | 0.77              |
| 3:H:519:UNK:HA   | 3:H:522:UNK:CB   | 2.13                     | 0.77              |
| 4:J:161:UNK:O    | 4:J:165:UNK:N    | 2.17                     | 0.77              |
| 1:E:426:GLU:OE1  | 1:E:428:GLU:N    | 2.17                     | 0.77              |
| 1:A:138:VAL:H    | 2:B:433:PHE:HB2  | 1.50                     | 0.77              |
| 2:D:165:THR:HG23 | 2:D:167:GLU:H    | 1.48                     | 0.77              |
| 4:J:350:UNK:CB   | 4:J:355:UNK:CB   | 2.63                     | 0.77              |
| 3:H:159:UNK:O    | 3:H:164:UNK:CB   | 2.33                     | 0.77              |
| 2:B:80:GLY:HA2   | 2:B:83:LYS:HE2   | 1.68                     | 0.77              |
| 4:J:319:UNK:O    | 4:J:323:UNK:CA   | 2.33                     | 0.76              |
| 1:E:201:LYS:HD2  | 1:E:203:GLN:HB2  | 1.67                     | 0.76              |
| 2:D:197:LYS:HD2  | 2:D:199:THR:H    | 1.50                     | 0.76              |
| 2:B:23:GLY:HA2   | 2:B:404:GLN:HE22 | 1.48                     | 0.76              |
| 1:C:48:ALA:HB1   | 1:C:358:VAL:H    | 1.50                     | 0.76              |
| 2:B:437:SER:O    | 2:B:440:THR:OG1  | 2.01                     | 0.76              |
| 2:F:29:ARG:HA    | 2:F:92:GLN:HE21  | 1.51                     | 0.76              |
| 2:F:306:ILE:HG21 | 2:F:335:ILE:HG22 | 1.67                     | 0.76              |
| 1:A:116:HIS:O    | 1:A:461:THR:OG1  | 2.02                     | 0.76              |
| 5:K:91:ALA:C     | 5:K:94:SER:CB    | 2.59                     | 0.76              |
| 1:A:219:GLY:N    | 1:A:421:ILE:O    | 2.16                     | 0.75              |
| 1:A:138:VAL:HG11 | 2:B:432:LEU:H    | 1.49                     | 0.75              |
| 2:B:78:GLN:OE1   | 2:B:78:GLN:N     | 2.18                     | 0.75              |
| 2:D:132:LYS:HB3  | 2:D:237:GLU:HG2  | 1.68                     | 0.75              |
| 2:D:170:THR:HA   | 2:D:200:GLY:HA2  | 1.68                     | 0.75              |
| 1:E:136:THR:OG1  | 1:E:137:GLU:OE1  | 2.03                     | 0.75              |
| 1:C:117:ARG:HB2  | 1:C:240:LEU:HB2  | 1.69                     | 0.75              |
| 1:E:193:ILE:HB   | 1:E:200:VAL:HB   | 1.68                     | 0.75              |
| 5:K:189:VAL:O    | 5:K:191:SER:O    | 2.04                     | 0.75              |
| 4:J:168:GLY:O    | 4:J:169:UNK:C    | 2.35                     | 0.74              |
| 1:A:131:LYS:HG2  | 2:B:418:GLY:O    | 1.86                     | 0.74              |
| 1:A:397:LEU:HD23 | 1:A:423:PRO:HG3  | 1.67                     | 0.74              |
| 1:C:132:GLU:O    | 1:C:168:LYS:NZ   | 2.18                     | 0.74              |
| 1:A:162:ARG:C    | 1:A:414:HIS:HA   | 2.11                     | 0.74              |
| 1:C:76:LYS:HG2   | 1:C:362:ARG:HG3  | 1.69                     | 0.74              |
| 4:J:143:UNK:O    | 4:J:147:UNK:N    | 2.19                     | 0.74              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:B:372:ARG:NH1  | 2:B:381:GLU:OE2 | 2.20                     | 0.74              |
| 2:D:434:LEU:HD12 | 2:D:438:ARG:HB3 | 1.69                     | 0.74              |
| 2:F:60:LEU:HA    | 2:F:63:ILE:HD12 | 1.68                     | 0.74              |
| 1:A:131:LYS:CG   | 2:B:418:GLY:O   | 2.36                     | 0.74              |
| 1:C:205:ARG:H    | 1:C:218:GLU:HG2 | 1.53                     | 0.74              |
| 1:E:125:LYS:NZ   | 1:E:127:THR:OG1 | 2.20                     | 0.74              |
| 4:J:183:UNK:O    | 4:J:187:UNK:N   | 2.21                     | 0.74              |
| 1:A:303:ARG:NH1  | 1:A:318:TYR:OH  | 2.20                     | 0.74              |
| 1:A:273:SER:HA   | 1:A:297:ALA:HB3 | 1.69                     | 0.74              |
| 2:B:146:GLN:NE2  | 2:B:185:ASP:O   | 2.20                     | 0.74              |
| 1:E:183:GLU:OE2  | 1:E:205:ARG:NH1 | 2.21                     | 0.74              |
| 2:F:400:ARG:NH1  | 6:F:501:ADP:O3A | 2.21                     | 0.74              |
| 1:E:162:LYS:HA   | 1:E:166:GLY:O   | 1.88                     | 0.73              |
| 1:A:177:LEU:HD21 | 1:A:194:MET:HB2 | 1.69                     | 0.73              |
| 2:D:160:LYS:HG3  | 2:D:171:ILE:HB  | 1.70                     | 0.73              |
| 3:H:191:UNK:O    | 3:H:193:UNK:N   | 2.20                     | 0.73              |
| 2:F:38:GLU:OE2   | 2:F:54:ARG:NH1  | 2.21                     | 0.73              |
| 2:F:112:GLU:OE2  | 2:F:267:GLU:N   | 2.20                     | 0.73              |
| 3:H:541:UNK:O    | 3:H:544:UNK:CB  | 2.35                     | 0.73              |
| 1:A:144:ARG:HH11 | 2:B:407:THR:N   | 1.84                     | 0.73              |
| 3:H:349:UNK:CB   | 3:H:384:UNK:CB  | 2.66                     | 0.73              |
| 1:A:203:GLU:HG2  | 2:F:308:SER:O   | 1.89                     | 0.73              |
| 1:A:274:ILE:HB   | 1:A:295:SER:HA  | 1.69                     | 0.73              |
| 1:A:417:LEU:O    | 1:A:455:ARG:NH1 | 2.21                     | 0.73              |
| 2:F:82:GLY:N     | 6:F:501:ADP:O2B | 2.22                     | 0.73              |
| 1:C:34:GLN:OE1   | 1:C:46:ARG:NH2  | 2.19                     | 0.73              |
| 1:C:354:LEU:HD12 | 1:C:357:ARG:HE  | 1.54                     | 0.73              |
| 1:A:144:ARG:HD2  | 2:B:407:THR:CG2 | 2.16                     | 0.73              |
| 1:C:63:GLY:N     | 1:C:315:LEU:O   | 2.21                     | 0.73              |
| 3:H:273:UNK:CB   | 3:H:302:UNK:C   | 2.66                     | 0.73              |
| 1:E:130:VAL:O    | 1:E:229:HIS:HA  | 1.89                     | 0.72              |
| 2:D:440:THR:OG1  | 2:D:441:GLN:OE1 | 2.07                     | 0.72              |
| 1:E:213:PHE:HE1  | 1:E:216:GLU:HG2 | 1.54                     | 0.72              |
| 4:J:173:UNK:O    | 4:J:174:UNK:CB  | 2.37                     | 0.72              |
| 1:A:405:LEU:HD13 | 1:A:409:CYS:HB2 | 1.72                     | 0.72              |
| 1:C:343:ASP:OD2  | 2:D:334:ARG:NH1 | 2.22                     | 0.72              |
| 1:A:183:GLN:NE2  | 1:A:184:GLU:OE2 | 2.23                     | 0.72              |
| 2:B:440:THR:OG1  | 2:B:441:GLN:NE2 | 2.22                     | 0.72              |
| 4:J:184:UNK:O    | 4:J:188:UNK:CB  | 2.37                     | 0.72              |
| 2:D:400:ARG:NH2  | 6:D:501:ADP:H2  | 1.87                     | 0.72              |
| 1:E:285:LYS:O    | 1:E:289:GLN:NE2 | 2.22                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:51:VAL:O     | 1:C:55:LEU:HG    | 1.89                     | 0.72              |
| 2:D:139:GLU:OE2  | 2:D:208:SER:OG   | 2.08                     | 0.72              |
| 4:J:217:UNK:O    | 4:J:220:UNK:CB   | 2.37                     | 0.72              |
| 2:F:195:ILE:HD12 | 2:F:211:ARG:HG3  | 1.72                     | 0.72              |
| 1:A:165:LEU:HD11 | 1:A:410:PHE:HB3  | 1.72                     | 0.72              |
| 2:B:34:ASP:OD1   | 2:B:38:GLU:N     | 2.19                     | 0.72              |
| 1:C:74:THR:OG1   | 1:C:362:ARG:NH2  | 2.23                     | 0.72              |
| 2:D:445:GLU:O    | 2:D:449:ALA:N    | 2.22                     | 0.72              |
| 2:F:311:PHE:O    | 2:F:315:ALA:N    | 2.19                     | 0.72              |
| 4:J:393:UNK:HA   | 4:J:400:GLY:HA2  | 1.72                     | 0.72              |
| 1:A:452:LEU:HG   | 1:A:454:ASP:HB2  | 1.72                     | 0.71              |
| 2:F:61:GLU:OE2   | 2:F:64:ARG:NH2   | 2.22                     | 0.71              |
| 1:A:205:LYS:NZ   | 1:A:208:GLU:OE1  | 2.15                     | 0.71              |
| 5:K:91:ALA:O     | 5:K:94:SER:CA    | 2.36                     | 0.71              |
| 5:K:124:GLN:O    | 5:K:127:PRO:CB   | 2.38                     | 0.71              |
| 1:A:231:GLY:H    | 1:A:260:LYS:HA   | 1.55                     | 0.71              |
| 1:A:451:ASP:OD1  | 1:A:452:LEU:N    | 2.23                     | 0.71              |
| 1:C:302:ASP:OD1  | 1:C:303:GLU:N    | 2.23                     | 0.71              |
| 5:K:189:VAL:O    | 5:K:191:SER:C    | 2.33                     | 0.71              |
| 4:J:217:UNK:O    | 4:J:221:UNK:N    | 2.24                     | 0.71              |
| 2:D:129:VAL:O    | 2:D:130:ARG:NE   | 2.23                     | 0.71              |
| 2:D:165:THR:HB   | 2:D:198:ALA:HB3  | 1.72                     | 0.71              |
| 3:H:191:UNK:C    | 3:H:193:UNK:N    | 2.53                     | 0.71              |
| 1:A:133:ALA:HB1  | 2:B:428:ARG:H    | 1.54                     | 0.71              |
| 1:A:204:ILE:N    | 2:F:308:SER:HB2  | 2.04                     | 0.71              |
| 2:D:78:GLN:O     | 2:D:81:THR:OG1   | 2.09                     | 0.71              |
| 2:D:139:GLU:OE2  | 2:D:210:THR:OG1  | 2.07                     | 0.71              |
| 1:A:111:GLN:OE1  | 1:A:502:ARG:NE   | 2.24                     | 0.71              |
| 1:A:138:VAL:HG11 | 2:B:432:LEU:N    | 2.05                     | 0.71              |
| 1:C:303:GLU:OE2  | 1:C:305:HIS:NE2  | 2.23                     | 0.71              |
| 1:E:203:GLN:O    | 1:E:205:ARG:NH1  | 2.24                     | 0.71              |
| 1:E:277:GLY:O    | 1:E:281:LYS:NZ   | 2.24                     | 0.71              |
| 1:A:140:GLN:O    | 1:A:142:ASN:N    | 2.23                     | 0.71              |
| 1:A:277:SER:HB3  | 1:A:298:VAL:HA   | 1.73                     | 0.71              |
| 2:B:416:ARG:CZ   | 2:B:418:GLY:HA3  | 2.21                     | 0.71              |
| 2:D:426:ILE:O    | 2:D:430:TYR:N    | 2.24                     | 0.71              |
| 2:B:141:GLU:HG2  | 2:B:165:THR:HG23 | 1.72                     | 0.71              |
| 2:B:132:LYS:HG2  | 2:B:237:GLU:HB3  | 1.73                     | 0.70              |
| 1:E:163:THR:HG22 | 1:E:164:ALA:H    | 1.56                     | 0.70              |
| 1:A:260:LYS:HZ1  | 1:A:262:ALA:HA   | 1.55                     | 0.70              |
| 3:H:91:UNK:CA    | 3:H:141:UNK:CB   | 2.70                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:123:GLY:CA   | 2:B:410:SER:CA   | 2.68                     | 0.70              |
| 1:A:201:SER:HB2  | 2:F:309:PHE:HB2  | 1.72                     | 0.70              |
| 3:H:637:UNK:O    | 3:H:641:UNK:N    | 2.24                     | 0.70              |
| 1:A:170:PRO:HG3  | 1:A:433:ASN:HB2  | 1.74                     | 0.70              |
| 2:D:443:MET:HA   | 2:D:446:TYR:HB2  | 1.74                     | 0.70              |
| 1:E:110:GLU:OE1  | 1:E:110:GLU:N    | 2.20                     | 0.70              |
| 1:C:193:ILE:HG22 | 1:C:201:LYS:H    | 1.57                     | 0.70              |
| 2:D:271:GLU:OE1  | 2:D:271:GLU:N    | 2.23                     | 0.70              |
| 1:A:465:THR:HG22 | 1:A:468:GLU:HB2  | 1.72                     | 0.70              |
| 2:B:384:GLU:OE1  | 2:B:384:GLU:N    | 2.25                     | 0.70              |
| 1:C:367:THR:N    | 1:C:370:GLU:OE2  | 2.22                     | 0.70              |
| 2:D:131:ILE:H    | 2:D:239:VAL:HG12 | 1.56                     | 0.70              |
| 2:F:368:LYS:HG3  | 2:F:372:ARG:HH12 | 1.57                     | 0.70              |
| 1:E:156:HIS:HD2  | 1:E:173:ASP:HA   | 1.55                     | 0.70              |
| 1:A:123:GLY:HA2  | 2:B:410:SER:CA   | 2.22                     | 0.69              |
| 2:D:138:ILE:HG12 | 2:D:205:LEU:HA   | 1.72                     | 0.69              |
| 2:D:364:GLU:O    | 2:D:367:THR:OG1  | 2.10                     | 0.69              |
| 1:A:204:ILE:HG12 | 2:F:311:PHE:HB2  | 1.74                     | 0.69              |
| 1:A:301:GLN:NE2  | 1:A:305:ASP:OD2  | 2.21                     | 0.69              |
| 2:B:43:SER:O     | 2:B:46:MET:N     | 2.24                     | 0.69              |
| 2:D:206:GLY:HA2  | 2:D:235:ARG:HD3  | 1.75                     | 0.69              |
| 1:A:210:LEU:O    | 1:A:214:PHE:N    | 2.22                     | 0.69              |
| 2:B:31:LEU:HB3   | 2:B:33:LEU:HD23  | 1.73                     | 0.69              |
| 1:C:65:ALA:H     | 1:C:354:LEU:N    | 1.85                     | 0.69              |
| 4:J:407:UNK:O    | 4:J:411:UNK:N    | 2.25                     | 0.69              |
| 2:D:366:ASP:N    | 2:D:366:ASP:OD1  | 2.22                     | 0.69              |
| 3:H:273:UNK:CB   | 3:H:302:UNK:CA   | 2.71                     | 0.69              |
| 1:A:468:GLU:HG2  | 1:A:472:ILE:HG22 | 1.72                     | 0.69              |
| 2:B:307:GLU:HA   | 1:C:102:TYR:O    | 1.92                     | 0.69              |
| 2:D:60:LEU:HA    | 2:D:63:ILE:HD12  | 1.73                     | 0.69              |
| 1:A:144:ARG:HD2  | 2:B:407:THR:H    | 1.58                     | 0.69              |
| 1:A:263:LYS:HD3  | 1:A:324:GLY:H    | 1.58                     | 0.69              |
| 2:F:283:TRP:HB3  | 2:F:289:ALA:HB3  | 1.74                     | 0.69              |
| 2:F:197:LYS:HG3  | 2:F:205:LEU:HD22 | 1.73                     | 0.69              |
| 3:H:494:UNK:O    | 3:H:496:UNK:N    | 2.26                     | 0.69              |
| 1:A:141:GLU:OE2  | 1:A:144:ARG:NE   | 2.25                     | 0.69              |
| 4:J:347:UNK:HA   | 4:J:454:UNK:O    | 1.93                     | 0.69              |
| 1:C:304:VAL:HG11 | 1:C:329:PHE:HB3  | 1.76                     | 0.68              |
| 1:E:184:ARG:HG2  | 1:E:212:GLU:HB3  | 1.75                     | 0.68              |
| 4:J:252:UNK:O    | 4:J:255:UNK:N    | 2.26                     | 0.68              |
| 1:A:369:ILE:HG13 | 1:A:373:LEU:HD12 | 1.75                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:338:THR:HG23 | 2:F:340:TYR:H    | 1.56                     | 0.68              |
| 1:E:376:LYS:HD2  | 1:E:380:GLN:HE22 | 1.58                     | 0.68              |
| 2:D:177:LYS:HE2  | 2:D:205:LEU:HD22 | 1.74                     | 0.68              |
| 2:F:186:LYS:O    | 2:F:213:ARG:NH2  | 2.26                     | 0.68              |
| 5:K:382:CYS:O    | 5:K:385:ASP:CB   | 2.41                     | 0.68              |
| 1:A:133:ALA:HB3  | 2:B:428:ARG:H    | 1.58                     | 0.68              |
| 1:E:126:GLU:OE1  | 1:E:128:LYS:NZ   | 2.26                     | 0.68              |
| 1:E:367:THR:N    | 1:E:370:GLU:OE1  | 2.22                     | 0.68              |
| 1:C:71:PRO:HB3   | 1:C:362:ARG:HB3  | 1.75                     | 0.68              |
| 1:C:124:ILE:HA   | 1:C:292:ALA:HA   | 1.76                     | 0.68              |
| 1:C:286:TYR:HB3  | 1:C:291:ILE:HG12 | 1.76                     | 0.68              |
| 1:C:315:LEU:HB3  | 1:C:319:LEU:HD11 | 1.76                     | 0.68              |
| 2:D:204:LYS:HD3  | 2:D:205:LEU:H    | 1.59                     | 0.68              |
| 2:F:149:ARG:NH2  | 2:F:180:GLU:OE2  | 2.27                     | 0.68              |
| 2:F:220:SER:OG   | 2:F:223:LYS:O    | 2.11                     | 0.68              |
| 2:F:137:ILE:HG13 | 2:F:206:GLY:HA2  | 1.74                     | 0.68              |
| 3:H:242:UNK:O    | 3:H:245:UNK:CB   | 2.42                     | 0.68              |
| 3:H:444:UNK:O    | 3:H:448:UNK:N    | 2.26                     | 0.68              |
| 1:C:34:GLN:NE2   | 1:C:39:LEU:O     | 2.26                     | 0.68              |
| 2:D:174:LEU:HD12 | 2:D:203:SER:HB3  | 1.76                     | 0.68              |
| 2:D:430:TYR:CZ   | 2:D:434:LEU:HA   | 2.29                     | 0.68              |
| 3:H:353:UNK:HA   | 3:H:388:UNK:HA   | 1.75                     | 0.68              |
| 1:C:194:GLU:HB3  | 1:C:197:SER:HB2  | 1.74                     | 0.67              |
| 2:D:316:LEU:HD11 | 2:D:353:ARG:HH12 | 1.57                     | 0.67              |
| 2:D:416:ARG:NH2  | 2:D:424:ASP:OD2  | 2.27                     | 0.67              |
| 2:D:160:LYS:HA   | 2:D:171:ILE:HA   | 1.75                     | 0.67              |
| 2:D:438:ARG:HA   | 2:D:442:TYR:HB3  | 1.74                     | 0.67              |
| 1:C:190:VAL:HG11 | 1:C:224:PRO:HB2  | 1.75                     | 0.67              |
| 1:A:135:SER:H    | 2:B:412:VAL:HB   | 1.58                     | 0.67              |
| 1:A:372:LYS:H    | 1:A:372:LYS:HD2  | 1.58                     | 0.67              |
| 1:C:13:GLN:OE1   | 1:C:13:GLN:N     | 2.26                     | 0.67              |
| 1:A:132:GLN:HG2  | 2:B:425:ASP:N    | 2.09                     | 0.67              |
| 2:F:194:THR:N    | 2:F:212:ALA:O    | 2.27                     | 0.67              |
| 1:A:123:GLY:HA3  | 2:B:412:VAL:H    | 1.58                     | 0.67              |
| 5:K:91:ALA:O     | 5:K:94:SER:N     | 2.26                     | 0.67              |
| 2:D:77:GLY:HA2   | 6:D:501:ADP:O1B  | 1.95                     | 0.67              |
| 2:F:37:LEU:O     | 2:F:54:ARG:NH1   | 2.27                     | 0.67              |
| 1:A:397:LEU:HB3  | 1:A:423:PRO:HB2  | 1.77                     | 0.67              |
| 1:C:283:VAL:HA   | 1:C:286:TYR:HB2  | 1.75                     | 0.67              |
| 1:E:63:GLY:O     | 1:E:357:ARG:NH2  | 2.27                     | 0.67              |
| 1:E:89:SER:O     | 1:E:123:ARG:NH2  | 2.28                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:61:MET:HG3   | 1:C:319:LEU:HD12 | 1.77                     | 0.67              |
| 2:F:428:ARG:O    | 2:F:431:SER:OG   | 2.13                     | 0.67              |
| 1:A:221:ARG:HH22 | 1:A:391:GLU:HB3  | 1.60                     | 0.66              |
| 1:A:549:GLN:OE1  | 2:F:78:GLN:NE2   | 2.25                     | 0.66              |
| 2:F:149:ARG:HH12 | 2:F:179:ILE:HG23 | 1.59                     | 0.66              |
| 1:A:204:ILE:HD13 | 2:F:311:PHE:HD1  | 1.59                     | 0.66              |
| 1:A:205:LYS:HG2  | 1:A:206:LYS:H    | 1.60                     | 0.66              |
| 1:A:487:GLU:O    | 1:A:525:LYS:NZ   | 2.28                     | 0.66              |
| 2:B:27:HIS:O     | 2:B:29:ARG:NH1   | 2.28                     | 0.66              |
| 2:B:29:ARG:HA    | 2:B:92:GLN:HG3   | 1.78                     | 0.66              |
| 2:B:157:LYS:HZ3  | 2:B:174:LEU:HB3  | 1.60                     | 0.66              |
| 2:B:383:SER:O    | 2:B:386:ALA:N    | 2.24                     | 0.66              |
| 2:D:396:GLU:OE1  | 2:D:397:THR:OG1  | 2.13                     | 0.66              |
| 2:F:34:ASP:OD1   | 2:F:40:ARG:NH2   | 2.28                     | 0.66              |
| 2:D:146:GLN:HE22 | 2:D:163:LEU:HG   | 1.59                     | 0.66              |
| 1:E:122:LEU:HB3  | 1:E:238:VAL:O    | 1.95                     | 0.66              |
| 2:F:192:VAL:HB   | 2:F:214:ASP:HB3  | 1.77                     | 0.66              |
| 1:A:144:ARG:HG2  | 2:B:405:LEU:HA   | 1.77                     | 0.66              |
| 3:H:444:UNK:O    | 3:H:447:UNK:CB   | 2.43                     | 0.66              |
| 5:K:383:ARG:O    | 5:K:386:SER:CB   | 2.43                     | 0.66              |
| 1:A:134:ALA:HB1  | 2:B:412:VAL:HG11 | 1.75                     | 0.66              |
| 1:E:135:VAL:HA   | 1:E:159:ILE:HG23 | 1.78                     | 0.66              |
| 4:J:219:UNK:O    | 4:J:223:UNK:N    | 2.28                     | 0.66              |
| 1:A:289:ILE:HB   | 1:A:301:GLN:HG2  | 1.78                     | 0.66              |
| 2:B:375:CYS:O    | 2:B:378:GLU:N    | 2.27                     | 0.66              |
| 1:C:346:SER:OG   | 1:C:350:ILE:O    | 2.13                     | 0.66              |
| 1:A:431:ARG:NH1  | 1:A:432:GLY:O    | 2.29                     | 0.66              |
| 2:F:179:ILE:HA   | 2:F:182:LEU:HD12 | 1.77                     | 0.66              |
| 5:K:386:SER:O    | 5:K:389:PRO:CA   | 2.44                     | 0.66              |
| 1:A:132:GLN:HG2  | 2:B:425:ASP:C    | 2.21                     | 0.65              |
| 1:A:132:GLN:HE21 | 2:B:423:VAL:C    | 2.05                     | 0.65              |
| 1:A:201:SER:O    | 2:F:308:SER:N    | 2.27                     | 0.65              |
| 1:A:225:THR:HA   | 1:A:331:GLU:HA   | 1.76                     | 0.65              |
| 1:E:369:GLN:OE1  | 1:E:369:GLN:N    | 2.23                     | 0.65              |
| 1:A:138:VAL:N    | 2:B:433:PHE:HB2  | 2.11                     | 0.65              |
| 2:D:381:GLU:HB2  | 2:D:420:GLU:HA   | 1.77                     | 0.65              |
| 5:K:123:GLN:C    | 5:K:127:PRO:N    | 2.54                     | 0.65              |
| 5:K:383:ARG:O    | 5:K:386:SER:N    | 2.29                     | 0.65              |
| 1:A:123:GLY:CA   | 2:B:411:LEU:H    | 2.08                     | 0.65              |
| 1:A:138:VAL:C    | 2:B:433:PHE:HB2  | 2.21                     | 0.65              |
| 1:A:141:GLU:OE2  | 1:A:144:ARG:NH2  | 2.30                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:176:THR:HB   | 2:D:177:LYS:HD3  | 1.76                     | 0.65              |
| 1:E:97:VAL:N     | 1:E:100:GLU:OE2  | 2.23                     | 0.65              |
| 1:E:177:PHE:O    | 1:E:202:ARG:NH1  | 2.29                     | 0.65              |
| 1:E:210:ALA:HA   | 1:E:213:PHE:HB3  | 1.79                     | 0.65              |
| 1:E:321:SER:OG   | 1:E:322:SER:N    | 2.28                     | 0.65              |
| 3:H:369:UNK:O    | 3:H:373:UNK:CB   | 2.44                     | 0.65              |
| 1:A:132:GLN:HG3  | 2:B:425:ASP:O    | 1.97                     | 0.65              |
| 1:A:203:GLU:HG3  | 2:F:311:PHE:N    | 2.11                     | 0.65              |
| 1:C:65:ALA:O     | 1:C:354:LEU:N    | 2.29                     | 0.65              |
| 1:E:390:ALA:O    | 1:E:394:LEU:N    | 2.23                     | 0.65              |
| 1:A:123:GLY:HA3  | 2:B:412:VAL:N    | 2.12                     | 0.65              |
| 1:A:135:SER:H    | 2:B:412:VAL:CB   | 2.09                     | 0.65              |
| 1:A:524:GLU:H    | 1:A:527:HIS:CE1  | 2.15                     | 0.65              |
| 1:A:546:ALA:O    | 1:A:550:ASP:N    | 2.23                     | 0.65              |
| 1:A:204:ILE:HB   | 2:F:116:THR:HG22 | 1.77                     | 0.65              |
| 2:B:24:ALA:HB3   | 6:B:501:ADP:O2'  | 1.97                     | 0.65              |
| 2:D:76:ALA:HB3   | 2:D:358:SER:HB2  | 1.79                     | 0.65              |
| 2:F:136:GLU:HB2  | 2:F:235:ARG:HE   | 1.61                     | 0.65              |
| 1:E:130:VAL:HG22 | 1:E:232:LYS:HD3  | 1.78                     | 0.65              |
| 1:A:117:SER:HA   | 1:A:462:MET:HB2  | 1.79                     | 0.65              |
| 1:E:373:GLN:OE1  | 1:E:373:GLN:N    | 2.22                     | 0.65              |
| 3:H:573:UNK:O    | 3:H:575:UNK:N    | 2.29                     | 0.65              |
| 1:C:396:GLU:OE1  | 1:C:396:GLU:N    | 2.29                     | 0.64              |
| 2:D:34:ASP:OD1   | 2:D:38:GLU:N     | 2.26                     | 0.64              |
| 4:J:199:UNK:O    | 4:J:202:UNK:CB   | 2.44                     | 0.64              |
| 4:J:327:UNK:HA   | 4:J:331:GLY:H    | 1.62                     | 0.64              |
| 2:B:61:GLU:OE2   | 2:B:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:B:164:LYS:HA   | 2:B:169:GLU:HG2  | 1.80                     | 0.64              |
| 2:B:280:VAL:HA   | 2:B:283:TRP:HD1  | 1.61                     | 0.64              |
| 2:D:73:VAL:HG13  | 2:D:325:ILE:HG22 | 1.79                     | 0.64              |
| 2:D:130:ARG:HH21 | 2:D:242:VAL:HG21 | 1.61                     | 0.64              |
| 2:F:32:GLY:HA3   | 2:F:43:SER:OG    | 1.98                     | 0.64              |
| 1:A:132:GLN:CG   | 2:B:425:ASP:C    | 2.70                     | 0.64              |
| 1:A:227:GLU:OE1  | 1:A:229:TYR:OH   | 2.15                     | 0.64              |
| 2:D:442:TYR:O    | 2:D:446:TYR:N    | 2.30                     | 0.64              |
| 1:E:194:GLU:OE1  | 1:E:194:GLU:N    | 2.29                     | 0.64              |
| 4:J:301:UNK:CA   | 4:J:308:UNK:CB   | 2.75                     | 0.64              |
| 2:B:362:TYR:CE2  | 6:B:501:ADP:N7   | 2.66                     | 0.64              |
| 2:B:428:ARG:HD2  | 2:B:431:SER:OG   | 1.98                     | 0.64              |
| 2:D:25:HIS:NE2   | 2:D:84:THR:OG1   | 2.29                     | 0.64              |
| 1:E:33:LYS:O     | 1:E:46:ARG:NH1   | 2.30                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:399:VAL:HB   | 1:A:425:VAL:HG11 | 1.77                     | 0.64              |
| 1:E:192:TYR:O    | 1:E:232:LYS:NZ   | 2.31                     | 0.64              |
| 2:F:188:GLN:HG3  | 2:F:191:ASP:HB2  | 1.77                     | 0.64              |
| 2:D:129:VAL:HG12 | 2:D:291:ILE:HG22 | 1.78                     | 0.64              |
| 5:K:59:LEU:HA    | 5:K:62:ALA:HB3   | 1.78                     | 0.64              |
| 2:D:157:LYS:HE3  | 2:D:174:LEU:HD23 | 1.80                     | 0.64              |
| 5:K:250:ASP:C    | 5:K:253:MET:CB   | 2.69                     | 0.64              |
| 1:A:110:THR:OG1  | 1:A:502:ARG:NH2  | 2.30                     | 0.64              |
| 1:A:134:ALA:CB   | 2:B:412:VAL:CG1  | 2.70                     | 0.64              |
| 1:A:433:ASN:OD1  | 1:A:434:CYS:N    | 2.30                     | 0.64              |
| 1:A:374:ARG:HH12 | 1:A:415:ARG:HH12 | 1.46                     | 0.64              |
| 1:C:44:ASN:HB3   | 1:C:68:LEU:HD11  | 1.78                     | 0.64              |
| 3:H:261:UNK:CA   | 3:H:265:UNK:CB   | 2.75                     | 0.64              |
| 1:A:165:LEU:N    | 1:A:451:ASP:OD1  | 2.30                     | 0.64              |
| 1:C:67:LEU:CD2   | 2:D:440:THR:HG21 | 2.27                     | 0.64              |
| 5:K:123:GLN:O    | 5:K:127:PRO:CB   | 2.46                     | 0.64              |
| 2:B:351:LEU:HA   | 2:B:354:LEU:HD12 | 1.80                     | 0.63              |
| 2:B:435:ASP:O    | 2:B:439:SER:N    | 2.24                     | 0.63              |
| 1:C:23:GLY:HA2   | 1:C:82:ALA:HB1   | 1.81                     | 0.63              |
| 2:F:193:ILE:HD12 | 2:F:213:ARG:HH11 | 1.63                     | 0.63              |
| 3:H:593:UNK:N    | 3:H:631:UNK:CB   | 2.61                     | 0.63              |
| 2:B:285:GLU:N    | 2:B:285:GLU:OE1  | 2.28                     | 0.63              |
| 1:C:128:LYS:HB2  | 1:C:232:LYS:HG2  | 1.80                     | 0.63              |
| 3:H:471:UNK:C    | 3:H:473:UNK:N    | 2.59                     | 0.63              |
| 1:E:426:GLU:HG3  | 1:E:429:HIS:CE1  | 2.32                     | 0.63              |
| 2:F:110:SER:OG   | 2:F:111:LEU:N    | 2.31                     | 0.63              |
| 2:F:381:GLU:N    | 2:F:381:GLU:OE1  | 2.32                     | 0.63              |
| 4:J:398:UNK:HA   | 4:J:453:UNK:CB   | 2.28                     | 0.63              |
| 5:K:302:PRO:C    | 5:K:305:GLN:CB   | 2.69                     | 0.63              |
| 1:C:356:ASP:H    | 1:C:357:ARG:HD3  | 1.64                     | 0.63              |
| 1:C:358:VAL:HG12 | 1:C:359:MET:H    | 1.61                     | 0.63              |
| 2:B:82:GLY:O     | 2:B:86:ILE:N     | 2.23                     | 0.63              |
| 1:C:130:VAL:HG21 | 1:C:232:LYS:HB3  | 1.79                     | 0.63              |
| 2:B:40:ARG:HB2   | 2:B:46:MET:HE1   | 1.80                     | 0.63              |
| 2:B:448:ASP:HA   | 2:B:451:LEU:HB2  | 1.80                     | 0.63              |
| 3:H:308:UNK:CB   | 3:H:358:UNK:CB   | 2.77                     | 0.63              |
| 5:K:383:ARG:CB   | 5:K:392:ARG:CB   | 2.77                     | 0.63              |
| 1:A:138:VAL:H    | 2:B:433:PHE:CB   | 2.12                     | 0.63              |
| 1:A:544:ILE:O    | 1:A:548:GLN:NE2  | 2.32                     | 0.63              |
| 2:F:382:MET:HG2  | 2:F:421:VAL:HB   | 1.81                     | 0.63              |
| 1:A:487:GLU:OE1  | 1:A:487:GLU:N    | 2.25                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:359:THR:N    | 6:D:501:ADP:O3B  | 2.32                     | 0.62              |
| 5:K:261:VAL:O    | 5:K:268:GLU:CB   | 2.46                     | 0.62              |
| 1:A:138:VAL:O    | 2:B:433:PHE:HB2  | 1.99                     | 0.62              |
| 1:A:151:VAL:HA   | 1:A:154:ILE:HG12 | 1.80                     | 0.62              |
| 1:E:42:GLN:HE22  | 1:E:364:MET:H    | 1.47                     | 0.62              |
| 2:F:299:ASP:OD1  | 2:F:300:GLU:N    | 2.31                     | 0.62              |
| 1:A:110:THR:O    | 1:A:502:ARG:NH2  | 2.31                     | 0.62              |
| 2:B:438:ARG:NH1  | 2:B:441:GLN:HB2  | 2.15                     | 0.62              |
| 2:D:239:VAL:HG23 | 2:D:240:HIS:H    | 1.64                     | 0.62              |
| 2:F:441:GLN:NE2  | 2:F:445:GLU:OE2  | 2.32                     | 0.62              |
| 3:H:637:UNK:O    | 3:H:640:UNK:N    | 2.32                     | 0.62              |
| 1:A:382:ASN:HA   | 1:A:385:ILE:HD12 | 1.82                     | 0.62              |
| 1:C:194:GLU:HB2  | 1:C:199:ALA:HB3  | 1.81                     | 0.62              |
| 3:H:471:UNK:O    | 3:H:473:UNK:N    | 2.33                     | 0.62              |
| 5:K:135:THR:HA   | 5:K:198:SER:CB   | 2.29                     | 0.62              |
| 2:B:382:MET:HE1  | 2:B:421:VAL:HG22 | 1.82                     | 0.62              |
| 1:C:183:GLU:OE1  | 1:C:202:ARG:N    | 2.25                     | 0.62              |
| 2:D:77:GLY:HA3   | 2:D:83:LYS:HD2   | 1.82                     | 0.62              |
| 1:A:464:TYR:CD2  | 1:A:472:ILE:HG21 | 2.35                     | 0.62              |
| 3:H:637:UNK:C    | 3:H:640:UNK:N    | 2.62                     | 0.62              |
| 1:E:424:SER:OG   | 1:E:425:ILE:N    | 2.30                     | 0.62              |
| 2:B:393:ILE:HA   | 2:B:396:GLU:HB2  | 1.82                     | 0.62              |
| 1:C:27:ASP:N     | 1:C:31:LEU:O     | 2.32                     | 0.62              |
| 2:D:428:ARG:HH11 | 2:D:429:VAL:HA   | 1.63                     | 0.62              |
| 1:E:205:ARG:HE   | 1:E:218:GLU:HA   | 1.63                     | 0.62              |
| 1:A:132:GLN:CB   | 2:B:425:ASP:HB3  | 2.20                     | 0.62              |
| 1:A:275:PHE:O    | 1:A:279:GLN:N    | 2.30                     | 0.62              |
| 1:A:495:ILE:HG13 | 1:A:498:LYS:HD2  | 1.81                     | 0.62              |
| 1:E:192:TYR:HB3  | 1:E:203:GLN:HB3  | 1.82                     | 0.62              |
| 1:A:403:HIS:CD2  | 1:A:404:MET:HB2  | 2.35                     | 0.61              |
| 1:A:527:HIS:HA   | 1:A:530:GLU:OE1  | 1.99                     | 0.61              |
| 2:B:174:LEU:HD22 | 2:B:179:ILE:HD13 | 1.80                     | 0.61              |
| 1:C:110:GLU:OE1  | 1:C:110:GLU:N    | 2.22                     | 0.61              |
| 1:A:134:ALA:CA   | 2:B:412:VAL:HG11 | 2.30                     | 0.61              |
| 2:B:23:GLY:HA2   | 2:B:404:GLN:NE2  | 2.13                     | 0.61              |
| 2:D:134:GLU:HA   | 2:D:207:ARG:HD3  | 1.81                     | 0.61              |
| 2:D:197:LYS:CD   | 2:D:199:THR:H    | 2.13                     | 0.61              |
| 2:F:142:VAL:HG13 | 2:F:161:LEU:HD21 | 1.82                     | 0.61              |
| 1:C:71:PRO:HB3   | 1:C:362:ARG:CB   | 2.31                     | 0.61              |
| 2:D:177:LYS:HB2  | 2:D:205:LEU:HD21 | 1.83                     | 0.61              |
| 2:D:282:GLU:HA   | 2:D:285:GLU:HG2  | 1.81                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:128:LYS:HZ1  | 1:E:234:ILE:HB   | 1.65                     | 0.61              |
| 2:F:149:ARG:HG3  | 2:F:183:THR:HG21 | 1.81                     | 0.61              |
| 1:A:141:GLU:HG2  | 1:A:144:ARG:HB2  | 1.83                     | 0.61              |
| 1:A:203:GLU:CG   | 2:F:311:PHE:H    | 2.11                     | 0.61              |
| 1:A:397:LEU:O    | 1:A:425:VAL:HB   | 2.00                     | 0.61              |
| 2:D:400:ARG:NH1  | 6:D:501:ADP:N3   | 2.49                     | 0.61              |
| 4:J:280:UNK:C    | 4:J:282:UNK:N    | 2.63                     | 0.61              |
| 1:A:203:GLU:CD   | 2:F:312:LEU:H    | 2.09                     | 0.61              |
| 2:D:144:GLU:OE2  | 2:D:188:GLN:N    | 2.27                     | 0.61              |
| 5:K:302:PRO:N    | 5:K:305:GLN:CB   | 2.61                     | 0.61              |
| 1:E:207:ASP:HB3  | 1:E:223:LEU:HD22 | 1.81                     | 0.61              |
| 1:E:40:VAL:O     | 6:E:501:ADP:N6   | 2.34                     | 0.61              |
| 1:C:168:LYS:HB3  | 1:C:170:LEU:HD13 | 1.81                     | 0.61              |
| 2:D:138:ILE:CG1  | 2:D:205:LEU:HA   | 2.31                     | 0.61              |
| 1:E:213:PHE:CE1  | 1:E:216:GLU:HG2  | 2.36                     | 0.61              |
| 2:F:31:LEU:O     | 2:F:53:ARG:NH2   | 2.31                     | 0.61              |
| 1:A:176:ALA:HB2  | 1:A:456:VAL:HA   | 1.81                     | 0.60              |
| 1:A:234:THR:OG1  | 1:A:256:ILE:O    | 2.17                     | 0.60              |
| 1:A:325:ASP:HB3  | 1:A:328:LYS:HB3  | 1.82                     | 0.60              |
| 2:B:376:GLU:N    | 2:B:376:GLU:OE1  | 2.33                     | 0.60              |
| 1:C:316:HIS:O    | 1:C:320:GLU:N    | 2.25                     | 0.60              |
| 2:D:400:ARG:NH2  | 6:D:501:ADP:C2   | 2.68                     | 0.60              |
| 1:E:162:LYS:HG2  | 1:E:167:THR:HA   | 1.83                     | 0.60              |
| 1:A:138:VAL:CA   | 2:B:433:PHE:HB2  | 2.31                     | 0.60              |
| 2:D:284:ARG:NH1  | 2:D:285:GLU:OE2  | 2.33                     | 0.60              |
| 2:F:388:THR:O    | 2:F:391:THR:OG1  | 2.17                     | 0.60              |
| 1:A:122:LEU:HD11 | 1:A:144:ARG:CZ   | 2.32                     | 0.60              |
| 1:A:302:GLY:HA3  | 1:A:316:GLU:CD   | 2.26                     | 0.60              |
| 2:F:196:ASP:HA   | 2:F:205:LEU:HD13 | 1.83                     | 0.60              |
| 3:H:493:UNK:O    | 3:H:496:UNK:N    | 2.34                     | 0.60              |
| 4:J:251:UNK:O    | 4:J:254:UNK:CB   | 2.49                     | 0.60              |
| 2:D:201:LYS:NZ   | 4:J:281:UNK:O    | 2.34                     | 0.60              |
| 1:E:17:SER:O     | 1:E:378:ARG:NH1  | 2.34                     | 0.60              |
| 2:D:149:ARG:HD3  | 2:D:182:LEU:HB3  | 1.83                     | 0.60              |
| 1:A:533:GLU:OE1  | 1:A:533:GLU:N    | 2.33                     | 0.60              |
| 2:B:42:ALA:N     | 2:B:46:MET:HE3   | 2.16                     | 0.60              |
| 2:B:97:ASP:N     | 2:B:97:ASP:OD1   | 2.31                     | 0.60              |
| 2:B:121:GLN:OE1  | 2:B:245:HIS:NE2  | 2.34                     | 0.60              |
| 1:C:162:LYS:O    | 1:C:208:THR:OG1  | 2.16                     | 0.60              |
| 1:A:146:ALA:HB3  | 1:A:454:ASP:HA   | 1.84                     | 0.60              |
| 2:D:374:ARG:NH2  | 2:D:378:GLU:OE2  | 2.35                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:183:GLN:HG3  | 1:A:184:GLU:HG2  | 1.82                     | 0.60              |
| 1:E:126:GLU:OE2  | 1:E:236:GLN:N    | 2.34                     | 0.60              |
| 4:J:393:UNK:CB   | 4:J:404:UNK:CB   | 2.80                     | 0.60              |
| 2:B:42:ALA:H     | 2:B:46:MET:HE3   | 1.66                     | 0.60              |
| 1:E:138:LEU:HA   | 1:E:157:VAL:HG13 | 1.84                     | 0.60              |
| 1:E:193:ILE:HG22 | 1:E:202:ARG:HA   | 1.83                     | 0.60              |
| 1:E:281:LYS:HA   | 1:E:284:ASN:HB2  | 1.83                     | 0.60              |
| 1:A:113:ILE:HG22 | 1:A:460:ARG:HB2  | 1.82                     | 0.60              |
| 1:A:116:HIS:H    | 1:A:461:THR:HA   | 1.67                     | 0.60              |
| 1:A:231:GLY:N    | 1:A:261:THR:H    | 2.00                     | 0.60              |
| 1:C:362:ARG:HD3  | 1:C:363:THR:O    | 2.02                     | 0.60              |
| 2:D:76:ALA:O     | 2:D:358:SER:OG   | 2.12                     | 0.60              |
| 3:H:261:UNK:C    | 3:H:265:UNK:CB   | 2.79                     | 0.60              |
| 1:A:134:ALA:CB   | 2:B:412:VAL:HG11 | 2.31                     | 0.59              |
| 2:B:305:ASP:O    | 2:B:308:SER:OG   | 2.15                     | 0.59              |
| 1:C:64:ARG:HH22  | 1:C:357:ARG:HH21 | 1.48                     | 0.59              |
| 2:D:84:THR:HG22  | 2:D:297:PHE:HE2  | 1.66                     | 0.59              |
| 3:H:637:UNK:O    | 3:H:640:UNK:CB   | 2.50                     | 0.59              |
| 1:A:181:ILE:HG12 | 1:A:455:ARG:HD3  | 1.83                     | 0.59              |
| 2:B:378:GLU:HG2  | 2:B:380:VAL:HG23 | 1.84                     | 0.59              |
| 2:D:146:GLN:NE2  | 2:D:196:ASP:HB2  | 2.17                     | 0.59              |
| 1:A:149:VAL:HA   | 1:A:152:GLU:CD   | 2.28                     | 0.59              |
| 1:A:210:LEU:HB3  | 1:A:214:PHE:CZ   | 2.37                     | 0.59              |
| 2:B:280:VAL:HA   | 2:B:283:TRP:CD1  | 2.36                     | 0.59              |
| 1:C:6:VAL:HG11   | 1:C:242:ASP:HB3  | 1.83                     | 0.59              |
| 2:D:138:ILE:HD12 | 2:D:178:MET:SD   | 2.42                     | 0.59              |
| 1:A:209:VAL:O    | 1:A:213:ASN:ND2  | 2.34                     | 0.59              |
| 1:C:319:LEU:HA   | 1:C:324:ALA:HB2  | 1.84                     | 0.59              |
| 2:D:383:SER:HG   | 2:D:386:ALA:H    | 1.48                     | 0.59              |
| 2:D:384:GLU:HA   | 2:D:387:TYR:HB2  | 1.84                     | 0.59              |
| 1:E:283:VAL:HG12 | 1:E:287:ILE:HD11 | 1.83                     | 0.59              |
| 1:A:135:SER:H    | 2:B:412:VAL:CG1  | 2.16                     | 0.59              |
| 4:J:350:UNK:O    | 4:J:355:UNK:HA   | 1.99                     | 0.59              |
| 2:F:174:LEU:HD22 | 2:F:182:LEU:HD13 | 1.85                     | 0.59              |
| 2:F:352:ASP:N    | 2:F:352:ASP:OD1  | 2.33                     | 0.59              |
| 3:H:514:UNK:C    | 3:H:516:UNK:N    | 2.65                     | 0.59              |
| 3:H:514:UNK:O    | 3:H:516:UNK:N    | 2.36                     | 0.59              |
| 4:J:330:UNK:C    | 4:J:332:UNK:N    | 2.62                     | 0.59              |
| 2:B:70:GLY:O     | 2:B:353:ARG:NH1  | 2.36                     | 0.59              |
| 1:C:279:ILE:HA   | 1:C:282:VAL:HG12 | 1.84                     | 0.59              |
| 1:A:399:VAL:H    | 1:A:425:VAL:CG2  | 2.13                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:480:GLU:OE1  | 1:A:480:GLU:N    | 2.35                     | 0.59              |
| 1:C:48:ALA:HB1   | 1:C:358:VAL:N    | 2.18                     | 0.59              |
| 2:D:374:ARG:O    | 2:D:378:GLU:HG2  | 2.03                     | 0.59              |
| 1:E:341:THR:O    | 1:E:342:GLU:HG2  | 2.03                     | 0.59              |
| 3:H:573:UNK:C    | 3:H:575:UNK:N    | 2.62                     | 0.59              |
| 1:A:132:GLN:NE2  | 2:B:423:VAL:O    | 2.36                     | 0.59              |
| 2:B:195:ILE:HG13 | 2:B:210:THR:H    | 1.68                     | 0.59              |
| 2:B:364:GLU:HB2  | 2:B:395:LEU:HD21 | 1.85                     | 0.59              |
| 1:A:231:GLY:H    | 1:A:261:THR:H    | 1.49                     | 0.59              |
| 1:A:494:GLU:HG3  | 1:A:498:LYS:NZ   | 2.17                     | 0.59              |
| 1:C:301:VAL:HG12 | 1:C:304:VAL:HG12 | 1.85                     | 0.59              |
| 2:D:132:LYS:HB3  | 2:D:237:GLU:CG   | 2.33                     | 0.59              |
| 2:D:386:ALA:HB2  | 2:D:422:GLN:C    | 2.27                     | 0.59              |
| 4:J:147:UNK:C    | 4:J:149:UNK:N    | 2.65                     | 0.59              |
| 2:B:194:THR:HG23 | 2:B:195:ILE:HG12 | 1.84                     | 0.58              |
| 2:B:233:GLN:NE2  | 2:B:234:LYS:O    | 2.36                     | 0.58              |
| 1:C:273:ASP:O    | 1:C:277:GLY:N    | 2.35                     | 0.58              |
| 2:D:206:GLY:HA3  | 2:D:235:ARG:HB2  | 1.85                     | 0.58              |
| 1:E:25:GLY:O     | 1:E:46:ARG:NH2   | 2.36                     | 0.58              |
| 1:A:204:ILE:O    | 2:F:308:SER:HA   | 2.03                     | 0.58              |
| 2:B:149:ARG:NH1  | 2:B:183:THR:O    | 2.37                     | 0.58              |
| 1:C:92:PRO:HD2   | 1:C:297:GLY:HA3  | 1.85                     | 0.58              |
| 2:D:279:LYS:HG2  | 2:D:283:TRP:HE1  | 1.67                     | 0.58              |
| 2:D:397:THR:HG23 | 2:D:436:GLU:HB2  | 1.85                     | 0.58              |
| 2:F:407:THR:O    | 2:F:410:SER:OG   | 2.16                     | 0.58              |
| 1:A:306:THR:HG22 | 1:A:321:LEU:H    | 1.68                     | 0.58              |
| 2:D:124:ARG:O    | 2:D:245:HIS:N    | 2.36                     | 0.58              |
| 1:A:441:ASP:N    | 1:A:441:ASP:OD1  | 2.35                     | 0.58              |
| 1:E:353:ASP:OD1  | 1:E:354:LEU:N    | 2.35                     | 0.58              |
| 2:F:81:THR:N     | 6:F:501:ADP:O2B  | 2.35                     | 0.58              |
| 3:H:444:UNK:HA   | 3:H:447:UNK:CB   | 2.33                     | 0.58              |
| 5:K:302:PRO:C    | 5:K:305:GLN:N    | 2.61                     | 0.58              |
| 1:A:109:LYS:HG2  | 1:A:427:PHE:O    | 2.03                     | 0.58              |
| 1:A:111:GLN:O    | 1:A:112:ARG:HG3  | 2.03                     | 0.58              |
| 1:C:43:GLU:O     | 1:C:47:GLU:HG2   | 2.03                     | 0.58              |
| 1:C:61:MET:N     | 1:C:320:GLU:OE1  | 2.37                     | 0.58              |
| 2:D:134:GLU:HG3  | 2:D:207:ARG:CZ   | 2.34                     | 0.58              |
| 1:E:42:GLN:HE22  | 1:E:364:MET:N    | 2.02                     | 0.58              |
| 1:E:178:GLU:O    | 1:E:182:LYS:NZ   | 2.27                     | 0.58              |
| 2:F:148:ASP:HB3  | 2:F:157:LYS:HB2  | 1.85                     | 0.58              |
| 4:J:345:UNK:O    | 4:J:349:UNK:N    | 2.36                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:163:ALA:HB2  | 1:A:414:HIS:N    | 2.18                     | 0.58              |
| 2:B:142:VAL:N    | 2:B:191:ASP:O    | 2.31                     | 0.58              |
| 1:C:314:TYR:CB   | 2:D:111:LEU:HD13 | 2.14                     | 0.58              |
| 2:F:135:THR:HA   | 2:F:207:ARG:HB2  | 1.84                     | 0.58              |
| 2:F:426:ILE:HA   | 2:F:429:VAL:HG12 | 1.84                     | 0.58              |
| 1:A:138:VAL:N    | 2:B:433:PHE:CD2  | 2.71                     | 0.58              |
| 1:A:190:PRO:HD3  | 1:A:394:PRO:HG3  | 1.86                     | 0.58              |
| 1:C:81:LEU:HG    | 1:C:85:GLN:HE22  | 1.69                     | 0.58              |
| 2:B:382:MET:HE3  | 2:B:383:SER:H    | 1.69                     | 0.58              |
| 1:C:27:ASP:H     | 1:C:31:LEU:N     | 2.01                     | 0.58              |
| 1:C:51:VAL:HG21  | 2:D:404:GLN:HE21 | 1.67                     | 0.58              |
| 1:C:63:GLY:HA2   | 1:C:315:LEU:HB2  | 1.86                     | 0.58              |
| 4:J:393:UNK:CA   | 4:J:400:GLY:CA   | 2.66                     | 0.58              |
| 1:A:124:LEU:HD23 | 1:A:135:SER:OG   | 2.02                     | 0.58              |
| 1:A:225:THR:HG22 | 1:A:329:LYS:HE3  | 1.86                     | 0.58              |
| 2:B:195:ILE:HG21 | 2:B:209:PHE:HA   | 1.85                     | 0.58              |
| 2:B:403:ILE:HG12 | 2:B:404:GLN:OE1  | 2.04                     | 0.58              |
| 1:C:123:ARG:HB3  | 1:C:293:GLU:HB3  | 1.86                     | 0.58              |
| 1:A:444:SER:OG   | 1:A:448:ILE:O    | 2.14                     | 0.57              |
| 1:C:106:ILE:C    | 1:C:107:LYS:HE2  | 2.28                     | 0.57              |
| 2:D:434:LEU:HD11 | 2:D:443:MET:HE3  | 1.86                     | 0.57              |
| 1:E:373:GLN:HA   | 1:E:376:LYS:HB3  | 1.86                     | 0.57              |
| 2:F:47:VAL:H     | 6:F:501:ADP:HN62 | 1.52                     | 0.57              |
| 3:H:175:UNK:C    | 3:H:177:UNK:H    | 2.16                     | 0.57              |
| 1:A:191:PHE:HD2  | 1:A:425:VAL:H    | 1.52                     | 0.57              |
| 2:B:130:ARG:HG3  | 2:B:241:THR:HG22 | 1.85                     | 0.57              |
| 2:D:334:ARG:HB2  | 2:D:341:GLN:HE22 | 1.69                     | 0.57              |
| 3:H:91:UNK:HA    | 3:H:141:UNK:CB   | 2.34                     | 0.57              |
| 2:B:352:ASP:O    | 1:C:408:GLN:NE2  | 2.36                     | 0.57              |
| 2:D:351:LEU:HA   | 2:D:354:LEU:HD12 | 1.85                     | 0.57              |
| 1:A:259:LEU:O    | 1:A:266:LYS:CB   | 2.51                     | 0.57              |
| 1:A:265:THR:HG22 | 1:A:267:GLN:HG2  | 1.86                     | 0.57              |
| 1:A:276:GLU:HG2  | 1:A:297:ALA:HA   | 1.86                     | 0.57              |
| 1:C:21:VAL:HG23  | 1:C:85:GLN:HG2   | 1.86                     | 0.57              |
| 1:C:55:LEU:HD11  | 1:C:354:LEU:HD11 | 1.87                     | 0.57              |
| 1:C:191:ILE:HG22 | 1:C:202:ARG:HD3  | 1.84                     | 0.57              |
| 2:F:187:VAL:HG22 | 2:F:213:ARG:HH12 | 1.69                     | 0.57              |
| 4:J:217:UNK:O    | 4:J:220:UNK:N    | 2.37                     | 0.57              |
| 1:A:229:TYR:HD2  | 1:A:259:LEU:HD22 | 1.68                     | 0.57              |
| 1:A:477:ALA:HB1  | 1:A:508:LEU:HD11 | 1.87                     | 0.57              |
| 1:C:27:ASP:OD1   | 1:C:28:GLU:N     | 2.38                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:82:GLY:O     | 6:D:501:ADP:O2'  | 2.22                     | 0.57              |
| 2:D:297:PHE:HD1  | 2:D:325:ILE:HG13 | 1.70                     | 0.57              |
| 2:F:142:VAL:HG21 | 2:F:193:ILE:HG22 | 1.86                     | 0.57              |
| 1:A:122:LEU:HB3  | 2:B:409:ALA:C    | 2.30                     | 0.57              |
| 2:D:137:ILE:HG12 | 2:D:211:ARG:HH11 | 1.70                     | 0.57              |
| 1:E:166:GLY:HA2  | 1:E:228:VAL:HG22 | 1.87                     | 0.57              |
| 1:E:338:ILE:HD11 | 1:E:346:SER:HB3  | 1.85                     | 0.57              |
| 3:H:648:UNK:C    | 3:H:650:UNK:N    | 2.64                     | 0.57              |
| 5:K:77:ASP:HA    | 5:K:80:PHE:CB    | 2.34                     | 0.57              |
| 2:D:440:THR:HG1  | 2:D:441:GLN:CD   | 2.11                     | 0.57              |
| 1:A:134:ALA:HA   | 2:B:412:VAL:HG11 | 1.85                     | 0.57              |
| 2:D:436:GLU:HA   | 2:D:439:SER:OG   | 2.05                     | 0.57              |
| 1:E:396:GLU:O    | 1:E:400:LYS:N    | 2.36                     | 0.57              |
| 3:H:125:UNK:CA   | 3:H:163:UNK:HA   | 2.34                     | 0.57              |
| 3:H:493:UNK:O    | 3:H:496:UNK:CA   | 2.53                     | 0.57              |
| 4:J:198:UNK:O    | 4:J:201:UNK:CB   | 2.52                     | 0.57              |
| 1:A:131:LYS:CE   | 2:B:413:CYS:CB   | 2.77                     | 0.57              |
| 1:A:431:ARG:NH1  | 1:A:434:CYS:SG   | 2.77                     | 0.57              |
| 2:B:104:ALA:N    | 2:B:107:GLU:OE2  | 2.30                     | 0.57              |
| 2:D:132:LYS:HA   | 2:D:238:VAL:O    | 2.05                     | 0.57              |
| 1:A:144:ARG:NH1  | 2:B:406:ILE:C    | 2.63                     | 0.57              |
| 1:A:412:TYR:HB2  | 2:B:111:LEU:HD23 | 1.87                     | 0.57              |
| 1:A:470:LYS:HG2  | 1:A:489:LEU:HD11 | 1.86                     | 0.57              |
| 1:C:311:CYS:HA   | 2:D:111:LEU:HD11 | 1.87                     | 0.57              |
| 1:C:428:GLU:OE1  | 1:C:428:GLU:N    | 2.29                     | 0.57              |
| 2:D:146:GLN:HB3  | 2:D:149:ARG:HB2  | 1.86                     | 0.57              |
| 2:D:180:GLU:O    | 2:D:184:LYS:N    | 2.37                     | 0.57              |
| 2:F:401:TYR:OH   | 2:F:433:PHE:O    | 2.16                     | 0.57              |
| 5:K:386:SER:O    | 5:K:389:PRO:N    | 2.38                     | 0.57              |
| 1:A:201:SER:O    | 2:F:308:SER:OG   | 2.22                     | 0.56              |
| 2:D:403:ILE:O    | 2:D:406:ILE:HG22 | 2.04                     | 0.56              |
| 1:E:439:ASP:N    | 1:E:439:ASP:OD1  | 2.36                     | 0.56              |
| 2:F:99:PRO:HG2   | 2:F:294:GLY:HA3  | 1.86                     | 0.56              |
| 3:H:472:UNK:O    | 3:H:475:UNK:N    | 2.38                     | 0.56              |
| 2:B:362:TYR:OH   | 6:B:501:ADP:N6   | 2.38                     | 0.56              |
| 1:C:168:LYS:HD2  | 1:C:228:VAL:HA   | 1.86                     | 0.56              |
| 1:C:414:ASN:HA   | 1:C:425:ILE:HD11 | 1.87                     | 0.56              |
| 2:D:156:SER:HA   | 2:D:174:LEU:H    | 1.70                     | 0.56              |
| 1:A:141:GLU:O    | 1:A:144:ARG:N    | 2.27                     | 0.56              |
| 1:C:129:GLU:HG2  | 1:C:231:LYS:HE3  | 1.87                     | 0.56              |
| 1:C:426:GLU:HB2  | 1:C:428:GLU:OE2  | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:142:VAL:HG23 | 2:D:164:LYS:HB3  | 1.88                     | 0.56              |
| 2:D:274:GLU:O    | 2:D:278:ALA:N    | 2.37                     | 0.56              |
| 2:F:185:ASP:OD2  | 2:F:213:ARG:NH1  | 2.38                     | 0.56              |
| 2:F:358:SER:OG   | 2:F:359:THR:N    | 2.37                     | 0.56              |
| 3:H:593:UNK:CB   | 3:H:631:UNK:HA   | 2.33                     | 0.56              |
| 4:J:121:UNK:C    | 4:J:123:UNK:H    | 2.18                     | 0.56              |
| 2:B:383:SER:HB3  | 2:B:423:VAL:HA   | 1.87                     | 0.56              |
| 1:C:396:GLU:HA   | 1:C:399:THR:HB   | 1.87                     | 0.56              |
| 2:D:170:THR:OG1  | 2:D:197:LYS:NZ   | 2.33                     | 0.56              |
| 2:D:439:SER:OG   | 2:D:440:THR:N    | 2.37                     | 0.56              |
| 1:A:116:HIS:HE1  | 1:A:118:HIS:O    | 1.88                     | 0.56              |
| 1:A:162:ARG:N    | 1:A:414:HIS:O    | 2.38                     | 0.56              |
| 1:C:14:ARG:NH1   | 1:C:95:PRO:O     | 2.37                     | 0.56              |
| 1:C:62:ALA:HB1   | 1:C:316:HIS:CE1  | 2.40                     | 0.56              |
| 2:D:422:GLN:HB2  | 2:D:424:ASP:H    | 1.71                     | 0.56              |
| 2:F:385:ASP:N    | 2:F:385:ASP:OD1  | 2.36                     | 0.56              |
| 4:J:168:GLY:O    | 4:J:170:UNK:N    | 2.38                     | 0.56              |
| 1:A:107:THR:O    | 1:A:427:PHE:N    | 2.38                     | 0.56              |
| 2:B:146:GLN:HE22 | 2:B:187:VAL:H    | 1.53                     | 0.56              |
| 1:C:307:LEU:HB3  | 1:C:311:CYS:SG   | 2.44                     | 0.56              |
| 2:D:428:ARG:NH1  | 2:D:429:VAL:HA   | 2.21                     | 0.56              |
| 2:D:190:GLY:HA3  | 2:D:215:TYR:HA   | 1.88                     | 0.56              |
| 2:D:218:MET:HG2  | 2:D:219:GLY:H    | 1.71                     | 0.56              |
| 1:A:133:ALA:HB1  | 2:B:428:ARG:N    | 2.21                     | 0.56              |
| 1:A:306:THR:HA   | 1:A:320:PRO:HA   | 1.88                     | 0.56              |
| 2:D:442:TYR:HA   | 2:D:445:GLU:HB2  | 1.87                     | 0.56              |
| 4:J:158:UNK:CB   | 4:J:197:UNK:CB   | 2.84                     | 0.56              |
| 1:A:196:GLY:H    | 1:A:402:VAL:N    | 2.04                     | 0.56              |
| 2:B:422:GLN:HB3  | 2:B:425:ASP:HB2  | 1.88                     | 0.56              |
| 1:C:44:ASN:OD1   | 2:D:439:SER:HA   | 2.05                     | 0.56              |
| 2:D:251:ASN:HD22 | 2:D:276:ILE:HD11 | 1.70                     | 0.56              |
| 4:J:59:UNK:O     | 4:J:60:UNK:C     | 2.51                     | 0.56              |
| 1:A:229:TYR:CE2  | 1:A:293:ALA:HA   | 2.40                     | 0.56              |
| 1:A:396:VAL:CA   | 1:A:424:ILE:HB   | 2.35                     | 0.56              |
| 2:B:352:ASP:OD1  | 2:B:352:ASP:N    | 2.38                     | 0.56              |
| 2:B:438:ARG:HA   | 2:B:441:GLN:HG2  | 1.88                     | 0.56              |
| 1:C:205:ARG:NE   | 1:C:215:LEU:O    | 2.38                     | 0.56              |
| 2:D:429:VAL:HB   | 2:D:433:PHE:CE2  | 2.41                     | 0.56              |
| 2:F:83:LYS:NZ    | 6:F:501:ADP:O1B  | 2.28                     | 0.56              |
| 2:F:319:ASP:N    | 2:F:319:ASP:OD1  | 2.36                     | 0.56              |
| 3:H:359:UNK:C    | 3:H:361:UNK:N    | 2.66                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:116:PHE:O    | 1:C:119:ALA:N    | 2.37                     | 0.55              |
| 1:C:189:ASP:HB3  | 1:C:205:ARG:HA   | 1.87                     | 0.55              |
| 2:D:312:LEU:O    | 2:D:315:ALA:N    | 2.38                     | 0.55              |
| 1:E:190:VAL:HG11 | 1:E:224:PRO:HG2  | 1.88                     | 0.55              |
| 1:E:219:GLU:O    | 1:E:221:VAL:N    | 2.36                     | 0.55              |
| 1:E:402:THR:HG22 | 1:E:405:TYR:H    | 1.71                     | 0.55              |
| 2:F:385:ASP:O    | 2:F:388:THR:OG1  | 2.18                     | 0.55              |
| 1:A:537:ASP:OD1  | 1:A:540:SER:OG   | 2.21                     | 0.55              |
| 2:B:374:ARG:HH22 | 2:B:406:ILE:HB   | 1.71                     | 0.55              |
| 1:C:125:LYS:HD2  | 1:C:233:GLU:HB3  | 1.88                     | 0.55              |
| 2:D:146:GLN:HG3  | 2:D:148:ASP:H    | 1.71                     | 0.55              |
| 2:D:382:MET:HE2  | 2:D:387:TYR:HA   | 1.88                     | 0.55              |
| 1:E:156:HIS:HB2  | 1:E:171:LYS:HB3  | 1.88                     | 0.55              |
| 1:A:237:THR:HG22 | 1:A:257:ILE:HG22 | 1.88                     | 0.55              |
| 1:A:414:HIS:CG   | 1:A:415:ARG:N    | 2.75                     | 0.55              |
| 2:B:130:ARG:HA   | 2:B:241:THR:HG22 | 1.88                     | 0.55              |
| 1:C:24:LEU:HD21  | 1:C:34:GLN:HA    | 1.88                     | 0.55              |
| 1:A:397:LEU:O    | 1:A:399:VAL:HG23 | 2.07                     | 0.55              |
| 1:C:193:ILE:HB   | 1:C:200:VAL:HA   | 1.88                     | 0.55              |
| 2:D:372:ARG:HG2  | 2:D:387:TYR:CE1  | 2.42                     | 0.55              |
| 2:D:389:VAL:HG13 | 2:D:426:ILE:HD11 | 1.88                     | 0.55              |
| 2:F:193:ILE:HG12 | 2:F:195:ILE:HG22 | 1.88                     | 0.55              |
| 2:B:299:ASP:OD1  | 2:B:300:GLU:N    | 2.37                     | 0.55              |
| 1:C:134:GLU:HG2  | 1:C:162:LYS:H    | 1.71                     | 0.55              |
| 1:C:374:ILE:HA   | 1:C:377:ILE:HD12 | 1.88                     | 0.55              |
| 1:C:381:THR:OG1  | 1:C:382:GLU:OE1  | 2.18                     | 0.55              |
| 1:C:393:HIS:N    | 1:C:427:LYS:HZ1  | 2.04                     | 0.55              |
| 2:D:381:GLU:O    | 2:D:421:VAL:N    | 2.34                     | 0.55              |
| 2:F:35:ASP:N     | 2:F:35:ASP:OD1   | 2.37                     | 0.55              |
| 1:A:278:LEU:HD13 | 1:A:301:GLN:HB3  | 1.88                     | 0.55              |
| 2:B:170:THR:HB   | 2:B:198:ALA:HA   | 1.88                     | 0.55              |
| 1:C:51:VAL:CG2   | 2:D:404:GLN:HE21 | 2.19                     | 0.55              |
| 1:C:248:ALA:HA   | 1:C:275:LEU:HD11 | 1.87                     | 0.55              |
| 1:E:36:ALA:O     | 1:E:39:LEU:N     | 2.37                     | 0.55              |
| 2:B:79:PRO:O     | 2:B:81:THR:N     | 2.39                     | 0.55              |
| 2:D:141:GLU:HG2  | 2:D:191:ASP:O    | 2.07                     | 0.55              |
| 2:D:448:ASP:HA   | 2:D:451:LEU:HG   | 1.87                     | 0.55              |
| 1:A:203:GLU:H    | 2:F:308:SER:C    | 2.15                     | 0.55              |
| 1:A:227:GLU:HB2  | 1:A:293:ALA:HB2  | 1.88                     | 0.55              |
| 1:A:278:LEU:HD21 | 1:A:289:ILE:HD12 | 1.87                     | 0.55              |
| 2:F:231:GLU:CD   | 2:F:232:LEU:H    | 2.15                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:309:PHE:O    | 2:B:313:ASN:ND2  | 2.39                     | 0.55              |
| 1:C:452:ASP:N    | 1:C:452:ASP:OD1  | 2.38                     | 0.55              |
| 2:D:283:TRP:O    | 2:D:288:LYS:HG2  | 2.06                     | 0.55              |
| 1:E:49:CYS:O     | 1:E:53:VAL:HG23  | 2.07                     | 0.55              |
| 1:E:373:GLN:O    | 1:E:377:ILE:N    | 2.35                     | 0.55              |
| 1:A:111:GLN:HE22 | 1:A:502:ARG:HG3  | 1.72                     | 0.55              |
| 2:F:306:ILE:HG23 | 2:F:336:ARG:O    | 2.07                     | 0.55              |
| 5:K:292:LEU:HA   | 5:K:295:LEU:O    | 2.07                     | 0.55              |
| 1:A:199:VAL:HA   | 1:A:206:LYS:HD2  | 1.89                     | 0.54              |
| 2:D:284:ARG:HG3  | 2:D:285:GLU:OE2  | 2.07                     | 0.54              |
| 2:D:393:ILE:HG23 | 2:D:435:ASP:CG   | 2.32                     | 0.54              |
| 1:A:237:THR:HG21 | 1:A:256:ILE:HD12 | 1.89                     | 0.54              |
| 2:D:28:ILE:O     | 2:D:29:ARG:NE    | 2.40                     | 0.54              |
| 3:H:602:UNK:O    | 3:H:605:UNK:CB   | 2.55                     | 0.54              |
| 1:C:337:VAL:HA   | 1:C:345:THR:HA   | 1.90                     | 0.54              |
| 2:D:182:LEU:HA   | 2:D:185:ASP:HB2  | 1.89                     | 0.54              |
| 2:D:394:GLY:O    | 2:D:397:THR:N    | 2.38                     | 0.54              |
| 3:H:278:UNK:CB   | 3:H:310:UNK:O    | 2.55                     | 0.54              |
| 5:K:280:LYS:O    | 5:K:285:GLN:CB   | 2.55                     | 0.54              |
| 1:A:203:GLU:HG3  | 2:F:311:PHE:CB   | 2.37                     | 0.54              |
| 2:D:161:LEU:O    | 2:D:170:THR:HG23 | 2.08                     | 0.54              |
| 5:K:170:PRO:O    | 5:K:173:TYR:CB   | 2.55                     | 0.54              |
| 1:C:418:LYS:HA   | 1:C:418:LYS:HE2  | 1.90                     | 0.54              |
| 1:A:232:GLU:OE2  | 1:A:260:LYS:NZ   | 2.41                     | 0.54              |
| 1:C:26:LEU:HA    | 1:C:31:LEU:C     | 2.33                     | 0.54              |
| 1:C:52:ILE:HG13  | 1:C:358:VAL:HA   | 1.90                     | 0.54              |
| 1:E:135:VAL:HG13 | 1:E:159:ILE:HG12 | 1.89                     | 0.54              |
| 3:H:96:UNK:O     | 3:H:100:UNK:CB   | 2.55                     | 0.54              |
| 3:H:496:UNK:O    | 3:H:498:UNK:N    | 2.39                     | 0.54              |
| 1:A:416:ALA:O    | 1:A:417:LEU:HD22 | 2.07                     | 0.54              |
| 1:C:157:VAL:HB   | 1:C:174:PRO:HG3  | 1.90                     | 0.54              |
| 1:C:328:ILE:HG12 | 1:C:359:MET:SD   | 2.47                     | 0.54              |
| 2:D:199:THR:OG1  | 2:D:233:GLN:NE2  | 2.41                     | 0.54              |
| 2:F:194:THR:HB   | 2:F:212:ALA:HB3  | 1.89                     | 0.54              |
| 3:H:273:UNK:O    | 3:H:306:UNK:CB   | 2.55                     | 0.54              |
| 1:A:218:ILE:N    | 1:A:423:PRO:HD3  | 2.23                     | 0.54              |
| 1:A:316:GLU:OE1  | 1:A:318:TYR:OH   | 2.13                     | 0.54              |
| 1:C:161:LEU:HD11 | 1:C:170:LEU:HD22 | 1.89                     | 0.54              |
| 2:D:140:GLY:HA2  | 2:D:231:GLU:O    | 2.07                     | 0.54              |
| 1:E:32:ALA:N     | 1:E:47:GLU:OE2   | 2.40                     | 0.54              |
| 2:F:117:GLU:O    | 2:F:120:THR:OG1  | 2.25                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:K:77:ASP:O     | 5:K:80:PHE:N     | 2.41                     | 0.54              |
| 1:A:124:LEU:HD12 | 1:A:125:ASP:O    | 2.07                     | 0.54              |
| 2:D:438:ARG:HA   | 2:D:442:TYR:CB   | 2.37                     | 0.54              |
| 2:D:438:ARG:O    | 2:D:443:MET:HG2  | 2.08                     | 0.54              |
| 1:A:171:GLY:HA2  | 1:A:431:ARG:H    | 1.72                     | 0.54              |
| 1:C:52:ILE:HG13  | 1:C:357:ARG:O    | 2.08                     | 0.54              |
| 1:C:77:THR:HG22  | 1:C:300:PHE:HE2  | 1.73                     | 0.54              |
| 2:D:146:GLN:H    | 2:D:149:ARG:HH21 | 1.55                     | 0.54              |
| 2:D:441:GLN:HA   | 2:D:444:LYS:HB2  | 1.90                     | 0.54              |
| 1:E:77:THR:N     | 6:E:501:ADP:O1A  | 2.41                     | 0.54              |
| 1:E:427:LYS:HG3  | 1:E:428:GLU:OE1  | 2.08                     | 0.54              |
| 3:H:667:UNK:C    | 3:H:669:UNK:N    | 2.69                     | 0.54              |
| 1:A:144:ARG:HG2  | 2:B:406:ILE:H    | 1.73                     | 0.53              |
| 1:A:203:GLU:C    | 2:F:308:SER:HB2  | 2.32                     | 0.53              |
| 1:A:221:ARG:NH2  | 1:A:391:GLU:HB3  | 2.23                     | 0.53              |
| 1:A:399:VAL:HG21 | 1:A:423:PRO:HG2  | 1.90                     | 0.53              |
| 2:B:298:ILE:HG22 | 2:B:299:ASP:H    | 1.73                     | 0.53              |
| 2:F:166:THR:HG23 | 2:F:229:ASP:HA   | 1.88                     | 0.53              |
| 2:F:271:GLU:H    | 2:F:271:GLU:CD   | 2.16                     | 0.53              |
| 1:C:51:VAL:HB    | 1:C:357:ARG:HB3  | 1.89                     | 0.53              |
| 2:D:61:GLU:HB3   | 1:E:415:LEU:HD23 | 1.90                     | 0.53              |
| 2:D:139:GLU:HB2  | 2:D:234:LYS:HB2  | 1.91                     | 0.53              |
| 3:H:452:UNK:O    | 3:H:455:UNK:N    | 2.42                     | 0.53              |
| 1:A:124:LEU:HD21 | 1:A:144:ARG:HH12 | 1.72                     | 0.53              |
| 1:A:164:VAL:HG21 | 1:A:454:ASP:HB3  | 1.90                     | 0.53              |
| 1:E:232:LYS:HD2  | 1:E:234:ILE:HD11 | 1.89                     | 0.53              |
| 2:F:124:ARG:HB3  | 2:F:245:HIS:HB2  | 1.89                     | 0.53              |
| 2:F:145:ILE:HG22 | 2:F:147:ILE:HG23 | 1.90                     | 0.53              |
| 2:F:416:ARG:NH1  | 2:F:418:GLY:HA3  | 2.23                     | 0.53              |
| 3:H:293:UNK:C    | 3:H:295:UNK:N    | 2.71                     | 0.53              |
| 4:J:330:UNK:O    | 4:J:332:UNK:N    | 2.42                     | 0.53              |
| 1:A:116:HIS:CE1  | 1:A:118:HIS:H    | 2.26                     | 0.53              |
| 1:A:260:LYS:H    | 1:A:291:ILE:HD11 | 1.72                     | 0.53              |
| 1:A:412:TYR:C    | 1:A:414:HIS:H    | 2.16                     | 0.53              |
| 2:B:364:GLU:HA   | 2:B:395:LEU:HD11 | 1.90                     | 0.53              |
| 2:B:413:CYS:HB2  | 2:B:418:GLY:O    | 2.08                     | 0.53              |
| 2:F:439:SER:OG   | 2:F:440:THR:N    | 2.39                     | 0.53              |
| 1:A:231:GLY:O    | 1:A:260:LYS:HA   | 2.08                     | 0.53              |
| 2:B:384:GLU:O    | 2:B:388:THR:HG23 | 2.09                     | 0.53              |
| 1:C:129:GLU:HB3  | 1:C:229:HIS:NE2  | 2.24                     | 0.53              |
| 2:D:319:ASP:N    | 2:D:319:ASP:OD1  | 2.40                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:102:TYR:OH   | 1:E:306:MET:O    | 2.20                     | 0.53              |
| 1:E:207:ASP:OD1  | 1:E:207:ASP:N    | 2.41                     | 0.53              |
| 2:F:124:ARG:NH1  | 2:F:273:ARG:HD2  | 2.22                     | 0.53              |
| 1:A:166:LEU:HD13 | 1:A:456:VAL:HG23 | 1.90                     | 0.53              |
| 2:B:275:GLN:O    | 2:B:279:LYS:N    | 2.38                     | 0.53              |
| 1:C:159:ILE:HG21 | 1:C:172:LEU:HD22 | 1.91                     | 0.53              |
| 1:C:348:HIS:HB2  | 1:C:350:ILE:HG13 | 1.90                     | 0.53              |
| 2:D:182:LEU:HD11 | 2:D:195:ILE:HA   | 1.91                     | 0.53              |
| 2:D:372:ARG:HG2  | 2:D:387:TYR:CZ   | 2.42                     | 0.53              |
| 3:H:131:UNK:C    | 3:H:133:UNK:N    | 2.71                     | 0.53              |
| 5:K:77:ASP:C     | 5:K:80:PHE:H     | 2.16                     | 0.53              |
| 5:K:90:ALA:O     | 5:K:94:SER:N     | 2.41                     | 0.53              |
| 1:A:166:LEU:HG   | 1:A:174:LYS:HD3  | 1.90                     | 0.53              |
| 1:A:377:ILE:HA   | 1:A:380:VAL:HG22 | 1.91                     | 0.53              |
| 2:D:279:LYS:O    | 2:D:283:TRP:HD1  | 1.90                     | 0.53              |
| 2:D:389:VAL:HG23 | 2:D:392:ARG:HE   | 1.73                     | 0.53              |
| 2:D:437:SER:HA   | 2:D:441:GLN:OE1  | 2.08                     | 0.53              |
| 1:E:443:SER:OG   | 1:E:444:ALA:N    | 2.42                     | 0.53              |
| 3:H:361:UNK:O    | 3:H:363:UNK:N    | 2.41                     | 0.53              |
| 3:H:493:UNK:O    | 3:H:496:UNK:HA   | 2.09                     | 0.53              |
| 1:A:133:ALA:C    | 2:B:428:ARG:HB3  | 2.33                     | 0.53              |
| 1:A:189:VAL:HB   | 1:A:394:PRO:HG2  | 1.91                     | 0.53              |
| 2:B:369:GLN:HA   | 2:B:372:ARG:CG   | 2.39                     | 0.53              |
| 1:C:145:ASN:HD21 | 1:C:152:LYS:HB3  | 1.74                     | 0.53              |
| 1:C:272:THR:OG1  | 1:C:274:LYS:NZ   | 2.35                     | 0.53              |
| 2:D:151:ALA:N    | 2:D:179:ILE:HB   | 2.24                     | 0.53              |
| 2:D:427:LYS:HA   | 2:D:430:TYR:HB2  | 1.91                     | 0.53              |
| 2:F:146:GLN:HB3  | 2:F:183:THR:HG23 | 1.91                     | 0.53              |
| 2:D:441:GLN:O    | 2:D:445:GLU:HG3  | 2.09                     | 0.53              |
| 2:F:134:GLU:O    | 2:F:207:ARG:NH1  | 2.42                     | 0.53              |
| 1:C:189:ASP:HB2  | 1:C:202:ARG:HD2  | 1.89                     | 0.53              |
| 1:C:205:ARG:HE   | 1:C:217:ALA:H    | 1.55                     | 0.53              |
| 1:C:430:VAL:HA   | 1:C:433:ILE:HG22 | 1.90                     | 0.53              |
| 1:E:188:GLY:HA3  | 1:E:208:THR:OG1  | 2.09                     | 0.53              |
| 1:E:286:TYR:HB3  | 1:E:292:ALA:HB2  | 1.90                     | 0.53              |
| 1:E:343:ASP:OD2  | 2:F:334:ARG:NH2  | 2.34                     | 0.53              |
| 2:F:141:GLU:HA   | 2:F:192:VAL:HG22 | 1.91                     | 0.53              |
| 4:J:199:UNK:O    | 4:J:202:UNK:N    | 2.42                     | 0.53              |
| 1:A:111:GLN:HG3  | 1:A:428:ALA:O    | 2.09                     | 0.52              |
| 1:A:140:GLN:C    | 1:A:142:ASN:H    | 2.17                     | 0.52              |
| 1:A:144:ARG:HH11 | 2:B:406:ILE:C    | 2.16                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:204:ILE:HD13 | 2:F:311:PHE:CD1  | 2.43                     | 0.52              |
| 1:C:61:MET:HB3   | 1:C:319:LEU:O    | 2.10                     | 0.52              |
| 2:D:138:ILE:HG13 | 2:D:205:LEU:HG   | 1.91                     | 0.52              |
| 1:E:356:ASP:OD1  | 1:E:357:ARG:N    | 2.42                     | 0.52              |
| 2:F:29:ARG:H     | 2:F:44:GLN:HB3   | 1.75                     | 0.52              |
| 2:F:384:GLU:O    | 2:F:388:THR:HG23 | 2.10                     | 0.52              |
| 3:H:368:UNK:O    | 3:H:372:UNK:CB   | 2.57                     | 0.52              |
| 1:A:131:LYS:HE3  | 2:B:413:CYS:HB2  | 1.89                     | 0.52              |
| 1:A:168:GLY:O    | 1:A:446:HIS:HB2  | 2.08                     | 0.52              |
| 1:A:190:PRO:CD   | 1:A:394:PRO:HG3  | 2.39                     | 0.52              |
| 2:B:142:VAL:HA   | 2:B:163:LEU:HD13 | 1.90                     | 0.52              |
| 1:C:343:ASP:OD1  | 1:C:344:ILE:HD12 | 2.09                     | 0.52              |
| 3:H:453:UNK:C    | 3:H:455:UNK:N    | 2.71                     | 0.52              |
| 1:A:195:VAL:HB   | 1:A:401:GLU:HA   | 1.92                     | 0.52              |
| 2:B:397:THR:HG23 | 2:B:398:SER:H    | 1.73                     | 0.52              |
| 2:D:216:ASP:HB3  | 2:D:229:ASP:OD1  | 2.10                     | 0.52              |
| 2:D:272:VAL:O    | 2:D:275:GLN:HG3  | 2.09                     | 0.52              |
| 1:E:139:THR:O    | 1:E:158:ILE:HG22 | 2.09                     | 0.52              |
| 1:E:317:ARG:HH22 | 2:F:112:GLU:HB3  | 1.74                     | 0.52              |
| 2:F:178:MET:HG3  | 2:F:211:ARG:HH21 | 1.75                     | 0.52              |
| 1:A:231:GLY:H    | 1:A:260:LYS:CA   | 2.22                     | 0.52              |
| 2:D:161:LEU:HB3  | 2:D:172:TYR:CE1  | 2.44                     | 0.52              |
| 2:F:245:HIS:O    | 2:F:249:VAL:HG23 | 2.09                     | 0.52              |
| 1:A:140:GLN:OE1  | 2:B:436:GLU:N    | 2.43                     | 0.52              |
| 1:A:180:ALA:HB3  | 1:A:455:ARG:HG2  | 1.92                     | 0.52              |
| 1:A:314:GLU:HB3  | 1:A:318:TYR:HE2  | 1.74                     | 0.52              |
| 2:B:143:VAL:O    | 2:B:164:LYS:NZ   | 2.40                     | 0.52              |
| 2:D:301:VAL:HG11 | 2:D:326:MET:HB3  | 1.92                     | 0.52              |
| 1:A:179:LEU:HD21 | 1:A:183:GLN:HA   | 1.91                     | 0.52              |
| 1:A:215:ARG:HH22 | 1:A:371:ASP:HA   | 1.74                     | 0.52              |
| 1:C:370:GLU:O    | 1:C:374:ILE:HG12 | 2.10                     | 0.52              |
| 2:D:148:ASP:HB3  | 2:D:178:MET:HG2  | 1.91                     | 0.52              |
| 2:D:430:TYR:OH   | 2:D:438:ARG:NE   | 2.42                     | 0.52              |
| 1:E:130:VAL:HB   | 1:E:230:LYS:HG2  | 1.92                     | 0.52              |
| 2:F:148:ASP:HB2  | 2:F:179:ILE:HG12 | 1.90                     | 0.52              |
| 4:J:162:UNK:O    | 4:J:165:UNK:CB   | 2.57                     | 0.52              |
| 1:A:170:PRO:HB3  | 1:A:432:GLY:C    | 2.35                     | 0.52              |
| 1:C:376:LYS:NZ   | 1:C:380:GLN:OE1  | 2.40                     | 0.52              |
| 2:D:130:ARG:O    | 2:D:289:ALA:HA   | 2.09                     | 0.52              |
| 2:D:145:ILE:HA   | 2:D:149:ARG:HH21 | 1.74                     | 0.52              |
| 2:D:147:ILE:HG13 | 2:D:161:LEU:HD11 | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:197:LYS:HD2  | 2:D:198:ALA:N    | 2.25                     | 0.52              |
| 1:E:428:GLU:N    | 1:E:428:GLU:OE1  | 2.43                     | 0.52              |
| 1:C:28:GLU:OE2   | 1:C:57:LYS:NZ    | 2.26                     | 0.52              |
| 1:E:386:ILE:HG22 | 1:E:425:ILE:HB   | 1.92                     | 0.52              |
| 1:C:396:GLU:O    | 1:C:400:LYS:N    | 2.32                     | 0.52              |
| 1:E:129:GLU:HG2  | 1:E:194:GLU:HA   | 1.91                     | 0.52              |
| 1:C:133:GLY:O    | 1:C:190:VAL:HA   | 2.09                     | 0.52              |
| 1:C:138:LEU:HA   | 1:C:157:VAL:HG21 | 1.91                     | 0.52              |
| 2:D:141:GLU:OE2  | 2:D:164:LYS:NZ   | 2.43                     | 0.52              |
| 2:D:141:GLU:HB2  | 2:D:230:GLY:HA3  | 1.92                     | 0.52              |
| 2:D:209:PHE:HA   | 2:D:211:ARG:CZ   | 2.40                     | 0.52              |
| 2:D:437:SER:O    | 2:D:441:GLN:N    | 2.43                     | 0.52              |
| 1:E:279:ILE:O    | 1:E:283:VAL:HG23 | 2.10                     | 0.52              |
| 3:H:582:UNK:O    | 3:H:586:UNK:N    | 2.43                     | 0.52              |
| 1:A:431:ARG:HD3  | 1:A:432:GLY:N    | 2.25                     | 0.51              |
| 2:B:234:LYS:HZ3  | 2:B:236:LYS:HA   | 1.75                     | 0.51              |
| 2:B:373:ILE:HG23 | 2:B:379:ASP:CG   | 2.34                     | 0.51              |
| 1:C:326:ILE:HD11 | 1:C:359:MET:HE1  | 1.92                     | 0.51              |
| 2:D:206:GLY:CA   | 2:D:235:ARG:HD3  | 2.40                     | 0.51              |
| 2:D:280:VAL:O    | 2:D:284:ARG:HG2  | 2.10                     | 0.51              |
| 2:D:383:SER:N    | 2:D:420:GLU:OE2  | 2.44                     | 0.51              |
| 1:E:163:THR:HG22 | 1:E:164:ALA:N    | 2.25                     | 0.51              |
| 3:H:470:UNK:O    | 3:H:473:UNK:CB   | 2.58                     | 0.51              |
| 5:K:77:ASP:O     | 5:K:80:PHE:C     | 2.52                     | 0.51              |
| 5:K:192:LEU:C    | 5:K:194:GLY:H    | 2.18                     | 0.51              |
| 1:A:201:SER:HB2  | 2:F:309:PHE:CG   | 2.45                     | 0.51              |
| 1:A:520:LYS:NZ   | 1:A:526:GLU:OE2  | 2.43                     | 0.51              |
| 2:B:61:GLU:HB3   | 1:C:415:LEU:HD13 | 1.93                     | 0.51              |
| 2:B:439:SER:HA   | 2:B:442:TYR:HB2  | 1.92                     | 0.51              |
| 2:B:441:GLN:O    | 2:B:445:GLU:HG3  | 2.11                     | 0.51              |
| 3:H:373:UNK:C    | 3:H:375:UNK:N    | 2.69                     | 0.51              |
| 2:B:434:LEU:HD13 | 2:B:439:SER:HB3  | 1.92                     | 0.51              |
| 2:D:179:ILE:O    | 2:D:183:THR:HG23 | 2.11                     | 0.51              |
| 2:D:182:LEU:HD21 | 2:D:195:ILE:HG12 | 1.92                     | 0.51              |
| 1:E:188:GLY:O    | 1:E:206:CYS:HB3  | 2.09                     | 0.51              |
| 1:E:234:ILE:HG22 | 1:E:235:ILE:H    | 1.75                     | 0.51              |
| 1:A:135:SER:O    | 1:A:144:ARG:NH2  | 2.44                     | 0.51              |
| 1:A:165:LEU:N    | 1:A:452:LEU:O    | 2.44                     | 0.51              |
| 2:B:388:THR:OG1  | 2:B:389:VAL:N    | 2.43                     | 0.51              |
| 1:C:11:LYS:HE2   | 1:C:14:ARG:HD2   | 1.92                     | 0.51              |
| 1:E:128:LYS:NZ   | 1:E:234:ILE:HB   | 2.26                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:185:VAL:HG12 | 1:E:189:ASP:OD1  | 2.10                     | 0.51              |
| 2:F:195:ILE:HG12 | 2:F:205:LEU:HD12 | 1.92                     | 0.51              |
| 3:H:538:UNK:C    | 3:H:540:UNK:N    | 2.66                     | 0.51              |
| 4:J:195:UNK:O    | 4:J:198:UNK:CB   | 2.59                     | 0.51              |
| 1:A:127:SER:O    | 1:A:127:SER:OG   | 2.24                     | 0.51              |
| 1:A:203:GLU:OE2  | 2:F:312:LEU:N    | 2.43                     | 0.51              |
| 2:B:362:TYR:OH   | 6:B:501:ADP:C6   | 2.61                     | 0.51              |
| 1:C:17:SER:HA    | 1:C:378:ARG:HH22 | 1.74                     | 0.51              |
| 2:F:166:THR:HG22 | 2:F:226:GLN:HE22 | 1.75                     | 0.51              |
| 1:C:17:SER:C     | 1:C:378:ARG:HH12 | 2.16                     | 0.51              |
| 1:C:378:ARG:HA   | 1:C:381:THR:OG1  | 2.11                     | 0.51              |
| 2:D:429:VAL:O    | 2:D:433:PHE:N    | 2.44                     | 0.51              |
| 1:A:132:GLN:HG2  | 2:B:425:ASP:CA   | 2.40                     | 0.51              |
| 2:B:129:VAL:HA   | 2:B:291:ILE:HA   | 1.92                     | 0.51              |
| 2:B:382:MET:HG3  | 2:B:383:SER:H    | 1.76                     | 0.51              |
| 2:D:182:LEU:HD21 | 2:D:195:ILE:HA   | 1.93                     | 0.51              |
| 2:D:188:GLN:HE22 | 2:D:213:ARG:C    | 2.19                     | 0.51              |
| 4:J:369:UNK:C    | 4:J:371:UNK:N    | 2.69                     | 0.51              |
| 1:A:123:GLY:N    | 2:B:411:LEU:H    | 2.08                     | 0.51              |
| 2:B:43:SER:H     | 2:B:46:MET:HG2   | 1.76                     | 0.51              |
| 1:C:427:LYS:HB3  | 1:C:431:GLU:OE1  | 2.10                     | 0.51              |
| 2:D:63:ILE:HG12  | 2:D:68:ILE:HD13  | 1.93                     | 0.51              |
| 2:D:181:SER:O    | 2:D:185:ASP:N    | 2.44                     | 0.51              |
| 2:D:439:SER:O    | 2:D:443:MET:HB2  | 2.10                     | 0.51              |
| 1:E:27:ASP:OD1   | 1:E:31:LEU:N     | 2.44                     | 0.51              |
| 1:E:302:ASP:OD1  | 1:E:303:GLU:N    | 2.43                     | 0.51              |
| 5:K:249:PRO:O    | 5:K:253:MET:N    | 2.44                     | 0.51              |
| 1:A:232:GLU:HA   | 1:A:260:LYS:HD3  | 1.92                     | 0.51              |
| 2:B:400:ARG:HD3  | 6:B:501:ADP:O1B  | 2.11                     | 0.51              |
| 2:B:123:PHE:O    | 2:B:126:SER:OG   | 2.21                     | 0.51              |
| 2:B:369:GLN:HA   | 2:B:372:ARG:HG2  | 1.92                     | 0.51              |
| 2:B:380:VAL:HG12 | 2:B:381:GLU:H    | 1.75                     | 0.51              |
| 2:D:172:TYR:HE2  | 2:D:174:LEU:HD13 | 1.76                     | 0.51              |
| 2:F:282:GLU:HA   | 2:F:285:GLU:HB3  | 1.92                     | 0.51              |
| 3:H:235:UNK:O    | 3:H:239:UNK:N    | 2.44                     | 0.51              |
| 1:A:221:ARG:HD2  | 1:A:222:ILE:N    | 2.25                     | 0.50              |
| 1:A:492:LEU:HD13 | 1:A:528:VAL:HG21 | 1.93                     | 0.50              |
| 2:B:43:SER:OG    | 2:B:46:MET:HE2   | 2.11                     | 0.50              |
| 1:C:42:GLN:O     | 1:C:45:ALA:HB3   | 2.10                     | 0.50              |
| 1:C:49:CYS:HB2   | 1:C:359:MET:HG3  | 1.93                     | 0.50              |
| 1:E:10:THR:OG1   | 1:E:11:LYS:N     | 2.43                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:190:VAL:O    | 1:E:204:GLY:HA3  | 2.11                     | 0.50              |
| 1:E:247:ASN:O    | 1:E:269:THR:N    | 2.44                     | 0.50              |
| 1:E:341:THR:HA   | 2:F:336:ARG:HH21 | 1.76                     | 0.50              |
| 2:F:286:GLU:OE2  | 2:F:288:LYS:HE3  | 2.11                     | 0.50              |
| 2:B:132:LYS:HG3  | 2:B:239:VAL:HG12 | 1.92                     | 0.50              |
| 2:B:236:LYS:NZ   | 2:B:238:VAL:HA   | 2.26                     | 0.50              |
| 2:B:348:ILE:O    | 2:B:351:LEU:N    | 2.44                     | 0.50              |
| 1:C:58:SER:C     | 1:C:59:LYS:HG3   | 2.37                     | 0.50              |
| 1:C:185:VAL:HG21 | 1:C:202:ARG:HE   | 1.77                     | 0.50              |
| 1:E:93:PHE:CD2   | 1:E:95:PRO:HD3   | 2.46                     | 0.50              |
| 1:E:129:GLU:OE2  | 1:E:196:ASN:N    | 2.44                     | 0.50              |
| 1:E:423:ASP:OD1  | 1:E:423:ASP:N    | 2.41                     | 0.50              |
| 1:E:426:GLU:HG3  | 1:E:429:HIS:ND1  | 2.27                     | 0.50              |
| 1:A:170:PRO:HG2  | 2:B:443:MET:HB3  | 1.94                     | 0.50              |
| 1:A:177:LEU:HD23 | 1:A:194:MET:HE2  | 1.94                     | 0.50              |
| 1:A:499:THR:OG1  | 1:A:500:THR:N    | 2.44                     | 0.50              |
| 2:B:50:LEU:O     | 2:B:53:ARG:N     | 2.44                     | 0.50              |
| 2:B:243:SER:OG   | 2:B:246:GLU:N    | 2.31                     | 0.50              |
| 3:H:85:UNK:O     | 3:H:90:UNK:N     | 2.44                     | 0.50              |
| 5:K:301:THR:O    | 5:K:305:GLN:CB   | 2.59                     | 0.50              |
| 1:A:201:SER:HB2  | 2:F:309:PHE:CB   | 2.39                     | 0.50              |
| 2:B:151:ALA:HA   | 2:B:179:ILE:HG13 | 1.94                     | 0.50              |
| 1:C:56:ILE:HG12  | 1:C:324:ALA:HB3  | 1.92                     | 0.50              |
| 2:D:81:THR:O     | 2:D:400:ARG:NH1  | 2.45                     | 0.50              |
| 2:F:424:ASP:OD1  | 2:F:424:ASP:N    | 2.43                     | 0.50              |
| 1:A:105:LYS:C    | 1:A:188:LYS:HD2  | 2.37                     | 0.50              |
| 4:J:217:UNK:HA   | 4:J:220:UNK:CB   | 2.41                     | 0.50              |
| 1:A:162:ARG:O    | 1:A:417:LEU:HD23 | 2.11                     | 0.50              |
| 1:A:487:GLU:HG2  | 1:A:525:LYS:HB2  | 1.93                     | 0.50              |
| 2:B:381:GLU:HG3  | 2:B:382:MET:H    | 1.76                     | 0.50              |
| 1:C:52:ILE:O     | 1:C:55:LEU:HB2   | 2.12                     | 0.50              |
| 1:C:61:MET:HB3   | 1:C:320:GLU:HA   | 1.94                     | 0.50              |
| 2:D:397:THR:CG2  | 2:D:436:GLU:H    | 2.24                     | 0.50              |
| 3:H:59:UNK:O     | 3:H:60:UNK:CB    | 2.60                     | 0.50              |
| 3:H:125:UNK:CB   | 3:H:163:UNK:N    | 2.75                     | 0.50              |
| 5:K:120:GLN:HA   | 5:K:123:GLN:CB   | 2.42                     | 0.50              |
| 5:K:249:PRO:O    | 5:K:253:MET:CB   | 2.60                     | 0.50              |
| 1:A:166:LEU:CD2  | 1:A:456:VAL:HB   | 2.40                     | 0.50              |
| 2:B:145:ILE:HG23 | 2:B:147:ILE:HG23 | 1.93                     | 0.50              |
| 2:B:161:LEU:HB3  | 2:B:172:TYR:CZ   | 2.47                     | 0.50              |
| 1:C:192:TYR:OH   | 1:C:230:LYS:HD2  | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:285:LYS:HG2  | 1:C:289:GLN:NE2  | 2.27                     | 0.50              |
| 1:E:280:ASN:O    | 1:E:284:ASN:N    | 2.32                     | 0.50              |
| 2:B:32:GLY:HA3   | 2:B:46:MET:SD    | 2.52                     | 0.50              |
| 1:C:46:ARG:O     | 1:C:49:CYS:HB3   | 2.12                     | 0.50              |
| 2:D:112:GLU:N    | 2:D:112:GLU:OE2  | 2.45                     | 0.50              |
| 1:A:161:GLY:O    | 1:A:414:HIS:HB2  | 2.12                     | 0.49              |
| 1:C:126:GLU:HB2  | 1:C:128:LYS:HZ2  | 1.75                     | 0.49              |
| 2:D:192:VAL:N    | 2:D:216:ASP:OD1  | 2.45                     | 0.49              |
| 2:D:280:VAL:HA   | 2:D:283:TRP:HB2  | 1.92                     | 0.49              |
| 2:F:282:GLU:O    | 2:F:286:GLU:N    | 2.28                     | 0.49              |
| 1:A:132:GLN:CG   | 2:B:425:ASP:O    | 2.60                     | 0.49              |
| 1:A:190:PRO:HG3  | 1:A:394:PRO:HG3  | 1.94                     | 0.49              |
| 1:A:472:ILE:HG23 | 1:A:473:ILE:HD12 | 1.94                     | 0.49              |
| 1:C:133:GLY:HA3  | 1:C:161:LEU:HB3  | 1.94                     | 0.49              |
| 1:C:389:GLU:OE1  | 1:C:427:LYS:HG3  | 2.11                     | 0.49              |
| 2:D:146:GLN:HE21 | 2:D:195:ILE:HG22 | 1.76                     | 0.49              |
| 2:D:170:THR:HG21 | 2:D:198:ALA:HA   | 1.94                     | 0.49              |
| 1:E:418:LYS:HE2  | 1:E:418:LYS:HA   | 1.94                     | 0.49              |
| 3:H:466:UNK:CB   | 3:H:507:UNK:HA   | 2.42                     | 0.49              |
| 1:A:132:GLN:HG3  | 2:B:425:ASP:C    | 2.37                     | 0.49              |
| 2:B:378:GLU:N    | 2:B:378:GLU:OE2  | 2.45                     | 0.49              |
| 1:C:390:ALA:HB2  | 1:C:426:GLU:HA   | 1.94                     | 0.49              |
| 2:D:149:ARG:HA   | 2:D:182:LEU:HB2  | 1.95                     | 0.49              |
| 2:D:389:VAL:HG11 | 2:D:423:VAL:HG13 | 1.94                     | 0.49              |
| 3:H:650:UNK:HA   | 3:H:653:UNK:CB   | 2.42                     | 0.49              |
| 1:A:148:GLY:O    | 1:A:151:VAL:HG22 | 2.12                     | 0.49              |
| 1:A:231:GLY:H    | 1:A:261:THR:N    | 2.10                     | 0.49              |
| 1:A:397:LEU:HB3  | 1:A:423:PRO:CB   | 2.40                     | 0.49              |
| 1:A:494:GLU:HG3  | 1:A:498:LYS:HZ1  | 1.77                     | 0.49              |
| 2:B:290:GLU:OE1  | 2:B:290:GLU:N    | 2.46                     | 0.49              |
| 2:B:304:LEU:O    | 2:B:336:ARG:HB2  | 2.11                     | 0.49              |
| 1:C:30:GLY:C     | 1:C:31:LEU:HD22  | 2.37                     | 0.49              |
| 2:D:199:THR:HG1  | 2:D:233:GLN:HE22 | 1.60                     | 0.49              |
| 2:D:447:GLN:HB3  | 2:D:451:LEU:HD23 | 1.93                     | 0.49              |
| 2:F:207:ARG:HE   | 2:F:235:ARG:HH21 | 1.59                     | 0.49              |
| 2:B:380:VAL:HG12 | 2:B:381:GLU:N    | 2.27                     | 0.49              |
| 1:C:67:LEU:HD23  | 2:D:440:THR:CG2  | 2.41                     | 0.49              |
| 1:C:386:ILE:HD11 | 1:C:391:LEU:HB2  | 1.93                     | 0.49              |
| 1:C:390:ALA:HA   | 1:C:427:LYS:HG2  | 1.94                     | 0.49              |
| 1:E:310:GLU:HB3  | 2:F:111:LEU:HD21 | 1.93                     | 0.49              |
| 2:F:41:GLN:NE2   | 2:F:41:GLN:O     | 2.45                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:84:THR:N     | 6:F:501:ADP:O2A  | 2.45                     | 0.49              |
| 2:B:186:LYS:NZ   | 2:B:188:GLN:OE1  | 2.31                     | 0.49              |
| 1:C:271:ILE:HG12 | 1:C:275:LEU:HD13 | 1.95                     | 0.49              |
| 1:E:177:PHE:O    | 1:E:181:GLN:HB2  | 2.13                     | 0.49              |
| 5:K:124:GLN:O    | 5:K:128:GLY:N    | 2.37                     | 0.49              |
| 5:K:159:ARG:O    | 5:K:163:GLU:N    | 2.42                     | 0.49              |
| 5:K:341:THR:CB   | 5:K:342:PRO:CD   | 2.90                     | 0.49              |
| 1:A:115:SER:OG   | 1:A:460:ARG:HG3  | 2.12                     | 0.49              |
| 1:A:183:GLN:NE2  | 1:A:183:GLN:O    | 2.46                     | 0.49              |
| 1:A:207:THR:O    | 1:A:210:LEU:HB2  | 2.12                     | 0.49              |
| 1:A:210:LEU:HD22 | 1:A:214:PHE:CE1  | 2.47                     | 0.49              |
| 1:A:314:GLU:HB3  | 1:A:318:TYR:CE2  | 2.48                     | 0.49              |
| 1:C:367:THR:O    | 1:C:370:GLU:HG2  | 2.13                     | 0.49              |
| 1:C:443:SER:OG   | 1:C:444:ALA:N    | 2.46                     | 0.49              |
| 2:D:81:THR:C     | 2:D:400:ARG:HE   | 2.21                     | 0.49              |
| 2:D:236:LYS:HE3  | 2:D:238:VAL:HA   | 1.94                     | 0.49              |
| 2:D:318:SER:OG   | 2:D:319:ASP:N    | 2.38                     | 0.49              |
| 1:A:115:SER:HB2  | 1:A:460:ARG:O    | 2.13                     | 0.49              |
| 1:A:216:ARG:NH2  | 1:A:397:LEU:HD21 | 2.28                     | 0.49              |
| 2:B:27:HIS:CD2   | 2:B:45:GLY:HA3   | 2.48                     | 0.49              |
| 2:B:59:VAL:O     | 2:B:63:ILE:HG12  | 2.12                     | 0.49              |
| 1:C:317:ARG:HH11 | 1:C:318:ALA:HB2  | 1.78                     | 0.49              |
| 1:C:361:ILE:O    | 1:C:361:ILE:HG13 | 2.13                     | 0.49              |
| 2:D:73:VAL:CG1   | 2:D:325:ILE:HG22 | 2.42                     | 0.49              |
| 1:A:111:GLN:HG2  | 1:A:428:ALA:HB3  | 1.94                     | 0.49              |
| 1:A:150:ILE:O    | 1:A:154:ILE:HG12 | 2.13                     | 0.49              |
| 1:A:208:GLU:OE1  | 1:A:208:GLU:N    | 2.28                     | 0.49              |
| 1:A:399:VAL:O    | 1:A:425:VAL:HG21 | 2.13                     | 0.49              |
| 1:A:525:LYS:O    | 1:A:529:GLU:HG2  | 2.11                     | 0.49              |
| 1:C:219:GLU:O    | 1:C:221:VAL:N    | 2.39                     | 0.49              |
| 1:C:363:THR:HG23 | 1:C:364:MET:O    | 2.13                     | 0.49              |
| 1:A:122:LEU:O    | 1:A:135:SER:HA   | 2.13                     | 0.49              |
| 1:C:122:LEU:HA   | 1:C:293:GLU:O    | 2.13                     | 0.49              |
| 1:C:426:GLU:OE1  | 1:C:426:GLU:N    | 2.45                     | 0.49              |
| 2:D:110:SER:OG   | 2:D:113:MET:N    | 2.46                     | 0.49              |
| 2:F:43:SER:O     | 2:F:46:MET:N     | 2.46                     | 0.49              |
| 2:F:149:ARG:HB2  | 2:F:150:PRO:HD3  | 1.95                     | 0.49              |
| 2:F:283:TRP:HA   | 2:F:286:GLU:OE2  | 2.13                     | 0.49              |
| 3:H:510:UNK:O    | 3:H:513:UNK:CB   | 2.60                     | 0.49              |
| 1:A:218:ILE:HB   | 1:A:338:LEU:HB3  | 1.94                     | 0.48              |
| 1:C:27:ASP:HB3   | 1:C:30:GLY:H     | 1.78                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:187:ALA:O    | 1:C:212:GLU:HB2  | 2.13                     | 0.48              |
| 1:A:142:ASN:H    | 1:A:142:ASN:ND2  | 2.10                     | 0.48              |
| 1:A:256:ILE:HG13 | 1:A:268:LEU:O    | 2.13                     | 0.48              |
| 1:C:134:GLU:OE1  | 1:C:209:TYR:HB2  | 2.12                     | 0.48              |
| 2:D:130:ARG:NH2  | 2:D:242:VAL:HG21 | 2.26                     | 0.48              |
| 2:D:311:PHE:HD2  | 2:D:312:LEU:HD23 | 1.78                     | 0.48              |
| 1:A:166:LEU:O    | 1:A:450:LEU:HA   | 2.13                     | 0.48              |
| 1:A:226:LYS:HE3  | 1:A:293:ALA:HB3  | 1.95                     | 0.48              |
| 2:B:105:GLY:N    | 2:B:300:GLU:OE2  | 2.46                     | 0.48              |
| 1:C:70:GLY:O     | 2:D:447:GLN:OE1  | 2.31                     | 0.48              |
| 1:C:128:LYS:O    | 1:C:231:LYS:HA   | 2.13                     | 0.48              |
| 1:C:134:GLU:OE1  | 1:C:208:THR:OG1  | 2.30                     | 0.48              |
| 2:D:139:GLU:CD   | 2:D:208:SER:HG   | 2.22                     | 0.48              |
| 2:D:316:LEU:HD21 | 2:D:353:ARG:HH22 | 1.78                     | 0.48              |
| 1:E:127:THR:OG1  | 1:E:233:GLU:OE1  | 2.30                     | 0.48              |
| 1:E:406:SER:O    | 1:E:406:SER:OG   | 2.31                     | 0.48              |
| 4:J:140:UNK:O    | 4:J:144:UNK:N    | 2.46                     | 0.48              |
| 1:A:135:SER:H    | 2:B:412:VAL:HG11 | 1.77                     | 0.48              |
| 2:B:39:PRO:HG2   | 2:B:50:LEU:HD23  | 1.95                     | 0.48              |
| 1:C:124:ILE:O    | 1:C:235:ILE:HG13 | 2.14                     | 0.48              |
| 2:D:102:ALA:HA   | 2:D:297:PHE:O    | 2.13                     | 0.48              |
| 1:E:24:LEU:O     | 1:E:46:ARG:NH2   | 2.35                     | 0.48              |
| 1:E:181:GLN:NE2  | 1:E:185:VAL:O    | 2.47                     | 0.48              |
| 1:A:465:THR:HG23 | 1:A:468:GLU:H    | 1.77                     | 0.48              |
| 1:A:546:ALA:HA   | 1:A:549:GLN:HB3  | 1.95                     | 0.48              |
| 2:B:124:ARG:HH21 | 2:B:244:LEU:HB3  | 1.79                     | 0.48              |
| 2:B:195:ILE:HD12 | 2:B:206:GLY:HA2  | 1.95                     | 0.48              |
| 2:B:427:LYS:O    | 2:B:431:SER:HB3  | 2.13                     | 0.48              |
| 1:C:69:ALA:HA    | 1:C:348:HIS:CE1  | 2.49                     | 0.48              |
| 3:H:97:UNK:O     | 3:H:101:UNK:N    | 2.47                     | 0.48              |
| 4:J:217:UNK:O    | 4:J:220:UNK:CA   | 2.61                     | 0.48              |
| 1:A:140:GLN:C    | 1:A:142:ASN:N    | 2.71                     | 0.48              |
| 1:A:218:ILE:H    | 1:A:423:PRO:HD3  | 1.77                     | 0.48              |
| 2:B:35:ASP:OD2   | 2:B:35:ASP:N     | 2.46                     | 0.48              |
| 2:B:43:SER:O     | 2:B:46:MET:HG2   | 2.14                     | 0.48              |
| 2:B:181:SER:OG   | 2:B:211:ARG:NE   | 2.37                     | 0.48              |
| 2:B:416:ARG:HH12 | 2:B:422:GLN:HE21 | 1.61                     | 0.48              |
| 1:C:40:VAL:HG12  | 1:C:41:GLY:N     | 2.28                     | 0.48              |
| 2:D:61:GLU:OE1   | 1:E:415:LEU:HD23 | 2.13                     | 0.48              |
| 2:D:390:LEU:HD13 | 2:D:426:ILE:HD12 | 1.96                     | 0.48              |
| 2:D:440:THR:O    | 2:D:444:LYS:HG2  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:53:VAL:HG12  | 1:E:57:LYS:HZ2   | 1.77                     | 0.48              |
| 1:E:137:GLU:OE1  | 1:E:137:GLU:N    | 2.46                     | 0.48              |
| 3:H:88:UNK:HA    | 3:H:91:UNK:CB    | 2.44                     | 0.48              |
| 3:H:176:UNK:CB   | 3:H:226:UNK:O    | 2.61                     | 0.48              |
| 5:K:192:LEU:C    | 5:K:194:GLY:N    | 2.71                     | 0.48              |
| 1:A:153:LEU:HB3  | 1:A:159:MET:SD   | 2.53                     | 0.48              |
| 2:B:24:ALA:N     | 2:B:403:ILE:HG21 | 2.28                     | 0.48              |
| 2:B:417:LYS:HD2  | 2:B:417:LYS:HA   | 1.70                     | 0.48              |
| 1:C:66:VAL:HG22  | 1:C:67:LEU:N     | 2.28                     | 0.48              |
| 1:C:123:ARG:CB   | 1:C:293:GLU:HB3  | 2.42                     | 0.48              |
| 2:D:29:ARG:C     | 2:D:44:GLN:HB3   | 2.39                     | 0.48              |
| 3:H:637:UNK:O    | 3:H:640:UNK:CA   | 2.62                     | 0.48              |
| 1:A:207:THR:O    | 1:A:211:MET:HG2  | 2.14                     | 0.48              |
| 2:B:134:GLU:O    | 2:B:207:ARG:NH1  | 2.47                     | 0.48              |
| 2:B:185:ASP:OD2  | 2:B:187:VAL:HB   | 2.13                     | 0.48              |
| 1:C:189:ASP:OD1  | 1:C:205:ARG:HG3  | 2.13                     | 0.48              |
| 2:D:81:THR:CB    | 6:D:501:ADP:HO3' | 2.27                     | 0.48              |
| 2:D:218:MET:HG2  | 2:D:219:GLY:N    | 2.29                     | 0.48              |
| 1:E:132:GLU:HG2  | 1:E:190:VAL:HG23 | 1.95                     | 0.48              |
| 5:K:31:THR:O     | 5:K:34:SER:CB    | 2.62                     | 0.48              |
| 2:B:159:GLY:HA3  | 2:B:174:LEU:HB2  | 1.95                     | 0.48              |
| 2:B:161:LEU:HD12 | 2:B:174:LEU:HD11 | 1.94                     | 0.48              |
| 1:E:431:GLU:O    | 1:E:435:GLU:HG2  | 2.14                     | 0.48              |
| 3:H:444:UNK:O    | 3:H:447:UNK:N    | 2.47                     | 0.48              |
| 1:A:133:ALA:CB   | 2:B:429:VAL:H    | 2.17                     | 0.48              |
| 1:A:163:ALA:HB2  | 1:A:413:LEU:C    | 2.39                     | 0.48              |
| 1:A:203:GLU:N    | 2:F:308:SER:OG   | 2.47                     | 0.48              |
| 1:A:211:MET:HA   | 1:A:214:PHE:CD2  | 2.49                     | 0.48              |
| 1:A:491:HIS:O    | 1:A:494:GLU:HG2  | 2.13                     | 0.48              |
| 2:B:272:VAL:O    | 2:B:276:ILE:HG13 | 2.14                     | 0.48              |
| 2:B:339:SER:O    | 2:B:339:SER:OG   | 2.25                     | 0.48              |
| 1:C:52:ILE:HD12  | 1:C:359:MET:HE3  | 1.96                     | 0.48              |
| 5:K:103:LEU:O    | 5:K:105:ALA:N    | 2.47                     | 0.48              |
| 2:D:126:SER:O    | 2:D:126:SER:OG   | 2.21                     | 0.47              |
| 2:D:351:LEU:HD23 | 2:D:354:LEU:HD12 | 1.96                     | 0.47              |
| 2:D:390:LEU:O    | 2:D:393:ILE:HB   | 2.13                     | 0.47              |
| 1:E:283:VAL:O    | 1:E:287:ILE:HD12 | 2.14                     | 0.47              |
| 1:A:169:PRO:HD2  | 1:A:458:ILE:HD12 | 1.96                     | 0.47              |
| 1:A:191:PHE:CE2  | 1:A:424:ILE:HG23 | 2.49                     | 0.47              |
| 1:A:205:LYS:HG2  | 1:A:206:LYS:N    | 2.26                     | 0.47              |
| 2:B:372:ARG:HD2  | 2:B:381:GLU:OE1  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:400:ARG:CZ   | 6:B:501:ADP:O3A  | 2.61                     | 0.47              |
| 1:C:122:LEU:O    | 1:C:237:ASP:HA   | 2.14                     | 0.47              |
| 1:E:20:HIS:O     | 1:E:22:LYS:NZ    | 2.34                     | 0.47              |
| 5:K:301:THR:C    | 5:K:305:GLN:CB   | 2.87                     | 0.47              |
| 1:A:196:GLY:N    | 1:A:403:HIS:H    | 2.12                     | 0.47              |
| 2:B:138:ILE:HD11 | 2:B:205:LEU:HD22 | 1.96                     | 0.47              |
| 2:B:142:VAL:HG22 | 2:B:163:LEU:HD13 | 1.95                     | 0.47              |
| 2:B:149:ARG:HH21 | 2:B:186:LYS:HD3  | 1.79                     | 0.47              |
| 2:B:201:LYS:HG3  | 2:B:202:ILE:H    | 1.80                     | 0.47              |
| 1:C:64:ARG:NH2   | 1:C:357:ARG:HH21 | 2.11                     | 0.47              |
| 2:D:124:ARG:NH2  | 2:D:273:ARG:HD2  | 2.29                     | 0.47              |
| 2:D:152:THR:H    | 2:D:157:LYS:HD2  | 1.80                     | 0.47              |
| 2:D:172:TYR:HA   | 2:D:201:LYS:O    | 2.15                     | 0.47              |
| 1:E:40:VAL:N     | 6:E:501:ADP:HN62 | 2.03                     | 0.47              |
| 1:E:184:ARG:NH2  | 1:E:217:ALA:O    | 2.46                     | 0.47              |
| 2:F:34:ASP:OD2   | 2:F:38:GLU:HB2   | 2.14                     | 0.47              |
| 4:J:217:UNK:C    | 4:J:220:UNK:N    | 2.77                     | 0.47              |
| 4:J:397:GLY:C    | 4:J:453:UNK:CB   | 2.87                     | 0.47              |
| 5:K:77:ASP:O     | 5:K:80:PHE:CA    | 2.63                     | 0.47              |
| 1:A:142:ASN:OD1  | 2:B:400:ARG:N    | 2.46                     | 0.47              |
| 1:A:204:ILE:HG23 | 2:F:119:LEU:HD12 | 1.96                     | 0.47              |
| 1:A:266:LYS:HD3  | 1:A:326:VAL:HG22 | 1.97                     | 0.47              |
| 1:A:275:PHE:N    | 1:A:296:GLY:H    | 1.97                     | 0.47              |
| 2:B:146:GLN:NE2  | 2:B:187:VAL:H    | 2.12                     | 0.47              |
| 2:B:400:ARG:NH2  | 6:B:501:ADP:PA   | 2.87                     | 0.47              |
| 2:D:138:ILE:HG22 | 2:D:139:GLU:N    | 2.29                     | 0.47              |
| 2:F:202:ILE:HG13 | 2:F:202:ILE:O    | 2.15                     | 0.47              |
| 1:A:133:ALA:HA   | 2:B:429:VAL:HG23 | 1.95                     | 0.47              |
| 1:A:170:PRO:HB3  | 1:A:433:ASN:N    | 2.29                     | 0.47              |
| 1:A:196:GLY:HA2  | 1:A:403:HIS:HB3  | 1.97                     | 0.47              |
| 1:A:203:GLU:HB3  | 2:F:312:LEU:HG   | 1.95                     | 0.47              |
| 1:A:483:ASN:HD22 | 1:A:521:ASP:CG   | 2.21                     | 0.47              |
| 2:B:161:LEU:HB2  | 2:B:174:LEU:HG   | 1.96                     | 0.47              |
| 2:B:383:SER:CB   | 2:B:423:VAL:HA   | 2.44                     | 0.47              |
| 2:B:397:THR:HG23 | 2:B:398:SER:N    | 2.29                     | 0.47              |
| 2:D:77:GLY:HA2   | 6:D:501:ADP:PB   | 2.54                     | 0.47              |
| 1:E:135:VAL:HG22 | 1:E:159:ILE:HD13 | 1.95                     | 0.47              |
| 1:E:285:LYS:HA   | 1:E:288:ASP:OD2  | 2.14                     | 0.47              |
| 2:F:138:ILE:HD12 | 2:F:233:GLN:HA   | 1.96                     | 0.47              |
| 3:H:362:UNK:O    | 3:H:366:UNK:N    | 2.47                     | 0.47              |
| 4:J:319:UNK:HA   | 4:J:322:UNK:CB   | 2.45                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:140:GLN:CD   | 2:B:434:LEU:HD12 | 2.39                     | 0.47              |
| 2:B:136:GLU:OE1  | 2:B:235:ARG:NH1  | 2.47                     | 0.47              |
| 2:B:393:ILE:O    | 2:B:397:THR:HG22 | 2.15                     | 0.47              |
| 1:C:112:LEU:HD23 | 1:C:112:LEU:HA   | 1.67                     | 0.47              |
| 2:D:60:LEU:HG    | 2:D:90:MET:HE3   | 1.96                     | 0.47              |
| 2:D:139:GLU:HB3  | 2:D:231:GLU:OE1  | 2.14                     | 0.47              |
| 2:D:170:THR:CG2  | 2:D:198:ALA:HA   | 2.45                     | 0.47              |
| 2:D:380:VAL:HG21 | 2:D:406:ILE:HD11 | 1.97                     | 0.47              |
| 1:A:120:LYS:O    | 1:A:183:GLN:HG2  | 2.15                     | 0.47              |
| 1:A:282:ARG:NH2  | 1:A:303:ARG:HB3  | 2.29                     | 0.47              |
| 2:B:141:GLU:O    | 2:B:165:THR:OG1  | 2.18                     | 0.47              |
| 2:B:383:SER:OG   | 2:B:421:VAL:HG13 | 2.15                     | 0.47              |
| 1:C:26:LEU:HD21  | 1:C:46:ARG:CZ    | 2.44                     | 0.47              |
| 2:D:142:VAL:HG21 | 2:D:163:LEU:HD12 | 1.95                     | 0.47              |
| 2:D:279:LYS:O    | 2:D:282:GLU:HG3  | 2.14                     | 0.47              |
| 2:D:368:LYS:NZ   | 2:D:388:THR:HA   | 2.30                     | 0.47              |
| 2:D:428:ARG:NH1  | 2:D:431:SER:OG   | 2.48                     | 0.47              |
| 1:E:14:ARG:NH1   | 1:E:95:PRO:O     | 2.48                     | 0.47              |
| 3:H:369:UNK:O    | 3:H:373:UNK:CA   | 2.61                     | 0.47              |
| 4:J:196:UNK:O    | 4:J:199:UNK:CB   | 2.63                     | 0.47              |
| 4:J:218:UNK:O    | 4:J:221:UNK:N    | 2.48                     | 0.47              |
| 5:K:76:ALA:O     | 5:K:79:ALA:HB3   | 2.15                     | 0.47              |
| 1:A:116:HIS:CG   | 1:A:117:SER:N    | 2.83                     | 0.47              |
| 1:A:144:ARG:HD2  | 2:B:407:THR:N    | 2.28                     | 0.47              |
| 1:A:256:ILE:HD11 | 1:A:269:LYS:HB3  | 1.97                     | 0.47              |
| 1:A:453:LEU:HB3  | 1:A:456:VAL:HG21 | 1.96                     | 0.47              |
| 1:A:470:LYS:HA   | 1:A:474:LYS:CB   | 2.35                     | 0.47              |
| 1:A:543:LYS:O    | 1:A:547:ASP:N    | 2.33                     | 0.47              |
| 1:C:26:LEU:HG    | 1:C:31:LEU:HA    | 1.96                     | 0.47              |
| 1:C:77:THR:HG22  | 1:C:300:PHE:CE2  | 2.49                     | 0.47              |
| 2:D:384:GLU:HA   | 2:D:387:TYR:HD2  | 1.80                     | 0.47              |
| 1:E:417:ALA:HB1  | 1:E:422:LYS:HB2  | 1.97                     | 0.47              |
| 2:F:130:ARG:HE   | 2:F:290:GLU:HB3  | 1.80                     | 0.47              |
| 4:J:457:UNK:O    | 4:J:460:UNK:CB   | 2.62                     | 0.47              |
| 1:A:138:VAL:HG21 | 2:B:432:LEU:H    | 1.79                     | 0.47              |
| 1:A:144:ARG:CD   | 2:B:407:THR:H    | 2.26                     | 0.47              |
| 2:B:120:THR:O    | 2:B:124:ARG:HG2  | 2.15                     | 0.47              |
| 2:B:136:GLU:HG3  | 2:B:233:GLN:NE2  | 2.30                     | 0.47              |
| 1:C:130:VAL:HA   | 1:C:193:ILE:O    | 2.15                     | 0.47              |
| 1:C:185:VAL:HG12 | 1:C:205:ARG:NH1  | 2.29                     | 0.47              |
| 1:C:240:LEU:O    | 1:C:243:LEU:HG   | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:315:LEU:C    | 1:C:319:LEU:HD21 | 2.40                     | 0.47              |
| 1:E:157:VAL:HG12 | 1:E:159:ILE:HG13 | 1.97                     | 0.47              |
| 1:E:180:LEU:HD12 | 1:E:202:ARG:H    | 1.80                     | 0.47              |
| 2:F:383:SER:N    | 2:F:420:GLU:OE2  | 2.48                     | 0.47              |
| 2:F:416:ARG:C    | 2:F:417:LYS:HG2  | 2.40                     | 0.47              |
| 4:J:352:UNK:O    | 4:J:355:UNK:N    | 2.47                     | 0.47              |
| 2:B:443:MET:O    | 2:B:447:GLN:N    | 2.46                     | 0.47              |
| 1:C:236:GLN:NE2  | 1:C:237:ASP:O    | 2.48                     | 0.47              |
| 1:C:236:GLN:OE1  | 1:C:238:VAL:HG13 | 2.14                     | 0.47              |
| 1:C:403:LEU:HD12 | 1:C:403:LEU:HA   | 1.74                     | 0.47              |
| 2:D:207:ARG:HG3  | 2:D:235:ARG:HD2  | 1.96                     | 0.47              |
| 2:D:383:SER:OG   | 2:D:422:GLN:HA   | 2.15                     | 0.47              |
| 2:F:310:SER:O    | 2:F:314:ARG:NE   | 2.40                     | 0.47              |
| 5:K:261:VAL:C    | 5:K:264:ALA:HB3  | 2.28                     | 0.47              |
| 1:A:124:LEU:HD23 | 1:A:135:SER:CB   | 2.45                     | 0.46              |
| 2:B:334:ARG:NH1  | 2:B:338:THR:O    | 2.47                     | 0.46              |
| 1:C:55:LEU:HD11  | 1:C:354:LEU:CD1  | 2.45                     | 0.46              |
| 1:C:138:LEU:HD12 | 1:C:174:PRO:HA   | 1.97                     | 0.46              |
| 2:D:434:LEU:CD1  | 2:D:438:ARG:HB3  | 2.42                     | 0.46              |
| 1:E:205:ARG:HB3  | 1:E:212:GLU:OE2  | 2.15                     | 0.46              |
| 2:F:389:VAL:HG11 | 2:F:423:VAL:HG23 | 1.97                     | 0.46              |
| 2:F:424:ASP:HA   | 2:F:427:LYS:HB2  | 1.97                     | 0.46              |
| 2:B:319:ASP:OD1  | 2:B:319:ASP:N    | 2.45                     | 0.46              |
| 2:D:197:LYS:HZ3  | 2:D:200:GLY:H    | 1.62                     | 0.46              |
| 2:F:134:GLU:HG3  | 2:F:237:GLU:HA   | 1.97                     | 0.46              |
| 4:J:196:UNK:O    | 4:J:199:UNK:N    | 2.49                     | 0.46              |
| 5:K:383:ARG:C    | 5:K:385:ASP:N    | 2.70                     | 0.46              |
| 1:A:402:VAL:O    | 1:A:402:VAL:HG12 | 2.15                     | 0.46              |
| 1:A:467:GLN:CD   | 1:A:467:GLN:N    | 2.73                     | 0.46              |
| 2:B:154:THR:HA   | 2:B:176:THR:HG23 | 1.97                     | 0.46              |
| 2:B:374:ARG:HH12 | 2:B:405:LEU:N    | 2.14                     | 0.46              |
| 1:C:190:VAL:O    | 1:C:202:ARG:HG3  | 2.15                     | 0.46              |
| 2:D:158:VAL:HG21 | 2:D:172:TYR:CE2  | 2.50                     | 0.46              |
| 2:D:440:THR:O    | 2:D:444:LYS:N    | 2.28                     | 0.46              |
| 1:E:132:GLU:O    | 1:E:166:GLY:HA3  | 2.15                     | 0.46              |
| 3:H:216:UNK:C    | 3:H:218:UNK:N    | 2.76                     | 0.46              |
| 4:J:327:UNK:HA   | 4:J:331:GLY:N    | 2.30                     | 0.46              |
| 1:A:133:ALA:CB   | 2:B:427:LYS:H    | 2.14                     | 0.46              |
| 1:A:191:PHE:CD2  | 1:A:424:ILE:HG23 | 2.50                     | 0.46              |
| 1:A:414:HIS:CG   | 1:A:415:ARG:H    | 2.32                     | 0.46              |
| 1:A:466:PRO:HB2  | 1:A:467:GLN:NE2  | 2.31                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:177:PHE:O    | 1:C:181:GLN:HB3  | 2.14                     | 0.46              |
| 2:D:84:THR:HG22  | 2:D:297:PHE:CE2  | 2.48                     | 0.46              |
| 2:D:299:ASP:OD1  | 2:D:299:ASP:N    | 2.45                     | 0.46              |
| 1:E:214:ASP:OD1  | 1:E:215:LEU:N    | 2.46                     | 0.46              |
| 3:H:125:UNK:HA   | 3:H:163:UNK:CA   | 2.46                     | 0.46              |
| 3:H:602:UNK:HA   | 3:H:605:UNK:CB   | 2.46                     | 0.46              |
| 4:J:323:UNK:HA   | 4:J:326:UNK:CB   | 2.44                     | 0.46              |
| 2:B:80:GLY:O     | 2:B:82:GLY:N     | 2.49                     | 0.46              |
| 2:B:84:THR:OG1   | 6:B:501:ADP:O1A  | 2.28                     | 0.46              |
| 2:B:142:VAL:HG13 | 2:B:163:LEU:HB2  | 1.96                     | 0.46              |
| 2:B:432:LEU:HD23 | 2:B:433:PHE:CE2  | 2.50                     | 0.46              |
| 2:B:443:MET:HA   | 2:B:446:TYR:HB3  | 1.97                     | 0.46              |
| 1:C:6:VAL:HG12   | 1:C:7:LYS:H      | 1.81                     | 0.46              |
| 1:C:45:ALA:HA    | 1:C:68:LEU:HD21  | 1.97                     | 0.46              |
| 2:D:168:MET:HG3  | 2:D:169:GLU:O    | 2.16                     | 0.46              |
| 1:E:128:LYS:O    | 1:E:231:LYS:HA   | 2.16                     | 0.46              |
| 2:F:140:GLY:O    | 2:F:142:VAL:HG23 | 2.15                     | 0.46              |
| 2:F:329:ASN:OD1  | 2:F:329:ASN:N    | 2.46                     | 0.46              |
| 1:A:165:LEU:O    | 1:A:453:LEU:HD23 | 2.16                     | 0.46              |
| 1:A:466:PRO:HB2  | 1:A:467:GLN:HE22 | 1.79                     | 0.46              |
| 2:B:374:ARG:NH1  | 2:B:405:LEU:H    | 2.13                     | 0.46              |
| 1:C:205:ARG:NE   | 1:C:217:ALA:H    | 2.14                     | 0.46              |
| 2:F:373:ILE:O    | 2:F:377:GLU:N    | 2.37                     | 0.46              |
| 4:J:472:UNK:C    | 4:J:474:UNK:N    | 2.76                     | 0.46              |
| 5:K:170:PRO:CA   | 5:K:173:TYR:CB   | 2.91                     | 0.46              |
| 1:A:132:GLN:HB2  | 2:B:422:GLN:O    | 2.16                     | 0.46              |
| 1:A:141:GLU:OE2  | 1:A:144:ARG:CZ   | 2.63                     | 0.46              |
| 1:A:149:VAL:O    | 1:A:153:LEU:HG   | 2.15                     | 0.46              |
| 1:A:418:GLU:O    | 1:A:420:SER:N    | 2.45                     | 0.46              |
| 2:B:247:ILE:HD12 | 2:B:247:ILE:HA   | 1.83                     | 0.46              |
| 2:F:349:ASP:OD1  | 2:F:349:ASP:N    | 2.46                     | 0.46              |
| 5:K:85:GLU:O     | 5:K:88:GLU:CB    | 2.63                     | 0.46              |
| 1:A:150:ILE:HG12 | 1:A:455:ARG:HH21 | 1.81                     | 0.46              |
| 1:A:341:LEU:HB3  | 1:A:377:ILE:HD13 | 1.98                     | 0.46              |
| 1:A:466:PRO:HA   | 1:A:469:MET:SD   | 2.56                     | 0.46              |
| 2:D:397:THR:OG1  | 2:D:435:ASP:HB3  | 2.16                     | 0.46              |
| 2:F:411:LEU:O    | 2:F:415:LYS:N    | 2.43                     | 0.46              |
| 1:A:275:PHE:H    | 1:A:296:GLY:N    | 1.97                     | 0.46              |
| 1:A:417:LEU:HD13 | 1:A:417:LEU:HA   | 1.81                     | 0.46              |
| 2:B:31:LEU:O     | 2:B:53:ARG:NH2   | 2.42                     | 0.46              |
| 2:B:146:GLN:OE1  | 2:B:187:VAL:N    | 2.49                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:51:VAL:HG21  | 2:D:404:GLN:HG2  | 1.97                     | 0.46              |
| 1:C:377:ILE:HA   | 1:C:380:GLN:NE2  | 2.31                     | 0.46              |
| 2:D:146:GLN:H    | 2:D:149:ARG:NH2  | 2.14                     | 0.46              |
| 2:F:139:GLU:H    | 2:F:234:LYS:NZ   | 2.13                     | 0.46              |
| 2:F:388:THR:OG1  | 2:F:389:VAL:N    | 2.49                     | 0.46              |
| 3:H:97:UNK:O     | 3:H:101:UNK:CB   | 2.64                     | 0.46              |
| 3:H:443:UNK:O    | 3:H:447:UNK:N    | 2.48                     | 0.46              |
| 1:A:109:LYS:HZ2  | 1:A:428:ALA:H    | 1.63                     | 0.46              |
| 1:A:162:ARG:NH2  | 1:A:418:GLU:HB3  | 2.17                     | 0.46              |
| 1:A:191:PHE:CG   | 1:A:427:PHE:HZ   | 2.33                     | 0.46              |
| 1:A:201:SER:CB   | 2:F:309:PHE:HB2  | 2.43                     | 0.46              |
| 1:A:380:VAL:HA   | 1:A:383:LYS:HD3  | 1.97                     | 0.46              |
| 1:A:425:VAL:HG22 | 1:A:426:ILE:N    | 2.31                     | 0.46              |
| 2:B:373:ILE:HB   | 2:B:403:ILE:HG13 | 1.98                     | 0.46              |
| 2:B:400:ARG:HG3  | 2:B:400:ARG:O    | 2.16                     | 0.46              |
| 1:C:117:ARG:HH12 | 1:C:276:ARG:CB   | 2.29                     | 0.46              |
| 2:D:122:ALA:HB1  | 2:D:296:LEU:HD11 | 1.98                     | 0.46              |
| 2:D:244:LEU:HD23 | 2:D:244:LEU:HA   | 1.68                     | 0.46              |
| 1:E:190:VAL:N    | 1:E:206:CYS:HB2  | 2.31                     | 0.46              |
| 1:E:378:ARG:HD2  | 1:E:378:ARG:HA   | 1.64                     | 0.46              |
| 4:J:251:UNK:O    | 4:J:254:UNK:N    | 2.49                     | 0.46              |
| 1:A:144:ARG:CD   | 2:B:407:THR:CG2  | 2.87                     | 0.45              |
| 1:A:270:LEU:HG   | 1:A:271:ASP:H    | 1.80                     | 0.45              |
| 2:B:268:ILE:HD11 | 2:B:273:ARG:HE   | 1.81                     | 0.45              |
| 2:B:425:ASP:OD1  | 2:B:427:LYS:HG2  | 2.16                     | 0.45              |
| 1:C:69:ALA:HB2   | 2:D:444:LYS:HD3  | 1.97                     | 0.45              |
| 2:D:161:LEU:HD12 | 2:D:162:THR:H    | 1.81                     | 0.45              |
| 2:D:213:ARG:HD3  | 2:D:213:ARG:H    | 1.81                     | 0.45              |
| 4:J:252:UNK:O    | 4:J:256:UNK:N    | 2.49                     | 0.45              |
| 1:A:179:LEU:HD12 | 1:A:182:ALA:HB3  | 1.99                     | 0.45              |
| 2:B:282:GLU:HA   | 2:B:285:GLU:HB2  | 1.98                     | 0.45              |
| 2:B:436:GLU:HA   | 2:B:439:SER:OG   | 2.17                     | 0.45              |
| 1:C:113:MET:HE2  | 1:C:276:ARG:NH2  | 2.31                     | 0.45              |
| 1:C:314:TYR:O    | 1:C:316:HIS:N    | 2.45                     | 0.45              |
| 2:D:349:ASP:OD1  | 2:D:350:LEU:N    | 2.48                     | 0.45              |
| 1:E:117:ARG:NH2  | 1:E:244:ASP:OD2  | 2.49                     | 0.45              |
| 1:E:123:ARG:HD3  | 1:E:235:ILE:HG21 | 1.97                     | 0.45              |
| 1:E:185:VAL:HG13 | 1:E:205:ARG:HG3  | 1.99                     | 0.45              |
| 2:F:141:GLU:HB3  | 2:F:164:LYS:HB2  | 1.97                     | 0.45              |
| 2:F:180:GLU:O    | 2:F:184:LYS:HG2  | 2.16                     | 0.45              |
| 1:A:171:GLY:HA2  | 1:A:431:ARG:N    | 2.31                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:162:THR:HG22 | 2:B:171:ILE:HG13 | 1.97                     | 0.45              |
| 2:B:368:LYS:O    | 2:B:372:ARG:HG2  | 2.16                     | 0.45              |
| 1:C:12:THR:O     | 1:C:16:ALA:N     | 2.50                     | 0.45              |
| 1:C:380:GLN:HG2  | 1:C:381:THR:N    | 2.31                     | 0.45              |
| 2:D:359:THR:O    | 6:D:501:ADP:O2B  | 2.34                     | 0.45              |
| 2:F:94:LEU:HD23  | 2:F:94:LEU:HA    | 1.63                     | 0.45              |
| 2:F:132:LYS:HZ2  | 2:F:239:VAL:HB   | 1.80                     | 0.45              |
| 1:A:208:GLU:HG2  | 1:A:209:VAL:H    | 1.82                     | 0.45              |
| 1:A:221:ARG:HG2  | 1:A:335:ASP:HA   | 1.97                     | 0.45              |
| 1:A:374:ARG:HH12 | 1:A:415:ARG:NH1  | 2.13                     | 0.45              |
| 2:B:32:GLY:HA2   | 2:B:44:GLN:NE2   | 2.31                     | 0.45              |
| 2:B:374:ARG:NH1  | 2:B:405:LEU:N    | 2.65                     | 0.45              |
| 2:D:99:PRO:HG2   | 2:D:294:GLY:HA3  | 1.97                     | 0.45              |
| 2:D:207:ARG:HG2  | 2:D:235:ARG:NH1  | 2.31                     | 0.45              |
| 2:D:444:LYS:O    | 2:D:447:GLN:HB2  | 2.17                     | 0.45              |
| 2:F:393:ILE:HD12 | 2:F:393:ILE:H    | 1.80                     | 0.45              |
| 3:H:366:UNK:HA   | 3:H:369:UNK:CB   | 2.47                     | 0.45              |
| 3:H:496:UNK:C    | 3:H:498:UNK:N    | 2.79                     | 0.45              |
| 1:C:183:GLU:O    | 1:C:185:VAL:HG13 | 2.17                     | 0.45              |
| 1:C:393:HIS:O    | 1:C:397:ILE:HG12 | 2.17                     | 0.45              |
| 2:D:35:ASP:N     | 2:D:35:ASP:OD1   | 2.47                     | 0.45              |
| 2:D:196:ASP:CG   | 2:D:197:LYS:H    | 2.25                     | 0.45              |
| 2:D:443:MET:O    | 2:D:447:GLN:N    | 2.42                     | 0.45              |
| 1:E:51:VAL:HG13  | 2:F:411:LEU:HD23 | 1.99                     | 0.45              |
| 1:E:187:ALA:N    | 1:E:209:TYR:OH   | 2.41                     | 0.45              |
| 2:F:129:VAL:O    | 2:F:241:THR:HA   | 2.16                     | 0.45              |
| 3:H:74:UNK:HA    | 3:H:77:UNK:CB    | 2.46                     | 0.45              |
| 3:H:188:UNK:O    | 3:H:193:UNK:HA   | 2.16                     | 0.45              |
| 3:H:558:UNK:C    | 3:H:560:UNK:N    | 2.78                     | 0.45              |
| 1:A:301:GLN:HE22 | 1:A:317:GLU:CG   | 2.30                     | 0.45              |
| 2:B:50:LEU:O     | 2:B:51:ALA:C     | 2.59                     | 0.45              |
| 1:C:185:VAL:HG11 | 1:C:202:ARG:HG2  | 1.98                     | 0.45              |
| 1:C:354:LEU:CD1  | 1:C:357:ARG:HB2  | 2.46                     | 0.45              |
| 2:D:188:GLN:HE22 | 2:D:214:ASP:N    | 2.14                     | 0.45              |
| 2:D:231:GLU:HG2  | 2:D:234:LYS:NZ   | 2.32                     | 0.45              |
| 2:F:306:ILE:HG12 | 2:F:337:GLY:HA3  | 1.97                     | 0.45              |
| 4:J:321:UNK:O    | 4:J:324:UNK:N    | 2.50                     | 0.45              |
| 1:A:133:ALA:CB   | 2:B:428:ARG:N    | 2.69                     | 0.45              |
| 1:A:164:VAL:C    | 1:A:165:LEU:HG   | 2.42                     | 0.45              |
| 1:A:207:THR:HA   | 1:A:210:LEU:HB2  | 1.99                     | 0.45              |
| 2:B:156:SER:OG   | 2:B:157:LYS:N    | 2.48                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:313:ASN:ND2  | 2:B:313:ASN:H    | 2.14                     | 0.45              |
| 2:B:368:LYS:HG3  | 2:B:387:TYR:HB3  | 1.98                     | 0.45              |
| 2:B:399:LEU:HG   | 2:B:399:LEU:O    | 2.17                     | 0.45              |
| 1:C:51:VAL:HG11  | 1:C:357:ARG:HG2  | 1.97                     | 0.45              |
| 1:C:71:PRO:O     | 1:C:332:ASN:HA   | 2.17                     | 0.45              |
| 1:C:343:ASP:OD1  | 1:C:343:ASP:N    | 2.47                     | 0.45              |
| 2:D:142:VAL:O    | 2:D:195:ILE:HD12 | 2.17                     | 0.45              |
| 2:D:148:ASP:CG   | 2:D:174:LEU:HD22 | 2.42                     | 0.45              |
| 4:J:393:UNK:CA   | 4:J:400:GLY:HA3  | 2.37                     | 0.45              |
| 5:K:155:UNK:HA   | 5:K:158:ASN:CB   | 2.47                     | 0.45              |
| 1:A:109:LYS:HZ2  | 1:A:428:ALA:N    | 2.14                     | 0.45              |
| 2:B:23:GLY:O     | 2:B:26:SER:N     | 2.41                     | 0.45              |
| 2:B:43:SER:O     | 2:B:45:GLY:N     | 2.50                     | 0.45              |
| 2:B:209:PHE:O    | 2:B:211:ARG:NH1  | 2.49                     | 0.45              |
| 1:C:27:ASP:OD1   | 1:C:29:SER:N     | 2.37                     | 0.45              |
| 2:D:104:ALA:HA   | 2:D:299:ASP:OD1  | 2.17                     | 0.45              |
| 2:D:232:LEU:HD23 | 2:D:232:LEU:HA   | 1.82                     | 0.45              |
| 2:D:368:LYS:HZ2  | 2:D:388:THR:HA   | 1.81                     | 0.45              |
| 2:D:437:SER:HA   | 2:D:441:GLN:HB2  | 1.99                     | 0.45              |
| 2:F:124:ARG:HD3  | 2:F:124:ARG:HA   | 1.70                     | 0.45              |
| 2:F:132:LYS:NZ   | 2:F:239:VAL:HB   | 2.32                     | 0.45              |
| 2:F:350:LEU:HD12 | 2:F:350:LEU:HA   | 1.75                     | 0.45              |
| 1:A:167:ALA:HB2  | 1:A:450:LEU:HB3  | 1.99                     | 0.45              |
| 1:A:216:ARG:HH21 | 1:A:397:LEU:HD21 | 1.82                     | 0.45              |
| 1:C:134:GLU:H    | 1:C:161:LEU:HA   | 1.82                     | 0.45              |
| 1:C:165:LYS:HG3  | 1:C:226:GLY:O    | 2.17                     | 0.45              |
| 1:C:189:ASP:C    | 1:C:206:CYS:HB2  | 2.42                     | 0.45              |
| 1:C:328:ILE:HG23 | 1:C:359:MET:HG2  | 1.99                     | 0.45              |
| 1:C:393:HIS:H    | 1:C:427:LYS:HZ1  | 1.65                     | 0.45              |
| 2:D:134:GLU:HG3  | 2:D:207:ARG:NH2  | 2.31                     | 0.45              |
| 2:D:156:SER:O    | 2:D:157:LYS:HG2  | 2.17                     | 0.45              |
| 2:D:204:LYS:HD3  | 2:D:205:LEU:N    | 2.28                     | 0.45              |
| 2:D:428:ARG:HD3  | 2:D:429:VAL:HG22 | 1.99                     | 0.45              |
| 1:A:223:LYS:HG2  | 1:A:333:ILE:HG23 | 1.99                     | 0.45              |
| 2:B:33:LEU:O     | 2:B:40:ARG:NH2   | 2.50                     | 0.45              |
| 2:B:143:VAL:O    | 2:B:164:LYS:HG2  | 2.17                     | 0.45              |
| 2:B:157:LYS:NZ   | 2:B:174:LEU:HB3  | 2.29                     | 0.45              |
| 2:B:383:SER:O    | 2:B:385:ASP:N    | 2.50                     | 0.45              |
| 1:C:207:ASP:OD1  | 1:C:207:ASP:N    | 2.49                     | 0.45              |
| 1:C:362:ARG:HG2  | 1:C:363:THR:H    | 1.82                     | 0.45              |
| 2:D:33:LEU:HG    | 2:D:39:PRO:HA    | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:243:SER:OG   | 2:D:246:GLU:N    | 2.44                     | 0.45              |
| 2:F:444:LYS:O    | 2:F:448:ASP:N    | 2.33                     | 0.45              |
| 1:A:162:ARG:H    | 1:A:162:ARG:HD3  | 1.83                     | 0.44              |
| 1:A:202:THR:HA   | 2:F:305:ASP:O    | 2.17                     | 0.44              |
| 1:C:117:ARG:HH12 | 1:C:276:ARG:HB3  | 1.81                     | 0.44              |
| 1:C:136:THR:HA   | 1:C:209:TYR:CE1  | 2.52                     | 0.44              |
| 2:D:81:THR:CB    | 6:D:501:ADP:O3'  | 2.65                     | 0.44              |
| 2:D:146:GLN:HG3  | 2:D:148:ASP:N    | 2.33                     | 0.44              |
| 2:D:311:PHE:O    | 2:D:315:ALA:N    | 2.46                     | 0.44              |
| 1:E:130:VAL:HG13 | 1:E:192:TYR:HA   | 1.98                     | 0.44              |
| 2:D:28:ILE:HD13  | 2:D:28:ILE:HA    | 1.81                     | 0.44              |
| 2:D:197:LYS:HD3  | 2:D:199:THR:OG1  | 2.18                     | 0.44              |
| 2:D:236:LYS:HD2  | 2:D:237:GLU:N    | 2.33                     | 0.44              |
| 2:D:318:SER:OG   | 2:D:319:ASP:OD1  | 2.35                     | 0.44              |
| 1:E:13:GLN:OE1   | 1:E:13:GLN:N     | 2.25                     | 0.44              |
| 1:E:60:LYS:HE2   | 1:E:60:LYS:HA    | 2.00                     | 0.44              |
| 1:E:219:GLU:CD   | 1:E:219:GLU:H    | 2.25                     | 0.44              |
| 2:F:379:ASP:OD1  | 2:F:379:ASP:C    | 2.60                     | 0.44              |
| 3:H:175:UNK:HA   | 3:H:181:UNK:CB   | 2.47                     | 0.44              |
| 5:K:91:ALA:C     | 5:K:94:SER:H     | 2.24                     | 0.44              |
| 2:B:177:LYS:NZ   | 2:B:209:PHE:O    | 2.50                     | 0.44              |
| 1:C:177:PHE:HE1  | 1:C:202:ARG:HH22 | 1.64                     | 0.44              |
| 1:C:311:CYS:O    | 1:C:314:TYR:HB3  | 2.17                     | 0.44              |
| 1:C:393:HIS:HB2  | 1:C:427:LYS:HD3  | 2.00                     | 0.44              |
| 2:D:82:GLY:O     | 2:D:400:ARG:NH1  | 2.48                     | 0.44              |
| 1:E:134:GLU:HG3  | 1:E:136:THR:HG23 | 1.99                     | 0.44              |
| 1:E:183:GLU:HG2  | 1:E:205:ARG:HD2  | 1.99                     | 0.44              |
| 2:F:124:ARG:HG2  | 2:F:248:ASP:OD2  | 2.17                     | 0.44              |
| 4:J:457:UNK:O    | 4:J:460:UNK:N    | 2.49                     | 0.44              |
| 1:A:482:ILE:HD12 | 1:A:512:ASN:HD22 | 1.81                     | 0.44              |
| 2:B:165:THR:HG22 | 2:B:167:GLU:H    | 1.81                     | 0.44              |
| 2:B:400:ARG:CZ   | 6:B:501:ADP:PB   | 3.05                     | 0.44              |
| 1:C:125:LYS:NZ   | 1:C:233:GLU:HB3  | 2.32                     | 0.44              |
| 2:D:306:ILE:HG13 | 2:D:307:GLU:N    | 2.32                     | 0.44              |
| 1:E:43:GLU:O     | 1:E:46:ARG:N     | 2.50                     | 0.44              |
| 1:E:386:ILE:HA   | 1:E:425:ILE:H    | 1.82                     | 0.44              |
| 5:K:48:UNK:HA    | 5:K:51:VAL:CB    | 2.48                     | 0.44              |
| 1:A:122:LEU:HD21 | 1:A:144:ARG:NH1  | 2.33                     | 0.44              |
| 1:A:203:GLU:CD   | 2:F:312:LEU:N    | 2.76                     | 0.44              |
| 1:A:468:GLU:HG3  | 1:A:471:GLN:HB3  | 1.99                     | 0.44              |
| 1:E:376:LYS:HD2  | 1:E:380:GLN:NE2  | 2.29                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:178:MET:SD   | 2:F:195:ILE:HD11 | 2.57                     | 0.44              |
| 4:J:257:UNK:CB   | 4:J:296:UNK:CB   | 2.96                     | 0.44              |
| 1:A:411:THR:OG1  | 2:B:109:PHE:O    | 2.35                     | 0.44              |
| 2:B:68:ILE:HD12  | 2:B:71:ARG:HB2   | 2.00                     | 0.44              |
| 2:B:295:VAL:HG12 | 2:B:323:VAL:CG1  | 2.48                     | 0.44              |
| 1:C:64:ARG:HA    | 1:C:353:ASP:HB2  | 1.99                     | 0.44              |
| 2:D:46:MET:HG2   | 2:D:53:ARG:CZ    | 2.48                     | 0.44              |
| 2:D:275:GLN:HA   | 2:D:278:ALA:HB3  | 1.99                     | 0.44              |
| 2:D:443:MET:O    | 2:D:447:GLN:HG2  | 2.18                     | 0.44              |
| 1:E:113:MET:O    | 1:E:117:ARG:HG2  | 2.18                     | 0.44              |
| 1:E:360:ILE:HG13 | 2:F:434:LEU:HB2  | 1.99                     | 0.44              |
| 5:K:263:ALA:O    | 5:K:265:LEU:N    | 2.51                     | 0.44              |
| 1:A:110:THR:HB   | 1:A:473:ILE:HG12 | 2.00                     | 0.44              |
| 1:A:166:LEU:HD13 | 1:A:456:VAL:CG2  | 2.48                     | 0.44              |
| 1:A:406:ASP:OD1  | 1:A:437:ARG:NE   | 2.50                     | 0.44              |
| 1:A:465:THR:OG1  | 1:A:466:PRO:HD2  | 2.18                     | 0.44              |
| 2:B:328:THR:HG21 | 2:B:344:HIS:HB3  | 2.00                     | 0.44              |
| 1:C:52:ILE:HD11  | 1:C:358:VAL:HG13 | 2.00                     | 0.44              |
| 1:C:53:VAL:HA    | 1:C:56:ILE:HG22  | 2.00                     | 0.44              |
| 1:C:66:VAL:HG22  | 1:C:67:LEU:H     | 1.82                     | 0.44              |
| 1:C:239:THR:O    | 1:C:242:ASP:HB2  | 2.17                     | 0.44              |
| 1:E:159:ILE:HD12 | 1:E:172:LEU:HB2  | 2.00                     | 0.44              |
| 1:A:218:ILE:HD12 | 1:A:339:HIS:HB2  | 2.00                     | 0.44              |
| 2:B:284:ARG:HA   | 2:B:289:ALA:O    | 2.17                     | 0.44              |
| 2:B:436:GLU:O    | 2:B:440:THR:HG23 | 2.18                     | 0.44              |
| 2:B:439:SER:HA   | 2:B:442:TYR:CD2  | 2.53                     | 0.44              |
| 1:C:281:LYS:HD3  | 1:C:281:LYS:HA   | 1.65                     | 0.44              |
| 2:D:86:ILE:H     | 2:D:86:ILE:HD12  | 1.82                     | 0.44              |
| 2:D:297:PHE:CD1  | 2:D:325:ILE:HG13 | 2.51                     | 0.44              |
| 1:E:12:THR:O     | 1:E:15:ILE:N     | 2.45                     | 0.44              |
| 1:E:13:GLN:H     | 1:E:13:GLN:CD    | 2.16                     | 0.44              |
| 1:E:131:TYR:HA   | 1:E:228:VAL:O    | 2.17                     | 0.44              |
| 1:E:283:VAL:O    | 1:E:286:TYR:N    | 2.51                     | 0.44              |
| 5:K:160:LEU:O    | 5:K:163:GLU:CB   | 2.66                     | 0.44              |
| 1:A:131:LYS:CE   | 2:B:413:CYS:HB2  | 2.48                     | 0.44              |
| 1:A:545:LEU:HA   | 1:A:548:GLN:OE1  | 2.17                     | 0.44              |
| 1:C:22:LYS:HB2   | 1:C:22:LYS:HE3   | 1.82                     | 0.44              |
| 2:D:82:GLY:HA3   | 2:D:400:ARG:HE   | 1.83                     | 0.44              |
| 2:D:397:THR:HG21 | 2:D:436:GLU:H    | 1.83                     | 0.44              |
| 1:E:76:LYS:HG2   | 1:E:363:THR:HG21 | 1.99                     | 0.44              |
| 1:E:212:GLU:OE2  | 1:E:218:GLU:HB3  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:426:GLU:OE2  | 1:E:429:HIS:N    | 2.42                     | 0.44              |
| 2:B:34:ASP:OD1   | 2:B:37:LEU:N     | 2.51                     | 0.43              |
| 2:B:73:VAL:HG23  | 2:B:355:LEU:O    | 2.18                     | 0.43              |
| 2:B:78:GLN:HB2   | 2:B:79:PRO:CD    | 2.41                     | 0.43              |
| 2:B:385:ASP:O    | 2:B:388:THR:OG1  | 2.35                     | 0.43              |
| 2:D:29:ARG:HB2   | 2:D:44:GLN:HA    | 2.00                     | 0.43              |
| 2:D:174:LEU:HG   | 2:D:175:GLY:H    | 1.82                     | 0.43              |
| 1:E:87:LEU:HD12  | 1:E:87:LEU:HA    | 1.78                     | 0.43              |
| 1:E:380:GLN:O    | 1:E:383:GLY:N    | 2.49                     | 0.43              |
| 3:H:496:UNK:O    | 3:H:497:UNK:C    | 2.66                     | 0.43              |
| 4:J:121:UNK:C    | 4:J:123:UNK:N    | 2.79                     | 0.43              |
| 4:J:321:UNK:O    | 4:J:324:UNK:CB   | 2.66                     | 0.43              |
| 1:A:220:LEU:H    | 1:A:337:THR:HA   | 1.82                     | 0.43              |
| 1:A:412:TYR:C    | 1:A:414:HIS:N    | 2.76                     | 0.43              |
| 1:A:414:HIS:C    | 1:A:416:ALA:H    | 2.26                     | 0.43              |
| 1:A:492:LEU:O    | 1:A:495:ILE:HG22 | 2.18                     | 0.43              |
| 2:B:130:ARG:HB3  | 2:B:290:GLU:OE1  | 2.18                     | 0.43              |
| 2:B:146:GLN:HE21 | 2:B:149:ARG:HG3  | 1.82                     | 0.43              |
| 2:B:236:LYS:HZ3  | 2:B:238:VAL:HA   | 1.81                     | 0.43              |
| 2:B:268:ILE:HD11 | 2:B:273:ARG:NE   | 2.32                     | 0.43              |
| 2:B:292:ILE:HD12 | 2:B:293:PRO:HD2  | 2.00                     | 0.43              |
| 2:B:367:THR:O    | 2:B:371:LEU:HD12 | 2.17                     | 0.43              |
| 1:C:25:GLY:C     | 1:C:32:ALA:HB2   | 2.43                     | 0.43              |
| 1:C:48:ALA:HB1   | 1:C:356:ASP:O    | 2.18                     | 0.43              |
| 1:C:162:LYS:NZ   | 1:C:168:LYS:O    | 2.49                     | 0.43              |
| 1:C:317:ARG:NH1  | 1:C:318:ALA:HB2  | 2.33                     | 0.43              |
| 2:D:29:ARG:HB2   | 2:D:44:GLN:HB3   | 1.99                     | 0.43              |
| 2:D:338:THR:OG1  | 2:D:339:SER:N    | 2.51                     | 0.43              |
| 2:D:359:THR:OG1  | 6:D:501:ADP:O1A  | 2.36                     | 0.43              |
| 2:D:428:ARG:HD3  | 2:D:429:VAL:CG2  | 2.48                     | 0.43              |
| 1:E:131:TYR:CZ   | 1:E:229:HIS:CD2  | 3.06                     | 0.43              |
| 1:E:395:GLY:O    | 1:E:399:THR:HG23 | 2.18                     | 0.43              |
| 2:F:247:ILE:HG22 | 2:F:276:ILE:HD13 | 2.00                     | 0.43              |
| 2:F:310:SER:O    | 2:F:310:SER:OG   | 2.37                     | 0.43              |
| 1:A:150:ILE:O    | 1:A:154:ILE:N    | 2.49                     | 0.43              |
| 1:A:231:GLY:HA3  | 1:A:265:THR:CA   | 2.48                     | 0.43              |
| 1:A:263:LYS:HA   | 1:A:323:LYS:HD2  | 2.00                     | 0.43              |
| 1:A:524:GLU:H    | 1:A:527:HIS:HD1  | 1.62                     | 0.43              |
| 1:C:97:VAL:O     | 1:C:100:GLU:HG2  | 2.18                     | 0.43              |
| 1:C:286:TYR:O    | 1:C:290:GLY:N    | 2.51                     | 0.43              |
| 1:C:372:LYS:HB3  | 1:C:391:LEU:HD21 | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:164:LYS:HB3  | 2:D:164:LYS:HE3  | 1.76                     | 0.43              |
| 2:F:77:GLY:HA3   | 2:F:359:THR:CG2  | 2.48                     | 0.43              |
| 2:F:165:THR:HG22 | 2:F:230:GLY:HA3  | 2.01                     | 0.43              |
| 2:F:166:THR:CG2  | 2:F:229:ASP:HA   | 2.47                     | 0.43              |
| 2:F:375:CYS:SG   | 2:F:376:GLU:N    | 2.91                     | 0.43              |
| 2:F:378:GLU:O    | 2:F:380:VAL:HG23 | 2.18                     | 0.43              |
| 1:A:131:LYS:CE   | 2:B:413:CYS:HB3  | 2.26                     | 0.43              |
| 1:A:165:LEU:HD13 | 1:A:449:PRO:HG2  | 2.00                     | 0.43              |
| 1:A:282:ARG:HH22 | 1:A:303:ARG:HB3  | 1.83                     | 0.43              |
| 1:A:487:GLU:HG2  | 1:A:488:ALA:N    | 2.33                     | 0.43              |
| 2:B:41:GLN:O     | 2:B:41:GLN:NE2   | 2.50                     | 0.43              |
| 2:B:422:GLN:O    | 2:B:424:ASP:N    | 2.50                     | 0.43              |
| 1:C:126:GLU:O    | 1:C:233:GLU:HA   | 2.18                     | 0.43              |
| 1:C:354:LEU:O    | 1:C:356:ASP:N    | 2.52                     | 0.43              |
| 1:C:418:LYS:NZ   | 1:C:423:ASP:HA   | 2.34                     | 0.43              |
| 2:D:86:ILE:O     | 2:D:90:MET:HG3   | 2.18                     | 0.43              |
| 2:D:112:GLU:HG2  | 2:D:113:MET:H    | 1.83                     | 0.43              |
| 2:D:137:ILE:HG21 | 2:D:211:ARG:NH1  | 2.33                     | 0.43              |
| 1:E:372:LYS:NZ   | 1:E:395:GLY:HA3  | 2.34                     | 0.43              |
| 2:F:130:ARG:HH21 | 2:F:290:GLU:HB3  | 1.82                     | 0.43              |
| 2:F:161:LEU:HD13 | 2:F:174:LEU:HD21 | 2.01                     | 0.43              |
| 3:H:238:UNK:C    | 3:H:240:UNK:N    | 2.81                     | 0.43              |
| 1:A:138:VAL:CG1  | 2:B:432:LEU:H    | 2.24                     | 0.43              |
| 1:A:158:LYS:HE2  | 1:A:158:LYS:HB3  | 1.74                     | 0.43              |
| 1:A:190:PRO:N    | 1:A:394:PRO:HB3  | 2.34                     | 0.43              |
| 1:A:206:LYS:O    | 1:A:208:GLU:N    | 2.52                     | 0.43              |
| 2:B:95:GLY:HA3   | 2:B:98:THR:HG23  | 2.00                     | 0.43              |
| 1:C:27:ASP:OD1   | 1:C:28:GLU:HG2   | 2.19                     | 0.43              |
| 1:C:64:ARG:HH22  | 1:C:357:ARG:NH2  | 2.16                     | 0.43              |
| 1:C:427:LYS:O    | 1:C:430:VAL:N    | 2.51                     | 0.43              |
| 2:D:31:LEU:HA    | 2:D:31:LEU:HD23  | 1.83                     | 0.43              |
| 1:E:6:VAL:HB     | 1:E:236:GLN:HE21 | 1.83                     | 0.43              |
| 5:K:76:ALA:HA    | 5:K:79:ALA:HB3   | 2.00                     | 0.43              |
| 5:K:162:GLN:O    | 5:K:164:ASN:N    | 2.52                     | 0.43              |
| 1:A:150:ILE:HG12 | 1:A:455:ARG:NH2  | 2.33                     | 0.43              |
| 1:A:174:LYS:HE3  | 1:A:174:LYS:HB3  | 1.88                     | 0.43              |
| 2:B:27:HIS:CE1   | 2:B:403:ILE:HD12 | 2.54                     | 0.43              |
| 2:B:382:MET:HE3  | 2:B:383:SER:OG   | 2.18                     | 0.43              |
| 1:C:132:GLU:OE1  | 1:C:163:THR:HG21 | 2.18                     | 0.43              |
| 1:E:191:ILE:HB   | 1:E:193:ILE:HG23 | 1.99                     | 0.43              |
| 1:E:213:PHE:CZ   | 1:E:222:PRO:HA   | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:H:510:UNK:O    | 3:H:513:UNK:N    | 2.52                     | 0.43              |
| 4:J:477:UNK:HA   | 4:J:478:UNK:HA   | 1.53                     | 0.43              |
| 1:A:133:ALA:O    | 2:B:428:ARG:CB   | 2.67                     | 0.43              |
| 1:A:330:LYS:HZ2  | 1:A:331:GLU:C    | 2.22                     | 0.43              |
| 2:B:306:ILE:HD12 | 1:C:102:TYR:CD1  | 2.54                     | 0.43              |
| 1:C:185:VAL:HB   | 1:C:189:ASP:OD2  | 2.18                     | 0.43              |
| 2:D:113:MET:SD   | 2:D:267:GLU:N    | 2.92                     | 0.43              |
| 2:D:275:GLN:O    | 2:D:279:LYS:N    | 2.37                     | 0.43              |
| 2:D:375:CYS:O    | 2:D:380:VAL:HG22 | 2.18                     | 0.43              |
| 1:E:79:LEU:HA    | 1:E:79:LEU:HD23  | 1.78                     | 0.43              |
| 1:E:129:GLU:CD   | 1:E:129:GLU:H    | 2.26                     | 0.43              |
| 2:F:161:LEU:HD23 | 2:F:162:THR:N    | 2.33                     | 0.43              |
| 5:K:263:ALA:C    | 5:K:265:LEU:N    | 2.77                     | 0.43              |
| 5:K:386:SER:O    | 5:K:389:PRO:CB   | 2.67                     | 0.43              |
| 1:A:170:PRO:HB2  | 1:A:432:GLY:HA2  | 2.01                     | 0.43              |
| 1:A:241:THR:HG22 | 1:A:242:GLU:N    | 2.33                     | 0.43              |
| 1:C:104:THR:O    | 1:C:107:LYS:NZ   | 2.34                     | 0.43              |
| 1:C:129:GLU:HB3  | 1:C:229:HIS:CE1  | 2.54                     | 0.43              |
| 1:C:389:GLU:OE2  | 1:C:427:LYS:HE2  | 2.19                     | 0.43              |
| 2:D:90:MET:HE2   | 2:D:90:MET:HB3   | 1.87                     | 0.43              |
| 2:D:409:ALA:O    | 2:D:412:VAL:HG22 | 2.19                     | 0.43              |
| 1:E:126:GLU:HB2  | 1:E:128:LYS:HZ2  | 1.84                     | 0.43              |
| 1:E:170:LEU:HD12 | 1:E:170:LEU:HA   | 1.84                     | 0.43              |
| 1:A:232:GLU:N    | 1:A:265:THR:HA   | 2.34                     | 0.43              |
| 2:B:28:ILE:HA    | 2:B:28:ILE:HD13  | 1.83                     | 0.43              |
| 2:B:157:LYS:HD3  | 2:B:174:LEU:O    | 2.19                     | 0.43              |
| 2:B:306:ILE:HG13 | 2:B:307:GLU:OE2  | 2.19                     | 0.43              |
| 1:C:385:ASN:O    | 1:C:424:SER:HA   | 2.19                     | 0.43              |
| 2:D:138:ILE:HG12 | 2:D:204:LYS:O    | 2.19                     | 0.43              |
| 2:D:201:LYS:HE3  | 4:J:281:UNK:C    | 2.29                     | 0.43              |
| 1:E:353:ASP:CG   | 1:E:354:LEU:H    | 2.27                     | 0.43              |
| 1:E:432:GLU:O    | 1:E:436:LEU:HG   | 2.19                     | 0.43              |
| 2:F:130:ARG:HB3  | 2:F:239:VAL:HG21 | 2.01                     | 0.43              |
| 2:F:160:LYS:HD3  | 2:F:172:TYR:O    | 2.19                     | 0.43              |
| 4:J:495:UNK:HA   | 4:J:496:UNK:HA   | 1.47                     | 0.43              |
| 1:A:172:THR:HG1  | 1:A:174:LYS:HZ2  | 1.65                     | 0.43              |
| 2:B:140:GLY:C    | 2:B:192:VAL:HG12 | 2.44                     | 0.43              |
| 1:E:96:MET:HE3   | 1:E:96:MET:HB2   | 1.96                     | 0.43              |
| 1:E:97:VAL:HG22  | 1:E:100:GLU:OE2  | 2.19                     | 0.43              |
| 1:E:234:ILE:HG22 | 1:E:235:ILE:N    | 2.33                     | 0.43              |
| 3:H:369:UNK:C    | 3:H:371:UNK:N    | 2.67                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:172:THR:OG1  | 1:A:174:LYS:N    | 2.52                     | 0.42              |
| 1:A:302:GLY:HA3  | 1:A:316:GLU:OE1  | 2.19                     | 0.42              |
| 2:B:374:ARG:HH12 | 2:B:405:LEU:C    | 2.27                     | 0.42              |
| 2:B:390:LEU:HA   | 2:B:390:LEU:HD23 | 1.73                     | 0.42              |
| 1:C:181:GLN:HG3  | 1:C:182:LYS:HD3  | 2.00                     | 0.42              |
| 2:D:94:LEU:HD23  | 2:D:94:LEU:HA    | 1.68                     | 0.42              |
| 2:D:121:GLN:HB3  | 2:D:125:ARG:HH21 | 1.83                     | 0.42              |
| 2:D:133:GLU:OE1  | 2:D:134:GLU:N    | 2.52                     | 0.42              |
| 2:D:137:ILE:HA   | 2:D:205:LEU:HD23 | 2.01                     | 0.42              |
| 2:F:306:ILE:O    | 2:F:306:ILE:HG13 | 2.16                     | 0.42              |
| 3:H:164:UNK:HA   | 3:H:167:UNK:CB   | 2.49                     | 0.42              |
| 1:A:436:ILE:HD11 | 1:A:449:PRO:HB3  | 2.00                     | 0.42              |
| 1:C:64:ARG:HB3   | 1:C:354:LEU:N    | 2.34                     | 0.42              |
| 2:D:132:LYS:HD3  | 2:D:237:GLU:HG2  | 1.99                     | 0.42              |
| 2:D:430:TYR:HA   | 2:D:433:PHE:CB   | 2.33                     | 0.42              |
| 1:E:37:SER:O     | 1:E:37:SER:OG    | 2.36                     | 0.42              |
| 1:E:279:ILE:HD12 | 1:E:279:ILE:H    | 1.84                     | 0.42              |
| 1:E:362:ARG:HD3  | 2:F:442:TYR:CD2  | 2.54                     | 0.42              |
| 2:F:326:MET:HE3  | 2:F:326:MET:HB2  | 1.73                     | 0.42              |
| 2:F:423:VAL:HG22 | 2:F:427:LYS:HG2  | 2.02                     | 0.42              |
| 1:A:172:THR:HG1  | 1:A:173:GLY:N    | 2.17                     | 0.42              |
| 1:A:544:ILE:CG2  | 1:A:548:GLN:HE22 | 2.33                     | 0.42              |
| 2:B:38:GLU:HA    | 2:B:39:PRO:HD3   | 1.94                     | 0.42              |
| 2:B:86:ILE:HD13  | 2:B:86:ILE:HA    | 1.81                     | 0.42              |
| 2:B:145:ILE:HD12 | 2:B:145:ILE:HA   | 1.91                     | 0.42              |
| 1:C:93:PHE:HD1   | 1:C:298:VAL:HG11 | 1.84                     | 0.42              |
| 1:C:122:LEU:HB2  | 1:C:238:VAL:HG23 | 2.00                     | 0.42              |
| 1:C:185:VAL:HG21 | 1:C:202:ARG:HB3  | 2.01                     | 0.42              |
| 2:D:32:GLY:CA    | 2:D:43:SER:HB2   | 2.49                     | 0.42              |
| 2:D:393:ILE:HG23 | 2:D:435:ASP:OD2  | 2.18                     | 0.42              |
| 2:D:444:LYS:O    | 2:D:448:ASP:N    | 2.33                     | 0.42              |
| 1:E:32:ALA:HB1   | 1:E:46:ARG:CZ    | 2.49                     | 0.42              |
| 1:E:160:GLY:HA3  | 1:E:162:LYS:NZ   | 2.34                     | 0.42              |
| 1:E:168:LYS:NZ   | 1:E:169:GLN:O    | 2.52                     | 0.42              |
| 2:F:195:ILE:HG23 | 2:F:196:ASP:OD1  | 2.19                     | 0.42              |
| 3:H:553:UNK:C    | 3:H:555:UNK:N    | 2.80                     | 0.42              |
| 2:D:145:ILE:O    | 2:D:145:ILE:HG13 | 2.19                     | 0.42              |
| 2:D:206:GLY:HA2  | 2:D:235:ARG:HH11 | 1.85                     | 0.42              |
| 2:D:436:GLU:O    | 2:D:440:THR:OG1  | 2.37                     | 0.42              |
| 1:E:234:ILE:O    | 1:E:235:ILE:HD13 | 2.20                     | 0.42              |
| 2:F:309:PHE:CE2  | 2:F:313:ASN:HB2  | 2.54                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:170:PRO:CB   | 1:A:432:GLY:HA2  | 2.48                     | 0.42              |
| 1:A:332:ILE:H    | 1:A:332:ILE:HG13 | 1.70                     | 0.42              |
| 2:B:375:CYS:C    | 2:B:377:GLU:N    | 2.77                     | 0.42              |
| 2:B:382:MET:HB3  | 2:B:387:TYR:CE1  | 2.54                     | 0.42              |
| 2:B:414:ARG:C    | 2:B:417:LYS:H    | 2.27                     | 0.42              |
| 1:C:54:GLU:O     | 1:C:58:SER:N     | 2.53                     | 0.42              |
| 1:C:370:GLU:HA   | 1:C:373:GLN:NE2  | 2.35                     | 0.42              |
| 2:D:32:GLY:C     | 2:D:33:LEU:HD12  | 2.44                     | 0.42              |
| 2:D:82:GLY:C     | 2:D:84:THR:H     | 2.26                     | 0.42              |
| 1:E:285:LYS:C    | 1:E:289:GLN:HE22 | 2.27                     | 0.42              |
| 3:H:558:UNK:O    | 3:H:560:UNK:N    | 2.53                     | 0.42              |
| 5:K:52:LEU:HA    | 5:K:55:LEU:CB    | 2.49                     | 0.42              |
| 5:K:91:ALA:CA    | 5:K:94:SER:CB    | 2.97                     | 0.42              |
| 1:A:116:HIS:HA   | 1:A:462:MET:HE3  | 2.01                     | 0.42              |
| 1:A:237:THR:HB   | 1:A:255:VAL:O    | 2.20                     | 0.42              |
| 1:A:256:ILE:HG23 | 1:A:267:GLN:OE1  | 2.19                     | 0.42              |
| 1:C:447:LEU:O    | 1:C:451:GLN:HG2  | 2.19                     | 0.42              |
| 2:D:78:GLN:HG3   | 2:D:79:PRO:HD2   | 2.00                     | 0.42              |
| 1:E:43:GLU:O     | 1:E:44:ASN:C     | 2.62                     | 0.42              |
| 1:E:212:GLU:OE1  | 1:E:218:GLU:N    | 2.53                     | 0.42              |
| 2:F:22:ILE:HG12  | 2:F:23:GLY:H     | 1.85                     | 0.42              |
| 4:J:249:UNK:O    | 4:J:253:UNK:N    | 2.53                     | 0.42              |
| 1:A:123:GLY:N    | 2:B:411:LEU:N    | 2.65                     | 0.42              |
| 2:B:23:GLY:O     | 2:B:26:SER:OG    | 2.25                     | 0.42              |
| 2:B:99:PRO:HG2   | 2:B:126:SER:O    | 2.20                     | 0.42              |
| 1:C:186:GLU:OE1  | 1:C:213:PHE:HA   | 2.19                     | 0.42              |
| 2:D:334:ARG:HA   | 2:D:340:TYR:O    | 2.20                     | 0.42              |
| 1:E:126:GLU:HB2  | 1:E:128:LYS:NZ   | 2.34                     | 0.42              |
| 1:E:365:LEU:HD23 | 1:E:365:LEU:HA   | 1.83                     | 0.42              |
| 1:E:372:LYS:HE3  | 1:E:392:ASN:HA   | 2.01                     | 0.42              |
| 1:E:403:LEU:HA   | 1:E:403:LEU:HD12 | 1.74                     | 0.42              |
| 2:F:435:ASP:H    | 2:F:438:ARG:HH21 | 1.67                     | 0.42              |
| 3:H:575:UNK:O    | 3:H:577:UNK:N    | 2.52                     | 0.42              |
| 1:A:222:ILE:HA   | 1:A:390:ALA:HB1  | 2.01                     | 0.42              |
| 1:A:277:SER:OG   | 1:A:299:LYS:N    | 2.53                     | 0.42              |
| 2:B:284:ARG:HD2  | 2:B:291:ILE:HG23 | 2.02                     | 0.42              |
| 2:B:382:MET:CG   | 2:B:383:SER:H    | 2.32                     | 0.42              |
| 2:D:143:VAL:HG23 | 2:D:145:ILE:HG12 | 2.02                     | 0.42              |
| 2:D:251:ASN:HD22 | 2:D:276:ILE:CD1  | 2.32                     | 0.42              |
| 1:E:125:LYS:CE   | 1:E:233:GLU:HB3  | 2.50                     | 0.42              |
| 1:E:313:THR:HG21 | 2:F:110:SER:HB2  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:317:ARG:HG3  | 1:E:318:ALA:N    | 2.35                     | 0.42              |
| 1:E:326:ILE:HD12 | 1:E:326:ILE:HA   | 1.91                     | 0.42              |
| 1:E:335:ASN:OD1  | 1:E:345:THR:HG22 | 2.20                     | 0.42              |
| 2:F:97:ASP:OD1   | 2:F:97:ASP:N     | 2.52                     | 0.42              |
| 2:F:119:LEU:HB3  | 2:F:311:PHE:CE2  | 2.55                     | 0.42              |
| 5:K:262:GLU:C    | 5:K:264:ALA:N    | 2.75                     | 0.42              |
| 1:A:118:HIS:HA   | 1:A:461:THR:OG1  | 2.20                     | 0.42              |
| 1:A:303:ARG:HG2  | 1:A:318:TYR:OH   | 2.20                     | 0.42              |
| 1:A:407:ILE:HD12 | 1:A:407:ILE:H    | 1.84                     | 0.42              |
| 1:C:81:LEU:HD12  | 1:C:81:LEU:HA    | 1.88                     | 0.42              |
| 1:C:241:HIS:O    | 1:C:245:VAL:HG12 | 2.20                     | 0.42              |
| 1:C:319:LEU:N    | 1:C:319:LEU:HD23 | 2.35                     | 0.42              |
| 1:A:175:THR:O    | 1:A:175:THR:OG1  | 2.28                     | 0.42              |
| 1:A:189:VAL:HB   | 1:A:394:PRO:CG   | 2.48                     | 0.42              |
| 1:A:200:TYR:C    | 2:F:306:ILE:O    | 2.63                     | 0.42              |
| 1:A:207:THR:OG1  | 1:A:211:MET:HE2  | 2.20                     | 0.42              |
| 1:A:535:PHE:HE1  | 2:F:55:ALA:HB1   | 1.84                     | 0.42              |
| 2:B:372:ARG:HA   | 2:B:387:TYR:CZ   | 2.55                     | 0.42              |
| 1:C:49:CYS:N     | 1:C:358:VAL:O    | 2.53                     | 0.42              |
| 1:C:95:PRO:HA    | 1:C:300:PHE:HB3  | 2.02                     | 0.42              |
| 2:D:142:VAL:HG21 | 2:D:163:LEU:HB3  | 2.01                     | 0.42              |
| 2:D:193:ILE:HG22 | 2:D:212:ALA:O    | 2.20                     | 0.42              |
| 1:E:12:THR:HA    | 1:E:15:ILE:HG12  | 2.02                     | 0.42              |
| 1:E:48:ALA:HB1   | 1:E:361:ILE:HD13 | 2.00                     | 0.42              |
| 2:F:30:GLY:O     | 2:F:31:LEU:HD23  | 2.20                     | 0.42              |
| 2:F:346:ILE:HG22 | 2:F:351:LEU:HG   | 2.02                     | 0.42              |
| 4:J:219:UNK:O    | 4:J:223:UNK:CB   | 2.68                     | 0.42              |
| 1:A:124:LEU:C    | 2:B:410:SER:OG   | 2.56                     | 0.41              |
| 2:B:434:LEU:HD13 | 2:B:439:SER:CB   | 2.50                     | 0.41              |
| 2:D:82:GLY:C     | 2:D:84:THR:N     | 2.78                     | 0.41              |
| 2:D:296:LEU:HD21 | 2:D:298:ILE:HD11 | 2.01                     | 0.41              |
| 2:D:329:ASN:C    | 1:E:447:LEU:HD21 | 2.45                     | 0.41              |
| 2:D:372:ARG:HA   | 2:D:387:TYR:OH   | 2.20                     | 0.41              |
| 1:E:209:TYR:HB3  | 1:E:212:GLU:HG3  | 2.01                     | 0.41              |
| 1:E:431:GLU:O    | 1:E:434:SER:OG   | 2.23                     | 0.41              |
| 1:A:149:VAL:HG23 | 1:A:152:GLU:OE1  | 2.19                     | 0.41              |
| 2:B:65:GLU:C     | 2:B:67:LYS:H     | 2.26                     | 0.41              |
| 1:C:185:VAL:HA   | 1:C:205:ARG:HH12 | 1.84                     | 0.41              |
| 1:C:354:LEU:HD12 | 1:C:357:ARG:NE   | 2.29                     | 0.41              |
| 2:D:81:THR:HB    | 6:D:501:ADP:O3'  | 2.19                     | 0.41              |
| 2:D:209:PHE:HA   | 2:D:211:ARG:NE   | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:282:GLU:O    | 2:D:283:TRP:C    | 2.63                     | 0.41              |
| 2:D:375:CYS:HA   | 2:D:406:ILE:HD11 | 2.02                     | 0.41              |
| 1:A:124:LEU:HB3  | 1:A:135:SER:CB   | 2.50                     | 0.41              |
| 1:A:164:VAL:HG22 | 1:A:417:LEU:HG   | 2.01                     | 0.41              |
| 1:A:177:LEU:HB3  | 1:A:192:CYS:O    | 2.21                     | 0.41              |
| 2:B:139:GLU:O    | 2:B:232:LEU:HD13 | 2.20                     | 0.41              |
| 2:B:248:ASP:HA   | 2:B:276:ILE:HD12 | 2.02                     | 0.41              |
| 1:C:69:ALA:HB2   | 2:D:444:LYS:CD   | 2.50                     | 0.41              |
| 1:C:128:LYS:HZ1  | 1:C:234:ILE:H    | 1.68                     | 0.41              |
| 1:C:293:GLU:HG3  | 2:D:221:GLN:OE1  | 2.20                     | 0.41              |
| 2:D:100:PHE:HD1  | 2:D:295:VAL:HG13 | 1.85                     | 0.41              |
| 1:E:43:GLU:OE1   | 1:E:43:GLU:N     | 2.47                     | 0.41              |
| 1:E:241:HIS:HA   | 1:E:244:ASP:OD2  | 2.21                     | 0.41              |
| 2:F:433:PHE:N    | 2:F:433:PHE:CD2  | 2.88                     | 0.41              |
| 1:A:190:PRO:CG   | 1:A:394:PRO:HG3  | 2.51                     | 0.41              |
| 1:A:191:PHE:HB2  | 1:A:425:VAL:H    | 1.85                     | 0.41              |
| 2:B:24:ALA:HA    | 2:B:27:HIS:CE1   | 2.56                     | 0.41              |
| 2:B:24:ALA:O     | 2:B:27:HIS:N     | 2.53                     | 0.41              |
| 2:B:244:LEU:O    | 2:B:247:ILE:HG22 | 2.20                     | 0.41              |
| 2:B:274:GLU:O    | 2:B:278:ALA:N    | 2.51                     | 0.41              |
| 2:B:385:ASP:HA   | 2:B:388:THR:OG1  | 2.21                     | 0.41              |
| 2:D:141:GLU:CB   | 2:D:230:GLY:HA3  | 2.51                     | 0.41              |
| 2:D:435:ASP:N    | 2:D:438:ARG:HB2  | 2.35                     | 0.41              |
| 1:E:178:GLU:HA   | 1:E:181:GLN:HB2  | 2.02                     | 0.41              |
| 5:K:272:ARG:HA   | 5:K:275:GLY:H    | 1.86                     | 0.41              |
| 1:A:408:GLU:HB3  | 2:B:111:LEU:CD2  | 2.51                     | 0.41              |
| 1:A:492:LEU:HD12 | 1:A:492:LEU:HA   | 1.73                     | 0.41              |
| 2:B:161:LEU:HD13 | 2:B:174:LEU:HD21 | 2.02                     | 0.41              |
| 2:B:371:LEU:C    | 2:B:373:ILE:N    | 2.79                     | 0.41              |
| 1:C:27:ASP:C     | 1:C:30:GLY:H     | 2.29                     | 0.41              |
| 1:C:441:LYS:HE3  | 1:C:441:LYS:HB2  | 1.82                     | 0.41              |
| 2:D:113:MET:N    | 2:D:113:MET:SD   | 2.93                     | 0.41              |
| 1:E:182:LYS:HB2  | 1:E:182:LYS:HE2  | 1.87                     | 0.41              |
| 2:B:438:ARG:HH22 | 2:B:445:GLU:HG2  | 1.85                     | 0.41              |
| 2:D:382:MET:HE2  | 2:D:387:TYR:CA   | 2.50                     | 0.41              |
| 2:D:412:VAL:HA   | 2:D:415:LYS:HB3  | 2.01                     | 0.41              |
| 1:E:20:HIS:HE1   | 6:E:501:ADP:O2'  | 2.03                     | 0.41              |
| 1:E:176:ILE:HA   | 1:E:179:SER:OG   | 2.21                     | 0.41              |
| 1:E:212:GLU:O    | 1:E:217:ALA:HB3  | 2.21                     | 0.41              |
| 1:E:283:VAL:O    | 1:E:284:ASN:C    | 2.64                     | 0.41              |
| 2:F:384:GLU:O    | 2:F:387:TYR:HB2  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:H:497:UNK:O    | 3:H:498:UNK:C    | 2.69                     | 0.41              |
| 5:K:197:ASP:C    | 5:K:199:SER:H    | 2.29                     | 0.41              |
| 5:K:302:PRO:C    | 5:K:305:GLN:CA   | 2.93                     | 0.41              |
| 1:A:110:THR:C    | 1:A:502:ARG:HH21 | 2.27                     | 0.41              |
| 1:A:231:GLY:N    | 1:A:260:LYS:HA   | 2.27                     | 0.41              |
| 1:A:509:THR:N    | 1:A:510:PRO:HD2  | 2.36                     | 0.41              |
| 2:B:424:ASP:N    | 2:B:424:ASP:OD2  | 2.46                     | 0.41              |
| 1:C:354:LEU:O    | 1:C:355:LEU:C    | 2.63                     | 0.41              |
| 1:C:448:ALA:HA   | 1:C:451:GLN:HB2  | 2.03                     | 0.41              |
| 2:D:156:SER:OG   | 2:D:173:ASP:HA   | 2.20                     | 0.41              |
| 2:D:177:LYS:HB2  | 2:D:205:LEU:CD2  | 2.50                     | 0.41              |
| 2:D:304:LEU:O    | 2:D:336:ARG:HB2  | 2.21                     | 0.41              |
| 2:D:421:VAL:HA   | 2:D:425:ASP:OD2  | 2.21                     | 0.41              |
| 2:F:60:LEU:HD12  | 2:F:63:ILE:HD12  | 2.03                     | 0.41              |
| 2:F:134:GLU:HG2  | 2:F:207:ARG:HH22 | 1.85                     | 0.41              |
| 2:F:214:ASP:CG   | 2:F:215:TYR:H    | 2.29                     | 0.41              |
| 2:F:309:PHE:HZ   | 2:F:350:LEU:HB2  | 1.85                     | 0.41              |
| 4:J:252:UNK:O    | 4:J:255:UNK:CA   | 2.69                     | 0.41              |
| 5:K:386:SER:CB   | 5:K:388:LEU:O    | 2.69                     | 0.41              |
| 1:A:106:SER:HB2  | 1:A:191:PHE:CZ   | 2.56                     | 0.41              |
| 1:A:230:GLU:HG3  | 1:A:261:THR:HB   | 2.03                     | 0.41              |
| 1:A:495:ILE:HA   | 1:A:498:LYS:HD2  | 2.03                     | 0.41              |
| 2:B:284:ARG:HG2  | 2:B:290:GLU:HA   | 2.02                     | 0.41              |
| 1:C:34:GLN:OE1   | 1:C:46:ARG:NH1   | 2.54                     | 0.41              |
| 1:C:54:GLU:HA    | 1:C:57:LYS:CB    | 2.50                     | 0.41              |
| 1:C:354:LEU:O    | 1:C:357:ARG:N    | 2.48                     | 0.41              |
| 2:D:31:LEU:HA    | 2:D:46:MET:HE1   | 2.02                     | 0.41              |
| 2:D:60:LEU:HA    | 2:D:60:LEU:HD23  | 1.84                     | 0.41              |
| 2:D:77:GLY:HA3   | 2:D:83:LYS:CD    | 2.50                     | 0.41              |
| 2:D:81:THR:HB    | 6:D:501:ADP:C3'  | 2.49                     | 0.41              |
| 2:D:137:ILE:CG2  | 2:D:209:PHE:H    | 2.33                     | 0.41              |
| 2:D:192:VAL:HG13 | 2:D:216:ASP:CG   | 2.46                     | 0.41              |
| 2:D:359:THR:HB   | 2:D:360:THR:H    | 1.71                     | 0.41              |
| 2:D:406:ILE:HG23 | 2:D:407:THR:N    | 2.36                     | 0.41              |
| 2:F:305:ASP:O    | 2:F:308:SER:OG   | 2.35                     | 0.41              |
| 3:H:379:UNK:C    | 3:H:381:UNK:N    | 2.83                     | 0.41              |
| 1:A:134:ALA:HB2  | 2:B:416:ARG:HH21 | 1.85                     | 0.41              |
| 1:A:408:GLU:H    | 1:A:408:GLU:CD   | 2.26                     | 0.41              |
| 2:B:33:LEU:HD13  | 2:B:38:GLU:C     | 2.46                     | 0.41              |
| 2:B:132:LYS:CG   | 2:B:237:GLU:HB3  | 2.46                     | 0.41              |
| 2:B:242:VAL:HG13 | 2:B:246:GLU:OE1  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:279:LYS:O    | 2:B:282:GLU:HG3  | 2.20                     | 0.41              |
| 2:B:384:GLU:O    | 2:B:387:TYR:HB2  | 2.21                     | 0.41              |
| 2:B:431:SER:H    | 2:B:431:SER:HG   | 1.63                     | 0.41              |
| 2:D:27:HIS:O     | 2:D:29:ARG:HG2   | 2.21                     | 0.41              |
| 2:D:30:GLY:N     | 2:D:44:GLN:HB3   | 2.36                     | 0.41              |
| 2:D:134:GLU:HA   | 2:D:207:ARG:CD   | 2.49                     | 0.41              |
| 2:D:401:TYR:O    | 2:D:404:GLN:HB3  | 2.20                     | 0.41              |
| 1:E:7:LYS:HD3    | 1:E:246:ALA:HB2  | 2.03                     | 0.41              |
| 1:E:160:GLY:O    | 1:E:162:LYS:N    | 2.54                     | 0.41              |
| 1:E:180:LEU:HD23 | 1:E:180:LEU:HA   | 1.90                     | 0.41              |
| 2:F:164:LYS:HB3  | 2:F:164:LYS:HE2  | 1.77                     | 0.41              |
| 2:F:442:TYR:HD1  | 2:F:442:TYR:HA   | 1.79                     | 0.41              |
| 3:H:86:UNK:O     | 3:H:88:UNK:N     | 2.54                     | 0.41              |
| 3:H:98:UNK:O     | 3:H:102:UNK:N    | 2.53                     | 0.41              |
| 3:H:293:UNK:O    | 3:H:295:UNK:N    | 2.54                     | 0.41              |
| 5:K:197:ASP:C    | 5:K:199:SER:N    | 2.77                     | 0.41              |
| 5:K:263:ALA:C    | 5:K:265:LEU:H    | 2.28                     | 0.41              |
| 1:A:143:ALA:HB1  | 1:A:456:VAL:O    | 2.21                     | 0.41              |
| 1:A:194:MET:HA   | 1:A:402:VAL:HB   | 2.03                     | 0.41              |
| 1:A:513:LEU:O    | 1:A:516:LYS:HB3  | 2.21                     | 0.41              |
| 2:B:368:LYS:NZ   | 2:B:372:ARG:HH12 | 2.19                     | 0.41              |
| 2:B:412:VAL:C    | 2:B:414:ARG:N    | 2.79                     | 0.41              |
| 1:C:55:LEU:HD13  | 1:C:60:LYS:O     | 2.21                     | 0.41              |
| 1:C:232:LYS:HG3  | 1:C:234:ILE:HG12 | 2.03                     | 0.41              |
| 2:D:82:GLY:C     | 6:D:501:ADP:O2'  | 2.64                     | 0.41              |
| 2:D:139:GLU:HB3  | 2:D:231:GLU:CD   | 2.46                     | 0.41              |
| 2:D:172:TYR:HB2  | 2:D:202:ILE:HA   | 2.02                     | 0.41              |
| 2:D:394:GLY:O    | 2:D:398:SER:N    | 2.54                     | 0.41              |
| 1:E:183:GLU:OE2  | 1:E:203:GLN:HA   | 2.21                     | 0.41              |
| 1:E:275:LEU:O    | 1:E:279:ILE:HD12 | 2.21                     | 0.41              |
| 1:E:355:LEU:HD12 | 1:E:355:LEU:HA   | 1.84                     | 0.41              |
| 1:E:432:GLU:CD   | 1:E:432:GLU:H    | 2.29                     | 0.41              |
| 4:J:343:UNK:O    | 4:J:347:UNK:N    | 2.54                     | 0.41              |
| 1:A:179:LEU:HD13 | 1:A:189:VAL:HG22 | 2.03                     | 0.40              |
| 1:A:243:ASN:HA   | 1:A:244:PRO:HD3  | 1.94                     | 0.40              |
| 1:A:328:LYS:NZ   | 1:A:330:LYS:HB2  | 2.37                     | 0.40              |
| 2:B:37:LEU:HD13  | 2:B:37:LEU:HA    | 1.90                     | 0.40              |
| 2:B:130:ARG:HB3  | 2:B:290:GLU:CD   | 2.46                     | 0.40              |
| 1:C:54:GLU:CD    | 1:C:57:LYS:HD3   | 2.46                     | 0.40              |
| 2:D:208:SER:O    | 2:D:210:THR:HG23 | 2.21                     | 0.40              |
| 2:D:318:SER:HG   | 2:D:319:ASP:H    | 1.67                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:11:LYS:HE3   | 1:E:11:LYS:HB3   | 1.95                     | 0.40              |
| 1:E:138:LEU:HA   | 1:E:157:VAL:CG1  | 2.49                     | 0.40              |
| 1:E:317:ARG:O    | 1:E:320:GLU:HG2  | 2.21                     | 0.40              |
| 1:E:343:ASP:OD1  | 1:E:343:ASP:N    | 2.52                     | 0.40              |
| 1:E:376:LYS:O    | 1:E:380:GLN:NE2  | 2.54                     | 0.40              |
| 2:F:283:TRP:HA   | 2:F:286:GLU:HG2  | 2.04                     | 0.40              |
| 1:A:162:ARG:HG2  | 1:A:417:LEU:HB2  | 2.03                     | 0.40              |
| 1:A:241:THR:HG22 | 1:A:242:GLU:H    | 1.84                     | 0.40              |
| 1:C:278:GLU:HG3  | 1:C:279:ILE:H    | 1.86                     | 0.40              |
| 1:C:287:ILE:HA   | 1:C:287:ILE:HD12 | 1.77                     | 0.40              |
| 2:D:46:MET:O     | 2:D:53:ARG:NH2   | 2.54                     | 0.40              |
| 2:D:127:ILE:HD11 | 2:D:322:PRO:HD3  | 2.02                     | 0.40              |
| 2:D:416:ARG:CZ   | 2:D:418:GLY:HA3  | 2.52                     | 0.40              |
| 1:E:128:LYS:HE2  | 1:E:128:LYS:HB2  | 1.92                     | 0.40              |
| 1:E:194:GLU:C    | 1:E:200:VAL:HG12 | 2.46                     | 0.40              |
| 1:E:394:LEU:HD12 | 1:E:394:LEU:HA   | 1.76                     | 0.40              |
| 2:F:188:GLN:NE2  | 2:F:216:ASP:OD1  | 2.54                     | 0.40              |
| 3:H:313:UNK:O    | 3:H:317:GLY:N    | 2.51                     | 0.40              |
| 5:K:145:UNK:O    | 5:K:149:UNK:N    | 2.55                     | 0.40              |
| 5:K:246:GLU:O    | 5:K:250:ASP:CB   | 2.69                     | 0.40              |
| 1:A:138:VAL:CB   | 2:B:433:PHE:HD2  | 2.33                     | 0.40              |
| 1:A:189:VAL:HB   | 1:A:190:PRO:HD3  | 2.04                     | 0.40              |
| 1:A:231:GLY:C    | 1:A:265:THR:HA   | 2.46                     | 0.40              |
| 2:B:24:ALA:H     | 2:B:403:ILE:HG21 | 1.85                     | 0.40              |
| 2:D:425:ASP:O    | 2:D:429:VAL:N    | 2.42                     | 0.40              |
| 1:E:218:GLU:HG3  | 1:E:219:GLU:O    | 2.21                     | 0.40              |
| 1:E:232:LYS:CD   | 1:E:234:ILE:HD11 | 2.51                     | 0.40              |
| 4:J:358:UNK:HA   | 4:J:361:UNK:CB   | 2.51                     | 0.40              |
| 5:K:146:UNK:O    | 5:K:150:UNK:N    | 2.54                     | 0.40              |
| 1:A:373:LEU:O    | 1:A:377:ILE:HG13 | 2.21                     | 0.40              |
| 1:A:407:ILE:O    | 1:A:408:GLU:C    | 2.65                     | 0.40              |
| 1:A:412:TYR:O    | 1:A:412:TYR:CG   | 2.75                     | 0.40              |
| 2:D:129:VAL:H    | 2:D:242:VAL:CG1  | 2.25                     | 0.40              |
| 2:D:135:THR:H    | 2:D:207:ARG:HH11 | 1.68                     | 0.40              |
| 2:D:429:VAL:O    | 2:D:432:LEU:N    | 2.55                     | 0.40              |
| 2:F:161:LEU:HB3  | 2:F:172:TYR:CE1  | 2.56                     | 0.40              |
| 3:H:175:UNK:C    | 3:H:177:UNK:N    | 2.83                     | 0.40              |
| 1:A:202:THR:HA   | 2:F:306:ILE:HA   | 2.02                     | 0.40              |
| 1:A:209:VAL:O    | 1:A:213:ASN:CG   | 2.65                     | 0.40              |
| 2:B:111:LEU:HD13 | 2:B:111:LEU:HA   | 1.87                     | 0.40              |
| 1:C:353:ASP:OD1  | 1:C:353:ASP:N    | 2.54                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:134:GLU:HA   | 2:D:207:ARG:CZ   | 2.50                     | 0.40              |
| 2:D:167:GLU:OE1  | 2:D:168:MET:HG2  | 2.21                     | 0.40              |
| 2:D:178:MET:HE2  | 2:D:195:ILE:O    | 2.21                     | 0.40              |
| 2:D:179:ILE:HG23 | 2:D:180:GLU:H    | 1.86                     | 0.40              |
| 2:D:425:ASP:O    | 2:D:429:VAL:HG23 | 2.21                     | 0.40              |
| 1:E:6:VAL:C      | 1:E:7:LYS:HD2    | 2.46                     | 0.40              |
| 1:E:184:ARG:HH12 | 1:E:217:ALA:HB1  | 1.87                     | 0.40              |
| 2:F:77:GLY:HA3   | 2:F:359:THR:HG22 | 2.02                     | 0.40              |
| 2:F:137:ILE:HG12 | 2:F:210:THR:OG1  | 2.22                     | 0.40              |
| 2:F:397:THR:OG1  | 2:F:398:SER:N    | 2.54                     | 0.40              |
| 4:J:436:UNK:O    | 4:J:440:UNK:N    | 2.55                     | 0.40              |
| 5:K:362:GLU:O    | 5:K:364:GLU:N    | 2.55                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 429/456 (94%)   | 316 (74%)  | 111 (26%) | 2 (0%)   | 24          | 54  |
| 1   | C     | 423/456 (93%)   | 353 (84%)  | 70 (16%)  | 0        | 100         | 100 |
| 1   | E     | 407/456 (89%)   | 347 (85%)  | 60 (15%)  | 0        | 100         | 100 |
| 2   | B     | 414/463 (89%)   | 340 (82%)  | 73 (18%)  | 1 (0%)   | 43          | 71  |
| 2   | D     | 415/463 (90%)   | 337 (81%)  | 78 (19%)  | 0        | 100         | 100 |
| 2   | F     | 415/463 (90%)   | 373 (90%)  | 42 (10%)  | 0        | 100         | 100 |
| 3   | H     | 6/1733 (0%)     | 6 (100%)   | 0         | 0        | 100         | 100 |
| 4   | J     | 6/964 (1%)      | 5 (83%)    | 0         | 1 (17%)  | 0           | 0   |
| 5   | K     | 356/491 (72%)   | 276 (78%)  | 59 (17%)  | 21 (6%)  | 1           | 9   |
| All | All   | 2871/5945 (48%) | 2353 (82%) | 493 (17%) | 25 (1%)  | 16          | 41  |

All (25) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | K     | 105 | ALA  |
| 5   | K     | 106 | ARG  |
| 5   | K     | 190 | ASP  |
| 5   | K     | 191 | SER  |
| 5   | K     | 283 | LYS  |
| 5   | K     | 296 | GLN  |
| 5   | K     | 318 | ARG  |
| 5   | K     | 342 | PRO  |
| 5   | K     | 388 | LEU  |
| 2   | B     | 80  | GLY  |
| 4   | J     | 194 | GLY  |
| 5   | K     | 104 | LEU  |
| 5   | K     | 163 | GLU  |
| 5   | K     | 343 | LEU  |
| 5   | K     | 216 | GLN  |
| 5   | K     | 244 | LEU  |
| 5   | K     | 297 | SER  |
| 5   | K     | 363 | PRO  |
| 1   | A     | 137 | LEU  |
| 5   | K     | 215 | ARG  |
| 5   | K     | 298 | ARG  |
| 5   | K     | 335 | SER  |
| 5   | K     | 360 | LEU  |
| 1   | A     | 428 | ALA  |
| 5   | K     | 341 | THR  |

### 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     | 364/387 (94%) | 361 (99%)  | 3 (1%)   | 73          | 76  |
| 1   | C     | 360/387 (93%) | 357 (99%)  | 3 (1%)   | 73          | 76  |
| 1   | E     | 343/387 (89%) | 342 (100%) | 1 (0%)   | 86          | 84  |
| 2   | B     | 343/390 (88%) | 343 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 2   | D     | 346/390 (89%)   | 345 (100%)  | 1 (0%)   | 86          | 84  |
| 2   | F     | 347/390 (89%)   | 347 (100%)  | 0        | 100         | 100 |
| 5   | K     | 1/383 (0%)      | 1 (100%)    | 0        | 100         | 100 |
| All | All   | 2104/2714 (78%) | 2096 (100%) | 8 (0%)   | 81          | 82  |

All (8) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 113 | ILE  |
| 1   | A     | 218 | ILE  |
| 1   | A     | 405 | LEU  |
| 1   | C     | 116 | PHE  |
| 1   | C     | 353 | ASP  |
| 1   | C     | 360 | ILE  |
| 2   | D     | 379 | ASP  |
| 1   | E     | 126 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 116 | HIS  |
| 1   | A     | 132 | GLN  |
| 1   | A     | 467 | GLN  |
| 1   | A     | 506 | GLN  |
| 1   | A     | 512 | ASN  |
| 1   | A     | 548 | GLN  |
| 2   | B     | 27  | HIS  |
| 2   | B     | 41  | GLN  |
| 2   | B     | 233 | GLN  |
| 2   | B     | 275 | GLN  |
| 2   | B     | 313 | ASN  |
| 2   | B     | 404 | GLN  |
| 2   | B     | 422 | GLN  |
| 2   | B     | 441 | GLN  |
| 1   | C     | 18  | HIS  |
| 1   | C     | 181 | GLN  |
| 1   | C     | 284 | ASN  |
| 1   | C     | 451 | GLN  |
| 2   | D     | 188 | GLN  |
| 2   | D     | 233 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 245 | HIS  |
| 2   | D     | 251 | ASN  |
| 2   | D     | 302 | HIS  |
| 2   | D     | 329 | ASN  |
| 2   | D     | 341 | GLN  |
| 2   | D     | 404 | GLN  |
| 1   | E     | 42  | GLN  |
| 1   | E     | 85  | GLN  |
| 1   | E     | 156 | HIS  |
| 1   | E     | 181 | GLN  |
| 1   | E     | 229 | HIS  |
| 1   | E     | 236 | GLN  |
| 1   | E     | 289 | GLN  |
| 2   | F     | 92  | GLN  |
| 2   | F     | 226 | GLN  |
| 2   | F     | 233 | GLN  |
| 2   | F     | 344 | 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](#)

5 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | ADP  | F     | 501 | -    | 28,29,29     | 1.40 | 6 (21%)  | 43,45,45    | 1.74 | 9 (20%)  |
| 6   | ADP  | B     | 501 | -    | 28,29,29     | 1.53 | 5 (17%)  | 43,45,45    | 1.71 | 7 (16%)  |
| 6   | ADP  | E     | 501 | -    | 28,29,29     | 1.36 | 5 (17%)  | 43,45,45    | 1.72 | 7 (16%)  |
| 6   | ADP  | C     | 501 | -    | 28,29,29     | 1.40 | 4 (14%)  | 43,45,45    | 2.07 | 9 (20%)  |
| 6   | ADP  | D     | 501 | -    | 28,29,29     | 1.32 | 4 (14%)  | 43,45,45    | 1.82 | 9 (20%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 6   | ADP  | F     | 501 | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 6   | ADP  | B     | 501 | -    | -       | 3/16/32/32 | 0/3/3/3 |
| 6   | ADP  | E     | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 6   | ADP  | C     | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 6   | ADP  | D     | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |

All (24) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | C     | 501 | ADP  | C5-C4 | 4.62  | 1.47        | 1.39     |
| 6   | D     | 501 | ADP  | C5-C4 | 4.15  | 1.46        | 1.39     |
| 6   | F     | 501 | ADP  | C5-C4 | 4.13  | 1.46        | 1.39     |
| 6   | E     | 501 | ADP  | C5-C4 | 4.07  | 1.46        | 1.39     |
| 6   | B     | 501 | ADP  | C5-C4 | 3.91  | 1.46        | 1.39     |
| 6   | B     | 501 | ADP  | C5-N7 | -3.46 | 1.32        | 1.39     |
| 6   | B     | 501 | ADP  | C4-N9 | -3.37 | 1.30        | 1.37     |
| 6   | D     | 501 | ADP  | C5-N7 | -2.81 | 1.33        | 1.39     |
| 6   | F     | 501 | ADP  | C4-N9 | -2.76 | 1.32        | 1.37     |
| 6   | C     | 501 | ADP  | C5-N7 | -2.65 | 1.34        | 1.39     |
| 6   | E     | 501 | ADP  | C4-N9 | -2.61 | 1.32        | 1.37     |
| 6   | F     | 501 | ADP  | C5-N7 | -2.54 | 1.34        | 1.39     |
| 6   | C     | 501 | ADP  | C8-N7 | 2.48  | 1.36        | 1.31     |
| 6   | E     | 501 | ADP  | C5-C6 | 2.36  | 1.47        | 1.41     |
| 6   | B     | 501 | ADP  | C8-N7 | 2.35  | 1.36        | 1.31     |
| 6   | F     | 501 | ADP  | C5-C6 | 2.33  | 1.47        | 1.41     |
| 6   | E     | 501 | ADP  | C5-N7 | -2.33 | 1.34        | 1.39     |
| 6   | B     | 501 | ADP  | C8-N9 | -2.24 | 1.33        | 1.37     |
| 6   | C     | 501 | ADP  | C5-C6 | 2.23  | 1.47        | 1.41     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | E     | 501 | ADP  | C8-N7 | 2.22  | 1.35        | 1.31     |
| 6   | D     | 501 | ADP  | C8-N7 | 2.14  | 1.35        | 1.31     |
| 6   | F     | 501 | ADP  | C8-N9 | -2.09 | 1.34        | 1.37     |
| 6   | F     | 501 | ADP  | C8-N7 | 2.09  | 1.35        | 1.31     |
| 6   | D     | 501 | ADP  | C4-N9 | -2.04 | 1.33        | 1.37     |

All (41) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | C     | 501 | ADP  | C5-C4-N3    | -6.46 | 117.82      | 126.72   |
| 6   | B     | 501 | ADP  | C5-C4-N3    | -5.70 | 118.87      | 126.72   |
| 6   | E     | 501 | ADP  | C5-C4-N3    | -5.53 | 119.10      | 126.72   |
| 6   | F     | 501 | ADP  | C5-C4-N3    | -5.31 | 119.40      | 126.72   |
| 6   | D     | 501 | ADP  | C5-C4-N3    | -5.26 | 119.47      | 126.72   |
| 6   | C     | 501 | ADP  | N3-C4-N9    | 5.13  | 135.88      | 127.17   |
| 6   | D     | 501 | ADP  | N3-C4-N9    | 4.62  | 135.03      | 127.17   |
| 6   | C     | 501 | ADP  | O4'-C1'-N9  | 4.26  | 116.28      | 108.09   |
| 6   | E     | 501 | ADP  | N3-C4-N9    | 4.26  | 134.41      | 127.17   |
| 6   | F     | 501 | ADP  | N3-C4-N9    | 4.02  | 134.00      | 127.17   |
| 6   | C     | 501 | ADP  | C2-N3-C4    | 3.87  | 121.28      | 111.83   |
| 6   | B     | 501 | ADP  | C4-C5-N7    | -3.68 | 106.37      | 110.58   |
| 6   | D     | 501 | ADP  | N3-C2-N1    | -3.67 | 123.03      | 128.58   |
| 6   | B     | 501 | ADP  | N3-C4-N9    | 3.64  | 133.35      | 127.17   |
| 6   | D     | 501 | ADP  | C2-N3-C4    | 3.57  | 120.55      | 111.83   |
| 6   | E     | 501 | ADP  | C2-N3-C4    | 3.53  | 120.45      | 111.83   |
| 6   | F     | 501 | ADP  | C2-N3-C4    | 3.46  | 120.27      | 111.83   |
| 6   | C     | 501 | ADP  | C4'-O4'-C1' | -3.45 | 101.86      | 109.47   |
| 6   | C     | 501 | ADP  | N3-C2-N1    | -3.30 | 123.58      | 128.58   |
| 6   | D     | 501 | ADP  | O4'-C1'-N9  | 3.30  | 114.42      | 108.09   |
| 6   | F     | 501 | ADP  | C4-C5-N7    | -3.17 | 106.95      | 110.58   |
| 6   | F     | 501 | ADP  | N3-C2-N1    | -3.01 | 124.02      | 128.58   |
| 6   | B     | 501 | ADP  | C2-N3-C4    | 2.96  | 119.07      | 111.83   |
| 6   | C     | 501 | ADP  | C4-C5-N7    | -2.92 | 107.24      | 110.58   |
| 6   | E     | 501 | ADP  | C4-C5-N7    | -2.91 | 107.26      | 110.58   |
| 6   | E     | 501 | ADP  | N3-C2-N1    | -2.77 | 124.39      | 128.58   |
| 6   | D     | 501 | ADP  | C4-N9-C8    | 2.72  | 108.59      | 105.74   |
| 6   | B     | 501 | ADP  | C5'-C4'-C3' | -2.52 | 106.15      | 115.21   |
| 6   | E     | 501 | ADP  | C3'-C2'-C1' | 2.44  | 106.08      | 101.46   |
| 6   | E     | 501 | ADP  | C4-N9-C8    | 2.42  | 108.28      | 105.74   |
| 6   | F     | 501 | ADP  | C4-N9-C8    | 2.40  | 108.26      | 105.74   |
| 6   | D     | 501 | ADP  | C4-C5-N7    | -2.18 | 108.09      | 110.58   |
| 6   | C     | 501 | ADP  | C5-N7-C8    | 2.17  | 106.86      | 103.45   |

*Continued on next page...*

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | F     | 501 | ADP  | C6-C5-N7    | 2.12  | 136.18      | 132.09   |
| 6   | C     | 501 | ADP  | O3B-PB-O2B  | 2.12  | 115.73      | 107.80   |
| 6   | D     | 501 | ADP  | C2-N1-C6    | 2.10  | 122.18      | 118.73   |
| 6   | B     | 501 | ADP  | O3B-PB-O2B  | 2.09  | 115.65      | 107.80   |
| 6   | F     | 501 | ADP  | C3'-C2'-C1' | 2.06  | 105.36      | 101.46   |
| 6   | D     | 501 | ADP  | C2'-C1'-N9  | -2.05 | 108.21      | 113.30   |
| 6   | B     | 501 | ADP  | C5-N7-C8    | 2.04  | 106.66      | 103.45   |
| 6   | F     | 501 | ADP  | O2A-PA-O1A  | 2.01  | 121.79      | 112.44   |

There are no chirality outliers.

All (20) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | D     | 501 | ADP  | C5'-O5'-PA-O1A  |
| 6   | D     | 501 | ADP  | C5'-O5'-PA-O2A  |
| 6   | D     | 501 | ADP  | C5'-O5'-PA-O3A  |
| 6   | F     | 501 | ADP  | C5'-O5'-PA-O1A  |
| 6   | B     | 501 | ADP  | O4'-C4'-C5'-O5' |
| 6   | B     | 501 | ADP  | C3'-C4'-C5'-O5' |
| 6   | C     | 501 | ADP  | O4'-C4'-C5'-O5' |
| 6   | C     | 501 | ADP  | C3'-C4'-C5'-O5' |
| 6   | E     | 501 | ADP  | O4'-C4'-C5'-O5' |
| 6   | E     | 501 | ADP  | C3'-C4'-C5'-O5' |
| 6   | F     | 501 | ADP  | O4'-C4'-C5'-O5' |
| 6   | F     | 501 | ADP  | C3'-C4'-C5'-O5' |
| 6   | F     | 501 | ADP  | PB-O3A-PA-O1A   |
| 6   | F     | 501 | ADP  | C5'-O5'-PA-O2A  |
| 6   | F     | 501 | ADP  | C5'-O5'-PA-O3A  |
| 6   | D     | 501 | ADP  | O4'-C4'-C5'-O5' |
| 6   | F     | 501 | ADP  | PB-O3A-PA-O2A   |
| 6   | C     | 501 | ADP  | C2'-C1'-N9-C8   |
| 6   | C     | 501 | ADP  | C4'-C5'-O5'-PA  |
| 6   | B     | 501 | ADP  | C4'-C5'-O5'-PA  |

There are no ring outliers.

4 monomers are involved in 45 short contacts:

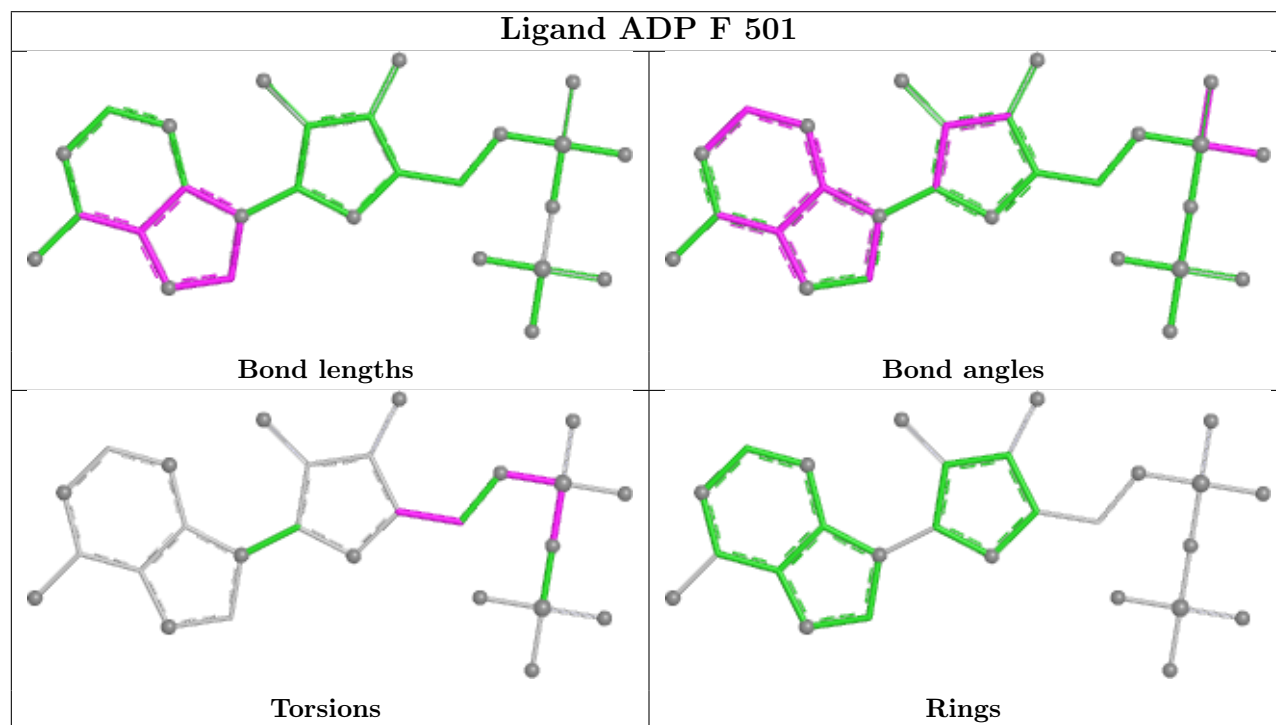
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | F     | 501 | ADP  | 6       | 0            |
| 6   | B     | 501 | ADP  | 13      | 0            |
| 6   | E     | 501 | ADP  | 5       | 0            |

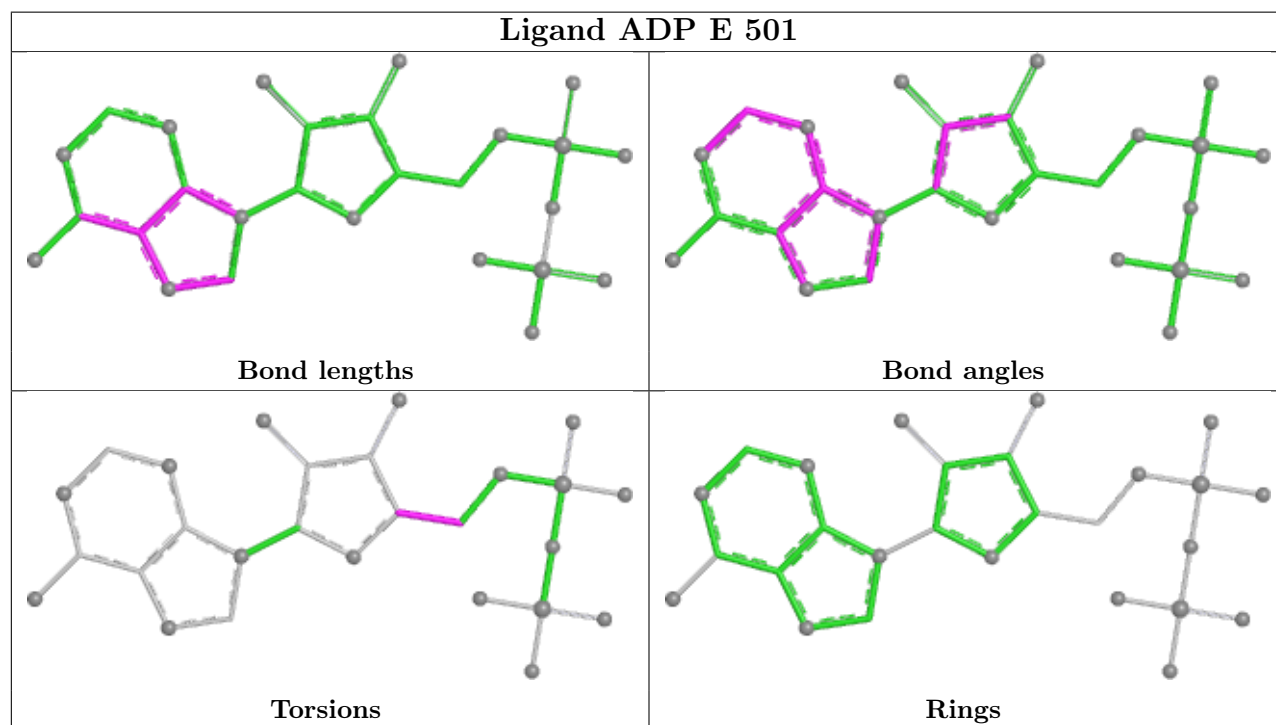
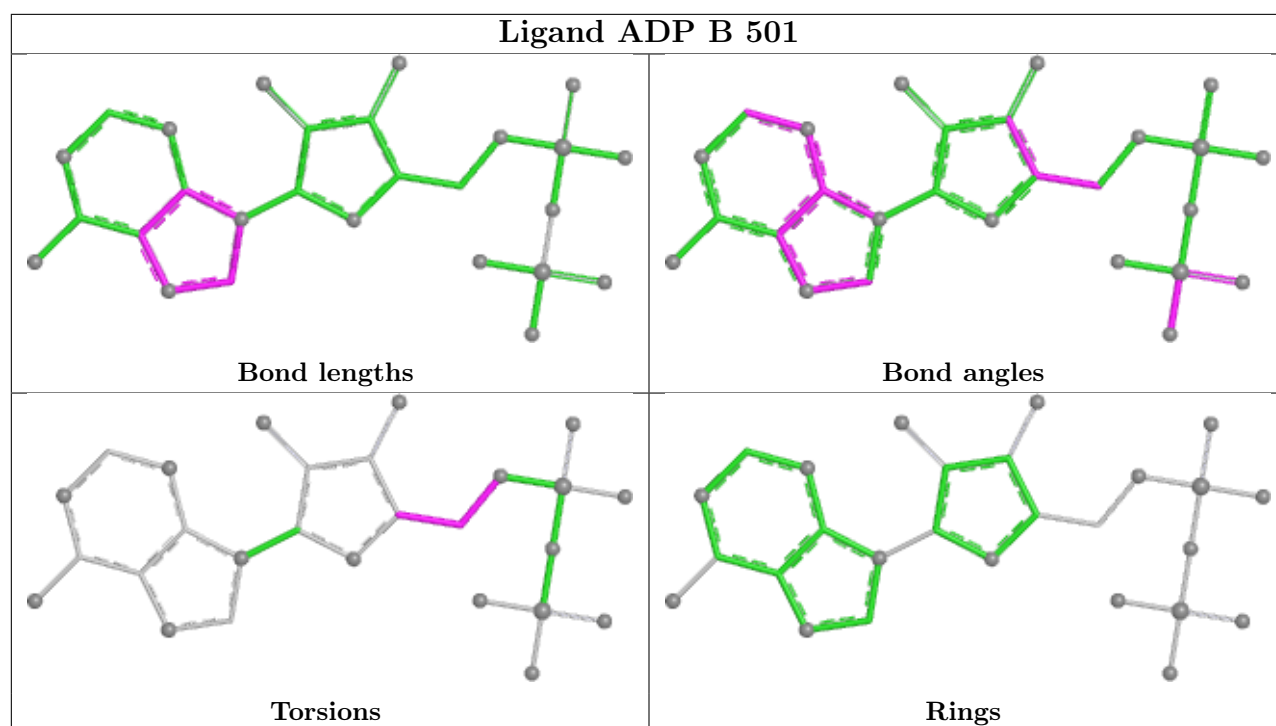
*Continued on next page...*

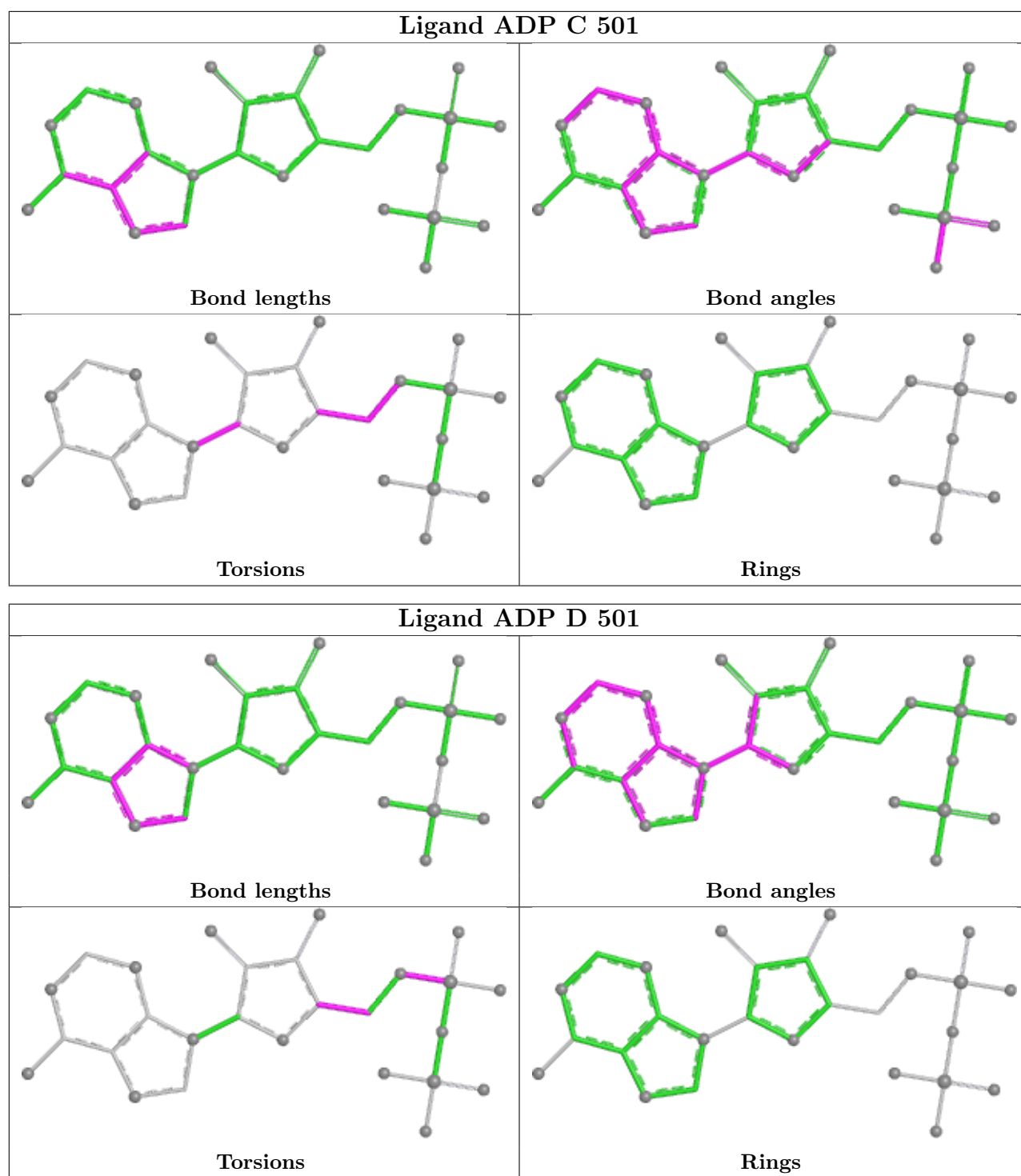
*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | D     | 501 | ADP  | 21      | 0            |

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 4   | J     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | J     | 60:UNK    | C      | 70:UNK    | N      | 9.60         |

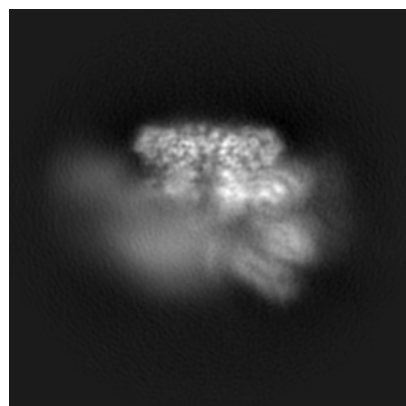
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12979. These allow visual inspection of the internal detail of the map and identification of artifacts.

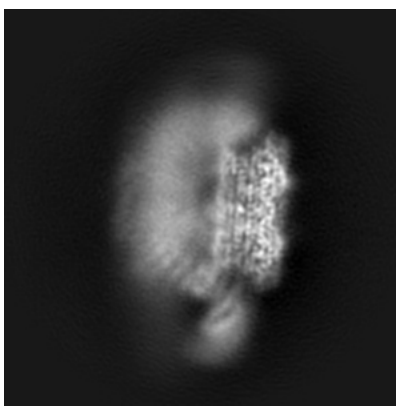
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

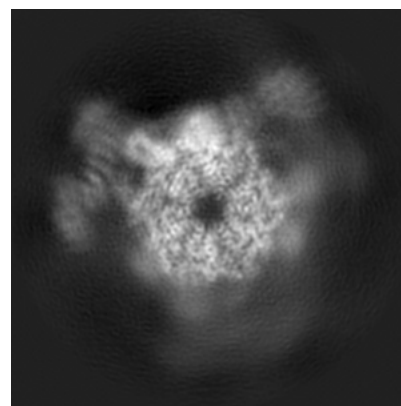
#### 6.1.1 Primary map



X

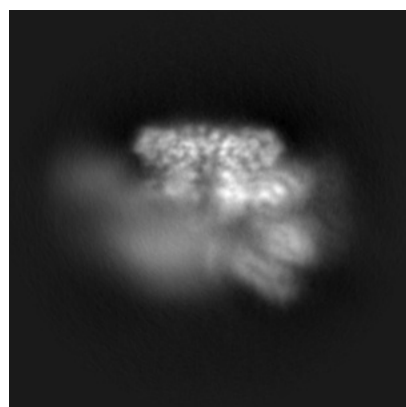


Y

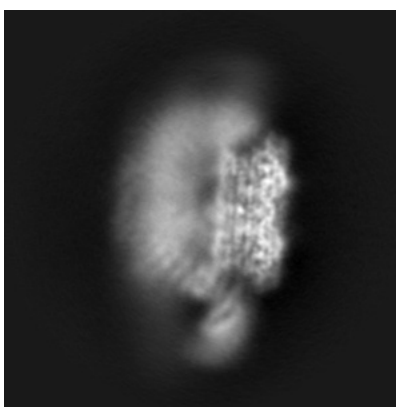


Z

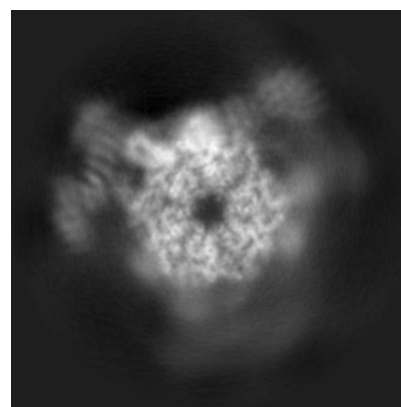
#### 6.1.2 Raw map



X



Y

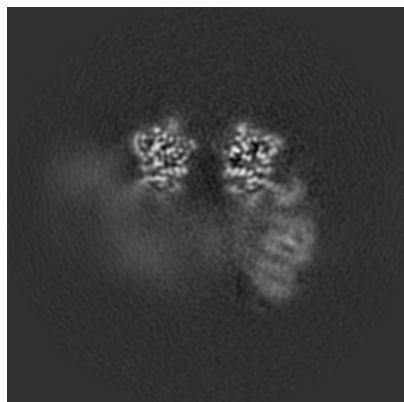


Z

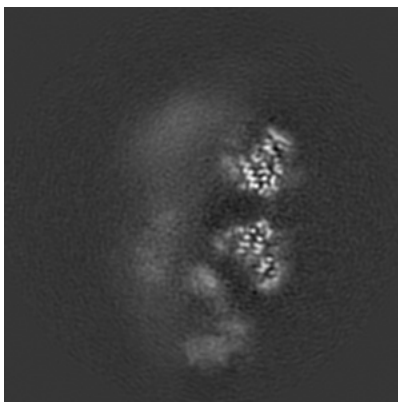
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

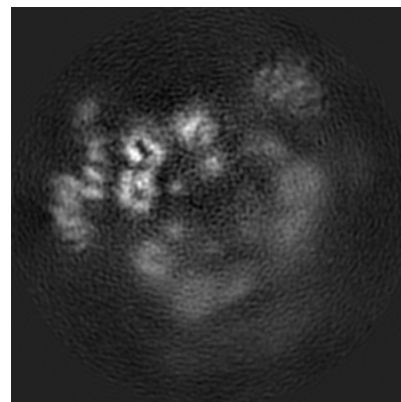
### 6.2.1 Primary map



X Index: 140

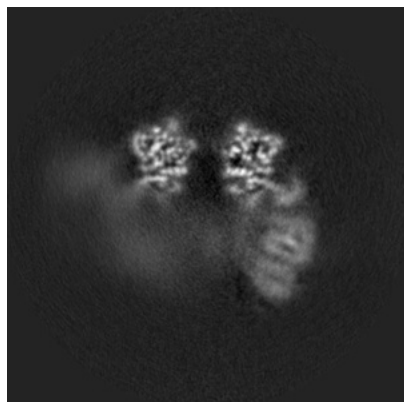


Y Index: 140

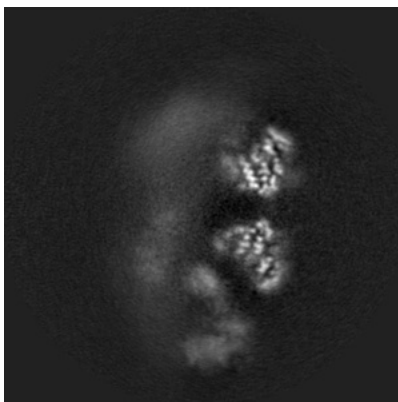


Z Index: 140

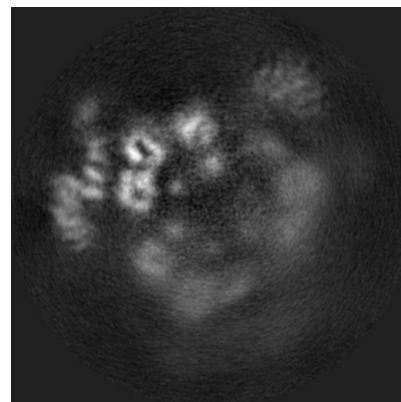
### 6.2.2 Raw map



X Index: 140



Y Index: 140

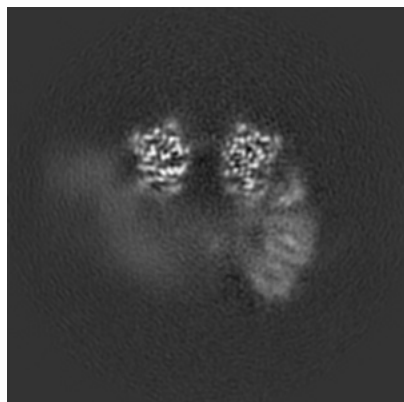


Z Index: 140

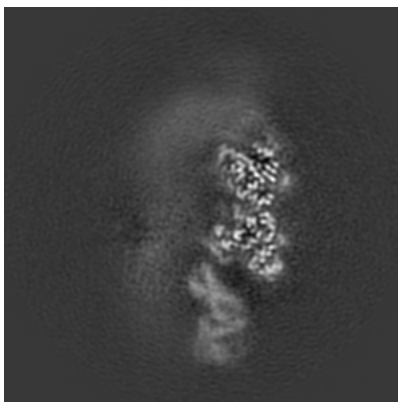
The images above show central slices of the map in three orthogonal directions.

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

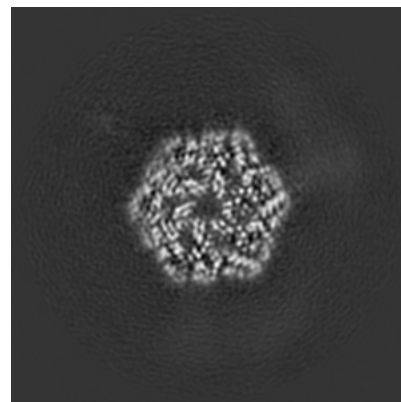
### 6.3.1 Primary map



X Index: 138

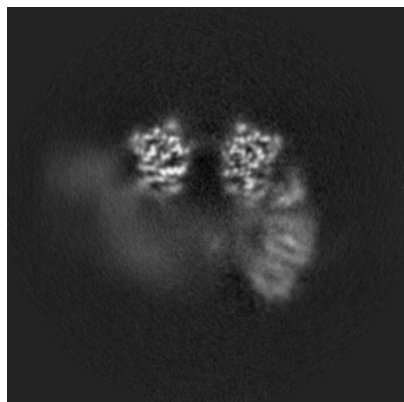


Y Index: 152

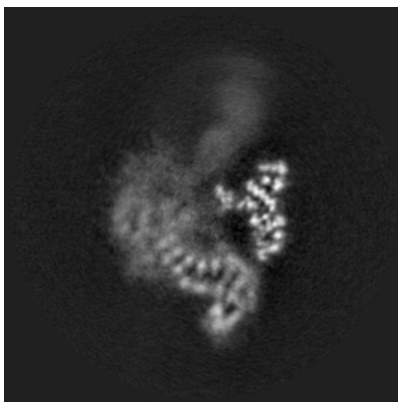


Z Index: 185

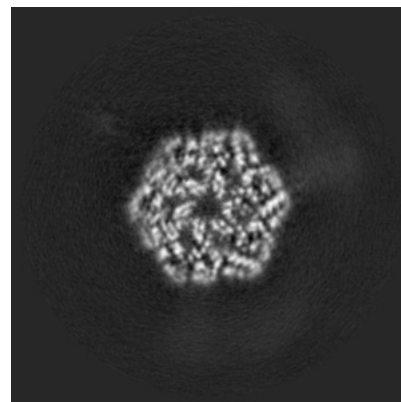
### 6.3.2 Raw map



X Index: 138



Y Index: 181

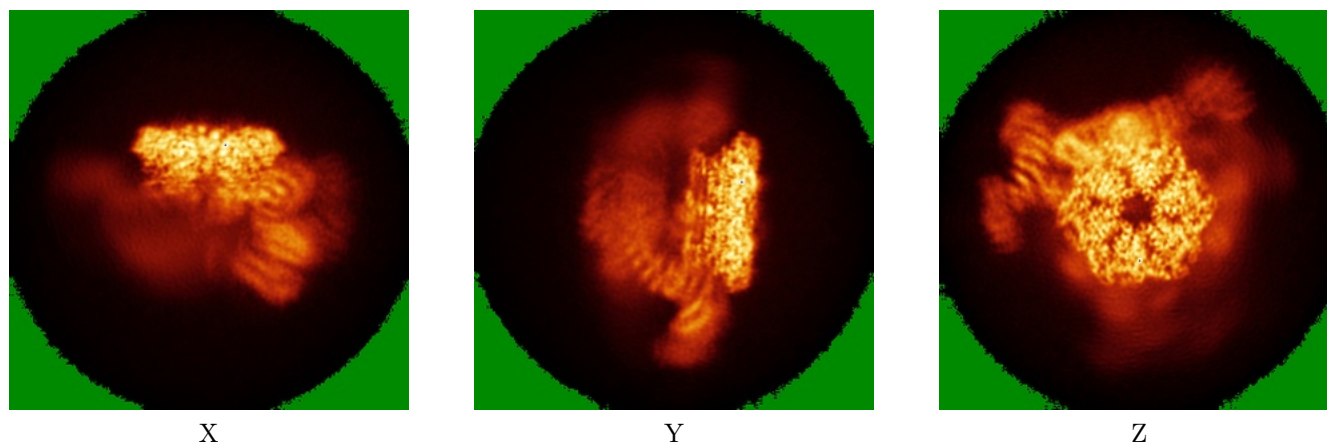


Z Index: 185

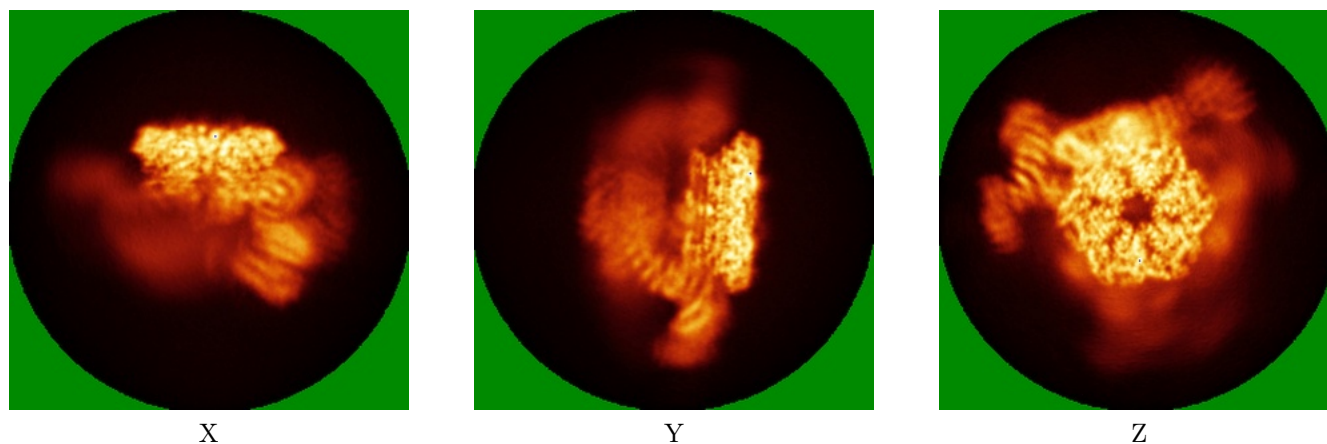
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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](#)

This section was not generated.

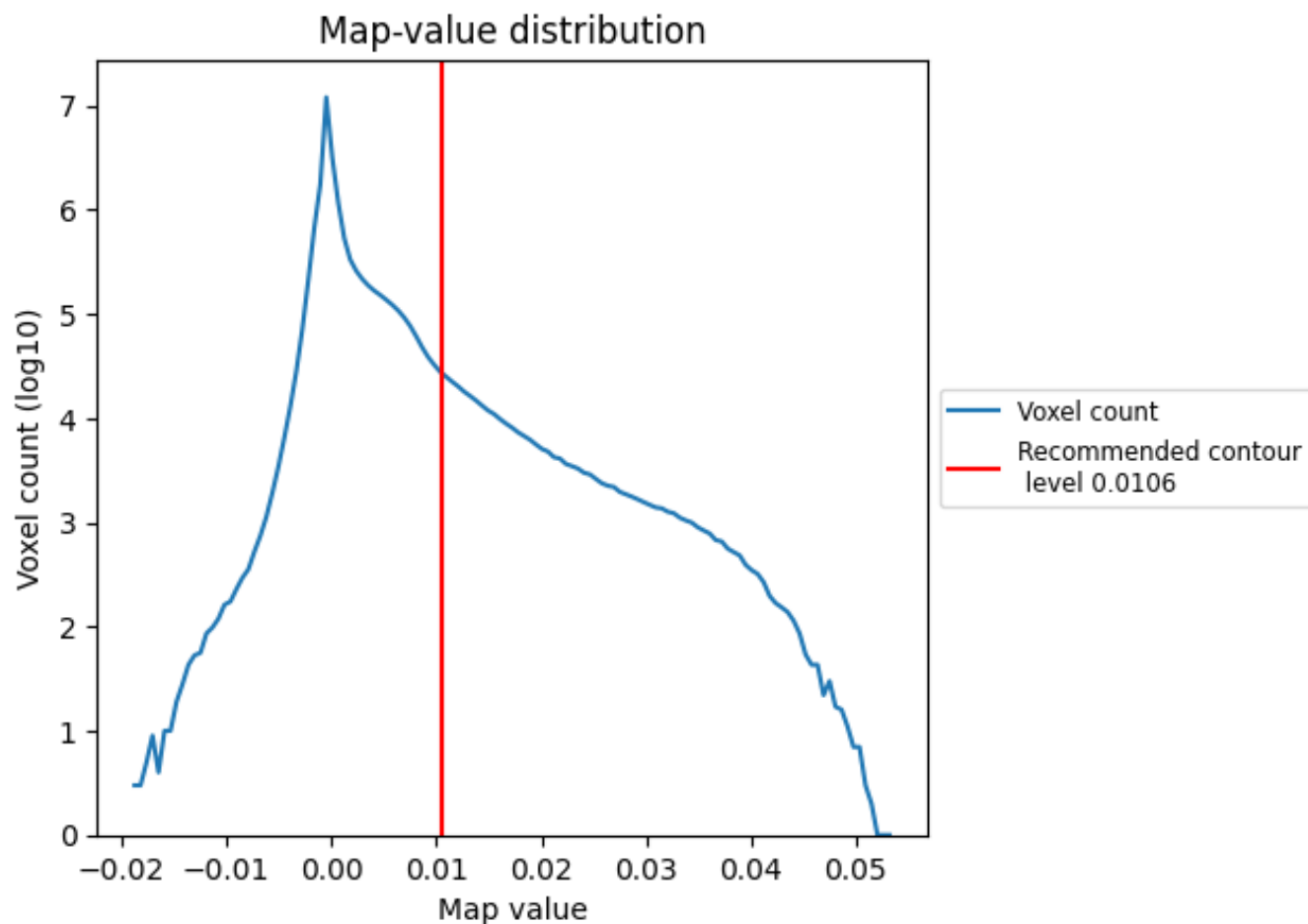
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

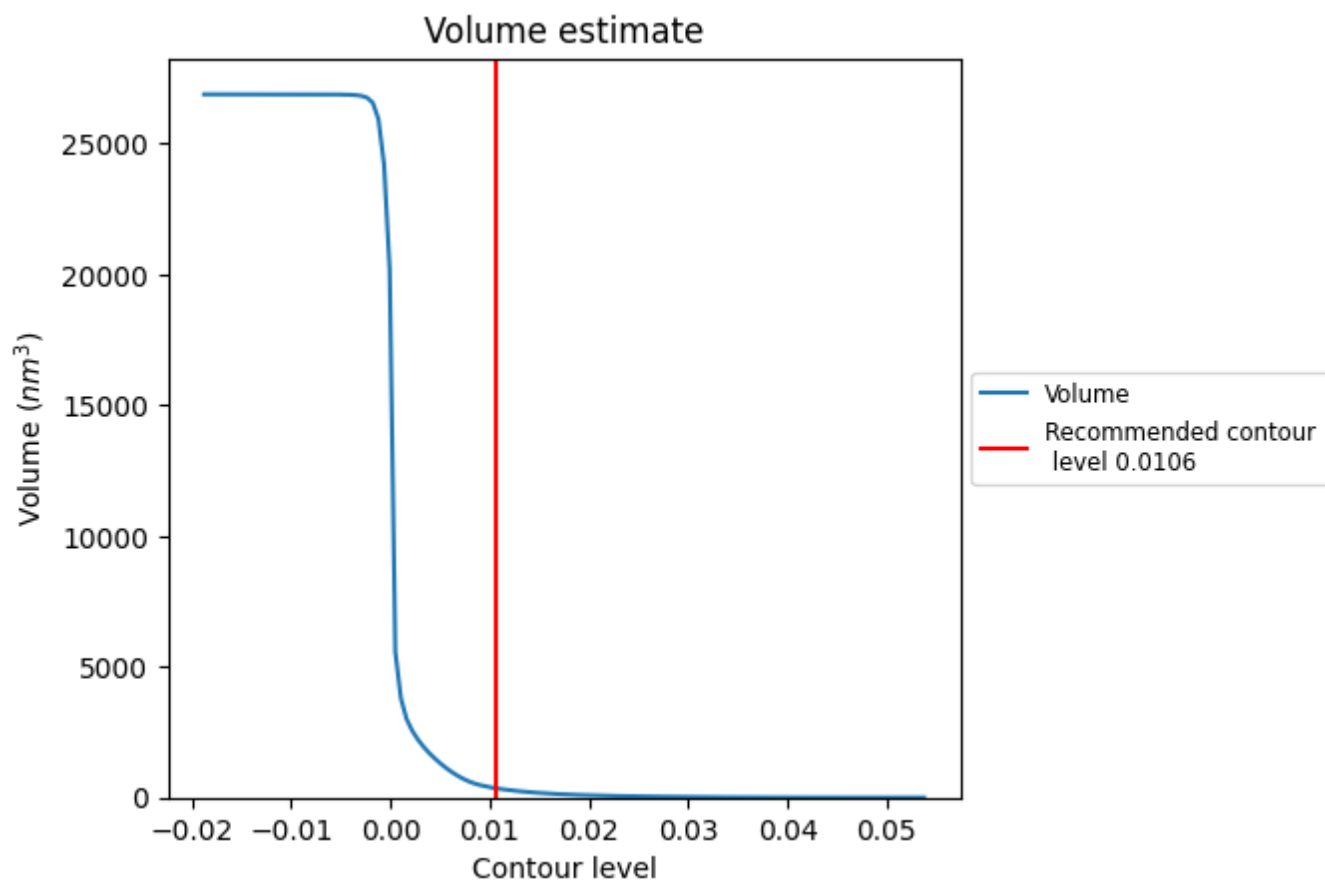
This section contains the results of statistical analysis of the map.

### 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.

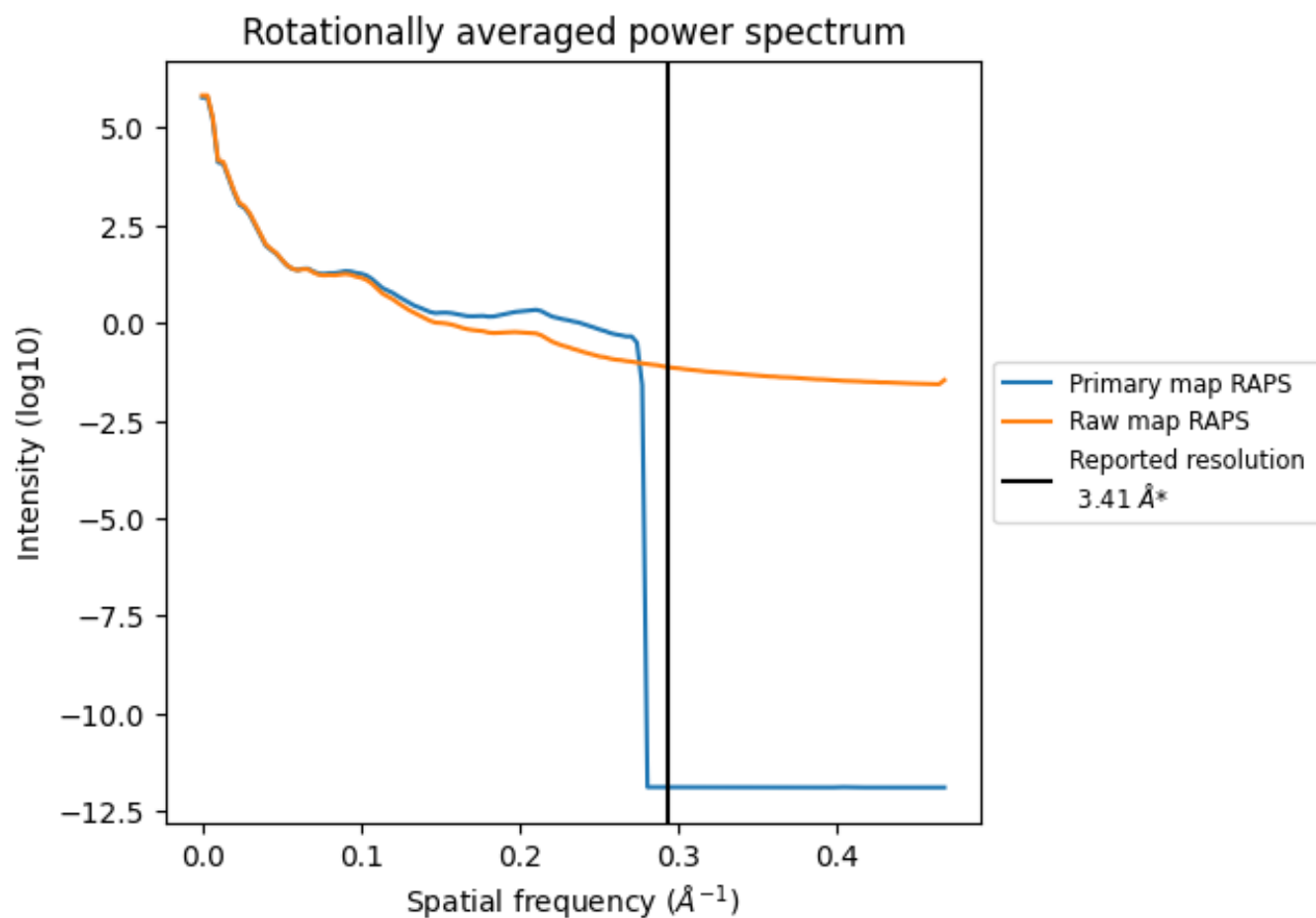
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 357  $\text{nm}^3$ ; this corresponds to an approximate mass of 323 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 ⓘ



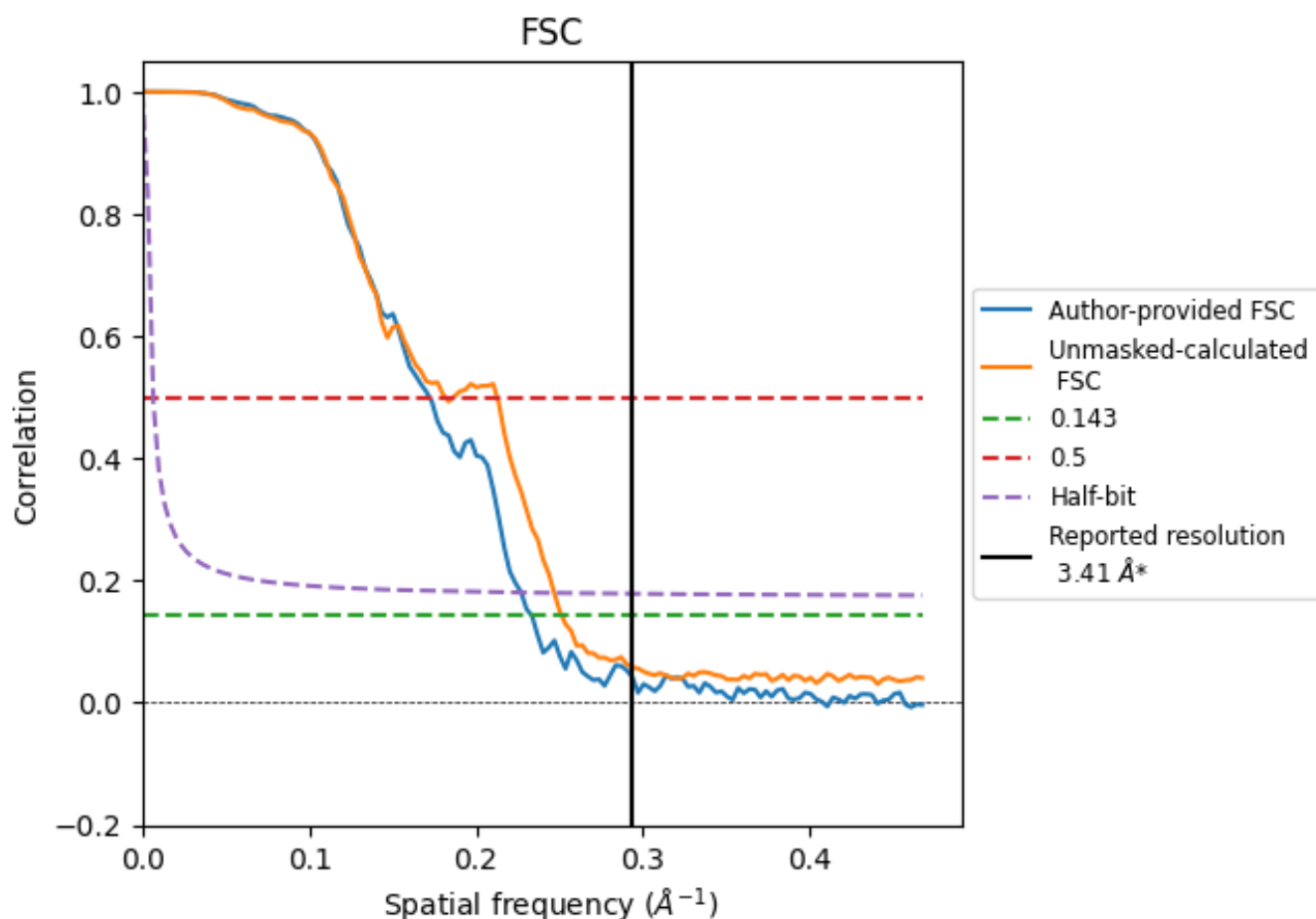
\*Reported resolution corresponds to spatial frequency of 0.293 Å<sup>-1</sup>



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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.293  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.41                               | -    | -        |
| Author-provided FSC curve | 4.28                               | 5.81 | 4.40     |
| Unmasked-calculated*      | 3.98                               | 5.51 | 4.05     |

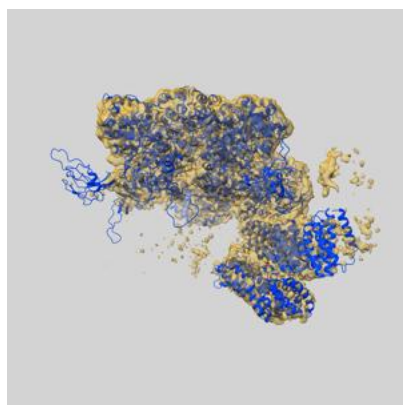
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.28 differs from the reported value 3.41 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.41 by more than 10 %

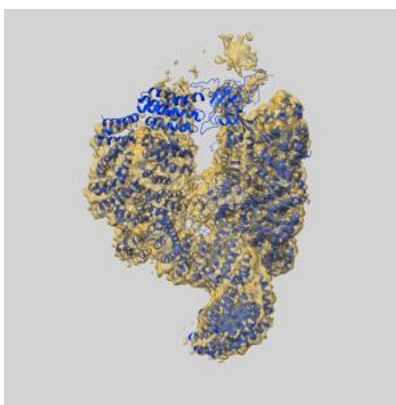
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12979 and PDB model 7OLE. Per-residue inclusion information can be found in section 3 on page 6.

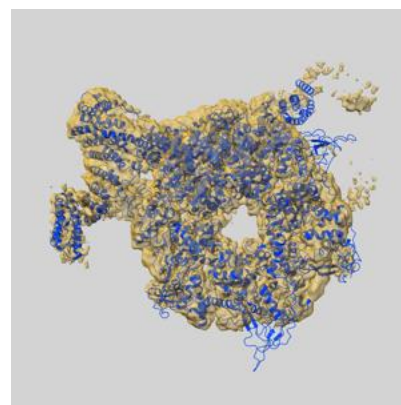
### 9.1 Map-model overlay [i](#)



X



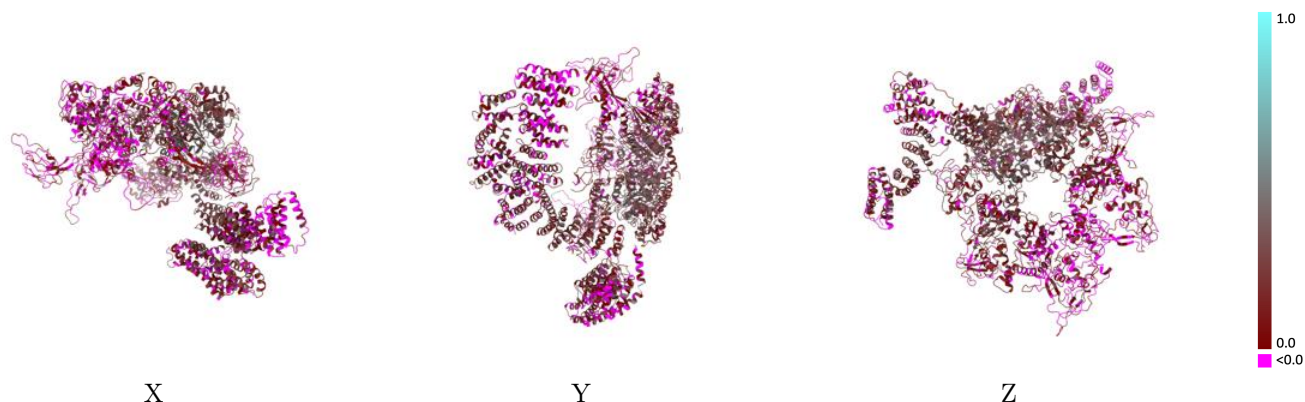
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0106 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

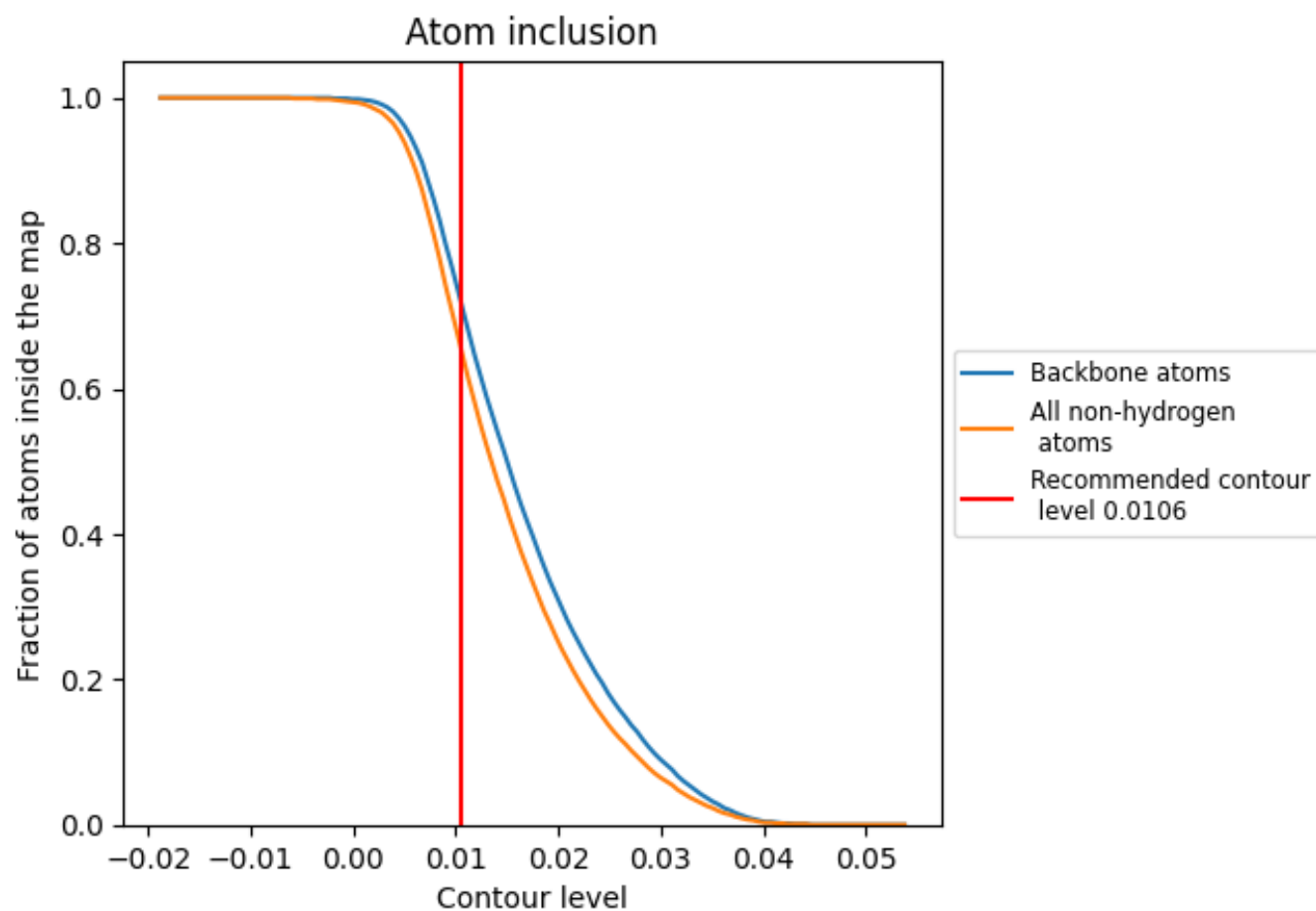


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 65% 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 (0.0106) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.6490 | <div></div> 0.1430 |
| A     | <div></div> 0.5180 | <div></div> 0.0430 |
| B     | <div></div> 0.4750 | <div></div> 0.0510 |
| C     | <div></div> 0.6130 | <div></div> 0.1630 |
| D     | <div></div> 0.8200 | <div></div> 0.2490 |
| E     | <div></div> 0.8770 | <div></div> 0.2790 |
| F     | <div></div> 0.5630 | <div></div> 0.1220 |
| H     | <div></div> 0.6830 | <div></div> 0.1170 |
| J     | <div></div> 0.6830 | <div></div> 0.1370 |
| K     | <div></div> 0.6170 | <div></div> 0.1210 |

