



## Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 08:47 PM UTC

PDB ID : 9OFC / pdb\_00009ofc  
EMDB ID : EMD-70428  
Title : CryoEM structure of Cad1 bound with cA4 and ATP, hexamer with three intact dimers  
Authors : Zhao, Y.; Li, H.  
Deposited on : 2025-04-29  
Resolution : 3.17 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

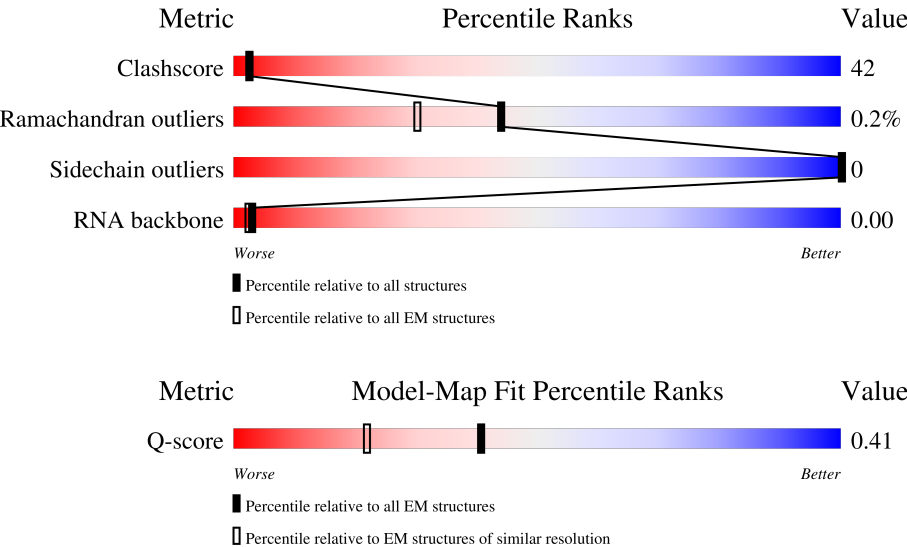
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.17 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                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 14465 ( 2.67 - 3.67 )                                    |

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     | 625    |                  |
| 1   | B     | 625    |                  |
| 1   | G     | 625    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | H     | 625    |                  |
| 1   | K     | 625    |                  |
| 1   | L     | 625    |                  |
| 2   | C     | 2      |                  |
| 2   | D     | 2      |                  |
| 2   | I     | 2      |                  |
| 2   | J     | 2      |                  |
| 2   | M     | 2      |                  |
| 2   | N     | 2      |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | A23  | C     | 708 | -         | -        | X       | -                |
| 2   | A23  | I     | 718 | -         | -        | X       | -                |
| 2   | A23  | M     | 728 | -         | -        | X       | -                |
| 2   | A23  | N     | 730 | -         | -        | X       | -                |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 29042 atoms, of which 72 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.

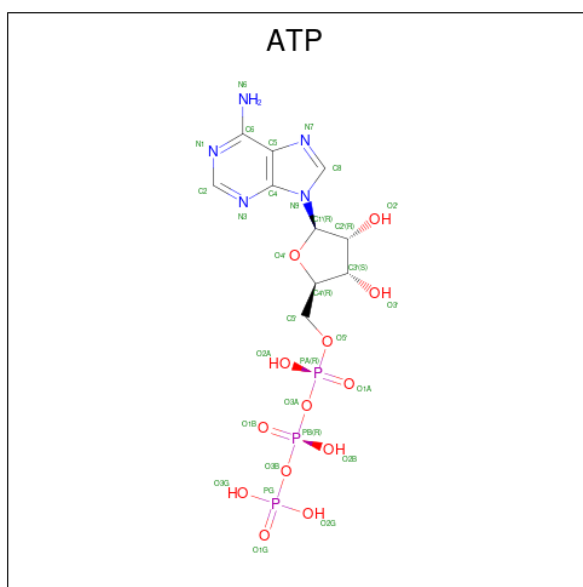
- Molecule 1 is a protein called CRISPR-associated ring nuclease and adenosine deaminase, subunit A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 605      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4735  | 3000 | 861 | 853 | 21 |         |       |
| 1   | B     | 611      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4784  | 3027 | 872 | 864 | 21 |         |       |
| 1   | G     | 604      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 4745  | 3008 | 862 | 855 | 20 |         |       |
| 1   | H     | 603      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 4735  | 3003 | 860 | 851 | 21 |         |       |
| 1   | K     | 604      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 4745  | 3008 | 862 | 855 | 20 |         |       |
| 1   | L     | 603      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 4735  | 3003 | 860 | 851 | 21 |         |       |

- Molecule 2 is a RNA chain called cA4 cleavage product, A2>P.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 2   | C     | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 44    | 20 | 10 | 12 | 2 |         |       |
| 2   | D     | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 44    | 20 | 10 | 12 | 2 |         |       |
| 2   | I     | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 44    | 20 | 10 | 12 | 2 |         |       |
| 2   | J     | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 44    | 20 | 10 | 12 | 2 |         |       |
| 2   | M     | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 44    | 20 | 10 | 12 | 2 |         |       |
| 2   | N     | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 44    | 20 | 10 | 12 | 2 |         |       |

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms       |         |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|
| 3   | A     | 1        | Total<br>43 | C<br>10 | H<br>12 | N<br>5 | O<br>13 | P<br>3 | 0       |
| 3   | B     | 1        | Total<br>43 | C<br>10 | H<br>12 | N<br>5 | O<br>13 | P<br>3 | 0       |
| 3   | G     | 1        | Total<br>43 | C<br>10 | H<br>12 | N<br>5 | O<br>13 | P<br>3 | 0       |
| 3   | H     | 1        | Total<br>43 | C<br>10 | H<br>12 | N<br>5 | O<br>13 | P<br>3 | 0       |
| 3   | K     | 1        | Total<br>43 | C<br>10 | H<br>12 | N<br>5 | O<br>13 | P<br>3 | 0       |
| 3   | L     | 1        | Total<br>43 | C<br>10 | H<br>12 | N<br>5 | O<br>13 | P<br>3 | 0       |

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 4   | A     | 1        | Total Zn<br>1 1 | 0       |
| 4   | B     | 1        | Total Zn<br>1 1 | 0       |
| 4   | G     | 1        | Total Zn<br>1 1 | 0       |
| 4   | H     | 1        | Total Zn<br>1 1 | 0       |
| 4   | K     | 1        | Total Zn<br>1 1 | 0       |

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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 4   | L     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 5   | G     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 5   | H     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 5   | K     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 5   | L     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |

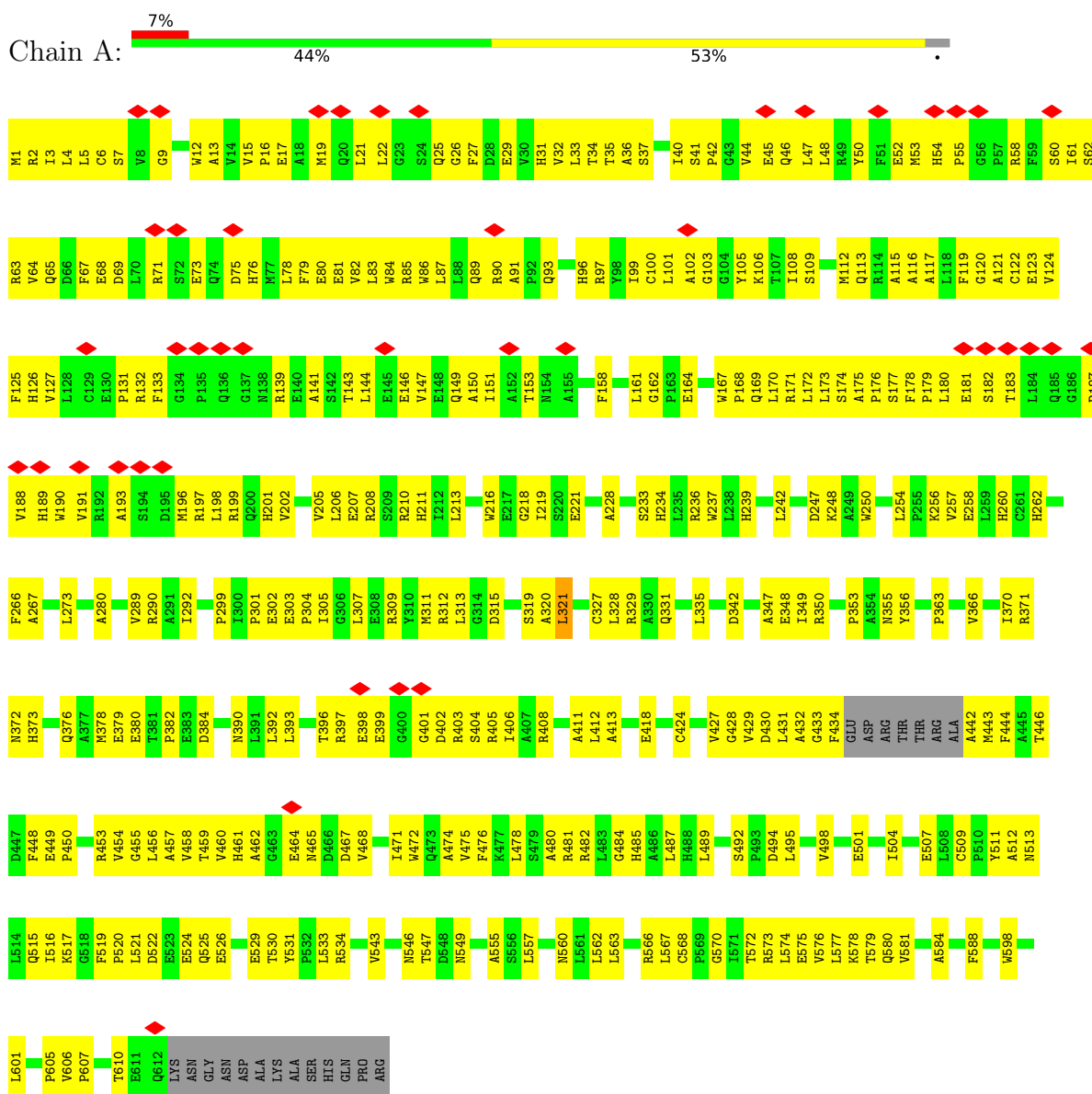
- Molecule 6 is water.

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 6   | A     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 6   | B     | 2        | Total | O | 0       |
|     |       |          | 2     | 2 |         |
| 6   | G     | 6        | Total | O | 0       |
|     |       |          | 6     | 6 |         |
| 6   | H     | 6        | Total | O | 0       |
|     |       |          | 6     | 6 |         |
| 6   | K     | 6        | Total | O | 0       |
|     |       |          | 6     | 6 |         |
| 6   | L     | 6        | Total | O | 0       |
|     |       |          | 6     | 6 |         |

### 3 Residue-property plots

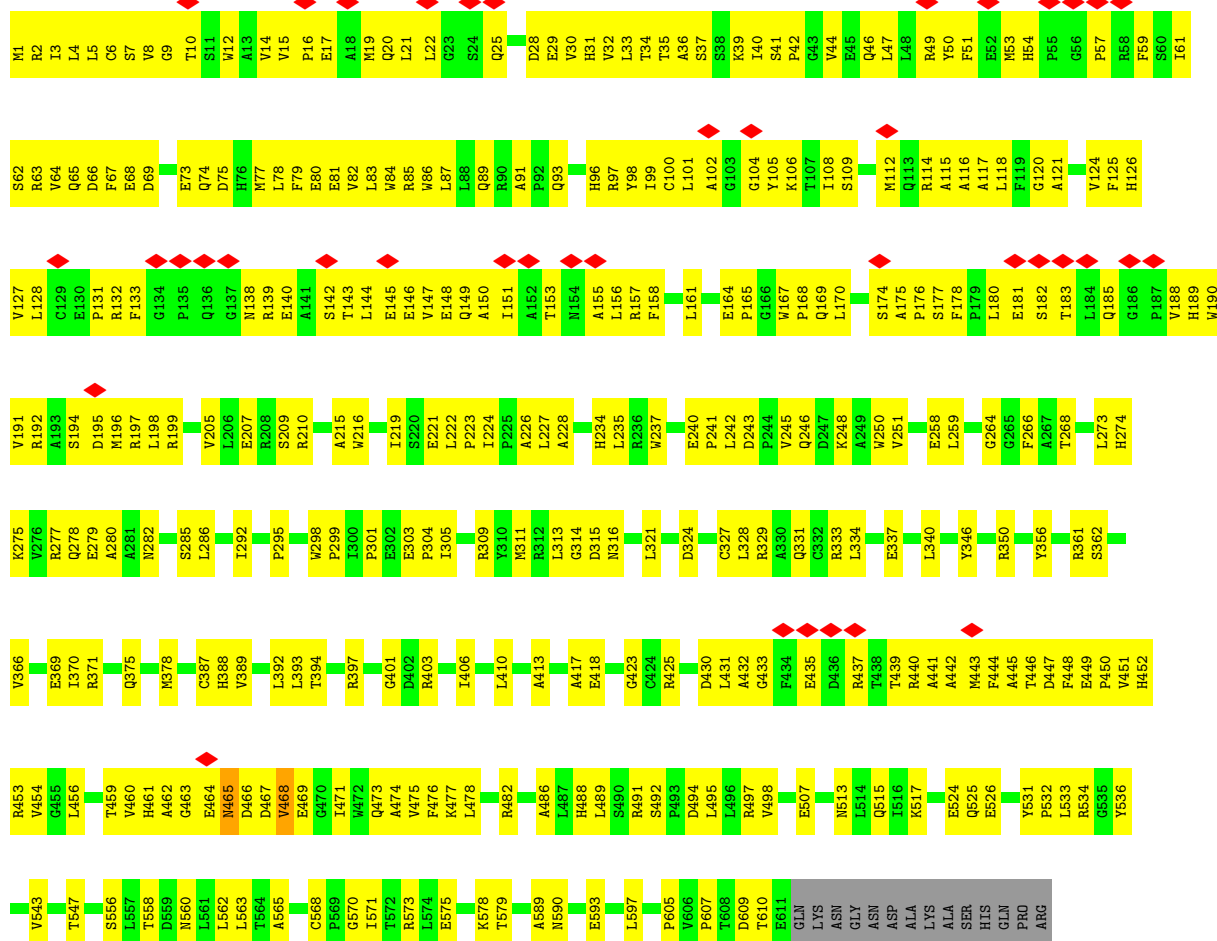
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: CRISPR-associated ring nuclease and adenosine deaminase, subunit A



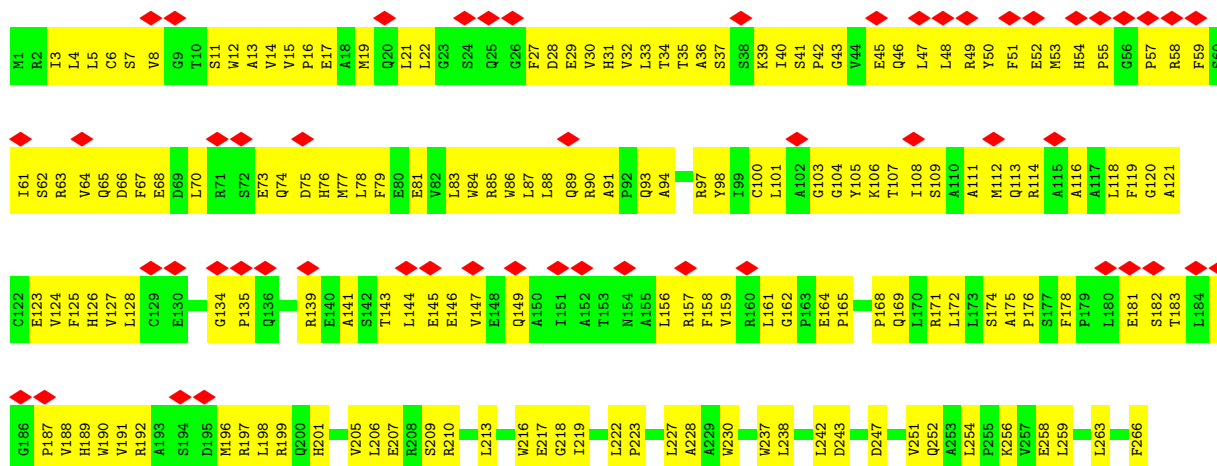
- Molecule 1: CRISPR-associated ring nuclease and adenosine deaminase, subunit A

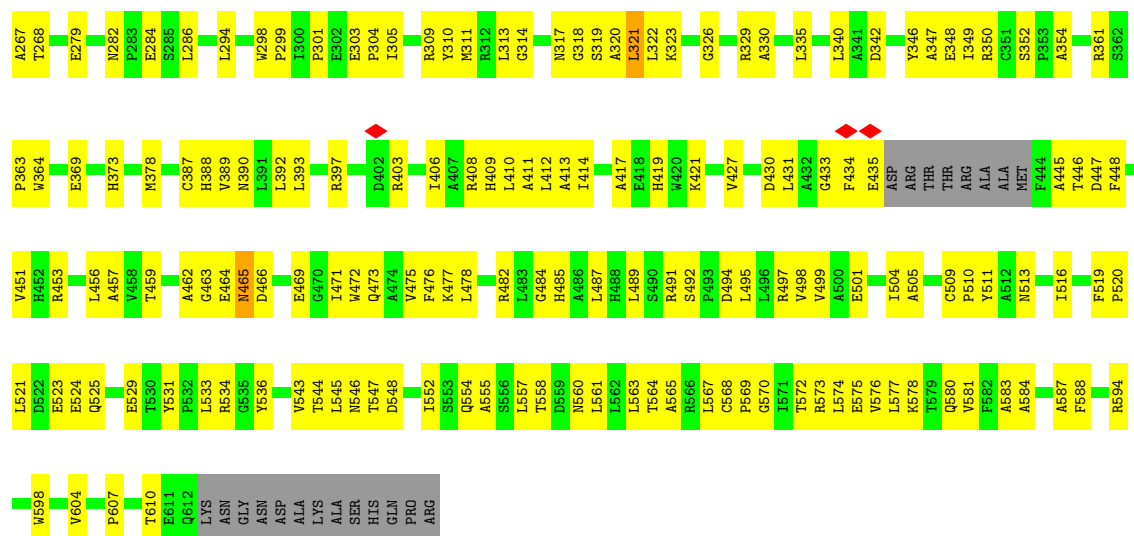
Chain B: 



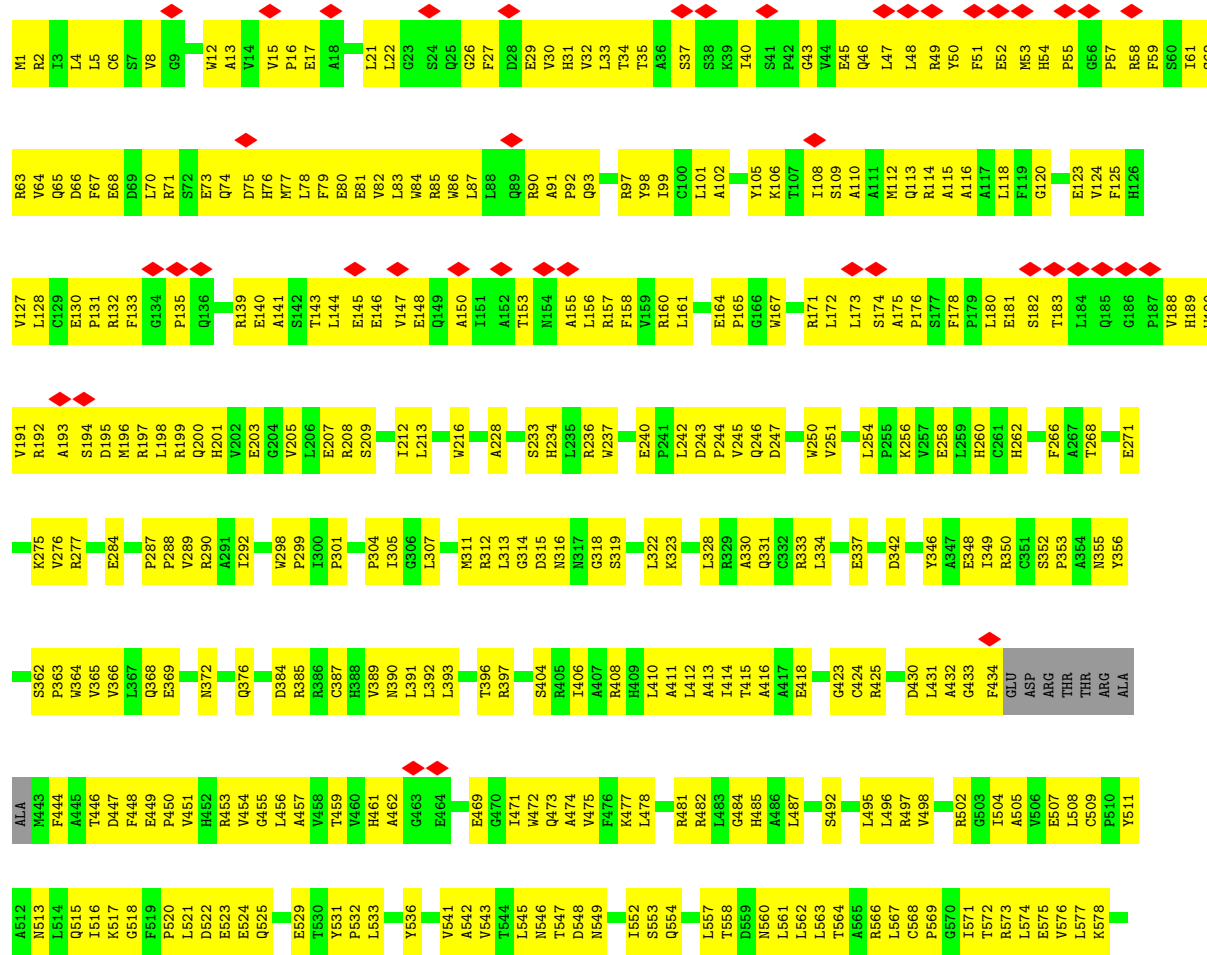
• Molecule 1: CRISPR-associated ring nuclease and adenosine deaminase, subunit A

Chain G: 



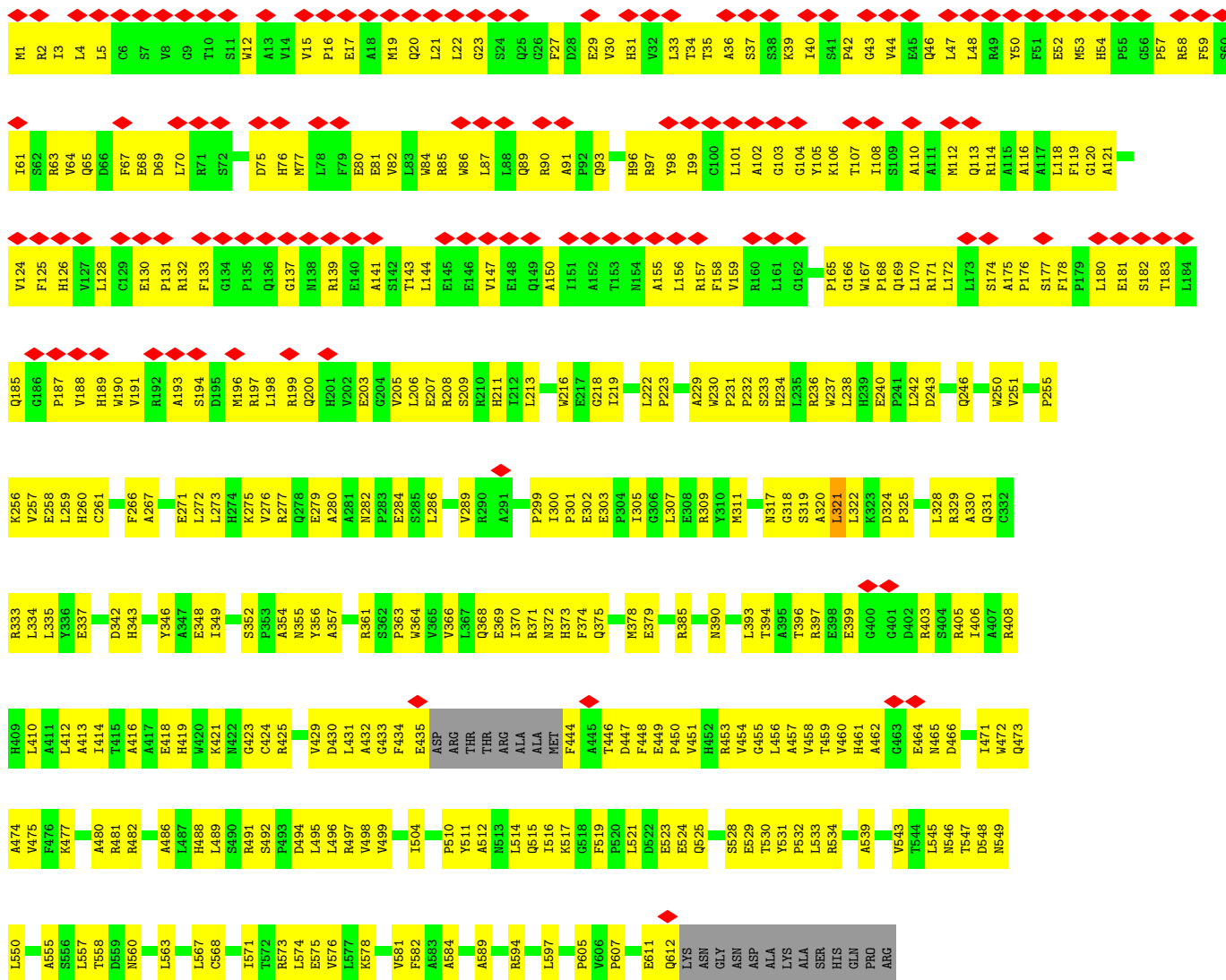


• Molecule 1: CRISPR-associated ring nuclease and adenosine deaminase, subunit A

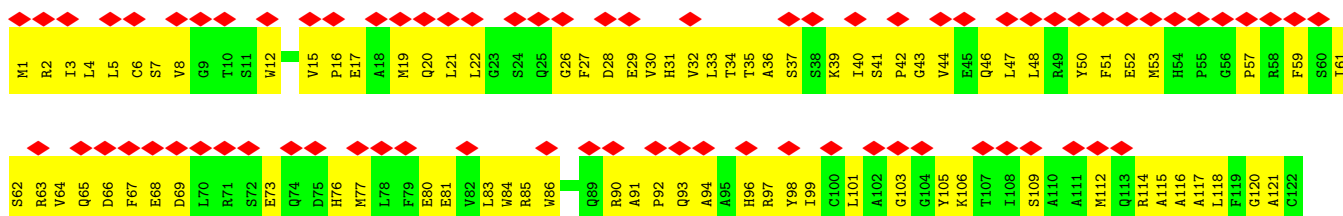


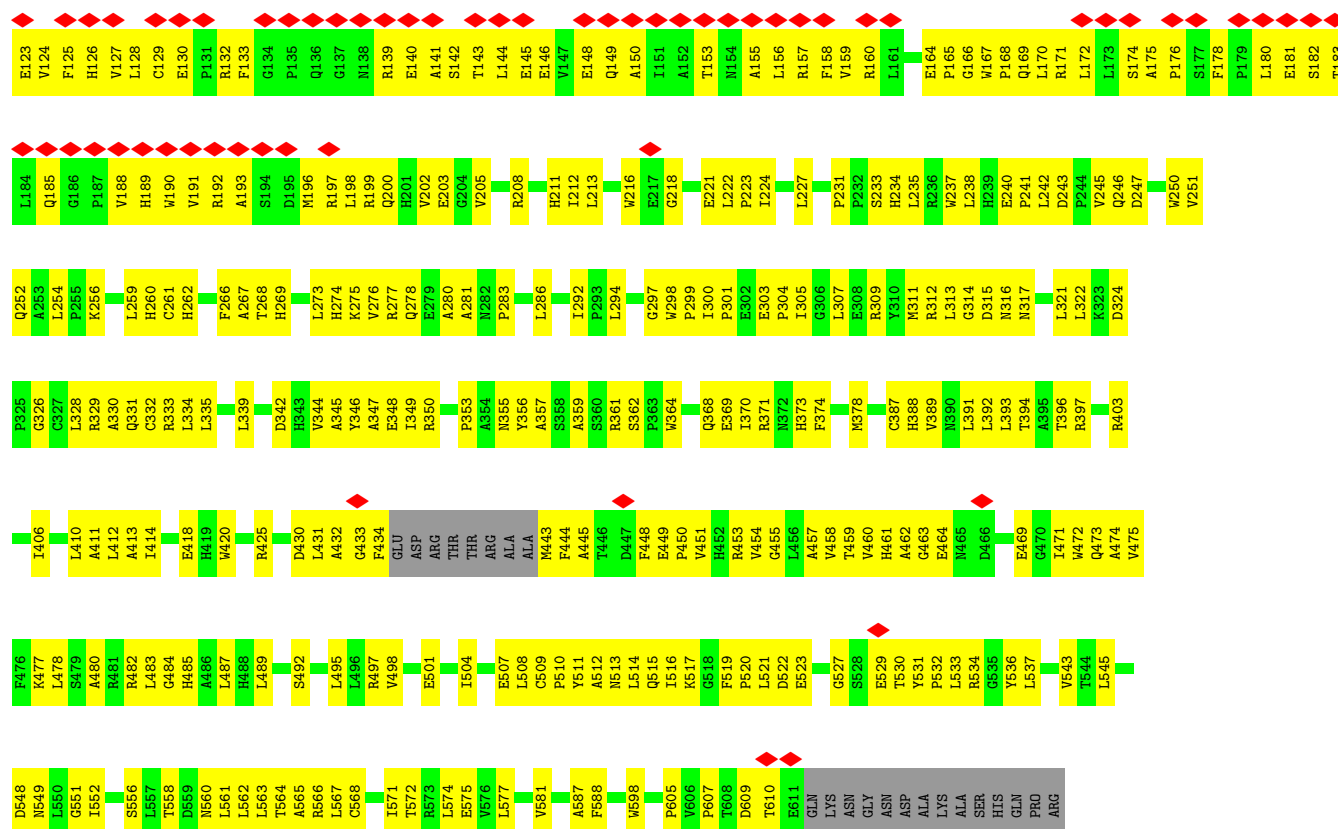


• Molecule 1: CRISPR-associated ring nuclease and adenosine deaminase, subunit A



• Molecule 1: CRISPR-associated ring nuclease and adenosine deaminase, subunit A





- Molecule 2: cA4 cleavage product, A2>P

Chain C: 50% 50%

A707  
A708

- Molecule 2: cA4 cleavage product, A2>P

Chain D: 50% 50%

A709  
A710

- Molecule 2: cA4 cleavage product, A2>P

Chain I: 50% 50%

A717  
A718

- Molecule 2: cA4 cleavage product, A2>P

Chain J: 50% 50%

A719  
A720

- Molecule 2: cA4 cleavage product, A2>P



- Molecule 2: cA4 cleavage product, A2>P



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 41951                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                                      | Depositor |
| Minimum defocus (nm)                 | 820                                     | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 QUANTUM (4k x 4k)              | Depositor |
| Maximum map value                    | 1.048                                   | Depositor |
| Minimum map value                    | -0.569                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.032                                   | Depositor |
| Recommended contour level            | 0.12                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 318.72, 318.72, 318.72                  | wwPDB     |
| Map dimensions                       | 384, 384, 384                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.83, 0.83, 0.83                        | 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: A23, ZN, ATP, MG

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     | 0.14         | 0/4854  | 0.29        | 0/6612  |
| 1   | B     | 0.12         | 0/4904  | 0.26        | 0/6681  |
| 1   | G     | 0.13         | 0/4866  | 0.28        | 0/6630  |
| 1   | H     | 0.14         | 0/4856  | 0.28        | 0/6616  |
| 1   | K     | 0.12         | 0/4866  | 0.25        | 0/6630  |
| 1   | L     | 0.12         | 0/4856  | 0.28        | 0/6616  |
| 2   | C     | 0.04         | 0/21    | 0.09        | 0/31    |
| 2   | D     | 0.05         | 0/21    | 0.10        | 0/31    |
| 2   | I     | 0.13         | 0/21    | 0.33        | 0/31    |
| 2   | J     | 0.04         | 0/21    | 0.09        | 0/31    |
| 2   | M     | 0.12         | 0/21    | 0.39        | 0/31    |
| 2   | N     | 0.04         | 0/21    | 0.09        | 0/31    |
| All | All   | 0.13         | 0/29328 | 0.27        | 0/39971 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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     | 4735  | 0        | 4698     | 375     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 4784  | 0        | 4746     | 405     | 0            |
| 1   | G     | 4745  | 0        | 4699     | 395     | 0            |
| 1   | H     | 4735  | 0        | 4694     | 428     | 0            |
| 1   | K     | 4745  | 0        | 4699     | 420     | 0            |
| 1   | L     | 4735  | 0        | 4694     | 435     | 0            |
| 2   | C     | 44    | 0        | 21       | 10      | 0            |
| 2   | D     | 44    | 0        | 22       | 9       | 0            |
| 2   | I     | 44    | 0        | 22       | 7       | 0            |
| 2   | J     | 44    | 0        | 22       | 7       | 0            |
| 2   | M     | 44    | 0        | 22       | 13      | 0            |
| 2   | N     | 44    | 0        | 21       | 10      | 0            |
| 3   | A     | 31    | 12       | 12       | 2       | 0            |
| 3   | B     | 31    | 12       | 12       | 5       | 0            |
| 3   | G     | 31    | 12       | 12       | 2       | 0            |
| 3   | H     | 31    | 12       | 12       | 3       | 0            |
| 3   | K     | 31    | 12       | 12       | 0       | 0            |
| 3   | L     | 31    | 12       | 12       | 4       | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | G     | 1     | 0        | 0        | 0       | 0            |
| 4   | H     | 1     | 0        | 0        | 0       | 0            |
| 4   | K     | 1     | 0        | 0        | 0       | 0            |
| 4   | L     | 1     | 0        | 0        | 0       | 0            |
| 5   | G     | 2     | 0        | 0        | 0       | 0            |
| 5   | H     | 2     | 0        | 0        | 0       | 0            |
| 5   | K     | 2     | 0        | 0        | 0       | 0            |
| 5   | L     | 2     | 0        | 0        | 0       | 0            |
| 6   | A     | 1     | 0        | 0        | 1       | 0            |
| 6   | B     | 2     | 0        | 0        | 1       | 0            |
| 6   | G     | 6     | 0        | 0        | 3       | 0            |
| 6   | H     | 6     | 0        | 0        | 4       | 0            |
| 6   | K     | 6     | 0        | 0        | 3       | 0            |
| 6   | L     | 6     | 0        | 0        | 3       | 0            |
| All | All   | 28970 | 72       | 28432    | 2419    | 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 (2419) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:435:GLU:HG2  | 1:G:462:ALA:HA   | 1.21                     | 1.19              |
| 2:I:718:A23:C4'  | 2:I:718:A23:O4'  | 1.74                     | 1.15              |
| 2:M:728:A23:O4'  | 2:M:728:A23:C4'  | 1.73                     | 1.14              |
| 1:G:101:LEU:HA   | 1:G:112:MET:HE1  | 1.29                     | 1.11              |
| 2:C:708:A23:O4'  | 2:C:708:A23:C4'  | 1.74                     | 1.11              |
| 2:J:720:A23:C4'  | 2:J:720:A23:O4'  | 1.74                     | 1.10              |
| 2:D:710:A23:O4'  | 2:D:710:A23:C4'  | 1.74                     | 1.08              |
| 2:N:730:A23:O4'  | 2:N:730:A23:C4'  | 1.74                     | 1.07              |
| 1:A:105:TYR:HB2  | 1:A:108:ILE:HG12 | 1.36                     | 1.06              |
| 1:K:29:GLU:HG2   | 1:K:58:ARG:HB3   | 1.39                     | 1.04              |
| 1:G:91:ALA:HB1   | 1:G:97:ARG:HG2   | 1.38                     | 1.04              |
| 1:H:4:LEU:HB3    | 1:H:30:VAL:HG12  | 1.38                     | 1.03              |
| 1:A:449:GLU:HG3  | 1:A:450:PRO:HD3  | 1.43                     | 1.00              |
| 1:L:283:PRO:HA   | 1:L:286:LEU:HD23 | 1.43                     | 1.00              |
| 1:B:124:VAL:HG13 | 1:B:161:LEU:HB2  | 1.44                     | 1.00              |
| 1:A:97:ARG:HG2   | 1:A:99:ILE:HD11  | 1.44                     | 0.99              |
| 1:A:511:TYR:HE1  | 1:A:563:LEU:HD13 | 1.24                     | 0.99              |
| 1:G:17:GLU:HB3   | 1:G:127:VAL:HG21 | 1.41                     | 0.98              |
| 1:H:21:LEU:HD11  | 1:H:160:ARG:HD2  | 1.43                     | 0.98              |
| 1:K:36:ALA:HA    | 1:K:63:ARG:HD3   | 1.44                     | 0.98              |
| 1:A:33:LEU:HD11  | 1:A:64:VAL:HG13  | 1.45                     | 0.98              |
| 1:A:36:ALA:HA    | 1:A:63:ARG:HD3   | 1.43                     | 0.97              |
| 1:G:124:VAL:HG23 | 1:G:161:LEU:HB2  | 1.45                     | 0.97              |
| 1:H:589:ALA:HB1  | 1:H:593:GLU:HB2  | 1.46                     | 0.97              |
| 1:K:35:THR:HA    | 1:K:64:VAL:HG22  | 1.47                     | 0.96              |
| 1:L:94:ALA:HA    | 1:L:97:ARG:HE    | 1.28                     | 0.96              |
| 1:H:572:THR:OG1  | 1:H:575:GLU:OE1  | 1.84                     | 0.96              |
| 1:B:132:ARG:HH21 | 1:B:155:ALA:HB2  | 1.31                     | 0.95              |
| 1:B:4:LEU:HB3    | 1:B:30:VAL:HG12  | 1.47                     | 0.95              |
| 1:B:397:ARG:HD3  | 1:B:443:MET:HE3  | 1.49                     | 0.95              |
| 1:H:195:ASP:OD2  | 1:H:196:MET:N    | 2.00                     | 0.94              |
| 1:K:435:GLU:HG3  | 1:K:465:ASN:HD21 | 1.32                     | 0.93              |
| 1:G:88:LEU:HD13  | 1:G:175:ALA:HA   | 1.51                     | 0.93              |
| 1:K:85:ARG:HB2   | 1:K:180:LEU:HD13 | 1.51                     | 0.93              |
| 1:B:181:GLU:HG2  | 1:B:192:ARG:HB3  | 1.52                     | 0.92              |
| 1:A:76:HIS:HA    | 1:A:79:PHE:CE1   | 2.05                     | 0.91              |
| 1:A:462:ALA:HB1  | 1:A:465:ASN:HD21 | 1.33                     | 0.91              |
| 1:B:101:LEU:HD13 | 1:B:109:SER:HB2  | 1.51                     | 0.90              |
| 1:G:41:SER:HA    | 1:G:63:ARG:HH12  | 1.33                     | 0.90              |
| 1:L:101:LEU:HD21 | 1:L:126:HIS:HB2  | 1.53                     | 0.89              |
| 1:L:463:GLY:O    | 1:L:517:LYS:NZ   | 2.05                     | 0.89              |
| 1:L:146:GLU:HA   | 1:L:149:GLN:HE21 | 1.37                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:16:PRO:HA    | 1:L:19:MET:HE3   | 1.53                     | 0.88              |
| 1:H:105:TYR:H    | 1:H:108:ILE:HD12 | 1.38                     | 0.88              |
| 1:A:511:TYR:CE1  | 1:A:563:LEU:HD13 | 2.09                     | 0.88              |
| 1:B:482:ARG:NE   | 1:B:507:GLU:OE2  | 2.06                     | 0.87              |
| 1:H:63:ARG:HH12  | 1:H:188:VAL:HB   | 1.36                     | 0.87              |
| 1:L:127:VAL:HG22 | 1:L:156:LEU:HD11 | 1.53                     | 0.87              |
| 1:A:35:THR:HA    | 1:A:64:VAL:HG22  | 1.56                     | 0.87              |
| 1:H:516:ILE:HG22 | 1:H:517:LYS:HD2  | 1.55                     | 0.87              |
| 1:H:431:LEU:HD11 | 1:H:448:PHE:HZ   | 1.39                     | 0.87              |
| 1:K:414:ILE:HG23 | 1:K:454:VAL:HG21 | 1.57                     | 0.87              |
| 1:A:432:ALA:HA   | 1:A:461:HIS:HB3  | 1.57                     | 0.86              |
| 1:B:378:MET:HE3  | 1:B:388:HIS:HA   | 1.57                     | 0.86              |
| 1:B:394:THR:HA   | 1:B:430:ASP:OD1  | 1.75                     | 0.85              |
| 1:G:85:ARG:HG3   | 1:G:198:LEU:HD13 | 1.58                     | 0.85              |
| 1:B:83:LEU:HD22  | 1:B:112:MET:HE2  | 1.56                     | 0.85              |
| 1:H:158:PHE:HB2  | 1:H:160:ARG:HH11 | 1.39                     | 0.85              |
| 1:H:82:VAL:HG22  | 1:H:193:ALA:HB2  | 1.58                     | 0.85              |
| 1:B:361:ARG:NH2  | 1:B:369:GLU:OE1  | 2.10                     | 0.84              |
| 1:H:31:HIS:CD2   | 1:H:90:ARG:HD2   | 2.12                     | 0.84              |
| 1:G:435:GLU:HG2  | 1:G:462:ALA:CA   | 2.07                     | 0.84              |
| 1:G:135:PRO:HD2  | 1:G:139:ARG:HH22 | 1.43                     | 0.84              |
| 1:G:74:GLN:HA    | 1:G:77:MET:HE2   | 1.58                     | 0.84              |
| 1:L:509:CYS:HB2  | 1:L:512:ALA:HB3  | 1.59                     | 0.83              |
| 1:A:213:LEU:HD11 | 1:B:209:SER:OG   | 1.79                     | 0.83              |
| 1:L:256:LYS:HE2  | 1:L:558:THR:HG22 | 1.57                     | 0.83              |
| 1:G:393:LEU:HD12 | 1:G:413:ALA:HB2  | 1.60                     | 0.83              |
| 1:A:498:VAL:HA   | 1:A:501:GLU:HG2  | 1.60                     | 0.83              |
| 1:L:101:LEU:O    | 1:L:109:SER:OG   | 1.96                     | 0.83              |
| 1:L:268:THR:HG21 | 1:L:314:GLY:HA2  | 1.61                     | 0.82              |
| 1:H:17:GLU:HB2   | 1:H:156:LEU:CD2  | 2.09                     | 0.82              |
| 1:B:431:LEU:HB2  | 1:B:448:PHE:CZ   | 2.14                     | 0.82              |
| 1:G:191:VAL:O    | 1:G:192:ARG:NE   | 2.12                     | 0.82              |
| 1:L:166:GLY:HA3  | 1:L:171:ARG:HD2  | 1.61                     | 0.82              |
| 1:H:16:PRO:HD3   | 1:H:47:LEU:HD21  | 1.60                     | 0.82              |
| 1:H:356:TYR:HB2  | 1:H:366:VAL:HG11 | 1.61                     | 0.82              |
| 1:L:394:THR:HG23 | 1:L:432:ALA:HB3  | 1.61                     | 0.82              |
| 1:H:393:LEU:HD12 | 1:H:413:ALA:HB2  | 1.62                     | 0.81              |
| 1:H:434:PHE:HE2  | 1:H:444:PHE:HB2  | 1.44                     | 0.81              |
| 1:K:19:MET:HE1   | 1:K:57:PRO:HG3   | 1.61                     | 0.81              |
| 1:B:403:ARG:HB2  | 1:K:453:ARG:HD3  | 1.61                     | 0.81              |
| 1:K:280:ALA:HB2  | 1:K:286:LEU:HD11 | 1.60                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:435:GLU:HG2  | 1:K:462:ALA:HA   | 1.63                     | 0.81              |
| 1:B:85:ARG:HH12  | 1:B:195:ASP:H    | 1.26                     | 0.81              |
| 1:A:411:ALA:HB2  | 1:H:414:ILE:HD11 | 1.63                     | 0.81              |
| 1:K:17:GLU:HB3   | 1:K:156:LEU:HD13 | 1.62                     | 0.81              |
| 1:K:418:GLU:O    | 1:K:421:LYS:NZ   | 2.13                     | 0.81              |
| 1:H:85:ARG:HH22  | 1:H:197:ARG:HD2  | 1.45                     | 0.81              |
| 1:H:547:THR:HA   | 1:H:560:ASN:HD21 | 1.45                     | 0.81              |
| 1:L:34:THR:O     | 1:L:64:VAL:N     | 2.13                     | 0.81              |
| 1:A:478:LEU:O    | 1:A:478:LEU:HD12 | 1.80                     | 0.81              |
| 1:K:65:GLN:HG2   | 1:K:190:TRP:HB3  | 1.61                     | 0.81              |
| 1:K:242:LEU:HD22 | 1:K:576:VAL:HG21 | 1.60                     | 0.81              |
| 1:K:563:LEU:HG   | 1:K:567:LEU:HD23 | 1.63                     | 0.81              |
| 1:K:48:LEU:HD13  | 1:K:187:PRO:HG2  | 1.61                     | 0.80              |
| 1:L:322:LEU:HB2  | 1:L:356:TYR:CE1  | 2.16                     | 0.80              |
| 1:A:482:ARG:NE   | 1:A:507:GLU:OE2  | 2.13                     | 0.80              |
| 1:G:101:LEU:HD13 | 1:H:106:LYS:HE2  | 1.63                     | 0.80              |
| 1:B:85:ARG:NH1   | 1:B:195:ASP:O    | 2.13                     | 0.80              |
| 1:B:40:ILE:HG13  | 1:B:63:ARG:HH12  | 1.46                     | 0.80              |
| 1:H:240:GLU:HG3  | 1:H:573:ARG:NH1  | 1.96                     | 0.80              |
| 1:K:511:TYR:CD1  | 1:K:563:LEU:HD22 | 2.14                     | 0.80              |
| 1:A:397:ARG:NE   | 1:A:433:GLY:O    | 2.14                     | 0.80              |
| 1:A:431:LEU:HD11 | 1:A:448:PHE:HE1  | 1.47                     | 0.80              |
| 1:L:167:TRP:HE3  | 1:L:168:PRO:HD3  | 1.47                     | 0.80              |
| 1:L:531:TYR:CD2  | 1:L:567:LEU:HD13 | 2.17                     | 0.80              |
| 1:B:181:GLU:OE1  | 1:B:194:SER:OG   | 1.99                     | 0.80              |
| 1:G:66:ASP:HB3   | 1:G:78:LEU:HD11  | 1.64                     | 0.80              |
| 3:H:703:ATP:O1A  | 6:H:801:HOH:O    | 1.98                     | 0.80              |
| 1:H:431:LEU:HD21 | 1:H:448:PHE:HE2  | 1.47                     | 0.79              |
| 1:A:402:ASP:OD2  | 1:A:404:SER:OG   | 2.01                     | 0.79              |
| 1:G:417:ALA:HB2  | 1:G:456:LEU:HD21 | 1.63                     | 0.79              |
| 1:B:50:TYR:HA    | 1:B:53:MET:HE2   | 1.63                     | 0.79              |
| 1:G:143:THR:OG1  | 1:G:146:GLU:OE1  | 2.00                     | 0.79              |
| 1:H:80:GLU:HA    | 1:H:83:LEU:HB3   | 1.63                     | 0.79              |
| 1:L:378:MET:HE3  | 1:L:388:HIS:HA   | 1.65                     | 0.79              |
| 3:G:701:ATP:O1A  | 6:G:2001:HOH:O   | 2.00                     | 0.79              |
| 1:H:258:GLU:OE2  | 1:H:547:THR:OG1  | 1.99                     | 0.79              |
| 1:A:472:TRP:HD1  | 1:A:495:LEU:HD11 | 1.48                     | 0.79              |
| 1:G:511:TYR:CD1  | 1:G:563:LEU:HD22 | 2.18                     | 0.79              |
| 1:B:393:LEU:HD12 | 1:B:413:ALA:HB2  | 1.64                     | 0.79              |
| 1:B:73:GLU:HG2   | 1:B:77:MET:HE1   | 1.64                     | 0.79              |
| 1:G:101:LEU:CA   | 1:G:112:MET:HE1  | 2.10                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:85:ARG:O     | 1:B:89:GLN:HG2   | 1.83                     | 0.79              |
| 1:H:350:ARG:NH1  | 1:H:430:ASP:OD2  | 2.15                     | 0.79              |
| 1:A:266:PHE:HB3  | 1:A:331:GLN:NE2  | 1.99                     | 0.78              |
| 1:B:53:MET:HG3   | 1:B:54:HIS:HD2   | 1.47                     | 0.78              |
| 1:B:274:HIS:O    | 1:B:278:GLN:NE2  | 2.16                     | 0.78              |
| 1:K:106:LYS:HD3  | 2:N:729:A:H5'    | 1.64                     | 0.78              |
| 1:H:196:MET:SD   | 1:H:199:ARG:HB3  | 2.24                     | 0.78              |
| 1:A:21:LEU:HD22  | 1:A:125:PHE:CE1  | 2.19                     | 0.78              |
| 1:B:440:ARG:HE   | 1:B:442:ALA:HB3  | 1.47                     | 0.78              |
| 1:K:511:TYR:HD1  | 1:K:563:LEU:HD22 | 1.48                     | 0.78              |
| 1:H:268:THR:CG2  | 1:H:314:GLY:HA2  | 2.14                     | 0.78              |
| 2:M:728:A23:O1C  | 2:N:729:A:O5'    | 2.02                     | 0.78              |
| 1:L:51:PHE:HE2   | 1:L:61:ILE:HD11  | 1.48                     | 0.78              |
| 1:L:414:ILE:HG23 | 1:L:454:VAL:HG21 | 1.66                     | 0.78              |
| 1:G:178:PHE:CG   | 1:G:198:LEU:HD12 | 2.19                     | 0.77              |
| 1:L:94:ALA:HA    | 1:L:97:ARG:NE    | 1.99                     | 0.77              |
| 1:L:126:HIS:O    | 1:L:159:VAL:N    | 2.14                     | 0.77              |
| 1:L:167:TRP:HB2  | 1:L:170:LEU:HD12 | 1.65                     | 0.77              |
| 1:B:440:ARG:HG2  | 1:B:442:ALA:H    | 1.48                     | 0.77              |
| 1:A:546:ASN:O    | 1:A:560:ASN:ND2  | 2.18                     | 0.77              |
| 1:K:435:GLU:HG3  | 1:K:465:ASN:ND2  | 1.99                     | 0.77              |
| 1:L:260:HIS:CD2  | 1:L:548:ASP:HA   | 2.19                     | 0.77              |
| 1:A:91:ALA:O     | 1:A:97:ARG:NH2   | 2.17                     | 0.77              |
| 1:K:534:ARG:NH1  | 1:K:575:GLU:OE1  | 2.17                     | 0.77              |
| 1:H:4:LEU:HD12   | 1:H:98:TYR:O     | 1.83                     | 0.77              |
| 1:H:304:PRO:HG3  | 1:H:518:GLY:HA3  | 1.67                     | 0.77              |
| 1:A:53:MET:HE1   | 1:A:54:HIS:NE2   | 1.99                     | 0.77              |
| 1:B:185:GLN:HB2  | 1:B:190:TRP:HE1  | 1.49                     | 0.77              |
| 1:H:521:LEU:HD13 | 1:H:566:ARG:HH12 | 1.48                     | 0.77              |
| 1:K:435:GLU:HG2  | 1:K:462:ALA:CB   | 2.15                     | 0.77              |
| 1:H:66:ASP:OD1   | 1:H:192:ARG:NH1  | 2.17                     | 0.77              |
| 1:B:16:PRO:HA    | 1:B:19:MET:CE    | 2.15                     | 0.77              |
| 1:H:16:PRO:HB2   | 1:H:147:VAL:HG11 | 1.66                     | 0.76              |
| 1:H:448:PHE:O    | 1:H:451:VAL:HG22 | 1.85                     | 0.76              |
| 1:K:266:PHE:HB3  | 1:K:331:GLN:NE2  | 2.01                     | 0.76              |
| 1:K:546:ASN:O    | 1:K:560:ASN:ND2  | 2.17                     | 0.76              |
| 1:A:393:LEU:HD12 | 1:A:413:ALA:HB2  | 1.66                     | 0.76              |
| 1:A:431:LEU:HD11 | 1:A:448:PHE:CE1  | 2.20                     | 0.76              |
| 1:H:53:MET:HE1   | 1:H:144:LEU:HB3  | 1.68                     | 0.76              |
| 1:A:119:PHE:HE1  | 1:A:173:LEU:HD12 | 1.50                     | 0.76              |
| 1:B:224:ILE:HB   | 1:B:227:LEU:HD13 | 1.66                     | 0.76              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:K:19:MET:SD      | 1:K:30:VAL:HG11  | 2.25                     | 0.76              |
| 1:L:4:LEU:HD22     | 1:L:27:PHE:CE2   | 2.20                     | 0.76              |
| 1:L:361:ARG:NH2    | 1:L:369:GLU:OE1  | 2.18                     | 0.76              |
| 1:B:397:ARG:HG3    | 1:B:433:GLY:HA2  | 1.67                     | 0.76              |
| 1:H:546:ASN:O      | 1:H:560:ASN:ND2  | 2.19                     | 0.76              |
| 1:K:492:SER:HB2    | 1:K:495:LEU:HB3  | 1.66                     | 0.76              |
| 1:B:106:LYS:HD2    | 2:C:707:A:H4'    | 1.68                     | 0.76              |
| 1:A:76:HIS:HA      | 1:A:79:PHE:HE1   | 1.48                     | 0.76              |
| 3:A:701:ATP:O1A    | 6:A:801:HOH:O    | 2.04                     | 0.76              |
| 1:L:132:ARG:HH21   | 1:L:155:ALA:HB2  | 1.51                     | 0.76              |
| 1:A:105:TYR:CB     | 1:A:108:ILE:HG12 | 2.13                     | 0.76              |
| 1:G:64:VAL:CG2     | 1:G:67:PHE:HB3   | 2.15                     | 0.75              |
| 1:H:17:GLU:HB2     | 1:H:156:LEU:HD21 | 1.66                     | 0.75              |
| 1:L:91:ALA:O       | 1:L:97:ARG:NH2   | 2.19                     | 0.75              |
| 1:L:101:LEU:HB2    | 1:L:109:SER:HB3  | 1.67                     | 0.75              |
| 1:B:444:PHE:O      | 1:B:447:ASP:N    | 2.17                     | 0.75              |
| 1:K:44:VAL:CG1     | 1:K:188:VAL:HG11 | 2.16                     | 0.75              |
| 1:B:460:VAL:HG21   | 1:B:474:ALA:HB1  | 1.68                     | 0.75              |
| 1:H:431:LEU:HD21   | 1:H:448:PHE:CE2  | 2.22                     | 0.75              |
| 1:B:83:LEU:HD13    | 1:B:112:MET:HE1  | 1.69                     | 0.75              |
| 1:G:141:ALA:HB1    | 1:G:146:GLU:HB3  | 1.69                     | 0.75              |
| 1:H:34:THR:O       | 1:H:63:ARG:HA    | 1.85                     | 0.75              |
| 1:K:431:LEU:HD21   | 1:K:448:PHE:CZ   | 2.22                     | 0.75              |
| 1:K:431:LEU:HD11   | 1:K:448:PHE:HZ   | 1.51                     | 0.75              |
| 1:B:234:HIS:HD2    | 1:B:607:PRO:HD2  | 1.52                     | 0.75              |
| 1:K:133:PHE:CE2    | 1:K:150:ALA:HB2  | 2.22                     | 0.74              |
| 1:L:433:GLY:O      | 1:L:434:PHE:HB2  | 1.87                     | 0.74              |
| 1:G:36:ALA:HB2     | 1:G:64:VAL:O     | 1.88                     | 0.74              |
| 1:L:274:HIS:O      | 1:L:278:GLN:HG2  | 1.88                     | 0.74              |
| 1:L:292:ILE:HD11   | 1:L:315:ASP:HB2  | 1.68                     | 0.74              |
| 1:K:276:VAL:HG13   | 1:K:330:ALA:HB3  | 1.69                     | 0.74              |
| 1:K:472[A]:TRP:HZ2 | 1:L:453:ARG:HA   | 1.53                     | 0.74              |
| 1:B:53:MET:HE2     | 1:B:144:LEU:HD22 | 1.70                     | 0.74              |
| 1:H:50:TYR:HA      | 1:H:53:MET:HE2   | 1.70                     | 0.74              |
| 1:H:35:THR:O       | 1:H:40:ILE:HD11  | 1.87                     | 0.73              |
| 1:K:368:GLN:O      | 1:K:372:ASN:ND2  | 2.21                     | 0.73              |
| 1:L:106:LYS:HG3    | 2:M:728:A23:H4'  | 1.70                     | 0.73              |
| 1:K:133:PHE:CD2    | 1:K:141:ALA:HB2  | 2.24                     | 0.73              |
| 1:L:73:GLU:HA      | 1:L:76:HIS:HB3   | 1.69                     | 0.73              |
| 1:A:472:TRP:CD1    | 1:A:495:LEU:HD11 | 2.23                     | 0.73              |
| 1:L:531:TYR:CE2    | 1:L:567:LEU:HD13 | 2.23                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:320:ALA:O    | 1:A:321:LEU:HB2  | 1.89                     | 0.73              |
| 1:G:174:SER:HB2  | 1:G:176:PRO:HD2  | 1.70                     | 0.73              |
| 1:G:397:ARG:HB3  | 1:G:433:GLY:HA3  | 1.71                     | 0.73              |
| 1:H:53:MET:HG3   | 1:H:54:HIS:HD2   | 1.53                     | 0.73              |
| 1:A:167:TRP:CD2  | 1:A:168:PRO:HD2  | 2.24                     | 0.73              |
| 1:A:266:PHE:HB3  | 1:A:331:GLN:HE22 | 1.54                     | 0.73              |
| 1:A:69:ASP:OD2   | 1:A:71:ARG:NH1   | 2.22                     | 0.73              |
| 1:G:64:VAL:HG21  | 1:G:67:PHE:HB3   | 1.71                     | 0.73              |
| 1:G:350:ARG:NH1  | 1:G:430:ASP:OD1  | 2.21                     | 0.73              |
| 1:G:403:ARG:HG3  | 1:G:406:ILE:HD12 | 1.70                     | 0.73              |
| 1:H:173:LEU:HD11 | 1:H:201:HIS:CE1  | 2.24                     | 0.73              |
| 1:L:311:MET:O    | 6:L:801:HOH:O    | 2.07                     | 0.73              |
| 1:B:16:PRO:HA    | 1:B:19:MET:HE2   | 1.71                     | 0.73              |
| 1:G:197:ARG:NH1  | 1:G:201:HIS:HB2  | 2.04                     | 0.73              |
| 1:H:482:ARG:NE   | 1:H:507:GLU:OE2  | 2.22                     | 0.73              |
| 1:L:64:VAL:HG11  | 1:L:67:PHE:HB3   | 1.71                     | 0.73              |
| 1:B:14:VAL:HG12  | 2:D:709:A:C2     | 2.24                     | 0.73              |
| 1:H:144:LEU:O    | 1:H:148:GLU:HG2  | 1.88                     | 0.73              |
| 1:K:65:GLN:CG    | 1:K:190:TRP:HB3  | 2.19                     | 0.73              |
| 1:B:102:ALA:HB2  | 1:B:127:VAL:HG12 | 1.71                     | 0.72              |
| 1:B:292:ILE:HD11 | 1:B:315:ASP:HB2  | 1.70                     | 0.72              |
| 1:G:183:THR:OG1  | 1:G:190:TRP:HB2  | 1.89                     | 0.72              |
| 1:H:178:PHE:HD2  | 1:H:198:LEU:HD13 | 1.53                     | 0.72              |
| 1:K:53:MET:HG2   | 1:K:54:HIS:CD2   | 2.24                     | 0.72              |
| 1:A:378:MET:CE   | 1:A:424:CYS:HB2  | 2.19                     | 0.72              |
| 1:K:406:ILE:O    | 1:K:410:LEU:HD23 | 1.87                     | 0.72              |
| 1:K:528:SER:OG   | 1:K:529:GLU:OE1  | 2.07                     | 0.72              |
| 1:L:2:ARG:HG2    | 1:L:98:TYR:CE1   | 2.23                     | 0.72              |
| 1:B:105:TYR:H    | 1:B:108:ILE:HD12 | 1.53                     | 0.72              |
| 1:H:63:ARG:HH22  | 1:H:188:VAL:HG21 | 1.53                     | 0.72              |
| 1:B:462:ALA:HB1  | 1:B:466:ASP:OD1  | 1.89                     | 0.72              |
| 1:H:311:MET:SD   | 6:H:806:HOH:O    | 2.47                     | 0.72              |
| 1:K:19:MET:HA    | 1:K:27:PHE:HE2   | 1.54                     | 0.72              |
| 1:K:279:GLU:HG3  | 1:K:330:ALA:HB2  | 1.71                     | 0.72              |
| 1:B:83:LEU:HD22  | 1:B:112:MET:CE   | 2.19                     | 0.72              |
| 1:A:258:GLU:OE2  | 1:A:547:THR:OG1  | 2.07                     | 0.72              |
| 1:H:81:GLU:O     | 1:H:85:ARG:HG3   | 1.90                     | 0.72              |
| 1:H:93:GLN:O     | 1:H:97:ARG:HD3   | 1.88                     | 0.72              |
| 1:B:87:LEU:HD21  | 1:B:97:ARG:HD3   | 1.72                     | 0.72              |
| 1:B:486:ALA:O    | 1:B:536:TYR:OH   | 2.04                     | 0.72              |
| 1:G:123:GLU:HG3  | 1:G:125:PHE:HD1  | 1.55                     | 0.72              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:G:5:LEU:HD23     | 1:G:31:HIS:HB2   | 1.69                     | 0.72              |
| 1:H:62:SER:HA      | 1:H:189:HIS:O    | 1.89                     | 0.72              |
| 1:L:445:ALA:HB1    | 1:L:448:PHE:HD2  | 1.53                     | 0.72              |
| 2:D:709:A:H4'      | 2:D:710:A23:OP2  | 1.90                     | 0.72              |
| 1:H:29:GLU:CB      | 1:H:58:ARG:HB2   | 2.20                     | 0.72              |
| 1:H:181:GLU:OE1    | 1:H:194:SER:HB3  | 1.90                     | 0.72              |
| 1:K:472[A]:TRP:CE3 | 1:K:495:LEU:HD13 | 2.25                     | 0.72              |
| 1:L:268:THR:CG2    | 1:L:314:GLY:HA2  | 2.19                     | 0.72              |
| 1:L:342:ASP:OD2    | 1:L:556:SER:HB3  | 1.88                     | 0.72              |
| 1:L:4:LEU:HB3      | 1:L:30:VAL:HG12  | 1.71                     | 0.71              |
| 1:A:531:TYR:HB2    | 1:A:567:LEU:HG   | 1.71                     | 0.71              |
| 1:B:3:ILE:HD13     | 1:B:96:HIS:ND1   | 2.05                     | 0.71              |
| 1:H:32:VAL:HB      | 1:H:61:ILE:HG12  | 1.72                     | 0.71              |
| 1:K:22:LEU:HD13    | 1:K:27:PHE:CE1   | 2.24                     | 0.71              |
| 1:A:35:THR:O       | 1:A:63:ARG:NH1   | 2.23                     | 0.71              |
| 1:B:219:ILE:HD12   | 1:B:222:LEU:HD12 | 1.70                     | 0.71              |
| 1:H:549:ASN:O      | 1:H:553:SER:OG   | 2.07                     | 0.71              |
| 1:K:61:ILE:O       | 1:K:189:HIS:N    | 2.19                     | 0.71              |
| 1:A:21:LEU:HA      | 1:A:158:PHE:CE2  | 2.26                     | 0.71              |
| 1:B:185:GLN:HB2    | 1:B:190:TRP:NE1  | 2.06                     | 0.71              |
| 1:G:489:LEU:HD13   | 1:G:499:VAL:HG11 | 1.73                     | 0.71              |
| 1:H:4:LEU:HB3      | 1:H:30:VAL:CG1   | 2.20                     | 0.71              |
| 1:K:35:THR:HA      | 1:K:64:VAL:CG2   | 2.19                     | 0.71              |
| 1:K:431:LEU:HD11   | 1:K:448:PHE:CZ   | 2.25                     | 0.71              |
| 1:L:64:VAL:CG1     | 1:L:67:PHE:HB3   | 2.21                     | 0.71              |
| 1:A:44:VAL:HG21    | 1:A:63:ARG:NH2   | 2.06                     | 0.71              |
| 1:A:36:ALA:HA      | 1:A:63:ARG:HH11  | 1.56                     | 0.71              |
| 1:A:63:ARG:O       | 1:A:191:VAL:HG22 | 1.89                     | 0.71              |
| 1:G:352:SER:N      | 6:G:2001:HOH:O   | 2.24                     | 0.71              |
| 1:B:65:GLN:HG3     | 1:B:192:ARG:CZ   | 2.21                     | 0.71              |
| 1:H:73:GLU:O       | 1:H:77:MET:N     | 2.20                     | 0.71              |
| 1:K:267:ALA:O      | 1:K:317:ASN:ND2  | 2.22                     | 0.71              |
| 1:L:53:MET:HE1     | 1:L:148:GLU:OE2  | 1.91                     | 0.71              |
| 1:B:74:GLN:HA      | 1:B:77:MET:HE2   | 1.73                     | 0.70              |
| 1:L:522:ASP:OD2    | 1:L:566:ARG:NH2  | 2.23                     | 0.70              |
| 1:A:462:ALA:HB1    | 1:A:465:ASN:ND2  | 2.06                     | 0.70              |
| 1:A:531:TYR:HB3    | 1:A:568:CYS:SG   | 2.31                     | 0.70              |
| 1:G:93:GLN:O       | 1:G:97:ARG:HG3   | 1.91                     | 0.70              |
| 1:G:584:ALA:O      | 1:G:594:ARG:NH1  | 2.24                     | 0.70              |
| 1:B:53:MET:HG3     | 1:B:54:HIS:CD2   | 2.26                     | 0.70              |
| 1:L:22:LEU:HD12    | 1:L:26:GLY:O     | 1.90                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:31:HIS:CE1   | 1:A:90:ARG:HD2   | 2.26                     | 0.70              |
| 1:A:449:GLU:HG3  | 1:A:450:PRO:CD   | 2.18                     | 0.70              |
| 1:G:35:THR:HA    | 1:G:64:VAL:CG2   | 2.21                     | 0.70              |
| 1:H:5:LEU:HD23   | 1:H:31:HIS:HB2   | 1.73                     | 0.70              |
| 1:H:85:ARG:HD3   | 1:H:180:LEU:HD13 | 1.73                     | 0.70              |
| 1:H:533:LEU:HB3  | 1:H:568:CYS:SG   | 2.32                     | 0.70              |
| 1:K:196:MET:O    | 1:K:200:GLN:HG3  | 1.91                     | 0.70              |
| 1:H:182:SER:OG   | 1:H:191:VAL:HG12 | 1.92                     | 0.70              |
| 1:H:507:GLU:OE1  | 6:H:802:HOH:O    | 2.08                     | 0.70              |
| 1:G:576:VAL:O    | 1:G:580:GLN:NE2  | 2.24                     | 0.70              |
| 1:K:414:ILE:CG2  | 1:K:454:VAL:HG21 | 2.22                     | 0.70              |
| 1:L:322:LEU:HD21 | 1:L:331:GLN:HG2  | 1.73                     | 0.70              |
| 1:B:22:LEU:HB3   | 1:B:25:GLN:HB2   | 1.72                     | 0.70              |
| 1:G:37:SER:HB2   | 1:G:68:GLU:O     | 1.91                     | 0.70              |
| 1:H:165:PRO:O    | 1:H:171:ARG:NH2  | 2.24                     | 0.70              |
| 1:B:77:MET:O     | 1:B:80:GLU:HG3   | 1.92                     | 0.70              |
| 1:G:141:ALA:CB   | 1:G:146:GLU:HB3  | 2.22                     | 0.69              |
| 1:L:3:ILE:O      | 1:L:98:TYR:N     | 2.25                     | 0.69              |
| 1:L:243:ASP:OD1  | 1:L:245:VAL:HG22 | 1.92                     | 0.69              |
| 1:G:91:ALA:HB1   | 1:G:97:ARG:CG    | 2.20                     | 0.69              |
| 1:A:81:GLU:OE2   | 1:A:85:ARG:NE    | 2.26                     | 0.69              |
| 1:A:301:PRO:HD3  | 1:A:515:GLN:HG2  | 1.74                     | 0.69              |
| 1:H:6:CYS:HB3    | 1:H:15:VAL:HG22  | 1.72                     | 0.69              |
| 1:K:213:LEU:CB   | 1:L:168:PRO:HG2  | 2.23                     | 0.69              |
| 1:G:46:GLN:HA    | 1:G:49:ARG:HG2   | 1.75                     | 0.69              |
| 1:H:91:ALA:HB1   | 1:H:97:ARG:HD2   | 1.73                     | 0.69              |
| 1:L:196:MET:HE3  | 1:L:199:ARG:HB2  | 1.74                     | 0.69              |
| 1:A:60:SER:HB2   | 1:A:189:HIS:CE1  | 2.27                     | 0.69              |
| 1:K:133:PHE:HD2  | 1:K:141:ALA:HB2  | 1.57                     | 0.69              |
| 1:K:435:GLU:HG2  | 1:K:462:ALA:CA   | 2.22                     | 0.69              |
| 1:B:37:SER:O     | 1:B:63:ARG:NH2   | 2.23                     | 0.69              |
| 1:H:6:CYS:O      | 1:H:33:LEU:N     | 2.16                     | 0.69              |
| 1:L:34:THR:O     | 1:L:64:VAL:HG23  | 1.92                     | 0.69              |
| 1:G:408:ARG:HD2  | 1:L:418:GLU:OE1  | 1.92                     | 0.69              |
| 1:K:97:ARG:HB3   | 1:K:121:ALA:HA   | 1.73                     | 0.69              |
| 1:L:534:ARG:HG3  | 1:L:568:CYS:HB3  | 1.75                     | 0.69              |
| 1:A:182:SER:HA   | 1:A:190:TRP:O    | 1.92                     | 0.69              |
| 1:B:268:THR:OG1  | 1:B:314:GLY:HA2  | 1.92                     | 0.69              |
| 1:H:414:ILE:HG22 | 1:H:456:LEU:HD12 | 1.74                     | 0.69              |
| 1:G:97:ARG:NH2   | 1:G:120:GLY:O    | 2.24                     | 0.69              |
| 1:G:121:ALA:O    | 1:G:164:GLU:N    | 2.22                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:473:GLN:O    | 1:G:477:LYS:HB2  | 1.92                     | 0.69              |
| 1:L:129:CYS:H    | 2:N:729:A:H2     | 1.40                     | 0.69              |
| 1:A:183:THR:OG1  | 1:A:190:TRP:HB2  | 1.93                     | 0.68              |
| 1:B:181:GLU:CG   | 1:B:192:ARG:HB3  | 2.22                     | 0.68              |
| 1:G:35:THR:HA    | 1:G:64:VAL:HG22  | 1.74                     | 0.68              |
| 1:G:98:TYR:CD2   | 1:G:123:GLU:HB3  | 2.28                     | 0.68              |
| 1:H:431:LEU:HD11 | 1:H:448:PHE:CZ   | 2.25                     | 0.68              |
| 1:K:319:SER:OG   | 6:K:802:HOH:O    | 2.10                     | 0.68              |
| 1:A:35:THR:HA    | 1:A:64:VAL:CG2   | 2.22                     | 0.68              |
| 1:B:467:ASP:O    | 1:B:469:GLU:N    | 2.24                     | 0.68              |
| 1:G:3:ILE:HG13   | 1:G:29:GLU:HB2   | 1.74                     | 0.68              |
| 1:G:50:TYR:HD1   | 1:G:53:MET:HE3   | 1.59                     | 0.68              |
| 1:H:545:LEU:HD12 | 1:H:561:LEU:HD22 | 1.75                     | 0.68              |
| 1:H:561:LEU:O    | 1:H:564:THR:OG1  | 2.10                     | 0.68              |
| 1:K:174:SER:HB3  | 1:K:176:PRO:HD2  | 1.75                     | 0.68              |
| 1:K:356:TYR:HB2  | 1:K:366:VAL:HG11 | 1.75                     | 0.68              |
| 1:A:443:MET:O    | 1:A:478:LEU:HD23 | 1.92                     | 0.68              |
| 1:L:123:GLU:OE2  | 1:L:160:ARG:HB2  | 1.94                     | 0.68              |
| 1:L:433:GLY:HA2  | 3:L:703:ATP:H1'  | 1.75                     | 0.68              |
| 1:L:545:LEU:HD12 | 1:L:561:LEU:HD22 | 1.75                     | 0.68              |
| 1:A:34:THR:OG1   | 1:A:40:ILE:HG21  | 1.93                     | 0.68              |
| 1:A:307:LEU:HB2  | 1:A:464:GLU:HB2  | 1.76                     | 0.68              |
| 1:G:101:LEU:HA   | 1:G:112:MET:CE   | 2.18                     | 0.68              |
| 1:G:114:ARG:NH2  | 1:H:113:GLN:OE1  | 2.27                     | 0.68              |
| 1:L:16:PRO:O     | 1:L:19:MET:HG2   | 1.92                     | 0.68              |
| 1:L:145:GLU:O    | 1:L:149:GLN:HG2  | 1.92                     | 0.68              |
| 1:A:76:HIS:O     | 1:A:80:GLU:HG3   | 1.94                     | 0.68              |
| 1:B:439:THR:C    | 1:B:440:ARG:HD3  | 2.19                     | 0.68              |
| 1:H:37:SER:HB2   | 1:H:68:GLU:O     | 1.94                     | 0.68              |
| 1:H:145:GLU:OE2  | 1:H:146:GLU:HG3  | 1.93                     | 0.68              |
| 1:K:183:THR:OG1  | 1:K:190:TRP:HB2  | 1.93                     | 0.68              |
| 1:K:397:ARG:HD2  | 1:K:434:PHE:H    | 1.58                     | 0.68              |
| 1:H:173:LEU:HD11 | 1:H:201:HIS:HE1  | 1.59                     | 0.68              |
| 1:H:333:ARG:O    | 1:H:337:GLU:HG2  | 1.94                     | 0.68              |
| 1:K:20:GLN:OE1   | 1:K:23:GLY:HA2   | 1.94                     | 0.68              |
| 1:L:211:HIS:ND1  | 1:L:231:PRO:HA   | 2.08                     | 0.68              |
| 1:G:5:LEU:CD2    | 1:G:31:HIS:HB2   | 2.24                     | 0.68              |
| 1:G:106:LYS:O    | 1:G:109:SER:OG   | 2.09                     | 0.68              |
| 1:H:475:VAL:HG13 | 1:H:504:ILE:CD1  | 2.23                     | 0.68              |
| 1:L:105:TYR:HA   | 2:M:728:A23:H1'  | 1.76                     | 0.68              |
| 1:K:5:LEU:N      | 1:K:98:TYR:O     | 2.21                     | 0.67              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:L:101:LEU:HD21   | 1:L:126:HIS:CB   | 2.23                     | 0.67              |
| 1:L:394:THR:OG1    | 6:L:802:HOH:O    | 2.11                     | 0.67              |
| 1:A:141:ALA:HB1    | 1:A:146:GLU:HB3  | 1.76                     | 0.67              |
| 1:A:180:LEU:HD12   | 1:A:193:ALA:HA   | 1.76                     | 0.67              |
| 1:B:67:PHE:CD1     | 1:B:75:ASP:HB3   | 2.30                     | 0.67              |
| 1:B:533:LEU:HD12   | 1:B:543:VAL:HG11 | 1.76                     | 0.67              |
| 1:L:267:ALA:O      | 1:L:317:ASN:ND2  | 2.27                     | 0.67              |
| 1:L:507:GLU:OE1    | 6:L:803:HOH:O    | 2.11                     | 0.67              |
| 1:H:97:ARG:NH2     | 1:H:120:GLY:O    | 2.27                     | 0.67              |
| 1:L:126:HIS:HB3    | 1:L:159:VAL:HB   | 1.76                     | 0.67              |
| 1:L:126:HIS:N      | 1:L:159:VAL:O    | 2.21                     | 0.67              |
| 1:L:128:LEU:HB2    | 1:L:157:ARG:HG3  | 1.74                     | 0.67              |
| 1:A:36:ALA:HA      | 1:A:63:ARG:CD    | 2.23                     | 0.67              |
| 1:A:408:ARG:HH12   | 1:H:454:VAL:HG12 | 1.59                     | 0.67              |
| 1:G:12:TRP:HH2     | 1:G:144:LEU:HD23 | 1.58                     | 0.67              |
| 1:L:34:THR:N       | 1:L:62:SER:O     | 2.25                     | 0.67              |
| 1:A:100:CYS:O      | 1:A:112:MET:HE1  | 1.94                     | 0.67              |
| 1:B:93:GLN:HB2     | 1:B:96:HIS:CD2   | 2.29                     | 0.67              |
| 1:H:53:MET:HE2     | 1:H:144:LEU:HD22 | 1.76                     | 0.67              |
| 1:K:12:TRP:NE1     | 1:K:46:GLN:OE1   | 2.28                     | 0.67              |
| 1:L:65:GLN:HB2     | 1:L:190:TRP:HE3  | 1.60                     | 0.67              |
| 1:A:378:MET:HE1    | 1:A:424:CYS:HB2  | 1.76                     | 0.67              |
| 1:B:106:LYS:HD2    | 2:C:707:A:C4'    | 2.25                     | 0.67              |
| 1:B:234:HIS:CD2    | 1:B:607:PRO:HD2  | 2.29                     | 0.67              |
| 1:H:139:ARG:HG2    | 1:H:140:GLU:H    | 1.58                     | 0.67              |
| 1:B:494:ASP:O      | 1:B:498:VAL:HG23 | 1.93                     | 0.67              |
| 1:G:65:GLN:HB3     | 1:G:192:ARG:HD2  | 1.75                     | 0.67              |
| 1:H:473:GLN:OE1    | 1:H:477:LYS:HD2  | 1.95                     | 0.67              |
| 1:K:97:ARG:NH1     | 1:K:119:PHE:O    | 2.27                     | 0.67              |
| 1:K:167:TRP:CD2    | 1:K:168:PRO:HD2  | 2.30                     | 0.67              |
| 1:K:460:VAL:HG23   | 1:K:480:ALA:HB2  | 1.77                     | 0.67              |
| 1:K:578:LYS:HE3    | 1:K:582:PHE:CZ   | 2.30                     | 0.67              |
| 1:B:471:ILE:HG21   | 1:B:489:LEU:CD1  | 2.24                     | 0.67              |
| 1:G:12:TRP:CH2     | 1:G:144:LEU:HD23 | 2.29                     | 0.67              |
| 1:H:268:THR:HG21   | 1:H:314:GLY:HA2  | 1.77                     | 0.67              |
| 1:K:114:ARG:HA     | 1:K:114:ARG:NE   | 2.09                     | 0.67              |
| 1:K:472[A]:TRP:CZ2 | 1:L:453:ARG:HA   | 2.28                     | 0.67              |
| 1:K:531:TYR:HB3    | 1:K:568:CYS:SG   | 2.35                     | 0.67              |
| 1:L:298:TRP:CD2    | 1:L:299:PRO:HA   | 2.28                     | 0.67              |
| 1:A:15:VAL:O       | 1:A:19:MET:HG2   | 1.94                     | 0.67              |
| 1:B:62:SER:HA      | 1:B:189:HIS:O    | 1.95                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:320:ALA:O    | 1:G:321:LEU:HB2  | 1.95                     | 0.67              |
| 1:G:50:TYR:HA    | 1:G:53:MET:HE2   | 1.76                     | 0.67              |
| 1:G:85:ARG:HA    | 1:G:88:LEU:HD21  | 1.75                     | 0.67              |
| 1:G:434:PHE:CE2  | 1:G:478:LEU:HD21 | 2.31                     | 0.67              |
| 1:H:520:PRO:HG3  | 1:H:529:GLU:HG3  | 1.77                     | 0.67              |
| 1:K:57:PRO:HG2   | 1:K:59:PHE:CE1   | 2.30                     | 0.67              |
| 1:K:272:LEU:O    | 1:K:276:VAL:HG23 | 1.94                     | 0.67              |
| 1:L:3:ILE:N      | 1:L:96:HIS:O     | 2.26                     | 0.67              |
| 1:L:531:TYR:HB2  | 1:L:567:LEU:HB3  | 1.77                     | 0.67              |
| 1:L:572:THR:OG1  | 1:L:575:GLU:OE1  | 2.10                     | 0.67              |
| 2:N:729:A:H4'    | 2:N:730:A23:OP1  | 1.95                     | 0.67              |
| 1:B:329:ARG:O    | 1:B:333:ARG:HG2  | 1.95                     | 0.66              |
| 1:H:132:ARG:HH21 | 1:H:155:ALA:HB2  | 1.60                     | 0.66              |
| 1:H:292:ILE:O    | 1:H:292:ILE:HG13 | 1.94                     | 0.66              |
| 1:A:3:ILE:HG13   | 1:A:29:GLU:HB2   | 1.77                     | 0.66              |
| 1:A:403:ARG:HA   | 1:A:406:ILE:HD13 | 1.77                     | 0.66              |
| 1:A:449:GLU:CG   | 1:A:450:PRO:HD3  | 2.21                     | 0.66              |
| 1:A:467:ASP:OD1  | 1:A:468:VAL:N    | 2.28                     | 0.66              |
| 1:B:375:GLN:HE22 | 1:B:423:GLY:HA3  | 1.58                     | 0.66              |
| 1:G:85:ARG:HA    | 1:G:88:LEU:CD2   | 2.26                     | 0.66              |
| 1:G:435:GLU:CG   | 1:G:462:ALA:HA   | 2.12                     | 0.66              |
| 1:L:273:LEU:O    | 1:L:277:ARG:HG3  | 1.95                     | 0.66              |
| 1:G:268:THR:OG1  | 1:G:314:GLY:HA2  | 1.94                     | 0.66              |
| 1:G:511:TYR:CE1  | 1:G:563:LEU:HD22 | 2.30                     | 0.66              |
| 1:K:48:LEU:CD1   | 1:K:187:PRO:HG2  | 2.24                     | 0.66              |
| 1:L:431:LEU:HD11 | 1:L:448:PHE:CE1  | 2.29                     | 0.66              |
| 1:B:5:LEU:HD22   | 1:B:31:HIS:HB2   | 1.76                     | 0.66              |
| 1:G:50:TYR:CD1   | 1:G:53:MET:HE3   | 2.30                     | 0.66              |
| 1:L:355:ASN:ND2  | 3:L:703:ATP:O1B  | 2.28                     | 0.66              |
| 1:L:378:MET:CE   | 1:L:388:HIS:HA   | 2.25                     | 0.66              |
| 1:B:144:LEU:O    | 1:B:148:GLU:HG2  | 1.96                     | 0.66              |
| 1:G:578:LYS:HA   | 1:G:581:VAL:HG12 | 1.78                     | 0.66              |
| 1:H:29:GLU:HB3   | 1:H:58:ARG:HB2   | 1.77                     | 0.66              |
| 1:H:471:ILE:O    | 1:H:475:VAL:HG23 | 1.94                     | 0.66              |
| 1:K:260:HIS:CD2  | 1:K:548:ASP:HA   | 2.30                     | 0.66              |
| 1:G:445:ALA:HB2  | 1:G:478:LEU:CD2  | 2.26                     | 0.66              |
| 1:K:31:HIS:CD2   | 1:K:90:ARG:HB3   | 2.31                     | 0.66              |
| 1:K:167:TRP:CD1  | 1:K:170:LEU:HG   | 2.30                     | 0.66              |
| 1:K:352:SER:N    | 6:K:803:HOH:O    | 2.13                     | 0.66              |
| 1:L:94:ALA:O     | 1:L:97:ARG:HG2   | 1.96                     | 0.66              |
| 1:L:448:PHE:O    | 1:L:451:VAL:HG22 | 1.95                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:174:SER:HB3  | 1:A:176:PRO:HD2  | 1.78                     | 0.66              |
| 1:A:516:ILE:HG22 | 1:A:517:LYS:HG3  | 1.77                     | 0.66              |
| 1:B:65:GLN:OE1   | 1:B:65:GLN:N     | 2.23                     | 0.66              |
| 1:K:307:LEU:CD2  | 1:K:464:GLU:HB2  | 2.25                     | 0.66              |
| 1:L:2:ARG:HG2    | 1:L:98:TYR:HE1   | 1.59                     | 0.66              |
| 1:A:299:PRO:O    | 1:A:515:GLN:NE2  | 2.27                     | 0.66              |
| 1:G:4:LEU:HD13   | 1:G:125:PHE:CZ   | 2.31                     | 0.66              |
| 1:G:165:PRO:O    | 1:G:171:ARG:NH1  | 2.29                     | 0.66              |
| 1:G:445:ALA:HB2  | 1:G:478:LEU:HD23 | 1.76                     | 0.66              |
| 1:H:91:ALA:CB    | 1:H:97:ARG:HD2   | 2.24                     | 0.66              |
| 1:L:350:ARG:HB3  | 1:L:392:LEU:HB2  | 1.77                     | 0.66              |
| 1:A:307:LEU:CB   | 1:A:464:GLU:HB2  | 2.26                     | 0.66              |
| 1:B:66:ASP:HB2   | 1:B:78:LEU:HD21  | 1.78                     | 0.66              |
| 1:G:237:TRP:CZ3  | 1:G:607:PRO:HG3  | 2.31                     | 0.66              |
| 1:H:200:GLN:HA   | 1:H:203:GLU:CD   | 2.21                     | 0.66              |
| 1:H:268:THR:HG23 | 1:H:314:GLY:HA2  | 1.77                     | 0.66              |
| 1:K:61:ILE:HD12  | 1:K:188:VAL:HG12 | 1.76                     | 0.66              |
| 1:K:410:LEU:HD12 | 1:K:451:VAL:CG2  | 2.25                     | 0.66              |
| 1:K:455:GLY:HA3  | 1:L:497:ARG:HH21 | 1.60                     | 0.66              |
| 1:L:17:GLU:HB3   | 1:L:156:LEU:CD2  | 2.25                     | 0.66              |
| 1:L:312:ARG:NE   | 1:L:312:ARG:HA   | 2.10                     | 0.66              |
| 1:K:393:LEU:HD12 | 1:K:413:ALA:HB2  | 1.77                     | 0.66              |
| 1:L:240:GLU:OE1  | 1:L:241:PRO:HD2  | 1.96                     | 0.66              |
| 1:L:473:GLN:O    | 1:L:477:LYS:HB2  | 1.95                     | 0.66              |
| 1:H:85:ARG:HH21  | 1:H:178:PHE:HB3  | 1.61                     | 0.65              |
| 1:K:430:ASP:C    | 1:K:431:LEU:HD22 | 2.21                     | 0.65              |
| 1:G:101:LEU:CD1  | 1:H:106:LYS:HE2  | 2.27                     | 0.65              |
| 1:H:67:PHE:HE1   | 1:H:75:ASP:HB3   | 1.61                     | 0.65              |
| 1:H:549:ASN:HD22 | 1:H:552:ILE:HD12 | 1.61                     | 0.65              |
| 1:L:167:TRP:O    | 1:L:171:ARG:NE   | 2.30                     | 0.65              |
| 1:A:7:SER:O      | 1:A:103:GLY:HA3  | 1.97                     | 0.65              |
| 1:B:248:LYS:HD2  | 1:B:562:LEU:CD1  | 2.27                     | 0.65              |
| 1:G:509:CYS:SG   | 1:G:548:ASP:HB2  | 2.37                     | 0.65              |
| 1:L:445:ALA:HB1  | 1:L:448:PHE:CD2  | 2.31                     | 0.65              |
| 1:A:29:GLU:OE1   | 1:A:58:ARG:HB3   | 1.96                     | 0.65              |
| 1:B:589:ALA:HB1  | 1:B:593:GLU:HB2  | 1.78                     | 0.65              |
| 1:G:430:ASP:O    | 1:G:431:LEU:HD23 | 1.97                     | 0.65              |
| 1:A:481:ARG:O    | 1:A:482:ARG:HG2  | 1.97                     | 0.65              |
| 1:H:174:SER:HB3  | 1:H:176:PRO:HD2  | 1.79                     | 0.65              |
| 1:B:124:VAL:HG13 | 1:B:161:LEU:CB   | 2.25                     | 0.65              |
| 1:B:133:PHE:CE2  | 1:B:149:GLN:HG3  | 2.31                     | 0.65              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:G:294:LEU:HD23   | 1:G:313:LEU:HD22 | 1.79                     | 0.65              |
| 1:L:256:LYS:HE2    | 1:L:558:THR:CG2  | 2.26                     | 0.65              |
| 1:B:417:ALA:HB2    | 1:B:456:LEU:HD11 | 1.79                     | 0.65              |
| 1:B:513:ASN:ND2    | 1:B:531:TYR:OH   | 2.21                     | 0.65              |
| 1:H:314:GLY:O      | 6:H:804:HOH:O    | 2.13                     | 0.65              |
| 1:L:259:LEU:HB3    | 1:L:482:ARG:NH1  | 2.12                     | 0.65              |
| 1:A:455:GLY:HA3    | 1:B:497:ARG:HH21 | 1.61                     | 0.65              |
| 1:L:307:LEU:O      | 1:L:311:MET:N    | 2.25                     | 0.65              |
| 1:G:94:ALA:HA      | 1:G:97:ARG:HE    | 1.61                     | 0.65              |
| 1:K:12:TRP:HB3     | 1:K:43:GLY:HA3   | 1.78                     | 0.65              |
| 1:K:320:ALA:O      | 1:K:321:LEU:HB2  | 1.95                     | 0.65              |
| 1:L:182:SER:HB2    | 1:L:191:VAL:HG12 | 1.78                     | 0.65              |
| 1:B:473:GLN:OE1    | 1:B:477:LYS:HG3  | 1.96                     | 0.64              |
| 1:G:462:ALA:HB3    | 1:G:484:GLY:O    | 1.97                     | 0.64              |
| 1:H:63:ARG:NH1     | 1:H:188:VAL:HB   | 2.12                     | 0.64              |
| 1:H:156:LEU:HD23   | 1:H:158:PHE:CZ   | 2.32                     | 0.64              |
| 1:H:492:SER:O      | 1:H:495:LEU:N    | 2.29                     | 0.64              |
| 1:G:88:LEU:HD12    | 1:G:89:GLN:N     | 2.11                     | 0.64              |
| 1:K:167:TRP:HB3    | 1:K:170:LEU:HB2  | 1.77                     | 0.64              |
| 1:L:196:MET:HE3    | 1:L:199:ARG:CB   | 2.27                     | 0.64              |
| 1:G:169:GLN:OE1    | 1:G:169:GLN:N    | 2.29                     | 0.64              |
| 1:K:511:TYR:HE1    | 1:K:563:LEU:HD13 | 1.61                     | 0.64              |
| 1:A:102:ALA:HA     | 1:A:126:HIS:CE1  | 2.33                     | 0.64              |
| 1:B:53:MET:CE      | 1:B:144:LEU:HD22 | 2.27                     | 0.64              |
| 1:G:197:ARG:HH12   | 1:G:201:HIS:HB2  | 1.60                     | 0.64              |
| 1:H:250:TRP:CD1    | 1:H:605:PRO:HG2  | 2.33                     | 0.64              |
| 1:A:69:ASP:OD1     | 1:A:105:TYR:OH   | 2.13                     | 0.64              |
| 1:B:435:GLU:OE2    | 1:B:465:ASN:N    | 2.30                     | 0.64              |
| 1:H:101:LEU:HB2    | 1:H:109:SER:OG   | 1.97                     | 0.64              |
| 1:K:354:ALA:HB1    | 1:K:405:ARG:HH11 | 1.62                     | 0.64              |
| 1:K:472[A]:TRP:HZ3 | 1:K:495:LEU:HB2  | 1.62                     | 0.64              |
| 1:A:85:ARG:NH1     | 1:A:179:PRO:O    | 2.30                     | 0.64              |
| 1:H:17:GLU:HB2     | 1:H:156:LEU:HD22 | 1.78                     | 0.64              |
| 1:H:53:MET:CE      | 1:H:144:LEU:HD22 | 2.27                     | 0.64              |
| 1:K:12:TRP:HB2     | 1:K:47:LEU:HG    | 1.79                     | 0.64              |
| 1:K:85:ARG:CB      | 1:K:180:LEU:HD13 | 2.23                     | 0.64              |
| 1:L:307:LEU:HB2    | 1:L:464:GLU:OE2  | 1.96                     | 0.64              |
| 1:G:378:MET:HE3    | 1:G:388:HIS:HA   | 1.80                     | 0.64              |
| 1:G:31:HIS:ND1     | 1:G:90:ARG:HD2   | 2.12                     | 0.64              |
| 1:G:242:LEU:HD23   | 1:G:565:ALA:HB2  | 1.80                     | 0.64              |
| 1:K:81:GLU:HG2     | 1:K:196:MET:CE   | 2.28                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:21:LEU:HB3   | 1:L:27:PHE:HZ    | 1.62                     | 0.64              |
| 1:A:399:GLU:OE1  | 1:A:399:GLU:N    | 2.31                     | 0.64              |
| 1:B:1:MET:HG3    | 1:B:3:ILE:HD11   | 1.78                     | 0.64              |
| 1:B:266:PHE:HB3  | 1:B:331:GLN:NE2  | 2.13                     | 0.64              |
| 1:H:135:PRO:HD2  | 1:H:139:ARG:HH12 | 1.63                     | 0.64              |
| 1:H:453:ARG:O    | 1:H:453:ARG:HG3  | 1.97                     | 0.64              |
| 1:A:15:VAL:HG13  | 1:A:19:MET:HE3   | 1.80                     | 0.63              |
| 1:H:158:PHE:HB2  | 1:H:160:ARG:NH1  | 2.11                     | 0.63              |
| 1:A:167:TRP:CG   | 1:A:168:PRO:HD2  | 2.33                     | 0.63              |
| 1:A:408:ARG:NH1  | 1:H:454:VAL:HG12 | 2.12                     | 0.63              |
| 1:A:524:GLU:OE1  | 1:A:524:GLU:N    | 2.22                     | 0.63              |
| 1:B:34:THR:O     | 1:B:63:ARG:HA    | 1.97                     | 0.63              |
| 1:B:128:LEU:HB2  | 1:B:157:ARG:HG3  | 1.80                     | 0.63              |
| 1:L:84:TRP:HE1   | 1:L:115:ALA:HB2  | 1.63                     | 0.63              |
| 1:L:165:PRO:O    | 1:L:171:ARG:NH1  | 2.29                     | 0.63              |
| 1:A:131:PRO:HD2  | 1:A:132:ARG:HH11 | 1.63                     | 0.63              |
| 1:B:2:ARG:N      | 1:B:28:ASP:OD2   | 2.27                     | 0.63              |
| 1:B:85:ARG:NH2   | 1:B:195:ASP:OD1  | 2.23                     | 0.63              |
| 1:B:432:ALA:HA   | 1:B:461:HIS:HB2  | 1.80                     | 0.63              |
| 1:G:7:SER:O      | 1:G:103:GLY:HA3  | 1.99                     | 0.63              |
| 1:G:39:LYS:NZ    | 1:G:40:ILE:HD11  | 2.13                     | 0.63              |
| 1:H:53:MET:HE3   | 1:H:148:GLU:OE2  | 1.98                     | 0.63              |
| 1:L:394:THR:CG2  | 1:L:432:ALA:HB3  | 2.28                     | 0.63              |
| 1:B:34:THR:O     | 1:B:64:VAL:HG23  | 1.98                     | 0.63              |
| 1:B:266:PHE:HB3  | 1:B:331:GLN:HE21 | 1.64                     | 0.63              |
| 1:H:15:VAL:HB    | 1:H:47:LEU:HD21  | 1.81                     | 0.63              |
| 1:A:397:ARG:HD3  | 1:A:444:PHE:HE2  | 1.63                     | 0.63              |
| 1:B:219:ILE:CD1  | 1:B:222:LEU:HD12 | 2.28                     | 0.63              |
| 1:B:378:MET:CE   | 1:B:388:HIS:HA   | 2.27                     | 0.63              |
| 1:G:91:ALA:CB    | 1:G:97:ARG:HG2   | 2.23                     | 0.63              |
| 1:H:208:ARG:HH11 | 1:H:212:ILE:HD12 | 1.62                     | 0.63              |
| 1:K:328:LEU:HD11 | 1:K:370:ILE:HG12 | 1.80                     | 0.63              |
| 1:L:21:LEU:HB3   | 1:L:27:PHE:CZ    | 2.33                     | 0.63              |
| 1:L:335:LEU:HD21 | 1:L:349:ILE:HG12 | 1.80                     | 0.63              |
| 1:A:100:CYS:C    | 1:A:112:MET:HE1  | 2.24                     | 0.63              |
| 1:B:84:TRP:HB3   | 1:B:198:LEU:HD21 | 1.81                     | 0.63              |
| 1:A:472:TRP:CD1  | 1:A:495:LEU:HD21 | 2.33                     | 0.63              |
| 1:G:34:THR:O     | 1:G:64:VAL:HG22  | 1.98                     | 0.63              |
| 1:G:143:THR:O    | 1:G:147:VAL:HG23 | 1.98                     | 0.63              |
| 1:H:200:GLN:HA   | 1:H:203:GLU:HG2  | 1.79                     | 0.63              |
| 1:K:431:LEU:HD21 | 1:K:448:PHE:CE1  | 2.34                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:523:GLU:OE2  | 1:K:530:THR:HG23 | 1.98                     | 0.63              |
| 1:L:242:LEU:HD23 | 1:L:565:ALA:HB2  | 1.80                     | 0.63              |
| 1:H:509:CYS:O    | 1:H:513:ASN:ND2  | 2.32                     | 0.63              |
| 1:K:302:GLU:HG2  | 1:K:303:GLU:OE1  | 1.98                     | 0.63              |
| 1:L:283:PRO:HA   | 1:L:286:LEU:CD2  | 2.25                     | 0.63              |
| 1:A:100:CYS:HA   | 1:A:125:PHE:O    | 1.98                     | 0.63              |
| 1:G:510:PRO:HD2  | 1:G:560:ASN:OD1  | 1.98                     | 0.63              |
| 1:K:238:LEU:HG   | 1:K:574:LEU:HB2  | 1.81                     | 0.63              |
| 1:G:494:ASP:O    | 1:G:498:VAL:HG23 | 1.99                     | 0.62              |
| 1:H:304:PRO:HB3  | 1:H:516:ILE:O    | 1.98                     | 0.62              |
| 1:K:101:LEU:HD11 | 1:K:126:HIS:HB2  | 1.81                     | 0.62              |
| 1:A:33:LEU:HD11  | 1:A:64:VAL:CG1   | 2.23                     | 0.62              |
| 1:A:247:ASP:OD2  | 1:A:573:ARG:NH2  | 2.27                     | 0.62              |
| 1:B:3:ILE:HG23   | 1:B:29:GLU:O     | 1.99                     | 0.62              |
| 1:K:533:LEU:HD12 | 1:K:543:VAL:HG11 | 1.80                     | 0.62              |
| 1:L:489:LEU:HB2  | 1:L:536:TYR:HE2  | 1.62                     | 0.62              |
| 1:A:256:LYS:NZ   | 1:A:342:ASP:O    | 2.31                     | 0.62              |
| 1:G:266:PHE:CD1  | 1:G:335:LEU:HD13 | 2.34                     | 0.62              |
| 1:A:475:VAL:HG13 | 1:A:504:ILE:CD1  | 2.30                     | 0.62              |
| 1:B:439:THR:O    | 1:B:440:ARG:HD3  | 1.98                     | 0.62              |
| 1:H:237:TRP:CZ3  | 1:H:607:PRO:HG3  | 2.34                     | 0.62              |
| 1:K:132:ARG:HA   | 1:K:137:GLY:O    | 1.99                     | 0.62              |
| 1:L:332:CYS:SG   | 1:L:370:ILE:HG23 | 2.40                     | 0.62              |
| 1:L:394:THR:HA   | 1:L:430:ASP:OD1  | 2.00                     | 0.62              |
| 1:G:128:LEU:HB2  | 1:G:157:ARG:HB2  | 1.81                     | 0.62              |
| 1:H:245:VAL:HG13 | 1:H:246:GLN:CD   | 2.24                     | 0.62              |
| 1:K:259:LEU:HB3  | 1:K:482:ARG:HH12 | 1.63                     | 0.62              |
| 1:G:49:ARG:HG3   | 1:G:144:LEU:HD11 | 1.81                     | 0.62              |
| 1:G:63:ARG:O     | 1:G:190:TRP:HA   | 1.99                     | 0.62              |
| 1:G:354:ALA:HA   | 1:G:363:PRO:HB3  | 1.81                     | 0.62              |
| 1:G:499:VAL:HG23 | 1:G:504:ILE:HB   | 1.81                     | 0.62              |
| 1:H:57:PRO:HG2   | 1:H:59:PHE:CZ    | 2.35                     | 0.62              |
| 1:L:510:PRO:HG2  | 1:L:560:ASN:O    | 2.00                     | 0.62              |
| 1:A:207:GLU:O    | 1:A:210:ARG:HG2  | 2.00                     | 0.62              |
| 1:B:440:ARG:HG2  | 1:B:441:ALA:N    | 2.15                     | 0.62              |
| 1:H:172:LEU:HD12 | 1:H:173:LEU:HD12 | 1.82                     | 0.62              |
| 1:G:63:ARG:N     | 1:G:189:HIS:O    | 2.22                     | 0.62              |
| 1:K:256:LYS:NZ   | 1:K:342:ASP:OD1  | 2.22                     | 0.62              |
| 1:K:280:ALA:CB   | 1:K:286:LEU:HD11 | 2.30                     | 0.62              |
| 1:B:449:GLU:O    | 1:B:453:ARG:HG3  | 2.00                     | 0.62              |
| 1:G:43:GLY:HA2   | 1:G:46:GLN:OE1   | 1.99                     | 0.62              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:G:97:ARG:NH2     | 1:G:119:PHE:O    | 2.33                     | 0.62              |
| 1:L:472[A]:TRP:CD1 | 1:L:495:LEU:HD22 | 2.35                     | 0.62              |
| 1:H:53:MET:HG3     | 1:H:54:HIS:CD2   | 2.34                     | 0.61              |
| 1:L:50:TYR:HD1     | 1:L:144:LEU:HD23 | 1.65                     | 0.61              |
| 1:L:509:CYS:CB     | 1:L:512:ALA:HB3  | 2.30                     | 0.61              |
| 1:B:240:GLU:HB3    | 1:B:241:PRO:HD2  | 1.82                     | 0.61              |
| 1:B:387:CYS:O      | 1:B:389:VAL:HG23 | 2.00                     | 0.61              |
| 1:K:307:LEU:HD23   | 1:K:464:GLU:HB2  | 1.80                     | 0.61              |
| 1:K:399:GLU:OE1    | 1:K:399:GLU:HA   | 2.00                     | 0.61              |
| 1:L:430:ASP:HB3    | 1:L:459:THR:CG2  | 2.29                     | 0.61              |
| 1:L:533:LEU:HD23   | 1:L:564:THR:HG21 | 1.82                     | 0.61              |
| 1:A:73:GLU:O       | 1:A:76:HIS:HB3   | 2.00                     | 0.61              |
| 1:B:131:PRO:HB3    | 1:B:140:GLU:OE2  | 2.00                     | 0.61              |
| 1:G:4:LEU:HD13     | 1:G:125:PHE:HZ   | 1.65                     | 0.61              |
| 1:G:524:GLU:HG2    | 1:G:525:GLN:OE1  | 1.99                     | 0.61              |
| 1:H:116:ALA:HB1    | 1:H:164:GLU:HG3  | 1.81                     | 0.61              |
| 1:K:258:GLU:O      | 1:K:259:LEU:HD23 | 2.00                     | 0.61              |
| 1:L:259:LEU:HD13   | 1:L:482:ARG:HH11 | 1.66                     | 0.61              |
| 1:B:224:ILE:HG22   | 1:B:226:ALA:H    | 1.65                     | 0.61              |
| 1:G:31:HIS:ND1     | 1:G:90:ARG:HB3   | 2.15                     | 0.61              |
| 1:G:182:SER:HA     | 1:G:190:TRP:O    | 2.00                     | 0.61              |
| 1:G:305:ILE:O      | 1:G:309:ARG:HB2  | 2.01                     | 0.61              |
| 1:H:34:THR:CG2     | 1:H:40:ILE:HD12  | 2.30                     | 0.61              |
| 1:K:133:PHE:HE2    | 1:K:150:ALA:HB2  | 1.62                     | 0.61              |
| 1:K:512:ALA:O      | 1:K:516:ILE:HG12 | 2.01                     | 0.61              |
| 1:L:99:ILE:HB      | 1:L:124:VAL:HG22 | 1.83                     | 0.61              |
| 1:K:584:ALA:O      | 1:K:594:ARG:NH1  | 2.33                     | 0.61              |
| 1:A:141:ALA:CB     | 1:A:146:GLU:HB3  | 2.29                     | 0.61              |
| 1:A:487:LEU:HD11   | 1:A:513:ASN:CG   | 2.25                     | 0.61              |
| 1:B:12:TRP:HH2     | 1:B:144:LEU:HD23 | 1.64                     | 0.61              |
| 1:B:417:ALA:CB     | 1:B:456:LEU:HD11 | 2.30                     | 0.61              |
| 1:G:135:PRO:HD2    | 1:G:139:ARG:NH2  | 2.12                     | 0.61              |
| 1:G:181:GLU:O      | 1:G:191:VAL:HA   | 2.00                     | 0.61              |
| 1:K:234:HIS:O      | 1:K:237:TRP:HB3  | 2.01                     | 0.61              |
| 1:K:410:LEU:HD12   | 1:K:451:VAL:HG21 | 1.81                     | 0.61              |
| 1:B:448:PHE:O      | 1:B:451:VAL:HG22 | 2.00                     | 0.61              |
| 1:G:48:LEU:HD13    | 1:G:187:PRO:HG2  | 1.82                     | 0.61              |
| 1:G:314:GLY:HA3    | 1:G:552:ILE:HD11 | 1.81                     | 0.61              |
| 1:K:37:SER:HB3     | 1:K:40:ILE:HG12  | 1.81                     | 0.61              |
| 1:K:213:LEU:HB3    | 1:L:168:PRO:HG2  | 1.83                     | 0.61              |
| 1:L:475:VAL:HG13   | 1:L:504:ILE:CD1  | 2.31                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:418:GLU:OE2  | 1:H:408:ARG:NE   | 2.34                     | 0.61              |
| 1:A:454:VAL:HG23 | 1:A:456:LEU:CD1  | 2.31                     | 0.61              |
| 1:G:13:ALA:O     | 1:G:17:GLU:HG3   | 2.00                     | 0.61              |
| 1:G:79:PHE:CE2   | 1:G:108:ILE:HG23 | 2.36                     | 0.61              |
| 1:H:133:PHE:HE2  | 1:H:150:ALA:HB2  | 1.65                     | 0.61              |
| 1:K:31:HIS:CE1   | 1:K:90:ARG:HD2   | 2.35                     | 0.61              |
| 1:L:510:PRO:CB   | 1:L:563:LEU:HD23 | 2.31                     | 0.61              |
| 1:A:471:ILE:HG21 | 1:A:489:LEU:HD13 | 1.83                     | 0.61              |
| 1:G:65:GLN:HB3   | 1:G:192:ARG:CD   | 2.30                     | 0.61              |
| 1:K:17:GLU:OE2   | 2:M:727:A:N6     | 2.34                     | 0.61              |
| 1:K:172:LEU:H    | 1:K:172:LEU:HD23 | 1.66                     | 0.61              |
| 1:K:547:THR:HG21 | 1:K:550:LEU:CD2  | 2.30                     | 0.61              |
| 1:G:100:CYS:HA   | 1:G:125:PHE:O    | 2.01                     | 0.61              |
| 1:H:16:PRO:HD3   | 1:H:47:LEU:CD2   | 2.31                     | 0.61              |
| 1:H:266:PHE:HB3  | 1:H:331:GLN:NE2  | 2.15                     | 0.61              |
| 1:K:65:GLN:HG2   | 1:K:190:TRP:HE3  | 1.66                     | 0.61              |
| 1:K:67:PHE:CE1   | 1:K:75:ASP:HB3   | 2.36                     | 0.61              |
| 1:L:4:LEU:HD12   | 1:L:98:TYR:O     | 2.01                     | 0.61              |
| 1:L:305:ILE:HG23 | 1:L:309:ARG:HE   | 1.65                     | 0.61              |
| 1:A:534:ARG:NH1  | 1:A:570:GLY:O    | 2.34                     | 0.60              |
| 1:B:63:ARG:HD3   | 1:B:190:TRP:CH2  | 2.36                     | 0.60              |
| 1:K:494:ASP:O    | 1:K:498:VAL:HG23 | 2.00                     | 0.60              |
| 1:B:73:GLU:CG    | 1:B:77:MET:HE1   | 2.31                     | 0.60              |
| 1:H:29:GLU:HB2   | 1:H:58:ARG:HB2   | 1.83                     | 0.60              |
| 1:H:522:ASP:OD2  | 1:H:566:ARG:NH2  | 2.34                     | 0.60              |
| 1:H:531:TYR:CD1  | 1:H:532:PRO:HD2  | 2.36                     | 0.60              |
| 1:K:213:LEU:HB2  | 1:L:168:PRO:HG2  | 1.82                     | 0.60              |
| 1:B:1:MET:HG3    | 1:B:3:ILE:CD1    | 2.31                     | 0.60              |
| 1:B:178:PHE:HE2  | 1:B:198:LEU:HA   | 1.66                     | 0.60              |
| 1:G:216:TRP:CZ2  | 1:H:228:ALA:HB3  | 2.36                     | 0.60              |
| 1:H:22:LEU:HD12  | 1:H:26:GLY:O     | 2.00                     | 0.60              |
| 1:H:533:LEU:HD13 | 1:H:543:VAL:HG11 | 1.82                     | 0.60              |
| 1:L:62:SER:HA    | 1:L:189:HIS:O    | 2.01                     | 0.60              |
| 1:A:348:GLU:HA   | 1:A:390:ASN:O    | 2.02                     | 0.60              |
| 1:A:397:ARG:HG2  | 1:A:433:GLY:HA3  | 1.84                     | 0.60              |
| 1:B:8:VAL:HG23   | 1:B:32:VAL:HG13  | 1.82                     | 0.60              |
| 1:B:87:LEU:O     | 1:B:91:ALA:N     | 2.34                     | 0.60              |
| 1:G:8:VAL:O      | 1:G:34:THR:OG1   | 2.07                     | 0.60              |
| 1:G:28:ASP:OD1   | 1:G:29:GLU:N     | 2.34                     | 0.60              |
| 1:H:80:GLU:O     | 1:H:84:TRP:N     | 2.29                     | 0.60              |
| 1:K:89:GLN:OE1   | 1:K:180:LEU:HB3  | 2.01                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:167:TRP:HB2  | 1:L:170:LEU:CD1  | 2.32                     | 0.60              |
| 2:M:727:A:O2'    | 2:M:728:A23:OP1  | 2.18                     | 0.60              |
| 1:A:397:ARG:HD3  | 1:A:444:PHE:CE2  | 2.36                     | 0.60              |
| 1:A:495:LEU:HA   | 1:A:498:VAL:HG22 | 1.84                     | 0.60              |
| 1:B:533:LEU:HB3  | 1:B:568:CYS:SG   | 2.42                     | 0.60              |
| 1:G:31:HIS:CE1   | 1:G:90:ARG:HD2   | 2.37                     | 0.60              |
| 1:G:172:LEU:HD23 | 1:G:172:LEU:H    | 1.65                     | 0.60              |
| 1:H:247:ASP:O    | 1:H:251:VAL:HG23 | 2.02                     | 0.60              |
| 1:K:305:ILE:HG22 | 1:K:305:ILE:O    | 2.01                     | 0.60              |
| 1:B:524:GLU:OE1  | 1:B:524:GLU:N    | 2.27                     | 0.60              |
| 1:K:208:ARG:HE   | 1:K:229:ALA:HB1  | 1.66                     | 0.60              |
| 1:A:65:GLN:HG2   | 1:A:190:TRP:HB3  | 1.84                     | 0.60              |
| 1:G:17:GLU:HB3   | 1:G:156:LEU:HD13 | 1.83                     | 0.60              |
| 1:G:87:LEU:HD12  | 1:G:88:LEU:N     | 2.17                     | 0.60              |
| 1:H:183:THR:O    | 1:H:190:TRP:HB2  | 2.02                     | 0.60              |
| 1:A:9:GLY:O      | 1:A:40:ILE:HD12  | 2.01                     | 0.60              |
| 1:H:79:PHE:CE2   | 1:H:108:ILE:HG12 | 2.37                     | 0.60              |
| 1:H:87:LEU:CD2   | 1:H:115:ALA:HB1  | 2.31                     | 0.60              |
| 1:H:393:LEU:HD12 | 1:H:413:ALA:CB   | 2.30                     | 0.60              |
| 1:B:65:GLN:NE2   | 1:B:192:ARG:HA   | 2.16                     | 0.60              |
| 1:B:128:LEU:HB3  | 1:B:157:ARG:CZ   | 2.32                     | 0.60              |
| 1:B:181:GLU:O    | 1:B:192:ARG:N    | 2.35                     | 0.60              |
| 1:H:348:GLU:HA   | 1:H:390:ASN:O    | 2.02                     | 0.60              |
| 1:K:44:VAL:HG13  | 1:K:188:VAL:HG11 | 1.81                     | 0.60              |
| 1:K:97:ARG:HD2   | 1:K:120:GLY:O    | 2.02                     | 0.60              |
| 1:K:178:PHE:CE2  | 1:K:198:LEU:HA   | 2.36                     | 0.60              |
| 1:L:133:PHE:CE2  | 1:L:150:ALA:HB2  | 2.37                     | 0.60              |
| 1:L:145:GLU:OE2  | 1:L:146:GLU:HG3  | 2.02                     | 0.60              |
| 1:L:430:ASP:HB3  | 1:L:459:THR:HG23 | 1.84                     | 0.60              |
| 1:B:133:PHE:HE2  | 1:B:149:GLN:HG3  | 1.66                     | 0.60              |
| 1:G:57:PRO:HG2   | 1:G:59:PHE:CE1   | 2.37                     | 0.60              |
| 1:K:423:GLY:O    | 1:K:425:ARG:HG3  | 2.02                     | 0.60              |
| 1:B:441:ALA:HB3  | 1:B:473:GLN:HG3  | 1.83                     | 0.59              |
| 1:B:445:ALA:O    | 1:B:446:THR:OG1  | 2.17                     | 0.59              |
| 1:G:57:PRO:HG2   | 1:G:59:PHE:CZ    | 2.36                     | 0.59              |
| 1:K:150:ALA:HA   | 1:K:155:ALA:HB3  | 1.84                     | 0.59              |
| 1:L:213:LEU:HA   | 1:L:216:TRP:HB3  | 1.84                     | 0.59              |
| 1:L:432:ALA:HA   | 1:L:461:HIS:HB2  | 1.84                     | 0.59              |
| 1:A:99:ILE:HG22  | 1:A:112:MET:HE3  | 1.84                     | 0.59              |
| 1:B:251:VAL:HG21 | 1:B:562:LEU:HD21 | 1.84                     | 0.59              |
| 1:G:17:GLU:CB    | 1:G:127:VAL:HG21 | 2.23                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:79:PHE:CD2   | 1:G:108:ILE:HG12 | 2.37                     | 0.59              |
| 1:G:393:LEU:HD12 | 1:G:413:ALA:CB   | 2.32                     | 0.59              |
| 1:G:534:ARG:NH1  | 1:G:570:GLY:O    | 2.36                     | 0.59              |
| 1:L:276:VAL:HG23 | 1:L:330:ALA:HB3  | 1.84                     | 0.59              |
| 1:L:420:TRP:O    | 1:L:425:ARG:HG2  | 2.01                     | 0.59              |
| 1:A:234:HIS:CD2  | 1:A:607:PRO:HD2  | 2.37                     | 0.59              |
| 1:B:12:TRP:NE1   | 1:B:142:SER:O    | 2.34                     | 0.59              |
| 1:B:329:ARG:HH11 | 1:B:329:ARG:HG2  | 1.67                     | 0.59              |
| 1:H:65:GLN:HG2   | 1:H:190:TRP:HE3  | 1.66                     | 0.59              |
| 1:H:101:LEU:HB3  | 1:H:112:MET:SD   | 2.42                     | 0.59              |
| 1:H:487:LEU:HD11 | 1:H:513:ASN:OD1  | 2.01                     | 0.59              |
| 1:K:82:VAL:HG22  | 1:K:193:ALA:HB2  | 1.84                     | 0.59              |
| 1:L:487:LEU:HD11 | 1:L:513:ASN:HB3  | 1.84                     | 0.59              |
| 1:A:292:ILE:CD1  | 1:A:315:ASP:HB2  | 2.32                     | 0.59              |
| 1:G:87:LEU:O     | 1:G:91:ALA:N     | 2.32                     | 0.59              |
| 1:G:217:GLU:HG2  | 1:G:218:GLY:N    | 2.17                     | 0.59              |
| 1:L:28:ASP:O     | 1:L:57:PRO:HB3   | 2.01                     | 0.59              |
| 1:L:322:LEU:HD21 | 1:L:331:GLN:CG   | 2.32                     | 0.59              |
| 1:A:16:PRO:HB3   | 1:A:50:TYR:CZ    | 2.37                     | 0.59              |
| 1:A:42:PRO:O     | 1:A:46:GLN:HG2   | 2.02                     | 0.59              |
| 1:B:87:LEU:HD21  | 1:B:97:ARG:CD    | 2.31                     | 0.59              |
| 1:G:348:GLU:HA   | 1:G:390:ASN:O    | 2.02                     | 0.59              |
| 1:G:578:LYS:O    | 1:G:581:VAL:HG12 | 2.02                     | 0.59              |
| 1:A:305:ILE:O    | 1:A:309:ARG:HB2  | 2.03                     | 0.59              |
| 1:B:8:VAL:CG2    | 1:B:32:VAL:HG13  | 2.32                     | 0.59              |
| 1:G:13:ALA:C     | 1:G:16:PRO:HD2   | 2.27                     | 0.59              |
| 1:L:243:ASP:O    | 1:L:247:ASP:HB2  | 2.02                     | 0.59              |
| 1:H:63:ARG:HH22  | 1:H:188:VAL:CG2  | 2.15                     | 0.59              |
| 1:K:209:SER:HB3  | 1:L:213:LEU:HD11 | 1.85                     | 0.59              |
| 1:K:259:LEU:HB3  | 1:K:482:ARG:NH1  | 2.18                     | 0.59              |
| 1:L:531:TYR:CD1  | 1:L:532:PRO:HD2  | 2.37                     | 0.59              |
| 1:B:34:THR:N     | 1:B:62:SER:O     | 2.34                     | 0.59              |
| 1:K:101:LEU:HD12 | 1:K:101:LEU:O    | 2.03                     | 0.59              |
| 1:K:514:LEU:HD13 | 1:K:521:LEU:HD11 | 1.83                     | 0.59              |
| 1:L:260:HIS:NE2  | 1:L:548:ASP:OD1  | 2.36                     | 0.59              |
| 1:L:374:PHE:O    | 1:L:378:MET:HG3  | 2.03                     | 0.59              |
| 1:A:48:LEU:HD22  | 1:A:187:PRO:HG2  | 1.85                     | 0.59              |
| 1:A:468:VAL:HG11 | 1:A:492:SER:HB2  | 1.85                     | 0.59              |
| 1:B:393:LEU:HD12 | 1:B:413:ALA:CB   | 2.32                     | 0.59              |
| 1:G:16:PRO:HB2   | 1:G:147:VAL:HG11 | 1.85                     | 0.59              |
| 1:H:110:ALA:O    | 1:H:113:GLN:HG3  | 2.03                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:5:LEU:O      | 1:K:99:ILE:HA    | 2.03                     | 0.59              |
| 1:K:5:LEU:HD23   | 1:K:31:HIS:HB2   | 1.84                     | 0.59              |
| 1:K:329:ARG:O    | 1:K:333:ARG:HG3  | 2.03                     | 0.59              |
| 1:K:460:VAL:HG21 | 1:K:474:ALA:HB1  | 1.85                     | 0.59              |
| 1:L:7:SER:O      | 1:L:103:GLY:HA3  | 2.02                     | 0.59              |
| 1:L:12:TRP:CE2   | 1:L:46:GLN:HG2   | 2.38                     | 0.59              |
| 1:L:346:TYR:HE2  | 1:L:587:ALA:HB1  | 1.68                     | 0.59              |
| 1:L:403:ARG:HA   | 1:L:406:ILE:HD13 | 1.85                     | 0.59              |
| 1:B:37:SER:HB2   | 1:B:68:GLU:O     | 2.03                     | 0.58              |
| 1:B:102:ALA:HA   | 1:B:126:HIS:CE1  | 2.38                     | 0.58              |
| 1:G:169:GLN:HB2  | 1:G:205:VAL:HG11 | 1.85                     | 0.58              |
| 1:H:83:LEU:HD21  | 1:H:112:MET:HA   | 1.85                     | 0.58              |
| 1:H:197:ARG:HA   | 1:H:200:GLN:OE1  | 2.03                     | 0.58              |
| 1:H:397:ARG:CZ   | 1:H:433:GLY:HA3  | 2.32                     | 0.58              |
| 1:H:430:ASP:OD1  | 1:H:431:LEU:N    | 2.36                     | 0.58              |
| 1:L:218:GLY:O    | 1:L:221:GLU:HG3  | 2.03                     | 0.58              |
| 1:L:234:HIS:CE1  | 1:L:610:THR:HG1  | 2.20                     | 0.58              |
| 1:A:53:MET:SD    | 1:A:54:HIS:N     | 2.76                     | 0.58              |
| 1:A:86:TRP:O     | 1:A:90:ARG:HG2   | 2.04                     | 0.58              |
| 1:G:434:PHE:HD2  | 1:G:478:LEU:HD11 | 1.69                     | 0.58              |
| 1:L:537:LEU:HD21 | 1:L:543:VAL:HG22 | 1.84                     | 0.58              |
| 1:A:169:GLN:HE22 | 1:A:208:ARG:HH12 | 1.51                     | 0.58              |
| 1:A:242:LEU:HD12 | 1:A:247:ASP:OD2  | 2.03                     | 0.58              |
| 1:A:454:VAL:HG23 | 1:A:456:LEU:HD13 | 1.85                     | 0.58              |
| 1:G:7:SER:HA     | 1:G:33:LEU:O     | 2.03                     | 0.58              |
| 1:G:403:ARG:HG2  | 1:G:403:ARG:O    | 2.01                     | 0.58              |
| 1:H:5:LEU:CD1    | 1:H:87:LEU:HD12  | 2.33                     | 0.58              |
| 1:H:200:GLN:HG2  | 1:H:201:HIS:N    | 2.19                     | 0.58              |
| 1:G:223:PRO:HD3  | 1:G:574:LEU:HD11 | 1.83                     | 0.58              |
| 1:K:2:ARG:HA     | 1:K:96:HIS:HB2   | 1.84                     | 0.58              |
| 1:L:5:LEU:HD13   | 1:L:86:TRP:CZ3   | 2.37                     | 0.58              |
| 1:L:512:ALA:O    | 1:L:516:ILE:HG22 | 2.02                     | 0.58              |
| 1:B:12:TRP:CH2   | 1:B:144:LEU:HD23 | 2.38                     | 0.58              |
| 1:B:54:HIS:NE2   | 1:B:148:GLU:OE2  | 2.28                     | 0.58              |
| 1:B:91:ALA:O     | 1:B:97:ARG:NH2   | 2.36                     | 0.58              |
| 1:A:99:ILE:CG2   | 1:A:112:MET:HE3  | 2.33                     | 0.58              |
| 1:G:311:MET:HE1  | 3:G:701:ATP:C8   | 2.38                     | 0.58              |
| 1:H:5:LEU:HD13   | 1:H:87:LEU:HD12  | 1.86                     | 0.58              |
| 1:K:84:TRP:HB3   | 1:K:198:LEU:HD21 | 1.85                     | 0.58              |
| 1:B:91:ALA:HB1   | 1:B:97:ARG:HE    | 1.69                     | 0.58              |
| 1:B:295:PRO:HG2  | 1:B:298:TRP:CE3  | 2.38                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:13:ALA:O     | 1:G:16:PRO:HD2   | 2.04                     | 0.58              |
| 1:G:21:LEU:HD22  | 1:G:125:PHE:CD2  | 2.38                     | 0.58              |
| 1:K:87:LEU:O     | 1:K:91:ALA:HB3   | 2.03                     | 0.58              |
| 1:L:531:TYR:CB   | 1:L:567:LEU:HB3  | 2.33                     | 0.58              |
| 1:A:216:TRP:CH2  | 1:B:228:ALA:HB3  | 2.39                     | 0.58              |
| 1:H:434:PHE:CE2  | 1:H:444:PHE:HB2  | 2.31                     | 0.58              |
| 1:G:114:ARG:HB3  | 1:G:118:LEU:HD13 | 1.86                     | 0.58              |
| 1:K:403:ARG:O    | 1:K:403:ARG:HG2  | 2.04                     | 0.58              |
| 1:L:234:HIS:NE2  | 1:L:610:THR:OG1  | 2.37                     | 0.58              |
| 1:A:1:MET:C      | 1:A:2:ARG:HD2    | 2.29                     | 0.58              |
| 1:B:5:LEU:CD2    | 1:B:31:HIS:HB2   | 2.34                     | 0.58              |
| 1:G:19:MET:HE2   | 1:G:57:PRO:HG3   | 1.85                     | 0.58              |
| 1:G:168:PRO:HG2  | 1:G:169:GLN:OE1  | 2.03                     | 0.58              |
| 1:H:262:HIS:CE1  | 1:H:350:ARG:HD2  | 2.38                     | 0.58              |
| 1:K:276:VAL:HG22 | 1:K:334:LEU:HD12 | 1.85                     | 0.58              |
| 1:L:222:LEU:HD12 | 1:L:227:LEU:CB   | 2.34                     | 0.58              |
| 1:A:13:ALA:C     | 1:A:16:PRO:HD2   | 2.29                     | 0.57              |
| 1:A:429:VAL:HG22 | 1:A:458:VAL:HG12 | 1.86                     | 0.57              |
| 1:B:89:GLN:NE2   | 1:B:175:ALA:HB1  | 2.18                     | 0.57              |
| 1:B:311:MET:HE1  | 3:B:701:ATP:C8   | 2.39                     | 0.57              |
| 1:H:349:ILE:O    | 1:H:391:LEU:HA   | 2.03                     | 0.57              |
| 1:A:100:CYS:HB2  | 1:A:125:PHE:CE2  | 2.39                     | 0.57              |
| 1:A:434:PHE:HE1  | 1:A:442:ALA:HB1  | 1.68                     | 0.57              |
| 1:B:100:CYS:HA   | 1:B:125:PHE:O    | 2.03                     | 0.57              |
| 1:H:32:VAL:CB    | 1:H:61:ILE:HG12  | 2.35                     | 0.57              |
| 1:K:251:VAL:HG12 | 1:K:558:THR:OG1  | 2.04                     | 0.57              |
| 1:L:4:LEU:HD22   | 1:L:27:PHE:HE2   | 1.66                     | 0.57              |
| 1:L:21:LEU:HD13  | 1:L:125:PHE:CD2  | 2.39                     | 0.57              |
| 1:L:510:PRO:HD2  | 1:L:560:ASN:OD1  | 2.04                     | 0.57              |
| 1:A:99:ILE:HG22  | 1:A:112:MET:CE   | 2.35                     | 0.57              |
| 1:A:301:PRO:CD   | 1:A:515:GLN:HG2  | 2.35                     | 0.57              |
| 1:B:67:PHE:HD1   | 1:B:75:ASP:HB3   | 1.68                     | 0.57              |
| 1:H:33:LEU:HB2   | 1:H:86:TRP:CZ3   | 2.39                     | 0.57              |
| 1:B:108:ILE:O    | 1:B:112:MET:HG2  | 2.03                     | 0.57              |
| 1:G:50:TYR:HB2   | 1:G:144:LEU:CD2  | 2.34                     | 0.57              |
| 1:G:417:ALA:CB   | 1:G:456:LEU:HD21 | 2.32                     | 0.57              |
| 1:G:531:TYR:HB2  | 1:G:567:LEU:HG   | 1.86                     | 0.57              |
| 1:H:34:THR:HG22  | 1:H:40:ILE:HD12  | 1.86                     | 0.57              |
| 1:H:178:PHE:HD2  | 1:H:198:LEU:CD1  | 2.16                     | 0.57              |
| 1:K:3:ILE:HA     | 1:K:29:GLU:O     | 2.05                     | 0.57              |
| 1:L:139:ARG:HG2  | 1:L:140:GLU:H    | 1.69                     | 0.57              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:L:463:GLY:HA2    | 1:L:485:HIS:O    | 2.05                     | 0.57              |
| 1:A:21:LEU:HG      | 1:A:22:LEU:HD12  | 1.86                     | 0.57              |
| 1:H:472[A]:TRP:CE2 | 1:H:495:LEU:HD13 | 2.39                     | 0.57              |
| 1:K:12:TRP:HB3     | 1:K:43:GLY:CA    | 2.34                     | 0.57              |
| 1:B:63:ARG:HB2     | 1:B:190:TRP:CZ3  | 2.40                     | 0.57              |
| 1:B:89:GLN:CD      | 1:B:175:ALA:HB1  | 2.29                     | 0.57              |
| 1:B:99:ILE:HD12    | 1:B:116:ALA:HB2  | 1.85                     | 0.57              |
| 1:G:88:LEU:CD1     | 1:G:175:ALA:HA   | 2.32                     | 0.57              |
| 1:H:200:GLN:O      | 1:H:203:GLU:HG2  | 2.04                     | 0.57              |
| 1:H:521:LEU:HD23   | 1:H:567:LEU:HD23 | 1.86                     | 0.57              |
| 1:L:346:TYR:CE2    | 1:L:587:ALA:HB1  | 2.39                     | 0.57              |
| 1:A:207:GLU:OE2    | 1:A:211:HIS:NE2  | 2.38                     | 0.57              |
| 1:A:547:THR:HA     | 1:A:560:ASN:ND2  | 2.19                     | 0.57              |
| 1:G:36:ALA:HB3     | 1:G:68:GLU:HG3   | 1.87                     | 0.57              |
| 1:H:141:ALA:HA     | 1:H:146:GLU:OE1  | 2.05                     | 0.57              |
| 1:H:524:GLU:HG2    | 1:H:525:GLN:N    | 2.19                     | 0.57              |
| 1:K:63:ARG:O       | 1:K:191:VAL:HG22 | 2.05                     | 0.57              |
| 1:K:128:LEU:HB2    | 1:K:157:ARG:HB2  | 1.85                     | 0.57              |
| 1:A:172:LEU:HD23   | 1:A:172:LEU:H    | 1.68                     | 0.57              |
| 1:B:133:PHE:N      | 1:B:139:ARG:O    | 2.35                     | 0.57              |
| 1:B:142:SER:N      | 1:B:146:GLU:OE1  | 2.36                     | 0.57              |
| 1:H:124:VAL:O      | 1:H:161:LEU:HB2  | 2.05                     | 0.57              |
| 1:K:496:LEU:HD21   | 1:K:539:ALA:CB   | 2.35                     | 0.57              |
| 1:L:262:HIS:HB2    | 1:L:549:ASN:OD1  | 2.05                     | 0.57              |
| 1:A:25:GLN:NE2     | 1:A:26:GLY:O     | 2.38                     | 0.57              |
| 1:A:50:TYR:HB2     | 1:A:144:LEU:HD11 | 1.87                     | 0.57              |
| 1:A:290:ARG:NH2    | 1:A:315:ASP:HB3  | 2.20                     | 0.57              |
| 1:B:221:GLU:O      | 1:B:221:GLU:HG2  | 2.05                     | 0.57              |
| 1:B:440:ARG:NE     | 1:B:442:ALA:HB3  | 2.18                     | 0.57              |
| 1:B:464:GLU:O      | 1:B:465:ASN:CB   | 2.52                     | 0.57              |
| 1:G:53:MET:CE      | 1:G:144:LEU:HD22 | 2.34                     | 0.57              |
| 1:H:33:LEU:HB2     | 1:H:86:TRP:CH2   | 2.40                     | 0.57              |
| 1:L:197:ARG:HA     | 1:L:200:GLN:CD   | 2.30                     | 0.57              |
| 1:A:64:VAL:CG2     | 1:A:67:PHE:HB3   | 2.35                     | 0.57              |
| 1:A:86:TRP:CD1     | 1:A:90:ARG:HG3   | 2.40                     | 0.57              |
| 1:A:353:PRO:HG2    | 1:A:412:LEU:HD23 | 1.86                     | 0.57              |
| 1:G:113:GLN:OE1    | 1:H:110:ALA:HB1  | 2.03                     | 0.57              |
| 1:K:211:HIS:ND1    | 1:K:232:PRO:HD3  | 2.20                     | 0.57              |
| 1:L:224:ILE:HD13   | 1:L:577:LEU:HD12 | 1.86                     | 0.57              |
| 1:L:307:LEU:HD22   | 1:L:464:GLU:OE2  | 2.04                     | 0.57              |
| 1:L:369:GLU:O      | 1:L:373:HIS:ND1  | 2.37                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:529:GLU:O    | 1:G:529:GLU:HG3  | 2.05                     | 0.56              |
| 1:B:133:PHE:CZ   | 1:B:150:ALA:HB2  | 2.39                     | 0.56              |
| 1:B:248:LYS:HD2  | 1:B:562:LEU:HD13 | 1.86                     | 0.56              |
| 1:B:258:GLU:O    | 1:B:259:LEU:HD23 | 2.05                     | 0.56              |
| 1:G:86:TRP:HE1   | 1:G:90:ARG:HE    | 1.52                     | 0.56              |
| 1:H:292:ILE:HG21 | 1:H:315:ASP:OD1  | 2.05                     | 0.56              |
| 1:K:178:PHE:HE2  | 1:K:198:LEU:HA   | 1.69                     | 0.56              |
| 1:L:251:VAL:HG21 | 1:L:562:LEU:HD21 | 1.87                     | 0.56              |
| 1:A:22:LEU:HD13  | 1:A:27:PHE:CZ    | 2.40                     | 0.56              |
| 1:A:398:GLU:HB2  | 1:A:401:GLY:HA3  | 1.85                     | 0.56              |
| 1:B:64:VAL:CG1   | 1:B:67:PHE:HB3   | 2.35                     | 0.56              |
| 1:B:81:GLU:OE1   | 1:B:196:MET:HA   | 2.06                     | 0.56              |
| 1:G:342:ASP:OD1  | 1:G:558:THR:OG1  | 2.22                     | 0.56              |
| 1:H:307:LEU:HD23 | 1:H:307:LEU:O    | 2.05                     | 0.56              |
| 1:K:19:MET:CE    | 1:K:57:PRO:HG3   | 2.32                     | 0.56              |
| 1:L:256:LYS:NZ   | 1:L:342:ASP:O    | 2.38                     | 0.56              |
| 1:A:84:TRP:HE1   | 1:A:115:ALA:HB2  | 1.71                     | 0.56              |
| 1:A:403:ARG:HB2  | 1:H:453:ARG:CZ   | 2.36                     | 0.56              |
| 1:B:459:THR:O    | 1:B:459:THR:HG23 | 2.06                     | 0.56              |
| 1:G:8:VAL:HG23   | 1:G:32:VAL:CG1   | 2.35                     | 0.56              |
| 1:K:37:SER:HB2   | 1:K:68:GLU:O     | 2.05                     | 0.56              |
| 1:K:299:PRO:O    | 1:K:301:PRO:HD3  | 2.06                     | 0.56              |
| 1:L:127:VAL:CG2  | 1:L:156:LEU:HD21 | 2.35                     | 0.56              |
| 1:L:298:TRP:CG   | 1:L:299:PRO:HA   | 2.40                     | 0.56              |
| 1:B:16:PRO:HA    | 1:B:19:MET:HE3   | 1.86                     | 0.56              |
| 1:B:181:GLU:HG2  | 1:B:181:GLU:O    | 2.05                     | 0.56              |
| 1:H:574:LEU:HD23 | 1:H:578:LYS:HG3  | 1.87                     | 0.56              |
| 1:L:8:VAL:HG23   | 1:L:32:VAL:HG13  | 1.87                     | 0.56              |
| 1:L:8:VAL:HG23   | 1:L:32:VAL:CG1   | 2.35                     | 0.56              |
| 1:A:302:GLU:OE1  | 1:A:303:GLU:HG2  | 2.06                     | 0.56              |
| 1:B:84:TRP:HB3   | 1:B:198:LEU:CD2  | 2.35                     | 0.56              |
| 1:B:128:LEU:HD23 | 2:D:709:A:O2'    | 2.06                     | 0.56              |
| 1:G:106:LYS:HE2  | 1:H:101:LEU:HD13 | 1.87                     | 0.56              |
| 1:H:200:GLN:HA   | 1:H:203:GLU:CG   | 2.36                     | 0.56              |
| 1:H:311:MET:HE1  | 3:H:703:ATP:C4   | 2.40                     | 0.56              |
| 1:K:116:ALA:O    | 1:K:120:GLY:N    | 2.39                     | 0.56              |
| 1:K:346:TYR:OH   | 1:K:589:ALA:HB2  | 2.06                     | 0.56              |
| 1:L:116:ALA:HB1  | 1:L:121:ALA:HB2  | 1.86                     | 0.56              |
| 1:L:256:LYS:CE   | 1:L:558:THR:HG22 | 2.34                     | 0.56              |
| 1:H:174:SER:CB   | 1:H:176:PRO:HD2  | 2.35                     | 0.56              |
| 1:H:342:ASP:OD1  | 1:H:558:THR:OG1  | 2.24                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:35:THR:HG21  | 2:N:730:A23:N1   | 2.21                     | 0.56              |
| 1:L:44:VAL:HA    | 1:L:47:LEU:HD12  | 1.88                     | 0.56              |
| 1:L:266:PHE:HE2  | 1:L:334:LEU:HB3  | 1.70                     | 0.56              |
| 1:A:350:ARG:NH1  | 1:A:430:ASP:OD1  | 2.39                     | 0.56              |
| 1:B:93:GLN:HB2   | 1:B:96:HIS:NE2   | 2.20                     | 0.56              |
| 1:B:183:THR:OG1  | 1:B:190:TRP:HB2  | 2.06                     | 0.56              |
| 1:G:243:ASP:O    | 1:G:247:ASP:HB2  | 2.05                     | 0.56              |
| 1:H:536:TYR:HB3  | 1:H:543:VAL:HG21 | 1.86                     | 0.56              |
| 1:A:83:LEU:HD21  | 1:A:112:MET:HA   | 1.86                     | 0.56              |
| 1:A:86:TRP:NE1   | 1:A:90:ARG:HG3   | 2.21                     | 0.56              |
| 1:A:147:VAL:O    | 1:A:151:ILE:HG13 | 2.05                     | 0.56              |
| 1:A:511:TYR:CD2  | 1:A:555:ALA:HB3  | 2.41                     | 0.56              |
| 1:B:251:VAL:HG12 | 1:B:558:THR:HG23 | 1.88                     | 0.56              |
| 1:H:78:LEU:O     | 1:H:82:VAL:HG23  | 2.06                     | 0.56              |
| 1:H:449:GLU:N    | 1:H:450:PRO:HD2  | 2.20                     | 0.56              |
| 1:L:4:LEU:HA     | 1:L:98:TYR:O     | 2.06                     | 0.56              |
| 1:G:46:GLN:HA    | 1:G:49:ARG:NE    | 2.21                     | 0.56              |
| 1:G:123:GLU:HA   | 1:G:162:GLY:O    | 2.06                     | 0.56              |
| 1:K:1:MET:O      | 1:K:96:HIS:HB3   | 2.06                     | 0.56              |
| 1:B:83:LEU:HD13  | 1:B:112:MET:CE   | 2.36                     | 0.55              |
| 1:G:79:PHE:CE2   | 1:G:108:ILE:HG12 | 2.41                     | 0.55              |
| 1:K:430:ASP:O    | 1:K:431:LEU:HD22 | 2.06                     | 0.55              |
| 1:G:421:LYS:NZ   | 1:L:359:ALA:O    | 2.25                     | 0.55              |
| 1:H:12:TRP:HZ2   | 1:H:143:THR:HA   | 1.71                     | 0.55              |
| 1:K:85:ARG:HE    | 1:K:198:LEU:HB2  | 1.71                     | 0.55              |
| 1:A:219:ILE:O    | 1:A:219:ILE:HG13 | 2.07                     | 0.55              |
| 1:A:292:ILE:HD13 | 1:A:315:ASP:HB2  | 1.88                     | 0.55              |
| 1:B:65:GLN:HE21  | 1:B:192:ARG:HG3  | 1.71                     | 0.55              |
| 1:B:124:VAL:HG22 | 1:B:161:LEU:HD22 | 1.87                     | 0.55              |
| 1:G:29:GLU:OE1   | 1:G:58:ARG:HD3   | 2.06                     | 0.55              |
| 1:G:36:ALA:N     | 1:G:67:PHE:O     | 2.33                     | 0.55              |
| 1:G:116:ALA:HB1  | 1:G:121:ALA:HB2  | 1.88                     | 0.55              |
| 1:H:6:CYS:HB2    | 1:H:32:VAL:HA    | 1.88                     | 0.55              |
| 1:H:131:PRO:HB3  | 1:H:140:GLU:OE2  | 2.06                     | 0.55              |
| 1:K:431:LEU:O    | 1:K:461:HIS:HB3  | 2.06                     | 0.55              |
| 1:K:459:THR:HG23 | 1:K:459:THR:O    | 2.06                     | 0.55              |
| 1:K:486:ALA:HB1  | 1:K:489:LEU:HD11 | 1.89                     | 0.55              |
| 1:L:19:MET:HA    | 1:L:27:PHE:CE2   | 2.42                     | 0.55              |
| 1:A:101:LEU:HA   | 1:A:112:MET:SD   | 2.46                     | 0.55              |
| 1:B:182:SER:OG   | 1:B:191:VAL:HG12 | 2.06                     | 0.55              |
| 1:B:397:ARG:HH12 | 1:B:403:ARG:NE   | 2.05                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:145:GLU:O    | 1:G:149:GLN:HG3  | 2.06                     | 0.55              |
| 1:H:240:GLU:HG3  | 1:H:573:ARG:HH12 | 1.71                     | 0.55              |
| 1:K:131:PRO:O    | 1:K:139:ARG:N    | 2.40                     | 0.55              |
| 1:A:106:LYS:HD3  | 1:B:106:LYS:HG2  | 1.89                     | 0.55              |
| 1:B:145:GLU:OE2  | 1:B:146:GLU:HG3  | 2.06                     | 0.55              |
| 1:G:74:GLN:HA    | 1:G:77:MET:CE    | 2.34                     | 0.55              |
| 1:A:178:PHE:HA   | 1:A:197:ARG:HH22 | 1.71                     | 0.55              |
| 1:H:67:PHE:CE1   | 1:H:75:ASP:HB3   | 2.40                     | 0.55              |
| 2:I:717:A:HI'    | 2:I:718:A23:P    | 2.47                     | 0.55              |
| 1:K:12:TRP:HE3   | 1:K:47:LEU:HG    | 1.72                     | 0.55              |
| 1:K:39:LYS:O     | 1:K:42:PRO:HD2   | 2.07                     | 0.55              |
| 1:K:337:GLU:O    | 1:K:337:GLU:HG2  | 2.07                     | 0.55              |
| 1:L:430:ASP:CB   | 1:L:459:THR:HG23 | 2.36                     | 0.55              |
| 1:B:350:ARG:HA   | 1:B:392:LEU:O    | 2.06                     | 0.55              |
| 1:H:83:LEU:O     | 1:H:87:LEU:HB2   | 2.07                     | 0.55              |
| 1:H:397:ARG:HB3  | 1:H:434:PHE:HE1  | 1.72                     | 0.55              |
| 1:K:259:LEU:HD13 | 1:K:482:ARG:HH11 | 1.70                     | 0.55              |
| 1:L:20:GLN:HB3   | 1:L:158:PHE:HZ   | 1.71                     | 0.55              |
| 1:L:133:PHE:HE2  | 1:L:150:ALA:HB2  | 1.71                     | 0.55              |
| 1:L:254:LEU:O    | 1:L:256:LYS:HG3  | 2.06                     | 0.55              |
| 1:L:259:LEU:HB3  | 1:L:482:ARG:HH12 | 1.70                     | 0.55              |
| 1:L:445:ALA:CB   | 1:L:478:LEU:HD21 | 2.36                     | 0.55              |
| 1:A:5:LEU:HA     | 1:A:31:HIS:O     | 2.06                     | 0.55              |
| 1:A:109:SER:O    | 1:A:112:MET:HG2  | 2.07                     | 0.55              |
| 1:A:526:GLU:HG3  | 1:A:530:THR:OG1  | 2.07                     | 0.55              |
| 1:B:37:SER:OG    | 1:B:39:LYS:HE2   | 2.07                     | 0.55              |
| 1:B:397:ARG:HH11 | 1:B:406:ILE:HD13 | 1.72                     | 0.55              |
| 1:G:196:MET:SD   | 1:G:196:MET:O    | 2.64                     | 0.55              |
| 1:H:431:LEU:HD12 | 1:H:434:PHE:HB2  | 1.89                     | 0.55              |
| 1:K:12:TRP:HH2   | 1:K:144:LEU:HD13 | 1.71                     | 0.55              |
| 1:K:457:ALA:HB2  | 1:K:481:ARG:NH1  | 2.21                     | 0.55              |
| 1:L:128:LEU:HB2  | 1:L:157:ARG:CG   | 2.37                     | 0.55              |
| 1:L:283:PRO:CA   | 1:L:286:LEU:HD23 | 2.26                     | 0.55              |
| 1:A:393:LEU:HD12 | 1:A:413:ALA:CB   | 2.33                     | 0.55              |
| 1:B:397:ARG:HG3  | 1:B:433:GLY:CA   | 2.35                     | 0.55              |
| 1:G:85:ARG:O     | 1:G:88:LEU:HG    | 2.06                     | 0.55              |
| 1:H:237:TRP:CH2  | 1:H:573:ARG:HD3  | 2.41                     | 0.55              |
| 1:K:57:PRO:HG2   | 1:K:59:PHE:CZ    | 2.41                     | 0.55              |
| 1:K:118:LEU:CD1  | 1:K:206:LEU:HD21 | 2.36                     | 0.55              |
| 1:L:116:ALA:HB1  | 1:L:121:ALA:CB   | 2.37                     | 0.55              |
| 1:A:87:LEU:HD21  | 1:A:97:ARG:HD3   | 1.89                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:105:TYR:HA   | 2:C:708:A23:O4'  | 2.07                     | 0.55              |
| 1:G:258:GLU:OE1  | 1:G:557:LEU:HD22 | 2.07                     | 0.55              |
| 1:H:81:GLU:OE2   | 1:H:85:ARG:HD2   | 2.07                     | 0.55              |
| 1:H:485:HIS:ND1  | 1:H:513:ASN:OD1  | 2.37                     | 0.55              |
| 1:K:185:GLN:HB2  | 1:K:190:TRP:CD1  | 2.42                     | 0.55              |
| 1:L:121:ALA:HB3  | 1:L:164:GLU:HB2  | 1.89                     | 0.55              |
| 1:L:197:ARG:O    | 1:L:200:GLN:HG2  | 2.07                     | 0.55              |
| 1:A:6:CYS:O      | 1:A:32:VAL:HA    | 2.07                     | 0.54              |
| 1:A:36:ALA:CA    | 1:A:63:ARG:HD3   | 2.28                     | 0.54              |
| 1:B:264:GLY:HA3  | 3:B:701:ATP:O2A  | 2.07                     | 0.54              |
| 1:G:52:GLU:HG2   | 1:G:53:MET:N     | 2.21                     | 0.54              |
| 1:H:549:ASN:ND2  | 1:H:552:ILE:HD12 | 2.21                     | 0.54              |
| 1:K:86:TRP:NE1   | 1:K:90:ARG:HG3   | 2.22                     | 0.54              |
| 1:K:266:PHE:HB3  | 1:K:331:GLN:HE22 | 1.68                     | 0.54              |
| 1:K:496:LEU:HD23 | 1:K:496:LEU:O    | 2.07                     | 0.54              |
| 1:L:523:GLU:OE1  | 1:L:530:THR:HG22 | 2.06                     | 0.54              |
| 1:A:141:ALA:HA   | 1:A:146:GLU:OE1  | 2.08                     | 0.54              |
| 1:K:101:LEU:HD12 | 1:K:126:HIS:ND1  | 2.21                     | 0.54              |
| 1:L:37:SER:OG    | 1:L:39:LYS:HG2   | 2.08                     | 0.54              |
| 1:A:267:ALA:O    | 1:A:273:LEU:HB2  | 2.07                     | 0.54              |
| 1:B:526:GLU:HG3  | 1:B:526:GLU:O    | 2.07                     | 0.54              |
| 1:K:511:TYR:CE1  | 1:K:563:LEU:HB2  | 2.43                     | 0.54              |
| 1:L:234:HIS:O    | 1:L:237:TRP:HB3  | 2.07                     | 0.54              |
| 1:L:280:ALA:HB1  | 1:L:286:LEU:HD21 | 1.88                     | 0.54              |
| 1:L:281:ALA:HB3  | 1:L:324:ASP:OD1  | 2.07                     | 0.54              |
| 1:L:357:ALA:HB1  | 1:L:361:ARG:O    | 2.07                     | 0.54              |
| 1:A:61:ILE:O     | 1:A:189:HIS:N    | 2.26                     | 0.54              |
| 1:B:53:MET:HE1   | 1:B:144:LEU:HB3  | 1.89                     | 0.54              |
| 1:G:434:PHE:CD2  | 1:G:478:LEU:HD21 | 2.43                     | 0.54              |
| 1:H:99:ILE:HG22  | 1:H:112:MET:HE2  | 1.90                     | 0.54              |
| 1:H:254:LEU:HD21 | 1:H:577:LEU:HD21 | 1.89                     | 0.54              |
| 1:H:387:CYS:O    | 1:H:389:VAL:HG23 | 2.06                     | 0.54              |
| 1:K:258:GLU:OE1  | 1:K:557:LEU:HD22 | 2.07                     | 0.54              |
| 1:B:40:ILE:HG13  | 1:B:63:ARG:NH1   | 2.21                     | 0.54              |
| 1:G:101:LEU:HG   | 1:G:126:HIS:HB2  | 1.90                     | 0.54              |
| 1:G:223:PRO:CD   | 1:G:574:LEU:HD11 | 2.38                     | 0.54              |
| 1:H:180:LEU:CD1  | 1:H:193:ALA:HA   | 2.37                     | 0.54              |
| 1:H:396:THR:CB   | 1:H:432:ALA:HB3  | 2.36                     | 0.54              |
| 1:H:563:LEU:HD12 | 1:H:566:ARG:HD3  | 1.89                     | 0.54              |
| 1:L:81:GLU:OE2   | 1:L:85:ARG:HD2   | 2.06                     | 0.54              |
| 1:L:443:MET:HG2  | 1:L:444:PHE:N    | 2.22                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:7:SER:HA     | 1:A:33:LEU:O     | 2.06                     | 0.54              |
| 1:A:188:VAL:HG23 | 1:A:190:TRP:HE1  | 1.73                     | 0.54              |
| 1:B:33:LEU:HD22  | 1:B:86:TRP:CZ3   | 2.42                     | 0.54              |
| 1:B:309:ARG:O    | 1:B:313:LEU:HG   | 2.06                     | 0.54              |
| 1:G:8:VAL:HG23   | 1:G:32:VAL:HG13  | 1.90                     | 0.54              |
| 1:G:213:LEU:HD13 | 1:H:209:SER:OG   | 2.08                     | 0.54              |
| 1:G:477:LYS:NZ   | 1:H:449:GLU:OE2  | 2.32                     | 0.54              |
| 1:K:16:PRO:HB2   | 1:K:147:VAL:HG11 | 1.89                     | 0.54              |
| 1:K:108:ILE:O    | 1:K:112:MET:HG2  | 2.07                     | 0.54              |
| 1:K:223:PRO:CD   | 1:K:574:LEU:HD11 | 2.37                     | 0.54              |
| 1:L:175:ALA:N    | 1:L:176:PRO:HD2  | 2.22                     | 0.54              |
| 1:B:292:ILE:CD1  | 1:B:315:ASP:HB2  | 2.36                     | 0.54              |
| 1:G:51:PHE:HB3   | 1:G:59:PHE:CD2   | 2.42                     | 0.54              |
| 1:H:57:PRO:HG2   | 1:H:59:PHE:CE2   | 2.42                     | 0.54              |
| 1:K:68:GLU:HG2   | 1:K:69:ASP:N     | 2.23                     | 0.54              |
| 1:A:117:ALA:HA   | 1:A:164:GLU:OE1  | 2.08                     | 0.54              |
| 1:B:68:GLU:HG2   | 1:B:69:ASP:N     | 2.22                     | 0.54              |
| 1:B:305:ILE:O    | 1:B:309:ARG:HD3  | 2.08                     | 0.54              |
| 1:G:42:PRO:HA    | 1:G:45:GLU:OE1   | 2.08                     | 0.54              |
| 1:H:84:TRP:HB3   | 1:H:198:LEU:CD2  | 2.38                     | 0.54              |
| 1:K:4:LEU:HA     | 1:K:98:TYR:HB2   | 1.89                     | 0.54              |
| 1:G:105:TYR:HD2  | 1:G:107:THR:HG1  | 1.56                     | 0.54              |
| 1:H:105:TYR:N    | 1:H:108:ILE:HD12 | 2.17                     | 0.54              |
| 1:H:276:VAL:HG23 | 1:H:334:LEU:HD12 | 1.90                     | 0.54              |
| 1:H:547:THR:HG23 | 1:H:557:LEU:HD13 | 1.90                     | 0.54              |
| 1:K:76:HIS:CE1   | 1:K:107:THR:HB   | 2.43                     | 0.54              |
| 1:K:85:ARG:CZ    | 1:K:178:PHE:HB3  | 2.37                     | 0.54              |
| 1:K:277:ARG:NH1  | 1:K:289:VAL:HG22 | 2.22                     | 0.54              |
| 1:L:17:GLU:HB3   | 1:L:156:LEU:HD21 | 1.89                     | 0.54              |
| 1:L:309:ARG:O    | 1:L:313:LEU:HG   | 2.08                     | 0.54              |
| 1:A:511:TYR:HE1  | 1:A:563:LEU:CD1  | 2.09                     | 0.54              |
| 1:G:434:PHE:CD2  | 1:G:478:LEU:HD11 | 2.42                     | 0.54              |
| 1:L:41:SER:N     | 1:L:42:PRO:HD2   | 2.22                     | 0.54              |
| 1:L:68:GLU:HG2   | 1:L:69:ASP:N     | 2.22                     | 0.54              |
| 1:A:434:PHE:CE1  | 1:A:442:ALA:HB1  | 2.42                     | 0.53              |
| 1:B:36:ALA:HB2   | 1:B:64:VAL:O     | 2.08                     | 0.53              |
| 1:G:121:ALA:H    | 1:G:164:GLU:HB2  | 1.73                     | 0.53              |
| 1:G:349:ILE:HG12 | 1:G:389:VAL:HG13 | 1.90                     | 0.53              |
| 1:G:487:LEU:HD13 | 1:G:519:PHE:HZ   | 1.72                     | 0.53              |
| 1:K:181:GLU:O    | 1:K:191:VAL:HA   | 2.08                     | 0.53              |
| 1:K:223:PRO:HD2  | 1:K:574:LEU:HD11 | 1.88                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:431:LEU:HD22 | 1:L:478:LEU:CD1  | 2.38                     | 0.53              |
| 1:A:76:HIS:NE2   | 1:A:80:GLU:OE2   | 2.41                     | 0.53              |
| 1:A:250:TRP:HH2  | 1:A:577:LEU:HD11 | 1.73                     | 0.53              |
| 1:A:519:PHE:O    | 1:A:521:LEU:HD12 | 2.07                     | 0.53              |
| 1:G:182:SER:OG   | 1:G:189:HIS:HB3  | 2.07                     | 0.53              |
| 1:G:209:SER:OG   | 1:H:213:LEU:HD21 | 2.08                     | 0.53              |
| 1:G:310:TYR:CD1  | 1:G:516:ILE:HD11 | 2.43                     | 0.53              |
| 1:K:22:LEU:HD13  | 1:K:27:PHE:HE1   | 1.73                     | 0.53              |
| 1:L:48:LEU:O     | 1:L:52:GLU:HG3   | 2.08                     | 0.53              |
| 1:L:533:LEU:CD2  | 1:L:564:THR:HG21 | 2.37                     | 0.53              |
| 1:A:210:ARG:HH12 | 1:B:165:PRO:HG2  | 1.73                     | 0.53              |
| 1:B:4:LEU:HD12   | 1:B:98:TYR:O     | 2.08                     | 0.53              |
| 1:B:476:PHE:CZ   | 1:B:498:VAL:HG11 | 2.42                     | 0.53              |
| 1:B:533:LEU:CD1  | 1:B:543:VAL:HG11 | 2.38                     | 0.53              |
| 1:G:84:TRP:O     | 1:G:87:LEU:HG    | 2.08                     | 0.53              |
| 1:H:254:LEU:O    | 1:H:256:LYS:HG3  | 2.07                     | 0.53              |
| 1:K:5:LEU:HD22   | 1:K:86:TRP:CH2   | 2.43                     | 0.53              |
| 1:K:143:THR:O    | 1:K:147:VAL:HG23 | 2.07                     | 0.53              |
| 1:A:15:VAL:CG1   | 1:A:19:MET:HE3   | 2.38                     | 0.53              |
| 1:A:254:LEU:HD23 | 1:A:605:PRO:HD2  | 1.89                     | 0.53              |
| 1:G:123:GLU:HG3  | 1:G:125:PHE:CD1  | 2.41                     | 0.53              |
| 1:H:411:ALA:O    | 1:H:415:THR:HG22 | 2.09                     | 0.53              |
| 2:I:718:A23:O1C  | 2:J:719:A:O5'    | 2.24                     | 0.53              |
| 1:K:102:ALA:HA   | 1:K:126:HIS:CE1  | 2.43                     | 0.53              |
| 1:K:547:THR:HA   | 1:K:560:ASN:ND2  | 2.24                     | 0.53              |
| 1:L:178:PHE:HD2  | 1:L:198:LEU:HD12 | 1.73                     | 0.53              |
| 1:L:393:LEU:HD12 | 1:L:413:ALA:HB2  | 1.89                     | 0.53              |
| 1:G:520:PRO:HD3  | 1:G:529:GLU:HG3  | 1.91                     | 0.53              |
| 1:H:128:LEU:HB2  | 1:H:157:ARG:CG   | 2.38                     | 0.53              |
| 1:K:364:TRP:HE3  | 1:K:412:LEU:HD11 | 1.72                     | 0.53              |
| 1:L:144:LEU:O    | 1:L:148:GLU:HG2  | 2.09                     | 0.53              |
| 1:L:510:PRO:HB3  | 1:L:563:LEU:HD23 | 1.90                     | 0.53              |
| 1:B:34:THR:CG2   | 1:B:40:ILE:HD12  | 2.38                     | 0.53              |
| 1:B:34:THR:CG2   | 1:B:63:ARG:HG2   | 2.39                     | 0.53              |
| 1:B:34:THR:HB    | 1:B:63:ARG:HG2   | 1.90                     | 0.53              |
| 1:B:64:VAL:HG11  | 1:B:67:PHE:HB3   | 1.91                     | 0.53              |
| 1:G:40:ILE:HB    | 1:G:63:ARG:NH2   | 2.24                     | 0.53              |
| 1:G:216:TRP:CD1  | 1:H:212:ILE:HD13 | 2.44                     | 0.53              |
| 1:G:279:GLU:HG3  | 1:G:330:ALA:HB2  | 1.89                     | 0.53              |
| 1:H:98:TYR:HD1   | 1:H:123:GLU:HB3  | 1.73                     | 0.53              |
| 1:H:128:LEU:O    | 1:H:156:LEU:HD12 | 2.09                     | 0.53              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:K:97:ARG:HB3     | 1:K:121:ALA:CA   | 2.39                     | 0.53              |
| 1:L:51:PHE:CE2     | 1:L:61:ILE:HD11  | 2.36                     | 0.53              |
| 1:B:471:ILE:HG21   | 1:B:489:LEU:HD13 | 1.90                     | 0.53              |
| 1:G:98:TYR:HB3     | 1:G:125:PHE:CE1  | 2.44                     | 0.53              |
| 1:G:299:PRO:O      | 1:G:301:PRO:HD3  | 2.08                     | 0.53              |
| 1:K:70:LEU:HB3     | 1:K:105:TYR:CE2  | 2.44                     | 0.53              |
| 1:B:21:LEU:HD22    | 1:B:125:PHE:CD1  | 2.44                     | 0.53              |
| 1:G:70:LEU:HD12    | 1:G:75:ASP:HB2   | 1.91                     | 0.53              |
| 1:G:86:TRP:NE1     | 1:G:90:ARG:HG3   | 2.24                     | 0.53              |
| 1:G:411:ALA:HB1    | 1:L:411:ALA:HA   | 1.91                     | 0.53              |
| 1:H:80:GLU:HG2     | 1:H:81:GLU:N     | 2.24                     | 0.53              |
| 1:K:511:TYR:HB3    | 1:K:515:GLN:NE2  | 2.24                     | 0.53              |
| 1:L:5:LEU:HD22     | 1:L:86:TRP:CH2   | 2.44                     | 0.53              |
| 1:L:350:ARG:HH11   | 1:L:461:HIS:CE1  | 2.27                     | 0.53              |
| 1:A:106:LYS:HZ3    | 2:C:708:A23:H4'  | 1.74                     | 0.53              |
| 1:B:185:GLN:HB2    | 1:B:190:TRP:CD1  | 2.43                     | 0.53              |
| 1:G:101:LEU:HD12   | 1:G:126:HIS:ND1  | 2.23                     | 0.53              |
| 1:H:423:GLY:O      | 1:H:425:ARG:HG3  | 2.09                     | 0.53              |
| 1:K:519:PHE:O      | 1:K:521:LEU:HD12 | 2.09                     | 0.53              |
| 1:L:474:ALA:HA     | 1:L:478:LEU:HB2  | 1.90                     | 0.53              |
| 1:A:418:GLU:CD     | 1:H:408:ARG:HE   | 2.17                     | 0.53              |
| 1:B:34:THR:HG23    | 1:B:40:ILE:HD12  | 1.90                     | 0.53              |
| 1:H:99:ILE:HG22    | 1:H:112:MET:CE   | 2.39                     | 0.53              |
| 1:H:237:TRP:CZ3    | 1:H:573:ARG:HD3  | 2.44                     | 0.53              |
| 1:K:84:TRP:HB3     | 1:K:198:LEU:CD2  | 2.39                     | 0.53              |
| 1:L:259:LEU:HD13   | 1:L:482:ARG:NH1  | 2.23                     | 0.53              |
| 1:A:106:LYS:NZ     | 2:D:709:A:O5'    | 2.41                     | 0.52              |
| 1:G:33:LEU:HD11    | 1:G:64:VAL:HG13  | 1.90                     | 0.52              |
| 1:G:472[A]:TRP:CE2 | 1:G:495:LEU:HD13 | 2.43                     | 0.52              |
| 1:H:45:GLU:O       | 1:H:49:ARG:HG2   | 2.10                     | 0.52              |
| 1:H:547:THR:HA     | 1:H:560:ASN:ND2  | 2.21                     | 0.52              |
| 1:L:3:ILE:HG21     | 1:L:91:ALA:HB2   | 1.90                     | 0.52              |
| 1:L:508:LEU:HD13   | 1:L:531:TYR:HE1  | 1.74                     | 0.52              |
| 1:B:1:MET:HA       | 1:B:28:ASP:OD2   | 2.09                     | 0.52              |
| 1:B:467:ASP:C      | 1:B:468:VAL:HG22 | 2.34                     | 0.52              |
| 1:G:84:TRP:HA      | 1:G:87:LEU:HD21  | 1.90                     | 0.52              |
| 1:G:472[A]:TRP:CD2 | 1:G:495:LEU:HD13 | 2.44                     | 0.52              |
| 1:K:233:SER:HA     | 1:K:236:ARG:NE   | 2.24                     | 0.52              |
| 1:K:259:LEU:HD13   | 1:K:482:ARG:NH1  | 2.24                     | 0.52              |
| 1:A:188:VAL:HG23   | 1:A:190:TRP:NE1  | 2.24                     | 0.52              |
| 1:A:429:VAL:CG2    | 1:A:458:VAL:HG12 | 2.40                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:511:TYR:HD2  | 1:A:555:ALA:HB3  | 1.72                     | 0.52              |
| 1:B:121:ALA:H    | 1:B:164:GLU:HB2  | 1.75                     | 0.52              |
| 1:K:375:GLN:O    | 1:K:379:GLU:HG2  | 2.09                     | 0.52              |
| 1:L:181:GLU:O    | 1:L:181:GLU:HG2  | 2.09                     | 0.52              |
| 1:A:123:GLU:OE2  | 1:A:162:GLY:N    | 2.42                     | 0.52              |
| 1:A:350:ARG:NH2  | 1:A:459:THR:HG21 | 2.24                     | 0.52              |
| 1:B:5:LEU:HB3    | 1:B:86:TRP:CH2   | 2.45                     | 0.52              |
| 1:B:156:LEU:HD23 | 1:B:158:PHE:CZ   | 2.44                     | 0.52              |
| 1:G:258:GLU:OE1  | 1:G:557:LEU:HD13 | 2.10                     | 0.52              |
| 1:H:271:GLU:OE1  | 1:H:275:LYS:NZ   | 2.42                     | 0.52              |
| 1:L:495:LEU:HD12 | 1:L:495:LEU:O    | 2.09                     | 0.52              |
| 1:G:482:ARG:HG2  | 1:G:505:ALA:HB3  | 1.92                     | 0.52              |
| 1:H:404:SER:HB2  | 1:H:408:ARG:NH1  | 2.25                     | 0.52              |
| 1:L:21:LEU:HD22  | 1:L:125:PHE:CE1  | 2.44                     | 0.52              |
| 1:B:16:PRO:HD3   | 1:B:47:LEU:CD2   | 2.39                     | 0.52              |
| 1:B:28:ASP:O     | 1:B:57:PRO:HB3   | 2.09                     | 0.52              |
| 1:B:563:LEU:O    | 1:B:563:LEU:HG   | 2.09                     | 0.52              |
| 1:H:86:TRP:CE2   | 1:H:90:ARG:HG3   | 2.45                     | 0.52              |
| 1:H:318:GLY:O    | 1:H:322:LEU:HB2  | 2.10                     | 0.52              |
| 1:H:533:LEU:CD1  | 1:H:543:VAL:HG11 | 2.39                     | 0.52              |
| 1:K:166:GLY:HA3  | 1:K:171:ARG:HD2  | 1.92                     | 0.52              |
| 1:K:209:SER:O    | 1:K:213:LEU:HD23 | 2.10                     | 0.52              |
| 1:L:73:GLU:O     | 1:L:77:MET:N     | 2.25                     | 0.52              |
| 1:L:489:LEU:HD12 | 1:L:536:TYR:CE2  | 2.44                     | 0.52              |
| 1:B:301:PRO:HD3  | 1:B:515:GLN:HG2  | 1.92                     | 0.52              |
| 1:B:460:VAL:HG12 | 1:B:461:HIS:H    | 1.75                     | 0.52              |
| 1:G:3:ILE:HA     | 1:G:29:GLU:O     | 2.09                     | 0.52              |
| 1:G:469:GLU:O    | 1:G:473:GLN:HG3  | 2.09                     | 0.52              |
| 1:H:276:VAL:HG22 | 1:H:330:ALA:CB   | 2.39                     | 0.52              |
| 1:A:109:SER:HA   | 1:A:112:MET:HG2  | 1.92                     | 0.52              |
| 1:G:3:ILE:CG1    | 1:G:29:GLU:HB2   | 2.39                     | 0.52              |
| 1:G:523:GLU:O    | 1:G:569:PRO:HB3  | 2.10                     | 0.52              |
| 1:L:81:GLU:HB2   | 1:L:196:MET:SD   | 2.50                     | 0.52              |
| 1:G:49:ARG:CD    | 1:G:144:LEU:HD11 | 2.40                     | 0.52              |
| 1:G:303:GLU:CD   | 1:G:304:PRO:HD2  | 2.35                     | 0.52              |
| 1:H:85:ARG:NH2   | 1:H:178:PHE:HB3  | 2.23                     | 0.52              |
| 1:H:102:ALA:HB2  | 1:H:127:VAL:HG12 | 1.91                     | 0.52              |
| 1:L:259:LEU:O    | 1:L:350:ARG:NH2  | 2.43                     | 0.52              |
| 1:A:89:GLN:HA    | 1:A:175:ALA:HB2  | 1.92                     | 0.52              |
| 1:B:328:LEU:HD11 | 1:B:370:ILE:CG1  | 2.40                     | 0.52              |
| 1:G:98:TYR:HB3   | 1:G:125:PHE:CZ   | 2.45                     | 0.52              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:H:333:ARG:HG2  | 1:H:333:ARG:HH11   | 1.75                     | 0.52              |
| 1:K:318:GLY:O    | 1:K:322:LEU:HB2    | 2.10                     | 0.52              |
| 1:A:64:VAL:HG21  | 1:A:67:PHE:HB3     | 1.91                     | 0.51              |
| 1:A:196:MET:SD   | 1:A:196:MET:O      | 2.67                     | 0.51              |
| 1:G:258:GLU:O    | 1:G:259:LEU:HD23   | 2.10                     | 0.51              |
| 1:K:37:SER:HA    | 1:K:68:GLU:HB2     | 1.92                     | 0.51              |
| 1:K:97:ARG:NH1   | 1:K:120:GLY:O      | 2.43                     | 0.51              |
| 1:K:533:LEU:CD1  | 1:K:543:VAL:HG11   | 2.40                     | 0.51              |
| 1:L:251:VAL:HG21 | 1:L:562:LEU:CD2    | 2.40                     | 0.51              |
| 1:L:286:LEU:HD12 | 1:L:321:LEU:CD1    | 2.40                     | 0.51              |
| 1:L:301:PRO:HG3  | 1:L:515:GLN:HA     | 1.92                     | 0.51              |
| 1:G:83:LEU:HD21  | 1:G:112:MET:HB3    | 1.92                     | 0.51              |
| 1:H:48:LEU:O     | 1:H:52:GLU:HG3     | 2.10                     | 0.51              |
| 1:H:64:VAL:CG1   | 1:H:67:PHE:HB3     | 2.40                     | 0.51              |
| 1:H:397:ARG:NE   | 1:H:433:GLY:HA3    | 2.25                     | 0.51              |
| 1:H:410:LEU:HD22 | 1:H:451:VAL:HG11   | 1.91                     | 0.51              |
| 1:L:63:ARG:HD2   | 1:L:190:TRP:CZ2    | 2.46                     | 0.51              |
| 1:L:106:LYS:HD3  | 2:M:728:A23:H5'    | 1.92                     | 0.51              |
| 1:L:297:GLY:O    | 1:L:300:ILE:HG22   | 2.09                     | 0.51              |
| 1:L:449:GLU:N    | 1:L:450:PRO:HD2    | 2.24                     | 0.51              |
| 1:L:533:LEU:HB3  | 1:L:568:CYS:SG     | 2.51                     | 0.51              |
| 2:M:727:A:H1'    | 2:M:728:A23:P      | 2.50                     | 0.51              |
| 1:A:78:LEU:O     | 1:A:82:VAL:HG23    | 2.10                     | 0.51              |
| 1:A:335:LEU:HD21 | 1:A:349:ILE:HD12   | 1.91                     | 0.51              |
| 1:G:46:GLN:CA    | 1:G:49:ARG:HG2     | 2.39                     | 0.51              |
| 1:G:363:PRO:HG2  | 1:L:418:GLU:OE2    | 2.09                     | 0.51              |
| 1:H:46:GLN:O     | 1:H:50:TYR:N       | 2.39                     | 0.51              |
| 1:H:242:LEU:HD12 | 1:H:247:ASP:OD2    | 2.10                     | 0.51              |
| 1:K:167:TRP:H    | 1:K:171:ARG:HD3    | 1.75                     | 0.51              |
| 1:K:167:TRP:O    | 1:K:171:ARG:NE     | 2.42                     | 0.51              |
| 1:A:133:PHE:CZ   | 1:A:150:ALA:HB2    | 2.45                     | 0.51              |
| 1:B:15:VAL:O     | 1:B:19:MET:HG3     | 2.10                     | 0.51              |
| 1:B:183:THR:O    | 1:B:190:TRP:HB2    | 2.10                     | 0.51              |
| 1:H:83:LEU:O     | 1:H:87:LEU:N       | 2.36                     | 0.51              |
| 1:K:238:LEU:HD12 | 1:K:573:ARG:HG3    | 1.92                     | 0.51              |
| 1:L:35:THR:O     | 1:L:63:ARG:HG3     | 2.10                     | 0.51              |
| 1:L:167:TRP:CE3  | 1:L:168:PRO:HD3    | 2.37                     | 0.51              |
| 1:L:469:GLU:HA   | 1:L:472[A]:TRP:HB2 | 1.93                     | 0.51              |
| 1:A:80:GLU:OE1   | 1:A:199:ARG:NH1    | 2.43                     | 0.51              |
| 1:A:233:SER:HA   | 1:A:236:ARG:NH1    | 2.26                     | 0.51              |
| 1:A:446:THR:O    | 1:A:449:GLU:HG2    | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:441:ALA:HB3  | 1:B:473:GLN:CG   | 2.39                     | 0.51              |
| 1:G:192:ARG:NE   | 1:G:192:ARG:HA   | 2.26                     | 0.51              |
| 1:K:167:TRP:CG   | 1:K:168:PRO:HD2  | 2.45                     | 0.51              |
| 1:K:346:TYR:OH   | 1:K:390:ASN:ND2  | 2.43                     | 0.51              |
| 1:A:36:ALA:HB2   | 1:A:64:VAL:O     | 2.11                     | 0.51              |
| 1:A:76:HIS:HA    | 1:A:79:PHE:CD1   | 2.44                     | 0.51              |
| 1:B:16:PRO:HD3   | 1:B:47:LEU:HD21  | 1.92                     | 0.51              |
| 1:B:207:GLU:OE2  | 1:B:210:ARG:NH2  | 2.41                     | 0.51              |
| 1:B:280:ALA:HB1  | 1:B:324:ASP:OD2  | 2.09                     | 0.51              |
| 1:B:571:ILE:HD12 | 1:B:575:GLU:OE1  | 2.10                     | 0.51              |
| 1:G:223:PRO:HB3  | 1:G:581:VAL:HG11 | 1.93                     | 0.51              |
| 1:H:133:PHE:CE2  | 1:H:150:ALA:HB2  | 2.45                     | 0.51              |
| 1:H:143:THR:O    | 1:H:147:VAL:HG23 | 2.11                     | 0.51              |
| 1:L:17:GLU:HB3   | 1:L:156:LEU:HD22 | 1.92                     | 0.51              |
| 1:L:174:SER:HB2  | 1:L:176:PRO:HD2  | 1.92                     | 0.51              |
| 1:L:185:GLN:HB2  | 1:L:190:TRP:CD1  | 2.45                     | 0.51              |
| 1:A:22:LEU:HB2   | 1:A:25:GLN:HE21  | 1.76                     | 0.51              |
| 1:A:432:ALA:HA   | 1:A:461:HIS:CB   | 2.37                     | 0.51              |
| 1:B:418:GLU:CD   | 1:K:408:ARG:HH12 | 2.17                     | 0.51              |
| 1:G:199:ARG:HD2  | 1:G:199:ARG:O    | 2.11                     | 0.51              |
| 1:G:318:GLY:H    | 1:G:322:LEU:HD23 | 1.75                     | 0.51              |
| 1:H:114:ARG:O    | 1:H:118:LEU:HD23 | 2.10                     | 0.51              |
| 1:K:471:ILE:O    | 1:K:475:VAL:HG23 | 2.11                     | 0.51              |
| 1:L:222:LEU:HD12 | 1:L:227:LEU:HB3  | 1.92                     | 0.51              |
| 1:L:410:LEU:O    | 1:L:414:ILE:HG13 | 2.11                     | 0.51              |
| 1:L:520:PRO:HD2  | 1:L:529:GLU:O    | 2.10                     | 0.51              |
| 1:A:210:ARG:NH1  | 1:B:165:PRO:HG2  | 2.26                     | 0.51              |
| 1:A:408:ARG:HH12 | 1:H:454:VAL:CG1  | 2.23                     | 0.51              |
| 1:A:494:ASP:OD1  | 1:B:454:VAL:HA   | 2.11                     | 0.51              |
| 1:G:431:LEU:HD11 | 1:G:448:PHE:CE2  | 2.46                     | 0.51              |
| 1:G:471:ILE:CG2  | 1:G:495:LEU:HD21 | 2.41                     | 0.51              |
| 1:H:509:CYS:SG   | 1:H:548:ASP:HB2  | 2.51                     | 0.51              |
| 1:K:435:GLU:OE2  | 1:K:471:ILE:HG13 | 2.10                     | 0.51              |
| 1:A:16:PRO:CB    | 1:A:147:VAL:HG11 | 2.40                     | 0.51              |
| 1:A:167:TRP:O    | 1:A:171:ARG:HG3  | 2.11                     | 0.51              |
| 1:A:250:TRP:CH2  | 1:A:577:LEU:HD11 | 2.46                     | 0.51              |
| 1:A:460:VAL:HG21 | 1:A:474:ALA:HB1  | 1.93                     | 0.51              |
| 1:G:210:ARG:HG2  | 1:H:167:TRP:CZ3  | 2.46                     | 0.51              |
| 1:G:544:THR:O    | 1:G:545:LEU:HD23 | 2.10                     | 0.51              |
| 1:H:181:GLU:HG2  | 1:H:181:GLU:O    | 2.10                     | 0.51              |
| 1:H:284:GLU:OE1  | 1:H:284:GLU:N    | 2.42                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:167:TRP:H    | 1:K:171:ARG:CD   | 2.24                     | 0.51              |
| 1:A:48:LEU:CD2   | 1:A:187:PRO:HG2  | 2.40                     | 0.51              |
| 1:A:547:THR:HA   | 1:A:560:ASN:HD21 | 1.75                     | 0.51              |
| 1:B:435:GLU:OE2  | 1:B:464:GLU:N    | 2.44                     | 0.51              |
| 1:G:66:ASP:HB3   | 1:G:192:ARG:NH1  | 2.26                     | 0.51              |
| 1:H:496:LEU:HD11 | 1:H:541:VAL:HG21 | 1.92                     | 0.51              |
| 2:J:719:A:H4'    | 2:J:720:A23:OP2  | 2.10                     | 0.51              |
| 1:A:62:SER:HA    | 1:A:189:HIS:O    | 2.10                     | 0.50              |
| 1:A:89:GLN:CA    | 1:A:175:ALA:HB2  | 2.41                     | 0.50              |
| 1:A:431:LEU:HD21 | 1:A:448:PHE:CE1  | 2.45                     | 0.50              |
| 1:B:435:GLU:O    | 1:B:437:ARG:N    | 2.34                     | 0.50              |
| 1:G:125:PHE:HA   | 1:G:159:VAL:O    | 2.10                     | 0.50              |
| 1:H:85:ARG:HH21  | 1:H:178:PHE:CB   | 2.23                     | 0.50              |
| 1:H:127:VAL:HG22 | 1:H:156:LEU:HD11 | 1.93                     | 0.50              |
| 1:H:243:ASP:OD2  | 1:H:246:GLN:NE2  | 2.44                     | 0.50              |
| 1:G:497:ARG:NH2  | 1:H:455:GLY:HA3  | 2.26                     | 0.50              |
| 1:H:4:LEU:HA     | 1:H:98:TYR:O     | 2.11                     | 0.50              |
| 1:H:290:ARG:H    | 1:H:316:ASN:HD21 | 1.59                     | 0.50              |
| 1:K:17:GLU:CB    | 1:K:156:LEU:HD13 | 2.40                     | 0.50              |
| 1:K:61:ILE:HB    | 1:K:188:VAL:HG12 | 1.93                     | 0.50              |
| 1:K:238:LEU:HD11 | 1:K:574:LEU:HA   | 1.94                     | 0.50              |
| 1:L:396:THR:OG1  | 1:L:433:GLY:HA3  | 2.11                     | 0.50              |
| 1:L:520:PRO:C    | 1:L:521:LEU:HD12 | 2.36                     | 0.50              |
| 1:B:85:ARG:NH1   | 1:B:195:ASP:H    | 2.02                     | 0.50              |
| 1:B:175:ALA:N    | 1:B:176:PRO:HD2  | 2.27                     | 0.50              |
| 1:G:46:GLN:HA    | 1:G:49:ARG:CG    | 2.41                     | 0.50              |
| 1:H:352:SER:HB3  | 1:H:355:ASN:HD22 | 1.76                     | 0.50              |
| 1:L:30:VAL:HG22  | 1:L:59:PHE:HE1   | 1.77                     | 0.50              |
| 1:B:78:LEU:O     | 1:B:82:VAL:HG23  | 2.11                     | 0.50              |
| 1:B:454:VAL:HG23 | 1:B:456:LEU:HD13 | 1.93                     | 0.50              |
| 1:H:233:SER:HA   | 1:H:236:ARG:CZ   | 2.41                     | 0.50              |
| 1:K:35:THR:O     | 1:K:63:ARG:HG3   | 2.11                     | 0.50              |
| 1:K:271:GLU:O    | 1:K:275:LYS:N    | 2.44                     | 0.50              |
| 1:L:245:VAL:HG23 | 1:L:246:GLN:CD   | 2.36                     | 0.50              |
| 1:L:394:THR:HG21 | 3:L:703:ATP:H5'1 | 1.94                     | 0.50              |
| 1:A:521:LEU:HD23 | 1:A:566:ARG:NH1  | 2.26                     | 0.50              |
| 1:G:4:LEU:HD12   | 1:G:98:TYR:O     | 2.11                     | 0.50              |
| 1:G:282:ASN:HB2  | 1:G:284:GLU:OE2  | 2.12                     | 0.50              |
| 1:G:431:LEU:CD2  | 1:G:448:PHE:HZ   | 2.24                     | 0.50              |
| 1:G:607:PRO:HB2  | 1:G:610:THR:CG2  | 2.42                     | 0.50              |
| 1:H:266:PHE:HB3  | 1:H:331:GLN:HE21 | 1.77                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:16:PRO:HD3   | 1:K:47:LEU:HD21  | 1.93                     | 0.50              |
| 1:K:29:GLU:CG    | 1:K:58:ARG:HB3   | 2.28                     | 0.50              |
| 1:K:105:TYR:H    | 1:K:108:ILE:HD12 | 1.77                     | 0.50              |
| 1:L:117:ALA:HB2  | 1:L:164:GLU:OE2  | 2.10                     | 0.50              |
| 1:L:182:SER:OG   | 1:L:189:HIS:HB3  | 2.12                     | 0.50              |
| 1:A:239:HIS:CD2  | 1:A:574:LEU:HD22 | 2.46                     | 0.50              |
| 1:A:311:MET:HE2  | 3:A:701:ATP:C4   | 2.47                     | 0.50              |
| 1:B:99:ILE:CD1   | 1:B:116:ALA:HB2  | 2.41                     | 0.50              |
| 1:B:273:LEU:O    | 1:B:277:ARG:HG3  | 2.11                     | 0.50              |
| 1:G:63:ARG:HD3   | 1:G:190:TRP:CZ2  | 2.47                     | 0.50              |
| 1:G:258:GLU:OE2  | 1:G:546:ASN:HB3  | 2.12                     | 0.50              |
| 1:G:410:LEU:HD23 | 1:G:447:ASP:O    | 2.12                     | 0.50              |
| 1:H:128:LEU:HB2  | 1:H:157:ARG:HG3  | 1.94                     | 0.50              |
| 1:H:200:GLN:HA   | 1:H:203:GLU:OE2  | 2.10                     | 0.50              |
| 1:K:307:LEU:HD22 | 1:K:464:GLU:HB2  | 1.94                     | 0.50              |
| 1:K:429:VAL:CG2  | 1:K:458:VAL:HG22 | 2.42                     | 0.50              |
| 1:L:185:GLN:O    | 1:L:188:VAL:HG22 | 2.12                     | 0.50              |
| 1:L:489:LEU:HB2  | 1:L:536:TYR:CE2  | 2.45                     | 0.50              |
| 1:A:44:VAL:HG11  | 1:A:188:VAL:HG11 | 1.94                     | 0.50              |
| 1:A:84:TRP:NE1   | 1:A:115:ALA:HB2  | 2.27                     | 0.50              |
| 1:G:207:GLU:HA   | 1:G:210:ARG:NH1  | 2.27                     | 0.50              |
| 1:G:519:PHE:HB2  | 1:G:567:LEU:HD11 | 1.94                     | 0.50              |
| 1:K:50:TYR:HA    | 1:K:53:MET:SD    | 2.52                     | 0.50              |
| 1:K:211:HIS:ND1  | 1:K:231:PRO:HA   | 2.27                     | 0.50              |
| 1:K:325:PRO:HG3  | 1:K:361:ARG:HD2  | 1.94                     | 0.50              |
| 1:L:133:PHE:CD2  | 1:L:141:ALA:HB2  | 2.47                     | 0.50              |
| 1:B:8:VAL:HG22   | 1:B:15:VAL:CG2   | 2.41                     | 0.50              |
| 1:B:449:GLU:HG3  | 1:B:453:ARG:NE   | 2.26                     | 0.50              |
| 1:B:464:GLU:OE2  | 1:B:517:LYS:HG2  | 2.12                     | 0.50              |
| 1:G:435:GLU:HG3  | 1:G:465:ASN:ND2  | 2.27                     | 0.50              |
| 1:K:12:TRP:CH2   | 1:K:144:LEU:HD22 | 2.46                     | 0.50              |
| 1:K:548:ASP:OD1  | 1:K:549:ASN:ND2  | 2.45                     | 0.50              |
| 1:L:130:GLU:HB2  | 1:L:155:ALA:HB1  | 1.94                     | 0.50              |
| 1:A:5:LEU:HG     | 1:A:31:HIS:HB2   | 1.94                     | 0.50              |
| 1:G:326:GLY:O    | 1:G:329:ARG:HG2  | 2.12                     | 0.50              |
| 1:K:307:LEU:HG   | 1:K:311:MET:HE1  | 1.93                     | 0.50              |
| 1:L:1:MET:HG3    | 1:L:96:HIS:HB3   | 1.94                     | 0.50              |
| 1:L:335:LEU:HD23 | 1:L:374:PHE:HZ   | 1.77                     | 0.50              |
| 1:A:65:GLN:CD    | 1:A:190:TRP:HB3  | 2.37                     | 0.49              |
| 1:A:312:ARG:NE   | 1:A:312:ARG:HA   | 2.27                     | 0.49              |
| 1:G:206:LEU:O    | 1:G:210:ARG:HG3  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:32:VAL:CG1   | 1:H:61:ILE:HG12  | 2.42                     | 0.49              |
| 1:H:208:ARG:HH11 | 1:H:212:ILE:CD1  | 2.24                     | 0.49              |
| 1:K:89:GLN:N     | 1:K:175:ALA:HB2  | 2.27                     | 0.49              |
| 1:L:4:LEU:HB3    | 1:L:30:VAL:CG1   | 2.40                     | 0.49              |
| 1:A:581:VAL:HG13 | 1:A:598:TRP:HH2  | 1.76                     | 0.49              |
| 1:B:10:THR:HG23  | 2:C:708:A23:C5   | 2.42                     | 0.49              |
| 1:B:77:MET:HG3   | 1:B:199:ARG:NH1  | 2.27                     | 0.49              |
| 1:H:15:VAL:N     | 1:H:16:PRO:HD2   | 2.27                     | 0.49              |
| 1:K:82:VAL:HG13  | 1:K:180:LEU:HD11 | 1.94                     | 0.49              |
| 1:K:466:ASP:C    | 1:K:491:ARG:HH22 | 2.19                     | 0.49              |
| 1:A:117:ALA:HA   | 1:A:164:GLU:CD   | 2.37                     | 0.49              |
| 1:B:169:GLN:O    | 1:B:170:LEU:HD23 | 2.11                     | 0.49              |
| 1:B:575:GLU:O    | 1:B:579:THR:HG23 | 2.12                     | 0.49              |
| 1:G:531:TYR:CB   | 1:G:567:LEU:HG   | 2.41                     | 0.49              |
| 1:G:572:THR:OG1  | 1:G:575:GLU:OE1  | 2.23                     | 0.49              |
| 1:K:21:LEU:HD12  | 1:K:158:PHE:HD2  | 1.76                     | 0.49              |
| 1:K:61:ILE:HB    | 1:K:188:VAL:HA   | 1.94                     | 0.49              |
| 1:K:64:VAL:HG23  | 1:K:67:PHE:O     | 2.12                     | 0.49              |
| 1:K:216:TRP:O    | 1:K:219:ILE:HB   | 2.13                     | 0.49              |
| 1:K:396:THR:OG1  | 1:K:432:ALA:HB3  | 2.12                     | 0.49              |
| 1:A:525:GLN:HG2  | 1:A:526:GLU:N    | 2.28                     | 0.49              |
| 1:B:143:THR:O    | 1:B:147:VAL:HG23 | 2.13                     | 0.49              |
| 1:B:440:ARG:HG2  | 1:B:442:ALA:N    | 2.24                     | 0.49              |
| 1:G:16:PRO:HB3   | 1:G:50:TYR:CE2   | 2.47                     | 0.49              |
| 1:G:32:VAL:HB    | 1:G:61:ILE:HG12  | 1.94                     | 0.49              |
| 1:G:434:PHE:HE2  | 1:G:478:LEU:HD21 | 1.76                     | 0.49              |
| 1:G:453:ARG:HG3  | 1:G:453:ARG:O    | 2.12                     | 0.49              |
| 1:H:397:ARG:CB   | 1:H:406:ILE:HD11 | 2.43                     | 0.49              |
| 1:L:527:GLY:H    | 1:L:530:THR:CG2  | 2.26                     | 0.49              |
| 1:A:31:HIS:CE1   | 1:A:58:ARG:HH12  | 2.30                     | 0.49              |
| 1:A:202:VAL:O    | 1:A:206:LEU:HD23 | 2.13                     | 0.49              |
| 1:A:520:PRO:HD2  | 1:A:529:GLU:O    | 2.12                     | 0.49              |
| 1:A:533:LEU:HB3  | 1:A:568:CYS:SG   | 2.53                     | 0.49              |
| 2:D:709:A:O2'    | 2:D:710:A23:OP1  | 2.25                     | 0.49              |
| 1:G:258:GLU:OE2  | 1:G:547:THR:N    | 2.35                     | 0.49              |
| 1:G:282:ASN:HB2  | 1:G:284:GLU:CD   | 2.37                     | 0.49              |
| 1:G:397:ARG:NE   | 1:G:434:PHE:H    | 2.10                     | 0.49              |
| 1:K:197:ARG:HH21 | 1:K:200:GLN:CD   | 2.21                     | 0.49              |
| 1:K:489:LEU:HD21 | 1:K:499:VAL:HG21 | 1.93                     | 0.49              |
| 1:K:511:TYR:CE1  | 1:K:563:LEU:HD13 | 2.45                     | 0.49              |
| 1:L:80:GLU:HG2   | 1:L:114:ARG:HH21 | 1.77                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:99:ILE:CG2   | 1:L:112:MET:HE2  | 2.42                     | 0.49              |
| 1:L:130:GLU:OE1  | 1:L:132:ARG:NE   | 2.26                     | 0.49              |
| 1:L:457:ALA:HB1  | 1:L:588:PHE:CZ   | 2.48                     | 0.49              |
| 1:L:485:HIS:HE1  | 1:L:509:CYS:SG   | 2.35                     | 0.49              |
| 1:A:406:ILE:HD12 | 1:A:406:ILE:H    | 1.78                     | 0.49              |
| 1:B:65:GLN:NE2   | 1:B:192:ARG:HG3  | 2.27                     | 0.49              |
| 2:I:717:A:H1'    | 2:I:718:A23:OP1  | 2.12                     | 0.49              |
| 1:K:36:ALA:CA    | 1:K:63:ARG:HD3   | 2.29                     | 0.49              |
| 1:K:93:GLN:HB2   | 1:K:96:HIS:CE1   | 2.47                     | 0.49              |
| 1:L:182:SER:HA   | 1:L:190:TRP:O    | 2.13                     | 0.49              |
| 1:L:250:TRP:NE1  | 1:L:605:PRO:HG2  | 2.27                     | 0.49              |
| 1:A:89:GLN:HG3   | 1:A:90:ARG:HG2   | 1.94                     | 0.49              |
| 1:A:411:ALA:HB2  | 1:H:414:ILE:CD1  | 2.37                     | 0.49              |
| 1:B:609:ASP:O    | 1:B:610:THR:HB   | 2.12                     | 0.49              |
| 1:G:318:GLY:O    | 1:G:322:LEU:HD23 | 2.12                     | 0.49              |
| 1:H:130:GLU:CD   | 1:H:155:ALA:HA   | 2.37                     | 0.49              |
| 1:H:298:TRP:CG   | 1:H:299:PRO:HA   | 2.47                     | 0.49              |
| 1:H:362:SER:O    | 1:H:366:VAL:HG23 | 2.12                     | 0.49              |
| 1:K:243:ASP:OD2  | 1:K:246:GLN:HB2  | 2.13                     | 0.49              |
| 1:K:364:TRP:HZ3  | 1:K:416:ALA:HB2  | 1.77                     | 0.49              |
| 1:K:397:ARG:CD   | 1:K:434:PHE:H    | 2.23                     | 0.49              |
| 1:L:73:GLU:HA    | 1:L:76:HIS:CB    | 2.40                     | 0.49              |
| 1:A:398:GLU:OE2  | 1:A:405:ARG:HD2  | 2.12                     | 0.49              |
| 1:B:51:PHE:CD2   | 1:B:59:PHE:HB3   | 2.48                     | 0.49              |
| 1:B:311:MET:HE1  | 3:B:701:ATP:C2'  | 2.43                     | 0.49              |
| 1:H:251:VAL:HG11 | 1:H:562:LEU:CD1  | 2.43                     | 0.49              |
| 1:L:149:GLN:O    | 1:L:153:THR:HG23 | 2.13                     | 0.49              |
| 1:L:353:PRO:HG2  | 1:L:412:LEU:HD23 | 1.94                     | 0.49              |
| 1:A:54:HIS:N     | 1:A:55:PRO:HD3   | 2.28                     | 0.49              |
| 1:B:73:GLU:OE2   | 1:B:74:GLN:NE2   | 2.46                     | 0.49              |
| 1:G:219:ILE:HD12 | 1:G:222:LEU:HD12 | 1.95                     | 0.49              |
| 1:G:446:THR:O    | 1:G:447:ASP:OD2  | 2.31                     | 0.49              |
| 1:H:80:GLU:HA    | 1:H:83:LEU:CB    | 2.39                     | 0.49              |
| 1:K:182:SER:HA   | 1:K:190:TRP:O    | 2.13                     | 0.49              |
| 1:K:369:GLU:HG2  | 1:K:373:HIS:CE1  | 2.48                     | 0.49              |
| 1:K:514:LEU:CD1  | 1:K:521:LEU:HD11 | 2.42                     | 0.49              |
| 1:L:80:GLU:HG2   | 1:L:114:ARG:NH2  | 2.27                     | 0.49              |
| 1:L:208:ARG:O    | 1:L:212:ILE:HG13 | 2.12                     | 0.49              |
| 1:L:223:PRO:HB2  | 1:L:224:ILE:HD12 | 1.94                     | 0.49              |
| 1:A:124:VAL:O    | 1:A:161:LEU:HB2  | 2.12                     | 0.49              |
| 1:B:292:ILE:HD12 | 1:B:316:ASN:OD1  | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:460:VAL:HG12 | 1:B:461:HIS:N    | 2.28                     | 0.49              |
| 1:H:85:ARG:HH21  | 1:H:178:PHE:CA   | 2.25                     | 0.49              |
| 1:H:312:ARG:HA   | 1:H:312:ARG:NE   | 2.27                     | 0.49              |
| 1:K:329:ARG:HA   | 1:K:373:HIS:CE1  | 2.48                     | 0.49              |
| 1:L:81:GLU:HB2   | 1:L:196:MET:HE1  | 1.94                     | 0.49              |
| 1:L:125:PHE:HA   | 1:L:160:ARG:HA   | 1.94                     | 0.49              |
| 1:A:289:VAL:O    | 1:A:289:VAL:HG23 | 2.11                     | 0.48              |
| 1:A:449:GLU:O    | 1:A:453:ARG:HG3  | 2.13                     | 0.48              |
| 1:B:34:THR:O     | 1:B:64:VAL:N     | 2.45                     | 0.48              |
| 1:B:44:VAL:HG21  | 1:B:63:ARG:HH11  | 1.77                     | 0.48              |
| 1:G:64:VAL:HB    | 1:G:192:ARG:NH2  | 2.28                     | 0.48              |
| 1:G:85:ARG:HA    | 1:G:88:LEU:CG    | 2.43                     | 0.48              |
| 1:H:5:LEU:CD2    | 1:H:31:HIS:HB2   | 2.43                     | 0.48              |
| 1:H:84:TRP:HB3   | 1:H:198:LEU:HD21 | 1.94                     | 0.48              |
| 1:H:523:GLU:OE1  | 1:H:525:GLN:N    | 2.46                     | 0.48              |
| 1:K:15:VAL:HB    | 1:K:16:PRO:HD3   | 1.94                     | 0.48              |
| 1:K:167:TRP:HZ2  | 1:K:209:SER:CB   | 2.25                     | 0.48              |
| 1:L:167:TRP:HE3  | 1:L:168:PRO:CD   | 2.23                     | 0.48              |
| 1:A:468:VAL:O    | 1:A:468:VAL:CG1  | 2.61                     | 0.48              |
| 1:A:472:TRP:HD1  | 1:A:495:LEU:HD21 | 1.75                     | 0.48              |
| 1:B:17:GLU:HA    | 1:B:20:GLN:OE1   | 2.13                     | 0.48              |
| 1:B:397:ARG:CD   | 1:B:443:MET:HE3  | 2.34                     | 0.48              |
| 1:G:41:SER:HA    | 1:G:63:ARG:NH1   | 2.15                     | 0.48              |
| 1:G:471:ILE:O    | 1:G:475:VAL:HG23 | 2.13                     | 0.48              |
| 1:H:201:HIS:O    | 1:H:205:VAL:HG23 | 2.13                     | 0.48              |
| 1:K:397:ARG:HD2  | 1:K:433:GLY:HA3  | 1.94                     | 0.48              |
| 1:L:224:ILE:HB   | 1:L:227:LEU:HG   | 1.95                     | 0.48              |
| 1:A:119:PHE:CE1  | 1:A:173:LEU:HD12 | 2.40                     | 0.48              |
| 1:A:169:GLN:HE22 | 1:A:208:ARG:NH1  | 2.11                     | 0.48              |
| 1:A:484:GLY:O    | 1:A:485:HIS:HB2  | 2.13                     | 0.48              |
| 1:B:14:VAL:HG23  | 1:B:15:VAL:N     | 2.28                     | 0.48              |
| 1:B:15:VAL:N     | 1:B:16:PRO:HD2   | 2.28                     | 0.48              |
| 1:B:280:ALA:HB2  | 1:B:327:CYS:SG   | 2.53                     | 0.48              |
| 1:B:301:PRO:HG2  | 1:B:515:GLN:HA   | 1.95                     | 0.48              |
| 1:B:401:GLY:O    | 1:B:403:ARG:HG2  | 2.12                     | 0.48              |
| 1:B:461:HIS:O    | 1:B:462:ALA:C    | 2.55                     | 0.48              |
| 1:G:491:ARG:N    | 1:G:491:ARG:HD2  | 2.28                     | 0.48              |
| 1:H:385:ARG:NH1  | 1:H:385:ARG:HB3  | 2.28                     | 0.48              |
| 1:H:474:ALA:HA   | 1:H:478:LEU:HD12 | 1.95                     | 0.48              |
| 1:K:36:ALA:HA    | 1:K:63:ARG:HH11  | 1.78                     | 0.48              |
| 1:K:516:ILE:HG13 | 1:K:517:LYS:N    | 2.28                     | 0.48              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:A:12:TRP:CH2     | 1:A:144:LEU:HD22 | 2.49                     | 0.48              |
| 1:B:467:ASP:O      | 1:B:468:VAL:HG22 | 2.14                     | 0.48              |
| 1:G:19:MET:SD      | 1:G:30:VAL:HG11  | 2.54                     | 0.48              |
| 1:G:487:LEU:HD13   | 1:G:519:PHE:CZ   | 2.48                     | 0.48              |
| 1:G:544:THR:HG23   | 1:G:583:ALA:HB2  | 1.96                     | 0.48              |
| 1:H:150:ALA:HA     | 1:H:153:THR:OG1  | 2.13                     | 0.48              |
| 1:A:218:GLY:HA3    | 1:A:221:GLU:OE2  | 2.12                     | 0.48              |
| 1:A:372:ASN:O      | 1:A:376:GLN:HG2  | 2.13                     | 0.48              |
| 1:A:376:GLN:O      | 1:A:380:GLU:OE1  | 2.31                     | 0.48              |
| 1:A:403:ARG:HH21   | 1:A:444:PHE:HE1  | 1.61                     | 0.48              |
| 1:G:501:GLU:OE2    | 1:H:481:ARG:NH1  | 2.47                     | 0.48              |
| 1:K:397:ARG:HA     | 1:K:406:ILE:HD11 | 1.95                     | 0.48              |
| 1:B:1:MET:CG       | 1:B:3:ILE:HD11   | 2.43                     | 0.48              |
| 1:B:4:LEU:O        | 1:B:5:LEU:HD23   | 2.13                     | 0.48              |
| 1:G:16:PRO:HB2     | 1:G:147:VAL:CG1  | 2.43                     | 0.48              |
| 1:G:16:PRO:CB      | 1:G:147:VAL:HG11 | 2.43                     | 0.48              |
| 1:K:12:TRP:CZ2     | 1:K:144:LEU:HD22 | 2.48                     | 0.48              |
| 1:L:346:TYR:OH     | 1:L:348:GLU:OE2  | 2.17                     | 0.48              |
| 1:A:443:MET:SD     | 1:A:444:PHE:N    | 2.81                     | 0.48              |
| 1:A:509:CYS:HB2    | 1:A:512:ALA:HB3  | 1.96                     | 0.48              |
| 1:K:233:SER:HA     | 1:K:236:ARG:HE   | 1.79                     | 0.48              |
| 1:K:256:LYS:NZ     | 1:K:342:ASP:O    | 2.47                     | 0.48              |
| 1:K:472[A]:TRP:CZ3 | 1:K:495:LEU:HB2  | 2.48                     | 0.48              |
| 1:A:12:TRP:HE3     | 1:A:47:LEU:HG    | 1.78                     | 0.48              |
| 1:A:353:PRO:HG2    | 1:A:412:LEU:CD2  | 2.43                     | 0.48              |
| 1:A:431:LEU:HD21   | 1:A:448:PHE:CZ   | 2.49                     | 0.48              |
| 1:B:3:ILE:HD13     | 1:B:96:HIS:CG    | 2.48                     | 0.48              |
| 1:B:128:LEU:HD23   | 2:D:709:A:HO2'   | 1.78                     | 0.48              |
| 1:G:8:VAL:HG21     | 1:G:47:LEU:CD1   | 2.44                     | 0.48              |
| 1:K:97:ARG:HB3     | 1:K:121:ALA:CB   | 2.44                     | 0.48              |
| 1:K:511:TYR:HE1    | 1:K:563:LEU:HB2  | 1.78                     | 0.48              |
| 1:L:34:THR:O       | 1:L:63:ARG:HA    | 2.13                     | 0.48              |
| 1:L:172:LEU:HG     | 1:L:172:LEU:O    | 2.13                     | 0.48              |
| 1:L:197:ARG:HA     | 1:L:200:GLN:NE2  | 2.29                     | 0.48              |
| 1:L:433:GLY:O      | 1:L:434:PHE:CB   | 2.61                     | 0.48              |
| 1:L:458:VAL:O      | 1:L:480:ALA:HA   | 2.14                     | 0.48              |
| 1:A:42:PRO:HA      | 1:A:45:GLU:OE1   | 2.13                     | 0.48              |
| 1:B:12:TRP:CH2     | 1:B:46:GLN:HB3   | 2.48                     | 0.48              |
| 1:G:464:GLU:OE1    | 1:G:464:GLU:HA   | 2.14                     | 0.48              |
| 1:H:242:LEU:HD22   | 1:H:576:VAL:HG21 | 1.94                     | 0.48              |
| 1:H:277:ARG:HH22   | 1:H:288:PRO:HA   | 1.78                     | 0.48              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:K:397:ARG:CD     | 1:K:433:GLY:HA3  | 2.44                     | 0.48              |
| 1:A:17:GLU:HB3     | 1:A:127:VAL:HG21 | 1.96                     | 0.48              |
| 1:A:97:ARG:O       | 1:A:122:CYS:N    | 2.46                     | 0.48              |
| 1:A:174:SER:CB     | 1:A:176:PRO:HD2  | 2.43                     | 0.48              |
| 1:A:454:VAL:CG2    | 1:A:456:LEU:HD13 | 2.44                     | 0.48              |
| 1:B:67:PHE:CE1     | 1:B:75:ASP:HB3   | 2.49                     | 0.48              |
| 1:G:127:VAL:HG23   | 1:G:158:PHE:CE1  | 2.49                     | 0.48              |
| 1:G:134:GLY:HA3    | 1:G:139:ARG:NH2  | 2.29                     | 0.48              |
| 1:G:397:ARG:CB     | 1:G:433:GLY:HA3  | 2.42                     | 0.48              |
| 1:H:4:LEU:CB       | 1:H:30:VAL:HG12  | 2.27                     | 0.48              |
| 1:H:196:MET:SD     | 1:H:196:MET:O    | 2.71                     | 0.48              |
| 1:K:167:TRP:HD1    | 1:K:170:LEU:HG   | 1.75                     | 0.48              |
| 1:K:524:GLU:HG2    | 1:K:525:GLN:N    | 2.29                     | 0.48              |
| 1:L:322:LEU:HD23   | 1:L:328:LEU:HD12 | 1.95                     | 0.48              |
| 1:A:93:GLN:HB2     | 1:A:96:HIS:HD2   | 1.79                     | 0.47              |
| 1:A:521:LEU:HD23   | 1:A:566:ARG:HH12 | 1.78                     | 0.47              |
| 1:B:87:LEU:HD21    | 1:B:97:ARG:CZ    | 2.44                     | 0.47              |
| 1:B:102:ALA:HA     | 1:B:126:HIS:HE1  | 1.79                     | 0.47              |
| 1:G:318:GLY:CA     | 1:G:322:LEU:HD23 | 2.45                     | 0.47              |
| 1:H:245:VAL:HG13   | 1:H:246:GLN:OE1  | 2.12                     | 0.47              |
| 1:K:77:MET:O       | 1:K:80:GLU:HG2   | 2.13                     | 0.47              |
| 1:L:4:LEU:CB       | 1:L:30:VAL:HG12  | 2.41                     | 0.47              |
| 1:L:577:LEU:O      | 1:L:581:VAL:HG23 | 2.14                     | 0.47              |
| 1:B:177:SER:C      | 1:B:178:PHE:HD1  | 2.21                     | 0.47              |
| 1:B:467:ASP:C      | 1:B:469:GLU:H    | 2.19                     | 0.47              |
| 1:G:141:ALA:CA     | 1:G:146:GLU:HB3  | 2.44                     | 0.47              |
| 1:H:609:ASP:C      | 1:H:610:THR:HG23 | 2.39                     | 0.47              |
| 1:A:12:TRP:CE3     | 1:A:47:LEU:HG    | 2.50                     | 0.47              |
| 1:A:65:GLN:HG3     | 1:A:191:VAL:O    | 2.13                     | 0.47              |
| 1:A:233:SER:HA     | 1:A:236:ARG:HH12 | 1.79                     | 0.47              |
| 1:A:237:TRP:CG     | 1:A:610:THR:HG22 | 2.49                     | 0.47              |
| 1:H:472[A]:TRP:CZ2 | 1:H:495:LEU:HD13 | 2.50                     | 0.47              |
| 1:K:33:LEU:HD12    | 1:K:34:THR:N     | 2.29                     | 0.47              |
| 1:K:101:LEU:CD1    | 1:K:126:HIS:HB2  | 2.44                     | 0.47              |
| 1:L:1:MET:HA       | 1:L:28:ASP:OD2   | 2.14                     | 0.47              |
| 1:L:83:LEU:HD12    | 1:L:86:TRP:CE3   | 2.48                     | 0.47              |
| 1:L:86:TRP:CA      | 1:L:180:LEU:HD22 | 2.45                     | 0.47              |
| 1:L:192:ARG:HG2    | 1:L:193:ALA:H    | 1.79                     | 0.47              |
| 1:L:545:LEU:HD12   | 1:L:561:LEU:CD2  | 2.42                     | 0.47              |
| 1:A:304:PRO:HB3    | 1:A:517:LYS:O    | 2.14                     | 0.47              |
| 1:A:563:LEU:O      | 1:A:563:LEU:HD23 | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:78:LEU:HA    | 1:B:196:MET:CE   | 2.44                     | 0.47              |
| 1:B:610:THR:HG22 | 1:B:610:THR:O    | 2.14                     | 0.47              |
| 1:H:396:THR:OG1  | 1:H:432:ALA:HB3  | 2.14                     | 0.47              |
| 1:K:435:GLU:HG2  | 1:K:462:ALA:HB1  | 1.94                     | 0.47              |
| 1:K:466:ASP:OD1  | 1:K:488:HIS:NE2  | 2.48                     | 0.47              |
| 1:L:31:HIS:CD2   | 1:L:90:ARG:HD2   | 2.50                     | 0.47              |
| 1:L:183:THR:N    | 1:L:190:TRP:O    | 2.40                     | 0.47              |
| 1:L:454:VAL:O    | 1:L:454:VAL:HG12 | 2.14                     | 0.47              |
| 1:B:116:ALA:O    | 1:B:120:GLY:N    | 2.46                     | 0.47              |
| 1:B:303:GLU:CD   | 1:B:304:PRO:HD2  | 2.40                     | 0.47              |
| 1:B:394:THR:HG21 | 6:B:802:HOH:O    | 2.13                     | 0.47              |
| 1:B:397:ARG:HH11 | 1:B:406:ILE:CD1  | 2.26                     | 0.47              |
| 1:H:12:TRP:HB3   | 1:H:43:GLY:HA3   | 1.95                     | 0.47              |
| 1:H:245:VAL:HG13 | 1:H:246:GLN:N    | 2.29                     | 0.47              |
| 1:H:333:ARG:HG2  | 1:H:333:ARG:NH1  | 2.30                     | 0.47              |
| 1:H:365:VAL:O    | 1:H:369:GLU:HG3  | 2.15                     | 0.47              |
| 1:H:459:THR:HG23 | 1:H:459:THR:O    | 2.13                     | 0.47              |
| 1:K:84:TRP:HZ3   | 1:K:199:ARG:HA   | 1.79                     | 0.47              |
| 1:K:255:PRO:HA   | 1:K:343:HIS:O    | 2.14                     | 0.47              |
| 1:L:245:VAL:HG23 | 1:L:246:GLN:N    | 2.29                     | 0.47              |
| 1:A:363:PRO:HG2  | 1:H:418:GLU:OE2  | 2.14                     | 0.47              |
| 1:B:68:GLU:HG2   | 1:B:69:ASP:OD1   | 2.15                     | 0.47              |
| 1:B:73:GLU:O     | 1:B:77:MET:SD    | 2.73                     | 0.47              |
| 1:B:356:TYR:HB2  | 1:B:366:VAL:HG11 | 1.97                     | 0.47              |
| 1:H:337:GLU:OE1  | 1:H:337:GLU:HA   | 2.15                     | 0.47              |
| 1:K:4:LEU:HD12   | 1:K:98:TYR:C     | 2.39                     | 0.47              |
| 1:K:12:TRP:O     | 1:K:47:LEU:HD21  | 2.14                     | 0.47              |
| 1:K:63:ARG:N     | 1:K:189:HIS:O    | 2.45                     | 0.47              |
| 1:K:200:GLN:O    | 1:K:203:GLU:HB3  | 2.14                     | 0.47              |
| 1:K:233:SER:O    | 1:K:236:ARG:HG2  | 2.14                     | 0.47              |
| 1:A:4:LEU:HD23   | 1:A:19:MET:HE1   | 1.97                     | 0.47              |
| 1:A:16:PRO:HB2   | 1:A:147:VAL:HG11 | 1.95                     | 0.47              |
| 1:A:65:GLN:CG    | 1:A:190:TRP:HB3  | 2.44                     | 0.47              |
| 1:A:87:LEU:HD21  | 1:A:97:ARG:CD    | 2.45                     | 0.47              |
| 1:A:228:ALA:HB3  | 1:B:216:TRP:CH2  | 2.50                     | 0.47              |
| 1:B:147:VAL:O    | 1:B:151:ILE:HG13 | 2.15                     | 0.47              |
| 1:B:223:PRO:HB3  | 1:B:578:LYS:HD2  | 1.97                     | 0.47              |
| 1:B:469:GLU:OE1  | 1:B:469:GLU:HA   | 2.14                     | 0.47              |
| 1:G:17:GLU:HB3   | 1:G:127:VAL:CG2  | 2.28                     | 0.47              |
| 1:G:35:THR:HG22  | 1:G:67:PHE:CE2   | 2.50                     | 0.47              |
| 1:G:46:GLN:HA    | 1:G:49:ARG:CD    | 2.45                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:46:GLN:O     | 1:G:49:ARG:HG2   | 2.14                     | 0.47              |
| 1:G:84:TRP:CZ3   | 1:G:199:ARG:HG2  | 2.49                     | 0.47              |
| 1:G:533:LEU:HB3  | 1:G:568:CYS:SG   | 2.55                     | 0.47              |
| 1:H:109:SER:O    | 1:H:112:MET:HG3  | 2.15                     | 0.47              |
| 1:H:311:MET:HE1  | 3:H:703:ATP:N9   | 2.30                     | 0.47              |
| 1:K:86:TRP:CD1   | 1:K:90:ARG:HG3   | 2.49                     | 0.47              |
| 1:K:209:SER:HB3  | 1:L:213:LEU:CD1  | 2.44                     | 0.47              |
| 1:K:230:TRP:CH2  | 1:K:607:PRO:HD3  | 2.50                     | 0.47              |
| 1:K:348:GLU:HA   | 1:K:390:ASN:O    | 2.15                     | 0.47              |
| 1:L:12:TRP:CZ2   | 1:L:46:GLN:HG2   | 2.49                     | 0.47              |
| 1:L:198:LEU:O    | 1:L:202:VAL:HG23 | 2.15                     | 0.47              |
| 1:L:241:PRO:HA   | 1:L:572:THR:HA   | 1.97                     | 0.47              |
| 1:L:261:CYS:HA   | 1:L:548:ASP:O    | 2.14                     | 0.47              |
| 1:L:432:ALA:HB2  | 1:L:461:HIS:CD2  | 2.50                     | 0.47              |
| 1:A:170:LEU:HD22 | 1:A:173:LEU:HD11 | 1.97                     | 0.47              |
| 1:A:584:ALA:HB2  | 1:A:601:LEU:HD11 | 1.97                     | 0.47              |
| 1:B:84:TRP:HE1   | 1:B:115:ALA:HB2  | 1.80                     | 0.47              |
| 1:B:449:GLU:N    | 1:B:450:PRO:HD2  | 2.30                     | 0.47              |
| 1:G:67:PHE:HB2   | 1:G:78:LEU:HD22  | 1.97                     | 0.47              |
| 1:G:126:HIS:O    | 1:G:158:PHE:HA   | 2.14                     | 0.47              |
| 1:K:33:LEU:HB2   | 1:K:86:TRP:CE2   | 2.50                     | 0.47              |
| 1:G:101:LEU:CG   | 1:G:126:HIS:HB2  | 2.45                     | 0.47              |
| 1:G:319:SER:O    | 1:G:323:LYS:HG3  | 2.15                     | 0.47              |
| 1:K:257:VAL:HG13 | 1:K:346:TYR:HB3  | 1.96                     | 0.47              |
| 1:L:349:ILE:O    | 1:L:391:LEU:HA   | 2.14                     | 0.47              |
| 1:A:87:LEU:HD21  | 1:A:97:ARG:NH1   | 2.30                     | 0.47              |
| 1:A:376:GLN:O    | 1:A:379:GLU:N    | 2.48                     | 0.47              |
| 1:A:606:VAL:HG12 | 1:A:607:PRO:O    | 2.14                     | 0.47              |
| 1:B:19:MET:SD    | 1:B:30:VAL:HG21  | 2.54                     | 0.47              |
| 1:B:34:THR:C     | 1:B:63:ARG:HA    | 2.40                     | 0.47              |
| 1:B:61:ILE:HB    | 1:B:188:VAL:HG12 | 1.97                     | 0.47              |
| 1:B:182:SER:HA   | 1:B:190:TRP:O    | 2.15                     | 0.47              |
| 1:B:397:ARG:HE   | 1:B:439:THR:HB   | 1.79                     | 0.47              |
| 1:G:62:SER:HA    | 1:G:189:HIS:O    | 2.15                     | 0.47              |
| 1:G:228:ALA:HB3  | 1:H:216:TRP:CH2  | 2.50                     | 0.47              |
| 1:H:1:MET:O      | 1:H:2:ARG:HG3    | 2.14                     | 0.47              |
| 1:H:4:LEU:HD11   | 1:H:125:PHE:CZ   | 2.50                     | 0.47              |
| 1:H:127:VAL:HG23 | 1:H:158:PHE:CE1  | 2.50                     | 0.47              |
| 1:A:6:CYS:SG     | 1:A:100:CYS:HB3  | 2.55                     | 0.46              |
| 1:A:304:PRO:HB3  | 1:A:517:LYS:C    | 2.39                     | 0.46              |
| 1:B:237:TRP:CZ3  | 1:B:607:PRO:HG3  | 2.49                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:49:ARG:CG    | 1:G:144:LEU:HD11 | 2.44                     | 0.46              |
| 1:G:364:TRP:HE3  | 1:G:412:LEU:HD11 | 1.80                     | 0.46              |
| 1:G:397:ARG:NH1  | 1:G:434:PHE:HA   | 2.30                     | 0.46              |
| 1:G:533:LEU:CD1  | 1:G:545:LEU:HD21 | 2.45                     | 0.46              |
| 1:H:571:ILE:HG23 | 1:H:571:ILE:O    | 2.16                     | 0.46              |
| 1:K:324:ASP:OD1  | 1:K:325:PRO:HD2  | 2.16                     | 0.46              |
| 1:K:449:GLU:O    | 1:K:453:ARG:HG3  | 2.15                     | 0.46              |
| 1:L:127:VAL:CG2  | 1:L:156:LEU:HD11 | 2.36                     | 0.46              |
| 1:L:146:GLU:HA   | 1:L:149:GLN:NE2  | 2.19                     | 0.46              |
| 1:L:182:SER:HA   | 1:L:191:VAL:HA   | 1.96                     | 0.46              |
| 1:L:292:ILE:CD1  | 1:L:315:ASP:HB2  | 2.43                     | 0.46              |
| 1:A:248:LYS:HG3  | 1:A:562:LEU:CD1  | 2.46                     | 0.46              |
| 1:G:41:SER:CA    | 1:G:63:ARG:HH12  | 2.17                     | 0.46              |
| 1:G:85:ARG:HA    | 1:G:88:LEU:HG    | 1.97                     | 0.46              |
| 1:G:101:LEU:HD12 | 1:G:126:HIS:HD1  | 1.80                     | 0.46              |
| 1:H:180:LEU:HD11 | 1:H:193:ALA:HA   | 1.97                     | 0.46              |
| 1:K:63:ARG:HD2   | 1:K:190:TRP:CZ3  | 2.50                     | 0.46              |
| 1:K:594:ARG:O    | 1:K:597:LEU:N    | 2.46                     | 0.46              |
| 1:L:12:TRP:NE1   | 1:L:142:SER:O    | 2.40                     | 0.46              |
| 1:L:549:ASN:CB   | 1:L:552:ILE:HD12 | 2.46                     | 0.46              |
| 1:A:237:TRP:CZ3  | 1:A:607:PRO:HG3  | 2.51                     | 0.46              |
| 1:B:131:PRO:HB2  | 1:B:138:ASN:O    | 2.14                     | 0.46              |
| 1:G:318:GLY:O    | 1:G:322:LEU:HB2  | 2.16                     | 0.46              |
| 1:K:167:TRP:CD1  | 1:K:169:GLN:H    | 2.32                     | 0.46              |
| 1:L:2:ARG:HD2    | 1:L:22:LEU:HD11  | 1.97                     | 0.46              |
| 1:A:106:LYS:NZ   | 2:C:708:A23:H4'  | 2.31                     | 0.46              |
| 1:G:94:ALA:HA    | 1:G:97:ARG:NE    | 2.30                     | 0.46              |
| 1:G:298:TRP:CG   | 1:G:299:PRO:HA   | 2.50                     | 0.46              |
| 1:G:554:GLN:O    | 1:G:554:GLN:HG2  | 2.15                     | 0.46              |
| 1:H:384:ASP:OD1  | 1:H:385:ARG:HG3  | 2.15                     | 0.46              |
| 1:H:511:TYR:CE1  | 1:H:563:LEU:HD22 | 2.51                     | 0.46              |
| 1:K:97:ARG:HD2   | 1:K:121:ALA:HB2  | 1.97                     | 0.46              |
| 1:K:237:TRP:HA   | 1:K:240:GLU:OE1  | 2.16                     | 0.46              |
| 1:K:460:VAL:CG2  | 1:K:480:ALA:HB2  | 2.44                     | 0.46              |
| 1:L:240:GLU:C    | 1:L:572:THR:HG22 | 2.41                     | 0.46              |
| 1:A:572:THR:O    | 1:A:575:GLU:N    | 2.41                     | 0.46              |
| 1:B:12:TRP:HZ2   | 1:B:143:THR:HA   | 1.81                     | 0.46              |
| 1:B:65:GLN:HG2   | 1:B:66:ASP:N     | 2.31                     | 0.46              |
| 1:B:534:ARG:NH2  | 1:B:570:GLY:O    | 2.49                     | 0.46              |
| 1:B:590:ASN:OD1  | 1:B:590:ASN:C    | 2.58                     | 0.46              |
| 1:G:354:ALA:HB3  | 1:G:409:HIS:NE2  | 2.30                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:21:LEU:HD22  | 1:K:125:PHE:CD1  | 2.51                     | 0.46              |
| 1:K:113:GLN:OE1  | 1:K:124:VAL:HG11 | 2.15                     | 0.46              |
| 1:K:237:TRP:O    | 1:K:573:ARG:NH1  | 2.43                     | 0.46              |
| 1:A:572:THR:O    | 1:A:575:GLU:HB2  | 2.15                     | 0.46              |
| 1:B:41:SER:N     | 1:B:42:PRO:HD2   | 2.30                     | 0.46              |
| 1:B:431:LEU:HD23 | 1:B:478:LEU:HD13 | 1.98                     | 0.46              |
| 1:G:123:GLU:OE2  | 1:G:162:GLY:N    | 2.49                     | 0.46              |
| 1:K:318:GLY:O    | 1:K:322:LEU:HD13 | 2.16                     | 0.46              |
| 1:L:77:MET:HE1   | 1:L:199:ARG:NH2  | 2.30                     | 0.46              |
| 1:A:319:SER:HB2  | 1:A:355:ASN:HB3  | 1.97                     | 0.46              |
| 1:A:468:VAL:O    | 1:A:468:VAL:HG12 | 2.15                     | 0.46              |
| 1:A:575:GLU:OE1  | 1:A:578:LYS:HD2  | 2.15                     | 0.46              |
| 1:B:17:GLU:CB    | 1:B:156:LEU:HD21 | 2.45                     | 0.46              |
| 1:B:99:ILE:HD12  | 1:B:116:ALA:CB   | 2.45                     | 0.46              |
| 1:B:406:ILE:O    | 1:B:410:LEU:HD13 | 2.16                     | 0.46              |
| 2:D:709:A:HO2'   | 2:D:710:A23:P    | 2.37                     | 0.46              |
| 1:G:22:LEU:HD13  | 1:G:27:PHE:CZ    | 2.50                     | 0.46              |
| 1:G:247:ASP:O    | 1:G:251:VAL:HG23 | 2.16                     | 0.46              |
| 1:G:543:VAL:HG12 | 1:G:544:THR:N    | 2.31                     | 0.46              |
| 2:I:717:A:C1'    | 2:I:718:A23:P    | 3.03                     | 0.46              |
| 1:B:223:PRO:HB2  | 1:B:224:ILE:HD12 | 1.96                     | 0.46              |
| 1:G:39:LYS:HZ1   | 1:G:40:ILE:HD11  | 1.81                     | 0.46              |
| 1:H:6:CYS:N      | 1:H:31:HIS:O     | 2.40                     | 0.46              |
| 1:H:22:LEU:HG    | 1:H:27:PHE:CZ    | 2.51                     | 0.46              |
| 1:H:536:TYR:HB3  | 1:H:543:VAL:CG2  | 2.46                     | 0.46              |
| 1:K:12:TRP:CE3   | 1:K:47:LEU:HG    | 2.50                     | 0.46              |
| 1:K:33:LEU:HD22  | 1:K:86:TRP:CD2   | 2.50                     | 0.46              |
| 1:L:114:ARG:CD   | 1:L:118:LEU:HD22 | 2.46                     | 0.46              |
| 1:L:178:PHE:CD2  | 1:L:198:LEU:HD12 | 2.50                     | 0.46              |
| 1:L:371:ARG:HG3  | 1:L:420:TRP:CE3  | 2.51                     | 0.46              |
| 1:L:406:ILE:O    | 1:L:406:ILE:HG22 | 2.15                     | 0.46              |
| 1:B:6:CYS:SG     | 1:B:15:VAL:HG13  | 2.56                     | 0.46              |
| 1:B:371:ARG:HD3  | 1:B:371:ARG:C    | 2.41                     | 0.46              |
| 1:B:556:SER:O    | 1:B:560:ASN:ND2  | 2.44                     | 0.46              |
| 1:G:53:MET:HE1   | 1:G:144:LEU:HD13 | 1.97                     | 0.46              |
| 1:H:6:CYS:HB2    | 1:H:32:VAL:HG22  | 1.98                     | 0.46              |
| 1:H:116:ALA:CB   | 1:H:164:GLU:HG3  | 2.46                     | 0.46              |
| 1:H:276:VAL:HA   | 1:H:330:ALA:CB   | 2.46                     | 0.46              |
| 1:H:545:LEU:HD12 | 1:H:561:LEU:CD2  | 2.45                     | 0.46              |
| 1:K:394:THR:OG1  | 6:K:801:HOH:O    | 2.00                     | 0.46              |
| 1:L:275:LYS:HE2  | 1:L:334:LEU:HD21 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:12:TRP:HB2   | 1:A:47:LEU:HG    | 1.98                     | 0.46              |
| 1:A:234:HIS:HD2  | 1:A:607:PRO:HD2  | 1.81                     | 0.46              |
| 1:A:256:LYS:HA   | 1:A:580:GLN:HE21 | 1.81                     | 0.46              |
| 1:A:520:PRO:HG2  | 1:A:529:GLU:HB3  | 1.96                     | 0.46              |
| 1:G:8:VAL:HG21   | 1:G:47:LEU:HD11  | 1.98                     | 0.46              |
| 1:G:22:LEU:HD13  | 1:G:27:PHE:CE1   | 2.51                     | 0.46              |
| 1:H:64:VAL:HG11  | 1:H:67:PHE:HB3   | 1.98                     | 0.46              |
| 1:H:178:PHE:CD2  | 1:H:198:LEU:HD13 | 2.43                     | 0.46              |
| 1:H:350:ARG:HA   | 1:H:392:LEU:O    | 2.16                     | 0.46              |
| 1:K:64:VAL:HG23  | 1:K:64:VAL:O     | 2.16                     | 0.46              |
| 1:K:511:TYR:HB3  | 1:K:515:GLN:HE22 | 1.80                     | 0.46              |
| 1:L:30:VAL:HG22  | 1:L:59:PHE:CE1   | 2.50                     | 0.46              |
| 1:B:275:LYS:O    | 1:B:279:GLU:HG2  | 2.16                     | 0.45              |
| 1:B:464:GLU:O    | 1:B:464:GLU:HG3  | 2.17                     | 0.45              |
| 1:B:524:GLU:HG2  | 1:B:525:GLN:N    | 2.29                     | 0.45              |
| 1:H:21:LEU:HA    | 1:H:158:PHE:CE2  | 2.51                     | 0.45              |
| 1:H:63:ARG:HH12  | 1:H:188:VAL:CB   | 2.19                     | 0.45              |
| 1:H:554:GLN:HG2  | 1:H:554:GLN:O    | 2.17                     | 0.45              |
| 1:K:40:ILE:O     | 1:K:44:VAL:HG23  | 2.15                     | 0.45              |
| 1:L:200:GLN:O    | 1:L:203:GLU:HG2  | 2.16                     | 0.45              |
| 1:L:250:TRP:CH2  | 1:L:577:LEU:HD21 | 2.51                     | 0.45              |
| 1:B:50:TYR:HA    | 1:B:53:MET:CE    | 2.41                     | 0.45              |
| 1:B:121:ALA:H    | 1:B:164:GLU:CB   | 2.29                     | 0.45              |
| 1:B:282:ASN:ND2  | 1:B:285:SER:HB3  | 2.31                     | 0.45              |
| 1:B:333:ARG:O    | 1:B:337:GLU:HG2  | 2.16                     | 0.45              |
| 1:G:4:LEU:HA     | 1:G:98:TYR:O     | 2.15                     | 0.45              |
| 1:G:81:GLU:OE2   | 1:G:85:ARG:NE    | 2.49                     | 0.45              |
| 1:G:116:ALA:HB1  | 1:G:121:ALA:CB   | 2.47                     | 0.45              |
| 1:G:258:GLU:O    | 1:G:347:ALA:HA   | 2.15                     | 0.45              |
| 1:G:286:LEU:HD23 | 1:G:286:LEU:H    | 1.81                     | 0.45              |
| 1:G:329:ARG:HB3  | 1:G:373:HIS:NE2  | 2.31                     | 0.45              |
| 1:G:361:ARG:NH2  | 1:G:369:GLU:OE1  | 2.42                     | 0.45              |
| 1:G:457:ALA:HB1  | 1:G:588:PHE:CZ   | 2.51                     | 0.45              |
| 1:H:65:GLN:HG2   | 1:H:190:TRP:CE3  | 2.48                     | 0.45              |
| 1:A:52:GLU:HA    | 1:A:52:GLU:OE1   | 2.17                     | 0.45              |
| 1:A:101:LEU:HA   | 1:A:112:MET:CE   | 2.46                     | 0.45              |
| 1:A:398:GLU:CB   | 1:A:401:GLY:HA3  | 2.47                     | 0.45              |
| 1:B:84:TRP:HZ3   | 1:B:199:ARG:HA   | 1.82                     | 0.45              |
| 1:K:17:GLU:O     | 1:K:158:PHE:HZ   | 1.99                     | 0.45              |
| 1:K:125:PHE:HB2  | 1:K:159:VAL:O    | 2.16                     | 0.45              |
| 1:K:169:GLN:OE1  | 1:K:205:VAL:HG13 | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:271:GLU:O    | 1:K:275:LYS:HG3  | 2.16                     | 0.45              |
| 1:K:497:ARG:HH21 | 1:L:455:GLY:HA3  | 1.81                     | 0.45              |
| 1:A:15:VAL:HB    | 1:A:16:PRO:HD3   | 1.98                     | 0.45              |
| 1:G:29:GLU:CD    | 1:G:58:ARG:HB3   | 2.41                     | 0.45              |
| 1:G:185:GLN:O    | 1:G:188:VAL:HG22 | 2.16                     | 0.45              |
| 1:G:492:SER:OG   | 1:G:495:LEU:HB3  | 2.17                     | 0.45              |
| 1:K:65:GLN:HG2   | 1:K:190:TRP:CE3  | 2.49                     | 0.45              |
| 1:K:103:GLY:HA2  | 2:N:730:A23:O1C  | 2.17                     | 0.45              |
| 1:K:223:PRO:HB2  | 1:K:581:VAL:HG21 | 1.97                     | 0.45              |
| 1:K:273:LEU:O    | 1:K:277:ARG:HG3  | 2.17                     | 0.45              |
| 1:K:496:LEU:HD21 | 1:K:539:ALA:HB3  | 1.99                     | 0.45              |
| 1:L:471:ILE:HG23 | 1:L:483:LEU:HD13 | 1.98                     | 0.45              |
| 1:A:36:ALA:CA    | 1:A:63:ARG:HH11  | 2.26                     | 0.45              |
| 1:A:82:VAL:HG22  | 1:A:193:ALA:HB2  | 1.98                     | 0.45              |
| 1:A:84:TRP:HE3   | 1:A:198:LEU:HD22 | 1.82                     | 0.45              |
| 1:B:104:GLY:HA2  | 2:C:708:A23:N3   | 2.31                     | 0.45              |
| 1:B:178:PHE:CE2  | 1:B:198:LEU:HA   | 2.51                     | 0.45              |
| 1:B:362:SER:OG   | 1:K:419:HIS:HD2  | 1.99                     | 0.45              |
| 1:G:106:LYS:HE2  | 1:H:101:LEU:CD1  | 2.46                     | 0.45              |
| 1:G:459:THR:OG1  | 6:G:2004:HOH:O   | 2.21                     | 0.45              |
| 1:H:364:TRP:HZ3  | 1:H:416:ALA:HB2  | 1.80                     | 0.45              |
| 1:K:2:ARG:HD2    | 1:K:98:TYR:OH    | 2.17                     | 0.45              |
| 1:L:85:ARG:HB2   | 1:L:180:LEU:HD13 | 1.98                     | 0.45              |
| 1:L:97:ARG:HD2   | 1:L:121:ALA:HA   | 1.99                     | 0.45              |
| 1:L:238:LEU:HG   | 1:L:574:LEU:HB2  | 1.99                     | 0.45              |
| 1:L:329:ARG:HH11 | 1:L:333:ARG:NH2  | 2.15                     | 0.45              |
| 1:L:492:SER:HB3  | 1:L:495:LEU:HB3  | 1.98                     | 0.45              |
| 1:A:75:ASP:O     | 1:A:79:PHE:HD1   | 2.00                     | 0.45              |
| 1:A:404:SER:O    | 1:A:408:ARG:HG2  | 2.15                     | 0.45              |
| 1:A:430:ASP:OD1  | 1:A:459:THR:HG23 | 2.17                     | 0.45              |
| 1:A:475:VAL:HG13 | 1:A:504:ILE:HD11 | 1.99                     | 0.45              |
| 1:G:581:VAL:HG23 | 1:G:598:TRP:CH2  | 2.52                     | 0.45              |
| 1:H:473:GLN:O    | 1:H:477:LYS:HB2  | 2.17                     | 0.45              |
| 1:L:37:SER:HB3   | 1:L:40:ILE:HG12  | 1.98                     | 0.45              |
| 1:L:269:HIS:CD2  | 1:L:294:LEU:HD11 | 2.51                     | 0.45              |
| 1:L:350:ARG:HD3  | 1:L:430:ASP:OD2  | 2.16                     | 0.45              |
| 1:L:534:ARG:HG2  | 1:L:571:ILE:HD13 | 1.99                     | 0.45              |
| 1:A:408:ARG:NH1  | 1:H:454:VAL:CG1  | 2.78                     | 0.45              |
| 1:B:21:LEU:HD22  | 1:B:125:PHE:CG   | 2.52                     | 0.45              |
| 1:B:157:ARG:HG3  | 1:B:157:ARG:O    | 2.17                     | 0.45              |
| 1:G:340:LEU:CD2  | 1:G:387:CYS:HB2  | 2.46                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:372:ASN:O    | 1:H:376:GLN:HG2  | 2.17                     | 0.45              |
| 1:K:1:MET:CE     | 1:K:3:ILE:HD11   | 2.46                     | 0.45              |
| 1:K:271:GLU:HG3  | 1:K:272:LEU:HD22 | 1.99                     | 0.45              |
| 1:K:393:LEU:HD12 | 1:K:413:ALA:CB   | 2.43                     | 0.45              |
| 1:K:488:HIS:CG   | 1:K:491:ARG:HH21 | 2.35                     | 0.45              |
| 1:A:5:LEU:HD21   | 1:A:90:ARG:HB2   | 1.97                     | 0.45              |
| 1:B:446:THR:HG21 | 1:K:446:THR:CB   | 2.47                     | 0.45              |
| 1:G:263:LEU:O    | 1:G:263:LEU:HG   | 2.17                     | 0.45              |
| 1:G:561:LEU:O    | 1:G:564:THR:OG1  | 2.29                     | 0.45              |
| 1:H:73:GLU:HG2   | 1:H:74:GLN:N     | 2.31                     | 0.45              |
| 1:H:192:ARG:HG2  | 1:H:193:ALA:N    | 2.32                     | 0.45              |
| 1:H:200:GLN:CA   | 1:H:203:GLU:HG2  | 2.47                     | 0.45              |
| 1:H:305:ILE:HG12 | 1:H:515:GLN:O    | 2.17                     | 0.45              |
| 1:K:352:SER:HB3  | 1:K:355:ASN:OD1  | 2.17                     | 0.45              |
| 1:K:357:ALA:HB1  | 1:K:361:ARG:O    | 2.17                     | 0.45              |
| 1:K:473:GLN:OE1  | 1:K:477:LYS:HG3  | 2.17                     | 0.45              |
| 1:L:610:THR:O    | 1:L:610:THR:HG22 | 2.17                     | 0.45              |
| 1:A:371:ARG:C    | 1:A:371:ARG:HD3  | 2.41                     | 0.45              |
| 1:B:87:LEU:HD11  | 1:B:97:ARG:HD3   | 1.98                     | 0.45              |
| 1:B:311:MET:HE1  | 3:B:701:ATP:N9   | 2.32                     | 0.45              |
| 1:K:385:ARG:HG2  | 1:K:385:ARG:O    | 2.17                     | 0.45              |
| 1:L:19:MET:HA    | 1:L:27:PHE:CD2   | 2.51                     | 0.45              |
| 1:L:21:LEU:HD13  | 1:L:125:PHE:CG   | 2.52                     | 0.45              |
| 1:A:12:TRP:CZ2   | 1:A:46:GLN:HB3   | 2.52                     | 0.45              |
| 1:A:120:GLY:HA2  | 1:A:164:GLU:OE2  | 2.16                     | 0.45              |
| 1:A:460:VAL:CG2  | 1:A:478:LEU:HD11 | 2.47                     | 0.45              |
| 1:B:311:MET:HE1  | 3:B:701:ATP:H2'  | 1.99                     | 0.45              |
| 1:B:328:LEU:HD11 | 1:B:370:ILE:HD11 | 1.99                     | 0.45              |
| 1:B:403:ARG:CB   | 1:K:453:ARG:HD3  | 2.41                     | 0.45              |
| 1:G:463:GLY:O    | 1:G:464:GLU:HB3  | 2.16                     | 0.45              |
| 1:G:520:PRO:HD3  | 1:G:529:GLU:CG   | 2.47                     | 0.45              |
| 1:K:371:ARG:HG2  | 1:K:424:CYS:SG   | 2.57                     | 0.45              |
| 1:L:344:VAL:O    | 1:L:387:CYS:HB3  | 2.17                     | 0.45              |
| 1:L:460:VAL:O    | 1:L:484:GLY:N    | 2.46                     | 0.45              |
| 1:A:12:TRP:CE2   | 1:A:46:GLN:HB3   | 2.52                     | 0.44              |
| 1:B:2:ARG:O      | 1:B:28:ASP:HB2   | 2.17                     | 0.44              |
| 1:B:81:GLU:OE2   | 1:B:85:ARG:HD2   | 2.17                     | 0.44              |
| 1:B:242:LEU:HD13 | 1:B:573:ARG:HG2  | 1.99                     | 0.44              |
| 1:B:488:HIS:HB3  | 1:B:491:ARG:HE   | 1.82                     | 0.44              |
| 1:G:451:VAL:HG13 | 1:G:456:LEU:HB2  | 1.99                     | 0.44              |
| 1:G:578:LYS:CA   | 1:G:581:VAL:HG12 | 2.46                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:461:HIS:NE2  | 1:H:485:HIS:HD2  | 2.15                     | 0.44              |
| 1:K:207:GLU:HG2  | 1:K:211:HIS:NE2  | 2.32                     | 0.44              |
| 1:K:218:GLY:O    | 1:K:222:LEU:HD13 | 2.17                     | 0.44              |
| 1:L:339:LEU:HD11 | 1:L:349:ILE:HD11 | 1.97                     | 0.44              |
| 1:L:471:ILE:HG21 | 1:L:489:LEU:HD21 | 1.99                     | 0.44              |
| 1:A:443:MET:CG   | 1:A:444:PHE:N    | 2.80                     | 0.44              |
| 1:B:471:ILE:O    | 1:B:475:VAL:HG23 | 2.16                     | 0.44              |
| 1:B:492:SER:HB3  | 1:B:495:LEU:HD13 | 1.98                     | 0.44              |
| 1:G:230:TRP:CZ3  | 1:G:238:LEU:HD22 | 2.53                     | 0.44              |
| 1:H:110:ALA:HA   | 1:H:113:GLN:CG   | 2.47                     | 0.44              |
| 1:K:4:LEU:HD12   | 1:K:98:TYR:O     | 2.18                     | 0.44              |
| 1:K:31:HIS:HB3   | 1:K:86:TRP:CZ2   | 2.51                     | 0.44              |
| 1:K:35:THR:HG22  | 1:K:64:VAL:HG21  | 1.99                     | 0.44              |
| 1:K:530:THR:HG22 | 1:K:531:TYR:N    | 2.31                     | 0.44              |
| 1:A:396:THR:O    | 1:A:396:THR:HG23 | 2.17                     | 0.44              |
| 1:B:177:SER:O    | 1:B:178:PHE:HD1  | 2.00                     | 0.44              |
| 1:B:423:GLY:O    | 1:B:425:ARG:HG3  | 2.16                     | 0.44              |
| 1:B:565:ALA:HA   | 1:B:571:ILE:HG22 | 1.99                     | 0.44              |
| 1:K:69:ASP:HA    | 2:N:730:A23:N6   | 2.33                     | 0.44              |
| 1:K:133:PHE:CZ   | 1:K:150:ALA:HB2  | 2.52                     | 0.44              |
| 1:L:311:MET:HE2  | 3:L:703:ATP:O2'  | 2.18                     | 0.44              |
| 1:L:364:TRP:O    | 1:L:368:GLN:HB2  | 2.17                     | 0.44              |
| 1:A:3:ILE:HG22   | 1:A:5:LEU:CD1    | 2.46                     | 0.44              |
| 1:A:498:VAL:HA   | 1:A:501:GLU:CG   | 2.40                     | 0.44              |
| 1:B:215:ALA:HB2  | 1:B:235:LEU:CD1  | 2.48                     | 0.44              |
| 1:B:245:VAL:HG23 | 1:B:246:GLN:N    | 2.32                     | 0.44              |
| 1:B:446:THR:HG21 | 1:K:446:THR:HB   | 1.99                     | 0.44              |
| 1:H:51:PHE:CD2   | 1:H:59:PHE:HB3   | 2.53                     | 0.44              |
| 1:H:105:TYR:HA   | 2:I:718:A23:O4'  | 2.18                     | 0.44              |
| 1:H:113:GLN:NE2  | 1:H:114:ARG:HG3  | 2.33                     | 0.44              |
| 1:H:451:VAL:O    | 1:H:454:VAL:HG22 | 2.16                     | 0.44              |
| 1:K:63:ARG:HD2   | 1:K:190:TRP:CH2  | 2.52                     | 0.44              |
| 1:L:121:ALA:HB1  | 1:L:124:VAL:HG23 | 1.99                     | 0.44              |
| 1:L:281:ALA:HB2  | 1:L:326:GLY:HA3  | 1.99                     | 0.44              |
| 1:L:339:LEU:HD13 | 1:L:347:ALA:CB   | 2.47                     | 0.44              |
| 1:A:1:MET:O      | 1:A:2:ARG:HD2    | 2.16                     | 0.44              |
| 1:B:149:GLN:O    | 1:B:153:THR:HG23 | 2.17                     | 0.44              |
| 1:B:468:VAL:HG11 | 1:B:491:ARG:HB2  | 1.99                     | 0.44              |
| 1:H:92:PRO:HG2   | 1:H:93:GLN:CD    | 2.42                     | 0.44              |
| 1:H:105:TYR:H    | 1:H:108:ILE:CD1  | 2.20                     | 0.44              |
| 1:H:109:SER:HA   | 1:H:112:MET:HG3  | 2.00                     | 0.44              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:K:305:ILE:O      | 1:K:309:ARG:HB2  | 2.17                     | 0.44              |
| 1:L:7:SER:HA       | 1:L:33:LEU:O     | 2.17                     | 0.44              |
| 1:L:81:GLU:HB2     | 1:L:196:MET:CE   | 2.48                     | 0.44              |
| 1:L:266:PHE:O      | 1:L:551:GLY:HA3  | 2.17                     | 0.44              |
| 1:L:273:LEU:O      | 1:L:276:VAL:HG12 | 2.18                     | 0.44              |
| 2:M:727:A:C1'      | 2:M:728:A23:P    | 3.05                     | 0.44              |
| 1:A:64:VAL:O       | 1:A:64:VAL:HG23  | 2.16                     | 0.44              |
| 1:B:33:LEU:HD22    | 1:B:86:TRP:CE3   | 2.52                     | 0.44              |
| 1:B:250:TRP:NE1    | 1:B:605:PRO:O    | 2.49                     | 0.44              |
| 1:B:442:ALA:C      | 1:B:444:PHE:H    | 2.25                     | 0.44              |
| 1:G:431:LEU:HD21   | 1:G:448:PHE:CZ   | 2.52                     | 0.44              |
| 1:G:459:THR:HG23   | 1:G:459:THR:O    | 2.18                     | 0.44              |
| 1:H:34:THR:OG1     | 1:H:61:ILE:HG23  | 2.18                     | 0.44              |
| 1:H:234:HIS:O      | 1:H:237:TRP:N    | 2.50                     | 0.44              |
| 1:H:574:LEU:CD2    | 1:H:578:LYS:HE3  | 2.47                     | 0.44              |
| 1:K:410:LEU:O      | 1:K:414:ILE:HG13 | 2.18                     | 0.44              |
| 1:L:44:VAL:O       | 1:L:48:LEU:HD23  | 2.17                     | 0.44              |
| 1:L:183:THR:O      | 1:L:190:TRP:HB2  | 2.17                     | 0.44              |
| 1:L:511:TYR:CE1    | 1:L:563:LEU:HD13 | 2.52                     | 0.44              |
| 1:A:149:GLN:O      | 1:A:153:THR:HG23 | 2.18                     | 0.44              |
| 1:B:195:ASP:CG     | 1:B:197:ARG:HG3  | 2.43                     | 0.44              |
| 1:G:35:THR:HG21    | 2:J:720:A23:N1   | 2.33                     | 0.44              |
| 1:G:267:ALA:HB3    | 1:G:317:ASN:ND2  | 2.32                     | 0.44              |
| 1:H:8:VAL:HG23     | 1:H:33:LEU:O     | 2.17                     | 0.44              |
| 1:L:237:TRP:CD1    | 1:L:607:PRO:HG2  | 2.53                     | 0.44              |
| 1:L:286:LEU:HD12   | 1:L:321:LEU:HD13 | 1.98                     | 0.44              |
| 2:M:727:A:H1'      | 2:M:728:A23:OP2  | 2.18                     | 0.44              |
| 1:A:260:HIS:CE1    | 1:A:461:HIS:NE2  | 2.86                     | 0.44              |
| 1:B:101:LEU:O      | 1:B:101:LEU:HD12 | 2.17                     | 0.44              |
| 1:B:124:VAL:O      | 1:B:161:LEU:HB2  | 2.18                     | 0.44              |
| 1:G:52:GLU:O       | 1:G:55:PRO:HG3   | 2.18                     | 0.44              |
| 1:G:73:GLU:O       | 1:G:76:HIS:N     | 2.50                     | 0.44              |
| 1:H:87:LEU:HD22    | 1:H:115:ALA:HB1  | 1.99                     | 0.44              |
| 1:H:128:LEU:HB2    | 1:H:157:ARG:HG2  | 2.00                     | 0.44              |
| 2:J:719:A:O2'      | 2:J:720:A23:OP1  | 2.36                     | 0.44              |
| 1:K:208:ARG:HH21   | 1:K:229:ALA:CB   | 2.31                     | 0.44              |
| 1:L:350:ARG:HA     | 1:L:392:LEU:O    | 2.18                     | 0.44              |
| 1:L:472[A]:TRP:HE1 | 1:L:495:LEU:HB2  | 1.82                     | 0.44              |
| 1:A:41:SER:HB2     | 1:A:42:PRO:HD3   | 2.00                     | 0.44              |
| 1:B:170:LEU:HD21   | 1:B:205:VAL:HG11 | 2.00                     | 0.44              |
| 1:B:280:ALA:CB     | 1:B:286:LEU:HD21 | 2.48                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:431:LEU:HB2  | 1:B:448:PHE:CE2  | 2.52                     | 0.44              |
| 1:B:565:ALA:HA   | 1:B:571:ILE:CG2  | 2.48                     | 0.44              |
| 1:G:410:LEU:O    | 1:G:414:ILE:HD12 | 2.18                     | 0.44              |
| 1:H:244:PRO:O    | 1:H:562:LEU:HD23 | 2.18                     | 0.44              |
| 1:K:5:LEU:HB2    | 1:K:99:ILE:HG12  | 2.00                     | 0.44              |
| 1:K:563:LEU:HG   | 1:K:563:LEU:O    | 2.16                     | 0.44              |
| 1:L:39:LYS:CE    | 2:M:728:A23:HN62 | 2.31                     | 0.44              |
| 1:A:476:PHE:CE2  | 1:B:452:HIS:HB3  | 2.53                     | 0.43              |
| 1:B:146:GLU:HA   | 1:B:149:GLN:HG2  | 2.00                     | 0.43              |
| 1:G:141:ALA:HA   | 1:G:146:GLU:HB3  | 2.00                     | 0.43              |
| 1:H:91:ALA:HB3   | 1:H:97:ARG:HD2   | 1.99                     | 0.43              |
| 1:K:29:GLU:HG2   | 1:K:58:ARG:CB    | 2.28                     | 0.43              |
| 1:K:238:LEU:HD21 | 1:K:574:LEU:CD1  | 2.47                     | 0.43              |
| 1:L:322:LEU:HD23 | 1:L:328:LEU:CD1  | 2.48                     | 0.43              |
| 1:L:532:PRO:HB2  | 1:L:536:TYR:CE1  | 2.53                     | 0.43              |
| 1:A:91:ALA:HB1   | 1:A:97:ARG:HE    | 1.84                     | 0.43              |
| 1:B:531:TYR:HA   | 1:B:532:PRO:HD3  | 1.89                     | 0.43              |
| 1:G:78:LEU:HD21  | 1:G:192:ARG:HH12 | 1.83                     | 0.43              |
| 1:H:397:ARG:HB3  | 1:H:406:ILE:HD11 | 2.00                     | 0.43              |
| 1:K:21:LEU:HD22  | 1:K:125:PHE:CE1  | 2.53                     | 0.43              |
| 1:K:510:PRO:HG3  | 1:K:545:LEU:HD22 | 2.00                     | 0.43              |
| 1:L:106:LYS:CD   | 2:M:728:A23:H5'  | 2.47                     | 0.43              |
| 1:L:212:ILE:O    | 1:L:216:TRP:N    | 2.51                     | 0.43              |
| 1:L:329:ARG:HH11 | 1:L:333:ARG:HH21 | 1.64                     | 0.43              |
| 1:L:397:ARG:NH2  | 1:L:443:MET:SD   | 2.91                     | 0.43              |
| 1:L:445:ALA:HB3  | 1:L:478:LEU:HD21 | 2.00                     | 0.43              |
| 1:A:37:SER:HA    | 1:A:68:GLU:OE1   | 2.18                     | 0.43              |
| 1:A:531:TYR:CD2  | 1:A:567:LEU:HD23 | 2.52                     | 0.43              |
| 1:B:140:GLU:N    | 1:B:140:GLU:OE1  | 2.52                     | 0.43              |
| 1:G:6:CYS:O      | 1:G:32:VAL:HA    | 2.18                     | 0.43              |
| 1:G:217:GLU:HG2  | 1:G:218:GLY:H    | 1.84                     | 0.43              |
| 1:H:82:VAL:HG22  | 1:H:193:ALA:CB   | 2.41                     | 0.43              |
| 1:H:106:LYS:HD2  | 2:I:718:A23:OP2  | 2.18                     | 0.43              |
| 1:H:276:VAL:CG2  | 1:H:334:LEU:HD12 | 2.48                     | 0.43              |
| 1:H:301:PRO:HD3  | 1:H:515:GLN:HG2  | 2.00                     | 0.43              |
| 1:H:558:THR:O    | 1:H:562:LEU:HD13 | 2.18                     | 0.43              |
| 1:K:67:PHE:CZ    | 1:K:70:LEU:HA    | 2.53                     | 0.43              |
| 1:K:97:ARG:O     | 1:K:121:ALA:HB1  | 2.18                     | 0.43              |
| 1:L:98:TYR:CD2   | 1:L:123:GLU:HB3  | 2.53                     | 0.43              |
| 1:L:510:PRO:HB3  | 1:L:567:LEU:HD12 | 1.99                     | 0.43              |
| 1:A:113:GLN:NE2  | 1:B:114:ARG:HD2  | 2.34                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:213:LEU:HB2  | 1:B:168:PRO:HG3  | 1.99                     | 0.43              |
| 1:A:290:ARG:NH2  | 1:A:315:ASP:O    | 2.46                     | 0.43              |
| 1:A:581:VAL:HG13 | 1:A:598:TRP:CH2  | 2.53                     | 0.43              |
| 1:B:7:SER:HA     | 1:B:33:LEU:HB3   | 2.00                     | 0.43              |
| 1:G:11:SER:O     | 1:G:14:VAL:HG22  | 2.18                     | 0.43              |
| 1:G:497:ARG:HH21 | 1:H:455:GLY:HA3  | 1.83                     | 0.43              |
| 1:G:511:TYR:CD2  | 1:G:555:ALA:CB   | 3.01                     | 0.43              |
| 1:H:27:PHE:HE2   | 1:H:98:TYR:CD2   | 2.36                     | 0.43              |
| 1:H:362:SER:HB2  | 1:H:363:PRO:HD2  | 2.01                     | 0.43              |
| 1:H:508:LEU:HB3  | 1:H:531:TYR:OH   | 2.17                     | 0.43              |
| 1:K:242:LEU:HD22 | 1:K:576:VAL:CG2  | 2.38                     | 0.43              |
| 1:K:305:ILE:HG22 | 1:K:309:ARG:HB2  | 2.01                     | 0.43              |
| 1:K:374:PHE:O    | 1:K:378:MET:HG3  | 2.17                     | 0.43              |
| 1:L:43:GLY:O     | 1:L:47:LEU:HG    | 2.19                     | 0.43              |
| 1:L:116:ALA:O    | 1:L:120:GLY:N    | 2.51                     | 0.43              |
| 1:A:116:ALA:O    | 1:A:120:GLY:N    | 2.42                     | 0.43              |
| 1:A:181:GLU:O    | 1:A:191:VAL:HA   | 2.18                     | 0.43              |
| 1:A:356:TYR:HB2  | 1:A:366:VAL:HG11 | 2.00                     | 0.43              |
| 1:A:458:VAL:HG23 | 1:A:480:ALA:HA   | 1.99                     | 0.43              |
| 1:B:117:ALA:HA   | 1:B:164:GLU:OE1  | 2.19                     | 0.43              |
| 1:B:133:PHE:HB2  | 1:B:139:ARG:O    | 2.18                     | 0.43              |
| 1:B:329:ARG:HG2  | 1:B:329:ARG:NH1  | 2.32                     | 0.43              |
| 1:G:64:VAL:HG23  | 1:G:67:PHE:O     | 2.18                     | 0.43              |
| 1:G:107:THR:O    | 1:G:111:ALA:N    | 2.49                     | 0.43              |
| 1:G:310:TYR:CG   | 1:G:516:ILE:HD11 | 2.54                     | 0.43              |
| 1:G:511:TYR:HD2  | 1:G:555:ALA:CB   | 2.31                     | 0.43              |
| 1:H:319:SER:O    | 1:H:323:LYS:HG3  | 2.18                     | 0.43              |
| 1:H:397:ARG:HD3  | 1:H:397:ARG:H    | 1.83                     | 0.43              |
| 1:H:457:ALA:HB1  | 1:H:588:PHE:CZ   | 2.54                     | 0.43              |
| 1:K:208:ARG:NE   | 1:K:229:ALA:HB1  | 2.30                     | 0.43              |
| 1:G:51:PHE:CE2   | 1:G:61:ILE:HD11  | 2.53                     | 0.43              |
| 1:H:12:TRP:HB3   | 1:H:43:GLY:CA    | 2.49                     | 0.43              |
| 1:H:79:PHE:CE2   | 1:H:108:ILE:HG23 | 2.54                     | 0.43              |
| 1:H:523:GLU:O    | 1:H:569:PRO:HG3  | 2.19                     | 0.43              |
| 1:K:3:ILE:HD13   | 1:K:96:HIS:CD2   | 2.54                     | 0.43              |
| 1:K:65:GLN:CD    | 1:K:190:TRP:HB3  | 2.43                     | 0.43              |
| 1:K:81:GLU:HG2   | 1:K:196:MET:SD   | 2.59                     | 0.43              |
| 1:L:101:LEU:HD23 | 1:L:101:LEU:H    | 1.82                     | 0.43              |
| 1:L:127:VAL:HG21 | 1:L:156:LEU:HD21 | 2.00                     | 0.43              |
| 1:B:49:ARG:O     | 1:B:53:MET:HG2   | 2.18                     | 0.43              |
| 1:H:70:LEU:HB2   | 1:H:105:TYR:CE2  | 2.54                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:70:LEU:HD11  | 1:H:76:HIS:HB2   | 2.01                     | 0.43              |
| 1:H:127:VAL:HG21 | 1:H:156:LEU:HD21 | 2.01                     | 0.43              |
| 1:H:183:THR:N    | 1:H:190:TRP:O    | 2.38                     | 0.43              |
| 1:H:410:LEU:HD22 | 1:H:451:VAL:CG1  | 2.49                     | 0.43              |
| 1:K:578:LYS:HG3  | 1:K:582:PHE:CE2  | 2.52                     | 0.43              |
| 1:L:252:GLN:HG3  | 1:L:252:GLN:O    | 2.18                     | 0.43              |
| 1:L:259:LEU:HD22 | 1:L:482:ARG:HH12 | 1.83                     | 0.43              |
| 1:L:277:ARG:NH2  | 1:L:286:LEU:HB3  | 2.34                     | 0.43              |
| 1:L:312:ARG:NE   | 1:L:312:ARG:CA   | 2.80                     | 0.43              |
| 1:L:345:ALA:O    | 1:L:387:CYS:HA   | 2.19                     | 0.43              |
| 2:N:729:A:H5''   | 2:N:730:A23:OP2  | 2.18                     | 0.43              |
| 1:A:13:ALA:O     | 1:A:16:PRO:HD2   | 2.17                     | 0.43              |
| 1:A:329:ARG:HB2  | 1:A:373:HIS:CE1  | 2.53                     | 0.43              |
| 1:B:37:SER:O     | 1:B:40:ILE:HG12  | 2.19                     | 0.43              |
| 1:B:403:ARG:NH1  | 1:B:447:ASP:OD2  | 2.52                     | 0.43              |
| 1:B:437:ARG:NE   | 1:B:437:ARG:HA   | 2.34                     | 0.43              |
| 1:G:254:LEU:O    | 1:G:256:LYS:HG3  | 2.18                     | 0.43              |
| 1:G:267:ALA:C    | 1:G:317:ASN:HD22 | 2.27                     | 0.43              |
| 1:G:533:LEU:HD23 | 1:G:533:LEU:C    | 2.44                     | 0.43              |
| 1:G:536:TYR:HB3  | 1:G:543:VAL:CG2  | 2.49                     | 0.43              |
| 1:H:8:VAL:N      | 1:H:33:LEU:O     | 2.52                     | 0.43              |
| 1:H:140:GLU:OE1  | 1:H:140:GLU:N    | 2.52                     | 0.43              |
| 1:H:180:LEU:HD12 | 1:H:193:ALA:HA   | 1.99                     | 0.43              |
| 1:H:203:GLU:O    | 1:H:207:GLU:HG3  | 2.18                     | 0.43              |
| 1:L:471:ILE:O    | 1:L:471:ILE:HG22 | 2.18                     | 0.43              |
| 1:L:510:PRO:HB2  | 1:L:563:LEU:HD23 | 2.01                     | 0.43              |
| 1:B:4:LEU:O      | 1:B:30:VAL:HA    | 2.18                     | 0.43              |
| 1:B:298:TRP:CG   | 1:B:299:PRO:HA   | 2.53                     | 0.43              |
| 1:B:375:GLN:NE2  | 1:B:423:GLY:HA3  | 2.31                     | 0.43              |
| 1:B:534:ARG:HH21 | 1:B:570:GLY:C    | 2.26                     | 0.43              |
| 1:B:547:THR:HG22 | 1:B:560:ASN:ND2  | 2.34                     | 0.43              |
| 1:G:46:GLN:C     | 1:G:49:ARG:HG2   | 2.44                     | 0.43              |
| 1:G:51:PHE:HE2   | 1:G:61:ILE:HD11  | 1.82                     | 0.43              |
| 1:G:419:HIS:HD2  | 1:L:362:SER:OG   | 2.02                     | 0.43              |
| 1:H:174:SER:C    | 1:H:176:PRO:HD2  | 2.44                     | 0.43              |
| 1:K:35:THR:O     | 1:K:40:ILE:HG21  | 2.19                     | 0.43              |
| 1:K:242:LEU:HD13 | 1:K:573:ARG:HB3  | 2.00                     | 0.43              |
| 1:A:1:MET:O      | 1:A:96:HIS:ND1   | 2.52                     | 0.43              |
| 1:A:258:GLU:OE1  | 1:A:557:LEU:HD13 | 2.19                     | 0.43              |
| 1:A:520:PRO:HD3  | 1:A:529:GLU:HG3  | 2.00                     | 0.43              |
| 1:B:431:LEU:HB2  | 1:B:448:PHE:HZ   | 1.73                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:578:LYS:HA   | 1:G:581:VAL:CG1  | 2.48                     | 0.43              |
| 1:H:55:PRO:C     | 1:H:57:PRO:HD2   | 2.44                     | 0.43              |
| 1:H:368:GLN:O    | 1:H:372:ASN:ND2  | 2.51                     | 0.43              |
| 1:K:4:LEU:HA     | 1:K:98:TYR:O     | 2.18                     | 0.43              |
| 1:K:48:LEU:HD21  | 1:K:61:ILE:HD12  | 2.01                     | 0.43              |
| 1:K:511:TYR:HE2  | 1:K:555:ALA:HB1  | 1.83                     | 0.43              |
| 1:L:233:SER:OG   | 1:L:610:THR:HG22 | 2.18                     | 0.43              |
| 1:L:235:LEU:HD23 | 1:L:235:LEU:O    | 2.19                     | 0.43              |
| 1:L:609:ASP:O    | 1:L:610:THR:HB   | 2.19                     | 0.43              |
| 1:A:575:GLU:OE1  | 1:A:575:GLU:HA   | 2.19                     | 0.42              |
| 1:B:17:GLU:HB3   | 1:B:156:LEU:CD2  | 2.48                     | 0.42              |
| 1:B:273:LEU:CD2  | 1:B:316:ASN:HD22 | 2.32                     | 0.42              |
| 1:B:298:TRP:CZ3  | 1:B:301:PRO:HG3  | 2.53                     | 0.42              |
| 1:B:316:ASN:O    | 1:B:321:LEU:HD13 | 2.18                     | 0.42              |
| 1:H:322:LEU:HD12 | 1:H:328:LEU:CD1  | 2.49                     | 0.42              |
| 1:H:498:VAL:O    | 1:H:502:ARG:HG3  | 2.19                     | 0.42              |
| 1:K:563:LEU:CG   | 1:K:567:LEU:HD23 | 2.39                     | 0.42              |
| 1:L:349:ILE:HD13 | 1:L:389:VAL:HG13 | 2.01                     | 0.42              |
| 1:B:89:GLN:HG3   | 1:B:180:LEU:HB3  | 2.00                     | 0.42              |
| 1:B:118:LEU:O    | 1:B:167:TRP:HB2  | 2.19                     | 0.42              |
| 1:B:430:ASP:O    | 1:B:431:LEU:C    | 2.62                     | 0.42              |
| 1:G:54:HIS:N     | 1:G:55:PRO:HD3   | 2.34                     | 0.42              |
| 1:G:68:GLU:N     | 1:G:68:GLU:OE1   | 2.52                     | 0.42              |
| 1:G:510:PRO:CB   | 1:G:563:LEU:HD23 | 2.49                     | 0.42              |
| 1:H:508:LEU:O    | 1:H:545:LEU:HA   | 2.19                     | 0.42              |
| 1:K:504:ILE:H    | 1:K:504:ILE:HD12 | 1.83                     | 0.42              |
| 1:K:511:TYR:CE2  | 1:K:555:ALA:HB1  | 2.54                     | 0.42              |
| 1:L:92:PRO:HG2   | 1:L:93:GLN:NE2   | 2.33                     | 0.42              |
| 1:L:431:LEU:HD22 | 1:L:478:LEU:HD13 | 2.01                     | 0.42              |
| 1:L:432:ALA:HA   | 1:L:461:HIS:CB   | 2.49                     | 0.42              |
| 1:A:257:VAL:H    | 1:A:580:GLN:HE22 | 1.67                     | 0.42              |
| 1:A:258:GLU:O    | 1:A:347:ALA:HA   | 2.18                     | 0.42              |
| 1:A:390:ASN:HB3  | 1:A:427:VAL:HG13 | 2.01                     | 0.42              |
| 1:A:457:ALA:HB1  | 1:A:588:PHE:CZ   | 2.54                     | 0.42              |
| 1:B:251:VAL:CG1  | 1:B:558:THR:HG23 | 2.47                     | 0.42              |
| 1:B:464:GLU:O    | 1:B:465:ASN:HB2  | 2.18                     | 0.42              |
| 1:G:36:ALA:CB    | 1:G:68:GLU:HG3   | 2.47                     | 0.42              |
| 1:G:243:ASP:HB3  | 1:G:247:ASP:OD2  | 2.18                     | 0.42              |
| 1:G:578:LYS:C    | 1:G:581:VAL:HG12 | 2.45                     | 0.42              |
| 1:H:195:ASP:CG   | 1:H:196:MET:H    | 2.12                     | 0.42              |
| 1:K:33:LEU:HD22  | 1:K:86:TRP:CG    | 2.54                     | 0.42              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:K:167:TRP:HZ2  | 1:K:209:SER:OG     | 2.02                     | 0.42              |
| 1:K:242:LEU:HD13 | 1:K:573:ARG:CB     | 2.49                     | 0.42              |
| 1:K:453:ARG:HG2  | 1:L:472[B]:TRP:CZ2 | 2.53                     | 0.42              |
| 1:K:547:THR:HG21 | 1:K:550:LEU:HG     | 2.00                     | 0.42              |
| 1:L:114:ARG:HD3  | 1:L:118:LEU:HD22   | 2.01                     | 0.42              |
| 1:A:53:MET:SD    | 1:A:53:MET:C       | 3.02                     | 0.42              |
| 1:A:262:HIS:HB2  | 1:A:549:ASN:ND2    | 2.34                     | 0.42              |
| 1:A:449:GLU:OE2  | 1:H:447:ASP:HB3    | 2.18                     | 0.42              |
| 1:G:318:GLY:N    | 1:G:322:LEU:HD23   | 2.34                     | 0.42              |
| 1:G:361:ARG:HH12 | 1:G:369:GLU:CD     | 2.26                     | 0.42              |
| 1:G:392:LEU:HD23 | 1:G:427:VAL:HG23   | 1.99                     | 0.42              |
| 1:H:198:LEU:O    | 1:H:198:LEU:HG     | 2.20                     | 0.42              |
| 1:K:488:HIS:HB3  | 1:K:491:ARG:HH21   | 1.85                     | 0.42              |
| 1:L:307:LEU:CB   | 1:L:464:GLU:OE2    | 2.67                     | 0.42              |
| 1:L:322:LEU:HB2  | 1:L:356:TYR:CD1    | 2.54                     | 0.42              |
| 1:L:511:TYR:CD1  | 1:L:563:LEU:HD22   | 2.54                     | 0.42              |
| 1:L:514:LEU:CD1  | 1:L:519:PHE:H      | 2.32                     | 0.42              |
| 1:A:280:ALA:HB2  | 1:A:327:CYS:SG     | 2.59                     | 0.42              |
| 1:A:446:THR:HG21 | 1:H:446:THR:HB     | 2.00                     | 0.42              |
| 1:B:127:VAL:HG13 | 2:D:709:A:N3       | 2.34                     | 0.42              |
| 1:G:104:GLY:O    | 2:J:720:A23:O1C    | 2.37                     | 0.42              |
| 1:G:128:LEU:O    | 1:G:156:LEU:HA     | 2.19                     | 0.42              |
| 1:G:169:GLN:HB2  | 1:G:205:VAL:CG1    | 2.48                     | 0.42              |
| 1:H:71:ARG:HB2   | 1:H:75:ASP:OD2     | 2.19                     | 0.42              |
| 1:H:79:PHE:O     | 1:H:83:LEU:N       | 2.46                     | 0.42              |
| 1:H:449:GLU:OE1  | 1:H:449:GLU:HA     | 2.18                     | 0.42              |
| 1:K:181:GLU:OE2  | 1:K:194:SER:N      | 2.52                     | 0.42              |
| 1:K:300:ILE:HD13 | 1:K:514:LEU:HD21   | 2.02                     | 0.42              |
| 1:K:446:THR:O    | 1:K:449:GLU:HG3    | 2.20                     | 0.42              |
| 1:K:547:THR:HG21 | 1:K:550:LEU:HD23   | 2.02                     | 0.42              |
| 1:L:182:SER:CB   | 1:L:191:VAL:HG12   | 2.48                     | 0.42              |
| 1:L:192:ARG:HG2  | 1:L:193:ALA:N      | 2.34                     | 0.42              |
| 1:A:16:PRO:HB2   | 1:A:147:VAL:CG1    | 2.49                     | 0.42              |
| 1:A:22:LEU:HD13  | 1:A:27:PHE:HZ      | 1.83                     | 0.42              |
| 1:H:79:PHE:CZ    | 1:H:108:ILE:HG23   | 2.55                     | 0.42              |
| 1:H:158:PHE:CB   | 1:H:160:ARG:HH11   | 2.21                     | 0.42              |
| 1:H:353:PRO:HG2  | 1:H:412:LEU:CD2    | 2.50                     | 0.42              |
| 1:K:36:ALA:HA    | 1:K:63:ARG:CD      | 2.32                     | 0.42              |
| 1:K:511:TYR:CE1  | 1:K:563:LEU:HD22   | 2.52                     | 0.42              |
| 1:K:611:GLU:HG2  | 1:K:612:GLN:N      | 2.33                     | 0.42              |
| 1:L:90:ARG:HH22  | 1:L:189:HIS:CD2    | 2.37                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:520:PRO:HB2  | 1:L:523:GLU:CD   | 2.44                     | 0.42              |
| 1:A:576:VAL:O    | 1:A:579:THR:OG1  | 2.32                     | 0.42              |
| 1:B:536:TYR:HB3  | 1:B:543:VAL:CG2  | 2.50                     | 0.42              |
| 1:G:15:VAL:HB    | 1:G:16:PRO:HD3   | 2.02                     | 0.42              |
| 1:G:64:VAL:HG23  | 1:G:67:PHE:HB3   | 2.00                     | 0.42              |
| 1:G:101:LEU:CD1  | 1:G:126:HIS:HB2  | 2.50                     | 0.42              |
| 1:H:260:HIS:O    | 1:H:548:ASP:N    | 2.40                     | 0.42              |
| 1:K:33:LEU:HD12  | 1:K:34:THR:H     | 1.83                     | 0.42              |
| 1:K:44:VAL:O     | 1:K:48:LEU:HG    | 2.20                     | 0.42              |
| 1:K:250:TRP:CD1  | 1:K:605:PRO:HB2  | 2.55                     | 0.42              |
| 1:L:4:LEU:O      | 1:L:5:LEU:HD23   | 2.19                     | 0.42              |
| 1:L:231:PRO:HD2  | 1:L:234:HIS:HB2  | 2.01                     | 0.42              |
| 1:A:393:LEU:HD12 | 1:A:413:ALA:CA   | 2.48                     | 0.42              |
| 1:B:87:LEU:HD21  | 1:B:97:ARG:NE    | 2.33                     | 0.42              |
| 1:B:476:PHE:HZ   | 1:B:498:VAL:HG11 | 1.84                     | 0.42              |
| 1:G:49:ARG:HA    | 1:G:52:GLU:OE1   | 2.19                     | 0.42              |
| 1:G:124:VAL:HG23 | 1:G:161:LEU:CB   | 2.33                     | 0.42              |
| 1:H:15:VAL:HB    | 1:H:47:LEU:CD2   | 2.49                     | 0.42              |
| 1:H:277:ARG:NH2  | 1:H:287:PRO:O    | 2.53                     | 0.42              |
| 1:K:571:ILE:HG23 | 1:K:571:ILE:O    | 2.19                     | 0.42              |
| 1:L:498:VAL:HA   | 1:L:501:GLU:HG2  | 2.01                     | 0.42              |
| 1:A:21:LEU:HD23  | 1:A:27:PHE:HZ    | 1.85                     | 0.42              |
| 1:A:22:LEU:HB2   | 1:A:25:GLN:NE2   | 2.34                     | 0.42              |
| 1:A:65:GLN:HG3   | 1:A:191:VAL:C    | 2.45                     | 0.42              |
| 1:A:382:PRO:HB2  | 1:A:384:ASP:OD1  | 2.19                     | 0.42              |
| 1:A:522:ASP:N    | 1:A:566:ARG:O    | 2.53                     | 0.42              |
| 1:G:84:TRP:HA    | 1:G:87:LEU:CD2   | 2.50                     | 0.42              |
| 1:H:34:THR:HG22  | 1:H:40:ILE:CD1   | 2.49                     | 0.42              |
| 1:H:462:ALA:HB3  | 1:H:484:GLY:O    | 2.19                     | 0.42              |
| 1:H:505:ALA:HA   | 1:H:542:ALA:HB3  | 2.02                     | 0.42              |
| 1:K:130:GLU:HG3  | 1:K:155:ALA:O    | 2.19                     | 0.42              |
| 1:K:397:ARG:HD2  | 1:K:434:PHE:N    | 2.28                     | 0.42              |
| 1:L:15:VAL:HG11  | 1:L:32:VAL:HG21  | 2.01                     | 0.42              |
| 1:L:34:THR:HG23  | 1:L:40:ILE:HD12  | 2.02                     | 0.42              |
| 1:A:121:ALA:N    | 1:A:164:GLU:OE2  | 2.53                     | 0.42              |
| 1:A:533:LEU:HD12 | 1:A:543:VAL:HG11 | 2.02                     | 0.42              |
| 1:B:5:LEU:HD22   | 1:B:86:TRP:CZ2   | 2.55                     | 0.42              |
| 1:B:9:GLY:HA2    | 2:C:708:A23:C2   | 2.49                     | 0.42              |
| 1:B:12:TRP:CZ2   | 1:B:46:GLN:HB3   | 2.54                     | 0.42              |
| 1:G:408:ARG:O    | 1:G:412:LEU:N    | 2.49                     | 0.42              |
| 1:H:85:ARG:HH21  | 1:H:178:PHE:C    | 2.28                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:110:ALA:O    | 1:K:114:ARG:HG2  | 2.20                     | 0.42              |
| 1:K:447:ASP:O    | 1:K:450:PRO:HD2  | 2.19                     | 0.42              |
| 1:K:451:VAL:HG13 | 1:K:456:LEU:HB2  | 2.01                     | 0.42              |
| 1:L:83:LEU:HD12  | 1:L:86:TRP:HE3   | 1.83                     | 0.42              |
| 1:L:273:LEU:HD21 | 1:L:316:ASN:HB3  | 2.01                     | 0.42              |
| 1:A:143:THR:O    | 1:A:147:VAL:HG23 | 2.19                     | 0.41              |
| 1:A:213:LEU:CB   | 1:B:168:PRO:HG3  | 2.49                     | 0.41              |
| 1:A:511:TYR:CE2  | 1:A:555:ALA:CB   | 3.03                     | 0.41              |
| 1:B:133:PHE:HE2  | 1:B:149:GLN:CG   | 2.30                     | 0.41              |
| 1:B:442:ALA:C    | 1:B:444:PHE:N    | 2.78                     | 0.41              |
| 1:G:8:VAL:CG2    | 1:G:32:VAL:HG11  | 2.50                     | 0.41              |
| 1:G:63:ARG:HB3   | 1:G:190:TRP:CZ3  | 2.55                     | 0.41              |
| 1:G:227:LEU:HD11 | 1:G:577:LEU:HD13 | 2.01                     | 0.41              |
| 1:H:13:ALA:O     | 1:H:17:GLU:HG2   | 2.20                     | 0.41              |
| 1:H:21:LEU:HD12  | 1:H:158:PHE:CD2  | 2.55                     | 0.41              |
| 1:H:84:TRP:CB    | 1:H:198:LEU:HD23 | 2.50                     | 0.41              |
| 1:K:177:SER:O    | 1:K:178:PHE:HD1  | 2.02                     | 0.41              |
| 1:L:15:VAL:N     | 1:L:16:PRO:HD2   | 2.35                     | 0.41              |
| 1:L:29:GLU:HG3   | 1:L:29:GLU:O     | 2.19                     | 0.41              |
| 1:L:33:LEU:HD22  | 1:L:83:LEU:HD13  | 2.02                     | 0.41              |
| 1:L:66:ASP:OD1   | 1:L:192:ARG:NH1  | 2.53                     | 0.41              |
| 1:L:430:ASP:OD1  | 1:L:430:ASP:N    | 2.53                     | 0.41              |
| 1:G:169:GLN:HE22 | 1:H:213:LEU:HG   | 1.85                     | 0.41              |
| 1:G:237:TRP:CH2  | 1:G:573:ARG:HD3  | 2.55                     | 0.41              |
| 1:H:116:ALA:O    | 1:H:164:GLU:HB3  | 2.20                     | 0.41              |
| 1:H:128:LEU:HB3  | 1:H:157:ARG:CZ   | 2.50                     | 0.41              |
| 1:K:282:ASN:O    | 1:K:284:GLU:N    | 2.41                     | 0.41              |
| 1:A:84:TRP:CD1   | 1:A:115:ALA:HB2  | 2.56                     | 0.41              |
| 1:A:91:ALA:CB    | 1:A:97:ARG:HE    | 2.32                     | 0.41              |
| 1:B:83:LEU:HD13  | 1:B:112:MET:SD   | 2.60                     | 0.41              |
| 1:G:3:ILE:HG23   | 1:G:29:GLU:O     | 2.20                     | 0.41              |
| 1:G:519:PHE:O    | 1:G:521:LEU:HD12 | 2.20                     | 0.41              |
| 1:H:64:VAL:HB    | 1:H:67:PHE:HB3   | 2.02                     | 0.41              |
| 1:K:130:GLU:HB3  | 1:K:132:ARG:HG2  | 2.02                     | 0.41              |
| 1:K:207:GLU:HG2  | 1:K:211:HIS:HE2  | 1.84                     | 0.41              |
| 1:K:242:LEU:CD2  | 1:K:576:VAL:HG21 | 2.40                     | 0.41              |
| 1:K:357:ALA:HB2  | 1:K:363:PRO:HA   | 2.02                     | 0.41              |
| 1:A:131:PRO:HD2  | 1:A:132:ARG:NH1  | 2.33                     | 0.41              |
| 1:B:435:GLU:OE2  | 1:B:463:GLY:C    | 2.63                     | 0.41              |
| 1:G:88:LEU:HD13  | 1:G:175:ALA:CA   | 2.35                     | 0.41              |
| 1:H:132:ARG:NH2  | 1:H:155:ALA:HB2  | 2.32                     | 0.41              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:K:21:LEU:CD1     | 1:K:158:PHE:HD2  | 2.33                     | 0.41              |
| 1:K:167:TRP:CH2    | 1:L:167:TRP:HH2  | 2.38                     | 0.41              |
| 1:K:321:LEU:HD23   | 1:K:321:LEU:C    | 2.46                     | 0.41              |
| 1:L:35:THR:HG21    | 1:L:67:PHE:HE2   | 1.85                     | 0.41              |
| 1:L:168:PRO:HA     | 1:L:171:ARG:HH21 | 1.85                     | 0.41              |
| 1:L:169:GLN:HE21   | 1:L:205:VAL:CG1  | 2.32                     | 0.41              |
| 1:L:303:GLU:HB3    | 1:L:304:PRO:HD2  | 2.01                     | 0.41              |
| 1:L:329:ARG:HG3    | 1:L:373:HIS:NE2  | 2.35                     | 0.41              |
| 1:B:10:THR:HG23    | 2:C:708:A23:N7   | 2.35                     | 0.41              |
| 1:B:46:GLN:O       | 1:B:144:LEU:HD21 | 2.20                     | 0.41              |
| 1:B:73:GLU:O       | 1:B:77:MET:CE    | 2.69                     | 0.41              |
| 1:B:243:ASP:OD1    | 1:B:245:VAL:HG22 | 2.20                     | 0.41              |
| 1:B:346:TYR:HB2    | 1:B:597:LEU:HD13 | 2.02                     | 0.41              |
| 1:G:251:VAL:HG12   | 1:G:558:THR:HG23 | 2.01                     | 0.41              |
| 1:H:85:ARG:NH2     | 1:H:197:ARG:HD2  | 2.25                     | 0.41              |
| 1:H:260:HIS:CD2    | 1:H:548:ASP:HA   | 2.55                     | 0.41              |
| 1:K:199:ARG:NH1    | 1:K:203:GLU:OE1  | 2.53                     | 0.41              |
| 1:K:486:ALA:HB1    | 1:K:489:LEU:CD1  | 2.50                     | 0.41              |
| 1:L:28:ASP:C       | 1:L:57:PRO:HB3   | 2.46                     | 0.41              |
| 1:L:350:ARG:CB     | 1:L:392:LEU:HB2  | 2.48                     | 0.41              |
| 1:A:34:THR:O       | 1:A:63:ARG:HA    | 2.21                     | 0.41              |
| 1:A:102:ALA:HA     | 1:A:126:HIS:HE1  | 1.82                     | 0.41              |
| 1:G:252:GLN:O      | 1:G:252:GLN:HG3  | 2.20                     | 0.41              |
| 1:G:305:ILE:HD11   | 1:G:310:TYR:HA   | 2.03                     | 0.41              |
| 1:H:487:LEU:HD11   | 1:H:513:ASN:CG   | 2.44                     | 0.41              |
| 1:H:533:LEU:HD22   | 1:H:545:LEU:HD21 | 2.03                     | 0.41              |
| 1:H:609:ASP:O      | 1:H:610:THR:OG1  | 2.28                     | 0.41              |
| 1:K:5:LEU:CD2      | 1:K:31:HIS:HB2   | 2.51                     | 0.41              |
| 1:L:3:ILE:CD1      | 1:L:96:HIS:HB3   | 2.51                     | 0.41              |
| 1:L:132:ARG:NH2    | 1:L:155:ALA:HB2  | 2.26                     | 0.41              |
| 1:A:309:ARG:O      | 1:A:313:LEU:HG   | 2.21                     | 0.41              |
| 1:A:328:LEU:HD11   | 1:A:370:ILE:HD11 | 2.02                     | 0.41              |
| 1:B:132:ARG:NH2    | 1:B:155:ALA:HB2  | 2.14                     | 0.41              |
| 1:B:449:GLU:HG3    | 1:B:453:ARG:HE   | 1.85                     | 0.41              |
| 1:G:8:VAL:HG23     | 1:G:32:VAL:HG11  | 2.03                     | 0.41              |
| 1:G:207:GLU:HA     | 1:G:210:ARG:HH11 | 1.84                     | 0.41              |
| 1:G:472[A]:TRP:CZ3 | 1:G:476:PHE:HE2  | 2.39                     | 0.41              |
| 1:H:15:VAL:CG1     | 1:H:47:LEU:HD22  | 2.50                     | 0.41              |
| 1:H:175:ALA:N      | 1:H:176:PRO:CD   | 2.83                     | 0.41              |
| 1:H:234:HIS:HD2    | 1:H:607:PRO:HG2  | 1.85                     | 0.41              |
| 1:H:364:TRP:NE1    | 1:H:368:GLN:OE1  | 2.53                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:521:LEU:HD22 | 1:H:566:ARG:NH1  | 2.36                     | 0.41              |
| 1:K:31:HIS:NE2   | 1:K:90:ARG:HD2   | 2.36                     | 0.41              |
| 1:K:52:GLU:HA    | 1:K:52:GLU:OE1   | 2.21                     | 0.41              |
| 1:K:104:GLY:N    | 2:N:730:A23:O1C  | 2.54                     | 0.41              |
| 1:K:305:ILE:HG22 | 1:K:309:ARG:CB   | 2.51                     | 0.41              |
| 1:L:34:THR:HG22  | 1:L:35:THR:N     | 2.35                     | 0.41              |
| 1:L:77:MET:CE    | 1:L:199:ARG:HH21 | 2.34                     | 0.41              |
| 1:L:273:LEU:HA   | 1:L:276:VAL:HG12 | 2.03                     | 0.41              |
| 1:A:177:SER:C    | 1:A:179:PRO:HD3  | 2.46                     | 0.41              |
| 1:A:607:PRO:HB2  | 1:A:610:THR:HG23 | 2.02                     | 0.41              |
| 1:H:290:ARG:HB2  | 1:H:316:ASN:HD21 | 1.85                     | 0.41              |
| 1:H:497:ARG:HG2  | 1:H:497:ARG:HH11 | 1.85                     | 0.41              |
| 1:H:521:LEU:CD2  | 1:H:567:LEU:HD23 | 2.51                     | 0.41              |
| 1:K:17:GLU:CD    | 2:M:727:A:H62    | 2.29                     | 0.41              |
| 1:K:114:ARG:O    | 1:K:118:LEU:HD23 | 2.21                     | 0.41              |
| 1:K:346:TYR:HB2  | 1:K:597:LEU:HD13 | 2.03                     | 0.41              |
| 1:K:435:GLU:CG   | 1:K:462:ALA:HA   | 2.41                     | 0.41              |
| 1:K:531:TYR:CD1  | 1:K:532:PRO:HD2  | 2.56                     | 0.41              |
| 1:L:50:TYR:HD1   | 1:L:144:LEU:CD2  | 2.33                     | 0.41              |
| 1:L:143:THR:H    | 1:L:146:GLU:HB2  | 1.84                     | 0.41              |
| 1:L:267:ALA:O    | 1:L:317:ASN:HB2  | 2.21                     | 0.41              |
| 1:L:368:GLN:HG3  | 1:L:420:TRP:HZ2  | 1.85                     | 0.41              |
| 1:A:86:TRP:O     | 1:A:89:GLN:HG2   | 2.20                     | 0.41              |
| 1:A:133:PHE:N    | 1:A:139:ARG:O    | 2.53                     | 0.41              |
| 1:A:149:GLN:NE2  | 1:A:153:THR:HG21 | 2.36                     | 0.41              |
| 1:B:19:MET:HE1   | 1:B:51:PHE:HE1   | 1.85                     | 0.41              |
| 1:B:79:PHE:CZ    | 1:B:108:ILE:HG23 | 2.56                     | 0.41              |
| 1:B:83:LEU:HD12  | 1:B:86:TRP:CZ3   | 2.56                     | 0.41              |
| 1:B:174:SER:HB2  | 1:B:176:PRO:HD2  | 2.03                     | 0.41              |
| 1:B:280:ALA:HB2  | 1:B:286:LEU:HD21 | 2.03                     | 0.41              |
| 1:B:340:LEU:HA   | 1:B:340:LEU:HD23 | 1.79                     | 0.41              |
| 1:B:440:ARG:CG   | 1:B:441:ALA:N    | 2.81                     | 0.41              |
| 1:G:21:LEU:HD22  | 1:G:125:PHE:CE2  | 2.56                     | 0.41              |
| 1:G:346:TYR:CE2  | 1:G:587:ALA:HB1  | 2.55                     | 0.41              |
| 1:H:12:TRP:CH2   | 1:H:46:GLN:HB3   | 2.56                     | 0.41              |
| 1:H:181:GLU:OE2  | 1:H:194:SER:N    | 2.54                     | 0.41              |
| 1:H:290:ARG:H    | 1:H:316:ASN:ND2  | 2.18                     | 0.41              |
| 1:H:364:TRP:HE3  | 1:H:412:LEU:CD1  | 2.34                     | 0.41              |
| 1:H:469:GLU:O    | 1:H:473:GLN:HG2  | 2.21                     | 0.41              |
| 1:H:610:THR:O    | 1:H:611:GLU:HB3  | 2.21                     | 0.41              |
| 1:K:165:PRO:O    | 1:K:171:ARG:NH1  | 2.53                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:238:LEU:HD21 | 1:K:574:LEU:HD12 | 2.03                     | 0.41              |
| 1:K:300:ILE:HD13 | 1:K:514:LEU:CD2  | 2.51                     | 0.41              |
| 1:K:335:LEU:HD21 | 1:K:349:ILE:HD12 | 2.03                     | 0.41              |
| 1:L:4:LEU:HD22   | 1:L:27:PHE:CD2   | 2.56                     | 0.41              |
| 1:L:15:VAL:HG11  | 1:L:32:VAL:CG2   | 2.51                     | 0.41              |
| 1:L:36:ALA:HB2   | 1:L:64:VAL:O     | 2.21                     | 0.41              |
| 1:L:46:GLN:OE1   | 1:L:144:LEU:HG   | 2.21                     | 0.41              |
| 1:L:462:ALA:CB   | 1:L:471:ILE:HD11 | 2.51                     | 0.41              |
| 1:L:487:LEU:HD11 | 1:L:513:ASN:CB   | 2.50                     | 0.41              |
| 1:A:40:ILE:O     | 1:A:44:VAL:HG23  | 2.21                     | 0.41              |
| 1:G:4:LEU:HD11   | 1:G:6:CYS:SG     | 2.60                     | 0.41              |
| 1:H:139:ARG:HG2  | 1:H:140:GLU:N    | 2.31                     | 0.41              |
| 1:H:277:ARG:NH1  | 1:H:289:VAL:HG23 | 2.36                     | 0.41              |
| 1:H:389:VAL:O    | 1:H:424:CYS:HA   | 2.21                     | 0.41              |
| 1:H:397:ARG:HB3  | 1:H:434:PHE:CE1  | 2.53                     | 0.41              |
| 1:K:434:PHE:HB2  | 1:K:444:PHE:CE2  | 2.56                     | 0.41              |
| 1:L:527:GLY:H    | 1:L:530:THR:HG21 | 1.84                     | 0.41              |
| 1:A:392:LEU:HD23 | 1:A:428:GLY:O    | 2.20                     | 0.40              |
| 1:B:3:ILE:HG22   | 1:B:4:LEU:N      | 2.36                     | 0.40              |
| 1:B:35:THR:HA    | 1:B:64:VAL:H     | 1.86                     | 0.40              |
| 1:B:79:PHE:CE2   | 1:B:108:ILE:HG23 | 2.56                     | 0.40              |
| 1:B:89:GLN:HA    | 1:B:175:ALA:CB   | 2.51                     | 0.40              |
| 1:H:84:TRP:HB3   | 1:H:198:LEU:HD23 | 2.03                     | 0.40              |
| 1:H:404:SER:HB2  | 1:H:408:ARG:HH12 | 1.86                     | 0.40              |
| 1:H:557:LEU:O    | 1:H:560:ASN:HB2  | 2.20                     | 0.40              |
| 2:J:720:A23:O1C  | 2:J:720:A23:H1'  | 2.21                     | 0.40              |
| 1:K:132:ARG:O    | 1:K:133:PHE:HD1  | 2.04                     | 0.40              |
| 1:L:196:MET:HE3  | 1:L:199:ARG:HB3  | 2.00                     | 0.40              |
| 1:L:245:VAL:HG23 | 1:L:246:GLN:NE2  | 2.36                     | 0.40              |
| 1:L:485:HIS:HB3  | 1:L:513:ASN:HD21 | 1.86                     | 0.40              |
| 1:A:180:LEU:CD1  | 1:A:193:ALA:HA   | 2.48                     | 0.40              |
| 1:A:572:THR:OG1  | 1:A:575:GLU:HG2  | 2.21                     | 0.40              |
| 1:B:430:ASP:CB   | 1:B:459:THR:HG23 | 2.52                     | 0.40              |
| 1:G:101:LEU:HD11 | 1:G:126:HIS:HB2  | 2.01                     | 0.40              |
| 1:G:465:ASN:O    | 1:G:466:ASP:HB3  | 2.21                     | 0.40              |
| 1:G:485:HIS:CD2  | 1:G:513:ASN:HD21 | 2.39                     | 0.40              |
| 1:H:4:LEU:HD12   | 1:H:98:TYR:C     | 2.45                     | 0.40              |
| 1:H:346:TYR:HB2  | 1:H:597:LEU:HD13 | 2.02                     | 0.40              |
| 1:A:201:HIS:O    | 1:A:205:VAL:HG23 | 2.21                     | 0.40              |
| 1:A:213:LEU:HD23 | 1:A:213:LEU:HA   | 1.90                     | 0.40              |
| 1:A:371:ARG:HD3  | 1:A:371:ARG:O    | 2.21                     | 0.40              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:A:547:THR:HG23   | 1:A:557:LEU:HD13 | 2.03                     | 0.40              |
| 1:B:34:THR:CB      | 1:B:63:ARG:HG2   | 2.52                     | 0.40              |
| 1:H:4:LEU:HD13     | 1:H:98:TYR:HB2   | 2.03                     | 0.40              |
| 1:H:34:THR:HG22    | 1:H:35:THR:N     | 2.37                     | 0.40              |
| 1:H:175:ALA:N      | 1:H:176:PRO:HD2  | 2.36                     | 0.40              |
| 1:H:313:LEU:HB2    | 1:H:552:ILE:HG23 | 2.03                     | 0.40              |
| 1:K:533:LEU:HB3    | 1:K:568:CYS:SG   | 2.62                     | 0.40              |
| 1:K:547:THR:O      | 1:K:548:ASP:HB3  | 2.22                     | 0.40              |
| 1:L:6:CYS:O        | 1:L:33:LEU:N     | 2.43                     | 0.40              |
| 1:L:84:TRP:CE3     | 1:L:198:LEU:HD22 | 2.56                     | 0.40              |
| 1:L:128:LEU:CD1    | 1:L:157:ARG:HE   | 2.34                     | 0.40              |
| 1:L:581:VAL:HG13   | 1:L:598:TRP:CH2  | 2.57                     | 0.40              |
| 1:B:17:GLU:HB3     | 1:B:156:LEU:HD21 | 2.02                     | 0.40              |
| 1:B:85:ARG:HH12    | 1:B:195:ASP:N    | 2.07                     | 0.40              |
| 1:G:84:TRP:HZ3     | 1:G:199:ARG:HA   | 1.86                     | 0.40              |
| 1:G:431:LEU:HD22   | 1:G:448:PHE:HZ   | 1.87                     | 0.40              |
| 1:G:453:ARG:NH1    | 1:H:469:GLU:OE1  | 2.39                     | 0.40              |
| 1:H:200:GLN:C      | 1:H:203:GLU:HG2  | 2.46                     | 0.40              |
| 1:K:12:TRP:HE3     | 1:K:47:LEU:CG    | 2.33                     | 0.40              |
| 1:K:61:ILE:CD1     | 1:K:188:VAL:HG12 | 2.48                     | 0.40              |
| 1:K:82:VAL:CG2     | 1:K:193:ALA:HB2  | 2.49                     | 0.40              |
| 1:K:261:CYS:SG     | 1:K:550:LEU:HD12 | 2.62                     | 0.40              |
| 1:K:282:ASN:O      | 1:K:282:ASN:OD1  | 2.39                     | 0.40              |
| 1:K:354:ALA:HB1    | 1:K:405:ARG:NH1  | 2.33                     | 0.40              |
| 1:L:17:GLU:CD      | 1:L:156:LEU:HD13 | 2.47                     | 0.40              |
| 1:L:414:ILE:CG2    | 1:L:454:VAL:HG21 | 2.44                     | 0.40              |
| 1:A:392:LEU:HD23   | 1:A:428:GLY:C    | 2.46                     | 0.40              |
| 1:A:471:ILE:O      | 1:A:475:VAL:HG23 | 2.21                     | 0.40              |
| 1:B:39:LYS:HD3     | 1:B:39:LYS:N     | 2.37                     | 0.40              |
| 1:B:139:ARG:HG2    | 1:B:140:GLU:N    | 2.37                     | 0.40              |
| 1:B:266:PHE:HE2    | 1:B:334:LEU:HB3  | 1.87                     | 0.40              |
| 1:G:64:VAL:O       | 1:G:64:VAL:HG23  | 2.22                     | 0.40              |
| 1:G:114:ARG:HH22   | 1:H:114:ARG:HA   | 1.86                     | 0.40              |
| 1:G:227:LEU:HD21   | 1:G:604:VAL:HG21 | 2.04                     | 0.40              |
| 1:G:472[A]:TRP:HZ3 | 1:G:476:PHE:HE2  | 1.69                     | 0.40              |
| 1:H:276:VAL:HG22   | 1:H:330:ALA:HB1  | 2.03                     | 0.40              |
| 1:K:37:SER:CA      | 1:K:68:GLU:HB2   | 2.51                     | 0.40              |
| 1:L:130:GLU:HG3    | 1:L:155:ALA:O    | 2.22                     | 0.40              |
| 1:L:183:THR:OG1    | 1:L:190:TRP:HB2  | 2.22                     | 0.40              |
| 1:L:196:MET:CE     | 1:L:199:ARG:HB2  | 2.48                     | 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     | 601/625 (96%)   | 572 (95%)  | 28 (5%)  | 1 (0%)   | 43          | 72  |
| 1   | B     | 609/625 (97%)   | 579 (95%)  | 28 (5%)  | 2 (0%)   | 36          | 66  |
| 1   | G     | 601/625 (96%)   | 568 (94%)  | 31 (5%)  | 2 (0%)   | 36          | 66  |
| 1   | H     | 600/625 (96%)   | 579 (96%)  | 21 (4%)  | 0        | 100         | 100 |
| 1   | K     | 601/625 (96%)   | 578 (96%)  | 22 (4%)  | 1 (0%)   | 43          | 72  |
| 1   | L     | 600/625 (96%)   | 573 (96%)  | 27 (4%)  | 0        | 100         | 100 |
| All | All   | 3612/3750 (96%) | 3449 (96%) | 157 (4%) | 6 (0%)   | 44          | 72  |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 321 | LEU  |
| 1   | B     | 465 | ASN  |
| 1   | G     | 321 | LEU  |
| 1   | G     | 465 | ASN  |
| 1   | K     | 321 | LEU  |
| 1   | B     | 468 | VAL  |

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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     | 495/511 (97%) | 495 (100%) | 0        | 100         | 100 |
| 1   | B     | 500/511 (98%) | 500 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | G     | 496/511 (97%)   | 496 (100%)  | 0        | 100         | 100 |
| 1   | H     | 495/511 (97%)   | 495 (100%)  | 0        | 100         | 100 |
| 1   | K     | 496/511 (97%)   | 496 (100%)  | 0        | 100         | 100 |
| 1   | L     | 495/511 (97%)   | 495 (100%)  | 0        | 100         | 100 |
| All | All   | 2977/3066 (97%) | 2977 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 25  | GLN  |
| 1   | A     | 169 | GLN  |
| 1   | A     | 189 | HIS  |
| 1   | A     | 239 | HIS  |
| 1   | A     | 343 | HIS  |
| 1   | A     | 373 | HIS  |
| 1   | A     | 419 | HIS  |
| 1   | A     | 580 | GLN  |
| 1   | B     | 46  | GLN  |
| 1   | B     | 89  | GLN  |
| 1   | B     | 126 | HIS  |
| 1   | B     | 149 | GLN  |
| 1   | B     | 252 | GLN  |
| 1   | B     | 278 | GLN  |
| 1   | B     | 316 | ASN  |
| 1   | B     | 375 | GLN  |
| 1   | B     | 376 | GLN  |
| 1   | B     | 465 | ASN  |
| 1   | G     | 200 | GLN  |
| 1   | G     | 211 | HIS  |
| 1   | G     | 269 | HIS  |
| 1   | G     | 419 | HIS  |
| 1   | G     | 488 | HIS  |
| 1   | G     | 513 | ASN  |
| 1   | G     | 549 | ASN  |
| 1   | G     | 612 | GLN  |
| 1   | H     | 31  | HIS  |
| 1   | H     | 54  | HIS  |
| 1   | H     | 65  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 76  | HIS  |
| 1   | H     | 211 | HIS  |
| 1   | H     | 316 | ASN  |
| 1   | H     | 355 | ASN  |
| 1   | H     | 419 | HIS  |
| 1   | H     | 560 | ASN  |
| 1   | K     | 20  | GLN  |
| 1   | K     | 54  | HIS  |
| 1   | K     | 76  | HIS  |
| 1   | K     | 96  | HIS  |
| 1   | K     | 239 | HIS  |
| 1   | K     | 372 | ASN  |
| 1   | K     | 390 | ASN  |
| 1   | K     | 419 | HIS  |
| 1   | K     | 465 | ASN  |
| 1   | K     | 485 | HIS  |
| 1   | K     | 513 | ASN  |
| 1   | K     | 515 | GLN  |
| 1   | K     | 603 | GLN  |
| 1   | L     | 31  | HIS  |
| 1   | L     | 126 | HIS  |
| 1   | L     | 138 | ASN  |
| 1   | L     | 149 | GLN  |
| 1   | L     | 189 | HIS  |
| 1   | L     | 201 | HIS  |
| 1   | L     | 252 | GLN  |
| 1   | L     | 269 | HIS  |
| 1   | L     | 419 | HIS  |
| 1   | L     | 461 | HIS  |
| 1   | L     | 485 | HIS  |
| 1   | L     | 513 | ASN  |
| 1   | L     | 580 | GLN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed  | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------|-------------------|-----------------|
| 2   | C     | 1/2 (50%) | 1 (100%)          | 0               |
| 2   | D     | 1/2 (50%) | 1 (100%)          | 0               |
| 2   | I     | 1/2 (50%) | 1 (100%)          | 0               |
| 2   | J     | 1/2 (50%) | 1 (100%)          | 0               |
| 2   | M     | 1/2 (50%) | 1 (100%)          | 0               |

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| Mol | Chain | Analysed   | Backbone Outliers | Pucker Outliers |
|-----|-------|------------|-------------------|-----------------|
| 2   | N     | 1/2 (50%)  | 1 (100%)          | 0               |
| All | All   | 6/12 (50%) | 6 (100%)          | 0               |

All (6) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 708 | A23  |
| 2   | D     | 710 | A23  |
| 2   | I     | 718 | A23  |
| 2   | J     | 720 | A23  |
| 2   | M     | 728 | A23  |
| 2   | N     | 730 | A23  |

There are no RNA pucker outliers to report.

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

6 non-standard protein/DNA/RNA residues 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 |
| 2   | A23  | C     | 708 | 2    | 23,28,29     | 4.22 | 8 (34%)  | 32,43,46    | 2.27 | 11 (34%) |
| 2   | A23  | D     | 710 | 2    | 23,28,29     | 4.20 | 8 (34%)  | 32,43,46    | 2.21 | 11 (34%) |
| 2   | A23  | M     | 728 | 2    | 23,28,29     | 4.19 | 8 (34%)  | 32,43,46    | 2.25 | 11 (34%) |
| 2   | A23  | I     | 718 | 2    | 23,28,29     | 4.20 | 8 (34%)  | 32,43,46    | 2.22 | 11 (34%) |
| 2   | A23  | J     | 720 | 2    | 23,28,29     | 4.20 | 8 (34%)  | 32,43,46    | 2.20 | 11 (34%) |
| 2   | A23  | N     | 730 | 2    | 23,28,29     | 4.21 | 8 (34%)  | 32,43,46    | 2.24 | 12 (37%) |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | A23  | C     | 708 | 2    | -       | 0/7/35/36 | 0/4/4/4 |
| 2   | A23  | D     | 710 | 2    | -       | 1/7/35/36 | 0/4/4/4 |
| 2   | A23  | M     | 728 | 2    | -       | 2/7/35/36 | 0/4/4/4 |
| 2   | A23  | I     | 718 | 2    | -       | 1/7/35/36 | 0/4/4/4 |
| 2   | A23  | J     | 720 | 2    | -       | 1/7/35/36 | 0/4/4/4 |
| 2   | A23  | N     | 730 | 2    | -       | 1/7/35/36 | 0/4/4/4 |

All (48) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 710 | A23  | O4'-C4' | 13.14 | 1.74        | 1.45     |
| 2   | J     | 720 | A23  | O4'-C4' | 13.09 | 1.74        | 1.45     |
| 2   | C     | 708 | A23  | O4'-C4' | 13.09 | 1.74        | 1.45     |
| 2   | N     | 730 | A23  | O4'-C4' | 13.07 | 1.74        | 1.45     |
| 2   | I     | 718 | A23  | O4'-C4' | 13.06 | 1.74        | 1.45     |
| 2   | M     | 728 | A23  | O4'-C4' | 12.81 | 1.73        | 1.45     |
| 2   | C     | 708 | A23  | C3'-C4' | -9.71 | 1.27        | 1.52     |
| 2   | J     | 720 | A23  | C3'-C4' | -9.61 | 1.28        | 1.52     |
| 2   | D     | 710 | A23  | C3'-C4' | -9.57 | 1.28        | 1.52     |
| 2   | M     | 728 | A23  | C3'-C4' | -9.57 | 1.28        | 1.52     |
| 2   | I     | 718 | A23  | C3'-C4' | -9.51 | 1.28        | 1.52     |
| 2   | N     | 730 | A23  | C3'-C4' | -9.50 | 1.28        | 1.52     |
| 2   | M     | 728 | A23  | C2'-C3' | 8.48  | 1.71        | 1.53     |
| 2   | N     | 730 | A23  | C2'-C3' | 8.46  | 1.71        | 1.53     |
| 2   | I     | 718 | A23  | C2'-C3' | 8.39  | 1.71        | 1.53     |
| 2   | C     | 708 | A23  | C2'-C3' | 8.33  | 1.71        | 1.53     |
| 2   | J     | 720 | A23  | C2'-C3' | 8.13  | 1.70        | 1.53     |
| 2   | D     | 710 | A23  | C2'-C3' | 8.07  | 1.70        | 1.53     |
| 2   | N     | 730 | A23  | C6-N6   | 4.55  | 1.45        | 1.34     |
| 2   | D     | 710 | A23  | C6-N6   | 4.53  | 1.45        | 1.34     |
| 2   | J     | 720 | A23  | C6-N6   | 4.50  | 1.45        | 1.34     |
| 2   | I     | 718 | A23  | C6-N6   | 4.50  | 1.45        | 1.34     |
| 2   | C     | 708 | A23  | C6-N6   | 4.49  | 1.45        | 1.34     |
| 2   | M     | 728 | A23  | C6-N6   | 4.42  | 1.45        | 1.34     |
| 2   | M     | 728 | A23  | PC-O1C  | 4.16  | 1.65        | 1.50     |
| 2   | D     | 710 | A23  | PC-O1C  | 4.16  | 1.65        | 1.50     |
| 2   | C     | 708 | A23  | PC-O1C  | 4.16  | 1.65        | 1.50     |
| 2   | J     | 720 | A23  | PC-O1C  | 4.16  | 1.65        | 1.50     |
| 2   | N     | 730 | A23  | PC-O1C  | 4.15  | 1.65        | 1.50     |
| 2   | I     | 718 | A23  | PC-O1C  | 4.14  | 1.65        | 1.50     |
| 2   | D     | 710 | A23  | O2'-C2' | -3.17 | 1.22        | 1.46     |
| 2   | J     | 720 | A23  | O2'-C2' | -3.16 | 1.22        | 1.46     |
| 2   | C     | 708 | A23  | O2'-C2' | -3.13 | 1.22        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | M     | 728 | A23  | O2'-C2' | -3.11 | 1.23        | 1.46     |
| 2   | N     | 730 | A23  | O2'-C2' | -3.08 | 1.23        | 1.46     |
| 2   | I     | 718 | A23  | O2'-C2' | -3.06 | 1.23        | 1.46     |
| 2   | J     | 720 | A23  | C8-N9   | -2.96 | 1.32        | 1.37     |
| 2   | M     | 728 | A23  | C8-N9   | -2.94 | 1.32        | 1.37     |
| 2   | I     | 718 | A23  | C8-N9   | -2.93 | 1.32        | 1.37     |
| 2   | D     | 710 | A23  | C8-N9   | -2.92 | 1.32        | 1.37     |
| 2   | N     | 730 | A23  | C8-N9   | -2.91 | 1.32        | 1.37     |
| 2   | C     | 708 | A23  | C8-N9   | -2.91 | 1.32        | 1.37     |
| 2   | C     | 708 | A23  | C5-N7   | -2.41 | 1.34        | 1.39     |
| 2   | J     | 720 | A23  | C5-N7   | -2.40 | 1.34        | 1.39     |
| 2   | I     | 718 | A23  | C5-N7   | -2.38 | 1.34        | 1.39     |
| 2   | N     | 730 | A23  | C5-N7   | -2.38 | 1.34        | 1.39     |
| 2   | D     | 710 | A23  | C5-N7   | -2.37 | 1.34        | 1.39     |
| 2   | M     | 728 | A23  | C5-N7   | -2.36 | 1.34        | 1.39     |

All (67) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | C     | 708 | A23  | C5-C4-N3   | -5.61 | 118.99      | 126.72   |
| 2   | J     | 720 | A23  | C5-C4-N3   | -5.41 | 119.27      | 126.72   |
| 2   | I     | 718 | A23  | C5-C4-N3   | -5.36 | 119.33      | 126.72   |
| 2   | N     | 730 | A23  | C5-C4-N3   | -5.35 | 119.35      | 126.72   |
| 2   | D     | 710 | A23  | C5-C4-N3   | -5.27 | 119.46      | 126.72   |
| 2   | M     | 728 | A23  | C5-C4-N3   | -5.22 | 119.53      | 126.72   |
| 2   | M     | 728 | A23  | N3-C2-N1   | -4.18 | 122.26      | 128.58   |
| 2   | D     | 710 | A23  | N3-C2-N1   | -4.12 | 122.34      | 128.58   |
| 2   | I     | 718 | A23  | N3-C2-N1   | -4.12 | 122.35      | 128.58   |
| 2   | C     | 708 | A23  | N3-C2-N1   | -4.11 | 122.36      | 128.58   |
| 2   | J     | 720 | A23  | N3-C2-N1   | -4.11 | 122.37      | 128.58   |
| 2   | C     | 708 | A23  | N3-C4-N9   | 4.06  | 134.08      | 127.17   |
| 2   | N     | 730 | A23  | N3-C2-N1   | -4.06 | 122.44      | 128.58   |
| 2   | C     | 708 | A23  | C2'-C1'-N9 | -3.96 | 107.24      | 113.75   |
| 2   | I     | 718 | A23  | N3-C4-N9   | 3.86  | 133.74      | 127.17   |
| 2   | J     | 720 | A23  | N3-C4-N9   | 3.83  | 133.68      | 127.17   |
| 2   | M     | 728 | A23  | N3-C4-N9   | 3.81  | 133.65      | 127.17   |
| 2   | D     | 710 | A23  | N3-C4-N9   | 3.79  | 133.62      | 127.17   |
| 2   | N     | 730 | A23  | C4-C5-N7   | -3.76 | 106.29      | 110.58   |
| 2   | N     | 730 | A23  | N3-C4-N9   | 3.75  | 133.55      | 127.17   |
| 2   | J     | 720 | A23  | C4-C5-N7   | -3.74 | 106.31      | 110.58   |
| 2   | M     | 728 | A23  | N9-C8-N7   | -3.73 | 108.64      | 113.94   |
| 2   | C     | 708 | A23  | C2-N3-C4   | 3.69  | 120.83      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | C     | 708 | A23  | C4-C5-N7    | -3.62 | 106.44      | 110.58   |
| 2   | J     | 720 | A23  | C5-N7-C8    | 3.62  | 109.14      | 103.45   |
| 2   | I     | 718 | A23  | C4-C5-N7    | -3.61 | 106.45      | 110.58   |
| 2   | D     | 710 | A23  | C4-C5-N7    | -3.61 | 106.45      | 110.58   |
| 2   | J     | 720 | A23  | C2-N3-C4    | 3.60  | 120.62      | 111.83   |
| 2   | N     | 730 | A23  | C5-N7-C8    | 3.60  | 109.10      | 103.45   |
| 2   | D     | 710 | A23  | N9-C8-N7    | -3.59 | 108.84      | 113.94   |
| 2   | I     | 718 | A23  | C2-N3-C4    | 3.59  | 120.60      | 111.83   |
| 2   | J     | 720 | A23  | N9-C8-N7    | -3.59 | 108.85      | 113.94   |
| 2   | I     | 718 | A23  | N9-C8-N7    | -3.58 | 108.85      | 113.94   |
| 2   | C     | 708 | A23  | C5-N7-C8    | 3.57  | 109.07      | 103.45   |
| 2   | M     | 728 | A23  | C5-N7-C8    | 3.57  | 109.06      | 103.45   |
| 2   | M     | 728 | A23  | C4-C5-N7    | -3.57 | 106.50      | 110.58   |
| 2   | D     | 710 | A23  | C2-N3-C4    | 3.55  | 120.51      | 111.83   |
| 2   | N     | 730 | A23  | N9-C8-N7    | -3.55 | 108.90      | 113.94   |
| 2   | M     | 728 | A23  | C2-N3-C4    | 3.55  | 120.50      | 111.83   |
| 2   | N     | 730 | A23  | C2-N3-C4    | 3.54  | 120.48      | 111.83   |
| 2   | I     | 718 | A23  | C5-N7-C8    | 3.54  | 109.02      | 103.45   |
| 2   | D     | 710 | A23  | C5-N7-C8    | 3.53  | 109.00      | 103.45   |
| 2   | C     | 708 | A23  | N9-C8-N7    | -3.51 | 108.96      | 113.94   |
| 2   | M     | 728 | A23  | C4'-O4'-C1' | -3.21 | 102.37      | 109.47   |
| 2   | M     | 728 | A23  | C4-N9-C8    | 3.08  | 108.97      | 105.74   |
| 2   | D     | 710 | A23  | C4-N9-C8    | 2.90  | 108.78      | 105.74   |
| 2   | I     | 718 | A23  | C4-N9-C8    | 2.87  | 108.75      | 105.74   |
| 2   | J     | 720 | A23  | C4-N9-C8    | 2.78  | 108.66      | 105.74   |
| 2   | N     | 730 | A23  | C4-N9-C8    | 2.74  | 108.61      | 105.74   |
| 2   | C     | 708 | A23  | C4-N9-C8    | 2.72  | 108.60      | 105.74   |
| 2   | N     | 730 | A23  | O2'-PC-O1C  | -2.61 | 108.87      | 115.76   |
| 2   | I     | 718 | A23  | O3'-PC-O1C  | -2.60 | 108.89      | 115.76   |
| 2   | I     | 718 | A23  | O2'-PC-O1C  | -2.60 | 108.90      | 115.76   |
| 2   | J     | 720 | A23  | O2'-PC-O1C  | -2.58 | 108.96      | 115.76   |
| 2   | D     | 710 | A23  | O2'-PC-O1C  | -2.56 | 109.01      | 115.76   |
| 2   | M     | 728 | A23  | O2'-PC-O1C  | -2.56 | 109.01      | 115.76   |
| 2   | N     | 730 | A23  | O3'-PC-O1C  | -2.45 | 109.29      | 115.76   |
| 2   | D     | 710 | A23  | O3'-PC-O1C  | -2.44 | 109.31      | 115.76   |
| 2   | J     | 720 | A23  | O3'-PC-O1C  | -2.44 | 109.31      | 115.76   |
| 2   | M     | 728 | A23  | O3'-PC-O1C  | -2.44 | 109.32      | 115.76   |
| 2   | I     | 718 | A23  | C2'-C1'-N9  | -2.38 | 109.83      | 113.75   |
| 2   | C     | 708 | A23  | O3'-PC-O1C  | -2.32 | 109.64      | 115.76   |
| 2   | D     | 710 | A23  | C2'-C1'-N9  | -2.31 | 109.94      | 113.75   |
| 2   | C     | 708 | A23  | O2'-PC-O1C  | -2.22 | 109.90      | 115.76   |
| 2   | J     | 720 | A23  | C2'-C1'-N9  | -2.08 | 110.32      | 113.75   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | N     | 730 | A23  | C4'-O4'-C1' | -2.07 | 104.90      | 109.47   |
| 2   | N     | 730 | A23  | C2'-C1'-N9  | -2.06 | 110.36      | 113.75   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | M     | 728 | A23  | O4'-C4'-C5'-O5' |
| 2   | M     | 728 | A23  | C3'-C4'-C5'-O5' |
| 2   | J     | 720 | A23  | C4'-C5'-O5'-P   |
| 2   | I     | 718 | A23  | C3'-C4'-C5'-O5' |
| 2   | N     | 730 | A23  | C4'-C5'-O5'-P   |
| 2   | D     | 710 | A23  | C4'-C5'-O5'-P   |

There are no ring outliers.

6 monomers are involved in 43 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | C     | 708 | A23  | 8       | 0            |
| 2   | D     | 710 | A23  | 4       | 0            |
| 2   | M     | 728 | A23  | 11      | 0            |
| 2   | I     | 718 | A23  | 7       | 0            |
| 2   | J     | 720 | A23  | 6       | 0            |
| 2   | N     | 730 | A23  | 7       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 14 are monoatomic - leaving 6 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | ATP  | K     | 701 | 5    | 32,33,33     | 0.28 | 0        | 48,52,52    | 0.66 | 0        |
| 3   | ATP  | A     | 701 | -    | 32,33,33     | 0.27 | 0        | 48,52,52    | 0.66 | 0        |
| 3   | ATP  | B     | 701 | -    | 32,33,33     | 0.27 | 0        | 48,52,52    | 0.68 | 0        |
| 3   | ATP  | L     | 703 | 5    | 32,33,33     | 0.27 | 0        | 48,52,52    | 0.68 | 0        |
| 3   | ATP  | G     | 701 | 4,5  | 32,33,33     | 0.27 | 0        | 48,52,52    | 0.68 | 0        |
| 3   | ATP  | H     | 703 | 5    | 32,33,33     | 0.27 | 0        | 48,52,52    | 0.70 | 2 (4%)   |

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   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 3   | ATP  | K     | 701 | 5    | -       | 4/22/38/38  | 0/3/3/3 |
| 3   | ATP  | A     | 701 | -    | -       | 8/22/38/38  | 0/3/3/3 |
| 3   | ATP  | B     | 701 | -    | -       | 3/22/38/38  | 0/3/3/3 |
| 3   | ATP  | L     | 703 | 5    | -       | 2/22/38/38  | 0/3/3/3 |
| 3   | ATP  | G     | 701 | 4,5  | -       | 10/22/38/38 | 0/3/3/3 |
| 3   | ATP  | H     | 703 | 5    | -       | 9/22/38/38  | 0/3/3/3 |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | H     | 703 | ATP  | O2'-C2'-C3' | -2.45 | 103.97      | 111.82   |
| 3   | H     | 703 | ATP  | O3'-C3'-C2' | -2.13 | 104.98      | 111.82   |

There are no chirality outliers.

All (36) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 3   | A     | 701 | ATP  | C5'-O5'-PA-O1A |
| 3   | A     | 701 | ATP  | C5'-O5'-PA-O3A |
| 3   | G     | 701 | ATP  | C5'-O5'-PA-O2A |
| 3   | G     | 701 | ATP  | C5'-O5'-PA-O3A |
| 3   | H     | 703 | ATP  | PB-O3B-PG-O3G  |
| 3   | H     | 703 | ATP  | C5'-O5'-PA-O1A |
| 3   | K     | 701 | ATP  | C5'-O5'-PA-O1A |
| 3   | K     | 701 | ATP  | C5'-O5'-PA-O3A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | G     | 701 | ATP  | C3'-C4'-C5'-O5' |
| 3   | G     | 701 | ATP  | O4'-C4'-C5'-O5' |
| 3   | H     | 703 | ATP  | C3'-C4'-C5'-O5' |
| 3   | B     | 701 | ATP  | O4'-C4'-C5'-O5' |
| 3   | B     | 701 | ATP  | C3'-C4'-C5'-O5' |
| 3   | H     | 703 | ATP  | O4'-C4'-C5'-O5' |
| 3   | L     | 703 | ATP  | PB-O3A-PA-O1A   |
| 3   | A     | 701 | ATP  | C2'-C1'-N9-C8   |
| 3   | A     | 701 | ATP  | PB-O3A-PA-O5'   |
| 3   | G     | 701 | ATP  | PB-O3A-PA-O5'   |
| 3   | G     | 701 | ATP  | PB-O3B-PG-O2G   |
| 3   | G     | 701 | ATP  | C2'-C1'-N9-C8   |
| 3   | B     | 701 | ATP  | PB-O3A-PA-O2A   |
| 3   | H     | 703 | ATP  | PB-O3A-PA-O2A   |
| 3   | A     | 701 | ATP  | C5'-O5'-PA-O2A  |
| 3   | H     | 703 | ATP  | C5'-O5'-PA-O3A  |
| 3   | K     | 701 | ATP  | C5'-O5'-PA-O2A  |
| 3   | H     | 703 | ATP  | PA-O3A-PB-O2B   |
| 3   | A     | 701 | ATP  | C2'-C1'-N9-C4   |
| 3   | L     | 703 | ATP  | PB-O3A-PA-O2A   |
| 3   | G     | 701 | ATP  | PB-O3B-PG-O1G   |
| 3   | H     | 703 | ATP  | PB-O3B-PG-O1G   |
| 3   | A     | 701 | ATP  | PB-O3B-PG-O3G   |
| 3   | G     | 701 | ATP  | PB-O3B-PG-O3G   |
| 3   | K     | 701 | ATP  | PB-O3B-PG-O3G   |
| 3   | G     | 701 | ATP  | PB-O3A-PA-O2A   |
| 3   | H     | 703 | ATP  | PB-O3A-PA-O1A   |
| 3   | A     | 701 | ATP  | O4'-C1'-N9-C8   |

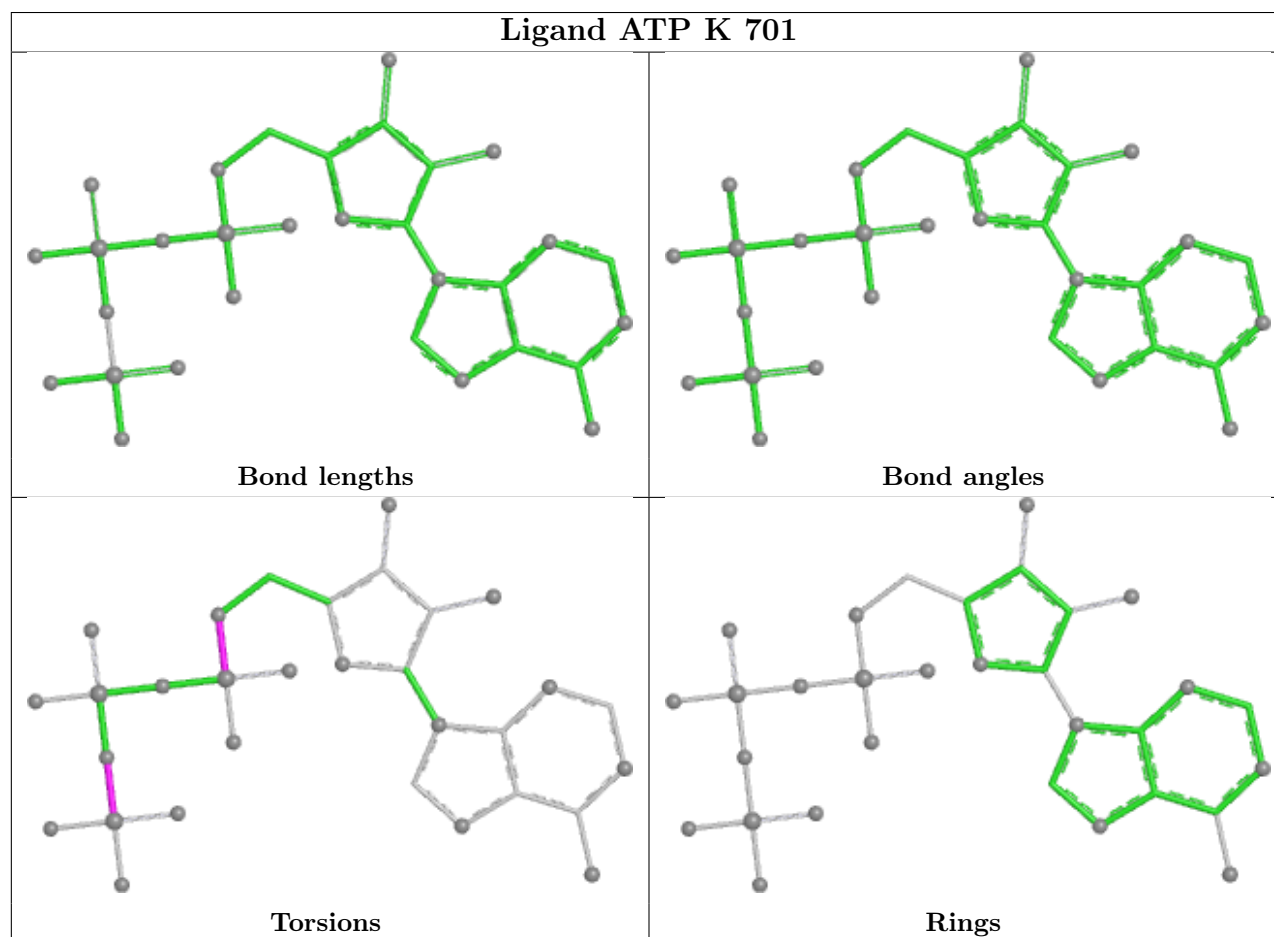
There are no ring outliers.

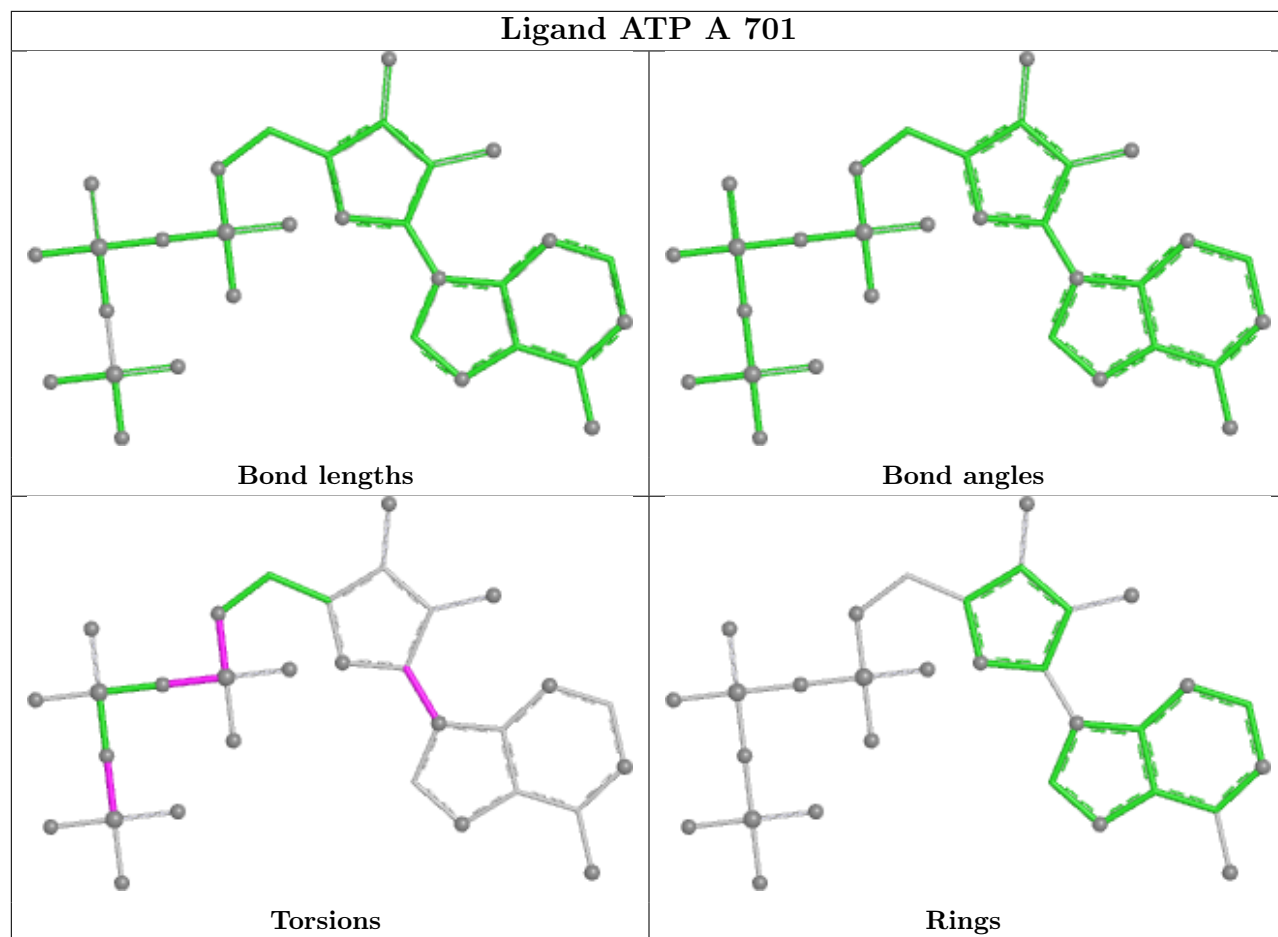
5 monomers are involved in 16 short contacts:

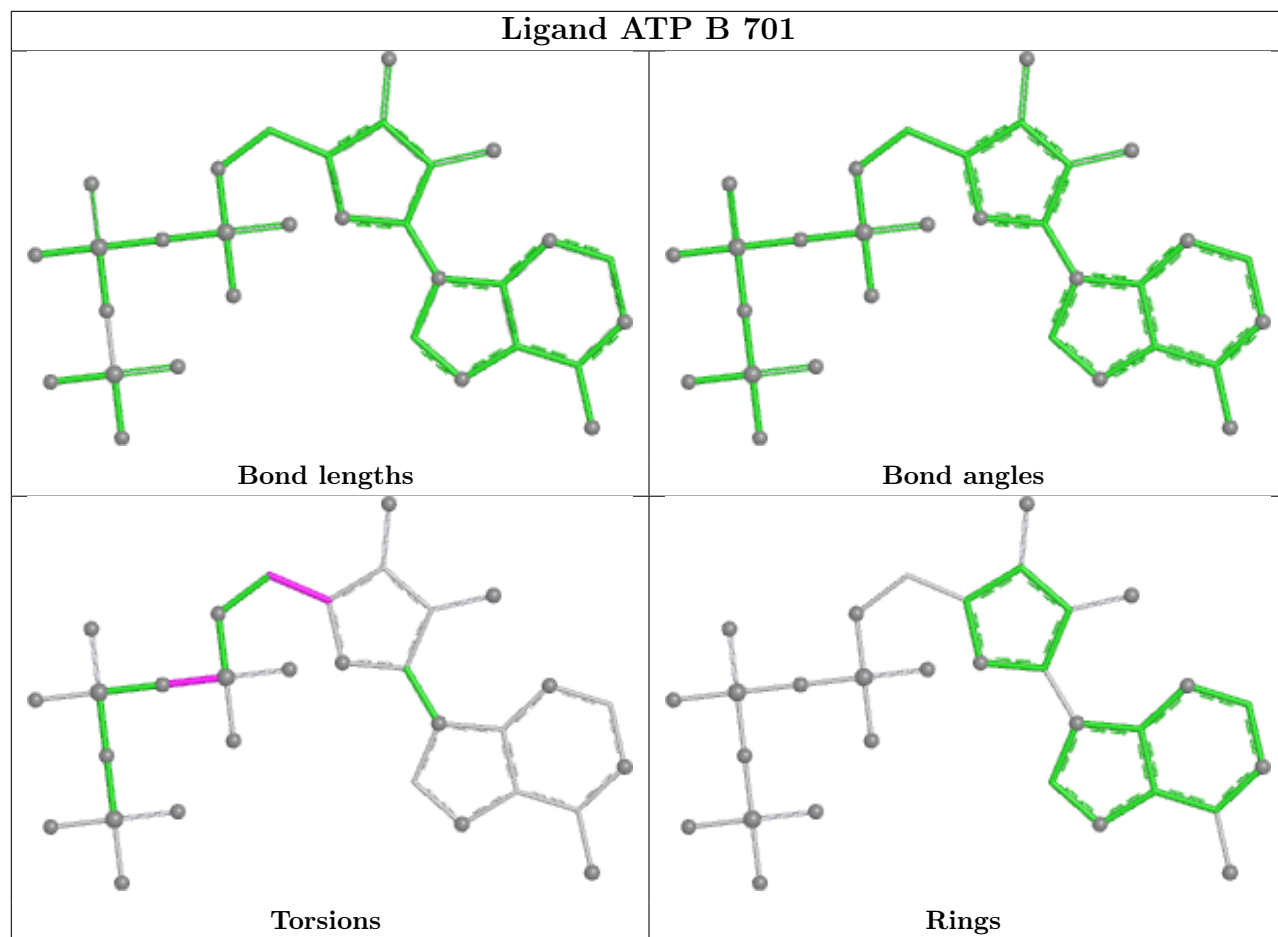
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 701 | ATP  | 2       | 0            |
| 3   | B     | 701 | ATP  | 5       | 0            |
| 3   | L     | 703 | ATP  | 4       | 0            |
| 3   | G     | 701 | ATP  | 2       | 0            |
| 3   | H     | 703 | ATP  | 3       | 0            |

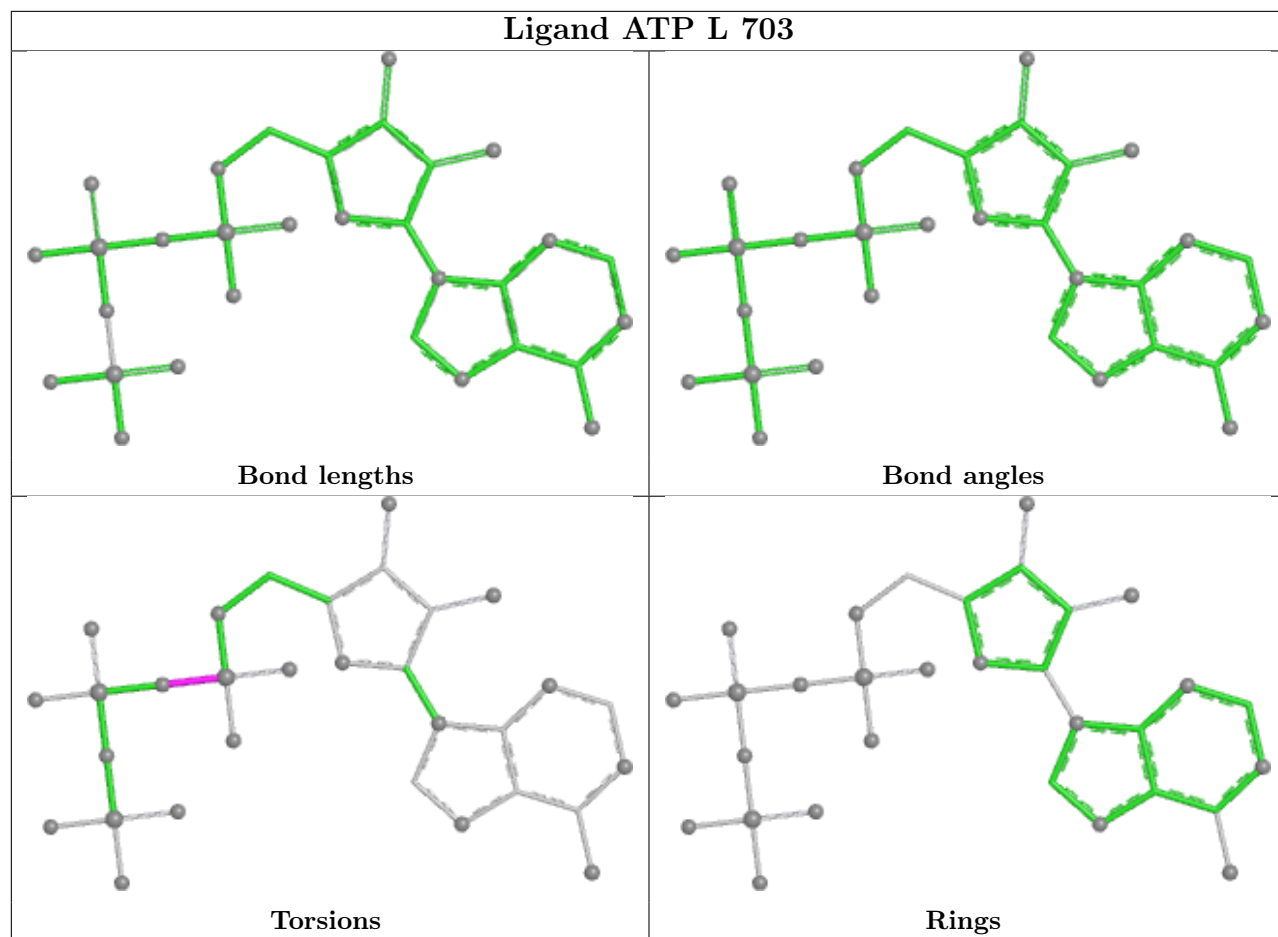
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

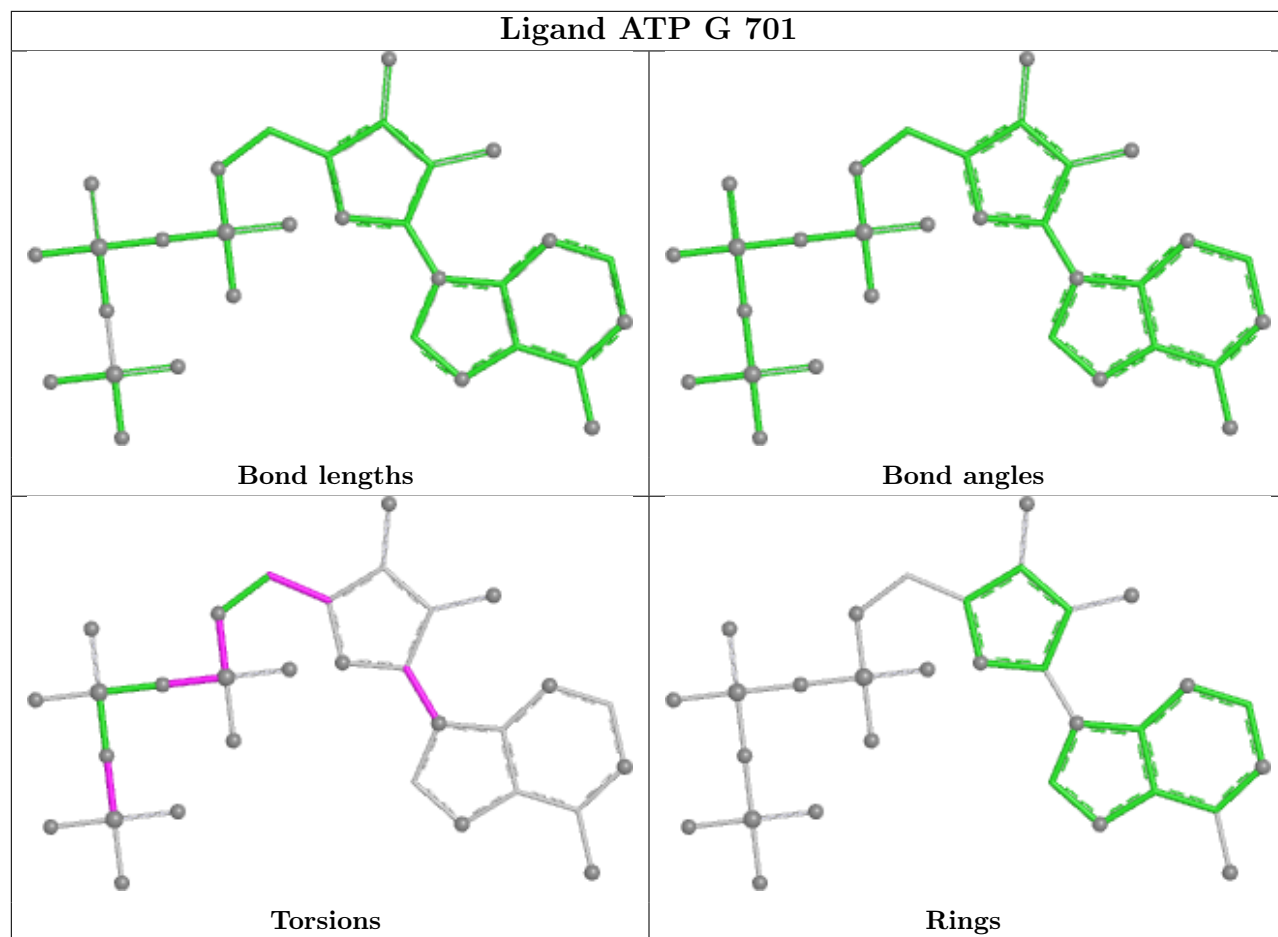
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

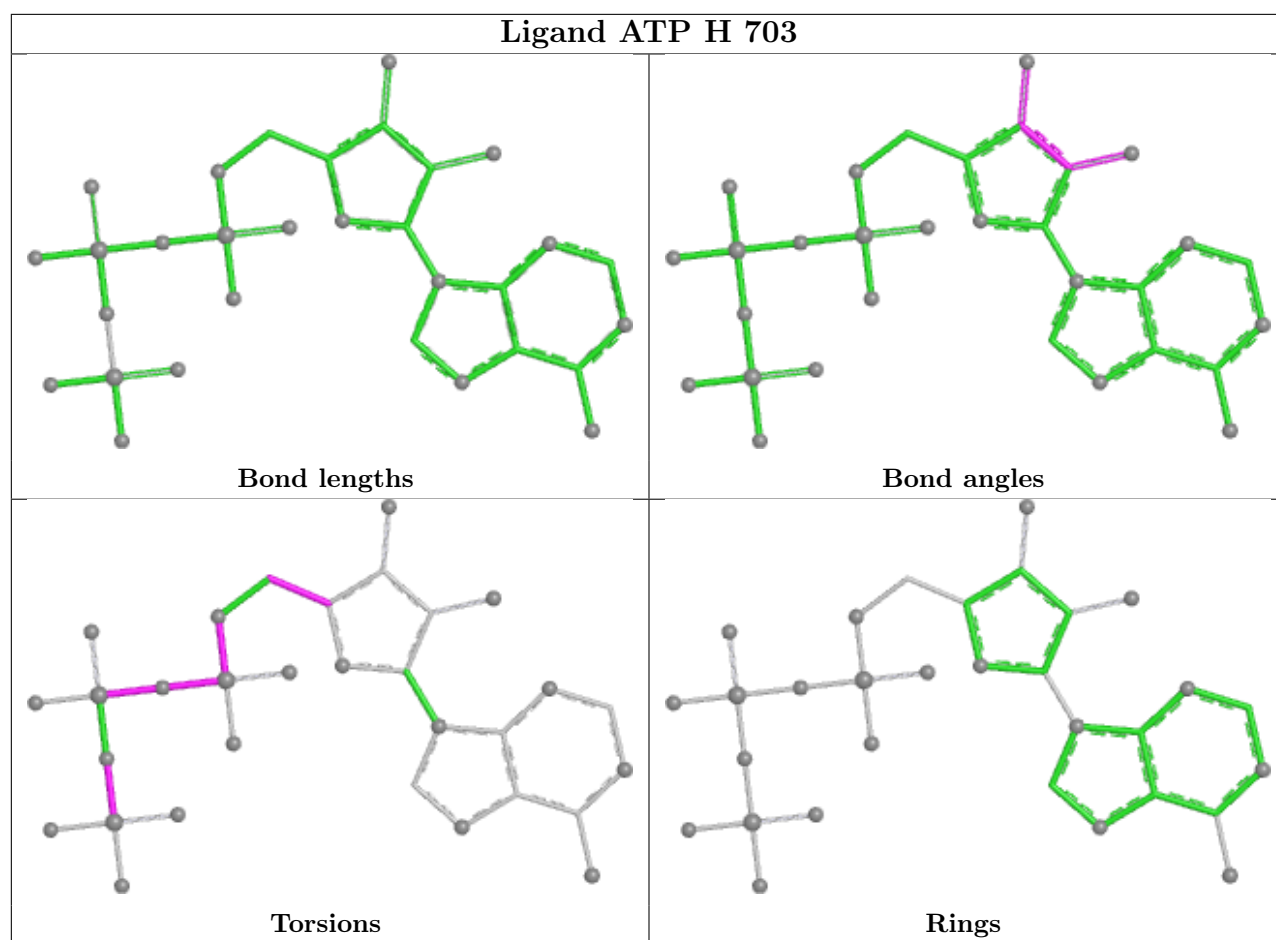












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

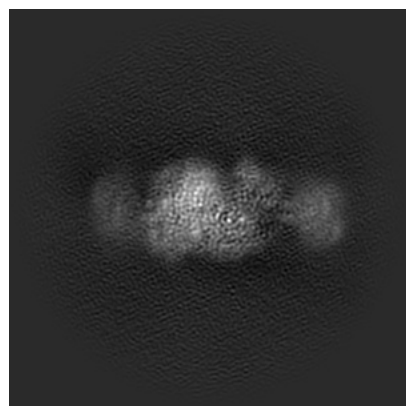
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70428. These allow visual inspection of the internal detail of the map and identification of artifacts.

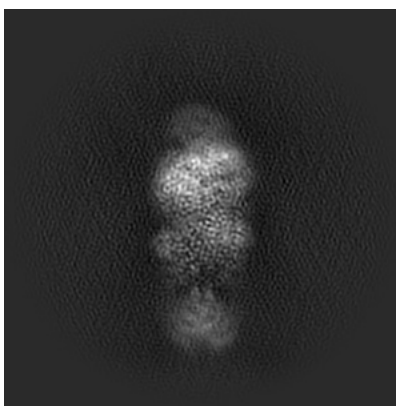
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

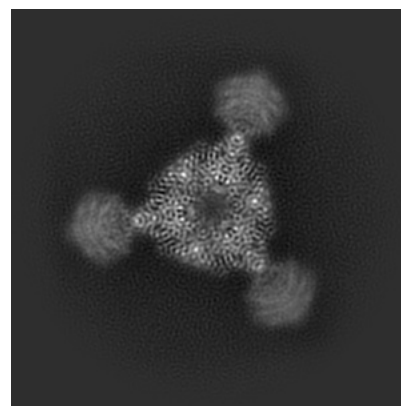
#### 6.1.1 Primary map



X

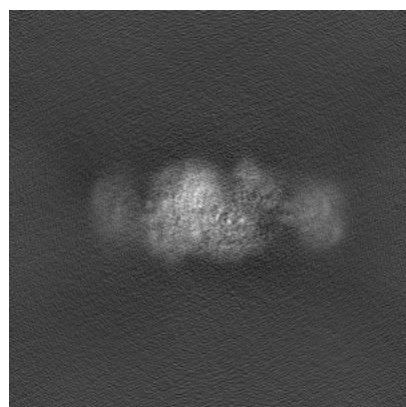


Y

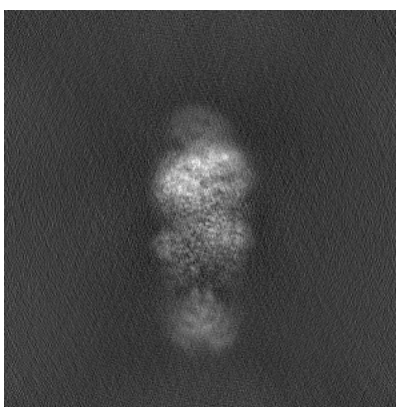


Z

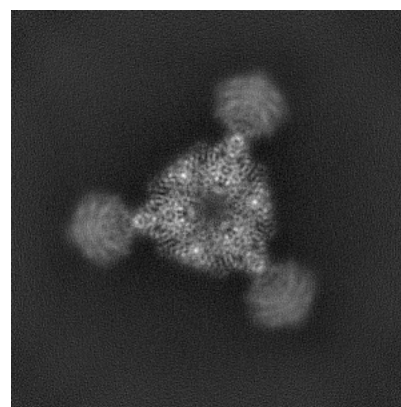
#### 6.1.2 Raw map



X



Y

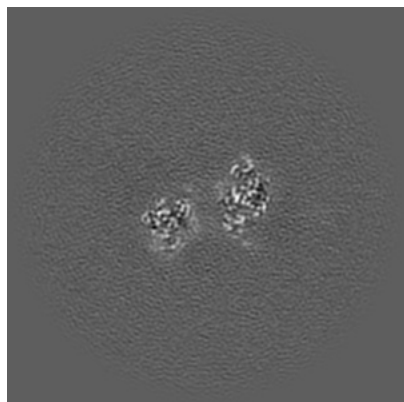


Z

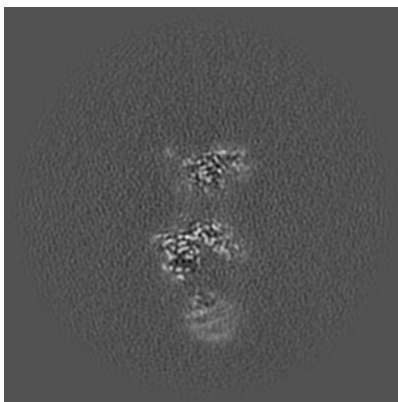
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

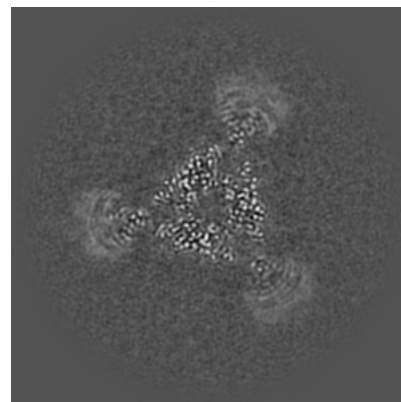
### 6.2.1 Primary map



X Index: 192

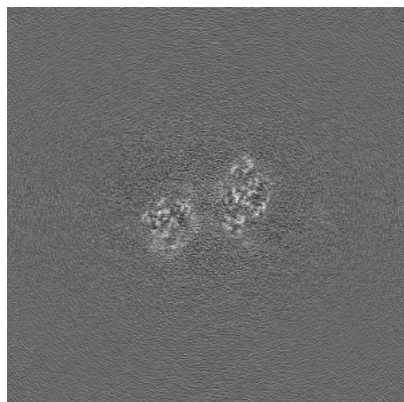


Y Index: 192

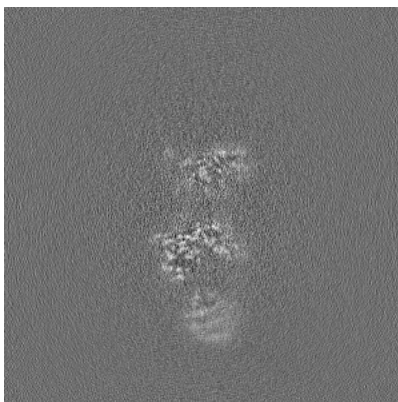


Z Index: 192

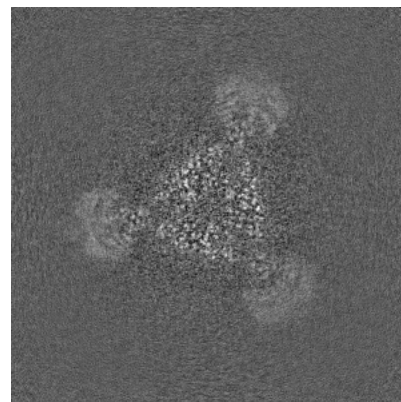
### 6.2.2 Raw map



X Index: 192



Y Index: 192

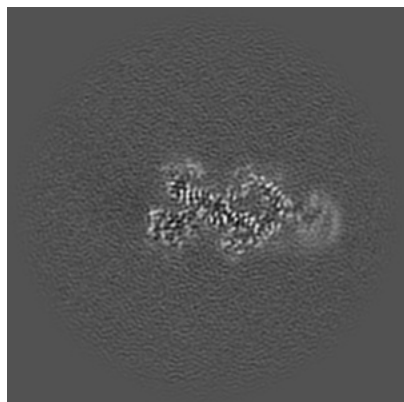


Z Index: 192

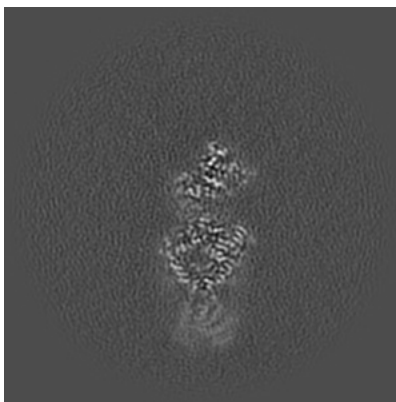
The images above show central slices of the map in three orthogonal directions.

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

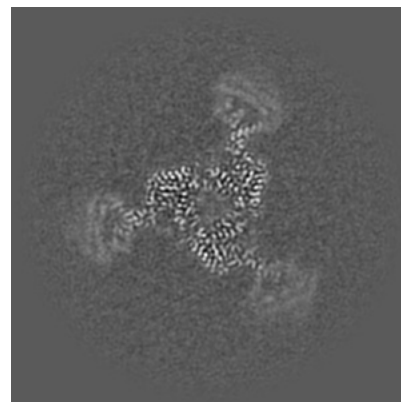
### 6.3.1 Primary map



X Index: 215

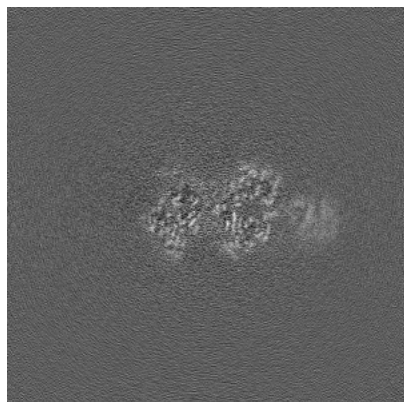


Y Index: 179

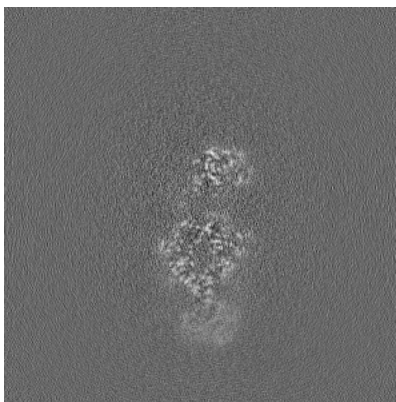


Z Index: 182

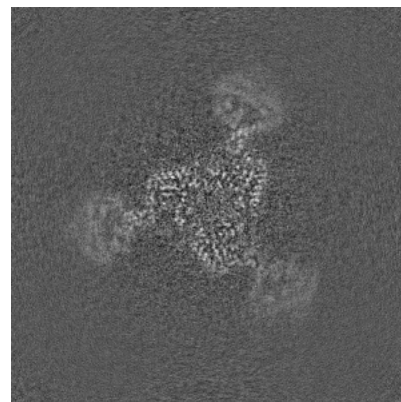
### 6.3.2 Raw map



X Index: 208



Y Index: 184

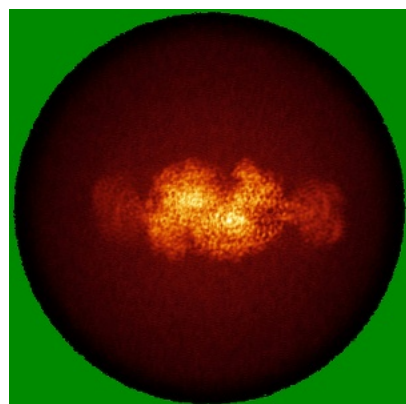


Z Index: 182

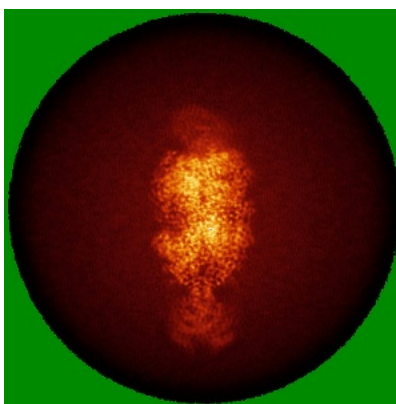
The images above show the largest variance slices of the map in three orthogonal directions.

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

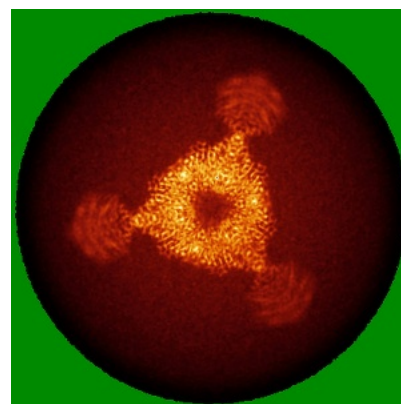
### 6.4.1 Primary map



X

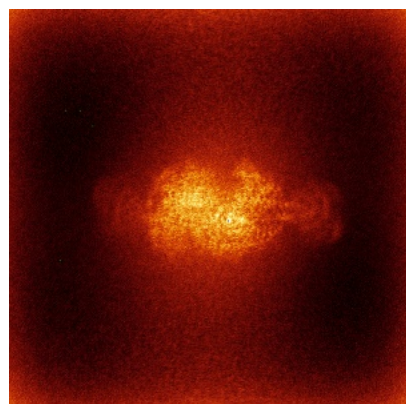


Y

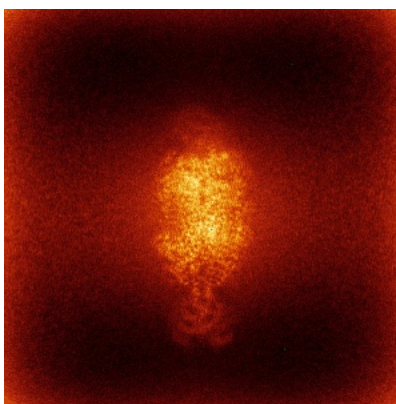


Z

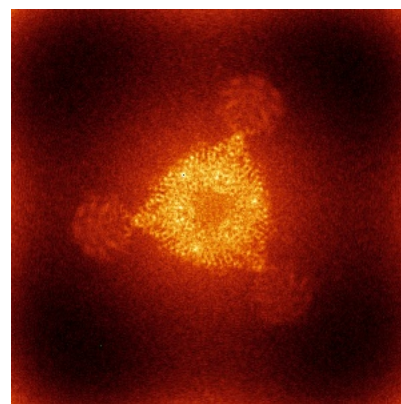
### 6.4.2 Raw map



X



Y

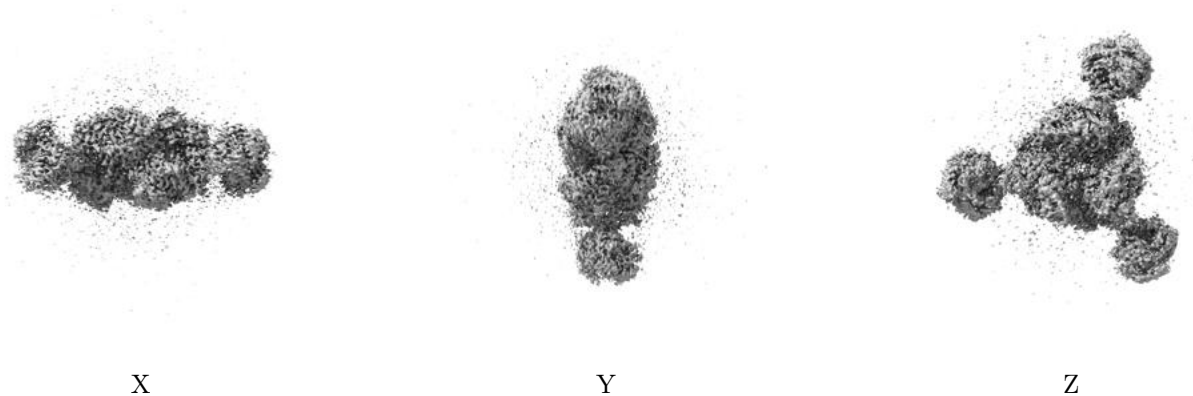


Z

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

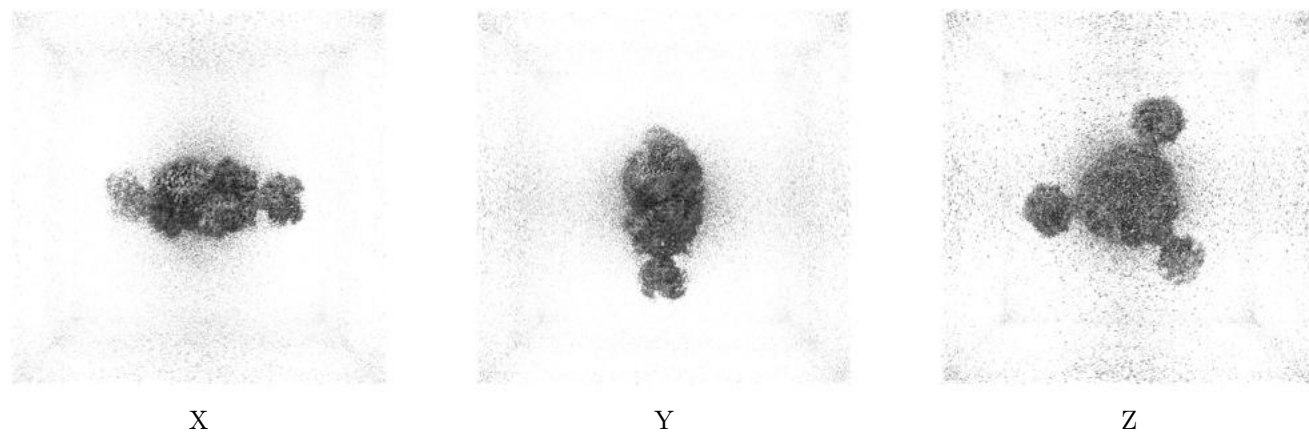
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

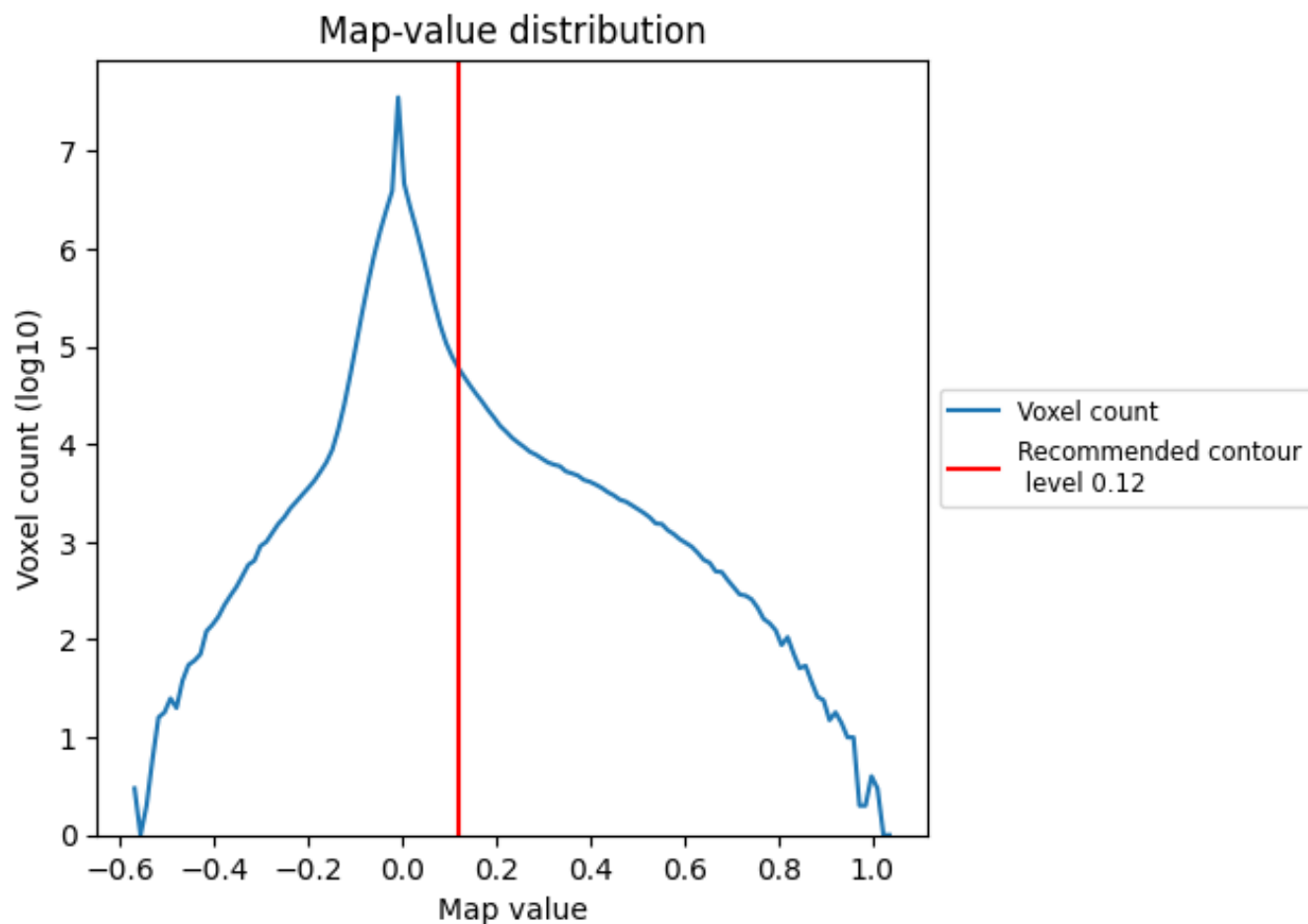
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

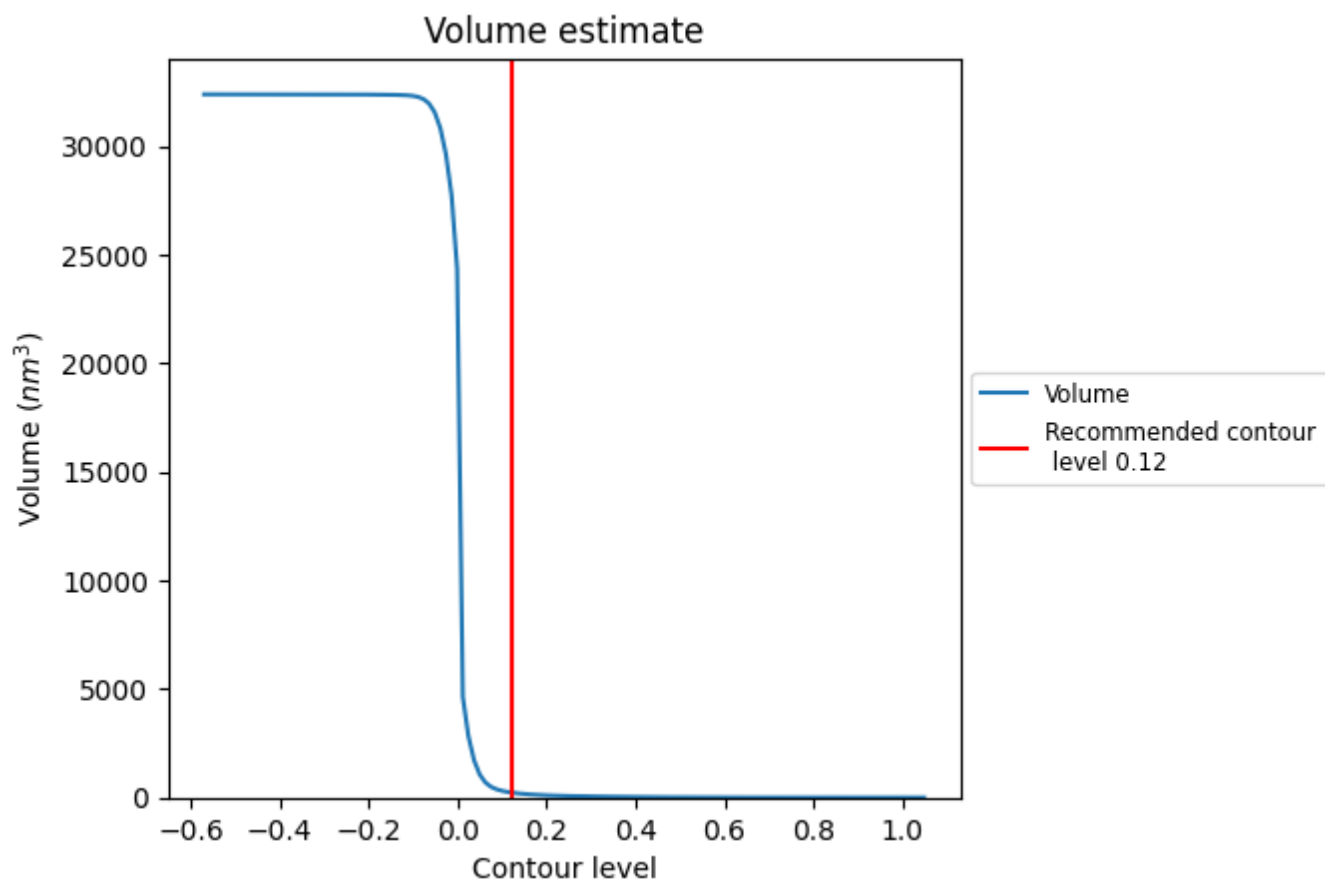
This section contains the results of statistical analysis of the map.

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



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

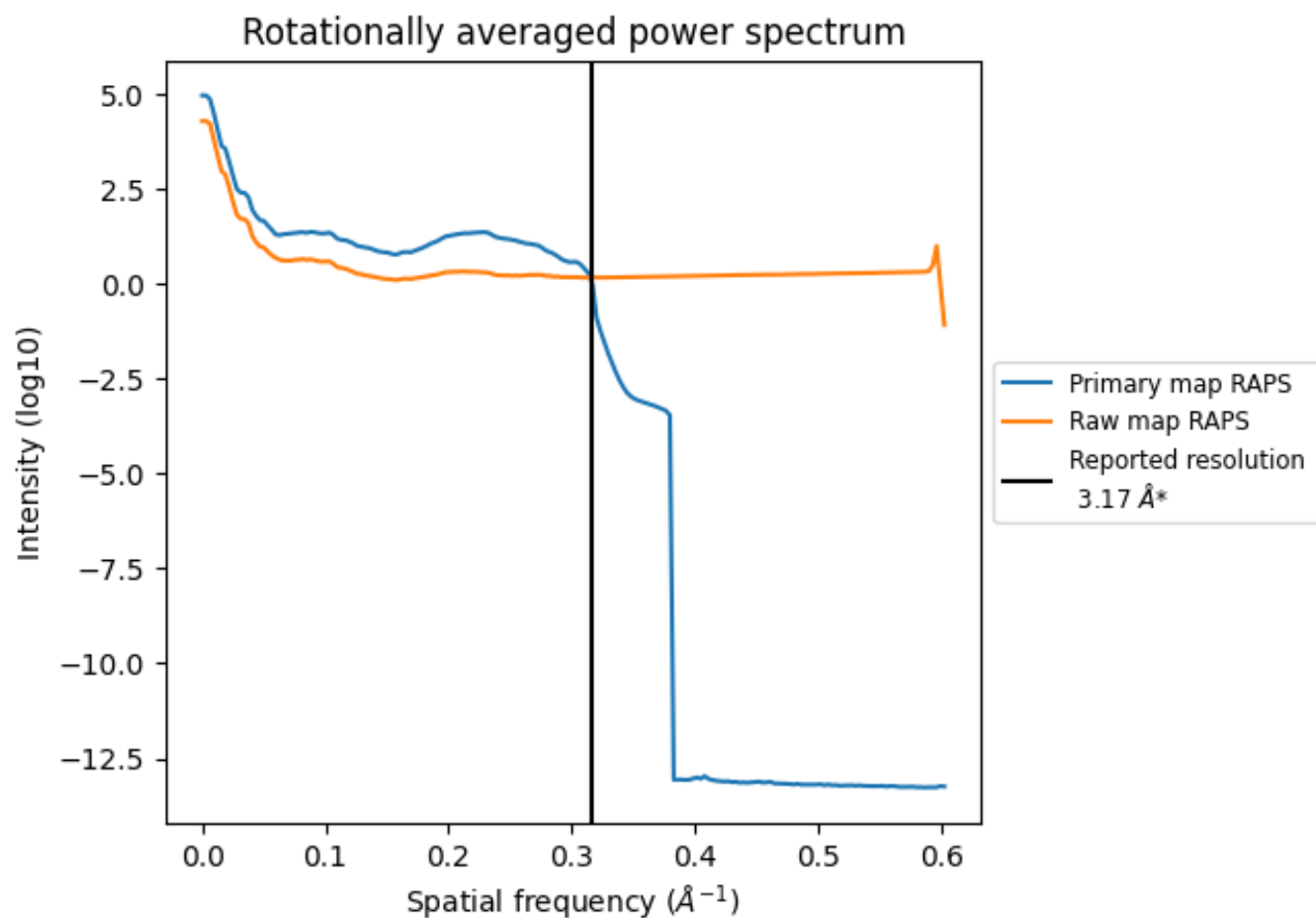
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 236 nm<sup>3</sup>; this corresponds to an approximate mass of 213 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 ⓘ

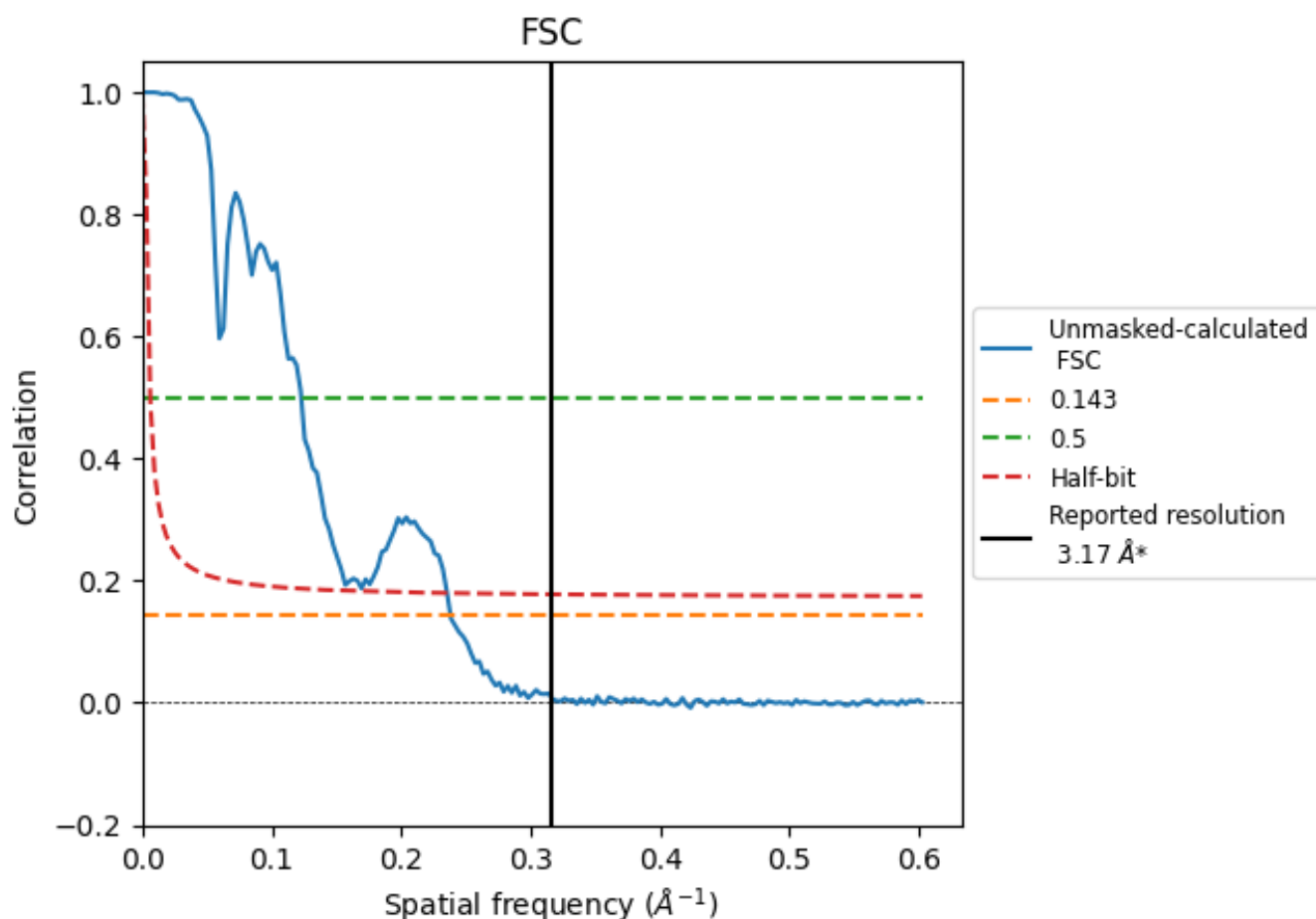


\*Reported resolution corresponds to spatial frequency of 0.315 Å<sup>-1</sup>

## 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 0.315  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

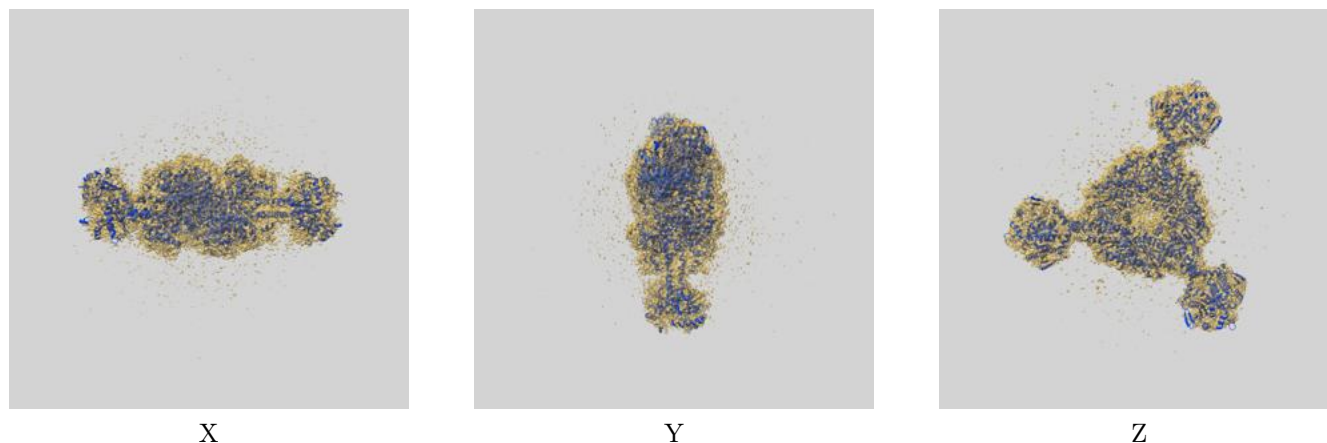
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.17                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 4.20                               | 8.14 | 4.25     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.20 differs from the reported value 3.17 by more than 10 %

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

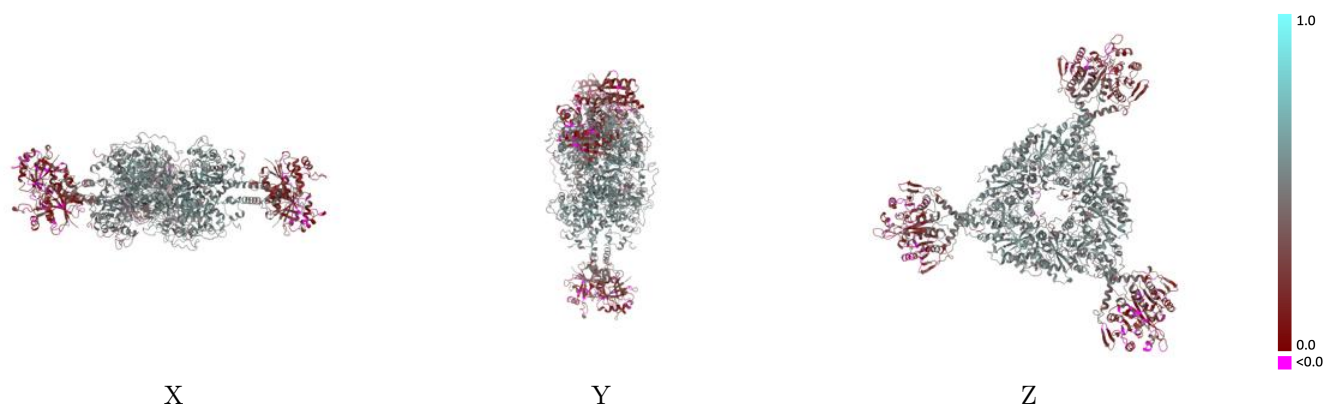
This section contains information regarding the fit between EMDB map EMD-70428 and PDB model 9OFC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



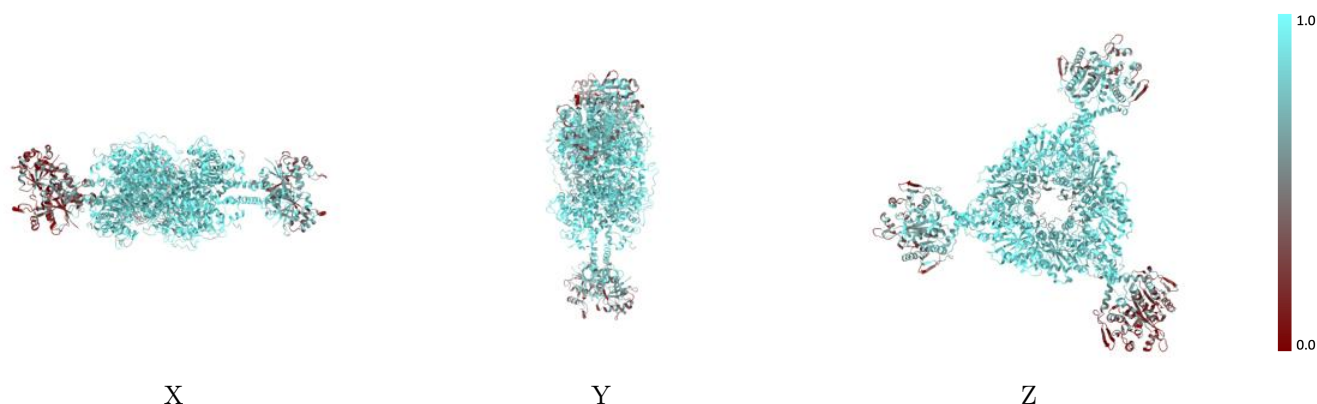
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



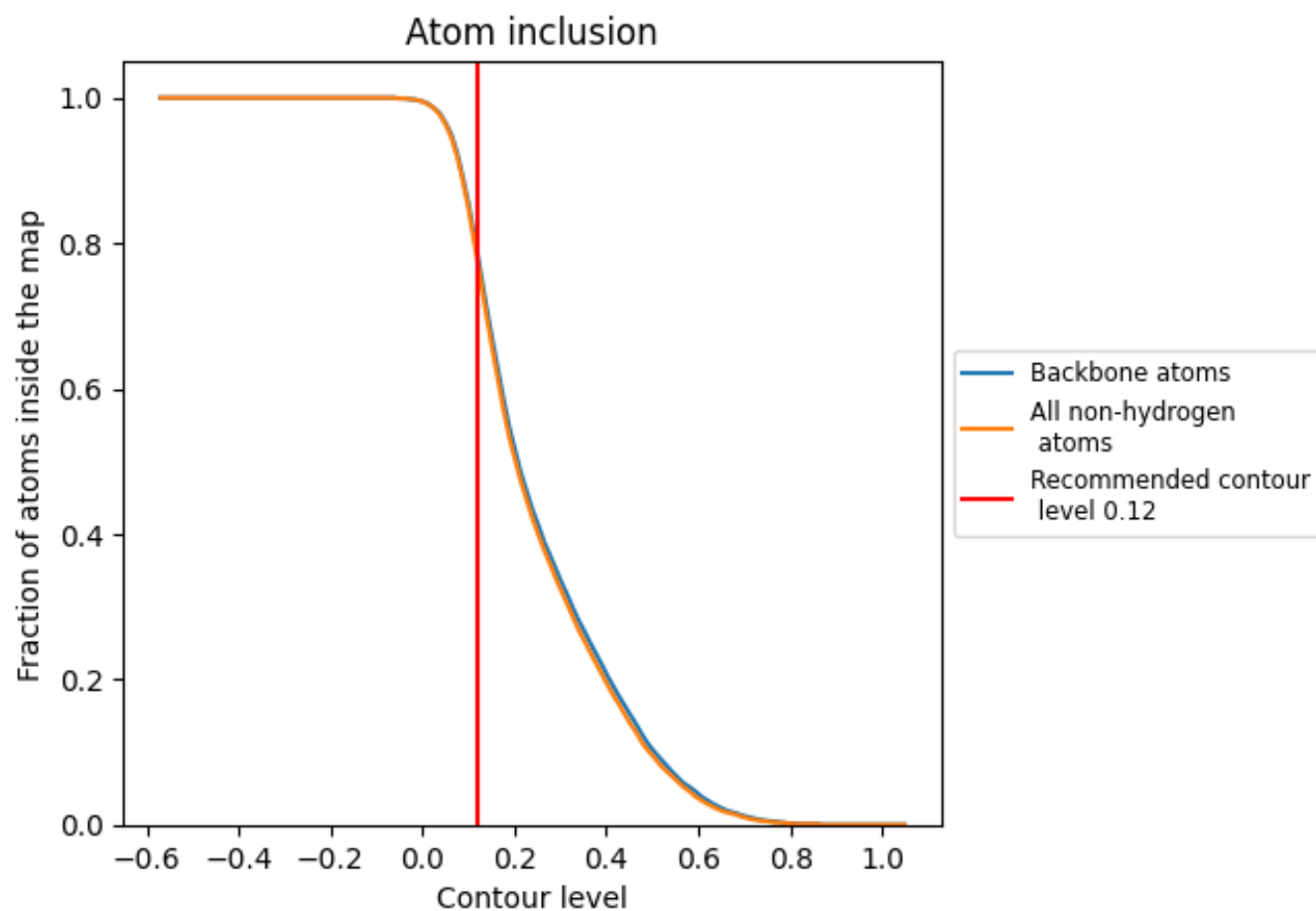
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (0.12) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.7750 | <div></div> 0.4100 |
| A     | <div></div> 0.8290 | <div></div> 0.4200 |
| B     | <div></div> 0.8190 | <div></div> 0.4250 |
| C     | <div></div> 0.7500 | <div></div> 0.2370 |
| D     | <div></div> 0.8640 | <div></div> 0.2650 |
| G     | <div></div> 0.8080 | <div></div> 0.4130 |
| H     | <div></div> 0.8220 | <div></div> 0.4240 |
| I     | <div></div> 0.8410 | <div></div> 0.3090 |
| J     | <div></div> 0.9770 | <div></div> 0.3520 |
| K     | <div></div> 0.7020 | <div></div> 0.4030 |
| L     | <div></div> 0.6920 | <div></div> 0.3800 |
| M     | <div></div> 0.5230 | <div></div> 0.2150 |
| N     | <div></div> 0.6360 | <div></div> 0.3060 |

