



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 10:26 PM EDT

PDB ID : 1Q3S  
Title : Crystal structure of the chaperonin from Thermococcus strain KS-1 (FormIII crystal complexed with ADP)  
Authors : Shomura, Y.; Yoshida, T.; Iizuka, R.; Maruyama, T.; Yohda, M.; Miki, K.  
Deposited on : 2003-07-31  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

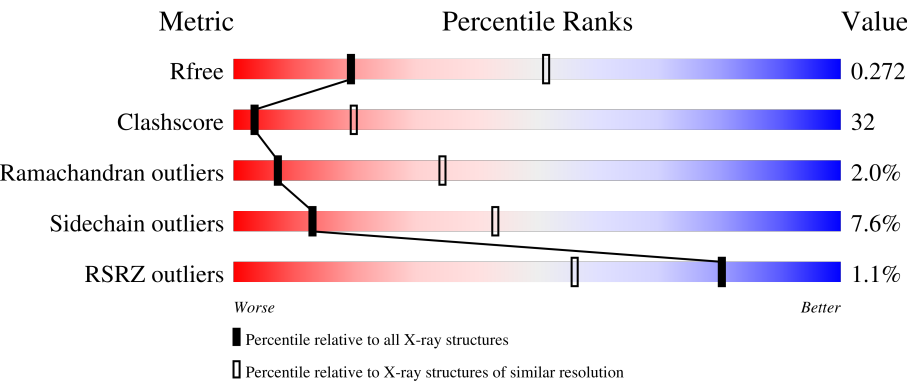
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R <sub>free</sub>     | 130704                      | 2092 (3.00-3.00)                                      |
| Clashscore            | 141614                      | 2416 (3.00-3.00)                                      |
| Ramachandran outliers | 138981                      | 2333 (3.00-3.00)                                      |
| Sidechain outliers    | 138945                      | 2336 (3.00-3.00)                                      |
| RSRZ outliers         | 127900                      | 1990 (3.00-3.00)                                      |

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

| Mol | Chain | Length | Quality of chain                             |
|-----|-------|--------|--|
| 1   | A     | 548    | <div><div>%</div><div>47%42%5%6%</div></div> |
| 1   | B     | 548    | <div><div>%</div><div>47%43%.6%</div></div>  |
| 1   | C     | 548    | <div><div>%</div><div>43%47%.6%</div></div>  |
| 1   | D     | 548    | <div><div>%</div><div>42%46%6%6%</div></div> |
| 1   | E     | 548    | <div><div>%</div><div>42%48%5%6%</div></div> |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | F     | 548    | <div><div><div>%</div><div><div></div><div>45%</div><div>44%</div><div>6%</div><div>6%</div></div></div></div> |
| 1   | G     | 548    | <div><div><div>%</div><div><div></div><div>49%</div><div>41%</div><div>•</div><div>6%</div></div></div></div>  |
| 1   | H     | 548    | <div><div><div>%</div><div><div></div><div>46%</div><div>45%</div><div>•</div><div>6%</div></div></div></div>  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31751 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Thermosome alpha subunit.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3941  | 2482 | 672 | 770 | 17 |         |         |       |
| 1   | B     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3941  | 2482 | 672 | 770 | 17 |         |         |       |
| 1   | C     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3941  | 2482 | 672 | 770 | 17 |         |         |       |
| 1   | D     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3941  | 2482 | 672 | 770 | 17 |         |         |       |
| 1   | E     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3941  | 2482 | 672 | 770 | 17 |         |         |       |
| 1   | F     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3941  | 2482 | 672 | 770 | 17 |         |         |       |
| 1   | G     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3941  | 2482 | 672 | 770 | 17 |         |         |       |
| 1   | H     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3941  | 2482 | 672 | 770 | 17 |         |         |       |

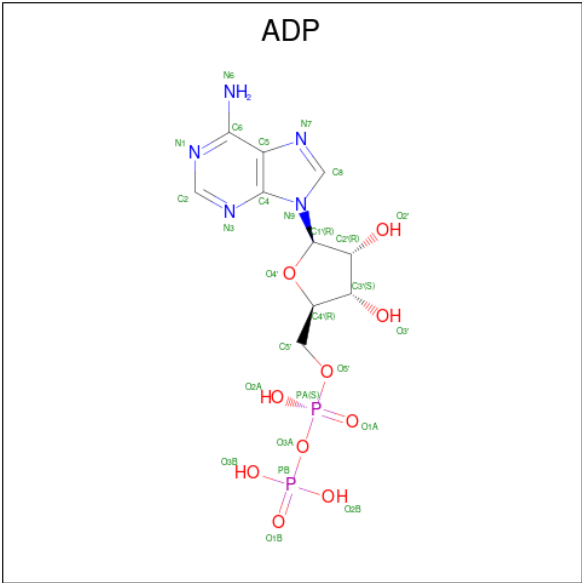
There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 65      | CYS      | GLY    | engineered mutation | UNP O24729 |
| B     | 65      | CYS      | GLY    | engineered mutation | UNP O24729 |
| C     | 65      | CYS      | GLY    | engineered mutation | UNP O24729 |
| D     | 65      | CYS      | GLY    | engineered mutation | UNP O24729 |
| E     | 65      | CYS      | GLY    | engineered mutation | UNP O24729 |
| F     | 65      | CYS      | GLY    | engineered mutation | UNP O24729 |
| G     | 65      | CYS      | GLY    | engineered mutation | UNP O24729 |
| H     | 65      | CYS      | GLY    | engineered mutation | UNP O24729 |

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | B     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | C     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | D     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | E     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | G     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | H     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |

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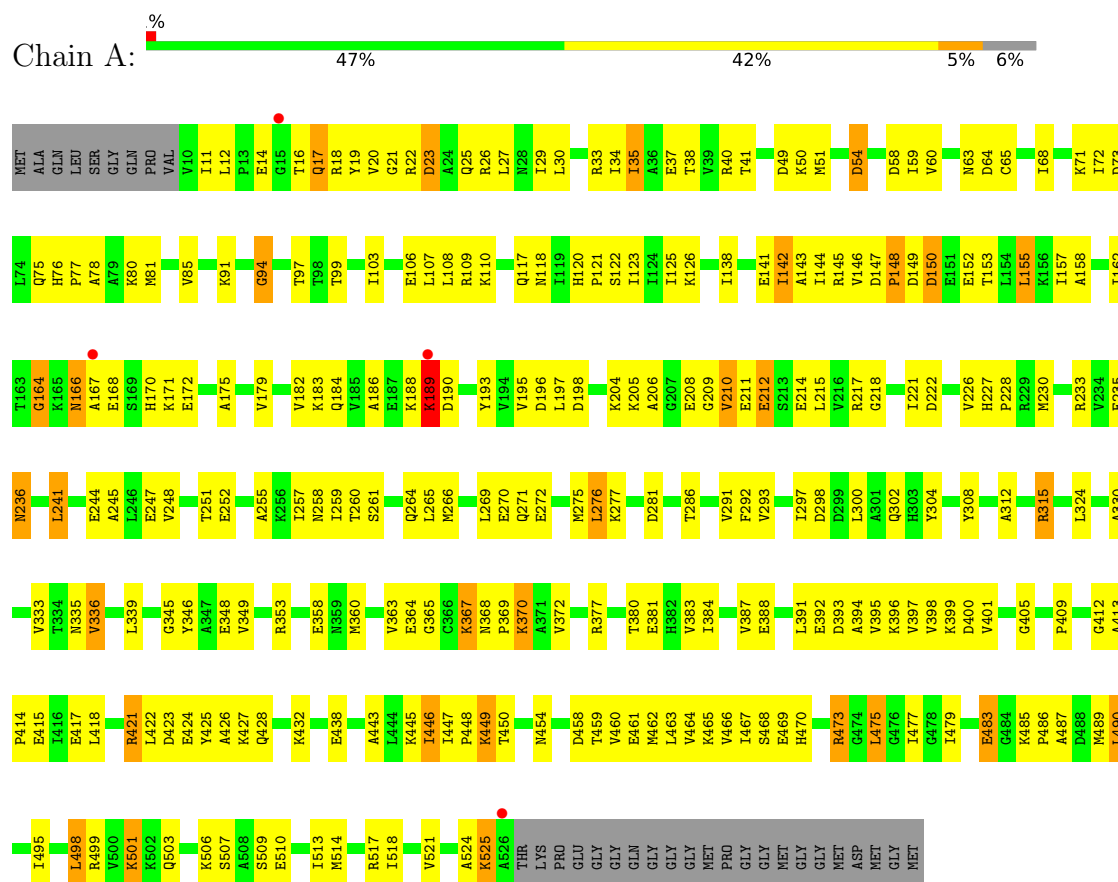
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| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | F     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | H     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |

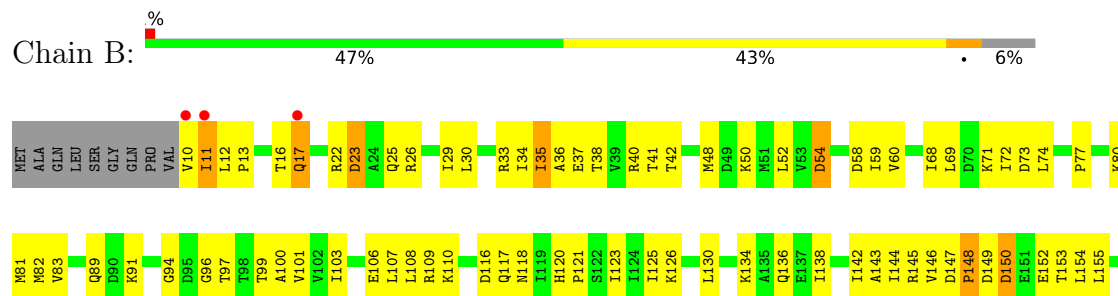
### 3 Residue-property plots

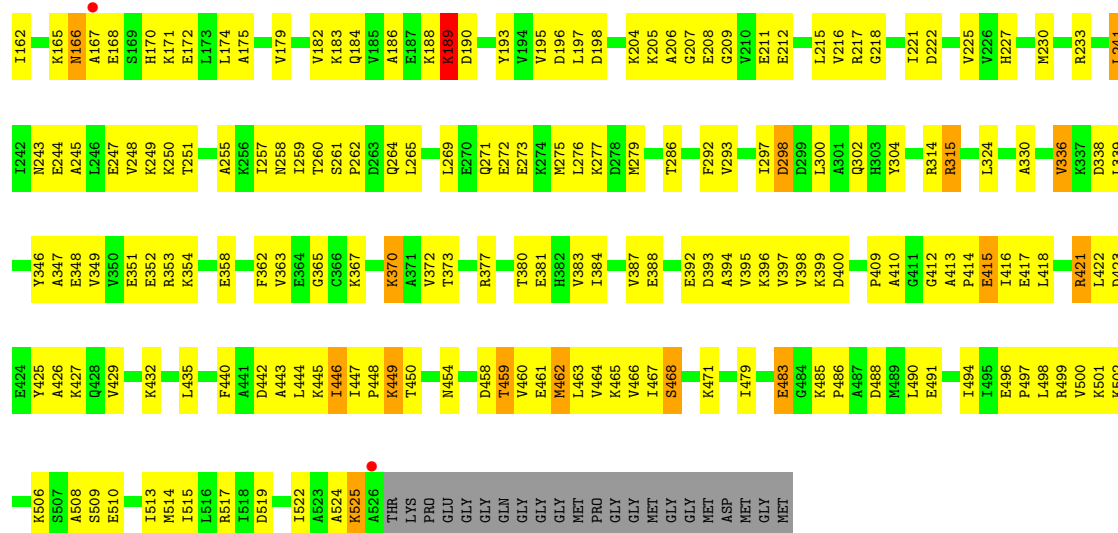
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Thermosome alpha subunit

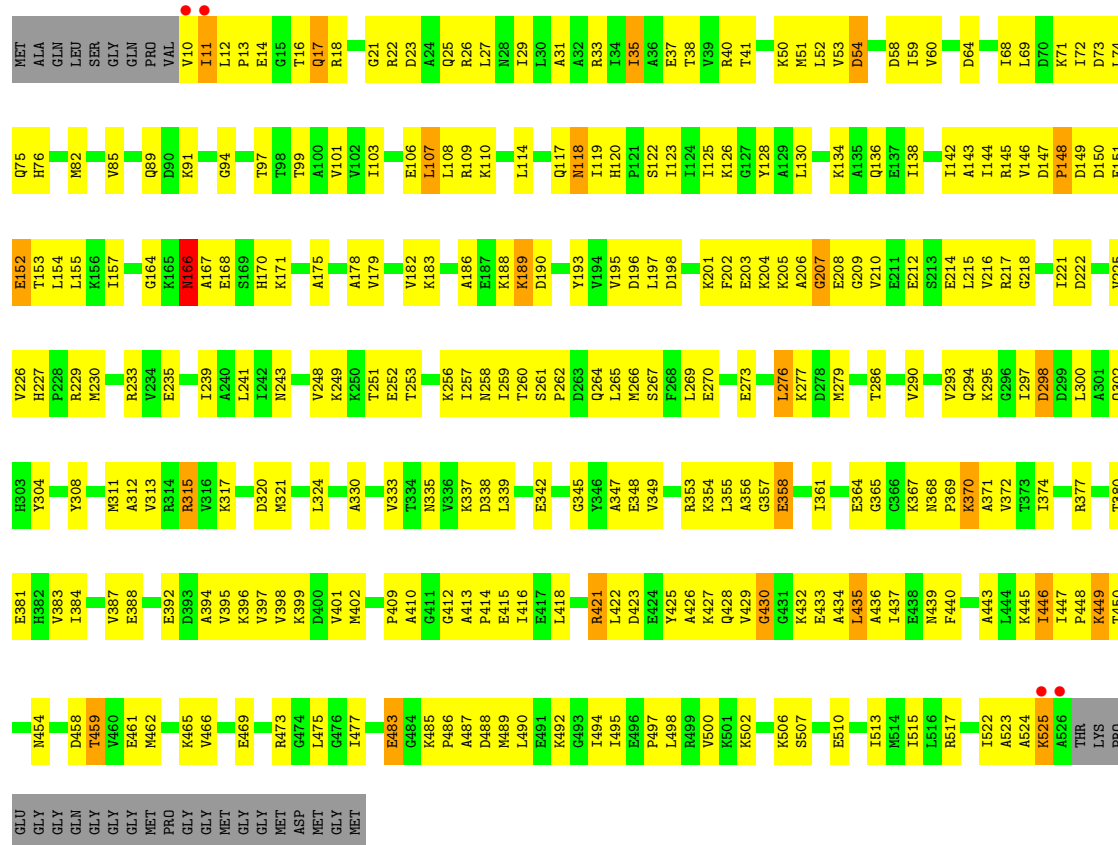


#### • Molecule 1: Thermosome alpha subunit





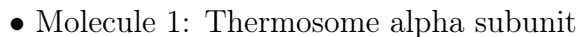
• Molecule 1: Thermosome alpha subunit

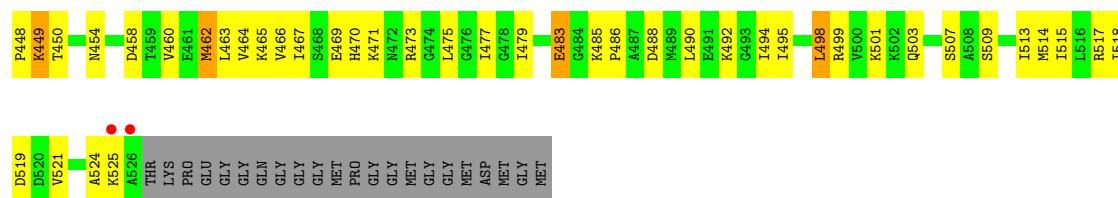


• Molecule 1: Thermosome alpha subunit

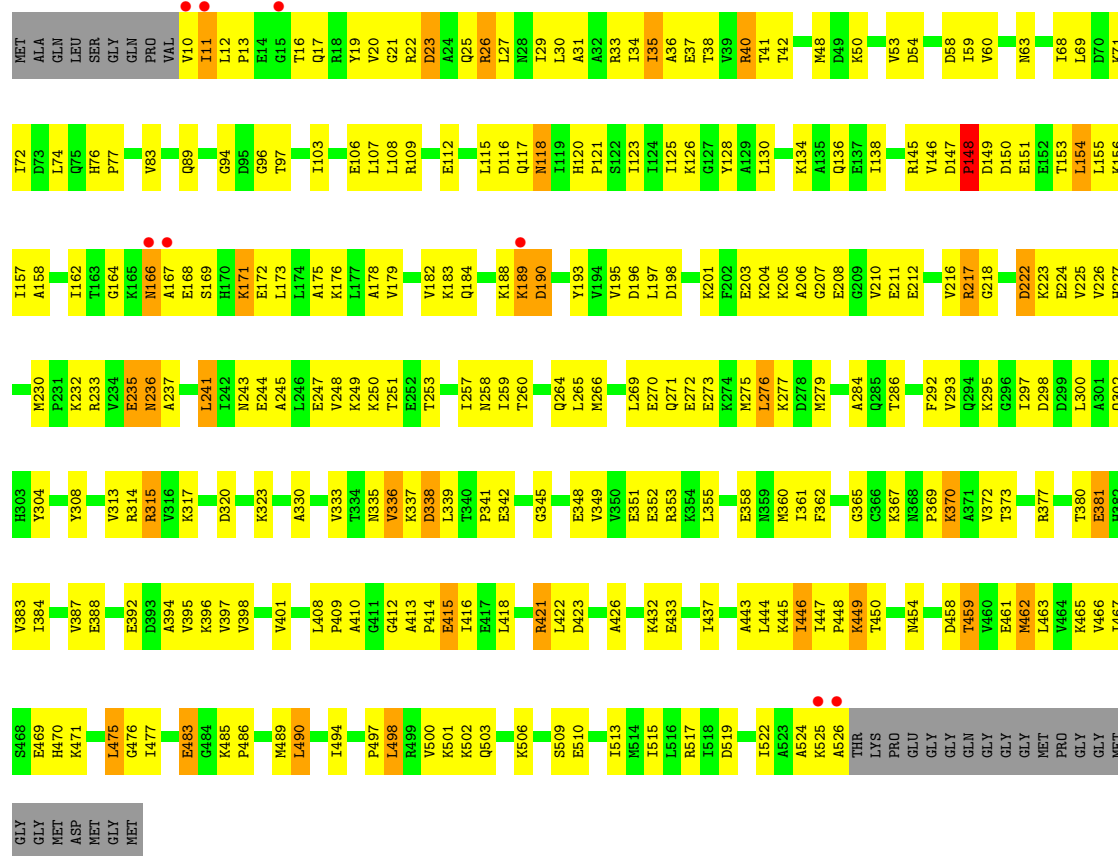
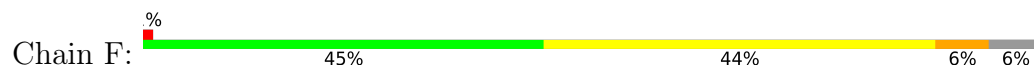




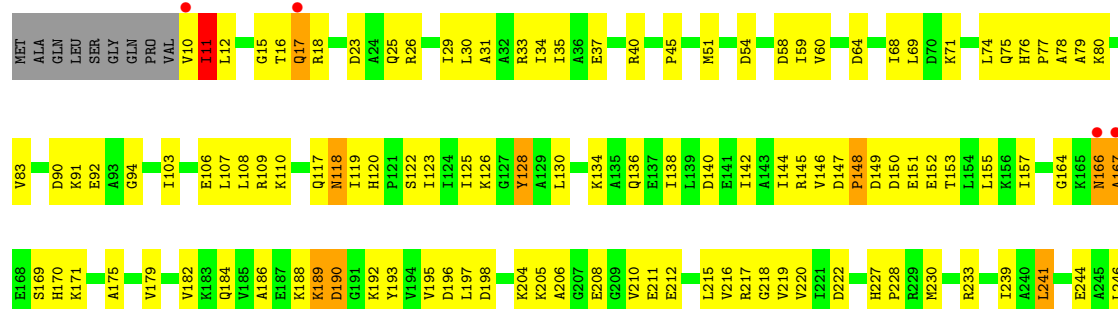


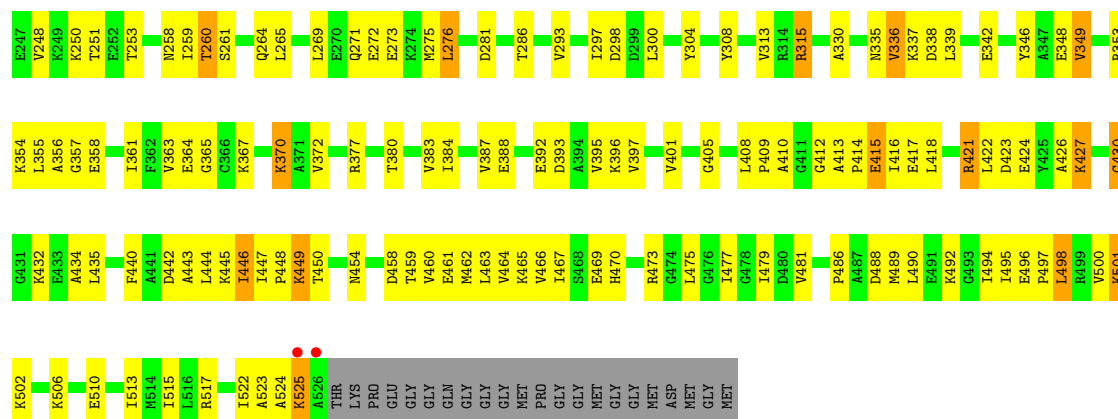


• Molecule 1: Thermosome alpha subunit

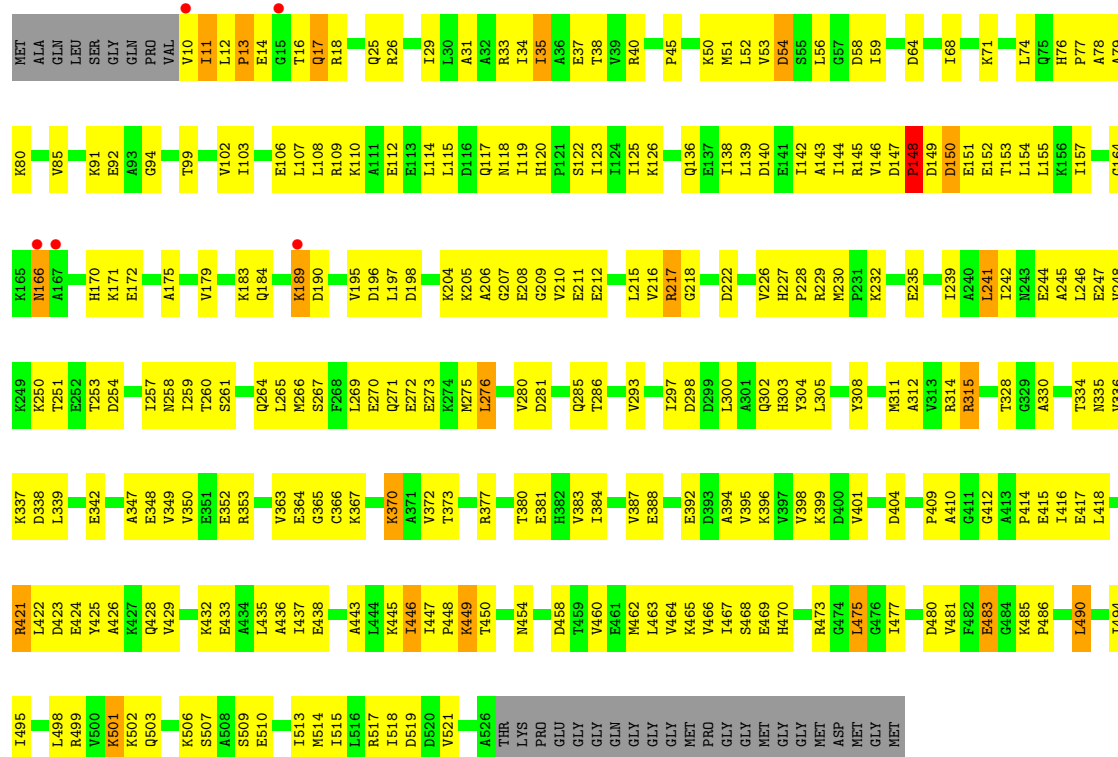


• Molecule 1: Thermosome alpha subunit





• Molecule 1: Thermosome alpha subunit



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 2 2 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 207.43Å 236.23Å 234.11Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 73.62 – 3.00<br>155.87 – 3.00                               | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.0 (73.62-3.00)<br>98.1 (155.87-3.00)                     | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.12  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.93 (at 3.01Å)   | Xtriage          |
| Refinement program  | CNS 1.1   | Depositor        |
| R, $R_{free}$   | 0.251 , 0.288<br>0.233 , 0.272                              | Depositor<br>DCC |
| $R_{free}$ test set   | 5646 reflections (5.03%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 42.2  | Xtriage          |
| Anisotropy  | 0.386   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 32.8   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.89  | EDS              |
| Total number of atoms   | 31751   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 38.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.43         | 0/3976  | 0.65        | 1/5358 (0.0%)  |
| 1   | B     | 0.43         | 0/3976  | 0.66        | 0/5358         |
| 1   | C     | 0.43         | 0/3976  | 0.65        | 1/5358 (0.0%)  |
| 1   | D     | 0.42         | 0/3976  | 0.64        | 1/5358 (0.0%)  |
| 1   | E     | 0.42         | 0/3976  | 0.66        | 0/5358         |
| 1   | F     | 0.42         | 0/3976  | 0.65        | 0/5358         |
| 1   | G     | 0.41         | 0/3976  | 0.64        | 0/5358         |
| 1   | H     | 0.41         | 0/3976  | 0.64        | 0/5358         |
| All | All   | 0.42         | 0/31808 | 0.65        | 3/42864 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | C     | 0                   | 1                   |
| 1   | E     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 207 | GLY  | O-C-N  | -8.59 | 108.95      | 122.70   |
| 1   | D     | 238 | LYS  | N-CA-C | -5.90 | 95.08       | 111.00   |
| 1   | A     | 164 | GLY  | N-CA-C | -5.45 | 99.48       | 113.10   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | C     | 207 | GLY  | Mainchain |
| 1   | E     | 207 | GLY  | Mainchain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3941  | 0        | 4122     | 274     | 0            |
| 1   | B     | 3941  | 0        | 4122     | 254     | 0            |
| 1   | C     | 3941  | 0        | 4122     | 271     | 0            |
| 1   | D     | 3941  | 0        | 4122     | 296     | 0            |
| 1   | E     | 3941  | 0        | 4122     | 333     | 0            |
| 1   | F     | 3941  | 0        | 4122     | 270     | 0            |
| 1   | G     | 3941  | 0        | 4122     | 248     | 0            |
| 1   | H     | 3941  | 0        | 4122     | 268     | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 2   | E     | 1     | 0        | 0        | 0       | 0            |
| 2   | G     | 1     | 0        | 0        | 0       | 0            |
| 2   | H     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 27    | 0        | 12       | 0       | 0            |
| 3   | B     | 27    | 0        | 12       | 1       | 0            |
| 3   | C     | 27    | 0        | 12       | 0       | 0            |
| 3   | D     | 27    | 0        | 12       | 0       | 0            |
| 3   | E     | 27    | 0        | 12       | 0       | 0            |
| 3   | F     | 27    | 0        | 12       | 1       | 0            |
| 3   | G     | 27    | 0        | 12       | 2       | 0            |
| 3   | H     | 27    | 0        | 12       | 1       | 0            |
| All | All   | 31751 | 0        | 33072    | 2088    | 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 32.

All (2088) 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:D:380:THR:HG22 | 1:D:383:VAL:HG23 | 1.26                     | 1.15              |
| 1:H:380:THR:HG22 | 1:H:383:VAL:HG23 | 1.27                     | 1.14              |
| 1:E:380:THR:HG22 | 1:E:383:VAL:HG23 | 1.23                     | 1.11              |
| 1:A:380:THR:HG22 | 1:A:383:VAL:HG23 | 1.10                     | 1.09              |
| 1:B:380:THR:HG22 | 1:B:383:VAL:HG23 | 1.34                     | 1.09              |
| 1:C:10:VAL:HG22  | 1:C:11:ILE:H     | 1.19                     | 1.07              |
| 1:H:106:GLU:HG3  | 1:H:446:ILE:HG12 | 1.07                     | 1.06              |
| 1:B:10:VAL:HG22  | 1:B:11:ILE:H     | 1.20                     | 1.05              |
| 1:C:380:THR:HG22 | 1:C:383:VAL:HG23 | 1.39                     | 1.05              |
| 1:D:10:VAL:HG22  | 1:D:11:ILE:H     | 1.22                     | 1.03              |
| 1:E:10:VAL:HG22  | 1:E:11:ILE:H     | 1.19                     | 1.03              |
| 1:C:258:ASN:HB3  | 1:D:258:ASN:HD21 | 1.25                     | 1.02              |
| 1:H:261:SER:H    | 1:H:264:GLN:HE21 | 1.03                     | 1.00              |
| 1:A:166:ASN:HA   | 1:B:517:ARG:HH12 | 1.25                     | 1.00              |
| 1:C:60:VAL:HG21  | 1:C:71:LYS:HE2   | 1.42                     | 0.99              |
| 1:A:258:ASN:HD21 | 1:H:258:ASN:HB3  | 1.27                     | 0.99              |
| 1:G:380:THR:HG22 | 1:G:383:VAL:HG23 | 1.42                     | 0.99              |
| 1:C:260:THR:H    | 1:C:264:GLN:HE21 | 1.01                     | 0.98              |
| 1:G:421:ARG:HB2  | 1:G:421:ARG:HH11 | 1.24                     | 0.98              |
| 1:E:421:ARG:HH11 | 1:E:421:ARG:HB2  | 1.23                     | 0.98              |
| 1:E:12:LEU:HD23  | 1:E:13:PRO:HD2   | 1.47                     | 0.97              |
| 1:F:10:VAL:HG22  | 1:F:11:ILE:H     | 1.30                     | 0.96              |
| 1:H:260:THR:H    | 1:H:264:GLN:NE2  | 1.62                     | 0.96              |
| 1:B:260:THR:H    | 1:B:264:GLN:HE22 | 1.01                     | 0.94              |
| 1:E:125:ILE:HG23 | 1:E:513:ILE:HG23 | 1.46                     | 0.94              |
| 1:F:421:ARG:HB2  | 1:F:421:ARG:HH11 | 1.29                     | 0.94              |
| 1:G:10:VAL:HG13  | 1:G:11:ILE:H     | 1.31                     | 0.94              |
| 1:D:258:ASN:HB3  | 1:E:258:ASN:HD21 | 1.30                     | 0.94              |
| 1:E:227:HIS:HB3  | 1:E:230:MET:HG3  | 1.50                     | 0.93              |
| 1:D:125:ILE:HG23 | 1:D:513:ILE:HG23 | 1.51                     | 0.93              |
| 1:A:260:THR:H    | 1:A:264:GLN:HE21 | 1.17                     | 0.92              |
| 1:D:260:THR:H    | 1:D:264:GLN:NE2  | 1.67                     | 0.92              |
| 1:H:106:GLU:HG3  | 1:H:446:ILE:CG1  | 1.98                     | 0.92              |
| 1:C:421:ARG:HB2  | 1:C:421:ARG:HH11 | 1.33                     | 0.91              |
| 1:F:380:THR:HG22 | 1:F:383:VAL:HG23 | 1.52                     | 0.91              |
| 1:F:125:ILE:HG23 | 1:F:513:ILE:HG23 | 1.50                     | 0.90              |
| 1:B:260:THR:H    | 1:B:264:GLN:NE2  | 1.71                     | 0.89              |
| 1:A:166:ASN:HA   | 1:B:517:ARG:NH1  | 1.88                     | 0.89              |
| 1:E:260:THR:H    | 1:E:264:GLN:NE2  | 1.69                     | 0.89              |
| 1:H:125:ILE:HG23 | 1:H:513:ILE:HG23 | 1.52                     | 0.89              |
| 1:H:260:THR:H    | 1:H:264:GLN:HE22 | 1.19                     | 0.89              |
| 1:A:125:ILE:HG23 | 1:A:513:ILE:HG23 | 1.55                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:106:GLU:CG   | 1:H:446:ILE:HG12 | 1.99                     | 0.88              |
| 1:D:383:VAL:O    | 1:D:387:VAL:HG23 | 1.74                     | 0.88              |
| 1:H:10:VAL:HG22  | 1:H:11:ILE:H     | 1.39                     | 0.88              |
| 1:H:380:THR:CG2  | 1:H:383:VAL:HG23 | 2.02                     | 0.88              |
| 1:G:258:ASN:HB3  | 1:H:258:ASN:HD21 | 1.36                     | 0.88              |
| 1:F:108:LEU:HD11 | 1:F:515:ILE:HD12 | 1.54                     | 0.87              |
| 1:B:184:GLN:NE2  | 1:B:217:ARG:HH21 | 1.72                     | 0.87              |
| 1:H:204:LYS:HB3  | 1:H:384:ILE:HG21 | 1.56                     | 0.87              |
| 1:A:212:GLU:HB2  | 1:A:377:ARG:HG3  | 1.56                     | 0.86              |
| 1:C:380:THR:CG2  | 1:C:383:VAL:HG23 | 2.03                     | 0.86              |
| 1:A:204:LYS:HD2  | 1:A:384:ILE:HG22 | 1.57                     | 0.86              |
| 1:E:293:VAL:HG21 | 1:E:297:ILE:HD11 | 1.56                     | 0.86              |
| 1:F:166:ASN:HA   | 1:G:517:ARG:HH12 | 1.41                     | 0.86              |
| 1:G:260:THR:H    | 1:G:264:GLN:HE21 | 1.21                     | 0.86              |
| 1:G:155:LEU:HD22 | 1:G:179:VAL:HG21 | 1.57                     | 0.85              |
| 1:G:54:ASP:OD1   | 1:G:58:ASP:HB3   | 1.76                     | 0.85              |
| 1:B:466:VAL:HG22 | 1:B:486:PRO:HG3  | 1.59                     | 0.85              |
| 1:D:421:ARG:HB2  | 1:D:421:ARG:HH11 | 1.42                     | 0.84              |
| 1:F:524:ALA:O    | 1:F:525:LYS:HG3  | 1.77                     | 0.84              |
| 1:C:380:THR:HG23 | 1:C:383:VAL:H    | 1.40                     | 0.84              |
| 1:D:212:GLU:HB2  | 1:D:377:ARG:HG3  | 1.58                     | 0.84              |
| 1:E:72:ILE:HD11  | 1:F:522:ILE:HD12 | 1.56                     | 0.84              |
| 1:G:462:MET:HA   | 1:G:462:MET:HE3  | 1.59                     | 0.84              |
| 1:A:370:LYS:HE2  | 1:A:370:LYS:HA   | 1.60                     | 0.84              |
| 1:G:123:ILE:HG21 | 1:G:432:LYS:HB3  | 1.60                     | 0.84              |
| 1:G:260:THR:H    | 1:G:264:GLN:NE2  | 1.76                     | 0.84              |
| 1:A:204:LYS:HD3  | 1:A:388:GLU:OE2  | 1.76                     | 0.84              |
| 1:B:204:LYS:HB3  | 1:B:384:ILE:HG21 | 1.61                     | 0.83              |
| 1:C:409:PRO:HB3  | 1:C:490:LEU:CD1  | 2.07                     | 0.83              |
| 1:D:269:LEU:HD12 | 1:E:251:THR:HG23 | 1.58                     | 0.83              |
| 1:C:260:THR:H    | 1:C:264:GLN:NE2  | 1.76                     | 0.83              |
| 1:B:145:ARG:HG2  | 1:B:145:ARG:HH11 | 1.43                     | 0.83              |
| 1:F:260:THR:H    | 1:F:264:GLN:NE2  | 1.76                     | 0.83              |
| 1:A:206:ALA:HA   | 1:A:384:ILE:HD11 | 1.62                     | 0.82              |
| 1:B:380:THR:HG23 | 1:B:383:VAL:H    | 1.43                     | 0.82              |
| 1:G:265:LEU:O    | 1:G:269:LEU:HD13 | 1.79                     | 0.82              |
| 1:G:206:ALA:HA   | 1:G:384:ILE:HD11 | 1.62                     | 0.82              |
| 1:E:380:THR:CG2  | 1:E:383:VAL:HG23 | 2.07                     | 0.82              |
| 1:F:370:LYS:HE2  | 1:F:370:LYS:HA   | 1.61                     | 0.82              |
| 1:F:388:GLU:O    | 1:F:392:GLU:HG3  | 1.80                     | 0.82              |
| 1:E:179:VAL:O    | 1:E:183:LYS:HG3  | 1.80                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:410:ALA:HB3  | 1:F:494:ILE:HG22 | 1.61                     | 0.82              |
| 1:H:227:HIS:HB3  | 1:H:230:MET:HG3  | 1.62                     | 0.82              |
| 1:A:469:GLU:HB2  | 1:A:477:ILE:HG21 | 1.60                     | 0.81              |
| 1:A:11:ILE:HG13  | 1:H:34:ILE:HG21  | 1.62                     | 0.81              |
| 1:B:421:ARG:HH11 | 1:B:421:ARG:HB2  | 1.44                     | 0.81              |
| 1:F:233:ARG:HH12 | 1:F:349:VAL:CG1  | 1.93                     | 0.81              |
| 1:F:380:THR:HG23 | 1:F:383:VAL:H    | 1.45                     | 0.81              |
| 1:F:445:LYS:O    | 1:F:449:LYS:HB2  | 1.81                     | 0.81              |
| 1:H:54:ASP:HB3   | 1:H:58:ASP:HB3   | 1.59                     | 0.81              |
| 1:A:138:ILE:HD13 | 1:A:421:ARG:HG2  | 1.61                     | 0.81              |
| 1:E:184:GLN:HA   | 1:E:184:GLN:HE21 | 1.45                     | 0.81              |
| 1:A:462:MET:O    | 1:A:466:VAL:HG23 | 1.81                     | 0.81              |
| 1:C:266:MET:O    | 1:C:270:GLU:HG3  | 1.81                     | 0.81              |
| 1:E:204:LYS:HD3  | 1:E:388:GLU:OE2  | 1.81                     | 0.81              |
| 1:A:38:THR:O     | 1:A:50:LYS:HE3   | 1.80                     | 0.80              |
| 1:F:184:GLN:NE2  | 1:F:217:ARG:HH21 | 1.79                     | 0.80              |
| 1:A:380:THR:CG2  | 1:A:383:VAL:HG23 | 2.03                     | 0.80              |
| 1:B:315:ARG:HG3  | 1:B:315:ARG:HH11 | 1.45                     | 0.80              |
| 1:F:269:LEU:HD12 | 1:G:251:THR:HG23 | 1.63                     | 0.80              |
| 1:G:421:ARG:HB2  | 1:G:421:ARG:NH1  | 1.96                     | 0.80              |
| 1:C:144:ILE:HD11 | 1:C:490:LEU:HD21 | 1.62                     | 0.80              |
| 1:E:272:GLU:HA   | 1:E:275:MET:HE3  | 1.62                     | 0.80              |
| 1:C:17:GLN:NE2   | 1:C:17:GLN:H     | 1.80                     | 0.80              |
| 1:G:380:THR:HG23 | 1:G:383:VAL:H    | 1.47                     | 0.80              |
| 1:G:370:LYS:HE2  | 1:G:370:LYS:HA   | 1.64                     | 0.80              |
| 1:D:204:LYS:HD2  | 1:D:384:ILE:HG22 | 1.64                     | 0.79              |
| 1:A:144:ILE:HD11 | 1:A:490:LEU:HD21 | 1.65                     | 0.79              |
| 1:A:269:LEU:HD12 | 1:B:251:THR:HG23 | 1.65                     | 0.79              |
| 1:E:348:GLU:HB3  | 1:E:365:GLY:HA3  | 1.64                     | 0.79              |
| 1:A:388:GLU:O    | 1:A:392:GLU:HG3  | 1.83                     | 0.79              |
| 1:A:421:ARG:HB2  | 1:A:421:ARG:HH11 | 1.48                     | 0.79              |
| 1:B:409:PRO:HB3  | 1:B:490:LEU:CD1  | 2.13                     | 0.79              |
| 1:D:241:LEU:HD22 | 1:D:330:ALA:HB3  | 1.65                     | 0.79              |
| 1:C:54:ASP:OD1   | 1:C:58:ASP:HB3   | 1.83                     | 0.78              |
| 1:C:483:GLU:HG3  | 1:C:485:LYS:NZ   | 1.97                     | 0.78              |
| 1:G:125:ILE:HD13 | 1:G:517:ARG:HG2  | 1.65                     | 0.78              |
| 1:B:445:LYS:O    | 1:B:448:PRO:HD2  | 1.82                     | 0.78              |
| 1:G:60:VAL:HG21  | 1:G:71:LYS:HE2   | 1.65                     | 0.78              |
| 1:G:125:ILE:HG23 | 1:G:513:ILE:HG23 | 1.66                     | 0.78              |
| 1:H:370:LYS:HA   | 1:H:370:LYS:HE2  | 1.66                     | 0.78              |
| 1:A:380:THR:HG22 | 1:A:383:VAL:CG2  | 2.05                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:409:PRO:HA   | 1:E:495:ILE:HG22 | 1.65                     | 0.77              |
| 1:A:204:LYS:HB3  | 1:A:384:ILE:CG2  | 2.15                     | 0.77              |
| 1:F:217:ARG:HA   | 1:F:372:VAL:HG23 | 1.67                     | 0.77              |
| 1:H:204:LYS:HD3  | 1:H:388:GLU:OE2  | 1.83                     | 0.77              |
| 1:C:10:VAL:HG22  | 1:C:11:ILE:N     | 1.99                     | 0.77              |
| 1:B:370:LYS:HE2  | 1:B:370:LYS:HA   | 1.64                     | 0.77              |
| 1:D:73:ASP:HB3   | 1:E:13:PRO:HG2   | 1.66                     | 0.77              |
| 1:E:233:ARG:HH12 | 1:E:349:VAL:CG1  | 1.97                     | 0.77              |
| 1:G:75:GLN:HG2   | 1:H:13:PRO:HD3   | 1.67                     | 0.77              |
| 1:E:10:VAL:HG22  | 1:E:11:ILE:N     | 1.98                     | 0.76              |
| 1:C:166:ASN:HA   | 1:D:517:ARG:HH12 | 1.50                     | 0.76              |
| 1:C:462:MET:O    | 1:C:466:VAL:HG23 | 1.84                     | 0.76              |
| 1:D:265:LEU:O    | 1:D:269:LEU:HD13 | 1.85                     | 0.76              |
| 1:B:166:ASN:HA   | 1:C:517:ARG:HH12 | 1.50                     | 0.76              |
| 1:C:348:GLU:O    | 1:C:349:VAL:HG23 | 1.85                     | 0.76              |
| 1:F:260:THR:H    | 1:F:264:GLN:HE21 | 1.33                     | 0.76              |
| 1:B:380:THR:CG2  | 1:B:383:VAL:HG23 | 2.16                     | 0.76              |
| 1:C:206:ALA:HA   | 1:C:384:ILE:HD11 | 1.67                     | 0.76              |
| 1:F:106:GLU:HG2  | 1:F:446:ILE:HG13 | 1.67                     | 0.76              |
| 1:E:466:VAL:HG22 | 1:E:486:PRO:HG3  | 1.68                     | 0.76              |
| 1:D:12:LEU:HD21  | 1:D:16:THR:HG21  | 1.68                     | 0.76              |
| 1:F:462:MET:O    | 1:F:466:VAL:HG23 | 1.85                     | 0.76              |
| 1:H:215:LEU:HD11 | 1:H:372:VAL:HG21 | 1.66                     | 0.76              |
| 1:G:204:LYS:HB3  | 1:G:384:ILE:HG21 | 1.67                     | 0.76              |
| 1:G:208:GLU:HB3  | 1:G:212:GLU:HG3  | 1.68                     | 0.76              |
| 1:C:125:ILE:HG23 | 1:C:513:ILE:HG23 | 1.67                     | 0.76              |
| 1:D:204:LYS:HB3  | 1:D:384:ILE:HG21 | 1.65                     | 0.76              |
| 1:B:10:VAL:HG22  | 1:B:11:ILE:N     | 1.98                     | 0.75              |
| 1:B:206:ALA:HA   | 1:B:384:ILE:HD11 | 1.68                     | 0.75              |
| 1:D:91:LYS:HB2   | 1:D:91:LYS:NZ    | 2.01                     | 0.75              |
| 1:E:380:THR:HG23 | 1:E:383:VAL:H    | 1.50                     | 0.75              |
| 1:G:144:ILE:HD11 | 1:G:490:LEU:HD21 | 1.66                     | 0.75              |
| 1:C:175:ALA:O    | 1:C:179:VAL:HG23 | 1.87                     | 0.75              |
| 1:D:217:ARG:HB3  | 1:D:217:ARG:NH1  | 2.00                     | 0.75              |
| 1:G:25:GLN:O     | 1:G:29:ILE:HG13  | 1.85                     | 0.75              |
| 1:G:244:GLU:OE1  | 1:G:336:VAL:HG22 | 1.85                     | 0.75              |
| 1:H:204:LYS:HB3  | 1:H:384:ILE:CG2  | 2.16                     | 0.75              |
| 1:A:369:PRO:O    | 1:A:370:LYS:HE2  | 1.85                     | 0.75              |
| 1:B:462:MET:HE1  | 1:B:486:PRO:HD3  | 1.67                     | 0.75              |
| 1:B:380:THR:HG22 | 1:B:383:VAL:CG2  | 2.14                     | 0.75              |
| 1:D:73:ASP:O     | 1:E:13:PRO:HD3   | 1.86                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:142:ILE:HB   | 1:G:475:LEU:HD22 | 1.69                     | 0.75              |
| 1:D:94:GLY:HA3   | 1:D:396:LYS:HD2  | 1.67                     | 0.75              |
| 1:E:462:MET:O    | 1:E:466:VAL:HG23 | 1.86                     | 0.75              |
| 1:C:204:LYS:HB3  | 1:C:384:ILE:HG21 | 1.68                     | 0.74              |
| 1:D:380:THR:CG2  | 1:D:383:VAL:HG23 | 2.12                     | 0.74              |
| 1:F:466:VAL:HG22 | 1:F:486:PRO:HG3  | 1.67                     | 0.74              |
| 1:D:10:VAL:HG22  | 1:D:11:ILE:N     | 2.02                     | 0.74              |
| 1:H:136:GLN:NE2  | 1:H:502:LYS:HE3  | 2.02                     | 0.74              |
| 1:B:410:ALA:HB3  | 1:B:494:ILE:HG22 | 1.68                     | 0.74              |
| 1:G:166:ASN:HA   | 1:H:517:ARG:HH12 | 1.52                     | 0.74              |
| 1:D:94:GLY:CA    | 1:D:396:LYS:HD2  | 2.18                     | 0.74              |
| 1:H:447:ILE:HB   | 1:H:448:PRO:HD3  | 1.68                     | 0.74              |
| 1:E:233:ARG:HH12 | 1:E:349:VAL:HG11 | 1.52                     | 0.74              |
| 1:D:469:GLU:HB2  | 1:D:477:ILE:HG21 | 1.69                     | 0.74              |
| 1:E:125:ILE:HG23 | 1:E:513:ILE:CG2  | 2.18                     | 0.74              |
| 1:A:447:ILE:HB   | 1:A:448:PRO:HD3  | 1.70                     | 0.74              |
| 1:F:446:ILE:O    | 1:F:450:THR:HG23 | 1.87                     | 0.74              |
| 1:D:205:LYS:HD2  | 1:D:356:ALA:HB3  | 1.69                     | 0.73              |
| 1:E:175:ALA:O    | 1:E:179:VAL:HG23 | 1.88                     | 0.73              |
| 1:F:315:ARG:HH11 | 1:F:315:ARG:HG3  | 1.52                     | 0.73              |
| 1:H:353:ARG:NH2  | 1:H:364:GLU:OE2  | 2.21                     | 0.73              |
| 1:A:251:THR:HG23 | 1:H:269:LEU:HD12 | 1.70                     | 0.73              |
| 1:G:138:ILE:HD13 | 1:G:421:ARG:HG2  | 1.70                     | 0.73              |
| 1:H:261:SER:H    | 1:H:264:GLN:NE2  | 1.83                     | 0.73              |
| 1:H:469:GLU:HB2  | 1:H:477:ILE:HG21 | 1.71                     | 0.73              |
| 1:A:258:ASN:HB3  | 1:B:258:ASN:HD21 | 1.52                     | 0.73              |
| 1:D:445:LYS:O    | 1:D:449:LYS:HB2  | 1.87                     | 0.73              |
| 1:G:466:VAL:HG22 | 1:G:486:PRO:HG3  | 1.69                     | 0.73              |
| 1:H:144:ILE:HD11 | 1:H:490:LEU:HD21 | 1.70                     | 0.73              |
| 1:C:447:ILE:HB   | 1:C:448:PRO:HD3  | 1.69                     | 0.73              |
| 1:H:206:ALA:HA   | 1:H:384:ILE:HD11 | 1.69                     | 0.73              |
| 1:E:204:LYS:HB3  | 1:E:384:ILE:HG21 | 1.68                     | 0.73              |
| 1:H:421:ARG:HH11 | 1:H:421:ARG:HB2  | 1.53                     | 0.73              |
| 1:A:155:LEU:HD22 | 1:A:179:VAL:HG21 | 1.71                     | 0.73              |
| 1:B:460:VAL:O    | 1:B:464:VAL:HG23 | 1.87                     | 0.73              |
| 1:A:204:LYS:HB3  | 1:A:384:ILE:HG21 | 1.69                     | 0.73              |
| 1:D:276:LEU:HD23 | 1:D:300:LEU:HB2  | 1.69                     | 0.73              |
| 1:B:488:ASP:HB3  | 1:B:491:GLU:HG3  | 1.71                     | 0.72              |
| 1:F:506:LYS:O    | 1:F:510:GLU:HG3  | 1.89                     | 0.72              |
| 1:H:443:ALA:O    | 1:H:446:ILE:HG13 | 1.89                     | 0.72              |
| 1:G:413:ALA:HB3  | 1:G:414:PRO:HD3  | 1.71                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:315:ARG:HH11 | 1:C:315:ARG:HG3  | 1.54                     | 0.72              |
| 1:H:462:MET:O    | 1:H:466:VAL:HG23 | 1.88                     | 0.72              |
| 1:B:204:LYS:HD3  | 1:B:388:GLU:OE2  | 1.89                     | 0.72              |
| 1:G:134:LYS:O    | 1:G:138:ILE:HG13 | 1.90                     | 0.72              |
| 1:E:146:VAL:HG22 | 1:E:147:ASP:H    | 1.55                     | 0.72              |
| 1:A:383:VAL:O    | 1:A:387:VAL:HG23 | 1.88                     | 0.72              |
| 1:E:103:ILE:O    | 1:E:107:LEU:HB2  | 1.89                     | 0.72              |
| 1:B:125:ILE:HG23 | 1:B:513:ILE:HG23 | 1.70                     | 0.72              |
| 1:B:506:LYS:O    | 1:B:510:GLU:HG3  | 1.89                     | 0.72              |
| 1:D:60:VAL:HG21  | 1:D:71:LYS:HE2   | 1.71                     | 0.72              |
| 1:D:125:ILE:HD13 | 1:D:517:ARG:HG2  | 1.69                     | 0.72              |
| 1:A:462:MET:HE3  | 1:A:462:MET:HA   | 1.72                     | 0.72              |
| 1:D:123:ILE:HG21 | 1:D:432:LYS:HB2  | 1.71                     | 0.72              |
| 1:E:258:ASN:HB3  | 1:F:258:ASN:HD21 | 1.54                     | 0.72              |
| 1:G:59:ILE:HD12  | 1:G:59:ILE:N     | 2.05                     | 0.72              |
| 1:H:483:GLU:HG3  | 1:H:485:LYS:NZ   | 2.05                     | 0.72              |
| 1:D:315:ARG:HH11 | 1:D:315:ARG:HG3  | 1.52                     | 0.71              |
| 1:H:513:ILE:O    | 1:H:517:ARG:HG3  | 1.90                     | 0.71              |
| 1:G:473:ARG:HB2  | 1:G:477:ILE:HG13 | 1.72                     | 0.71              |
| 1:H:143:ALA:HB3  | 1:H:145:ARG:HH12 | 1.55                     | 0.71              |
| 1:H:266:MET:O    | 1:H:270:GLU:HG3  | 1.90                     | 0.71              |
| 1:F:54:ASP:OD1   | 1:F:58:ASP:HB3   | 1.90                     | 0.71              |
| 1:D:37:GLU:HG2   | 1:D:40:ARG:NH1   | 2.05                     | 0.71              |
| 1:A:22:ARG:HG3   | 1:A:23:ASP:N     | 2.06                     | 0.71              |
| 1:C:506:LYS:O    | 1:C:510:GLU:HG3  | 1.91                     | 0.71              |
| 1:E:147:ASP:HB3  | 1:E:150:ASP:HB2  | 1.71                     | 0.71              |
| 1:G:108:LEU:HD11 | 1:G:515:ILE:HD12 | 1.71                     | 0.71              |
| 1:B:286:THR:HG21 | 1:B:339:LEU:HG   | 1.72                     | 0.71              |
| 1:D:380:THR:HG22 | 1:D:383:VAL:CG2  | 2.14                     | 0.71              |
| 1:E:184:GLN:HA   | 1:E:184:GLN:NE2  | 2.06                     | 0.71              |
| 1:D:123:ILE:HG21 | 1:D:432:LYS:CB   | 2.21                     | 0.71              |
| 1:F:11:ILE:O     | 1:F:11:ILE:HD13  | 1.90                     | 0.71              |
| 1:C:380:THR:HG22 | 1:C:383:VAL:CG2  | 2.19                     | 0.70              |
| 1:F:412:GLY:O    | 1:F:415:GLU:HG2  | 1.90                     | 0.70              |
| 1:F:29:ILE:O     | 1:F:33:ARG:HG3   | 1.91                     | 0.70              |
| 1:C:383:VAL:O    | 1:C:387:VAL:HG23 | 1.91                     | 0.70              |
| 1:F:178:ALA:O    | 1:F:182:VAL:HG23 | 1.92                     | 0.70              |
| 1:F:147:ASP:HB3  | 1:F:150:ASP:HB2  | 1.73                     | 0.70              |
| 1:G:383:VAL:O    | 1:G:387:VAL:HG23 | 1.92                     | 0.70              |
| 1:H:445:LYS:O    | 1:H:449:LYS:HB2  | 1.92                     | 0.70              |
| 1:B:73:ASP:HB3   | 1:C:13:PRO:HG2   | 1.72                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:392:GLU:O    | 1:B:396:LYS:HE3  | 1.92                     | 0.70              |
| 1:H:506:LYS:O    | 1:H:510:GLU:HG3  | 1.91                     | 0.70              |
| 1:C:25:GLN:O     | 1:C:29:ILE:HG13  | 1.92                     | 0.70              |
| 1:C:125:ILE:HD13 | 1:C:517:ARG:HG2  | 1.73                     | 0.70              |
| 1:C:466:VAL:HG22 | 1:C:486:PRO:HG3  | 1.71                     | 0.70              |
| 1:H:380:THR:HG22 | 1:H:383:VAL:CG2  | 2.16                     | 0.70              |
| 1:A:91:LYS:HB2   | 1:A:91:LYS:NZ    | 2.06                     | 0.70              |
| 1:B:446:ILE:O    | 1:B:450:THR:HG23 | 1.92                     | 0.70              |
| 1:E:483:GLU:HG3  | 1:E:485:LYS:NZ   | 2.06                     | 0.70              |
| 1:F:10:VAL:HG22  | 1:F:11:ILE:N     | 2.06                     | 0.70              |
| 1:F:509:SER:O    | 1:F:513:ILE:HG13 | 1.92                     | 0.70              |
| 1:G:460:VAL:O    | 1:G:464:VAL:HG23 | 1.91                     | 0.70              |
| 1:D:348:GLU:HB3  | 1:D:365:GLY:HA3  | 1.74                     | 0.70              |
| 1:B:462:MET:HA   | 1:B:462:MET:HE3  | 1.73                     | 0.70              |
| 1:H:261:SER:N    | 1:H:264:GLN:HE21 | 1.85                     | 0.70              |
| 1:A:244:GLU:OE1  | 1:A:336:VAL:HG22 | 1.91                     | 0.69              |
| 1:B:205:LYS:O    | 1:B:377:ARG:NH1  | 2.25                     | 0.69              |
| 1:F:233:ARG:HH12 | 1:F:349:VAL:HG11 | 1.54                     | 0.69              |
| 1:G:447:ILE:HB   | 1:G:448:PRO:HD3  | 1.74                     | 0.69              |
| 1:H:241:LEU:HD22 | 1:H:330:ALA:HB3  | 1.73                     | 0.69              |
| 1:H:394:ALA:O    | 1:H:398:VAL:HG23 | 1.91                     | 0.69              |
| 1:A:394:ALA:O    | 1:A:398:VAL:HG23 | 1.92                     | 0.69              |
| 1:B:42:THR:HG22  | 1:B:48:MET:O     | 1.90                     | 0.69              |
| 1:B:244:GLU:OE1  | 1:B:336:VAL:HG22 | 1.91                     | 0.69              |
| 1:C:412:GLY:O    | 1:C:415:GLU:HG2  | 1.91                     | 0.69              |
| 1:C:488:ASP:O    | 1:C:492:LYS:HG2  | 1.92                     | 0.69              |
| 1:D:37:GLU:HG2   | 1:D:40:ARG:HH12  | 1.58                     | 0.69              |
| 1:H:501:LYS:HA   | 1:H:501:LYS:HE3  | 1.74                     | 0.69              |
| 1:E:257:ILE:HG22 | 1:E:259:ILE:HD12 | 1.74                     | 0.69              |
| 1:E:276:LEU:HD23 | 1:E:300:LEU:HB2  | 1.75                     | 0.69              |
| 1:E:410:ALA:HB3  | 1:E:494:ILE:HG22 | 1.74                     | 0.69              |
| 1:D:204:LYS:HB3  | 1:D:384:ILE:CG2  | 2.21                     | 0.69              |
| 1:E:11:ILE:HD13  | 1:E:11:ILE:C     | 2.12                     | 0.69              |
| 1:F:380:THR:CG2  | 1:F:383:VAL:HG23 | 2.20                     | 0.69              |
| 1:B:30:LEU:O     | 1:B:34:ILE:HG13  | 1.93                     | 0.69              |
| 1:D:460:VAL:O    | 1:D:464:VAL:HG23 | 1.92                     | 0.69              |
| 1:F:227:HIS:HB3  | 1:F:230:MET:HG3  | 1.74                     | 0.69              |
| 1:G:409:PRO:HB3  | 1:G:490:LEU:CD1  | 2.22                     | 0.69              |
| 1:G:17:GLN:NE2   | 1:G:17:GLN:H     | 1.91                     | 0.69              |
| 1:E:12:LEU:HD23  | 1:E:13:PRO:CD    | 2.22                     | 0.69              |
| 1:E:421:ARG:HB2  | 1:E:421:ARG:NH1  | 2.05                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:466:VAL:HG21 | 1:E:479:ILE:HG12 | 1.75                     | 0.69              |
| 1:F:409:PRO:HB3  | 1:F:490:LEU:HD13 | 1.73                     | 0.69              |
| 1:G:498:LEU:O    | 1:G:498:LEU:HD22 | 1.93                     | 0.69              |
| 1:H:123:ILE:HG21 | 1:H:432:LYS:HB3  | 1.74                     | 0.69              |
| 1:C:410:ALA:HB3  | 1:C:494:ILE:HG22 | 1.73                     | 0.69              |
| 1:E:269:LEU:HD12 | 1:F:251:THR:HG23 | 1.74                     | 0.69              |
| 1:A:196:ASP:OD1  | 1:A:198:ASP:HB2  | 1.92                     | 0.69              |
| 1:B:204:LYS:HB3  | 1:B:384:ILE:CG2  | 2.22                     | 0.69              |
| 1:H:226:VAL:HG12 | 1:H:312:ALA:O    | 1.93                     | 0.69              |
| 1:G:29:ILE:HG23  | 1:G:108:LEU:HB3  | 1.74                     | 0.68              |
| 1:E:166:ASN:HA   | 1:F:517:ARG:NH1  | 2.09                     | 0.68              |
| 1:F:103:ILE:O    | 1:F:107:LEU:HB2  | 1.92                     | 0.68              |
| 1:A:258:ASN:ND2  | 1:H:258:ASN:HB3  | 2.05                     | 0.68              |
| 1:B:144:ILE:HD11 | 1:B:490:LEU:HD21 | 1.76                     | 0.68              |
| 1:H:304:TYR:O    | 1:H:308:TYR:HD1  | 1.76                     | 0.68              |
| 1:C:370:LYS:HE2  | 1:C:370:LYS:HA   | 1.74                     | 0.68              |
| 1:D:261:SER:O    | 1:D:264:GLN:HG3  | 1.92                     | 0.68              |
| 1:G:412:GLY:O    | 1:G:415:GLU:HG2  | 1.93                     | 0.68              |
| 1:A:175:ALA:O    | 1:A:179:VAL:HG23 | 1.93                     | 0.68              |
| 1:C:421:ARG:HB2  | 1:C:421:ARG:NH1  | 2.09                     | 0.68              |
| 1:F:272:GLU:HA   | 1:F:275:MET:HE3  | 1.75                     | 0.68              |
| 1:G:144:ILE:CD1  | 1:G:490:LEU:HD21 | 2.23                     | 0.68              |
| 1:C:75:GLN:HG3   | 1:D:10:VAL:HG13  | 1.76                     | 0.68              |
| 1:C:445:LYS:O    | 1:C:448:PRO:HD2  | 1.93                     | 0.68              |
| 1:G:380:THR:CG2  | 1:G:383:VAL:HG23 | 2.23                     | 0.68              |
| 1:D:506:LYS:O    | 1:D:510:GLU:HG3  | 1.94                     | 0.68              |
| 1:E:416:ILE:O    | 1:E:420:ILE:HG13 | 1.94                     | 0.68              |
| 1:A:260:THR:H    | 1:A:264:GLN:NE2  | 1.90                     | 0.68              |
| 1:D:217:ARG:HA   | 1:D:372:VAL:HG23 | 1.76                     | 0.68              |
| 1:D:443:ALA:O    | 1:D:446:ILE:HG13 | 1.93                     | 0.68              |
| 1:A:353:ARG:NH2  | 1:A:364:GLU:OE2  | 2.26                     | 0.68              |
| 1:C:446:ILE:O    | 1:C:450:THR:HG23 | 1.94                     | 0.68              |
| 1:D:370:LYS:HE2  | 1:D:370:LYS:HA   | 1.74                     | 0.68              |
| 1:A:75:GLN:HB2   | 1:B:11:ILE:C     | 2.14                     | 0.67              |
| 1:A:315:ARG:HH11 | 1:A:315:ARG:HG3  | 1.60                     | 0.67              |
| 1:F:125:ILE:HD13 | 1:F:517:ARG:HG2  | 1.77                     | 0.67              |
| 1:F:276:LEU:HD23 | 1:F:300:LEU:HB2  | 1.75                     | 0.67              |
| 1:F:449:LYS:HE3  | 1:F:459:THR:HG21 | 1.76                     | 0.67              |
| 1:D:144:ILE:HD11 | 1:D:490:LEU:HD21 | 1.76                     | 0.67              |
| 1:E:425:TYR:O    | 1:E:429:VAL:HG23 | 1.94                     | 0.67              |
| 1:F:447:ILE:HB   | 1:F:448:PRO:HD3  | 1.76                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:217:ARG:HB3  | 1:G:217:ARG:NH1  | 2.09                     | 0.67              |
| 1:G:315:ARG:HG3  | 1:G:315:ARG:HH11 | 1.59                     | 0.67              |
| 1:D:230:MET:HE2  | 1:D:312:ALA:H    | 1.59                     | 0.67              |
| 1:D:260:THR:H    | 1:D:264:GLN:HE21 | 1.40                     | 0.67              |
| 1:H:38:THR:O     | 1:H:50:LYS:HE3   | 1.95                     | 0.67              |
| 1:H:91:LYS:HB2   | 1:H:91:LYS:NZ    | 2.10                     | 0.67              |
| 1:C:150:ASP:OD2  | 1:C:152:GLU:HB3  | 1.94                     | 0.67              |
| 1:E:45:PRO:HA    | 1:E:164:GLY:HA2  | 1.75                     | 0.67              |
| 1:E:206:ALA:HA   | 1:E:384:ILE:HD11 | 1.76                     | 0.67              |
| 1:E:230:MET:HE1  | 1:E:312:ALA:HB3  | 1.76                     | 0.67              |
| 1:F:205:LYS:HZ3  | 1:F:358:GLU:HB2  | 1.60                     | 0.67              |
| 1:F:513:ILE:O    | 1:F:517:ARG:HG3  | 1.94                     | 0.67              |
| 1:H:157:ILE:HG13 | 1:H:401:VAL:HG21 | 1.77                     | 0.67              |
| 1:B:208:GLU:HB3  | 1:B:212:GLU:HG3  | 1.75                     | 0.67              |
| 1:D:244:GLU:OE1  | 1:D:336:VAL:HG22 | 1.95                     | 0.67              |
| 1:E:469:GLU:HB2  | 1:E:477:ILE:HG21 | 1.77                     | 0.67              |
| 1:F:166:ASN:HA   | 1:G:517:ARG:NH1  | 2.10                     | 0.67              |
| 1:H:265:LEU:O    | 1:H:269:LEU:HD13 | 1.95                     | 0.67              |
| 1:A:60:VAL:HG21  | 1:A:71:LYS:HE2   | 1.77                     | 0.67              |
| 1:G:348:GLU:O    | 1:G:349:VAL:HG23 | 1.93                     | 0.67              |
| 1:G:418:LEU:O    | 1:G:422:LEU:HB2  | 1.95                     | 0.67              |
| 1:E:35:ILE:HD11  | 1:E:74:LEU:HD21  | 1.77                     | 0.66              |
| 1:G:227:HIS:HB3  | 1:G:230:MET:HG3  | 1.76                     | 0.66              |
| 1:A:150:ASP:OD2  | 1:A:152:GLU:HB3  | 1.95                     | 0.66              |
| 1:B:59:ILE:HD12  | 1:B:59:ILE:N     | 2.10                     | 0.66              |
| 1:B:409:PRO:HB3  | 1:B:490:LEU:HD11 | 1.76                     | 0.66              |
| 1:D:204:LYS:HD3  | 1:D:388:GLU:OE2  | 1.96                     | 0.66              |
| 1:G:217:ARG:HB3  | 1:G:217:ARG:HH11 | 1.60                     | 0.66              |
| 1:G:335:ASN:OD1  | 1:G:337:LYS:HB2  | 1.95                     | 0.66              |
| 1:H:102:VAL:HG12 | 1:H:446:ILE:HD13 | 1.77                     | 0.66              |
| 1:B:272:GLU:HA   | 1:B:275:MET:HE3  | 1.77                     | 0.66              |
| 1:E:412:GLY:O    | 1:E:416:ILE:HG13 | 1.96                     | 0.66              |
| 1:A:257:ILE:HB   | 1:B:255:ALA:HB2  | 1.78                     | 0.66              |
| 1:H:125:ILE:HD13 | 1:H:517:ARG:HG2  | 1.76                     | 0.66              |
| 1:E:94:GLY:HA3   | 1:E:396:LYS:HD2  | 1.77                     | 0.66              |
| 1:G:29:ILE:O     | 1:G:33:ARG:HG3   | 1.96                     | 0.66              |
| 1:H:37:GLU:HG2   | 1:H:40:ARG:NH1   | 2.10                     | 0.66              |
| 1:A:109:ARG:NH2  | 1:A:110:LYS:HD3  | 2.10                     | 0.66              |
| 1:A:483:GLU:HG3  | 1:A:485:LYS:NZ   | 2.09                     | 0.66              |
| 1:H:35:ILE:HD11  | 1:H:74:LEU:HD21  | 1.78                     | 0.66              |
| 1:A:469:GLU:CB   | 1:A:477:ILE:HG21 | 2.25                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:462:MET:O    | 1:B:466:VAL:HG23 | 1.95                     | 0.66              |
| 1:A:230:MET:HE1  | 1:A:312:ALA:HB3  | 1.78                     | 0.66              |
| 1:A:443:ALA:O    | 1:A:446:ILE:HG13 | 1.94                     | 0.66              |
| 1:C:142:ILE:HB   | 1:C:475:LEU:CD2  | 2.26                     | 0.66              |
| 1:D:197:LEU:HD22 | 1:D:395:VAL:HG12 | 1.78                     | 0.66              |
| 1:E:59:ILE:N     | 1:E:59:ILE:HD12  | 2.11                     | 0.66              |
| 1:F:126:LYS:NZ   | 1:F:126:LYS:HB3  | 2.10                     | 0.66              |
| 1:E:370:LYS:HA   | 1:E:370:LYS:HE2  | 1.77                     | 0.65              |
| 1:D:91:LYS:HB2   | 1:D:91:LYS:HZ2   | 1.59                     | 0.65              |
| 1:E:94:GLY:CA    | 1:E:396:LYS:HD2  | 2.25                     | 0.65              |
| 1:H:261:SER:O    | 1:H:264:GLN:HG3  | 1.95                     | 0.65              |
| 1:B:94:GLY:HA3   | 1:B:396:LYS:HD2  | 1.77                     | 0.65              |
| 1:B:413:ALA:HB3  | 1:B:414:PRO:HD3  | 1.78                     | 0.65              |
| 1:E:383:VAL:O    | 1:E:387:VAL:HG23 | 1.95                     | 0.65              |
| 1:H:380:THR:HG23 | 1:H:383:VAL:H    | 1.62                     | 0.65              |
| 1:D:206:ALA:HA   | 1:D:384:ILE:HD11 | 1.76                     | 0.65              |
| 1:D:445:LYS:O    | 1:D:448:PRO:HD2  | 1.95                     | 0.65              |
| 1:E:307:LYS:HD2  | 1:F:338:ASP:OD2  | 1.97                     | 0.65              |
| 1:G:145:ARG:HG2  | 1:G:145:ARG:HH11 | 1.61                     | 0.65              |
| 1:B:445:LYS:O    | 1:B:449:LYS:HB2  | 1.96                     | 0.65              |
| 1:D:446:ILE:O    | 1:D:450:THR:HG23 | 1.95                     | 0.65              |
| 1:A:517:ARG:HH12 | 1:H:166:ASN:HA   | 1.61                     | 0.65              |
| 1:B:380:THR:CG2  | 1:B:383:VAL:H    | 2.08                     | 0.65              |
| 1:B:188:LYS:HB2  | 1:B:193:TYR:HA   | 1.79                     | 0.65              |
| 1:D:524:ALA:O    | 1:D:525:LYS:HG2  | 1.97                     | 0.65              |
| 1:E:380:THR:HG22 | 1:E:383:VAL:CG2  | 2.14                     | 0.65              |
| 1:A:517:ARG:NH1  | 1:H:166:ASN:HA   | 2.11                     | 0.65              |
| 1:B:108:LEU:HD11 | 1:B:515:ILE:HD12 | 1.79                     | 0.65              |
| 1:C:155:LEU:HD13 | 1:C:179:VAL:HG21 | 1.78                     | 0.65              |
| 1:E:73:ASP:O     | 1:F:13:PRO:HD3   | 1.97                     | 0.65              |
| 1:F:258:ASN:HB3  | 1:G:258:ASN:HD21 | 1.61                     | 0.65              |
| 1:F:272:GLU:HA   | 1:F:275:MET:CE   | 2.26                     | 0.65              |
| 1:C:108:LEU:HD11 | 1:C:515:ILE:HD12 | 1.77                     | 0.65              |
| 1:C:10:VAL:CG2   | 1:C:11:ILE:H     | 2.05                     | 0.64              |
| 1:D:241:LEU:HD22 | 1:D:330:ALA:CB   | 2.27                     | 0.64              |
| 1:D:304:TYR:O    | 1:D:308:TYR:HD1  | 1.80                     | 0.64              |
| 1:E:205:LYS:NZ   | 1:E:358:GLU:HG2  | 2.12                     | 0.64              |
| 1:E:394:ALA:O    | 1:E:398:VAL:HG23 | 1.96                     | 0.64              |
| 1:C:166:ASN:HA   | 1:D:517:ARG:NH1  | 2.12                     | 0.64              |
| 1:F:297:ILE:HG22 | 1:F:302:GLN:HG3  | 1.79                     | 0.64              |
| 1:G:11:ILE:HG23  | 1:G:12:LEU:N     | 2.12                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:123:ILE:HG21 | 1:C:432:LYS:HB3  | 1.79                     | 0.64              |
| 1:G:37:GLU:HG2   | 1:G:40:ARG:NH1   | 2.12                     | 0.64              |
| 1:A:208:GLU:HB3  | 1:A:212:GLU:HG3  | 1.77                     | 0.64              |
| 1:D:138:ILE:HD13 | 1:D:421:ARG:HG2  | 1.79                     | 0.64              |
| 1:D:465:LYS:O    | 1:D:469:GLU:HG2  | 1.97                     | 0.64              |
| 1:A:126:LYS:NZ   | 1:A:126:LYS:HB3  | 2.11                     | 0.64              |
| 1:H:372:VAL:HG22 | 1:H:373:THR:N    | 2.12                     | 0.64              |
| 1:B:466:VAL:HG21 | 1:B:479:ILE:HG12 | 1.80                     | 0.64              |
| 1:D:226:VAL:HG12 | 1:D:312:ALA:O    | 1.97                     | 0.64              |
| 1:D:230:MET:HE1  | 1:D:312:ALA:HB3  | 1.79                     | 0.64              |
| 1:C:189:LYS:HD2  | 1:C:189:LYS:C    | 2.18                     | 0.64              |
| 1:E:99:THR:O     | 1:E:103:ILE:HG13 | 1.97                     | 0.64              |
| 1:F:125:ILE:HG23 | 1:F:513:ILE:CG2  | 2.27                     | 0.64              |
| 1:F:205:LYS:HZ3  | 1:F:358:GLU:CB   | 2.11                     | 0.64              |
| 1:F:204:LYS:HD3  | 1:F:388:GLU:OE2  | 1.98                     | 0.64              |
| 1:H:409:PRO:HB3  | 1:H:490:LEU:HD13 | 1.79                     | 0.64              |
| 1:D:211:GLU:OE1  | 1:D:211:GLU:HA   | 1.98                     | 0.64              |
| 1:E:272:GLU:HA   | 1:E:275:MET:CE   | 2.27                     | 0.64              |
| 1:E:293:VAL:CG2  | 1:E:297:ILE:HD11 | 2.25                     | 0.64              |
| 1:A:217:ARG:HB3  | 1:A:217:ARG:NH1  | 2.12                     | 0.63              |
| 1:E:261:SER:H    | 1:E:264:GLN:HE21 | 1.45                     | 0.63              |
| 1:F:225:VAL:HG21 | 1:F:232:LYS:HD3  | 1.80                     | 0.63              |
| 1:G:423:ASP:OD1  | 1:G:427:LYS:HE2  | 1.98                     | 0.63              |
| 1:A:30:LEU:O     | 1:A:34:ILE:HG13  | 1.98                     | 0.63              |
| 1:D:11:ILE:HD13  | 1:D:12:LEU:HB2   | 1.80                     | 0.63              |
| 1:E:447:ILE:HB   | 1:E:448:PRO:HD3  | 1.80                     | 0.63              |
| 1:F:123:ILE:HG21 | 1:F:432:LYS:HB3  | 1.79                     | 0.63              |
| 1:A:257:ILE:HG22 | 1:A:259:ILE:HD12 | 1.80                     | 0.63              |
| 1:A:445:LYS:O    | 1:A:449:LYS:HB2  | 1.98                     | 0.63              |
| 1:B:483:GLU:HG3  | 1:B:485:LYS:NZ   | 2.13                     | 0.63              |
| 1:D:447:ILE:HB   | 1:D:448:PRO:HD3  | 1.79                     | 0.63              |
| 1:H:383:VAL:O    | 1:H:387:VAL:HG23 | 1.98                     | 0.63              |
| 1:B:60:VAL:HG21  | 1:B:71:LYS:HE2   | 1.78                     | 0.63              |
| 1:F:235:GLU:HA   | 1:F:235:GLU:OE2  | 1.99                     | 0.63              |
| 1:F:269:LEU:HD12 | 1:G:251:THR:CG2  | 2.28                     | 0.63              |
| 1:H:11:ILE:HD13  | 1:H:11:ILE:C     | 2.18                     | 0.63              |
| 1:B:11:ILE:C     | 1:B:11:ILE:HD13  | 2.19                     | 0.63              |
| 1:E:227:HIS:ND1  | 1:E:228:PRO:HD2  | 2.13                     | 0.63              |
| 1:F:277:LYS:HB2  | 1:F:304:TYR:CE2  | 2.33                     | 0.63              |
| 1:B:29:ILE:O     | 1:B:33:ARG:HG3   | 1.98                     | 0.63              |
| 1:C:142:ILE:HB   | 1:C:475:LEU:HD22 | 1.79                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:463:LEU:O    | 1:G:467:ILE:HG13 | 1.99                     | 0.63              |
| 1:E:166:ASN:HA   | 1:F:517:ARG:HH12 | 1.62                     | 0.63              |
| 1:E:513:ILE:O    | 1:E:517:ARG:HG3  | 1.99                     | 0.63              |
| 1:G:423:ASP:O    | 1:G:426:ALA:HB3  | 1.98                     | 0.63              |
| 1:A:85:VAL:HG13  | 1:A:507:SER:HB3  | 1.81                     | 0.63              |
| 1:E:29:ILE:O     | 1:E:33:ARG:HG3   | 1.98                     | 0.63              |
| 1:E:196:ASP:OD1  | 1:E:198:ASP:HB2  | 1.99                     | 0.63              |
| 1:E:212:GLU:HB2  | 1:E:377:ARG:HG3  | 1.81                     | 0.63              |
| 1:E:297:ILE:HG22 | 1:E:302:GLN:HG3  | 1.80                     | 0.63              |
| 1:F:188:LYS:HD3  | 1:F:193:TYR:CE1  | 2.34                     | 0.63              |
| 1:C:524:ALA:C    | 1:C:525:LYS:HD2  | 2.19                     | 0.62              |
| 1:F:30:LEU:O     | 1:F:34:ILE:HG13  | 1.99                     | 0.62              |
| 1:A:125:ILE:HG23 | 1:A:513:ILE:CG2  | 2.27                     | 0.62              |
| 1:A:217:ARG:HB3  | 1:A:217:ARG:HH11 | 1.62                     | 0.62              |
| 1:B:145:ARG:HG2  | 1:B:145:ARG:NH1  | 2.11                     | 0.62              |
| 1:C:513:ILE:O    | 1:C:517:ARG:HG3  | 1.99                     | 0.62              |
| 1:E:189:LYS:HD2  | 1:E:189:LYS:C    | 2.19                     | 0.62              |
| 1:G:10:VAL:HG13  | 1:G:11:ILE:N     | 2.10                     | 0.62              |
| 1:A:463:LEU:O    | 1:A:467:ILE:HG13 | 1.99                     | 0.62              |
| 1:B:166:ASN:HA   | 1:C:517:ARG:NH1  | 2.13                     | 0.62              |
| 1:D:409:PRO:HB3  | 1:D:490:LEU:HD13 | 1.80                     | 0.62              |
| 1:E:445:LYS:O    | 1:E:449:LYS:HB2  | 1.99                     | 0.62              |
| 1:F:383:VAL:O    | 1:F:387:VAL:HG23 | 1.99                     | 0.62              |
| 1:C:497:PRO:HB2  | 1:C:500:VAL:HG23 | 1.80                     | 0.62              |
| 1:E:265:LEU:O    | 1:E:269:LEU:HD13 | 1.99                     | 0.62              |
| 1:F:233:ARG:NH1  | 1:F:349:VAL:HG13 | 2.14                     | 0.62              |
| 1:C:22:ARG:HG3   | 1:C:23:ASP:N     | 2.14                     | 0.62              |
| 1:F:335:ASN:OD1  | 1:F:337:LYS:HB2  | 1.99                     | 0.62              |
| 1:G:465:LYS:O    | 1:G:469:GLU:HG2  | 1.99                     | 0.62              |
| 1:G:497:PRO:HB2  | 1:G:500:VAL:HG23 | 1.81                     | 0.62              |
| 1:A:59:ILE:HD12  | 1:A:59:ILE:N     | 2.15                     | 0.62              |
| 1:D:11:ILE:HD13  | 1:D:11:ILE:C     | 2.20                     | 0.62              |
| 1:G:204:LYS:HD2  | 1:G:384:ILE:HG22 | 1.81                     | 0.62              |
| 1:G:354:LYS:HA   | 1:G:358:GLU:O    | 2.00                     | 0.62              |
| 1:G:462:MET:HE1  | 1:G:486:PRO:HD3  | 1.80                     | 0.62              |
| 1:H:64:ASP:O     | 1:H:68:ILE:HG13  | 1.99                     | 0.62              |
| 1:D:109:ARG:NH2  | 1:D:110:LYS:HD3  | 2.13                     | 0.62              |
| 1:H:281:ASP:OD1  | 1:H:308:TYR:OH   | 2.13                     | 0.62              |
| 1:F:146:VAL:HG22 | 1:F:147:ASP:N    | 2.15                     | 0.62              |
| 1:F:286:THR:HG21 | 1:F:339:LEU:HG   | 1.82                     | 0.62              |
| 1:H:117:GLN:O    | 1:H:118:ASN:HB2  | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:125:ILE:HD13 | 1:A:517:ARG:HG2  | 1.82                     | 0.62              |
| 1:A:257:ILE:HB   | 1:B:255:ALA:CB   | 2.30                     | 0.62              |
| 1:B:249:LYS:HE2  | 1:B:279:MET:HE3  | 1.82                     | 0.62              |
| 1:D:179:VAL:O    | 1:D:183:LYS:HG3  | 2.00                     | 0.62              |
| 1:D:404:ASP:OD1  | 1:D:499:ARG:HB2  | 1.99                     | 0.62              |
| 1:D:416:ILE:HD13 | 1:D:466:VAL:HG12 | 1.81                     | 0.62              |
| 1:E:17:GLN:NE2   | 1:E:17:GLN:H     | 1.97                     | 0.62              |
| 1:A:409:PRO:HB3  | 1:A:490:LEU:HD13 | 1.81                     | 0.61              |
| 1:C:204:LYS:HD3  | 1:C:388:GLU:OE2  | 1.99                     | 0.61              |
| 1:C:265:LEU:O    | 1:C:269:LEU:HD13 | 2.00                     | 0.61              |
| 1:E:73:ASP:HB3   | 1:F:13:PRO:HG2   | 1.82                     | 0.61              |
| 1:F:394:ALA:O    | 1:F:398:VAL:HG23 | 2.00                     | 0.61              |
| 1:G:388:GLU:O    | 1:G:392:GLU:HG3  | 1.99                     | 0.61              |
| 1:H:388:GLU:O    | 1:H:392:GLU:HG3  | 1.99                     | 0.61              |
| 1:B:150:ASP:OD1  | 1:B:153:THR:HG23 | 1.99                     | 0.61              |
| 1:B:509:SER:O    | 1:B:513:ILE:HG13 | 2.00                     | 0.61              |
| 1:F:413:ALA:HB3  | 1:F:414:PRO:HD3  | 1.81                     | 0.61              |
| 1:A:145:ARG:HG2  | 1:A:145:ARG:HH11 | 1.65                     | 0.61              |
| 1:B:13:PRO:O     | 1:B:16:THR:HB    | 2.00                     | 0.61              |
| 1:C:11:ILE:HD13  | 1:C:11:ILE:O     | 2.00                     | 0.61              |
| 1:C:21:GLY:O     | 1:C:25:GLN:HG3   | 2.01                     | 0.61              |
| 1:B:524:ALA:C    | 1:B:525:LYS:HD2  | 2.21                     | 0.61              |
| 1:E:483:GLU:HG3  | 1:E:485:LYS:HZ3  | 1.64                     | 0.61              |
| 1:B:447:ILE:HB   | 1:B:448:PRO:HD3  | 1.82                     | 0.61              |
| 1:D:142:ILE:HB   | 1:D:475:LEU:HD22 | 1.81                     | 0.61              |
| 1:E:144:ILE:HD11 | 1:E:490:LEU:HD21 | 1.82                     | 0.61              |
| 1:A:11:ILE:HD11  | 1:H:31:ALA:HA    | 1.82                     | 0.61              |
| 1:H:175:ALA:O    | 1:H:179:VAL:HG23 | 2.01                     | 0.61              |
| 1:D:17:GLN:NE2   | 1:D:17:GLN:H     | 1.99                     | 0.61              |
| 1:E:388:GLU:O    | 1:E:392:GLU:HG3  | 2.00                     | 0.61              |
| 1:F:409:PRO:HB3  | 1:F:490:LEU:CD1  | 2.29                     | 0.61              |
| 1:F:445:LYS:O    | 1:F:448:PRO:HD2  | 2.01                     | 0.61              |
| 1:C:260:THR:N    | 1:C:264:GLN:HE21 | 1.86                     | 0.61              |
| 1:D:106:GLU:HG2  | 1:D:446:ILE:CG1  | 2.31                     | 0.61              |
| 1:E:125:ILE:HD13 | 1:E:517:ARG:HG2  | 1.82                     | 0.61              |
| 1:E:151:GLU:O    | 1:E:155:LEU:HD23 | 2.01                     | 0.61              |
| 1:H:125:ILE:HG23 | 1:H:513:ILE:CG2  | 2.27                     | 0.61              |
| 1:H:126:LYS:NZ   | 1:H:126:LYS:HB3  | 2.16                     | 0.61              |
| 1:B:120:HIS:ND1  | 1:B:121:PRO:HD2  | 2.15                     | 0.61              |
| 1:D:172:GLU:OE1  | 1:D:172:GLU:HA   | 2.01                     | 0.61              |
| 1:E:60:VAL:HG21  | 1:E:71:LYS:HE2   | 1.83                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:69:LEU:HB3   | 1:E:83:VAL:HG22  | 1.83                     | 0.61              |
| 1:G:348:GLU:HB3  | 1:G:365:GLY:HA3  | 1.82                     | 0.61              |
| 1:C:354:LYS:HE2  | 1:C:357:GLY:HA2  | 1.82                     | 0.60              |
| 1:C:445:LYS:O    | 1:C:449:LYS:HB2  | 2.01                     | 0.60              |
| 1:E:108:LEU:HD11 | 1:E:515:ILE:HD12 | 1.82                     | 0.60              |
| 1:H:211:GLU:OE1  | 1:H:211:GLU:HA   | 2.00                     | 0.60              |
| 1:B:103:ILE:O    | 1:B:107:LEU:HB2  | 2.00                     | 0.60              |
| 1:D:241:LEU:CD2  | 1:D:330:ALA:HB3  | 2.31                     | 0.60              |
| 1:F:106:GLU:HG2  | 1:F:446:ILE:CG1  | 2.31                     | 0.60              |
| 1:C:11:ILE:HD13  | 1:C:11:ILE:C     | 2.21                     | 0.60              |
| 1:E:354:LYS:HE2  | 1:E:357:GLY:HA2  | 1.83                     | 0.60              |
| 1:F:243:ASN:OD1  | 1:F:295:LYS:HE3  | 2.00                     | 0.60              |
| 1:A:106:GLU:HG2  | 1:A:446:ILE:HG13 | 1.82                     | 0.60              |
| 1:B:261:SER:O    | 1:B:264:GLN:HB2  | 2.00                     | 0.60              |
| 1:D:469:GLU:CB   | 1:D:477:ILE:HG21 | 2.31                     | 0.60              |
| 1:E:205:LYS:HZ1  | 1:E:358:GLU:HG2  | 1.66                     | 0.60              |
| 1:F:197:LEU:HD22 | 1:F:395:VAL:CG1  | 2.31                     | 0.60              |
| 1:F:208:GLU:HB3  | 1:F:212:GLU:HG3  | 1.81                     | 0.60              |
| 1:F:235:GLU:O    | 1:F:237:ALA:N    | 2.34                     | 0.60              |
| 1:G:126:LYS:HB3  | 1:G:126:LYS:NZ   | 2.17                     | 0.60              |
| 1:G:466:VAL:HG21 | 1:G:479:ILE:HG12 | 1.83                     | 0.60              |
| 1:H:155:LEU:HD22 | 1:H:179:VAL:HG21 | 1.84                     | 0.60              |
| 1:C:157:ILE:HG13 | 1:C:401:VAL:HG21 | 1.83                     | 0.60              |
| 1:F:244:GLU:OE1  | 1:F:336:VAL:HG22 | 2.01                     | 0.60              |
| 1:H:227:HIS:HD1  | 1:H:229:ARG:H    | 1.48                     | 0.60              |
| 1:C:269:LEU:HD12 | 1:D:251:THR:HG23 | 1.83                     | 0.60              |
| 1:D:151:GLU:O    | 1:D:155:LEU:HD23 | 2.02                     | 0.60              |
| 1:E:109:ARG:HG2  | 1:E:109:ARG:HH11 | 1.67                     | 0.60              |
| 1:A:179:VAL:O    | 1:A:183:LYS:HG3  | 2.02                     | 0.60              |
| 1:A:261:SER:H    | 1:A:264:GLN:HG3  | 1.66                     | 0.60              |
| 1:B:233:ARG:HD2  | 1:B:351:GLU:OE2  | 2.02                     | 0.60              |
| 1:D:217:ARG:HB3  | 1:D:217:ARG:HH11 | 1.66                     | 0.60              |
| 1:E:230:MET:HE2  | 1:E:312:ALA:N    | 2.17                     | 0.60              |
| 1:G:269:LEU:HD12 | 1:H:251:THR:HG23 | 1.84                     | 0.60              |
| 1:G:430:GLY:HA2  | 1:G:434:ALA:HB2  | 1.83                     | 0.60              |
| 1:F:157:ILE:HG13 | 1:F:401:VAL:HG21 | 1.84                     | 0.60              |
| 1:B:241:LEU:HD12 | 1:B:292:PHE:HB2  | 1.83                     | 0.60              |
| 1:A:77:PRO:HB2   | 1:H:51:MET:CE    | 2.31                     | 0.59              |
| 1:C:59:ILE:N     | 1:C:59:ILE:HD12  | 2.17                     | 0.59              |
| 1:C:64:ASP:O     | 1:C:68:ILE:HG13  | 2.02                     | 0.59              |
| 1:F:249:LYS:HE2  | 1:F:279:MET:HE3  | 1.83                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:260:THR:N    | 1:H:264:GLN:NE2  | 2.44                     | 0.59              |
| 1:H:465:LYS:O    | 1:H:469:GLU:HG2  | 2.01                     | 0.59              |
| 1:B:182:VAL:O    | 1:B:186:ALA:HB2  | 2.03                     | 0.59              |
| 1:B:348:GLU:HB3  | 1:B:365:GLY:HA3  | 1.84                     | 0.59              |
| 1:C:261:SER:O    | 1:C:264:GLN:HG3  | 2.02                     | 0.59              |
| 1:E:142:ILE:HB   | 1:E:475:LEU:HD22 | 1.82                     | 0.59              |
| 1:F:175:ALA:O    | 1:F:179:VAL:HG23 | 2.02                     | 0.59              |
| 1:A:197:LEU:HD22 | 1:A:395:VAL:CG1  | 2.31                     | 0.59              |
| 1:C:117:GLN:O    | 1:C:118:ASN:HB2  | 2.01                     | 0.59              |
| 1:C:483:GLU:HG3  | 1:C:485:LYS:HZ1  | 1.68                     | 0.59              |
| 1:H:59:ILE:N     | 1:H:59:ILE:HD12  | 2.16                     | 0.59              |
| 1:H:136:GLN:NE2  | 1:H:136:GLN:HA   | 2.17                     | 0.59              |
| 1:A:475:LEU:HD12 | 1:A:475:LEU:O    | 2.03                     | 0.59              |
| 1:C:205:LYS:O    | 1:C:377:ARG:NH1  | 2.35                     | 0.59              |
| 1:E:443:ALA:O    | 1:E:446:ILE:HG13 | 2.03                     | 0.59              |
| 1:F:22:ARG:HG3   | 1:F:23:ASP:N     | 2.18                     | 0.59              |
| 1:F:206:ALA:HA   | 1:F:384:ILE:HD11 | 1.83                     | 0.59              |
| 1:G:136:GLN:HA   | 1:G:136:GLN:HE21 | 1.67                     | 0.59              |
| 1:B:166:ASN:HD22 | 1:B:166:ASN:C    | 2.05                     | 0.59              |
| 1:E:106:GLU:HG2  | 1:E:446:ILE:CG1  | 2.33                     | 0.59              |
| 1:E:145:ARG:HG2  | 1:E:145:ARG:HH11 | 1.67                     | 0.59              |
| 1:H:418:LEU:O    | 1:H:422:LEU:HB2  | 2.03                     | 0.59              |
| 1:B:216:VAL:O    | 1:B:372:VAL:HG23 | 2.02                     | 0.59              |
| 1:D:348:GLU:O    | 1:D:349:VAL:HG23 | 2.02                     | 0.59              |
| 1:A:265:LEU:O    | 1:A:269:LEU:HD13 | 2.02                     | 0.59              |
| 1:A:423:ASP:O    | 1:A:426:ALA:HB3  | 2.02                     | 0.59              |
| 1:D:418:LEU:O    | 1:D:422:LEU:HB2  | 2.03                     | 0.59              |
| 1:E:271:GLN:O    | 1:E:275:MET:HG3  | 2.02                     | 0.59              |
| 1:F:257:ILE:HG22 | 1:F:259:ILE:HD12 | 1.85                     | 0.59              |
| 1:F:465:LYS:O    | 1:F:469:GLU:HG2  | 2.03                     | 0.59              |
| 1:A:12:LEU:HD13  | 1:A:16:THR:HG21  | 1.83                     | 0.59              |
| 1:E:109:ARG:NH2  | 1:E:110:LYS:HD3  | 2.17                     | 0.59              |
| 1:E:423:ASP:OD1  | 1:E:427:LYS:HE2  | 2.02                     | 0.59              |
| 1:A:466:VAL:HG21 | 1:A:479:ILE:HG12 | 1.85                     | 0.59              |
| 1:C:461:GLU:HG2  | 1:C:465:LYS:NZ   | 2.18                     | 0.59              |
| 1:G:126:LYS:O    | 1:G:130:LEU:HG   | 2.02                     | 0.59              |
| 1:G:353:ARG:NH2  | 1:G:364:GLU:OE2  | 2.35                     | 0.59              |
| 1:H:328:THR:HG22 | 1:H:366:CYS:SG   | 2.43                     | 0.59              |
| 1:H:509:SER:O    | 1:H:513:ILE:HG13 | 2.03                     | 0.59              |
| 1:A:450:THR:O    | 1:A:454:ASN:ND2  | 2.36                     | 0.59              |
| 1:C:433:GLU:O    | 1:C:437:ILE:HG13 | 2.02                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:227:HIS:HB3  | 1:E:230:MET:CG   | 2.30                     | 0.59              |
| 1:G:205:LYS:NZ   | 1:G:358:GLU:HG2  | 2.17                     | 0.59              |
| 1:G:409:PRO:HB3  | 1:G:490:LEU:HD13 | 1.85                     | 0.59              |
| 1:C:226:VAL:HG12 | 1:C:312:ALA:O    | 2.03                     | 0.58              |
| 1:D:182:VAL:O    | 1:D:186:ALA:HB2  | 2.03                     | 0.58              |
| 1:G:157:ILE:HG13 | 1:G:401:VAL:HG21 | 1.85                     | 0.58              |
| 1:G:276:LEU:HD23 | 1:G:300:LEU:HB2  | 1.84                     | 0.58              |
| 1:A:266:MET:O    | 1:A:270:GLU:HG3  | 2.02                     | 0.58              |
| 1:B:400:ASP:OD1  | 1:B:499:ARG:HD2  | 2.04                     | 0.58              |
| 1:G:170:HIS:CE1  | 1:G:210:VAL:HB   | 2.38                     | 0.58              |
| 1:G:416:ILE:HD13 | 1:G:466:VAL:HG12 | 1.84                     | 0.58              |
| 1:H:120:HIS:ND1  | 1:H:122:SER:HB3  | 2.18                     | 0.58              |
| 1:B:272:GLU:HA   | 1:B:275:MET:CE   | 2.33                     | 0.58              |
| 1:D:106:GLU:HG2  | 1:D:446:ILE:HG13 | 1.83                     | 0.58              |
| 1:E:91:LYS:HG2   | 1:E:91:LYS:O     | 2.04                     | 0.58              |
| 1:G:513:ILE:O    | 1:G:517:ARG:HG3  | 2.03                     | 0.58              |
| 1:C:204:LYS:HD2  | 1:C:384:ILE:HG22 | 1.86                     | 0.58              |
| 1:D:315:ARG:HG3  | 1:D:315:ARG:NH1  | 2.19                     | 0.58              |
| 1:F:233:ARG:NH1  | 1:F:349:VAL:CG1  | 2.65                     | 0.58              |
| 1:H:264:GLN:HA   | 1:H:267:SER:OG   | 2.04                     | 0.58              |
| 1:C:353:ARG:NH2  | 1:C:364:GLU:OE2  | 2.36                     | 0.58              |
| 1:F:150:ASP:OD1  | 1:F:153:THR:HG23 | 2.03                     | 0.58              |
| 1:F:271:GLN:O    | 1:F:275:MET:HG3  | 2.04                     | 0.58              |
| 1:B:297:ILE:HG22 | 1:B:302:GLN:HG3  | 1.84                     | 0.58              |
| 1:D:110:LYS:HE3  | 1:D:442:ASP:OD1  | 2.03                     | 0.58              |
| 1:G:445:LYS:O    | 1:G:448:PRO:HD2  | 2.04                     | 0.58              |
| 1:A:206:ALA:CA   | 1:A:384:ILE:HD11 | 2.32                     | 0.58              |
| 1:D:303:HIS:CD2  | 1:E:335:ASN:HB3  | 2.39                     | 0.58              |
| 1:D:409:PRO:HB3  | 1:D:490:LEU:CD1  | 2.33                     | 0.58              |
| 1:A:226:VAL:HG12 | 1:A:312:ALA:O    | 2.03                     | 0.58              |
| 1:A:400:ASP:OD1  | 1:A:499:ARG:HD2  | 2.04                     | 0.58              |
| 1:D:188:LYS:HB2  | 1:D:193:TYR:HA   | 1.86                     | 0.58              |
| 1:F:96:GLY:HA2   | 3:F:6528:ADP:O1B | 2.04                     | 0.58              |
| 1:F:184:GLN:NE2  | 1:F:217:ARG:NH2  | 2.52                     | 0.58              |
| 1:F:469:GLU:HB2  | 1:F:477:ILE:HG21 | 1.85                     | 0.58              |
| 1:G:370:LYS:HA   | 1:G:370:LYS:CE   | 2.34                     | 0.58              |
| 1:H:216:VAL:O    | 1:H:218:GLY:N    | 2.36                     | 0.58              |
| 1:B:277:LYS:HD2  | 1:B:304:TYR:CE1  | 2.39                     | 0.57              |
| 1:B:513:ILE:O    | 1:B:517:ARG:HG3  | 2.02                     | 0.57              |
| 1:D:29:ILE:HG23  | 1:D:108:LEU:HB3  | 1.86                     | 0.57              |
| 1:D:280:VAL:HG13 | 1:D:305:LEU:HG   | 1.84                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:276:LEU:HD23 | 1:A:300:LEU:HB2  | 1.86                     | 0.57              |
| 1:C:123:ILE:HG21 | 1:C:432:LYS:CB   | 2.34                     | 0.57              |
| 1:D:45:PRO:HA    | 1:D:164:GLY:HA2  | 1.85                     | 0.57              |
| 1:D:230:MET:HE2  | 1:D:312:ALA:N    | 2.19                     | 0.57              |
| 1:E:136:GLN:HA   | 1:E:136:GLN:NE2  | 2.18                     | 0.57              |
| 1:E:342:GLU:N    | 1:E:342:GLU:OE2  | 2.37                     | 0.57              |
| 1:F:233:ARG:HH12 | 1:F:349:VAL:HG13 | 1.65                     | 0.57              |
| 1:A:29:ILE:HG23  | 1:A:108:LEU:HB3  | 1.86                     | 0.57              |
| 1:B:277:LYS:HB2  | 1:B:304:TYR:CE2  | 2.39                     | 0.57              |
| 1:C:120:HIS:ND1  | 1:C:122:SER:HB3  | 2.18                     | 0.57              |
| 1:D:466:VAL:HG22 | 1:D:486:PRO:HG3  | 1.86                     | 0.57              |
| 1:E:154:LEU:HG   | 1:E:398:VAL:HG13 | 1.86                     | 0.57              |
| 1:H:29:ILE:HG23  | 1:H:108:LEU:HB3  | 1.86                     | 0.57              |
| 1:A:158:ALA:O    | 1:A:162:ILE:HG13 | 2.04                     | 0.57              |
| 1:A:304:TYR:O    | 1:A:308:TYR:HD1  | 1.88                     | 0.57              |
| 1:A:393:ASP:O    | 1:A:397:VAL:HG22 | 2.05                     | 0.57              |
| 1:C:150:ASP:OD1  | 1:C:153:THR:HG23 | 2.04                     | 0.57              |
| 1:H:280:VAL:HG13 | 1:H:305:LEU:HG   | 1.86                     | 0.57              |
| 1:H:417:GLU:OE2  | 1:H:470:HIS:NE2  | 2.28                     | 0.57              |
| 1:B:126:LYS:HB3  | 1:B:126:LYS:NZ   | 2.19                     | 0.57              |
| 1:C:146:VAL:HG22 | 1:C:147:ASP:N    | 2.19                     | 0.57              |
| 1:E:509:SER:O    | 1:E:513:ILE:HG13 | 2.05                     | 0.57              |
| 1:G:188:LYS:HG3  | 1:G:192:LYS:C    | 2.24                     | 0.57              |
| 1:A:230:MET:HE2  | 1:A:312:ALA:N    | 2.19                     | 0.57              |
| 1:C:37:GLU:HG2   | 1:C:40:ARG:NH1   | 2.19                     | 0.57              |
| 1:D:114:LEU:HD22 | 1:D:119:ILE:HD12 | 1.86                     | 0.57              |
| 1:F:497:PRO:HB2  | 1:F:500:VAL:HG23 | 1.86                     | 0.57              |
| 1:G:445:LYS:O    | 1:G:449:LYS:HB2  | 2.05                     | 0.57              |
| 1:A:38:THR:O     | 1:A:50:LYS:CE    | 2.52                     | 0.57              |
| 1:B:94:GLY:CA    | 1:B:396:LYS:HD2  | 2.34                     | 0.57              |
| 1:B:394:ALA:O    | 1:B:398:VAL:HG23 | 2.04                     | 0.57              |
| 1:D:388:GLU:O    | 1:D:392:GLU:HG3  | 2.05                     | 0.57              |
| 1:F:204:LYS:HD2  | 1:F:384:ILE:HG22 | 1.86                     | 0.57              |
| 1:G:11:ILE:CG2   | 1:G:12:LEU:N     | 2.67                     | 0.57              |
| 1:H:241:LEU:HD22 | 1:H:330:ALA:CB   | 2.35                     | 0.57              |
| 1:A:241:LEU:HD22 | 1:A:330:ALA:HB3  | 1.87                     | 0.57              |
| 1:B:12:LEU:HD21  | 1:B:16:THR:HG21  | 1.87                     | 0.57              |
| 1:B:227:HIS:HB3  | 1:B:230:MET:HG3  | 1.87                     | 0.57              |
| 1:B:412:GLY:O    | 1:B:415:GLU:HG2  | 2.05                     | 0.57              |
| 1:C:297:ILE:HG22 | 1:C:302:GLN:HG3  | 1.86                     | 0.57              |
| 1:C:425:TYR:O    | 1:C:429:VAL:HG23 | 2.05                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:443:ALA:O    | 1:C:446:ILE:HG13 | 2.04                     | 0.57              |
| 1:D:259:ILE:HG22 | 1:E:257:ILE:HG23 | 1.85                     | 0.57              |
| 1:D:261:SER:H    | 1:D:264:GLN:HE21 | 1.52                     | 0.57              |
| 1:E:138:ILE:HD13 | 1:E:421:ARG:HG2  | 1.87                     | 0.57              |
| 1:E:412:GLY:O    | 1:E:415:GLU:HG2  | 2.05                     | 0.57              |
| 1:A:75:GLN:HB2   | 1:B:11:ILE:CA    | 2.35                     | 0.57              |
| 1:H:205:LYS:O    | 1:H:377:ARG:NH1  | 2.38                     | 0.57              |
| 1:A:37:GLU:HG2   | 1:A:40:ARG:NH1   | 2.20                     | 0.56              |
| 1:D:197:LEU:HD22 | 1:D:395:VAL:CG1  | 2.35                     | 0.56              |
| 1:E:355:LEU:O    | 1:E:356:ALA:HB3  | 2.05                     | 0.56              |
| 1:F:59:ILE:HD12  | 1:F:59:ILE:N     | 2.20                     | 0.56              |
| 1:G:147:ASP:O    | 1:G:149:ASP:N    | 2.38                     | 0.56              |
| 1:G:261:SER:O    | 1:G:264:GLN:HG3  | 2.05                     | 0.56              |
| 1:A:509:SER:O    | 1:A:513:ILE:HG13 | 2.05                     | 0.56              |
| 1:F:13:PRO:O     | 1:F:16:THR:HB    | 2.05                     | 0.56              |
| 1:F:270:GLU:HA   | 1:F:273:GLU:HG3  | 1.86                     | 0.56              |
| 1:F:461:GLU:HG2  | 1:F:465:LYS:HZ2  | 1.71                     | 0.56              |
| 1:H:76:HIS:CD2   | 1:H:78:ALA:HB3   | 2.40                     | 0.56              |
| 1:H:125:ILE:CD1  | 1:H:517:ARG:HG2  | 2.34                     | 0.56              |
| 1:A:99:THR:O     | 1:A:103:ILE:HG13 | 2.04                     | 0.56              |
| 1:B:54:ASP:OD1   | 1:B:58:ASP:HB3   | 2.06                     | 0.56              |
| 1:B:91:LYS:HB2   | 1:B:91:LYS:NZ    | 2.20                     | 0.56              |
| 1:B:179:VAL:O    | 1:B:183:LYS:HG3  | 2.05                     | 0.56              |
| 1:B:197:LEU:HD22 | 1:B:395:VAL:CG1  | 2.35                     | 0.56              |
| 1:B:250:LYS:NZ   | 1:C:253:THR:HA   | 2.19                     | 0.56              |
| 1:B:462:MET:CE   | 1:B:486:PRO:HD3  | 2.35                     | 0.56              |
| 1:D:126:LYS:NZ   | 1:D:126:LYS:HB3  | 2.20                     | 0.56              |
| 1:D:147:ASP:HB3  | 1:D:150:ASP:HB2  | 1.88                     | 0.56              |
| 1:D:217:ARG:HH11 | 1:D:217:ARG:CB   | 2.17                     | 0.56              |
| 1:D:497:PRO:HB2  | 1:D:500:VAL:HG23 | 1.86                     | 0.56              |
| 1:F:134:LYS:O    | 1:F:138:ILE:HG13 | 2.05                     | 0.56              |
| 1:F:179:VAL:O    | 1:F:183:LYS:HG3  | 2.04                     | 0.56              |
| 1:H:189:LYS:HD2  | 1:H:189:LYS:C    | 2.25                     | 0.56              |
| 1:A:138:ILE:CD1  | 1:A:421:ARG:HG2  | 2.34                     | 0.56              |
| 1:C:413:ALA:HB3  | 1:C:414:PRO:HD3  | 1.87                     | 0.56              |
| 1:E:150:ASP:OD2  | 1:E:152:GLU:HB3  | 2.05                     | 0.56              |
| 1:E:266:MET:HG2  | 1:F:271:GLN:NE2  | 2.20                     | 0.56              |
| 1:F:123:ILE:HG21 | 1:F:432:LYS:CB   | 2.35                     | 0.56              |
| 1:F:204:LYS:HB3  | 1:F:384:ILE:HG21 | 1.87                     | 0.56              |
| 1:F:210:VAL:HA   | 1:F:377:ARG:O    | 2.05                     | 0.56              |
| 1:G:51:MET:HB2   | 1:H:518:ILE:HD13 | 1.86                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:64:ASP:O     | 1:G:68:ILE:HG13  | 2.05                     | 0.56              |
| 1:A:182:VAL:O    | 1:A:186:ALA:HB2  | 2.06                     | 0.56              |
| 1:C:409:PRO:HB3  | 1:C:490:LEU:HD12 | 1.88                     | 0.56              |
| 1:D:513:ILE:O    | 1:D:517:ARG:HG3  | 2.05                     | 0.56              |
| 1:H:348:GLU:O    | 1:H:349:VAL:HG23 | 2.06                     | 0.56              |
| 1:F:184:GLN:HE22 | 1:F:217:ARG:HH21 | 1.54                     | 0.56              |
| 1:B:241:LEU:CD2  | 1:B:330:ALA:HB3  | 2.35                     | 0.56              |
| 1:C:257:ILE:HG22 | 1:C:259:ILE:HD12 | 1.87                     | 0.56              |
| 1:D:175:ALA:O    | 1:D:179:VAL:HG23 | 2.06                     | 0.56              |
| 1:D:226:VAL:HG22 | 1:D:302:GLN:OE1  | 2.06                     | 0.56              |
| 1:E:233:ARG:HH11 | 1:E:233:ARG:HG3  | 1.71                     | 0.56              |
| 1:G:196:ASP:OD1  | 1:G:198:ASP:HB2  | 2.06                     | 0.56              |
| 1:B:276:LEU:HD23 | 1:B:300:LEU:HB2  | 1.87                     | 0.56              |
| 1:E:38:THR:O     | 1:E:50:LYS:HE3   | 2.06                     | 0.56              |
| 1:F:10:VAL:CG2   | 1:F:11:ILE:H     | 2.13                     | 0.56              |
| 1:F:483:GLU:HG3  | 1:F:485:LYS:NZ   | 2.21                     | 0.56              |
| 1:G:94:GLY:HA3   | 1:G:396:LYS:HD2  | 1.88                     | 0.56              |
| 1:C:151:GLU:O    | 1:C:155:LEU:HD23 | 2.06                     | 0.56              |
| 1:D:150:ASP:OD1  | 1:D:153:THR:HG23 | 2.06                     | 0.56              |
| 1:D:196:ASP:OD1  | 1:D:198:ASP:HB2  | 2.06                     | 0.56              |
| 1:E:11:ILE:HD13  | 1:E:11:ILE:O     | 2.05                     | 0.56              |
| 1:E:218:GLY:HA3  | 1:E:363:VAL:O    | 2.06                     | 0.56              |
| 1:H:54:ASP:OD1   | 1:H:56:LEU:HB2   | 2.06                     | 0.56              |
| 1:A:81:MET:HE3   | 1:A:514:MET:SD   | 2.46                     | 0.56              |
| 1:D:10:VAL:CG2   | 1:D:11:ILE:H     | 2.08                     | 0.56              |
| 1:E:17:GLN:H     | 1:E:17:GLN:HE21  | 1.54                     | 0.56              |
| 1:E:266:MET:O    | 1:E:270:GLU:HG3  | 2.06                     | 0.56              |
| 1:F:146:VAL:HG22 | 1:F:147:ASP:H    | 1.70                     | 0.56              |
| 1:G:125:ILE:CD1  | 1:G:517:ARG:HG2  | 2.33                     | 0.56              |
| 1:D:423:ASP:OD1  | 1:D:427:LYS:HE2  | 2.06                     | 0.55              |
| 1:E:372:VAL:HG22 | 1:E:373:THR:H    | 1.70                     | 0.55              |
| 1:E:450:THR:O    | 1:E:454:ASN:ND2  | 2.38                     | 0.55              |
| 1:G:315:ARG:HG3  | 1:G:315:ARG:NH1  | 2.20                     | 0.55              |
| 1:C:315:ARG:HG3  | 1:C:315:ARG:NH1  | 2.21                     | 0.55              |
| 1:D:501:LYS:HA   | 1:D:501:LYS:HE3  | 1.88                     | 0.55              |
| 1:F:348:GLU:HB3  | 1:F:365:GLY:HA3  | 1.88                     | 0.55              |
| 1:F:421:ARG:HH11 | 1:F:421:ARG:CB   | 2.11                     | 0.55              |
| 1:G:166:ASN:HA   | 1:H:517:ARG:NH1  | 2.19                     | 0.55              |
| 1:G:380:THR:HG22 | 1:G:383:VAL:CG2  | 2.26                     | 0.55              |
| 1:H:54:ASP:CB    | 1:H:58:ASP:HB3   | 2.33                     | 0.55              |
| 1:H:473:ARG:HB2  | 1:H:477:ILE:HG13 | 1.87                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:204:LYS:HD2  | 1:B:384:ILE:HG22 | 1.87                     | 0.55              |
| 1:C:233:ARG:HH12 | 1:C:349:VAL:HG11 | 1.71                     | 0.55              |
| 1:G:208:GLU:HB3  | 1:G:212:GLU:CG   | 2.36                     | 0.55              |
| 1:A:211:GLU:OE1  | 1:A:211:GLU:HA   | 2.06                     | 0.55              |
| 1:E:197:LEU:HD22 | 1:E:395:VAL:CG1  | 2.36                     | 0.55              |
| 1:G:204:LYS:HB3  | 1:G:384:ILE:CG2  | 2.36                     | 0.55              |
| 1:A:209:GLY:C    | 1:A:211:GLU:N    | 2.60                     | 0.55              |
| 1:E:123:ILE:HG21 | 1:E:432:LYS:HB3  | 1.89                     | 0.55              |
| 1:E:400:ASP:O    | 1:E:404:ASP:HB2  | 2.07                     | 0.55              |
| 1:E:409:PRO:HB3  | 1:E:490:LEU:CD1  | 2.36                     | 0.55              |
| 1:F:208:GLU:HB3  | 1:F:212:GLU:CG   | 2.37                     | 0.55              |
| 1:G:30:LEU:O     | 1:G:34:ILE:HG13  | 2.07                     | 0.55              |
| 1:G:401:VAL:O    | 1:G:405:GLY:N    | 2.37                     | 0.55              |
| 1:D:483:GLU:HG3  | 1:D:485:LYS:NZ   | 2.22                     | 0.55              |
| 1:E:260:THR:H    | 1:E:264:GLN:HE22 | 1.53                     | 0.55              |
| 1:F:60:VAL:HG21  | 1:F:71:LYS:HE2   | 1.89                     | 0.55              |
| 1:G:443:ALA:O    | 1:G:446:ILE:HG13 | 2.06                     | 0.55              |
| 1:B:463:LEU:O    | 1:B:467:ILE:HG13 | 2.07                     | 0.55              |
| 1:C:423:ASP:OD1  | 1:C:427:LYS:HE2  | 2.07                     | 0.55              |
| 1:D:250:LYS:NZ   | 1:E:253:THR:HA   | 2.22                     | 0.55              |
| 1:D:293:VAL:CG2  | 1:D:297:ILE:HD11 | 2.36                     | 0.55              |
| 1:D:394:ALA:O    | 1:D:398:VAL:HG23 | 2.07                     | 0.55              |
| 1:E:412:GLY:HA2  | 1:E:415:GLU:OE2  | 2.06                     | 0.55              |
| 1:G:269:LEU:HD12 | 1:H:251:THR:CG2  | 2.37                     | 0.55              |
| 1:H:140:ASP:OD1  | 1:H:502:LYS:HD2  | 2.07                     | 0.55              |
| 1:H:210:VAL:HA   | 1:H:377:ARG:O    | 2.07                     | 0.55              |
| 1:B:241:LEU:HD22 | 1:B:330:ALA:HB3  | 1.88                     | 0.55              |
| 1:C:16:THR:HG23  | 1:C:523:ALA:O    | 2.06                     | 0.55              |
| 1:F:204:LYS:HB3  | 1:F:384:ILE:CG2  | 2.37                     | 0.55              |
| 1:F:276:LEU:HD23 | 1:F:300:LEU:CB   | 2.36                     | 0.55              |
| 1:G:35:ILE:HG13  | 1:G:79:ALA:HB1   | 1.89                     | 0.55              |
| 1:G:128:TYR:CE2  | 1:G:440:PHE:HB2  | 2.42                     | 0.55              |
| 1:A:205:LYS:O    | 1:A:377:ARG:NH1  | 2.40                     | 0.55              |
| 1:D:392:GLU:O    | 1:D:396:LYS:HE3  | 2.07                     | 0.55              |
| 1:E:142:ILE:HB   | 1:E:475:LEU:CD2  | 2.37                     | 0.55              |
| 1:E:215:LEU:HD11 | 1:E:372:VAL:HG21 | 1.89                     | 0.55              |
| 1:A:209:GLY:C    | 1:A:211:GLU:H    | 2.10                     | 0.54              |
| 1:C:29:ILE:O     | 1:C:33:ARG:HG3   | 2.06                     | 0.54              |
| 1:C:136:GLN:NE2  | 1:C:136:GLN:HA   | 2.22                     | 0.54              |
| 1:G:125:ILE:HG23 | 1:G:513:ILE:CG2  | 2.37                     | 0.54              |
| 1:H:215:LEU:HD11 | 1:H:372:VAL:CG2  | 2.37                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:286:THR:HG21 | 1:A:339:LEU:HG   | 1.90                     | 0.54              |
| 1:D:350:VAL:HG13 | 1:D:363:VAL:HG22 | 1.89                     | 0.54              |
| 1:F:196:ASP:OD1  | 1:F:198:ASP:HB2  | 2.06                     | 0.54              |
| 1:H:11:ILE:HG23  | 1:H:12:LEU:H     | 1.72                     | 0.54              |
| 1:B:258:ASN:HB3  | 1:C:258:ASN:HD21 | 1.72                     | 0.54              |
| 1:C:227:HIS:HB3  | 1:C:230:MET:HG3  | 1.89                     | 0.54              |
| 1:D:238:LYS:HD2  | 1:D:287:GLY:O    | 2.08                     | 0.54              |
| 1:D:248:VAL:HG11 | 1:D:272:GLU:OE2  | 2.07                     | 0.54              |
| 1:D:466:VAL:HG21 | 1:D:479:ILE:HG12 | 1.89                     | 0.54              |
| 1:D:488:ASP:O    | 1:D:492:LYS:HG2  | 2.07                     | 0.54              |
| 1:F:461:GLU:HG2  | 1:F:465:LYS:NZ   | 2.22                     | 0.54              |
| 1:A:235:GLU:O    | 1:A:236:ASN:C    | 2.45                     | 0.54              |
| 1:A:417:GLU:OE2  | 1:A:470:HIS:NE2  | 2.34                     | 0.54              |
| 1:B:209:GLY:O    | 1:B:212:GLU:HG2  | 2.07                     | 0.54              |
| 1:D:380:THR:HG23 | 1:D:383:VAL:H    | 1.72                     | 0.54              |
| 1:G:217:ARG:HA   | 1:G:372:VAL:HG23 | 1.89                     | 0.54              |
| 1:G:370:LYS:HE2  | 1:G:370:LYS:CA   | 2.35                     | 0.54              |
| 1:A:260:THR:N    | 1:A:264:GLN:HE21 | 1.97                     | 0.54              |
| 1:D:166:ASN:HA   | 1:E:517:ARG:NH1  | 2.23                     | 0.54              |
| 1:E:239:ILE:HD13 | 1:E:328:THR:HG21 | 1.90                     | 0.54              |
| 1:E:488:ASP:O    | 1:E:492:LYS:HG2  | 2.07                     | 0.54              |
| 1:E:503:GLN:HA   | 1:E:503:GLN:NE2  | 2.23                     | 0.54              |
| 1:F:26:ARG:CB    | 1:F:26:ARG:HH11  | 2.20                     | 0.54              |
| 1:H:138:ILE:O    | 1:H:142:ILE:HG12 | 2.08                     | 0.54              |
| 1:D:108:LEU:HD11 | 1:D:515:ILE:HD12 | 1.89                     | 0.54              |
| 1:E:42:THR:HG22  | 1:E:48:MET:O     | 2.08                     | 0.54              |
| 1:H:206:ALA:CA   | 1:H:384:ILE:HD11 | 2.36                     | 0.54              |
| 1:B:445:LYS:C    | 1:B:448:PRO:HD2  | 2.28                     | 0.54              |
| 1:E:30:LEU:O     | 1:E:34:ILE:HG13  | 2.07                     | 0.54              |
| 1:G:94:GLY:CA    | 1:G:396:LYS:HD2  | 2.38                     | 0.54              |
| 1:A:233:ARG:HH12 | 1:A:349:VAL:HG11 | 1.72                     | 0.54              |
| 1:E:205:LYS:O    | 1:E:377:ARG:NH1  | 2.41                     | 0.54              |
| 1:G:142:ILE:HB   | 1:G:475:LEU:CD2  | 2.36                     | 0.54              |
| 1:G:430:GLY:CA   | 1:G:434:ALA:HB2  | 2.37                     | 0.54              |
| 1:A:462:MET:HE1  | 1:A:486:PRO:HD3  | 1.89                     | 0.54              |
| 1:B:117:GLN:O    | 1:B:118:ASN:HB2  | 2.06                     | 0.54              |
| 1:D:54:ASP:OD1   | 1:D:58:ASP:HB3   | 2.06                     | 0.54              |
| 1:E:230:MET:HE2  | 1:E:312:ALA:H    | 1.72                     | 0.54              |
| 1:F:380:THR:HG22 | 1:F:383:VAL:CG2  | 2.30                     | 0.54              |
| 1:H:143:ALA:HB3  | 1:H:145:ARG:NH1  | 2.22                     | 0.54              |
| 1:D:218:GLY:HA3  | 1:D:363:VAL:O    | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:355:LEU:HD11 | 1:D:377:ARG:NH2  | 2.23                     | 0.54              |
| 1:D:76:HIS:HB2   | 1:E:11:ILE:HA    | 1.91                     | 0.53              |
| 1:D:134:LYS:O    | 1:D:138:ILE:HG13 | 2.08                     | 0.53              |
| 1:E:372:VAL:HG22 | 1:E:373:THR:N    | 2.23                     | 0.53              |
| 1:E:446:ILE:HG22 | 1:E:450:THR:HG23 | 1.91                     | 0.53              |
| 1:H:348:GLU:HB3  | 1:H:365:GLY:HA3  | 1.91                     | 0.53              |
| 1:B:189:LYS:HD2  | 1:B:189:LYS:C    | 2.28                     | 0.53              |
| 1:C:136:GLN:HA   | 1:C:136:GLN:HE21 | 1.71                     | 0.53              |
| 1:E:258:ASN:HB3  | 1:F:258:ASN:ND2  | 2.23                     | 0.53              |
| 1:G:272:GLU:HA   | 1:G:275:MET:HE2  | 1.90                     | 0.53              |
| 1:H:146:VAL:HG22 | 1:H:147:ASP:N    | 2.22                     | 0.53              |
| 1:A:33:ARG:NH1   | 1:A:109:ARG:HG3  | 2.23                     | 0.53              |
| 1:D:35:ILE:HD11  | 1:D:74:LEU:CD2   | 2.37                     | 0.53              |
| 1:E:335:ASN:HD21 | 1:E:337:LYS:HB2  | 1.74                     | 0.53              |
| 1:F:217:ARG:HA   | 1:F:372:VAL:CG2  | 2.36                     | 0.53              |
| 1:F:317:LYS:O    | 1:F:320:ASP:N    | 2.41                     | 0.53              |
| 1:G:18:ARG:HG3   | 1:G:522:ILE:HG12 | 1.90                     | 0.53              |
| 1:G:146:VAL:HG22 | 1:G:147:ASP:N    | 2.24                     | 0.53              |
| 1:H:426:ALA:HB1  | 1:H:438:GLU:HG3  | 1.91                     | 0.53              |
| 1:A:94:GLY:CA    | 1:A:396:LYS:HD2  | 2.39                     | 0.53              |
| 1:A:501:LYS:HA   | 1:A:501:LYS:HE3  | 1.88                     | 0.53              |
| 1:B:216:VAL:O    | 1:B:372:VAL:CG2  | 2.56                     | 0.53              |
| 1:C:31:ALA:CB    | 1:C:76:HIS:CD2   | 2.91                     | 0.53              |
| 1:E:167:ALA:C    | 1:E:169:SER:H    | 2.11                     | 0.53              |
| 1:E:233:ARG:HH12 | 1:E:349:VAL:HG13 | 1.72                     | 0.53              |
| 1:F:11:ILE:HD13  | 1:F:11:ILE:C     | 2.29                     | 0.53              |
| 1:F:12:LEU:HD23  | 1:F:13:PRO:HD2   | 1.90                     | 0.53              |
| 1:F:138:ILE:HD13 | 1:F:421:ARG:HG2  | 1.91                     | 0.53              |
| 1:G:11:ILE:CG2   | 1:G:12:LEU:H     | 2.21                     | 0.53              |
| 1:H:151:GLU:O    | 1:H:155:LEU:HD23 | 2.08                     | 0.53              |
| 1:D:391:LEU:O    | 1:D:395:VAL:HG23 | 2.08                     | 0.53              |
| 1:E:50:LYS:HD2   | 1:E:68:ILE:HD13  | 1.90                     | 0.53              |
| 1:E:146:VAL:HG22 | 1:E:147:ASP:N    | 2.21                     | 0.53              |
| 1:F:38:THR:O     | 1:F:50:LYS:CE    | 2.57                     | 0.53              |
| 1:F:147:ASP:O    | 1:F:149:ASP:N    | 2.41                     | 0.53              |
| 1:F:418:LEU:O    | 1:F:422:LEU:HB2  | 2.09                     | 0.53              |
| 1:G:409:PRO:HB2  | 1:G:489:MET:HB2  | 1.91                     | 0.53              |
| 1:A:315:ARG:HG3  | 1:A:315:ARG:NH1  | 2.24                     | 0.53              |
| 1:A:466:VAL:HG22 | 1:A:486:PRO:HG3  | 1.91                     | 0.53              |
| 1:A:473:ARG:HB2  | 1:A:477:ILE:HG13 | 1.90                     | 0.53              |
| 1:B:82:MET:CE    | 1:B:101:VAL:HG13 | 2.39                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:232:LYS:HD2  | 1:H:352:GLU:OE2  | 2.09                     | 0.53              |
| 1:H:315:ARG:HH11 | 1:H:315:ARG:HG3  | 1.73                     | 0.53              |
| 1:C:259:ILE:HD12 | 1:C:259:ILE:N    | 2.24                     | 0.53              |
| 1:C:313:VAL:HG21 | 1:C:361:ILE:CD1  | 2.38                     | 0.53              |
| 1:C:354:LYS:HA   | 1:C:358:GLU:O    | 2.09                     | 0.53              |
| 1:D:146:VAL:HG22 | 1:D:147:ASP:N    | 2.23                     | 0.53              |
| 1:D:425:TYR:O    | 1:D:429:VAL:HG23 | 2.08                     | 0.53              |
| 1:E:460:VAL:O    | 1:E:464:VAL:HG23 | 2.07                     | 0.53              |
| 1:F:146:VAL:O    | 1:F:148:PRO:HD3  | 2.09                     | 0.53              |
| 1:G:408:LEU:HD12 | 1:G:498:LEU:HA   | 1.89                     | 0.53              |
| 1:G:417:GLU:OE2  | 1:G:470:HIS:NE2  | 2.42                     | 0.53              |
| 1:B:106:GLU:HG2  | 1:B:446:ILE:HG13 | 1.91                     | 0.53              |
| 1:E:184:GLN:NE2  | 1:E:217:ARG:NH2  | 2.57                     | 0.53              |
| 1:E:208:GLU:HB3  | 1:E:212:GLU:CG   | 2.39                     | 0.53              |
| 1:F:353:ARG:HD2  | 1:F:362:PHE:CD1  | 2.44                     | 0.53              |
| 1:H:10:VAL:HG22  | 1:H:11:ILE:N     | 2.15                     | 0.53              |
| 1:A:155:LEU:HA   | 1:A:179:VAL:HG21 | 1.91                     | 0.53              |
| 1:B:354:LYS:HA   | 1:B:358:GLU:O    | 2.08                     | 0.53              |
| 1:E:469:GLU:CB   | 1:E:477:ILE:HG21 | 2.38                     | 0.53              |
| 1:F:154:LEU:HG   | 1:F:398:VAL:HG13 | 1.89                     | 0.53              |
| 1:H:227:HIS:HB3  | 1:H:230:MET:CG   | 2.37                     | 0.53              |
| 1:A:22:ARG:CG    | 1:A:23:ASP:N     | 2.72                     | 0.52              |
| 1:A:189:LYS:HD2  | 1:A:189:LYS:C    | 2.28                     | 0.52              |
| 1:B:146:VAL:HG22 | 1:B:147:ASP:N    | 2.24                     | 0.52              |
| 1:D:463:LEU:O    | 1:D:467:ILE:HG13 | 2.09                     | 0.52              |
| 1:E:353:ARG:NH2  | 1:E:364:GLU:OE2  | 2.40                     | 0.52              |
| 1:E:421:ARG:HH11 | 1:E:421:ARG:CB   | 2.09                     | 0.52              |
| 1:A:221:ILE:CD1  | 1:A:324:LEU:HD11 | 2.39                     | 0.52              |
| 1:C:217:ARG:HA   | 1:C:372:VAL:HG23 | 1.90                     | 0.52              |
| 1:G:208:GLU:HG3  | 1:G:377:ARG:HH21 | 1.74                     | 0.52              |
| 1:H:245:ALA:HB1  | 1:H:247:GLU:OE1  | 2.09                     | 0.52              |
| 1:A:227:HIS:HB3  | 1:A:230:MET:HG3  | 1.90                     | 0.52              |
| 1:B:388:GLU:O    | 1:B:392:GLU:HG3  | 2.08                     | 0.52              |
| 1:D:227:HIS:HB3  | 1:D:230:MET:SD   | 2.49                     | 0.52              |
| 1:E:423:ASP:O    | 1:E:426:ALA:HB3  | 2.09                     | 0.52              |
| 1:F:370:LYS:HA   | 1:F:370:LYS:CE   | 2.36                     | 0.52              |
| 1:G:410:ALA:HB3  | 1:G:494:ILE:HG22 | 1.90                     | 0.52              |
| 1:A:184:GLN:NE2  | 1:A:184:GLN:HA   | 2.24                     | 0.52              |
| 1:A:465:LYS:O    | 1:A:468:SER:HB3  | 2.09                     | 0.52              |
| 1:B:22:ARG:CG    | 1:B:23:ASP:N     | 2.71                     | 0.52              |
| 1:B:425:TYR:O    | 1:B:429:VAL:HG23 | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:388:GLU:O    | 1:C:392:GLU:HG3  | 2.09                     | 0.52              |
| 1:D:286:THR:HG21 | 1:D:339:LEU:HG   | 1.92                     | 0.52              |
| 1:F:205:LYS:O    | 1:F:377:ARG:NH1  | 2.42                     | 0.52              |
| 1:H:372:VAL:HG22 | 1:H:373:THR:H    | 1.74                     | 0.52              |
| 1:A:217:ARG:HA   | 1:A:372:VAL:HG23 | 1.92                     | 0.52              |
| 1:B:25:GLN:O     | 1:B:29:ILE:HG13  | 2.10                     | 0.52              |
| 1:B:315:ARG:HG3  | 1:B:315:ARG:NH1  | 2.16                     | 0.52              |
| 1:C:506:LYS:O    | 1:C:510:GLU:CG   | 2.57                     | 0.52              |
| 1:D:31:ALA:CB    | 1:D:76:HIS:CD2   | 2.93                     | 0.52              |
| 1:H:38:THR:O     | 1:H:50:LYS:CE    | 2.57                     | 0.52              |
| 1:A:195:VAL:HB   | 1:A:399:LYS:HG3  | 1.89                     | 0.52              |
| 1:C:183:LYS:HG2  | 1:C:402:MET:HE3  | 1.92                     | 0.52              |
| 1:C:335:ASN:OD1  | 1:C:337:LYS:HB2  | 2.09                     | 0.52              |
| 1:D:293:VAL:HG21 | 1:D:297:ILE:HD11 | 1.92                     | 0.52              |
| 1:D:342:GLU:OE2  | 1:D:342:GLU:N    | 2.40                     | 0.52              |
| 1:E:286:THR:HA   | 1:E:341:PRO:HG3  | 1.91                     | 0.52              |
| 1:G:462:MET:O    | 1:G:466:VAL:HG23 | 2.10                     | 0.52              |
| 1:H:76:HIS:CD2   | 1:H:78:ALA:H     | 2.28                     | 0.52              |
| 1:H:170:HIS:CE1  | 1:H:210:VAL:HB   | 2.44                     | 0.52              |
| 1:H:460:VAL:O    | 1:H:464:VAL:HG23 | 2.09                     | 0.52              |
| 1:B:81:MET:HE3   | 1:B:514:MET:SD   | 2.50                     | 0.52              |
| 1:B:496:GLU:OE1  | 1:B:501:LYS:NZ   | 2.31                     | 0.52              |
| 1:C:230:MET:HE1  | 1:C:312:ALA:HB3  | 1.91                     | 0.52              |
| 1:C:368:ASN:ND2  | 1:C:370:LYS:HE3  | 2.24                     | 0.52              |
| 1:C:394:ALA:O    | 1:C:398:VAL:HG23 | 2.09                     | 0.52              |
| 1:D:209:GLY:C    | 1:D:211:GLU:H    | 2.11                     | 0.52              |
| 1:E:22:ARG:CG    | 1:E:23:ASP:N     | 2.72                     | 0.52              |
| 1:E:233:ARG:NH1  | 1:E:349:VAL:HG13 | 2.24                     | 0.52              |
| 1:E:260:THR:H    | 1:E:264:GLN:HE21 | 1.56                     | 0.52              |
| 1:F:380:THR:CG2  | 1:F:383:VAL:H    | 2.20                     | 0.52              |
| 1:C:445:LYS:C    | 1:C:448:PRO:HD2  | 2.30                     | 0.52              |
| 1:D:147:ASP:O    | 1:D:149:ASP:N    | 2.43                     | 0.52              |
| 1:E:31:ALA:HA    | 1:E:34:ILE:HD12  | 1.91                     | 0.52              |
| 1:G:227:HIS:HE2  | 1:H:334:THR:HB   | 1.75                     | 0.52              |
| 1:G:524:ALA:O    | 1:G:525:LYS:HD2  | 2.09                     | 0.52              |
| 1:A:182:VAL:HG22 | 1:A:395:VAL:HG13 | 1.92                     | 0.52              |
| 1:A:461:GLU:HG2  | 1:A:465:LYS:NZ   | 2.25                     | 0.52              |
| 1:C:13:PRO:O     | 1:C:16:THR:HB    | 2.10                     | 0.52              |
| 1:D:424:GLU:O    | 1:D:428:GLN:HG2  | 2.10                     | 0.52              |
| 1:F:29:ILE:HG23  | 1:F:108:LEU:HB3  | 1.92                     | 0.52              |
| 1:G:380:THR:CG2  | 1:G:383:VAL:H    | 2.19                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:423:ASP:OD1  | 1:A:427:LYS:HE2  | 2.10                     | 0.52              |
| 1:B:22:ARG:HG3   | 1:B:23:ASP:N     | 2.24                     | 0.52              |
| 1:B:383:VAL:O    | 1:B:387:VAL:HG23 | 2.09                     | 0.52              |
| 1:C:126:LYS:NZ   | 1:C:126:LYS:HB3  | 2.25                     | 0.52              |
| 1:F:151:GLU:O    | 1:F:155:LEU:HD23 | 2.10                     | 0.52              |
| 1:G:45:PRO:HA    | 1:G:164:GLY:HA2  | 1.92                     | 0.52              |
| 1:H:483:GLU:HG3  | 1:H:485:LYS:HZ3  | 1.75                     | 0.52              |
| 1:H:483:GLU:OE1  | 1:H:483:GLU:HA   | 2.09                     | 0.52              |
| 1:D:59:ILE:HD12  | 1:D:59:ILE:N     | 2.25                     | 0.51              |
| 1:E:330:ALA:HB2  | 1:E:345:GLY:HA3  | 1.92                     | 0.51              |
| 1:E:470:HIS:CE1  | 1:E:475:LEU:HA   | 2.45                     | 0.51              |
| 1:H:17:GLN:NE2   | 1:H:17:GLN:H     | 2.07                     | 0.51              |
| 1:H:92:GLU:O     | 1:H:499:ARG:HD3  | 2.11                     | 0.51              |
| 1:H:217:ARG:HB3  | 1:H:217:ARG:HH11 | 1.75                     | 0.51              |
| 1:H:293:VAL:HG21 | 1:H:297:ILE:HD11 | 1.92                     | 0.51              |
| 1:B:81:MET:CE    | 1:B:514:MET:SD   | 2.98                     | 0.51              |
| 1:B:184:GLN:HE22 | 1:B:217:ARG:HH21 | 1.54                     | 0.51              |
| 1:C:217:ARG:HB3  | 1:C:217:ARG:HH11 | 1.75                     | 0.51              |
| 1:D:370:LYS:HE2  | 1:D:370:LYS:CA   | 2.39                     | 0.51              |
| 1:E:327:ALA:O    | 1:E:366:CYS:HB3  | 2.10                     | 0.51              |
| 1:F:458:ASP:O    | 1:F:459:THR:C    | 2.48                     | 0.51              |
| 1:A:73:ASP:O     | 1:B:13:PRO:HD3   | 2.10                     | 0.51              |
| 1:A:106:GLU:HG2  | 1:A:446:ILE:CG1  | 2.40                     | 0.51              |
| 1:A:445:LYS:O    | 1:A:448:PRO:HD2  | 2.10                     | 0.51              |
| 1:B:257:ILE:HG22 | 1:B:259:ILE:HD12 | 1.93                     | 0.51              |
| 1:D:94:GLY:HA2   | 1:D:396:LYS:HD2  | 1.91                     | 0.51              |
| 1:E:59:ILE:HD12  | 1:E:59:ILE:H     | 1.73                     | 0.51              |
| 1:F:126:LYS:HB3  | 1:F:126:LYS:HZ2  | 1.74                     | 0.51              |
| 1:F:201:LYS:HB2  | 1:F:323:LYS:HE3  | 1.92                     | 0.51              |
| 1:A:170:HIS:HD2  | 1:A:211:GLU:OE1  | 1.93                     | 0.51              |
| 1:B:154:LEU:HG   | 1:B:398:VAL:HG13 | 1.92                     | 0.51              |
| 1:D:142:ILE:HB   | 1:D:475:LEU:CD2  | 2.41                     | 0.51              |
| 1:E:33:ARG:NH1   | 1:E:109:ARG:HG3  | 2.26                     | 0.51              |
| 1:E:94:GLY:HA2   | 1:E:396:LYS:HD2  | 1.93                     | 0.51              |
| 1:E:147:ASP:O    | 1:E:149:ASP:N    | 2.43                     | 0.51              |
| 1:G:184:GLN:NE2  | 1:G:217:ARG:NH2  | 2.59                     | 0.51              |
| 1:G:250:LYS:NZ   | 1:H:253:THR:HA   | 2.26                     | 0.51              |
| 1:D:75:GLN:HB2   | 1:E:10:VAL:C     | 2.31                     | 0.51              |
| 1:E:417:GLU:OE1  | 1:E:421:ARG:NH1  | 2.43                     | 0.51              |
| 1:H:136:GLN:HA   | 1:H:136:GLN:HE21 | 1.75                     | 0.51              |
| 1:H:335:ASN:OD1  | 1:H:337:LYS:HB2  | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:449:LYS:HE3  | 1:F:459:THR:CG2  | 2.40                     | 0.51              |
| 1:H:239:ILE:HD11 | 1:H:347:ALA:CB   | 2.39                     | 0.51              |
| 1:H:465:LYS:O    | 1:H:468:SER:HB3  | 2.09                     | 0.51              |
| 1:A:460:VAL:O    | 1:A:464:VAL:HG23 | 2.11                     | 0.51              |
| 1:B:217:ARG:HA   | 1:B:372:VAL:HG23 | 1.92                     | 0.51              |
| 1:B:409:PRO:HB3  | 1:B:490:LEU:HD13 | 1.93                     | 0.51              |
| 1:C:370:LYS:HE2  | 1:C:370:LYS:CA   | 2.41                     | 0.51              |
| 1:C:392:GLU:O    | 1:C:396:LYS:HE3  | 2.11                     | 0.51              |
| 1:D:188:LYS:HD3  | 1:D:193:TYR:CE1  | 2.45                     | 0.51              |
| 1:E:446:ILE:HD12 | 1:E:446:ILE:H    | 1.76                     | 0.51              |
| 1:G:136:GLN:HA   | 1:G:136:GLN:NE2  | 2.26                     | 0.51              |
| 1:G:210:VAL:HA   | 1:G:377:ARG:O    | 2.11                     | 0.51              |
| 1:G:313:VAL:HG21 | 1:G:361:ILE:HD13 | 1.92                     | 0.51              |
| 1:H:429:VAL:HG21 | 1:H:437:ILE:CD1  | 2.41                     | 0.51              |
| 1:B:348:GLU:CB   | 1:B:365:GLY:HA3  | 2.40                     | 0.51              |
| 1:B:372:VAL:HG22 | 1:B:373:THR:N    | 2.26                     | 0.51              |
| 1:C:22:ARG:CG    | 1:C:23:ASP:N     | 2.74                     | 0.51              |
| 1:C:145:ARG:HG2  | 1:C:145:ARG:HH11 | 1.76                     | 0.51              |
| 1:C:293:VAL:HG21 | 1:C:297:ILE:HD11 | 1.92                     | 0.51              |
| 1:H:138:ILE:HD13 | 1:H:421:ARG:HG2  | 1.92                     | 0.51              |
| 1:B:196:ASP:OD1  | 1:B:198:ASP:HB2  | 2.11                     | 0.51              |
| 1:D:397:VAL:O    | 1:D:401:VAL:HG23 | 2.11                     | 0.51              |
| 1:G:355:LEU:O    | 1:G:356:ALA:HB3  | 2.11                     | 0.51              |
| 1:B:258:ASN:HB3  | 1:C:258:ASN:ND2  | 2.26                     | 0.51              |
| 1:C:430:GLY:CA   | 1:C:434:ALA:HB2  | 2.41                     | 0.51              |
| 1:D:292:PHE:CD1  | 1:D:324:LEU:HD13 | 2.45                     | 0.51              |
| 1:E:51:MET:CE    | 1:F:77:PRO:HB2   | 2.41                     | 0.51              |
| 1:G:59:ILE:HD12  | 1:G:59:ILE:H     | 1.76                     | 0.51              |
| 1:A:146:VAL:HG22 | 1:A:147:ASP:H    | 1.75                     | 0.50              |
| 1:B:412:GLY:HA2  | 1:B:415:GLU:CG   | 2.41                     | 0.50              |
| 1:D:498:LEU:O    | 1:D:498:LEU:HD22 | 2.11                     | 0.50              |
| 1:F:266:MET:O    | 1:F:270:GLU:HG3  | 2.11                     | 0.50              |
| 1:F:498:LEU:O    | 1:F:498:LEU:HD22 | 2.11                     | 0.50              |
| 1:B:269:LEU:HD12 | 1:C:251:THR:HG23 | 1.91                     | 0.50              |
| 1:C:215:LEU:HD11 | 1:C:372:VAL:CG2  | 2.40                     | 0.50              |
| 1:D:72:ILE:HG22  | 1:D:73:ASP:N     | 2.26                     | 0.50              |
| 1:E:445:LYS:O    | 1:E:448:PRO:HD2  | 2.11                     | 0.50              |
| 1:F:297:ILE:HD12 | 1:F:314:ARG:HB3  | 1.92                     | 0.50              |
| 1:G:216:VAL:O    | 1:G:218:GLY:N    | 2.43                     | 0.50              |
| 1:G:259:ILE:HG23 | 1:G:264:GLN:HB2  | 1.93                     | 0.50              |
| 1:C:126:LYS:O    | 1:C:130:LEU:HG   | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:155:LEU:HD22 | 1:D:179:VAL:HG21 | 1.93                     | 0.50              |
| 1:D:210:VAL:O    | 1:D:210:VAL:HG12 | 2.12                     | 0.50              |
| 1:D:271:GLN:O    | 1:D:275:MET:HG3  | 2.10                     | 0.50              |
| 1:E:54:ASP:OD1   | 1:E:58:ASP:HB3   | 2.11                     | 0.50              |
| 1:G:188:LYS:HD3  | 1:G:193:TYR:CE1  | 2.46                     | 0.50              |
| 1:A:77:PRO:CG    | 1:H:53:VAL:HG21  | 2.41                     | 0.50              |
| 1:B:233:ARG:HH11 | 1:B:233:ARG:HG3  | 1.77                     | 0.50              |
| 1:B:461:GLU:HG2  | 1:B:465:LYS:NZ   | 2.25                     | 0.50              |
| 1:C:227:HIS:HD1  | 1:C:229:ARG:H    | 1.58                     | 0.50              |
| 1:E:106:GLU:HG2  | 1:E:446:ILE:HG13 | 1.93                     | 0.50              |
| 1:E:204:LYS:HB3  | 1:E:384:ILE:CG2  | 2.40                     | 0.50              |
| 1:E:315:ARG:HH11 | 1:E:315:ARG:HG3  | 1.76                     | 0.50              |
| 1:F:117:GLN:O    | 1:F:118:ASN:HB2  | 2.10                     | 0.50              |
| 1:G:17:GLN:NE2   | 1:G:17:GLN:N     | 2.57                     | 0.50              |
| 1:G:117:GLN:O    | 1:G:118:ASN:HB2  | 2.10                     | 0.50              |
| 1:G:189:LYS:HD2  | 1:G:189:LYS:C    | 2.32                     | 0.50              |
| 1:A:271:GLN:O    | 1:A:275:MET:HG3  | 2.11                     | 0.50              |
| 1:A:418:LEU:O    | 1:A:422:LEU:HB2  | 2.12                     | 0.50              |
| 1:C:215:LEU:HD11 | 1:C:372:VAL:HG21 | 1.93                     | 0.50              |
| 1:D:421:ARG:HB2  | 1:D:421:ARG:NH1  | 2.20                     | 0.50              |
| 1:E:82:MET:CE    | 1:E:101:VAL:HG13 | 2.42                     | 0.50              |
| 1:E:209:GLY:C    | 1:E:211:GLU:H    | 2.15                     | 0.50              |
| 1:E:221:ILE:CD1  | 1:E:324:LEU:HD11 | 2.41                     | 0.50              |
| 1:F:235:GLU:O    | 1:F:236:ASN:C    | 2.50                     | 0.50              |
| 1:G:239:ILE:H    | 1:G:239:ILE:HD12 | 1.75                     | 0.50              |
| 1:H:415:GLU:HG3  | 1:H:447:ILE:HB   | 1.94                     | 0.50              |
| 1:A:182:VAL:CG2  | 1:A:395:VAL:HG13 | 2.42                     | 0.50              |
| 1:D:51:MET:HB2   | 1:E:518:ILE:HD13 | 1.94                     | 0.50              |
| 1:D:258:ASN:CB   | 1:E:258:ASN:HD21 | 2.14                     | 0.50              |
| 1:D:450:THR:O    | 1:D:454:ASN:ND2  | 2.44                     | 0.50              |
| 1:A:147:ASP:O    | 1:A:149:ASP:N    | 2.45                     | 0.50              |
| 1:B:146:VAL:HG22 | 1:B:147:ASP:H    | 1.77                     | 0.50              |
| 1:C:256:LYS:HE3  | 1:D:254:ASP:OD1  | 2.11                     | 0.50              |
| 1:D:303:HIS:NE2  | 1:E:335:ASN:HB3  | 2.26                     | 0.50              |
| 1:E:35:ILE:HD11  | 1:E:74:LEU:CD2   | 2.42                     | 0.50              |
| 1:E:92:GLU:O     | 1:E:499:ARG:HD3  | 2.12                     | 0.50              |
| 1:E:462:MET:HE3  | 1:E:465:LYS:HD2  | 1.94                     | 0.50              |
| 1:G:138:ILE:O    | 1:G:142:ILE:HG23 | 2.12                     | 0.50              |
| 1:G:175:ALA:O    | 1:G:179:VAL:HG23 | 2.11                     | 0.50              |
| 1:H:29:ILE:O     | 1:H:33:ARG:HG3   | 2.11                     | 0.50              |
| 1:A:218:GLY:HA3  | 1:A:363:VAL:O    | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:125:ILE:HD13 | 1:B:517:ARG:HG2  | 1.93                     | 0.50              |
| 1:C:134:LYS:O    | 1:C:138:ILE:HG13 | 2.12                     | 0.50              |
| 1:D:89:GLN:OE1   | 1:D:503:GLN:HG3  | 2.11                     | 0.50              |
| 1:D:272:GLU:HA   | 1:D:275:MET:HE3  | 1.92                     | 0.50              |
| 1:D:462:MET:O    | 1:D:466:VAL:HG23 | 2.12                     | 0.50              |
| 1:E:277:LYS:HB2  | 1:E:304:TYR:CE2  | 2.47                     | 0.50              |
| 1:G:10:VAL:CG1   | 1:G:11:ILE:H     | 2.13                     | 0.50              |
| 1:G:215:LEU:HD11 | 1:G:372:VAL:HG21 | 1.94                     | 0.50              |
| 1:H:138:ILE:CD1  | 1:H:421:ARG:HG2  | 2.42                     | 0.50              |
| 1:H:286:THR:HG21 | 1:H:339:LEU:HG   | 1.93                     | 0.50              |
| 1:E:126:LYS:NZ   | 1:E:126:LYS:HB3  | 2.27                     | 0.50              |
| 1:E:167:ALA:O    | 1:E:169:SER:N    | 2.45                     | 0.50              |
| 1:G:408:LEU:O    | 1:G:495:ILE:HB   | 2.12                     | 0.50              |
| 1:A:91:LYS:HB2   | 1:A:91:LYS:HZ2   | 1.77                     | 0.49              |
| 1:B:175:ALA:O    | 1:B:179:VAL:HG23 | 2.12                     | 0.49              |
| 1:B:225:VAL:HG23 | 1:B:352:GLU:OE1  | 2.12                     | 0.49              |
| 1:B:461:GLU:HG2  | 1:B:465:LYS:HZ2  | 1.77                     | 0.49              |
| 1:C:217:ARG:HB3  | 1:C:217:ARG:NH1  | 2.27                     | 0.49              |
| 1:E:106:GLU:HG2  | 1:E:446:ILE:HG12 | 1.93                     | 0.49              |
| 1:E:462:MET:CE   | 1:E:486:PRO:HD3  | 2.42                     | 0.49              |
| 1:H:244:GLU:OE1  | 1:H:336:VAL:HG22 | 2.12                     | 0.49              |
| 1:A:150:ASP:OD1  | 1:A:153:THR:HG23 | 2.12                     | 0.49              |
| 1:A:462:MET:HE3  | 1:A:462:MET:CA   | 2.41                     | 0.49              |
| 1:A:513:ILE:O    | 1:A:517:ARG:HG3  | 2.12                     | 0.49              |
| 1:B:120:HIS:CG   | 1:B:121:PRO:HD2  | 2.48                     | 0.49              |
| 1:B:259:ILE:HD12 | 1:B:259:ILE:N    | 2.27                     | 0.49              |
| 1:C:72:ILE:HG22  | 1:C:74:LEU:HD23  | 1.92                     | 0.49              |
| 1:C:188:LYS:HD3  | 1:C:193:TYR:CE1  | 2.46                     | 0.49              |
| 1:C:498:LEU:HD13 | 1:C:502:LYS:HD3  | 1.95                     | 0.49              |
| 1:D:393:ASP:O    | 1:D:397:VAL:HG22 | 2.12                     | 0.49              |
| 1:E:11:ILE:C     | 1:E:11:ILE:CD1   | 2.80                     | 0.49              |
| 1:E:11:ILE:HG23  | 1:E:12:LEU:H     | 1.77                     | 0.49              |
| 1:E:81:MET:HE3   | 1:E:514:MET:SD   | 2.51                     | 0.49              |
| 1:E:110:LYS:HE3  | 1:E:442:ASP:OD1  | 2.11                     | 0.49              |
| 1:E:394:ALA:O    | 1:E:397:VAL:HG22 | 2.12                     | 0.49              |
| 1:F:72:ILE:HG22  | 1:F:74:LEU:HD23  | 1.95                     | 0.49              |
| 1:A:123:ILE:HG21 | 1:A:432:LYS:HB2  | 1.95                     | 0.49              |
| 1:A:227:HIS:ND1  | 1:A:228:PRO:HD2  | 2.28                     | 0.49              |
| 1:C:75:GLN:HB2   | 1:D:11:ILE:C     | 2.32                     | 0.49              |
| 1:E:247:GLU:HA   | 1:E:276:LEU:HD11 | 1.94                     | 0.49              |
| 1:F:476:GLY:HA3  | 1:F:490:LEU:HD22 | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:239:ILE:HD11 | 1:H:347:ALA:HB3  | 1.93                     | 0.49              |
| 1:H:241:LEU:CD2  | 1:H:330:ALA:HB3  | 2.42                     | 0.49              |
| 1:H:245:ALA:HB1  | 1:H:247:GLU:HG2  | 1.95                     | 0.49              |
| 1:A:188:LYS:HB2  | 1:A:193:TYR:HA   | 1.94                     | 0.49              |
| 1:A:209:GLY:O    | 1:A:211:GLU:N    | 2.45                     | 0.49              |
| 1:A:251:THR:HG23 | 1:H:269:LEU:CD1  | 2.40                     | 0.49              |
| 1:C:35:ILE:HD12  | 1:C:69:LEU:CD2   | 2.43                     | 0.49              |
| 1:C:125:ILE:CD1  | 1:C:517:ARG:HG2  | 2.41                     | 0.49              |
| 1:C:432:LYS:O    | 1:C:435:LEU:HB2  | 2.11                     | 0.49              |
| 1:E:99:THR:HG23  | 1:E:447:ILE:HD12 | 1.95                     | 0.49              |
| 1:F:216:VAL:O    | 1:F:218:GLY:N    | 2.45                     | 0.49              |
| 1:F:462:MET:CE   | 1:F:465:LYS:HD2  | 2.42                     | 0.49              |
| 1:C:138:ILE:O    | 1:C:142:ILE:HG23 | 2.12                     | 0.49              |
| 1:C:293:VAL:CG2  | 1:C:297:ILE:HD11 | 2.42                     | 0.49              |
| 1:C:304:TYR:O    | 1:C:308:TYR:HD1  | 1.96                     | 0.49              |
| 1:D:12:LEU:HD23  | 1:D:13:PRO:HD2   | 1.93                     | 0.49              |
| 1:D:409:PRO:HA   | 1:D:495:ILE:HG22 | 1.93                     | 0.49              |
| 1:G:462:MET:CE   | 1:G:486:PRO:HD3  | 2.42                     | 0.49              |
| 1:G:506:LYS:O    | 1:G:510:GLU:CG   | 2.60                     | 0.49              |
| 1:H:146:VAL:HG22 | 1:H:147:ASP:H    | 1.76                     | 0.49              |
| 1:A:205:LYS:HE3  | 1:A:360:MET:SD   | 2.52                     | 0.49              |
| 1:D:136:GLN:HA   | 1:D:136:GLN:HE21 | 1.78                     | 0.49              |
| 1:E:72:ILE:HD11  | 1:F:522:ILE:CD1  | 2.37                     | 0.49              |
| 1:E:413:ALA:N    | 1:E:414:PRO:CD   | 2.76                     | 0.49              |
| 1:A:103:ILE:O    | 1:A:107:LEU:HB2  | 2.12                     | 0.49              |
| 1:A:208:GLU:HB3  | 1:A:212:GLU:CG   | 2.42                     | 0.49              |
| 1:C:146:VAL:HG22 | 1:C:147:ASP:H    | 1.78                     | 0.49              |
| 1:D:81:MET:HE3   | 1:D:514:MET:SD   | 2.53                     | 0.49              |
| 1:E:170:HIS:HD2  | 1:E:211:GLU:OE1  | 1.96                     | 0.49              |
| 1:F:38:THR:O     | 1:F:50:LYS:HE3   | 2.12                     | 0.49              |
| 1:C:197:LEU:HD22 | 1:C:395:VAL:CG1  | 2.42                     | 0.49              |
| 1:C:369:PRO:HB2  | 1:C:371:ALA:O    | 2.13                     | 0.49              |
| 1:D:136:GLN:HA   | 1:D:136:GLN:NE2  | 2.27                     | 0.49              |
| 1:E:248:VAL:HG11 | 1:E:272:GLU:OE2  | 2.12                     | 0.49              |
| 1:E:400:ASP:OD1  | 1:E:499:ARG:HD2  | 2.12                     | 0.49              |
| 1:G:126:LYS:HB3  | 1:G:126:LYS:HZ2  | 1.77                     | 0.49              |
| 1:G:458:ASP:OD1  | 1:G:461:GLU:HB2  | 2.13                     | 0.49              |
| 1:H:242:ILE:HD11 | 1:H:339:LEU:HD22 | 1.94                     | 0.49              |
| 1:A:123:ILE:HG21 | 1:A:432:LYS:CB   | 2.43                     | 0.49              |
| 1:A:272:GLU:HA   | 1:A:275:MET:CE   | 2.43                     | 0.49              |
| 1:B:73:ASP:O     | 1:C:13:PRO:HD3   | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:166:ASN:C    | 1:B:166:ASN:ND2  | 2.65                     | 0.49              |
| 1:C:179:VAL:O    | 1:C:183:LYS:HG3  | 2.13                     | 0.49              |
| 1:D:18:ARG:HG3   | 1:D:522:ILE:HG12 | 1.95                     | 0.49              |
| 1:E:13:PRO:O     | 1:E:16:THR:HB    | 2.13                     | 0.49              |
| 1:F:204:LYS:HD2  | 1:F:384:ILE:CG2  | 2.43                     | 0.49              |
| 1:F:211:GLU:HA   | 1:F:211:GLU:OE1  | 2.13                     | 0.49              |
| 1:G:123:ILE:HG21 | 1:G:432:LYS:CB   | 2.36                     | 0.49              |
| 1:H:154:LEU:HG   | 1:H:398:VAL:HG13 | 1.93                     | 0.49              |
| 1:E:477:ILE:HD13 | 1:E:488:ASP:HA   | 1.94                     | 0.49              |
| 1:G:69:LEU:HB3   | 1:G:83:VAL:HG22  | 1.95                     | 0.49              |
| 1:G:182:VAL:HG13 | 1:G:195:VAL:HG11 | 1.94                     | 0.49              |
| 1:A:144:ILE:CD1  | 1:A:490:LEU:HD21 | 2.40                     | 0.48              |
| 1:B:91:LYS:HB2   | 1:B:91:LYS:HZ2   | 1.77                     | 0.48              |
| 1:C:99:THR:O     | 1:C:103:ILE:HG13 | 2.12                     | 0.48              |
| 1:C:430:GLY:HA2  | 1:C:434:ALA:HB2  | 1.94                     | 0.48              |
| 1:D:182:VAL:CG2  | 1:D:395:VAL:HG13 | 2.43                     | 0.48              |
| 1:D:503:GLN:HA   | 1:D:503:GLN:NE2  | 2.28                     | 0.48              |
| 1:E:109:ARG:HG2  | 1:E:109:ARG:NH1  | 2.24                     | 0.48              |
| 1:E:145:ARG:HG2  | 1:E:145:ARG:NH1  | 2.28                     | 0.48              |
| 1:F:333:VAL:HG21 | 1:F:339:LEU:HD13 | 1.95                     | 0.48              |
| 1:G:304:TYR:O    | 1:G:308:TYR:HD1  | 1.95                     | 0.48              |
| 1:H:404:ASP:OD1  | 1:H:499:ARG:HB2  | 2.13                     | 0.48              |
| 1:B:143:ALA:HB3  | 1:B:145:ARG:NH1  | 2.28                     | 0.48              |
| 1:B:215:LEU:HD11 | 1:B:372:VAL:HG21 | 1.96                     | 0.48              |
| 1:C:82:MET:CE    | 1:C:101:VAL:HG13 | 2.43                     | 0.48              |
| 1:C:348:GLU:O    | 1:C:349:VAL:CG2  | 2.59                     | 0.48              |
| 1:D:221:ILE:CD1  | 1:D:324:LEU:HD11 | 2.43                     | 0.48              |
| 1:G:54:ASP:OD1   | 1:G:58:ASP:CB    | 2.54                     | 0.48              |
| 1:B:52:LEU:HD11  | 1:B:68:ILE:HA    | 1.95                     | 0.48              |
| 1:B:91:LYS:HG2   | 1:B:91:LYS:O     | 2.14                     | 0.48              |
| 1:B:250:LYS:HZ3  | 1:C:253:THR:HA   | 1.78                     | 0.48              |
| 1:B:314:ARG:HD2  | 1:B:315:ARG:HD3  | 1.96                     | 0.48              |
| 1:B:423:ASP:OD1  | 1:B:427:LYS:HE2  | 2.12                     | 0.48              |
| 1:C:75:GLN:CG    | 1:D:10:VAL:HG13  | 2.42                     | 0.48              |
| 1:A:49:ASP:OD1   | 1:A:63:ASN:HB2   | 2.13                     | 0.48              |
| 1:A:94:GLY:HA3   | 1:A:396:LYS:HD2  | 1.94                     | 0.48              |
| 1:A:146:VAL:HG22 | 1:A:147:ASP:N    | 2.29                     | 0.48              |
| 1:A:197:LEU:HD22 | 1:A:395:VAL:HG12 | 1.96                     | 0.48              |
| 1:A:235:GLU:O    | 1:A:236:ASN:O    | 2.32                     | 0.48              |
| 1:D:123:ILE:HG21 | 1:D:432:LYS:HB3  | 1.91                     | 0.48              |
| 1:D:487:ALA:HB3  | 1:D:489:MET:CE   | 2.42                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:75:GLN:HE21  | 1:F:13:PRO:HA    | 1.79                     | 0.48              |
| 1:E:204:LYS:HD2  | 1:E:384:ILE:HG22 | 1.94                     | 0.48              |
| 1:E:232:LYS:HD2  | 1:E:352:GLU:OE2  | 2.13                     | 0.48              |
| 1:E:257:ILE:HG22 | 1:E:259:ILE:CD1  | 2.41                     | 0.48              |
| 1:F:23:ASP:O     | 1:F:27:LEU:HG    | 2.14                     | 0.48              |
| 1:G:450:THR:O    | 1:G:454:ASN:ND2  | 2.46                     | 0.48              |
| 1:G:501:LYS:HA   | 1:G:501:LYS:HE3  | 1.95                     | 0.48              |
| 1:A:397:VAL:HA   | 1:A:400:ASP:OD2  | 2.14                     | 0.48              |
| 1:C:166:ASN:O    | 1:C:168:GLU:HG2  | 2.14                     | 0.48              |
| 1:C:342:GLU:OE2  | 1:C:342:GLU:N    | 2.46                     | 0.48              |
| 1:D:63:ASN:O     | 1:D:63:ASN:ND2   | 2.47                     | 0.48              |
| 1:C:330:ALA:HB2  | 1:C:345:GLY:HA3  | 1.94                     | 0.48              |
| 1:C:370:LYS:HA   | 1:C:370:LYS:CE   | 2.43                     | 0.48              |
| 1:G:119:ILE:HD11 | 1:G:435:LEU:HD23 | 1.95                     | 0.48              |
| 1:G:219:VAL:HG12 | 1:G:220:VAL:N    | 2.29                     | 0.48              |
| 1:A:143:ALA:HB3  | 1:A:145:ARG:HH12 | 1.79                     | 0.48              |
| 1:A:409:PRO:HA   | 1:A:495:ILE:HG22 | 1.94                     | 0.48              |
| 1:B:35:ILE:HG21  | 1:B:82:MET:CB    | 2.44                     | 0.48              |
| 1:B:100:ALA:O    | 1:B:508:ALA:HB2  | 2.14                     | 0.48              |
| 1:B:450:THR:O    | 1:B:454:ASN:ND2  | 2.47                     | 0.48              |
| 1:C:243:ASN:OD1  | 1:C:295:LYS:HE3  | 2.14                     | 0.48              |
| 1:E:304:TYR:O    | 1:E:308:TYR:HD1  | 1.97                     | 0.48              |
| 1:E:475:LEU:HD12 | 1:E:475:LEU:O    | 2.13                     | 0.48              |
| 1:F:315:ARG:HG3  | 1:F:315:ARG:NH1  | 2.22                     | 0.48              |
| 1:F:369:PRO:O    | 1:F:370:LYS:HE2  | 2.13                     | 0.48              |
| 1:G:273:GLU:HG2  | 1:G:300:LEU:CD1  | 2.43                     | 0.48              |
| 1:A:297:ILE:HG22 | 1:A:302:GLN:HG3  | 1.96                     | 0.48              |
| 1:B:143:ALA:HB3  | 1:B:145:ARG:HH12 | 1.79                     | 0.48              |
| 1:B:212:GLU:HB2  | 1:B:377:ARG:HG3  | 1.96                     | 0.48              |
| 1:B:524:ALA:O    | 1:B:525:LYS:HD2  | 2.12                     | 0.48              |
| 1:C:120:HIS:ND1  | 1:C:122:SER:CB   | 2.76                     | 0.48              |
| 1:C:423:ASP:O    | 1:C:426:ALA:HB3  | 2.13                     | 0.48              |
| 1:D:158:ALA:O    | 1:D:162:ILE:HG13 | 2.13                     | 0.48              |
| 1:E:22:ARG:HG3   | 1:E:23:ASP:N     | 2.29                     | 0.48              |
| 1:E:158:ALA:O    | 1:E:162:ILE:HG13 | 2.12                     | 0.48              |
| 1:E:280:VAL:HG11 | 1:E:304:TYR:HB3  | 1.96                     | 0.48              |
| 1:E:317:LYS:O    | 1:E:320:ASP:N    | 2.47                     | 0.48              |
| 1:H:50:LYS:HD2   | 1:H:68:ILE:HD13  | 1.96                     | 0.48              |
| 1:B:269:LEU:HD12 | 1:C:251:THR:CG2  | 2.44                     | 0.48              |
| 1:E:432:LYS:O    | 1:E:435:LEU:HB2  | 2.13                     | 0.48              |
| 1:F:226:VAL:O    | 1:F:226:VAL:HG22 | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:241:LEU:HD22 | 1:F:330:ALA:HB3  | 1.95                     | 0.48              |
| 1:G:16:THR:HG23  | 1:G:523:ALA:O    | 2.14                     | 0.48              |
| 1:G:146:VAL:HG22 | 1:G:147:ASP:H    | 1.79                     | 0.48              |
| 1:H:99:THR:O     | 1:H:103:ILE:HG13 | 2.13                     | 0.48              |
| 1:C:524:ALA:O    | 1:C:525:LYS:HE2  | 2.14                     | 0.48              |
| 1:D:509:SER:O    | 1:D:513:ILE:HG13 | 2.13                     | 0.48              |
| 1:F:38:THR:HG22  | 1:F:50:LYS:HE3   | 1.95                     | 0.48              |
| 1:F:89:GLN:HG2   | 1:F:97:THR:HA    | 1.95                     | 0.48              |
| 1:F:233:ARG:HH11 | 1:F:233:ARG:HG3  | 1.78                     | 0.48              |
| 1:F:355:LEU:HB3  | 1:F:360:MET:SD   | 2.54                     | 0.48              |
| 1:F:421:ARG:HB2  | 1:F:421:ARG:NH1  | 2.12                     | 0.48              |
| 1:H:449:LYS:HG3  | 1:H:463:LEU:HD22 | 1.95                     | 0.48              |
| 1:A:424:GLU:OE1  | 1:A:424:GLU:HA   | 2.14                     | 0.47              |
| 1:B:37:GLU:HG2   | 1:B:40:ARG:NH1   | 2.29                     | 0.47              |
| 1:B:82:MET:HE2   | 1:B:101:VAL:HG13 | 1.96                     | 0.47              |
| 1:C:204:LYS:HB3  | 1:C:384:ILE:CG2  | 2.41                     | 0.47              |
| 1:E:465:LYS:O    | 1:E:469:GLU:HG2  | 2.13                     | 0.47              |
| 1:F:42:THR:HG22  | 1:F:48:MET:O     | 2.14                     | 0.47              |
| 1:G:189:LYS:HD2  | 1:G:190:ASP:N    | 2.28                     | 0.47              |
| 1:G:281:ASP:OD1  | 1:G:308:TYR:OH   | 2.20                     | 0.47              |
| 1:A:333:VAL:HG21 | 1:A:339:LEU:HD13 | 1.96                     | 0.47              |
| 1:C:11:ILE:HD13  | 1:C:12:LEU:HB2   | 1.96                     | 0.47              |
| 1:E:239:ILE:HD11 | 1:E:347:ALA:CB   | 2.43                     | 0.47              |
| 1:F:53:VAL:HG21  | 1:G:77:PRO:CG    | 2.44                     | 0.47              |
| 1:F:145:ARG:HH11 | 1:F:145:ARG:HG2  | 1.79                     | 0.47              |
| 1:F:207:GLY:HA2  | 1:G:92:GLU:OE1   | 2.14                     | 0.47              |
| 1:F:293:VAL:HG21 | 1:F:297:ILE:HD11 | 1.96                     | 0.47              |
| 1:F:463:LEU:O    | 1:F:467:ILE:HG13 | 2.14                     | 0.47              |
| 1:G:217:ARG:HH11 | 1:G:217:ARG:CB   | 2.24                     | 0.47              |
| 1:H:281:ASP:O    | 1:H:285:GLN:HG3  | 2.14                     | 0.47              |
| 1:A:412:GLY:O    | 1:A:415:GLU:HG2  | 2.14                     | 0.47              |
| 1:B:134:LYS:O    | 1:B:138:ILE:HG13 | 2.14                     | 0.47              |
| 1:C:249:LYS:HE2  | 1:C:279:MET:CE   | 2.45                     | 0.47              |
| 1:D:125:ILE:CD1  | 1:D:517:ARG:HG2  | 2.42                     | 0.47              |
| 1:D:311:MET:HE3  | 1:D:350:VAL:HG12 | 1.97                     | 0.47              |
| 1:F:498:LEU:HD13 | 1:F:502:LYS:HD3  | 1.95                     | 0.47              |
| 1:G:409:PRO:HA   | 1:G:495:ILE:HG22 | 1.95                     | 0.47              |
| 1:E:120:HIS:CG   | 1:E:121:PRO:HD2  | 2.49                     | 0.47              |
| 1:H:272:GLU:HA   | 1:H:275:MET:CE   | 2.43                     | 0.47              |
| 1:H:414:PRO:HD2  | 1:H:415:GLU:OE2  | 2.15                     | 0.47              |
| 1:A:487:ALA:HB3  | 1:A:489:MET:CE   | 2.44                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:241:LEU:HD22 | 1:B:330:ALA:CB   | 2.45                     | 0.47              |
| 1:E:197:LEU:HD22 | 1:E:395:VAL:HG12 | 1.96                     | 0.47              |
| 1:E:498:LEU:HD22 | 1:E:498:LEU:O    | 2.15                     | 0.47              |
| 1:G:150:ASP:OD1  | 1:G:153:THR:HG23 | 2.14                     | 0.47              |
| 1:G:481:VAL:HG22 | 3:G:7528:ADP:N1  | 2.29                     | 0.47              |
| 1:H:184:GLN:NE2  | 1:H:217:ARG:NH2  | 2.61                     | 0.47              |
| 1:A:230:MET:HE2  | 1:A:312:ALA:H    | 1.77                     | 0.47              |
| 1:A:272:GLU:HA   | 1:A:275:MET:HE3  | 1.96                     | 0.47              |
| 1:A:518:ILE:HD13 | 1:H:51:MET:HB2   | 1.96                     | 0.47              |
| 1:B:54:ASP:OD1   | 1:B:58:ASP:CB    | 2.62                     | 0.47              |
| 1:B:123:ILE:HG21 | 1:B:432:LYS:HB3  | 1.95                     | 0.47              |
| 1:C:51:MET:CE    | 1:D:77:PRO:HB2   | 2.44                     | 0.47              |
| 1:C:229:ARG:NH1  | 1:D:332:ILE:O    | 2.47                     | 0.47              |
| 1:C:286:THR:HG21 | 1:C:339:LEU:HG   | 1.95                     | 0.47              |
| 1:C:298:ASP:O    | 1:C:302:GLN:HG3  | 2.14                     | 0.47              |
| 1:F:22:ARG:CG    | 1:F:23:ASP:N     | 2.78                     | 0.47              |
| 1:F:370:LYS:HE2  | 1:F:370:LYS:CA   | 2.39                     | 0.47              |
| 1:G:91:LYS:HB2   | 1:G:91:LYS:NZ    | 2.29                     | 0.47              |
| 1:H:425:TYR:O    | 1:H:429:VAL:HG23 | 2.15                     | 0.47              |
| 1:A:257:ILE:HG12 | 1:H:259:ILE:HG21 | 1.95                     | 0.47              |
| 1:A:367:LYS:HG2  | 1:A:368:ASN:N    | 2.29                     | 0.47              |
| 1:B:150:ASP:OD2  | 1:B:152:GLU:HB3  | 2.14                     | 0.47              |
| 1:B:260:THR:N    | 1:B:264:GLN:HE22 | 1.86                     | 0.47              |
| 1:B:397:VAL:HG23 | 1:B:398:VAL:N    | 2.30                     | 0.47              |
| 1:B:497:PRO:HB2  | 1:B:500:VAL:HG23 | 1.95                     | 0.47              |
| 1:C:75:GLN:HG2   | 1:D:13:PRO:HD3   | 1.97                     | 0.47              |
| 1:C:94:GLY:CA    | 1:C:396:LYS:HD2  | 2.45                     | 0.47              |
| 1:C:276:LEU:HD23 | 1:C:300:LEU:HB2  | 1.97                     | 0.47              |
| 1:D:51:MET:CE    | 1:E:77:PRO:HB2   | 2.44                     | 0.47              |
| 1:E:103:ILE:O    | 1:E:103:ILE:HG22 | 2.14                     | 0.47              |
| 1:F:26:ARG:HH11  | 1:F:26:ARG:HB3   | 1.78                     | 0.47              |
| 1:F:37:GLU:HG2   | 1:F:40:ARG:NH1   | 2.30                     | 0.47              |
| 1:F:222:ASP:O    | 1:F:223:LYS:HG2  | 2.15                     | 0.47              |
| 1:G:59:ILE:HD11  | 1:H:80:LYS:HE2   | 1.96                     | 0.47              |
| 1:G:188:LYS:HB2  | 1:G:193:TYR:HA   | 1.97                     | 0.47              |
| 1:G:227:HIS:HE2  | 1:H:334:THR:CB   | 2.26                     | 0.47              |
| 1:G:269:LEU:CD1  | 1:H:251:THR:HG23 | 2.44                     | 0.47              |
| 1:H:13:PRO:O     | 1:H:16:THR:HB    | 2.15                     | 0.47              |
| 1:H:18:ARG:HA    | 1:H:521:VAL:O    | 2.15                     | 0.47              |
| 1:A:370:LYS:HE2  | 1:A:370:LYS:CA   | 2.40                     | 0.47              |
| 1:B:208:GLU:HB3  | 1:B:212:GLU:CG   | 2.44                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:413:ALA:HB3  | 1:D:414:PRO:HD3  | 1.95                     | 0.47              |
| 1:C:106:GLU:HB2  | 1:C:446:ILE:HG12 | 1.97                     | 0.47              |
| 1:C:208:GLU:OE2  | 1:C:212:GLU:HG3  | 2.15                     | 0.47              |
| 1:D:16:THR:HA    | 1:D:523:ALA:O    | 2.15                     | 0.47              |
| 1:D:38:THR:O     | 1:D:50:LYS:HE3   | 2.15                     | 0.47              |
| 1:D:215:LEU:HD11 | 1:D:372:VAL:CG2  | 2.45                     | 0.47              |
| 1:D:283:ILE:HA   | 1:D:339:LEU:HD23 | 1.96                     | 0.47              |
| 1:G:241:LEU:HD22 | 1:G:330:ALA:HB3  | 1.97                     | 0.47              |
| 1:H:208:GLU:HB3  | 1:H:212:GLU:HG3  | 1.95                     | 0.47              |
| 1:B:99:THR:O     | 1:B:103:ILE:HG13 | 2.14                     | 0.47              |
| 1:C:144:ILE:CD1  | 1:C:490:LEU:HD21 | 2.39                     | 0.47              |
| 1:D:25:GLN:O     | 1:D:29:ILE:HG13  | 2.15                     | 0.47              |
| 1:D:92:GLU:O     | 1:D:499:ARG:HD3  | 2.15                     | 0.47              |
| 1:E:29:ILE:HG23  | 1:E:108:LEU:HB3  | 1.97                     | 0.47              |
| 1:E:269:LEU:CD1  | 1:F:251:THR:HG23 | 2.45                     | 0.47              |
| 1:G:120:HIS:ND1  | 1:G:122:SER:HB3  | 2.30                     | 0.47              |
| 1:H:91:LYS:HG2   | 1:H:91:LYS:O     | 2.15                     | 0.47              |
| 1:H:150:ASP:OD1  | 1:H:153:THR:HG23 | 2.14                     | 0.47              |
| 1:A:146:VAL:HG21 | 1:A:153:THR:HG21 | 1.97                     | 0.46              |
| 1:A:370:LYS:HA   | 1:A:370:LYS:CE   | 2.40                     | 0.46              |
| 1:B:126:LYS:O    | 1:B:130:LEU:HG   | 2.14                     | 0.46              |
| 1:B:314:ARG:HD2  | 1:B:315:ARG:CD   | 2.45                     | 0.46              |
| 1:C:210:VAL:HA   | 1:C:377:ARG:O    | 2.15                     | 0.46              |
| 1:D:483:GLU:O    | 1:D:485:LYS:HG2  | 2.14                     | 0.46              |
| 1:F:446:ILE:N    | 1:F:446:ILE:HD12 | 2.29                     | 0.46              |
| 1:H:253:THR:O    | 1:H:254:ASP:C    | 2.54                     | 0.46              |
| 1:H:417:GLU:HG3  | 1:H:421:ARG:HH12 | 1.80                     | 0.46              |
| 1:A:221:ILE:HD11 | 1:A:324:LEU:HD11 | 1.96                     | 0.46              |
| 1:A:449:LYS:HE3  | 1:A:459:THR:HG21 | 1.98                     | 0.46              |
| 1:A:483:GLU:HG3  | 1:A:485:LYS:HZ1  | 1.78                     | 0.46              |
| 1:B:89:GLN:HG2   | 1:B:97:THR:HA    | 1.97                     | 0.46              |
| 1:C:18:ARG:HG3   | 1:C:522:ILE:HG12 | 1.98                     | 0.46              |
| 1:C:225:VAL:HG11 | 1:C:230:MET:HB2  | 1.97                     | 0.46              |
| 1:C:249:LYS:HE2  | 1:C:279:MET:HE3  | 1.97                     | 0.46              |
| 1:D:412:GLY:O    | 1:D:415:GLU:HG2  | 2.15                     | 0.46              |
| 1:G:15:GLY:O     | 1:G:525:LYS:HE2  | 2.14                     | 0.46              |
| 1:G:211:GLU:OE1  | 1:G:211:GLU:HA   | 2.15                     | 0.46              |
| 1:B:144:ILE:HG22 | 1:B:144:ILE:O    | 2.14                     | 0.46              |
| 1:C:35:ILE:HG13  | 1:C:74:LEU:HD13  | 1.97                     | 0.46              |
| 1:D:208:GLU:HB3  | 1:D:212:GLU:CG   | 2.45                     | 0.46              |
| 1:D:259:ILE:HG21 | 1:E:257:ILE:HG12 | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:205:LYS:HZ1  | 1:G:358:GLU:HG2  | 1.80                     | 0.46              |
| 1:G:239:ILE:HD12 | 1:G:239:ILE:N    | 2.30                     | 0.46              |
| 1:H:150:ASP:OD2  | 1:H:152:GLU:HB3  | 2.16                     | 0.46              |
| 1:H:432:LYS:O    | 1:H:435:LEU:HB2  | 2.14                     | 0.46              |
| 1:A:483:GLU:HG3  | 1:A:485:LYS:HZ3  | 1.79                     | 0.46              |
| 1:B:372:VAL:HG22 | 1:B:373:THR:H    | 1.79                     | 0.46              |
| 1:D:75:GLN:HG3   | 1:E:10:VAL:HG13  | 1.96                     | 0.46              |
| 1:G:59:ILE:N     | 1:G:59:ILE:CD1   | 2.76                     | 0.46              |
| 1:H:11:ILE:HG23  | 1:H:12:LEU:N     | 2.30                     | 0.46              |
| 1:H:450:THR:O    | 1:H:454:ASN:ND2  | 2.48                     | 0.46              |
| 1:B:348:GLU:O    | 1:B:349:VAL:HG23 | 2.15                     | 0.46              |
| 1:C:239:ILE:HD11 | 1:C:347:ALA:HB3  | 1.98                     | 0.46              |
| 1:D:182:VAL:HG22 | 1:D:395:VAL:HG13 | 1.98                     | 0.46              |
| 1:G:35:ILE:HD11  | 1:G:74:LEU:HD22  | 1.97                     | 0.46              |
| 1:G:106:GLU:HG2  | 1:G:446:ILE:HG13 | 1.97                     | 0.46              |
| 1:H:370:LYS:HE2  | 1:H:370:LYS:CA   | 2.43                     | 0.46              |
| 1:A:91:LYS:HB2   | 1:A:91:LYS:HZ3   | 1.79                     | 0.46              |
| 1:A:465:LYS:O    | 1:A:469:GLU:HG2  | 2.15                     | 0.46              |
| 1:B:421:ARG:HB2  | 1:B:421:ARG:NH1  | 2.21                     | 0.46              |
| 1:E:208:GLU:HB3  | 1:E:212:GLU:HG3  | 1.98                     | 0.46              |
| 1:E:229:ARG:HG2  | 1:E:229:ARG:HH11 | 1.81                     | 0.46              |
| 1:E:401:VAL:O    | 1:E:405:GLY:N    | 2.44                     | 0.46              |
| 1:F:293:VAL:CG2  | 1:F:297:ILE:HD11 | 2.46                     | 0.46              |
| 1:G:103:ILE:HG12 | 1:G:446:ILE:HD11 | 1.97                     | 0.46              |
| 1:G:271:GLN:O    | 1:G:275:MET:HG3  | 2.16                     | 0.46              |
| 1:G:286:THR:HG21 | 1:G:339:LEU:HG   | 1.97                     | 0.46              |
| 1:H:426:ALA:CB   | 1:H:438:GLU:HG3  | 2.45                     | 0.46              |
| 1:H:515:ILE:C    | 1:H:517:ARG:H    | 2.19                     | 0.46              |
| 1:A:392:GLU:O    | 1:A:396:LYS:HE3  | 2.16                     | 0.46              |
| 1:A:524:ALA:O    | 1:A:525:LYS:HD2  | 2.16                     | 0.46              |
| 1:B:154:LEU:HD12 | 1:B:154:LEU:HA   | 1.83                     | 0.46              |
| 1:B:162:ILE:HD13 | 1:B:174:LEU:HB2  | 1.98                     | 0.46              |
| 1:D:11:ILE:HD13  | 1:D:11:ILE:O     | 2.15                     | 0.46              |
| 1:D:106:GLU:HG2  | 1:D:446:ILE:HG12 | 1.97                     | 0.46              |
| 1:E:20:VAL:O     | 1:E:23:ASP:HB2   | 2.15                     | 0.46              |
| 1:G:103:ILE:O    | 1:G:107:LEU:HB2  | 2.16                     | 0.46              |
| 1:H:480:ASP:HB3  | 1:H:483:GLU:HB2  | 1.98                     | 0.46              |
| 1:A:170:HIS:HD2  | 1:A:211:GLU:CD   | 2.19                     | 0.46              |
| 1:B:498:LEU:O    | 1:B:498:LEU:HD22 | 2.16                     | 0.46              |
| 1:C:38:THR:O     | 1:C:50:LYS:HE3   | 2.16                     | 0.46              |
| 1:C:114:LEU:HG   | 1:C:439:ASN:ND2  | 2.31                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:29:ILE:O     | 1:D:33:ARG:HG3   | 2.15                     | 0.46              |
| 1:H:119:ILE:HD11 | 1:H:435:LEU:HD23 | 1.97                     | 0.46              |
| 1:A:126:LYS:HB3  | 1:A:126:LYS:HZ2  | 1.79                     | 0.46              |
| 1:A:276:LEU:HD23 | 1:A:300:LEU:CB   | 2.46                     | 0.46              |
| 1:B:443:ALA:O    | 1:B:446:ILE:HG13 | 2.16                     | 0.46              |
| 1:C:91:LYS:O     | 1:C:91:LYS:HG2   | 2.15                     | 0.46              |
| 1:C:154:LEU:HG   | 1:C:398:VAL:HG13 | 1.97                     | 0.46              |
| 1:E:424:GLU:O    | 1:E:428:GLN:HG2  | 2.16                     | 0.46              |
| 1:G:147:ASP:HB3  | 1:G:150:ASP:HB2  | 1.97                     | 0.46              |
| 1:H:514:MET:O    | 1:H:514:MET:HG2  | 2.16                     | 0.46              |
| 1:A:255:ALA:HB2  | 1:H:257:ILE:HB   | 1.98                     | 0.46              |
| 1:A:466:VAL:HG21 | 1:A:479:ILE:CG1  | 2.46                     | 0.46              |
| 1:B:11:ILE:HD13  | 1:B:11:ILE:O     | 2.16                     | 0.46              |
| 1:B:165:LYS:NZ   | 1:B:393:ASP:OD2  | 2.34                     | 0.46              |
| 1:D:188:LYS:HD3  | 1:D:193:TYR:CD1  | 2.51                     | 0.46              |
| 1:D:290:VAL:HG22 | 1:D:311:MET:HE2  | 1.98                     | 0.46              |
| 1:H:91:LYS:HB2   | 1:H:91:LYS:HZ2   | 1.79                     | 0.46              |
| 1:H:195:VAL:HB   | 1:H:399:LYS:HG3  | 1.98                     | 0.46              |
| 1:A:506:LYS:O    | 1:A:510:GLU:CG   | 2.63                     | 0.45              |
| 1:B:109:ARG:NH2  | 1:B:110:LYS:HD3  | 2.31                     | 0.45              |
| 1:C:290:VAL:HG13 | 1:C:311:MET:HE2  | 1.97                     | 0.45              |
| 1:D:38:THR:HG22  | 1:D:50:LYS:HE3   | 1.97                     | 0.45              |
| 1:D:99:THR:O     | 1:D:103:ILE:HG13 | 2.16                     | 0.45              |
| 1:D:432:LYS:O    | 1:D:435:LEU:HB2  | 2.16                     | 0.45              |
| 1:E:123:ILE:HG21 | 1:E:432:LYS:CB   | 2.46                     | 0.45              |
| 1:F:162:ILE:HG21 | 1:F:171:LYS:HA   | 1.98                     | 0.45              |
| 1:F:416:ILE:HD13 | 1:F:466:VAL:HG12 | 1.98                     | 0.45              |
| 1:H:412:GLY:O    | 1:H:416:ILE:HG13 | 2.17                     | 0.45              |
| 1:H:424:GLU:O    | 1:H:428:GLN:HG3  | 2.16                     | 0.45              |
| 1:A:252:GLU:O    | 1:H:250:LYS:NZ   | 2.47                     | 0.45              |
| 1:A:255:ALA:CB   | 1:H:257:ILE:HB   | 2.46                     | 0.45              |
| 1:A:461:GLU:HG2  | 1:A:465:LYS:HZ2  | 1.81                     | 0.45              |
| 1:C:128:TYR:CE2  | 1:C:440:PHE:HB2  | 2.51                     | 0.45              |
| 1:C:178:ALA:O    | 1:C:182:VAL:HG23 | 2.15                     | 0.45              |
| 1:D:272:GLU:HA   | 1:D:275:MET:CE   | 2.46                     | 0.45              |
| 1:E:134:LYS:O    | 1:E:138:ILE:HG13 | 2.16                     | 0.45              |
| 1:E:462:MET:HE1  | 1:E:485:LYS:HA   | 1.97                     | 0.45              |
| 1:A:120:HIS:ND1  | 1:A:122:SER:HB3  | 2.31                     | 0.45              |
| 1:A:469:GLU:HG3  | 1:A:486:PRO:CB   | 2.46                     | 0.45              |
| 1:B:211:GLU:OE1  | 1:B:211:GLU:HA   | 2.16                     | 0.45              |
| 1:C:369:PRO:O    | 1:C:370:LYS:HE2  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:123:ILE:HG23 | 1:D:433:GLU:OE2  | 2.15                     | 0.45              |
| 1:D:188:LYS:HD2  | 1:D:191:GLY:O    | 2.17                     | 0.45              |
| 1:D:410:ALA:HB3  | 1:D:494:ILE:HG22 | 1.97                     | 0.45              |
| 1:E:243:ASN:OD1  | 1:E:295:LYS:HE3  | 2.16                     | 0.45              |
| 1:E:245:ALA:HB1  | 1:E:247:GLU:HG2  | 1.97                     | 0.45              |
| 1:E:469:GLU:HA   | 1:E:469:GLU:OE2  | 2.16                     | 0.45              |
| 1:F:120:HIS:ND1  | 1:F:121:PRO:HD2  | 2.31                     | 0.45              |
| 1:G:488:ASP:O    | 1:G:492:LYS:HG2  | 2.16                     | 0.45              |
| 1:H:12:LEU:HD23  | 1:H:13:PRO:HD2   | 1.96                     | 0.45              |
| 1:H:139:LEU:HD23 | 1:H:142:ILE:HD11 | 1.98                     | 0.45              |
| 1:H:166:ASN:C    | 1:H:166:ASN:HD22 | 2.20                     | 0.45              |
| 1:A:37:GLU:HA    | 1:A:40:ARG:HG2   | 1.97                     | 0.45              |
| 1:A:54:ASP:OD1   | 1:A:58:ASP:HB3   | 2.15                     | 0.45              |
| 1:C:418:LEU:O    | 1:C:422:LEU:HB2  | 2.16                     | 0.45              |
| 1:D:35:ILE:HD11  | 1:D:74:LEU:HD22  | 1.98                     | 0.45              |
| 1:D:38:THR:O     | 1:D:50:LYS:CE    | 2.64                     | 0.45              |
| 1:E:466:VAL:HG21 | 1:E:479:ILE:CG1  | 2.46                     | 0.45              |
| 1:E:469:GLU:O    | 1:E:473:ARG:N    | 2.48                     | 0.45              |
| 1:F:116:ASP:C    | 1:F:118:ASN:H    | 2.19                     | 0.45              |
| 1:F:259:ILE:HD12 | 1:F:259:ILE:N    | 2.30                     | 0.45              |
| 1:G:182:VAL:O    | 1:G:186:ALA:HB2  | 2.16                     | 0.45              |
| 1:H:142:ILE:HB   | 1:H:475:LEU:HD22 | 1.99                     | 0.45              |
| 1:H:149:ASP:O    | 1:H:151:GLU:N    | 2.49                     | 0.45              |
| 1:H:297:ILE:HD12 | 1:H:314:ARG:HB3  | 1.98                     | 0.45              |
| 1:B:293:VAL:CG2  | 1:B:297:ILE:HD11 | 2.46                     | 0.45              |
| 1:C:91:LYS:HB2   | 1:C:91:LYS:NZ    | 2.31                     | 0.45              |
| 1:D:483:GLU:HG3  | 1:D:485:LYS:CE   | 2.47                     | 0.45              |
| 1:E:136:GLN:HA   | 1:E:136:GLN:HE21 | 1.81                     | 0.45              |
| 1:E:208:GLU:HB3  | 1:E:212:GLU:HG2  | 1.98                     | 0.45              |
| 1:G:313:VAL:HG21 | 1:G:361:ILE:CD1  | 2.47                     | 0.45              |
| 1:G:449:LYS:HG3  | 1:G:463:LEU:HD22 | 1.98                     | 0.45              |
| 1:G:470:HIS:HA   | 1:G:477:ILE:HB   | 1.99                     | 0.45              |
| 1:H:114:LEU:HD11 | 1:H:436:ALA:HA   | 1.98                     | 0.45              |
| 1:H:204:LYS:HD2  | 1:H:384:ILE:HG22 | 1.99                     | 0.45              |
| 1:A:77:PRO:HG2   | 1:H:53:VAL:HG21  | 1.98                     | 0.45              |
| 1:A:230:MET:CE   | 1:A:312:ALA:HB3  | 2.47                     | 0.45              |
| 1:A:458:ASP:C    | 1:A:458:ASP:OD2  | 2.55                     | 0.45              |
| 1:D:195:VAL:HB   | 1:D:399:LYS:HG3  | 1.98                     | 0.45              |
| 1:E:145:ARG:HD3  | 1:E:145:ARG:HA   | 1.76                     | 0.45              |
| 1:E:209:GLY:C    | 1:E:211:GLU:N    | 2.69                     | 0.45              |
| 1:E:394:ALA:O    | 1:E:397:VAL:CG2  | 2.65                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:201:LYS:HE2  | 1:F:203:GLU:OE1  | 2.17                     | 0.45              |
| 1:F:241:LEU:HD12 | 1:F:292:PHE:HB2  | 1.98                     | 0.45              |
| 1:F:276:LEU:CD2  | 1:F:300:LEU:HB2  | 2.43                     | 0.45              |
| 1:G:146:VAL:HG21 | 1:G:153:THR:HG21 | 1.99                     | 0.45              |
| 1:G:205:LYS:O    | 1:G:377:ARG:NH1  | 2.49                     | 0.45              |
| 1:G:393:ASP:O    | 1:G:397:VAL:HG13 | 2.17                     | 0.45              |
| 1:H:462:MET:HA   | 1:H:462:MET:HE3  | 1.98                     | 0.45              |
| 1:H:463:LEU:O    | 1:H:467:ILE:HG13 | 2.17                     | 0.45              |
| 1:A:76:HIS:CD2   | 1:A:78:ALA:H     | 2.35                     | 0.45              |
| 1:B:17:GLN:NE2   | 1:B:17:GLN:H     | 2.15                     | 0.45              |
| 1:B:123:ILE:HG21 | 1:B:432:LYS:CB   | 2.47                     | 0.45              |
| 1:D:12:LEU:CD2   | 1:D:16:THR:HG21  | 2.43                     | 0.45              |
| 1:D:35:ILE:HD13  | 1:D:35:ILE:HA    | 1.80                     | 0.45              |
| 1:F:408:LEU:HD11 | 1:F:498:LEU:HD23 | 1.99                     | 0.45              |
| 1:G:90:ASP:O     | 1:G:94:GLY:HA2   | 2.17                     | 0.45              |
| 1:G:109:ARG:NH2  | 1:G:110:LYS:HD3  | 2.32                     | 0.45              |
| 1:G:110:LYS:HE3  | 1:G:442:ASP:OD1  | 2.17                     | 0.45              |
| 1:H:45:PRO:HB2   | 1:H:481:VAL:HG21 | 1.99                     | 0.45              |
| 1:A:35:ILE:HD13  | 1:A:35:ILE:HA    | 1.82                     | 0.45              |
| 1:B:215:LEU:HD11 | 1:B:372:VAL:CG2  | 2.47                     | 0.45              |
| 1:B:265:LEU:O    | 1:B:269:LEU:HD13 | 2.16                     | 0.45              |
| 1:C:262:PRO:O    | 1:D:271:GLN:HG2  | 2.17                     | 0.45              |
| 1:D:235:GLU:O    | 1:D:348:GLU:O    | 2.35                     | 0.45              |
| 1:E:76:HIS:HB2   | 1:F:11:ILE:HA    | 1.98                     | 0.45              |
| 1:E:414:PRO:HD2  | 1:E:415:GLU:OE2  | 2.17                     | 0.45              |
| 1:G:410:ALA:O    | 1:G:489:MET:HG3  | 2.17                     | 0.45              |
| 1:H:260:THR:N    | 1:H:264:GLN:HE22 | 1.99                     | 0.45              |
| 1:H:372:VAL:CG2  | 1:H:373:THR:N    | 2.79                     | 0.45              |
| 1:A:77:PRO:HB2   | 1:H:51:MET:HE1   | 1.99                     | 0.45              |
| 1:B:69:LEU:HB3   | 1:B:83:VAL:HG22  | 1.98                     | 0.45              |
| 1:C:89:GLN:HG2   | 1:C:97:THR:HA    | 1.98                     | 0.45              |
| 1:C:143:ALA:HB3  | 1:C:145:ARG:NH1  | 2.31                     | 0.45              |
| 1:C:355:LEU:O    | 1:C:356:ALA:HB3  | 2.17                     | 0.45              |
| 1:C:461:GLU:HG2  | 1:C:465:LYS:HZ2  | 1.80                     | 0.45              |
| 1:D:241:LEU:HD12 | 1:D:292:PHE:HB2  | 1.99                     | 0.45              |
| 1:E:269:LEU:HD12 | 1:F:251:THR:CG2  | 2.43                     | 0.45              |
| 1:F:167:ALA:O    | 1:F:169:SER:N    | 2.50                     | 0.45              |
| 1:G:215:LEU:HD11 | 1:G:372:VAL:CG2  | 2.47                     | 0.45              |
| 1:A:25:GLN:O     | 1:A:29:ILE:HG13  | 2.16                     | 0.45              |
| 1:A:37:GLU:HG2   | 1:A:40:ARG:CZ    | 2.47                     | 0.45              |
| 1:A:117:GLN:O    | 1:A:118:ASN:HB2  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:141:GLU:O    | 1:A:143:ALA:N    | 2.50                     | 0.45              |
| 1:A:210:VAL:HA   | 1:A:377:ARG:O    | 2.16                     | 0.45              |
| 1:A:503:GLN:NE2  | 1:A:503:GLN:HA   | 2.32                     | 0.45              |
| 1:C:412:GLY:HA2  | 1:C:415:GLU:CG   | 2.47                     | 0.45              |
| 1:E:227:HIS:HD2  | 1:E:302:GLN:HB3  | 1.82                     | 0.45              |
| 1:E:286:THR:HG22 | 1:E:341:PRO:CD   | 2.47                     | 0.45              |
| 1:E:335:ASN:ND2  | 1:E:337:LYS:HB2  | 2.30                     | 0.45              |
| 1:F:409:PRO:HB2  | 1:F:489:MET:HB2  | 1.99                     | 0.45              |
| 1:G:17:GLN:H     | 1:G:17:GLN:HE21  | 1.62                     | 0.45              |
| 1:A:215:LEU:HD11 | 1:A:372:VAL:CG2  | 2.47                     | 0.44              |
| 1:B:29:ILE:HG23  | 1:B:108:LEU:HB3  | 1.97                     | 0.44              |
| 1:B:218:GLY:HA3  | 1:B:363:VAL:O    | 2.16                     | 0.44              |
| 1:B:353:ARG:HD2  | 1:B:362:PHE:CD1  | 2.52                     | 0.44              |
| 1:B:458:ASP:OD2  | 1:B:458:ASP:C    | 2.55                     | 0.44              |
| 1:C:52:LEU:HD11  | 1:C:68:ILE:HA    | 1.98                     | 0.44              |
| 1:C:415:GLU:HG3  | 1:C:447:ILE:HB   | 1.99                     | 0.44              |
| 1:D:144:ILE:CD1  | 1:D:490:LEU:HD21 | 2.45                     | 0.44              |
| 1:D:207:GLY:O    | 1:D:208:GLU:HB2  | 2.16                     | 0.44              |
| 1:E:17:GLN:NE2   | 1:E:17:GLN:N     | 2.63                     | 0.44              |
| 1:E:157:ILE:HD11 | 1:E:495:ILE:HD12 | 2.00                     | 0.44              |
| 1:F:206:ALA:HA   | 1:F:384:ILE:CD1  | 2.47                     | 0.44              |
| 1:F:225:VAL:HG23 | 1:F:352:GLU:OE1  | 2.18                     | 0.44              |
| 1:F:397:VAL:HG23 | 1:F:398:VAL:N    | 2.31                     | 0.44              |
| 1:H:11:ILE:HD13  | 1:H:12:LEU:HB2   | 1.99                     | 0.44              |
| 1:H:273:GLU:HG2  | 1:H:300:LEU:HD13 | 1.99                     | 0.44              |
| 1:A:281:ASP:OD1  | 1:A:308:TYR:OH   | 2.17                     | 0.44              |
| 1:B:221:ILE:HD11 | 1:B:324:LEU:HD11 | 1.99                     | 0.44              |
| 1:C:182:VAL:CG2  | 1:C:395:VAL:HG13 | 2.47                     | 0.44              |
| 1:D:13:PRO:O     | 1:D:16:THR:HB    | 2.17                     | 0.44              |
| 1:D:445:LYS:C    | 1:D:448:PRO:HD2  | 2.37                     | 0.44              |
| 1:E:38:THR:O     | 1:E:50:LYS:CE    | 2.64                     | 0.44              |
| 1:E:85:VAL:HG13  | 1:E:507:SER:HB3  | 1.99                     | 0.44              |
| 1:E:144:ILE:CD1  | 1:E:490:LEU:HD21 | 2.47                     | 0.44              |
| 1:E:216:VAL:O    | 1:E:372:VAL:HG23 | 2.17                     | 0.44              |
| 1:F:136:GLN:NE2  | 1:F:136:GLN:HA   | 2.33                     | 0.44              |
| 1:F:158:ALA:HB2  | 1:F:398:VAL:CG2  | 2.48                     | 0.44              |
| 1:F:333:VAL:HG12 | 1:F:335:ASN:H    | 1.82                     | 0.44              |
| 1:G:205:LYS:HD3  | 1:G:205:LYS:HA   | 1.74                     | 0.44              |
| 1:G:461:GLU:HG2  | 1:G:465:LYS:NZ   | 2.32                     | 0.44              |
| 1:H:52:LEU:HD11  | 1:H:68:ILE:HA    | 1.98                     | 0.44              |
| 1:A:142:ILE:HB   | 1:A:475:LEU:HD22 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:212:GLU:HB2  | 1:C:377:ARG:HG3  | 2.00                     | 0.44              |
| 1:C:230:MET:CE   | 1:C:312:ALA:HB3  | 2.47                     | 0.44              |
| 1:C:333:VAL:HG21 | 1:C:339:LEU:CD1  | 2.47                     | 0.44              |
| 1:C:498:LEU:O    | 1:C:498:LEU:HD22 | 2.17                     | 0.44              |
| 1:D:145:ARG:HG2  | 1:D:145:ARG:HH11 | 1.82                     | 0.44              |
| 1:E:446:ILE:H    | 1:E:446:ILE:CD1  | 2.28                     | 0.44              |
| 1:G:184:GLN:NE2  | 1:G:217:ARG:HH21 | 2.15                     | 0.44              |
| 1:H:108:LEU:HD11 | 1:H:515:ILE:HD12 | 1.99                     | 0.44              |
| 1:A:145:ARG:HG2  | 1:A:145:ARG:NH1  | 2.28                     | 0.44              |
| 1:B:245:ALA:HB1  | 1:B:247:GLU:HG2  | 1.98                     | 0.44              |
| 1:C:17:GLN:H     | 1:C:17:GLN:CD    | 2.21                     | 0.44              |
| 1:C:449:LYS:HE3  | 1:C:459:THR:CG2  | 2.48                     | 0.44              |
| 1:D:217:ARG:NH1  | 1:D:217:ARG:CB   | 2.74                     | 0.44              |
| 1:E:458:ASP:OD2  | 1:E:458:ASP:C    | 2.56                     | 0.44              |
| 1:F:412:GLY:O    | 1:F:416:ILE:HG13 | 2.17                     | 0.44              |
| 1:G:218:GLY:HA3  | 1:G:363:VAL:O    | 2.17                     | 0.44              |
| 1:G:354:LYS:HE2  | 1:G:357:GLY:HA2  | 2.00                     | 0.44              |
| 1:G:517:ARG:HE   | 1:G:517:ARG:HB3  | 1.65                     | 0.44              |
| 1:A:18:ARG:HA    | 1:A:521:VAL:O    | 2.17                     | 0.44              |
| 1:A:251:THR:CG2  | 1:H:269:LEU:HD12 | 2.45                     | 0.44              |
| 1:B:136:GLN:HE21 | 1:B:502:LYS:NZ   | 2.14                     | 0.44              |
| 1:B:446:ILE:HD12 | 1:B:446:ILE:N    | 2.33                     | 0.44              |
| 1:C:227:HIS:HB3  | 1:C:230:MET:SD   | 2.57                     | 0.44              |
| 1:D:215:LEU:HD11 | 1:D:372:VAL:HG21 | 2.00                     | 0.44              |
| 1:E:488:ASP:OD1  | 1:E:490:LEU:HB2  | 2.16                     | 0.44              |
| 1:F:156:LYS:O    | 1:F:157:ILE:C    | 2.56                     | 0.44              |
| 1:G:140:ASP:OD1  | 1:G:502:LYS:HD2  | 2.17                     | 0.44              |
| 1:G:145:ARG:HG2  | 1:G:145:ARG:NH1  | 2.30                     | 0.44              |
| 1:G:151:GLU:O    | 1:G:155:LEU:HD23 | 2.17                     | 0.44              |
| 1:H:37:GLU:HG2   | 1:H:40:ARG:HH12  | 1.79                     | 0.44              |
| 1:H:112:GLU:HA   | 1:H:115:LEU:HD12 | 2.00                     | 0.44              |
| 1:H:147:ASP:HB3  | 1:H:150:ASP:HB2  | 1.99                     | 0.44              |
| 1:A:142:ILE:HB   | 1:A:475:LEU:CD2  | 2.48                     | 0.44              |
| 1:A:204:LYS:HD2  | 1:A:384:ILE:CG2  | 2.40                     | 0.44              |
| 1:A:209:GLY:O    | 1:A:212:GLU:HG2  | 2.17                     | 0.44              |
| 1:B:35:ILE:HD12  | 1:B:69:LEU:CD2   | 2.47                     | 0.44              |
| 1:B:96:GLY:HA2   | 3:B:2528:ADP:O1B | 2.18                     | 0.44              |
| 1:C:202:PHE:CE2  | 1:C:374:ILE:HD12 | 2.53                     | 0.44              |
| 1:D:81:MET:CE    | 1:D:514:MET:SD   | 3.06                     | 0.44              |
| 1:D:154:LEU:HG   | 1:D:398:VAL:HG13 | 1.99                     | 0.44              |
| 1:D:209:GLY:C    | 1:D:211:GLU:N    | 2.70                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:10:VAL:CG2   | 1:E:11:ILE:N     | 2.72                     | 0.44              |
| 1:E:11:ILE:HG23  | 1:E:12:LEU:N     | 2.33                     | 0.44              |
| 1:E:75:GLN:HG3   | 1:F:12:LEU:C     | 2.38                     | 0.44              |
| 1:E:149:ASP:O    | 1:E:151:GLU:N    | 2.50                     | 0.44              |
| 1:F:35:ILE:HD13  | 1:F:35:ILE:HA    | 1.78                     | 0.44              |
| 1:F:205:LYS:HB3  | 1:F:377:ARG:NH1  | 2.33                     | 0.44              |
| 1:F:313:VAL:HG21 | 1:F:361:ILE:CD1  | 2.46                     | 0.44              |
| 1:G:424:GLU:OE1  | 1:G:424:GLU:HA   | 2.17                     | 0.44              |
| 1:H:217:ARG:HB3  | 1:H:217:ARG:NH1  | 2.32                     | 0.44              |
| 1:H:342:GLU:H    | 1:H:342:GLU:CD   | 2.21                     | 0.44              |
| 1:B:12:LEU:HD23  | 1:B:13:PRO:HD2   | 1.99                     | 0.44              |
| 1:B:146:VAL:O    | 1:B:148:PRO:HD3  | 2.18                     | 0.44              |
| 1:B:204:LYS:O    | 1:B:205:LYS:HD3  | 2.18                     | 0.44              |
| 1:B:416:ILE:CD1  | 1:B:466:VAL:HG12 | 2.48                     | 0.44              |
| 1:D:319:SER:O    | 1:D:323:LYS:HG3  | 2.18                     | 0.44              |
| 1:F:12:LEU:HD21  | 1:F:16:THR:HG21  | 2.00                     | 0.44              |
| 1:F:284:ALA:HB2  | 1:F:308:TYR:CD1  | 2.52                     | 0.44              |
| 1:F:372:VAL:HG22 | 1:F:373:THR:N    | 2.33                     | 0.44              |
| 1:F:415:GLU:HG3  | 1:F:447:ILE:HB   | 1.99                     | 0.44              |
| 1:H:272:GLU:HA   | 1:H:275:MET:HE3  | 1.98                     | 0.44              |
| 1:A:65:CYS:HB3   | 1:A:97:THR:OG1   | 2.17                     | 0.44              |
| 1:A:277:LYS:HB2  | 1:A:304:TYR:CE2  | 2.52                     | 0.44              |
| 1:C:109:ARG:HG2  | 1:C:109:ARG:HH11 | 1.83                     | 0.44              |
| 1:E:182:VAL:O    | 1:E:186:ALA:HB2  | 2.18                     | 0.44              |
| 1:E:208:GLU:HB2  | 1:E:377:ARG:HB3  | 1.99                     | 0.44              |
| 1:E:433:GLU:H    | 1:E:433:GLU:CD   | 2.21                     | 0.44              |
| 1:F:94:GLY:HA2   | 1:F:396:LYS:HD2  | 1.99                     | 0.44              |
| 1:G:80:LYS:O     | 1:G:83:VAL:HB    | 2.17                     | 0.44              |
| 1:G:205:LYS:HZ3  | 1:G:358:GLU:HG2  | 1.83                     | 0.44              |
| 1:G:233:ARG:HH12 | 1:G:349:VAL:HG11 | 1.83                     | 0.44              |
| 1:A:59:ILE:HD11  | 1:B:80:LYS:HE2   | 1.99                     | 0.44              |
| 1:B:233:ARG:HH12 | 1:B:349:VAL:CG1  | 2.29                     | 0.44              |
| 1:B:271:GLN:O    | 1:B:275:MET:HG3  | 2.18                     | 0.44              |
| 1:B:370:LYS:HA   | 1:B:370:LYS:CE   | 2.40                     | 0.44              |
| 1:C:450:THR:O    | 1:C:454:ASN:ND2  | 2.51                     | 0.44              |
| 1:C:483:GLU:HG3  | 1:C:485:LYS:CE   | 2.48                     | 0.44              |
| 1:D:119:ILE:HD11 | 1:D:435:LEU:HD23 | 1.99                     | 0.44              |
| 1:D:266:MET:O    | 1:D:270:GLU:HG3  | 2.18                     | 0.44              |
| 1:F:69:LEU:HB3   | 1:F:83:VAL:HG22  | 1.99                     | 0.44              |
| 1:F:450:THR:O    | 1:F:454:ASN:ND2  | 2.51                     | 0.44              |
| 1:H:245:ALA:HB1  | 1:H:247:GLU:CG   | 2.48                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:297:ILE:HG22 | 1:H:302:GLN:HG3  | 2.00                     | 0.44              |
| 1:A:380:THR:HG23 | 1:A:383:VAL:H    | 1.83                     | 0.43              |
| 1:A:425:TYR:O    | 1:A:428:GLN:HG3  | 2.18                     | 0.43              |
| 1:B:458:ASP:O    | 1:B:459:THR:C    | 2.57                     | 0.43              |
| 1:D:110:LYS:HB3  | 1:D:439:ASN:HD22 | 1.83                     | 0.43              |
| 1:E:233:ARG:NH1  | 1:E:349:VAL:CG1  | 2.72                     | 0.43              |
| 1:F:31:ALA:CB    | 1:F:76:HIS:CD2   | 3.01                     | 0.43              |
| 1:F:146:VAL:CG2  | 1:F:147:ASP:N    | 2.81                     | 0.43              |
| 1:F:416:ILE:CD1  | 1:F:466:VAL:HG12 | 2.48                     | 0.43              |
| 1:G:75:GLN:CG    | 1:H:13:PRO:HD3   | 2.41                     | 0.43              |
| 1:G:392:GLU:O    | 1:G:396:LYS:HB2  | 2.17                     | 0.43              |
| 1:A:19:TYR:HB3   | 1:A:23:ASP:HB3   | 2.00                     | 0.43              |
| 1:A:217:ARG:HH11 | 1:A:217:ARG:CB   | 2.30                     | 0.43              |
| 1:C:17:GLN:NE2   | 1:C:17:GLN:N     | 2.59                     | 0.43              |
| 1:D:62:THR:OG1   | 1:D:63:ASN:N     | 2.51                     | 0.43              |
| 1:D:430:GLY:CA   | 1:D:434:ALA:HB2  | 2.48                     | 0.43              |
| 1:E:35:ILE:HG21  | 1:E:82:MET:CB    | 2.47                     | 0.43              |
| 1:E:167:ALA:C    | 1:E:169:SER:N    | 2.71                     | 0.43              |
| 1:G:31:ALA:CB    | 1:G:76:HIS:CD2   | 3.01                     | 0.43              |
| 1:G:392:GLU:O    | 1:G:396:LYS:HE3  | 2.18                     | 0.43              |
| 1:A:64:ASP:O     | 1:A:68:ILE:HG13  | 2.18                     | 0.43              |
| 1:A:413:ALA:N    | 1:A:414:PRO:CD   | 2.81                     | 0.43              |
| 1:C:147:ASP:O    | 1:C:149:ASP:N    | 2.51                     | 0.43              |
| 1:D:201:LYS:HB2  | 1:D:323:LYS:HE3  | 2.00                     | 0.43              |
| 1:D:220:VAL:HG11 | 1:D:360:MET:CE   | 2.48                     | 0.43              |
| 1:E:143:ALA:HB3  | 1:E:145:ARG:NH1  | 2.34                     | 0.43              |
| 1:F:467:ILE:HG22 | 1:F:471:LYS:HD2  | 1.99                     | 0.43              |
| 1:G:138:ILE:O    | 1:G:142:ILE:HG12 | 2.18                     | 0.43              |
| 1:H:25:GLN:O     | 1:H:29:ILE:HG13  | 2.17                     | 0.43              |
| 1:A:80:LYS:HE2   | 1:H:59:ILE:HD11  | 1.99                     | 0.43              |
| 1:B:262:PRO:HG2  | 1:C:267:SER:HB2  | 2.01                     | 0.43              |
| 1:B:483:GLU:HG3  | 1:B:485:LYS:HZ3  | 1.80                     | 0.43              |
| 1:C:221:ILE:HD11 | 1:C:324:LEU:HD11 | 2.01                     | 0.43              |
| 1:C:262:PRO:HG2  | 1:D:267:SER:HB2  | 2.00                     | 0.43              |
| 1:C:446:ILE:HA   | 1:C:449:LYS:HB2  | 2.00                     | 0.43              |
| 1:D:180:GLU:HG2  | 1:D:215:LEU:CD2  | 2.48                     | 0.43              |
| 1:D:353:ARG:NH2  | 1:D:364:GLU:OE2  | 2.52                     | 0.43              |
| 1:E:393:ASP:O    | 1:E:397:VAL:HG22 | 2.19                     | 0.43              |
| 1:F:265:LEU:O    | 1:F:269:LEU:HD13 | 2.18                     | 0.43              |
| 1:H:458:ASP:OD2  | 1:H:458:ASP:C    | 2.56                     | 0.43              |
| 1:A:94:GLY:HA3   | 1:A:396:LYS:HB3  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:103:ILE:O    | 1:B:103:ILE:HG22 | 2.18                     | 0.43              |
| 1:B:106:GLU:HG2  | 1:B:446:ILE:CG1  | 2.48                     | 0.43              |
| 1:D:51:MET:HE1   | 1:E:77:PRO:HB2   | 2.00                     | 0.43              |
| 1:E:239:ILE:HD11 | 1:E:347:ALA:HB3  | 2.00                     | 0.43              |
| 1:E:446:ILE:HD12 | 1:E:446:ILE:N    | 2.33                     | 0.43              |
| 1:E:462:MET:HE3  | 1:E:462:MET:HA   | 2.00                     | 0.43              |
| 1:F:146:VAL:HG21 | 1:F:153:THR:HG21 | 1.99                     | 0.43              |
| 1:F:423:ASP:O    | 1:F:426:ALA:HB3  | 2.18                     | 0.43              |
| 1:G:106:GLU:OE1  | 1:G:106:GLU:HA   | 2.18                     | 0.43              |
| 1:H:94:GLY:HA2   | 1:H:396:LYS:HD2  | 1.99                     | 0.43              |
| 1:A:257:ILE:HG22 | 1:A:259:ILE:CD1  | 2.47                     | 0.43              |
| 1:B:155:LEU:HD22 | 1:B:179:VAL:HG21 | 1.99                     | 0.43              |
| 1:B:207:GLY:O    | 1:B:208:GLU:HB2  | 2.18                     | 0.43              |
| 1:C:206:ALA:CA   | 1:C:384:ILE:HD11 | 2.44                     | 0.43              |
| 1:E:286:THR:HG22 | 1:E:341:PRO:HG3  | 2.00                     | 0.43              |
| 1:E:392:GLU:O    | 1:E:396:LYS:HB2  | 2.19                     | 0.43              |
| 1:F:19:TYR:N     | 1:F:19:TYR:CD1   | 2.86                     | 0.43              |
| 1:F:20:VAL:HG12  | 1:F:21:GLY:N     | 2.33                     | 0.43              |
| 1:F:217:ARG:HB3  | 1:F:217:ARG:NH1  | 2.33                     | 0.43              |
| 1:A:261:SER:O    | 1:A:264:GLN:HG3  | 2.19                     | 0.43              |
| 1:A:426:ALA:HB1  | 1:A:438:GLU:HG3  | 2.00                     | 0.43              |
| 1:B:147:ASP:O    | 1:B:149:ASP:N    | 2.52                     | 0.43              |
| 1:C:300:LEU:HD23 | 1:C:300:LEU:HA   | 1.92                     | 0.43              |
| 1:C:333:VAL:HG21 | 1:C:339:LEU:HD13 | 2.00                     | 0.43              |
| 1:D:281:ASP:O    | 1:D:285:GLN:HG3  | 2.18                     | 0.43              |
| 1:E:297:ILE:CG2  | 1:E:302:GLN:HG3  | 2.47                     | 0.43              |
| 1:F:445:LYS:C    | 1:F:448:PRO:HD2  | 2.39                     | 0.43              |
| 1:H:35:ILE:HG13  | 1:H:79:ALA:HB1   | 2.01                     | 0.43              |
| 1:H:271:GLN:O    | 1:H:275:MET:HG3  | 2.19                     | 0.43              |
| 1:H:293:VAL:CG2  | 1:H:297:ILE:HD11 | 2.49                     | 0.43              |
| 1:A:409:PRO:HB3  | 1:A:490:LEU:CD1  | 2.46                     | 0.43              |
| 1:B:149:ASP:N    | 1:B:149:ASP:OD2  | 2.50                     | 0.43              |
| 1:B:195:VAL:HB   | 1:B:399:LYS:HG3  | 2.01                     | 0.43              |
| 1:D:156:LYS:O    | 1:D:157:ILE:C    | 2.56                     | 0.43              |
| 1:E:210:VAL:HA   | 1:E:377:ARG:O    | 2.19                     | 0.43              |
| 1:F:443:ALA:O    | 1:F:446:ILE:HG13 | 2.18                     | 0.43              |
| 1:H:207:GLY:O    | 1:H:208:GLU:HB2  | 2.18                     | 0.43              |
| 1:A:17:GLN:N     | 1:A:17:GLN:NE2   | 2.67                     | 0.43              |
| 1:E:81:MET:CE    | 1:E:514:MET:SD   | 3.07                     | 0.43              |
| 1:E:126:LYS:O    | 1:E:130:LEU:HG   | 2.19                     | 0.43              |
| 1:E:204:LYS:CD   | 1:E:388:GLU:OE2  | 2.62                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:189:LYS:HD2  | 1:F:190:ASP:N    | 2.33                     | 0.43              |
| 1:H:462:MET:O    | 1:H:462:MET:HE3  | 2.19                     | 0.43              |
| 1:H:469:GLU:O    | 1:H:473:ARG:N    | 2.52                     | 0.43              |
| 1:H:503:GLN:HA   | 1:H:503:GLN:NE2  | 2.33                     | 0.43              |
| 1:B:110:LYS:HE3  | 1:B:442:ASP:OD1  | 2.19                     | 0.43              |
| 1:D:205:LYS:O    | 1:D:377:ARG:NH1  | 2.51                     | 0.43              |
| 1:E:154:LEU:HD12 | 1:E:154:LEU:HA   | 1.88                     | 0.43              |
| 1:E:291:VAL:HG23 | 1:E:310:ILE:CG2  | 2.48                     | 0.43              |
| 1:F:224:GLU:O    | 1:F:313:VAL:HG13 | 2.19                     | 0.43              |
| 1:F:269:LEU:CD1  | 1:G:251:THR:HG23 | 2.40                     | 0.43              |
| 1:F:272:GLU:HA   | 1:F:275:MET:HE2  | 2.00                     | 0.43              |
| 1:F:433:GLU:O    | 1:F:437:ILE:HG13 | 2.18                     | 0.43              |
| 1:A:462:MET:CE   | 1:A:486:PRO:HD3  | 2.47                     | 0.42              |
| 1:B:59:ILE:HD12  | 1:B:59:ILE:H     | 1.81                     | 0.42              |
| 1:C:182:VAL:O    | 1:C:186:ALA:HB2  | 2.19                     | 0.42              |
| 1:E:300:LEU:HD23 | 1:E:300:LEU:HA   | 1.84                     | 0.42              |
| 1:C:75:GLN:HB2   | 1:D:11:ILE:CA    | 2.49                     | 0.42              |
| 1:C:196:ASP:OD1  | 1:C:198:ASP:HB2  | 2.19                     | 0.42              |
| 1:C:205:LYS:HZ1  | 1:C:358:GLU:HG2  | 1.84                     | 0.42              |
| 1:D:425:TYR:O    | 1:D:428:GLN:HG3  | 2.19                     | 0.42              |
| 1:D:517:ARG:HE   | 1:D:517:ARG:HB3  | 1.68                     | 0.42              |
| 1:E:72:ILE:HG22  | 1:E:74:LEU:HD23  | 2.01                     | 0.42              |
| 1:E:215:LEU:HD11 | 1:E:372:VAL:CG2  | 2.48                     | 0.42              |
| 1:E:217:ARG:HA   | 1:E:372:VAL:HG23 | 2.01                     | 0.42              |
| 1:E:221:ILE:HD11 | 1:E:324:LEU:HD11 | 2.00                     | 0.42              |
| 1:E:286:THR:CA   | 1:E:341:PRO:HG3  | 2.49                     | 0.42              |
| 1:E:404:ASP:OD1  | 1:E:499:ARG:HB2  | 2.18                     | 0.42              |
| 1:E:410:ALA:CB   | 1:E:494:ILE:HG22 | 2.46                     | 0.42              |
| 1:E:443:ALA:O    | 1:E:446:ILE:CD1  | 2.68                     | 0.42              |
| 1:F:50:LYS:HD2   | 1:F:68:ILE:HD13  | 2.01                     | 0.42              |
| 1:F:182:VAL:HG13 | 1:F:195:VAL:HG11 | 1.99                     | 0.42              |
| 1:G:197:LEU:HD22 | 1:G:395:VAL:CG1  | 2.49                     | 0.42              |
| 1:H:172:GLU:OE1  | 1:H:172:GLU:HA   | 2.19                     | 0.42              |
| 1:H:218:GLY:HA3  | 1:H:363:VAL:O    | 2.19                     | 0.42              |
| 1:H:446:ILE:O    | 1:H:450:THR:HG23 | 2.19                     | 0.42              |
| 1:A:269:LEU:CD1  | 1:B:251:THR:HG23 | 2.42                     | 0.42              |
| 1:A:348:GLU:HB3  | 1:A:365:GLY:HA3  | 2.00                     | 0.42              |
| 1:B:72:ILE:HG22  | 1:B:74:LEU:HD23  | 2.02                     | 0.42              |
| 1:B:116:ASP:C    | 1:B:118:ASN:H    | 2.22                     | 0.42              |
| 1:C:114:LEU:HD11 | 1:C:436:ALA:HA   | 2.01                     | 0.42              |
| 1:C:477:ILE:HA   | 1:C:487:ALA:O    | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:167:ALA:C    | 1:G:169:SER:H    | 2.23                     | 0.42              |
| 1:A:20:VAL:HG12  | 1:A:21:GLY:N     | 2.35                     | 0.42              |
| 1:A:391:LEU:O    | 1:A:394:ALA:HB3  | 2.19                     | 0.42              |
| 1:B:17:GLN:H     | 1:B:17:GLN:HE21  | 1.67                     | 0.42              |
| 1:B:144:ILE:CD1  | 1:B:490:LEU:HD21 | 2.47                     | 0.42              |
| 1:C:397:VAL:HG23 | 1:C:398:VAL:N    | 2.34                     | 0.42              |
| 1:C:449:LYS:HE2  | 1:C:449:LYS:HB3  | 1.85                     | 0.42              |
| 1:E:37:GLU:HG2   | 1:E:40:ARG:CZ    | 2.49                     | 0.42              |
| 1:E:503:GLN:HA   | 1:E:503:GLN:HE21 | 1.84                     | 0.42              |
| 1:E:524:ALA:O    | 1:E:525:LYS:HD3  | 2.19                     | 0.42              |
| 1:F:146:VAL:CG2  | 1:F:147:ASP:H    | 2.32                     | 0.42              |
| 1:F:197:LEU:HD22 | 1:F:395:VAL:HG12 | 2.01                     | 0.42              |
| 1:F:245:ALA:HB1  | 1:F:247:GLU:HG2  | 2.01                     | 0.42              |
| 1:F:503:GLN:NE2  | 1:F:506:LYS:HD2  | 2.35                     | 0.42              |
| 1:H:52:LEU:HD13  | 1:H:71:LYS:HB2   | 2.02                     | 0.42              |
| 1:A:23:ASP:O     | 1:A:27:LEU:HG    | 2.19                     | 0.42              |
| 1:A:94:GLY:HA2   | 1:A:396:LYS:HD2  | 2.00                     | 0.42              |
| 1:C:29:ILE:HG23  | 1:C:108:LEU:HB3  | 2.01                     | 0.42              |
| 1:C:209:GLY:H    | 1:C:212:GLU:HG2  | 1.83                     | 0.42              |
| 1:C:259:ILE:HG12 | 1:C:265:LEU:HD23 | 2.02                     | 0.42              |
| 1:C:261:SER:H    | 1:C:264:GLN:HG3  | 1.83                     | 0.42              |
| 1:D:74:LEU:HD13  | 1:D:79:ALA:HB1   | 2.01                     | 0.42              |
| 1:D:138:ILE:O    | 1:D:142:ILE:HG12 | 2.20                     | 0.42              |
| 1:D:144:ILE:O    | 1:D:144:ILE:HG22 | 2.19                     | 0.42              |
| 1:E:276:LEU:HD23 | 1:E:300:LEU:CB   | 2.46                     | 0.42              |
| 1:F:72:ILE:HG22  | 1:F:74:LEU:CD2   | 2.50                     | 0.42              |
| 1:F:109:ARG:HG2  | 1:F:109:ARG:HH11 | 1.84                     | 0.42              |
| 1:F:112:GLU:HA   | 1:F:115:LEU:HD12 | 2.00                     | 0.42              |
| 1:G:293:VAL:HG21 | 1:G:297:ILE:HD11 | 2.01                     | 0.42              |
| 1:H:91:LYS:O     | 1:H:91:LYS:CG    | 2.67                     | 0.42              |
| 1:C:270:GLU:HA   | 1:C:273:GLU:HG3  | 2.02                     | 0.42              |
| 1:E:250:LYS:NZ   | 1:F:253:THR:HA   | 2.35                     | 0.42              |
| 1:H:109:ARG:NH2  | 1:H:110:LYS:HD3  | 2.34                     | 0.42              |
| 1:H:147:ASP:O    | 1:H:149:ASP:N    | 2.53                     | 0.42              |
| 1:H:304:TYR:O    | 1:H:308:TYR:CD1  | 2.65                     | 0.42              |
| 1:H:462:MET:HE2  | 1:H:486:PRO:HG3  | 2.02                     | 0.42              |
| 1:A:236:ASN:HA   | 1:A:346:TYR:HE1  | 1.85                     | 0.42              |
| 1:B:35:ILE:HD13  | 1:B:35:ILE:HA    | 1.89                     | 0.42              |
| 1:C:23:ASP:O     | 1:C:27:LEU:HG    | 2.19                     | 0.42              |
| 1:C:462:MET:CE   | 1:C:486:PRO:HD3  | 2.50                     | 0.42              |
| 1:D:76:HIS:HA    | 1:D:77:PRO:HD3   | 1.91                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:126:LYS:O    | 1:F:130:LEU:HG   | 2.20                     | 0.42              |
| 1:F:286:THR:HA   | 1:F:341:PRO:HG3  | 2.01                     | 0.42              |
| 1:F:467:ILE:O    | 1:F:471:LYS:HG3  | 2.20                     | 0.42              |
| 1:G:45:PRO:HB2   | 1:G:481:VAL:HG21 | 2.00                     | 0.42              |
| 1:H:498:LEU:HD22 | 1:H:498:LEU:O    | 2.19                     | 0.42              |
| 1:A:76:HIS:CD2   | 1:A:78:ALA:HB3   | 2.55                     | 0.42              |
| 1:A:143:ALA:HB3  | 1:A:145:ARG:NH1  | 2.35                     | 0.42              |
| 1:A:245:ALA:HB1  | 1:A:247:GLU:HG2  | 2.00                     | 0.42              |
| 1:A:446:ILE:N    | 1:A:446:ILE:HD12 | 2.34                     | 0.42              |
| 1:B:35:ILE:HG22  | 1:B:36:ALA:N     | 2.35                     | 0.42              |
| 1:C:461:GLU:HG2  | 1:C:465:LYS:HZ1  | 1.83                     | 0.42              |
| 1:D:76:HIS:CD2   | 1:D:78:ALA:HB3   | 2.55                     | 0.42              |
| 1:E:239:ILE:HG23 | 1:E:290:VAL:HG12 | 2.01                     | 0.42              |
| 1:E:348:GLU:O    | 1:E:349:VAL:HG23 | 2.19                     | 0.42              |
| 1:F:25:GLN:O     | 1:F:29:ILE:HG13  | 2.20                     | 0.42              |
| 1:F:446:ILE:HD12 | 1:F:446:ILE:H    | 1.85                     | 0.42              |
| 1:H:433:GLU:CD   | 1:H:433:GLU:H    | 2.22                     | 0.42              |
| 1:A:227:HIS:HB3  | 1:A:230:MET:SD   | 2.59                     | 0.42              |
| 1:A:469:GLU:HG3  | 1:A:486:PRO:HB2  | 2.01                     | 0.42              |
| 1:B:370:LYS:HE2  | 1:B:370:LYS:CA   | 2.42                     | 0.42              |
| 1:B:446:ILE:HD12 | 1:B:446:ILE:H    | 1.85                     | 0.42              |
| 1:D:212:GLU:CA   | 1:D:212:GLU:OE2  | 2.68                     | 0.42              |
| 1:C:37:GLU:HA    | 1:C:40:ARG:HG2   | 2.01                     | 0.42              |
| 1:C:277:LYS:HB2  | 1:C:304:TYR:CE2  | 2.55                     | 0.42              |
| 1:C:315:ARG:NH1  | 1:C:315:ARG:CG   | 2.82                     | 0.42              |
| 1:C:409:PRO:HA   | 1:C:495:ILE:HG22 | 2.02                     | 0.42              |
| 1:E:114:LEU:HD22 | 1:E:119:ILE:HD12 | 2.00                     | 0.42              |
| 1:E:117:GLN:O    | 1:E:118:ASN:HB2  | 2.19                     | 0.42              |
| 1:E:152:GLU:HG3  | 1:E:153:THR:N    | 2.34                     | 0.42              |
| 1:E:188:LYS:HD3  | 1:E:193:TYR:CE1  | 2.54                     | 0.42              |
| 1:E:233:ARG:HG3  | 1:E:233:ARG:NH1  | 2.32                     | 0.42              |
| 1:F:37:GLU:HA    | 1:F:40:ARG:HG2   | 2.01                     | 0.42              |
| 1:F:342:GLU:OE2  | 1:F:342:GLU:N    | 2.50                     | 0.42              |
| 1:G:37:GLU:HA    | 1:G:40:ARG:HG2   | 2.01                     | 0.42              |
| 1:G:227:HIS:HA   | 1:G:228:PRO:HD3  | 1.91                     | 0.42              |
| 1:H:197:LEU:HD22 | 1:H:395:VAL:CG1  | 2.50                     | 0.42              |
| 1:H:370:LYS:HA   | 1:H:370:LYS:CE   | 2.45                     | 0.42              |
| 1:D:40:ARG:HE    | 1:D:450:THR:HG21 | 1.85                     | 0.41              |
| 1:D:462:MET:HE2  | 1:D:486:PRO:HG3  | 2.01                     | 0.41              |
| 1:E:340:THR:HG1  | 1:E:342:GLU:HB2  | 1.85                     | 0.41              |
| 1:F:250:LYS:NZ   | 1:G:253:THR:HA   | 2.34                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:330:ALA:HB2  | 1:F:345:GLY:HA3  | 2.01                     | 0.41              |
| 1:G:204:LYS:HD3  | 1:G:388:GLU:OE2  | 2.19                     | 0.41              |
| 1:G:481:VAL:HG13 | 3:G:7528:ADP:C2  | 2.55                     | 0.41              |
| 1:H:412:GLY:O    | 1:H:415:GLU:HG2  | 2.20                     | 0.41              |
| 1:C:51:MET:HB2   | 1:D:518:ILE:HD13 | 2.01                     | 0.41              |
| 1:D:208:GLU:HB3  | 1:D:212:GLU:HG3  | 2.01                     | 0.41              |
| 1:D:292:PHE:CE2  | 1:D:313:VAL:HG21 | 2.56                     | 0.41              |
| 1:E:144:ILE:O    | 1:E:144:ILE:HG22 | 2.19                     | 0.41              |
| 1:E:210:VAL:O    | 1:E:210:VAL:HG12 | 2.20                     | 0.41              |
| 1:G:208:GLU:CG   | 1:G:377:ARG:HH21 | 2.33                     | 0.41              |
| 1:G:412:GLY:HA2  | 1:G:415:GLU:CG   | 2.50                     | 0.41              |
| 1:A:17:GLN:NE2   | 1:A:17:GLN:H     | 2.18                     | 0.41              |
| 1:A:401:VAL:O    | 1:A:405:GLY:N    | 2.51                     | 0.41              |
| 1:B:106:GLU:CB   | 1:B:446:ILE:HG12 | 2.51                     | 0.41              |
| 1:C:94:GLY:HA2   | 1:C:396:LYS:HD2  | 2.01                     | 0.41              |
| 1:C:469:GLU:O    | 1:C:473:ARG:N    | 2.53                     | 0.41              |
| 1:E:463:LEU:O    | 1:E:467:ILE:HG13 | 2.21                     | 0.41              |
| 1:G:76:HIS:CD2   | 1:G:78:ALA:HB3   | 2.55                     | 0.41              |
| 1:G:346:TYR:OH   | 1:G:348:GLU:HA   | 2.20                     | 0.41              |
| 1:A:138:ILE:O    | 1:A:142:ILE:HG12 | 2.20                     | 0.41              |
| 1:A:241:LEU:HD12 | 1:A:292:PHE:HB2  | 2.02                     | 0.41              |
| 1:A:369:PRO:O    | 1:A:370:LYS:CE   | 2.62                     | 0.41              |
| 1:A:483:GLU:OE1  | 1:A:483:GLU:HA   | 2.21                     | 0.41              |
| 1:B:346:TYR:CG   | 1:B:347:ALA:N    | 2.88                     | 0.41              |
| 1:C:114:LEU:HD22 | 1:C:119:ILE:HD12 | 2.02                     | 0.41              |
| 1:D:145:ARG:HD3  | 1:D:145:ARG:HA   | 1.83                     | 0.41              |
| 1:D:216:VAL:O    | 1:D:372:VAL:CG2  | 2.68                     | 0.41              |
| 1:D:417:GLU:OE2  | 1:D:470:HIS:NE2  | 2.42                     | 0.41              |
| 1:D:462:MET:O    | 1:D:462:MET:HE3  | 2.21                     | 0.41              |
| 1:E:211:GLU:OE1  | 1:E:211:GLU:HA   | 2.21                     | 0.41              |
| 1:F:54:ASP:OD1   | 1:F:58:ASP:CB    | 2.64                     | 0.41              |
| 1:G:15:GLY:O     | 1:G:524:ALA:O    | 2.39                     | 0.41              |
| 1:G:167:ALA:HB2  | 1:G:387:VAL:HG22 | 2.01                     | 0.41              |
| 1:H:94:GLY:HA3   | 1:H:396:LYS:HB3  | 2.02                     | 0.41              |
| 1:A:72:ILE:HD11  | 1:B:522:ILE:HD12 | 2.02                     | 0.41              |
| 1:A:120:HIS:ND1  | 1:A:121:PRO:HD2  | 2.35                     | 0.41              |
| 1:A:293:VAL:HG21 | 1:A:297:ILE:HD11 | 2.03                     | 0.41              |
| 1:B:293:VAL:HG21 | 1:B:297:ILE:HD11 | 2.02                     | 0.41              |
| 1:B:483:GLU:HG3  | 1:B:485:LYS:HZ1  | 1.86                     | 0.41              |
| 1:C:35:ILE:HD12  | 1:C:69:LEU:HD22  | 2.02                     | 0.41              |
| 1:D:498:LEU:HD13 | 1:D:502:LYS:HD3  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:197:LEU:CD1  | 1:E:396:LYS:HG3  | 2.51                     | 0.41              |
| 1:E:420:ILE:HD13 | 1:E:471:LYS:HG3  | 2.02                     | 0.41              |
| 1:E:498:LEU:C    | 1:E:498:LEU:HD13 | 2.41                     | 0.41              |
| 1:F:94:GLY:HA3   | 1:F:396:LYS:HB3  | 2.02                     | 0.41              |
| 1:F:173:LEU:O    | 1:F:176:LYS:HB3  | 2.19                     | 0.41              |
| 1:G:524:ALA:O    | 1:G:525:LYS:CD   | 2.69                     | 0.41              |
| 1:H:273:GLU:HG2  | 1:H:300:LEU:CD1  | 2.50                     | 0.41              |
| 1:H:498:LEU:C    | 1:H:498:LEU:HD13 | 2.40                     | 0.41              |
| 1:A:51:MET:CE    | 1:B:77:PRO:HB2   | 2.50                     | 0.41              |
| 1:A:266:MET:HG2  | 1:B:271:GLN:NE2  | 2.36                     | 0.41              |
| 1:A:335:ASN:HB2  | 1:H:303:HIS:CD2  | 2.54                     | 0.41              |
| 1:B:91:LYS:O     | 1:B:91:LYS:CG    | 2.68                     | 0.41              |
| 1:C:12:LEU:HD23  | 1:C:13:PRO:N     | 2.34                     | 0.41              |
| 1:C:201:LYS:HE2  | 1:C:203:GLU:OE1  | 2.21                     | 0.41              |
| 1:C:259:ILE:N    | 1:C:259:ILE:CD1  | 2.84                     | 0.41              |
| 1:D:304:TYR:O    | 1:D:308:TYR:CD1  | 2.67                     | 0.41              |
| 1:E:35:ILE:HA    | 1:E:35:ILE:HD13  | 1.85                     | 0.41              |
| 1:E:75:GLN:HB2   | 1:F:11:ILE:C     | 2.41                     | 0.41              |
| 1:E:380:THR:CG2  | 1:E:383:VAL:H    | 2.28                     | 0.41              |
| 1:E:462:MET:HE1  | 1:E:486:PRO:HD3  | 2.02                     | 0.41              |
| 1:F:109:ARG:HG2  | 1:F:109:ARG:NH1  | 2.36                     | 0.41              |
| 1:F:470:HIS:CE1  | 1:F:475:LEU:HA   | 2.55                     | 0.41              |
| 1:G:192:LYS:HE2  | 1:G:192:LYS:HB3  | 1.87                     | 0.41              |
| 1:G:342:GLU:OE2  | 1:G:342:GLU:N    | 2.52                     | 0.41              |
| 1:H:209:GLY:C    | 1:H:211:GLU:H    | 2.24                     | 0.41              |
| 1:A:103:ILE:O    | 1:A:103:ILE:HG22 | 2.20                     | 0.41              |
| 1:A:157:ILE:HG13 | 1:A:401:VAL:HG21 | 2.03                     | 0.41              |
| 1:A:257:ILE:HG12 | 1:H:259:ILE:CG2  | 2.51                     | 0.41              |
| 1:A:291:VAL:O    | 1:A:312:ALA:HA   | 2.21                     | 0.41              |
| 1:B:142:ILE:HD13 | 1:B:417:GLU:HG2  | 2.03                     | 0.41              |
| 1:C:317:LYS:O    | 1:C:320:ASP:HB2  | 2.21                     | 0.41              |
| 1:C:409:PRO:HB2  | 1:C:489:MET:HB2  | 2.02                     | 0.41              |
| 1:C:458:ASP:O    | 1:C:459:THR:C    | 2.59                     | 0.41              |
| 1:D:126:LYS:O    | 1:D:130:LEU:HG   | 2.21                     | 0.41              |
| 1:D:317:LYS:O    | 1:D:320:ASP:N    | 2.53                     | 0.41              |
| 1:D:381:GLU:O    | 1:D:384:ILE:HB   | 2.21                     | 0.41              |
| 1:E:37:GLU:HA    | 1:E:40:ARG:HG2   | 2.03                     | 0.41              |
| 1:E:103:ILE:CG1  | 1:E:447:ILE:HD11 | 2.51                     | 0.41              |
| 1:F:35:ILE:HG22  | 1:F:36:ALA:N     | 2.35                     | 0.41              |
| 1:F:154:LEU:HD12 | 1:F:154:LEU:HA   | 1.83                     | 0.41              |
| 1:F:189:LYS:HD2  | 1:F:189:LYS:C    | 2.41                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:94:GLY:CA    | 1:H:396:LYS:HD2  | 2.51                     | 0.41              |
| 1:A:12:LEU:HD13  | 1:A:16:THR:CG2   | 2.50                     | 0.41              |
| 1:B:490:LEU:CD1  | 1:B:490:LEU:N    | 2.84                     | 0.41              |
| 1:C:103:ILE:O    | 1:C:107:LEU:HB2  | 2.21                     | 0.41              |
| 1:D:72:ILE:CG2   | 1:D:73:ASP:N     | 2.83                     | 0.41              |
| 1:D:73:ASP:O     | 1:E:13:PRO:CD    | 2.64                     | 0.41              |
| 1:D:114:LEU:CD1  | 1:D:436:ALA:HA   | 2.51                     | 0.41              |
| 1:D:206:ALA:CA   | 1:D:384:ILE:HD11 | 2.47                     | 0.41              |
| 1:E:146:VAL:HG21 | 1:E:153:THR:HG21 | 2.03                     | 0.41              |
| 1:F:31:ALA:HB2   | 1:F:76:HIS:CD2   | 2.56                     | 0.41              |
| 1:H:227:HIS:ND1  | 1:H:228:PRO:HD2  | 2.36                     | 0.41              |
| 1:H:311:MET:CE   | 1:H:350:VAL:HG12 | 2.50                     | 0.41              |
| 1:H:410:ALA:HB3  | 1:H:494:ILE:HG22 | 2.02                     | 0.41              |
| 1:A:81:MET:CE    | 1:A:514:MET:SD   | 3.09                     | 0.41              |
| 1:A:141:GLU:C    | 1:A:143:ALA:H    | 2.23                     | 0.41              |
| 1:A:330:ALA:HB2  | 1:A:345:GLY:HA3  | 2.03                     | 0.41              |
| 1:A:446:ILE:HD12 | 1:A:446:ILE:H    | 1.86                     | 0.41              |
| 1:A:498:LEU:HD13 | 1:A:498:LEU:C    | 2.41                     | 0.41              |
| 1:B:59:ILE:N     | 1:B:59:ILE:CD1   | 2.79                     | 0.41              |
| 1:C:85:VAL:HG13  | 1:C:507:SER:HB3  | 2.02                     | 0.41              |
| 1:C:202:PHE:HE2  | 1:C:374:ILE:HD12 | 1.86                     | 0.41              |
| 1:C:216:VAL:O    | 1:C:218:GLY:N    | 2.52                     | 0.41              |
| 1:D:65:CYS:HB3   | 1:D:97:THR:OG1   | 2.21                     | 0.41              |
| 1:D:188:LYS:HG3  | 1:D:192:LYS:C    | 2.40                     | 0.41              |
| 1:D:189:LYS:HD2  | 1:D:189:LYS:C    | 2.40                     | 0.41              |
| 1:D:483:GLU:HG3  | 1:D:485:LYS:HE2  | 2.03                     | 0.41              |
| 1:F:217:ARG:CA   | 1:F:372:VAL:HG23 | 2.44                     | 0.41              |
| 1:F:233:ARG:HD2  | 1:F:351:GLU:OE2  | 2.21                     | 0.41              |
| 1:G:75:GLN:NE2   | 1:H:13:PRO:HG3   | 2.36                     | 0.41              |
| 1:G:502:LYS:HB3  | 1:G:502:LYS:HE3  | 1.90                     | 0.41              |
| 1:H:29:ILE:CD1   | 1:H:112:GLU:HB2  | 2.50                     | 0.41              |
| 1:H:481:VAL:HG13 | 3:H:8528:ADP:C2  | 2.56                     | 0.41              |
| 1:C:109:ARG:HG2  | 1:C:109:ARG:NH1  | 2.36                     | 0.41              |
| 1:C:119:ILE:HD11 | 1:C:435:LEU:HD23 | 2.02                     | 0.41              |
| 1:D:18:ARG:HA    | 1:D:521:VAL:O    | 2.21                     | 0.41              |
| 1:D:64:ASP:O     | 1:D:68:ILE:HG13  | 2.21                     | 0.41              |
| 1:D:172:GLU:OE1  | 1:D:172:GLU:CA   | 2.69                     | 0.41              |
| 1:E:81:MET:HE2   | 1:E:515:ILE:HG12 | 2.03                     | 0.41              |
| 1:F:216:VAL:O    | 1:F:372:VAL:HG23 | 2.20                     | 0.41              |
| 1:H:209:GLY:C    | 1:H:211:GLU:N    | 2.73                     | 0.41              |
| 1:A:172:GLU:OE1  | 1:A:172:GLU:HA   | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:38:THR:O     | 1:B:50:LYS:CE    | 2.69                     | 0.40              |
| 1:B:166:ASN:O    | 1:B:168:GLU:N    | 2.54                     | 0.40              |
| 1:B:468:SER:O    | 1:B:471:LYS:N    | 2.54                     | 0.40              |
| 1:C:33:ARG:O     | 1:C:37:GLU:HG3   | 2.21                     | 0.40              |
| 1:C:82:MET:HE2   | 1:C:101:VAL:HG13 | 2.01                     | 0.40              |
| 1:D:348:GLU:O    | 1:D:349:VAL:CG2  | 2.67                     | 0.40              |
| 1:D:401:VAL:O    | 1:D:405:GLY:N    | 2.51                     | 0.40              |
| 1:E:232:LYS:HD3  | 1:E:232:LYS:HA   | 1.85                     | 0.40              |
| 1:F:13:PRO:HB2   | 1:F:16:THR:OG1   | 2.21                     | 0.40              |
| 1:F:300:LEU:HD23 | 1:F:300:LEU:HA   | 1.81                     | 0.40              |
| 1:G:136:GLN:HE21 | 1:G:136:GLN:CA   | 2.31                     | 0.40              |
| 1:G:524:ALA:C    | 1:G:525:LYS:HD2  | 2.42                     | 0.40              |
| 1:H:76:HIS:HA    | 1:H:77:PRO:HD3   | 1.86                     | 0.40              |
| 1:H:85:VAL:HG13  | 1:H:507:SER:HB3  | 2.03                     | 0.40              |
| 1:H:196:ASP:OD1  | 1:H:198:ASP:HB2  | 2.21                     | 0.40              |
| 1:H:276:LEU:HD23 | 1:H:300:LEU:HB2  | 2.03                     | 0.40              |
| 1:B:423:ASP:O    | 1:B:426:ALA:HB3  | 2.20                     | 0.40              |
| 1:C:53:VAL:HG21  | 1:D:77:PRO:HG2   | 2.02                     | 0.40              |
| 1:C:195:VAL:HB   | 1:C:399:LYS:HG3  | 2.03                     | 0.40              |
| 1:D:370:LYS:HA   | 1:D:370:LYS:CE   | 2.46                     | 0.40              |
| 1:E:116:ASP:C    | 1:E:118:ASN:H    | 2.24                     | 0.40              |
| 1:F:54:ASP:OD1   | 1:F:58:ASP:N     | 2.54                     | 0.40              |
| 1:F:380:THR:OG1  | 1:F:381:GLU:N    | 2.53                     | 0.40              |
| 1:G:75:GLN:HB2   | 1:H:11:ILE:C     | 2.42                     | 0.40              |
| 1:G:204:LYS:HB2  | 1:G:204:LYS:HE3  | 1.90                     | 0.40              |
| 1:G:496:GLU:OE1  | 1:G:501:LYS:NZ   | 2.48                     | 0.40              |
| 1:H:469:GLU:CB   | 1:H:477:ILE:HG21 | 2.46                     | 0.40              |
| 1:A:106:GLU:HB2  | 1:A:446:ILE:HG12 | 2.03                     | 0.40              |
| 1:A:184:GLN:HA   | 1:A:184:GLN:HE21 | 1.87                     | 0.40              |
| 1:B:273:GLU:HG2  | 1:B:300:LEU:CD1  | 2.51                     | 0.40              |
| 1:B:466:VAL:CG2  | 1:B:486:PRO:HG3  | 2.42                     | 0.40              |
| 1:B:488:ASP:HB3  | 1:B:491:GLU:CG   | 2.48                     | 0.40              |
| 1:C:73:ASP:O     | 1:D:13:PRO:HD3   | 2.21                     | 0.40              |
| 1:C:136:GLN:NE2  | 1:C:502:LYS:HG2  | 2.36                     | 0.40              |
| 1:C:462:MET:HE1  | 1:C:486:PRO:HD3  | 2.04                     | 0.40              |
| 1:C:469:GLU:HA   | 1:C:469:GLU:OE2  | 2.20                     | 0.40              |
| 1:D:475:LEU:HD12 | 1:D:475:LEU:O    | 2.21                     | 0.40              |
| 1:E:172:GLU:HA   | 1:E:172:GLU:OE1  | 2.21                     | 0.40              |
| 1:E:229:ARG:HG2  | 1:E:229:ARG:NH1  | 2.37                     | 0.40              |
| 1:E:311:MET:CE   | 1:E:350:VAL:HG12 | 2.51                     | 0.40              |
| 1:F:525:LYS:O    | 1:F:526:ALA:HB2  | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:35:ILE:HD13  | 1:H:35:ILE:HA    | 1.93                     | 0.40              |
| 1:A:490:LEU:HD12 | 1:A:490:LEU:HA   | 1.80                     | 0.40              |
| 1:B:81:MET:HE1   | 1:B:514:MET:SD   | 2.60                     | 0.40              |
| 1:B:145:ARG:NH1  | 1:B:145:ARG:CG   | 2.78                     | 0.40              |
| 1:C:304:TYR:O    | 1:C:308:TYR:CD1  | 2.75                     | 0.40              |
| 1:C:356:ALA:C    | 1:C:358:GLU:H    | 2.24                     | 0.40              |
| 1:C:483:GLU:HA   | 1:C:483:GLU:OE1  | 2.21                     | 0.40              |
| 1:C:525:LYS:HD2  | 1:C:525:LYS:N    | 2.35                     | 0.40              |
| 1:D:227:HIS:HB3  | 1:D:230:MET:HG3  | 2.03                     | 0.40              |
| 1:D:229:ARG:HH12 | 1:E:332:ILE:H    | 1.69                     | 0.40              |
| 1:D:451:LEU:HD23 | 1:D:451:LEU:HA   | 1.97                     | 0.40              |
| 1:E:18:ARG:HA    | 1:E:521:VAL:O    | 2.22                     | 0.40              |
| 1:E:225:VAL:CG1  | 1:E:230:MET:HB2  | 2.52                     | 0.40              |
| 1:E:311:MET:HE1  | 1:E:350:VAL:CG1  | 2.51                     | 0.40              |
| 1:H:76:HIS:HD2   | 1:H:78:ALA:HB3   | 1.84                     | 0.40              |
| 1:H:123:ILE:HG21 | 1:H:432:LYS:CB   | 2.45                     | 0.40              |
| 1:A:75:GLN:HG3   | 1:B:10:VAL:HG13  | 2.04                     | 0.40              |
| 1:A:227:HIS:HA   | 1:A:228:PRO:HD3  | 1.90                     | 0.40              |
| 1:B:243:ASN:O    | 1:B:243:ASN:CG   | 2.59                     | 0.40              |
| 1:B:418:LEU:O    | 1:B:422:LEU:HB2  | 2.22                     | 0.40              |
| 1:C:118:ASN:HD22 | 1:C:118:ASN:HA   | 1.57                     | 0.40              |
| 1:C:142:ILE:HB   | 1:C:475:LEU:HD21 | 2.01                     | 0.40              |
| 1:C:294:GLN:OE1  | 1:C:321:MET:HG3  | 2.21                     | 0.40              |
| 1:C:348:GLU:HB3  | 1:C:365:GLY:HA3  | 2.02                     | 0.40              |
| 1:C:416:ILE:HD13 | 1:C:466:VAL:HG12 | 2.03                     | 0.40              |
| 1:D:91:LYS:O     | 1:D:91:LYS:CG    | 2.70                     | 0.40              |
| 1:D:106:GLU:HG3  | 1:D:443:ALA:HB1  | 2.03                     | 0.40              |
| 1:D:106:GLU:HB2  | 1:D:446:ILE:HG12 | 2.03                     | 0.40              |
| 1:D:245:ALA:HB1  | 1:D:247:GLU:HG2  | 2.04                     | 0.40              |
| 1:D:257:ILE:HG22 | 1:D:259:ILE:HD12 | 2.04                     | 0.40              |
| 1:D:299:ASP:O    | 1:D:302:GLN:HB2  | 2.21                     | 0.40              |
| 1:E:26:ARG:CG    | 1:E:26:ARG:HH11  | 2.35                     | 0.40              |
| 1:E:143:ALA:HB3  | 1:E:145:ARG:HH12 | 1.87                     | 0.40              |
| 1:E:184:GLN:HE21 | 1:E:184:GLN:CA   | 2.11                     | 0.40              |
| 1:H:147:ASP:OD2  | 1:H:148:PRO:HD2  | 2.20                     | 0.40              |
| 1:H:179:VAL:O    | 1:H:183:LYS:HG3  | 2.22                     | 0.40              |
| 1:H:409:PRO:HA   | 1:H:495:ILE:HG22 | 2.03                     | 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 515/548 (94%)   | 468 (91%)  | 34 (7%)  | 13 (2%)  | 5           | 28 |
| 1   | B     | 515/548 (94%)   | 464 (90%)  | 41 (8%)  | 10 (2%)  | 8           | 36 |
| 1   | C     | 515/548 (94%)   | 463 (90%)  | 42 (8%)  | 10 (2%)  | 8           | 36 |
| 1   | D     | 515/548 (94%)   | 459 (89%)  | 46 (9%)  | 10 (2%)  | 8           | 36 |
| 1   | E     | 515/548 (94%)   | 468 (91%)  | 38 (7%)  | 9 (2%)   | 9           | 39 |
| 1   | F     | 515/548 (94%)   | 467 (91%)  | 36 (7%)  | 12 (2%)  | 6           | 30 |
| 1   | G     | 515/548 (94%)   | 452 (88%)  | 52 (10%) | 11 (2%)  | 7           | 33 |
| 1   | H     | 515/548 (94%)   | 459 (89%)  | 47 (9%)  | 9 (2%)   | 9           | 39 |
| All | All   | 4120/4384 (94%) | 3700 (90%) | 336 (8%) | 84 (2%)  | 7           | 34 |

All (84) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 148 | PRO  |
| 1   | A     | 367 | LYS  |
| 1   | B     | 167 | ALA  |
| 1   | B     | 248 | VAL  |
| 1   | C     | 148 | PRO  |
| 1   | C     | 167 | ALA  |
| 1   | D     | 148 | PRO  |
| 1   | D     | 367 | LYS  |
| 1   | E     | 150 | ASP  |
| 1   | E     | 248 | VAL  |
| 1   | E     | 367 | LYS  |
| 1   | F     | 148 | PRO  |
| 1   | F     | 367 | LYS  |
| 1   | G     | 11  | ILE  |
| 1   | G     | 148 | PRO  |
| 1   | H     | 367 | LYS  |
| 1   | A     | 236 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 473 | ARG  |
| 1   | A     | 475 | LEU  |
| 1   | B     | 367 | LYS  |
| 1   | C     | 152 | GLU  |
| 1   | C     | 235 | GLU  |
| 1   | C     | 367 | LYS  |
| 1   | C     | 430 | GLY  |
| 1   | D     | 167 | ALA  |
| 1   | D     | 248 | VAL  |
| 1   | E     | 47  | GLY  |
| 1   | E     | 148 | PRO  |
| 1   | E     | 168 | GLU  |
| 1   | E     | 235 | GLU  |
| 1   | F     | 168 | GLU  |
| 1   | F     | 236 | ASN  |
| 1   | F     | 459 | THR  |
| 1   | G     | 167 | ALA  |
| 1   | G     | 367 | LYS  |
| 1   | G     | 430 | GLY  |
| 1   | H     | 148 | PRO  |
| 1   | H     | 150 | ASP  |
| 1   | H     | 248 | VAL  |
| 1   | A     | 142 | ILE  |
| 1   | A     | 189 | LYS  |
| 1   | B     | 150 | ASP  |
| 1   | B     | 189 | LYS  |
| 1   | C     | 164 | GLY  |
| 1   | D     | 298 | ASP  |
| 1   | E     | 151 | GLU  |
| 1   | F     | 172 | GLU  |
| 1   | F     | 217 | ARG  |
| 1   | F     | 444 | LEU  |
| 1   | F     | 475 | LEU  |
| 1   | G     | 444 | LEU  |
| 1   | G     | 459 | THR  |
| 1   | H     | 164 | GLY  |
| 1   | H     | 235 | GLU  |
| 1   | H     | 475 | LEU  |
| 1   | A     | 167 | ALA  |
| 1   | B     | 459 | THR  |
| 1   | C     | 248 | VAL  |
| 1   | C     | 459 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 58  | ASP  |
| 1   | D     | 235 | GLU  |
| 1   | F     | 235 | GLU  |
| 1   | F     | 248 | VAL  |
| 1   | G     | 152 | GLU  |
| 1   | G     | 427 | LYS  |
| 1   | H     | 13  | PRO  |
| 1   | A     | 164 | GLY  |
| 1   | A     | 248 | VAL  |
| 1   | B     | 172 | GLU  |
| 1   | B     | 298 | ASP  |
| 1   | B     | 444 | LEU  |
| 1   | C     | 166 | ASN  |
| 1   | D     | 150 | ASP  |
| 1   | D     | 164 | GLY  |
| 1   | H     | 217 | ARG  |
| 1   | A     | 150 | ASP  |
| 1   | D     | 157 | ILE  |
| 1   | F     | 164 | GLY  |
| 1   | G     | 248 | VAL  |
| 1   | A     | 94  | GLY  |
| 1   | A     | 210 | VAL  |
| 1   | E     | 430 | GLY  |
| 1   | G     | 349 | VAL  |
| 1   | B     | 148 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 422/441 (96%) | 389 (92%) | 33 (8%)  | 12          | 42 |
| 1   | B     | 422/441 (96%) | 391 (93%) | 31 (7%)  | 14          | 44 |
| 1   | C     | 422/441 (96%) | 388 (92%) | 34 (8%)  | 11          | 40 |
| 1   | D     | 422/441 (96%) | 387 (92%) | 35 (8%)  | 11          | 39 |
| 1   | E     | 422/441 (96%) | 392 (93%) | 30 (7%)  | 14          | 46 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | F     | 422/441 (96%)   | 387 (92%)  | 35 (8%)  | 11          | 39 |
| 1   | G     | 422/441 (96%)   | 394 (93%)  | 28 (7%)  | 16          | 49 |
| 1   | H     | 422/441 (96%)   | 393 (93%)  | 29 (7%)  | 15          | 48 |
| All | All   | 3376/3528 (96%) | 3121 (92%) | 255 (8%) | 13          | 43 |

All (255) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | GLU  |
| 1   | A     | 17  | GLN  |
| 1   | A     | 23  | ASP  |
| 1   | A     | 26  | ARG  |
| 1   | A     | 35  | ILE  |
| 1   | A     | 41  | THR  |
| 1   | A     | 54  | ASP  |
| 1   | A     | 148 | PRO  |
| 1   | A     | 155 | LEU  |
| 1   | A     | 166 | ASN  |
| 1   | A     | 168 | GLU  |
| 1   | A     | 171 | LYS  |
| 1   | A     | 189 | LYS  |
| 1   | A     | 190 | ASP  |
| 1   | A     | 212 | GLU  |
| 1   | A     | 214 | GLU  |
| 1   | A     | 222 | ASP  |
| 1   | A     | 241 | LEU  |
| 1   | A     | 276 | LEU  |
| 1   | A     | 298 | ASP  |
| 1   | A     | 315 | ARG  |
| 1   | A     | 336 | VAL  |
| 1   | A     | 358 | GLU  |
| 1   | A     | 370 | LYS  |
| 1   | A     | 381 | GLU  |
| 1   | A     | 421 | ARG  |
| 1   | A     | 446 | ILE  |
| 1   | A     | 449 | LYS  |
| 1   | A     | 483 | GLU  |
| 1   | A     | 490 | LEU  |
| 1   | A     | 498 | LEU  |
| 1   | A     | 501 | LYS  |
| 1   | A     | 525 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 11  | ILE  |
| 1   | B     | 17  | GLN  |
| 1   | B     | 23  | ASP  |
| 1   | B     | 26  | ARG  |
| 1   | B     | 35  | ILE  |
| 1   | B     | 41  | THR  |
| 1   | B     | 54  | ASP  |
| 1   | B     | 166 | ASN  |
| 1   | B     | 170 | HIS  |
| 1   | B     | 171 | LYS  |
| 1   | B     | 189 | LYS  |
| 1   | B     | 190 | ASP  |
| 1   | B     | 222 | ASP  |
| 1   | B     | 241 | LEU  |
| 1   | B     | 298 | ASP  |
| 1   | B     | 315 | ARG  |
| 1   | B     | 336 | VAL  |
| 1   | B     | 338 | ASP  |
| 1   | B     | 370 | LYS  |
| 1   | B     | 381 | GLU  |
| 1   | B     | 415 | GLU  |
| 1   | B     | 421 | ARG  |
| 1   | B     | 435 | LEU  |
| 1   | B     | 440 | PHE  |
| 1   | B     | 446 | ILE  |
| 1   | B     | 449 | LYS  |
| 1   | B     | 462 | MET  |
| 1   | B     | 468 | SER  |
| 1   | B     | 483 | GLU  |
| 1   | B     | 519 | ASP  |
| 1   | B     | 525 | LYS  |
| 1   | C     | 11  | ILE  |
| 1   | C     | 14  | GLU  |
| 1   | C     | 17  | GLN  |
| 1   | C     | 26  | ARG  |
| 1   | C     | 35  | ILE  |
| 1   | C     | 41  | THR  |
| 1   | C     | 54  | ASP  |
| 1   | C     | 107 | LEU  |
| 1   | C     | 110 | LYS  |
| 1   | C     | 118 | ASN  |
| 1   | C     | 148 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 166 | ASN  |
| 1   | C     | 170 | HIS  |
| 1   | C     | 171 | LYS  |
| 1   | C     | 189 | LYS  |
| 1   | C     | 190 | ASP  |
| 1   | C     | 214 | GLU  |
| 1   | C     | 222 | ASP  |
| 1   | C     | 241 | LEU  |
| 1   | C     | 252 | GLU  |
| 1   | C     | 276 | LEU  |
| 1   | C     | 298 | ASP  |
| 1   | C     | 315 | ARG  |
| 1   | C     | 338 | ASP  |
| 1   | C     | 358 | GLU  |
| 1   | C     | 370 | LYS  |
| 1   | C     | 381 | GLU  |
| 1   | C     | 421 | ARG  |
| 1   | C     | 428 | GLN  |
| 1   | C     | 435 | LEU  |
| 1   | C     | 446 | ILE  |
| 1   | C     | 449 | LYS  |
| 1   | C     | 483 | GLU  |
| 1   | C     | 525 | LYS  |
| 1   | D     | 11  | ILE  |
| 1   | D     | 17  | GLN  |
| 1   | D     | 26  | ARG  |
| 1   | D     | 35  | ILE  |
| 1   | D     | 63  | ASN  |
| 1   | D     | 107 | LEU  |
| 1   | D     | 110 | LYS  |
| 1   | D     | 148 | PRO  |
| 1   | D     | 166 | ASN  |
| 1   | D     | 171 | LYS  |
| 1   | D     | 189 | LYS  |
| 1   | D     | 190 | ASP  |
| 1   | D     | 212 | GLU  |
| 1   | D     | 222 | ASP  |
| 1   | D     | 241 | LEU  |
| 1   | D     | 252 | GLU  |
| 1   | D     | 258 | ASN  |
| 1   | D     | 276 | LEU  |
| 1   | D     | 289 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 298 | ASP  |
| 1   | D     | 315 | ARG  |
| 1   | D     | 336 | VAL  |
| 1   | D     | 358 | GLU  |
| 1   | D     | 364 | GLU  |
| 1   | D     | 370 | LYS  |
| 1   | D     | 381 | GLU  |
| 1   | D     | 421 | ARG  |
| 1   | D     | 428 | GLN  |
| 1   | D     | 446 | ILE  |
| 1   | D     | 449 | LYS  |
| 1   | D     | 483 | GLU  |
| 1   | D     | 490 | LEU  |
| 1   | D     | 498 | LEU  |
| 1   | D     | 501 | LYS  |
| 1   | D     | 519 | ASP  |
| 1   | E     | 11  | ILE  |
| 1   | E     | 14  | GLU  |
| 1   | E     | 17  | GLN  |
| 1   | E     | 23  | ASP  |
| 1   | E     | 26  | ARG  |
| 1   | E     | 35  | ILE  |
| 1   | E     | 54  | ASP  |
| 1   | E     | 59  | ILE  |
| 1   | E     | 80  | LYS  |
| 1   | E     | 148 | PRO  |
| 1   | E     | 166 | ASN  |
| 1   | E     | 189 | LYS  |
| 1   | E     | 214 | GLU  |
| 1   | E     | 222 | ASP  |
| 1   | E     | 241 | LEU  |
| 1   | E     | 251 | THR  |
| 1   | E     | 276 | LEU  |
| 1   | E     | 286 | THR  |
| 1   | E     | 298 | ASP  |
| 1   | E     | 315 | ARG  |
| 1   | E     | 364 | GLU  |
| 1   | E     | 370 | LYS  |
| 1   | E     | 421 | ARG  |
| 1   | E     | 446 | ILE  |
| 1   | E     | 449 | LYS  |
| 1   | E     | 462 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 483 | GLU  |
| 1   | E     | 498 | LEU  |
| 1   | E     | 501 | LYS  |
| 1   | E     | 519 | ASP  |
| 1   | F     | 11  | ILE  |
| 1   | F     | 17  | GLN  |
| 1   | F     | 23  | ASP  |
| 1   | F     | 26  | ARG  |
| 1   | F     | 35  | ILE  |
| 1   | F     | 40  | ARG  |
| 1   | F     | 41  | THR  |
| 1   | F     | 63  | ASN  |
| 1   | F     | 118 | ASN  |
| 1   | F     | 128 | TYR  |
| 1   | F     | 148 | PRO  |
| 1   | F     | 154 | LEU  |
| 1   | F     | 166 | ASN  |
| 1   | F     | 171 | LYS  |
| 1   | F     | 189 | LYS  |
| 1   | F     | 190 | ASP  |
| 1   | F     | 222 | ASP  |
| 1   | F     | 241 | LEU  |
| 1   | F     | 276 | LEU  |
| 1   | F     | 298 | ASP  |
| 1   | F     | 315 | ARG  |
| 1   | F     | 336 | VAL  |
| 1   | F     | 338 | ASP  |
| 1   | F     | 370 | LYS  |
| 1   | F     | 381 | GLU  |
| 1   | F     | 415 | GLU  |
| 1   | F     | 421 | ARG  |
| 1   | F     | 446 | ILE  |
| 1   | F     | 449 | LYS  |
| 1   | F     | 462 | MET  |
| 1   | F     | 483 | GLU  |
| 1   | F     | 490 | LEU  |
| 1   | F     | 498 | LEU  |
| 1   | F     | 501 | LYS  |
| 1   | F     | 519 | ASP  |
| 1   | G     | 11  | ILE  |
| 1   | G     | 17  | GLN  |
| 1   | G     | 23  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 26  | ARG  |
| 1   | G     | 118 | ASN  |
| 1   | G     | 128 | TYR  |
| 1   | G     | 148 | PRO  |
| 1   | G     | 166 | ASN  |
| 1   | G     | 171 | LYS  |
| 1   | G     | 189 | LYS  |
| 1   | G     | 190 | ASP  |
| 1   | G     | 222 | ASP  |
| 1   | G     | 241 | LEU  |
| 1   | G     | 246 | LEU  |
| 1   | G     | 260 | THR  |
| 1   | G     | 276 | LEU  |
| 1   | G     | 298 | ASP  |
| 1   | G     | 315 | ARG  |
| 1   | G     | 336 | VAL  |
| 1   | G     | 338 | ASP  |
| 1   | G     | 370 | LYS  |
| 1   | G     | 415 | GLU  |
| 1   | G     | 421 | ARG  |
| 1   | G     | 446 | ILE  |
| 1   | G     | 449 | LYS  |
| 1   | G     | 498 | LEU  |
| 1   | G     | 501 | LYS  |
| 1   | G     | 525 | LYS  |
| 1   | H     | 11  | ILE  |
| 1   | H     | 14  | GLU  |
| 1   | H     | 17  | GLN  |
| 1   | H     | 26  | ARG  |
| 1   | H     | 35  | ILE  |
| 1   | H     | 54  | ASP  |
| 1   | H     | 107 | LEU  |
| 1   | H     | 148 | PRO  |
| 1   | H     | 166 | ASN  |
| 1   | H     | 171 | LYS  |
| 1   | H     | 189 | LYS  |
| 1   | H     | 190 | ASP  |
| 1   | H     | 222 | ASP  |
| 1   | H     | 241 | LEU  |
| 1   | H     | 246 | LEU  |
| 1   | H     | 276 | LEU  |
| 1   | H     | 298 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 315 | ARG  |
| 1   | H     | 338 | ASP  |
| 1   | H     | 370 | LYS  |
| 1   | H     | 381 | GLU  |
| 1   | H     | 421 | ARG  |
| 1   | H     | 423 | ASP  |
| 1   | H     | 446 | ILE  |
| 1   | H     | 449 | LYS  |
| 1   | H     | 483 | GLU  |
| 1   | H     | 490 | LEU  |
| 1   | H     | 501 | LYS  |
| 1   | H     | 519 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 17  | GLN  |
| 1   | A     | 28  | ASN  |
| 1   | A     | 63  | ASN  |
| 1   | A     | 75  | GLN  |
| 1   | A     | 76  | HIS  |
| 1   | A     | 117 | GLN  |
| 1   | A     | 118 | ASN  |
| 1   | A     | 136 | GLN  |
| 1   | A     | 166 | ASN  |
| 1   | A     | 184 | GLN  |
| 1   | A     | 258 | ASN  |
| 1   | A     | 264 | GLN  |
| 1   | A     | 285 | GLN  |
| 1   | A     | 439 | ASN  |
| 1   | A     | 503 | GLN  |
| 1   | B     | 17  | GLN  |
| 1   | B     | 28  | ASN  |
| 1   | B     | 76  | HIS  |
| 1   | B     | 118 | ASN  |
| 1   | B     | 136 | GLN  |
| 1   | B     | 166 | ASN  |
| 1   | B     | 170 | HIS  |
| 1   | B     | 184 | GLN  |
| 1   | B     | 258 | ASN  |
| 1   | B     | 264 | GLN  |
| 1   | B     | 285 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 503 | GLN  |
| 1   | C     | 17  | GLN  |
| 1   | C     | 28  | ASN  |
| 1   | C     | 75  | GLN  |
| 1   | C     | 76  | HIS  |
| 1   | C     | 118 | ASN  |
| 1   | C     | 136 | GLN  |
| 1   | C     | 166 | ASN  |
| 1   | C     | 258 | ASN  |
| 1   | C     | 264 | GLN  |
| 1   | C     | 285 | GLN  |
| 1   | C     | 368 | ASN  |
| 1   | D     | 17  | GLN  |
| 1   | D     | 28  | ASN  |
| 1   | D     | 63  | ASN  |
| 1   | D     | 76  | HIS  |
| 1   | D     | 118 | ASN  |
| 1   | D     | 136 | GLN  |
| 1   | D     | 166 | ASN  |
| 1   | D     | 170 | HIS  |
| 1   | D     | 184 | GLN  |
| 1   | D     | 258 | ASN  |
| 1   | D     | 264 | GLN  |
| 1   | D     | 285 | GLN  |
| 1   | D     | 439 | ASN  |
| 1   | E     | 17  | GLN  |
| 1   | E     | 28  | ASN  |
| 1   | E     | 75  | GLN  |
| 1   | E     | 76  | HIS  |
| 1   | E     | 118 | ASN  |
| 1   | E     | 136 | GLN  |
| 1   | E     | 166 | ASN  |
| 1   | E     | 170 | HIS  |
| 1   | E     | 184 | GLN  |
| 1   | E     | 258 | ASN  |
| 1   | E     | 264 | GLN  |
| 1   | E     | 285 | GLN  |
| 1   | E     | 335 | ASN  |
| 1   | E     | 439 | ASN  |
| 1   | F     | 17  | GLN  |
| 1   | F     | 28  | ASN  |
| 1   | F     | 63  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 76  | HIS  |
| 1   | F     | 118 | ASN  |
| 1   | F     | 136 | GLN  |
| 1   | F     | 166 | ASN  |
| 1   | F     | 170 | HIS  |
| 1   | F     | 184 | GLN  |
| 1   | F     | 258 | ASN  |
| 1   | F     | 264 | GLN  |
| 1   | F     | 271 | GLN  |
| 1   | F     | 285 | GLN  |
| 1   | F     | 503 | GLN  |
| 1   | G     | 17  | GLN  |
| 1   | G     | 28  | ASN  |
| 1   | G     | 76  | HIS  |
| 1   | G     | 118 | ASN  |
| 1   | G     | 136 | GLN  |
| 1   | G     | 166 | ASN  |
| 1   | G     | 184 | GLN  |
| 1   | G     | 258 | ASN  |
| 1   | G     | 264 | GLN  |
| 1   | G     | 285 | GLN  |
| 1   | G     | 503 | GLN  |
| 1   | H     | 17  | GLN  |
| 1   | H     | 28  | ASN  |
| 1   | H     | 76  | HIS  |
| 1   | H     | 118 | ASN  |
| 1   | H     | 136 | GLN  |
| 1   | H     | 166 | ASN  |
| 1   | H     | 170 | HIS  |
| 1   | H     | 184 | GLN  |
| 1   | H     | 258 | ASN  |
| 1   | H     | 264 | GLN  |
| 1   | H     | 285 | GLN  |
| 1   | H     | 503 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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   | ADP  | H     | 8528 | 2    | 24,29,29     | 1.60 | 7 (29%)     | 29,45,45    | 1.53 | 2 (6%)      |
| 3   | ADP  | E     | 5528 | 2    | 24,29,29     | 1.55 | 5 (20%)     | 29,45,45    | 1.57 | 2 (6%)      |
| 3   | ADP  | F     | 6528 | -    | 24,29,29     | 1.62 | 6 (25%)     | 29,45,45    | 1.55 | 2 (6%)      |
| 3   | ADP  | C     | 3528 | 2    | 24,29,29     | 1.52 | 5 (20%)     | 29,45,45    | 1.59 | 2 (6%)      |
| 3   | ADP  | B     | 2528 | 2    | 24,29,29     | 1.54 | 6 (25%)     | 29,45,45    | 1.57 | 2 (6%)      |
| 3   | ADP  | D     | 4528 | 2    | 24,29,29     | 1.64 | 4 (16%)     | 29,45,45    | 1.62 | 2 (6%)      |
| 3   | ADP  | G     | 7528 | 2    | 24,29,29     | 1.60 | 6 (25%)     | 29,45,45    | 1.54 | 2 (6%)      |
| 3   | ADP  | A     | 1528 | 2    | 24,29,29     | 1.62 | 6 (25%)     | 29,45,45    | 1.54 | 2 (6%)      |

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   | ADP  | H     | 8528 | 2    | -       | 2/12/32/32 | 0/3/3/3 |
| 3   | ADP  | E     | 5528 | 2    | -       | 2/12/32/32 | 0/3/3/3 |
| 3   | ADP  | F     | 6528 | -    | -       | 2/12/32/32 | 0/3/3/3 |
| 3   | ADP  | C     | 3528 | 2    | -       | 2/12/32/32 | 0/3/3/3 |
| 3   | ADP  | B     | 2528 | 2    | -       | 2/12/32/32 | 0/3/3/3 |
| 3   | ADP  | D     | 4528 | 2    | -       | 2/12/32/32 | 0/3/3/3 |
| 3   | ADP  | G     | 7528 | 2    | -       | 2/12/32/32 | 0/3/3/3 |
| 3   | ADP  | A     | 1528 | 2    | -       | 2/12/32/32 | 0/3/3/3 |

All (45) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | F     | 6528 | ADP  | C2-N3   | 3.97  | 1.38        | 1.32     |
| 3   | C     | 3528 | ADP  | C2-N3   | 3.97  | 1.38        | 1.32     |
| 3   | G     | 7528 | ADP  | C2-N3   | 3.96  | 1.38        | 1.32     |
| 3   | D     | 4528 | ADP  | C2-N3   | 3.89  | 1.38        | 1.32     |
| 3   | A     | 1528 | ADP  | C2-N3   | 3.79  | 1.38        | 1.32     |
| 3   | H     | 8528 | ADP  | C2-N3   | 3.72  | 1.38        | 1.32     |
| 3   | B     | 2528 | ADP  | C2-N3   | 3.54  | 1.37        | 1.32     |
| 3   | D     | 4528 | ADP  | PB-O3B  | 3.46  | 1.68        | 1.54     |
| 3   | E     | 5528 | ADP  | C2-N3   | 3.44  | 1.37        | 1.32     |
| 3   | H     | 8528 | ADP  | PB-O3B  | 3.32  | 1.67        | 1.54     |
| 3   | E     | 5528 | ADP  | PB-O3B  | 3.30  | 1.67        | 1.54     |
| 3   | C     | 3528 | ADP  | PB-O3B  | 3.25  | 1.67        | 1.54     |
| 3   | A     | 1528 | ADP  | PB-O3B  | 3.24  | 1.67        | 1.54     |
| 3   | F     | 6528 | ADP  | PB-O3B  | 3.24  | 1.67        | 1.54     |
| 3   | G     | 7528 | ADP  | C2'-C1' | -3.13 | 1.49        | 1.53     |
| 3   | D     | 4528 | ADP  | C4-N3   | 3.10  | 1.39        | 1.35     |
| 3   | B     | 2528 | ADP  | PB-O3B  | 3.03  | 1.66        | 1.54     |
| 3   | G     | 7528 | ADP  | PB-O3B  | 2.82  | 1.65        | 1.54     |
| 3   | B     | 2528 | ADP  | C2'-C1' | -2.56 | 1.49        | 1.53     |
| 3   | D     | 4528 | ADP  | C2-N1   | 2.54  | 1.38        | 1.33     |
| 3   | G     | 7528 | ADP  | C2-N1   | 2.54  | 1.38        | 1.33     |
| 3   | A     | 1528 | ADP  | C2-N1   | 2.52  | 1.38        | 1.33     |
| 3   | H     | 8528 | ADP  | O4'-C1' | 2.51  | 1.44        | 1.41     |
| 3   | F     | 6528 | ADP  | C4-N3   | 2.39  | 1.39        | 1.35     |
| 3   | F     | 6528 | ADP  | C2-N1   | 2.38  | 1.38        | 1.33     |
| 3   | B     | 2528 | ADP  | C2-N1   | 2.36  | 1.38        | 1.33     |
| 3   | F     | 6528 | ADP  | C5-N7   | -2.36 | 1.31        | 1.39     |
| 3   | E     | 5528 | ADP  | C2-N1   | 2.34  | 1.38        | 1.33     |
| 3   | A     | 1528 | ADP  | C5-N7   | -2.33 | 1.31        | 1.39     |
| 3   | H     | 8528 | ADP  | C2-N1   | 2.30  | 1.38        | 1.33     |
| 3   | E     | 5528 | ADP  | C4-N3   | 2.28  | 1.38        | 1.35     |
| 3   | A     | 1528 | ADP  | C4-N3   | 2.28  | 1.38        | 1.35     |
| 3   | B     | 2528 | ADP  | C4-N3   | 2.28  | 1.38        | 1.35     |
| 3   | H     | 8528 | ADP  | C4-N3   | 2.25  | 1.38        | 1.35     |
| 3   | H     | 8528 | ADP  | C5-N7   | -2.25 | 1.31        | 1.39     |
| 3   | G     | 7528 | ADP  | C4-N3   | 2.24  | 1.38        | 1.35     |
| 3   | B     | 2528 | ADP  | C5-N7   | -2.23 | 1.31        | 1.39     |
| 3   | C     | 3528 | ADP  | C2-N1   | 2.23  | 1.38        | 1.33     |
| 3   | A     | 1528 | ADP  | O4'-C1' | 2.16  | 1.44        | 1.41     |
| 3   | F     | 6528 | ADP  | O4'-C1' | 2.14  | 1.44        | 1.41     |
| 3   | H     | 8528 | ADP  | C2'-C1' | -2.13 | 1.50        | 1.53     |
| 3   | C     | 3528 | ADP  | C4-N3   | 2.06  | 1.38        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | G     | 7528 | ADP  | C5-N7   | -2.05 | 1.32        | 1.39     |
| 3   | C     | 3528 | ADP  | C5-N7   | -2.05 | 1.32        | 1.39     |
| 3   | E     | 5528 | ADP  | O3'-C3' | 2.02  | 1.47        | 1.43     |

All (16) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | H     | 8528 | ADP  | N3-C2-N1 | -6.61 | 118.35      | 128.68   |
| 3   | D     | 4528 | ADP  | N3-C2-N1 | -6.59 | 118.37      | 128.68   |
| 3   | A     | 1528 | ADP  | N3-C2-N1 | -6.54 | 118.45      | 128.68   |
| 3   | G     | 7528 | ADP  | N3-C2-N1 | -6.54 | 118.46      | 128.68   |
| 3   | B     | 2528 | ADP  | N3-C2-N1 | -6.54 | 118.46      | 128.68   |
| 3   | F     | 6528 | ADP  | N3-C2-N1 | -6.50 | 118.51      | 128.68   |
| 3   | C     | 3528 | ADP  | N3-C2-N1 | -6.49 | 118.53      | 128.68   |
| 3   | E     | 5528 | ADP  | N3-C2-N1 | -6.42 | 118.64      | 128.68   |
| 3   | E     | 5528 | ADP  | C4-C5-N7 | -3.15 | 106.12      | 109.40   |
| 3   | C     | 3528 | ADP  | C4-C5-N7 | -3.12 | 106.14      | 109.40   |
| 3   | D     | 4528 | ADP  | C4-C5-N7 | -3.10 | 106.17      | 109.40   |
| 3   | G     | 7528 | ADP  | C4-C5-N7 | -2.94 | 106.33      | 109.40   |
| 3   | H     | 8528 | ADP  | C4-C5-N7 | -2.92 | 106.36      | 109.40   |
| 3   | F     | 6528 | ADP  | C4-C5-N7 | -2.91 | 106.37      | 109.40   |
| 3   | B     | 2528 | ADP  | C4-C5-N7 | -2.86 | 106.42      | 109.40   |
| 3   | A     | 1528 | ADP  | C4-C5-N7 | -2.84 | 106.44      | 109.40   |

There are no chirality outliers.

All (16) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 3   | A     | 1528 | ADP  | PA-O3A-PB-O3B |
| 3   | B     | 2528 | ADP  | PA-O3A-PB-O3B |
| 3   | C     | 3528 | ADP  | PA-O3A-PB-O3B |
| 3   | D     | 4528 | ADP  | PA-O3A-PB-O3B |
| 3   | E     | 5528 | ADP  | PA-O3A-PB-O3B |
| 3   | F     | 6528 | ADP  | PA-O3A-PB-O3B |
| 3   | G     | 7528 | ADP  | PA-O3A-PB-O3B |
| 3   | H     | 8528 | ADP  | PA-O3A-PB-O3B |
| 3   | A     | 1528 | ADP  | PA-O3A-PB-O2B |
| 3   | B     | 2528 | ADP  | PA-O3A-PB-O2B |
| 3   | C     | 3528 | ADP  | PA-O3A-PB-O2B |
| 3   | D     | 4528 | ADP  | PA-O3A-PB-O2B |
| 3   | E     | 5528 | ADP  | PA-O3A-PB-O2B |
| 3   | F     | 6528 | ADP  | PA-O3A-PB-O2B |

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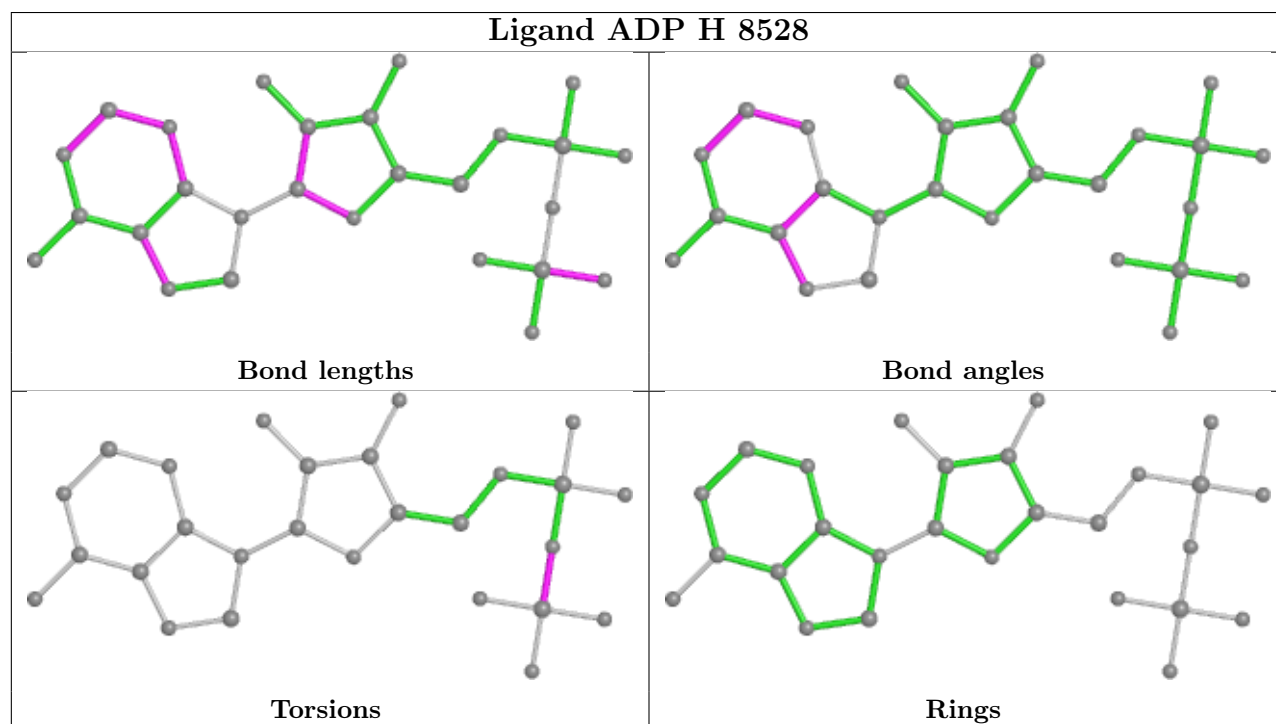
| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 3   | G     | 7528 | ADP  | PA-O3A-PB-O2B |
| 3   | H     | 8528 | ADP  | PA-O3A-PB-O2B |

There are no ring outliers.

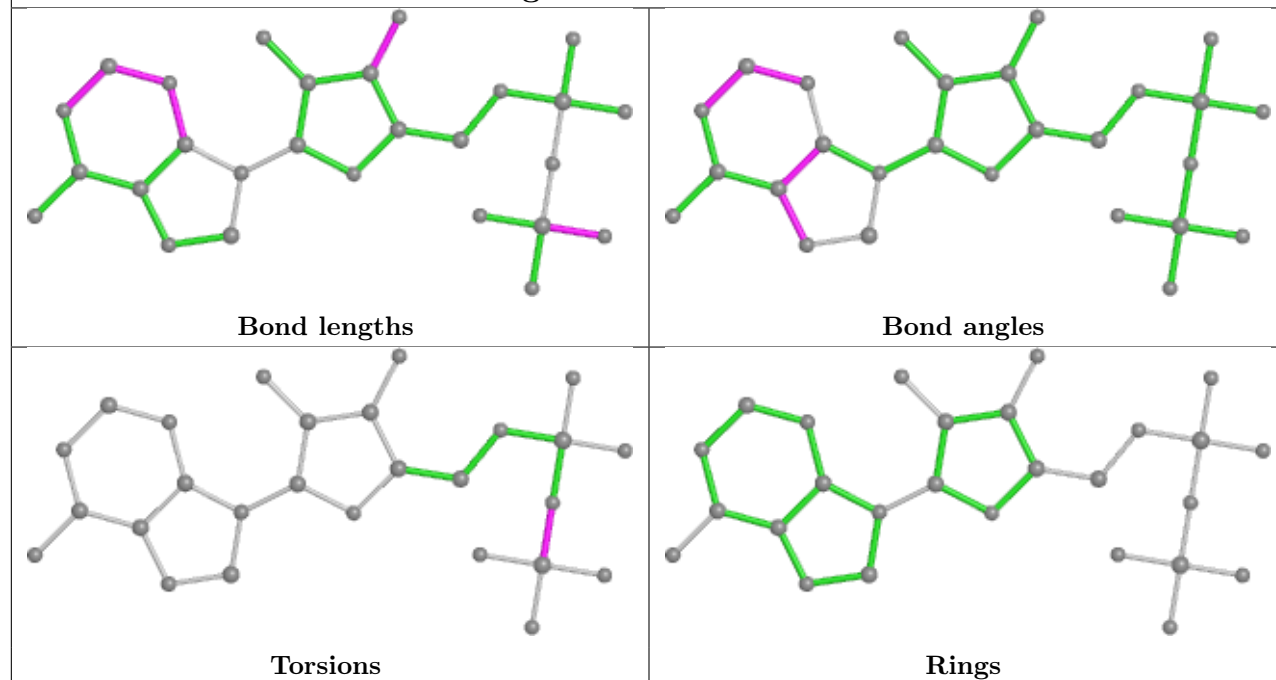
4 monomers are involved in 5 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | H     | 8528 | ADP  | 1       | 0            |
| 3   | F     | 6528 | ADP  | 1       | 0            |
| 3   | B     | 2528 | ADP  | 1       | 0            |
| 3   | G     | 7528 | ADP  | 2       | 0            |

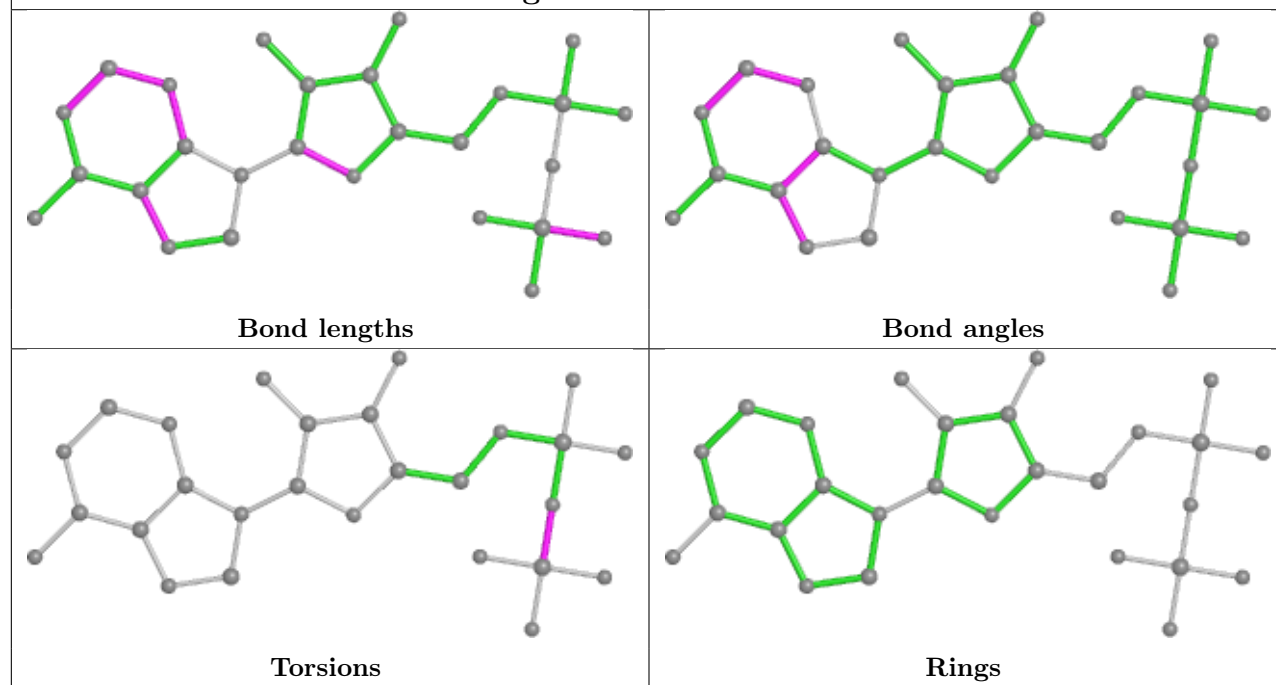
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



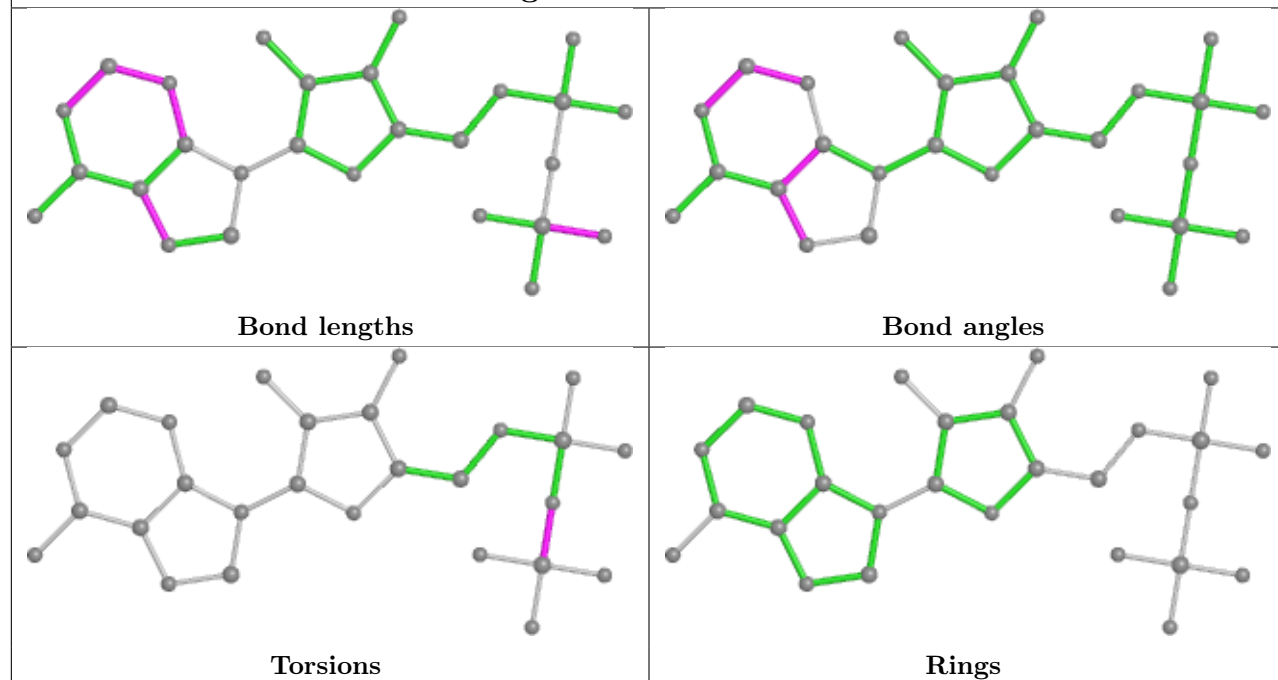
## Ligand ADP E 5528



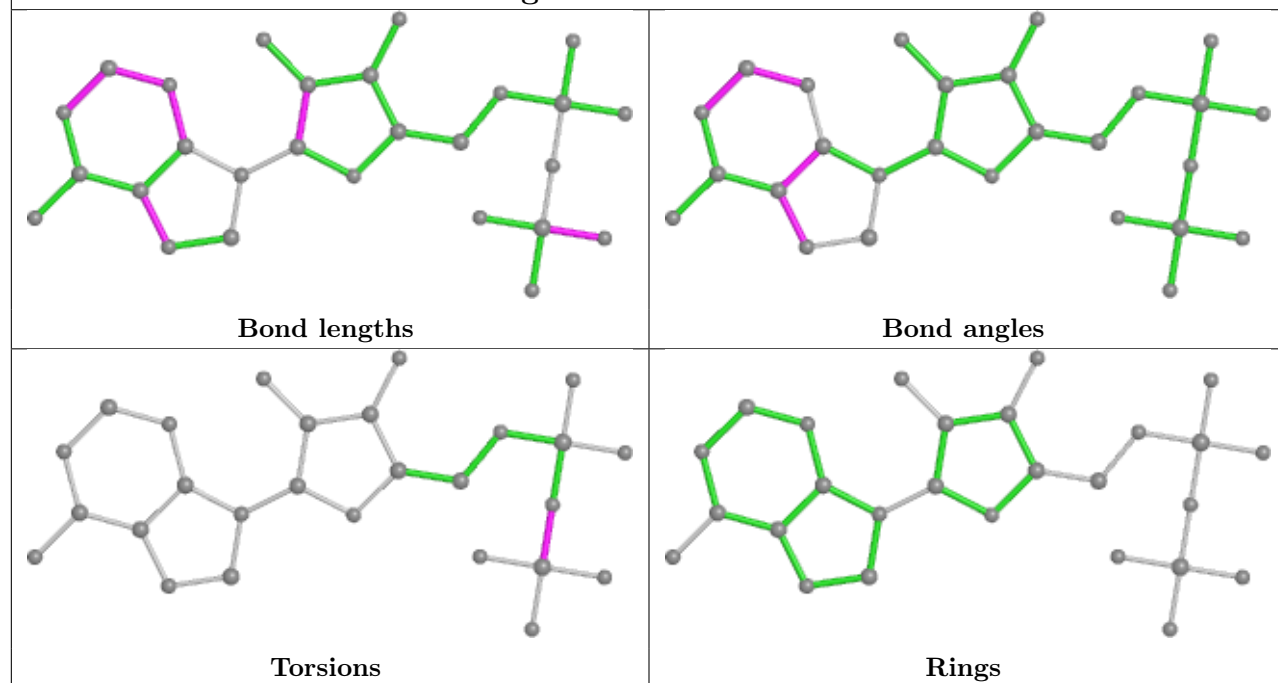
## Ligand ADP F 6528



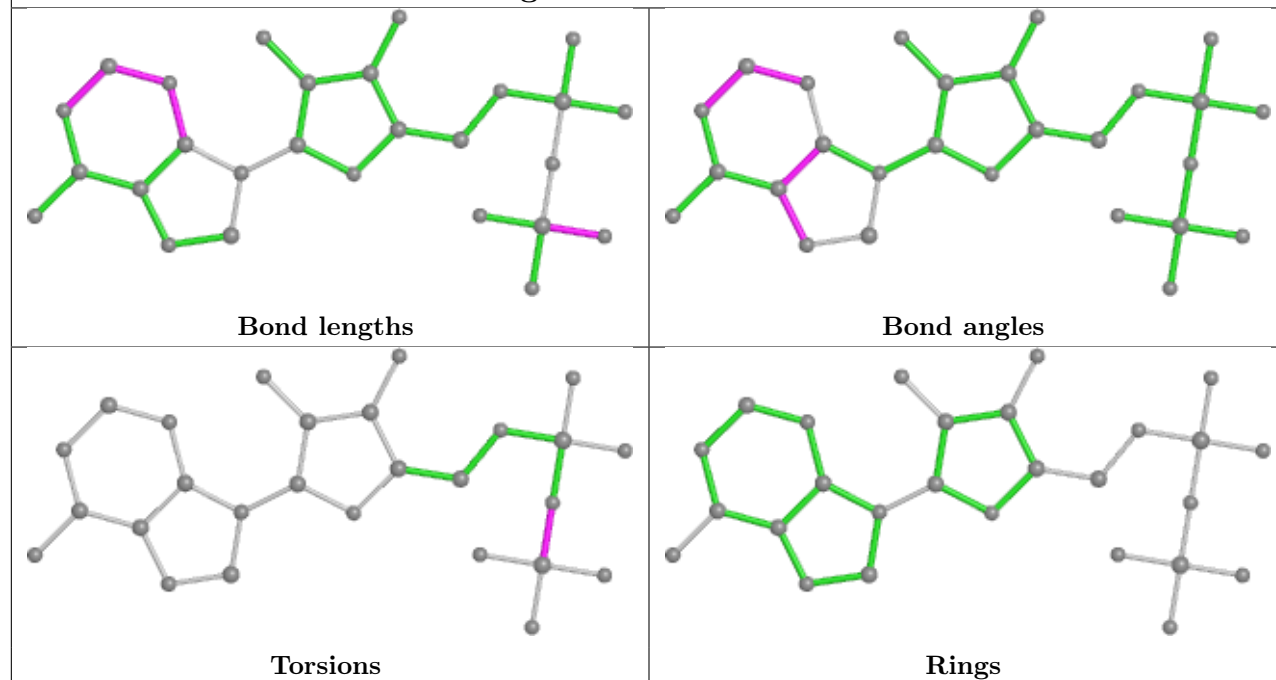
## Ligand ADP C 3528



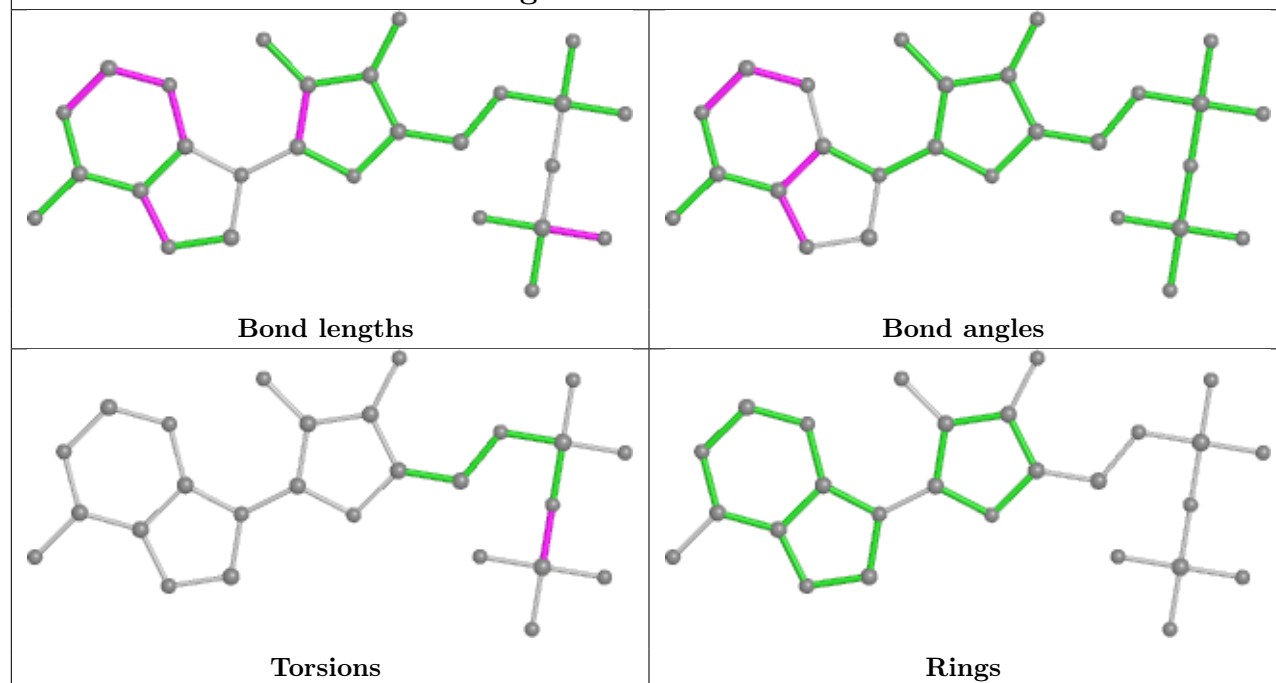
## Ligand ADP B 2528

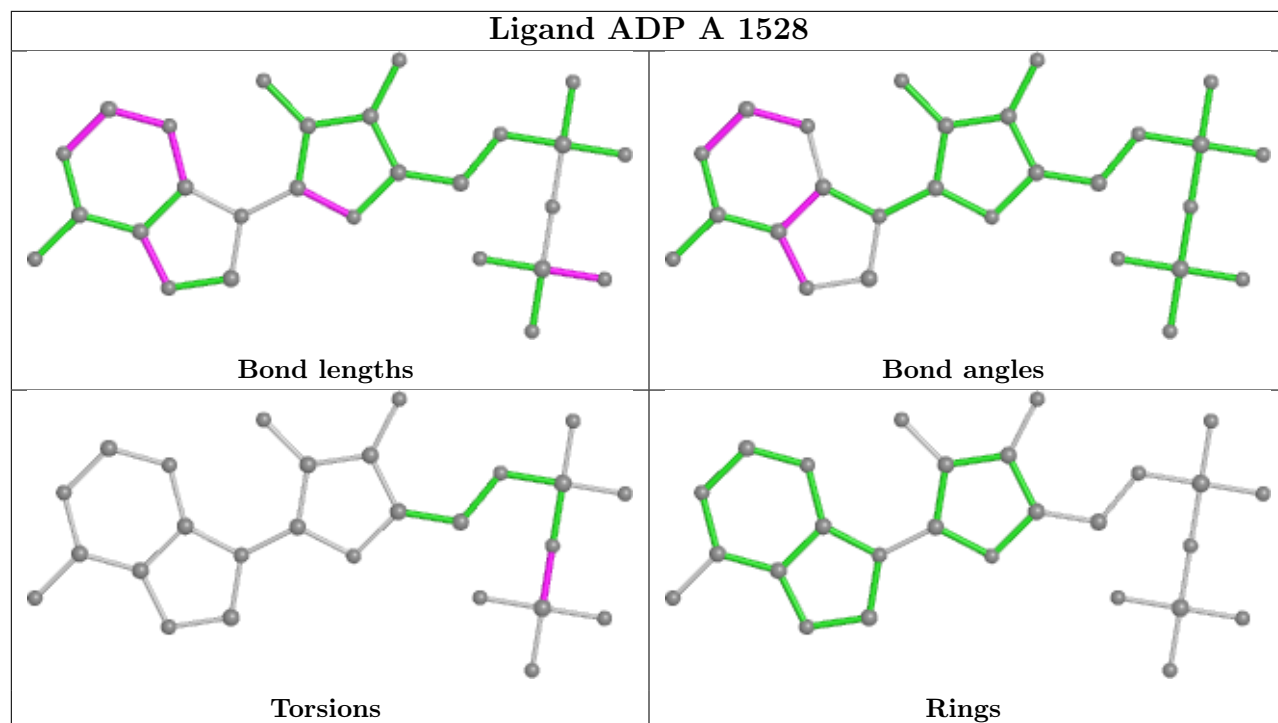


## Ligand ADP D 4528



## Ligand ADP G 7528





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2 |       | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|-----------|-------|-----------------------|---------|
| 1   | A     | 517/548 (94%)   | -0.17  | 4 (0%)    | 86 65 | 10, 30, 62, 102       | 0       |
| 1   | B     | 517/548 (94%)   | -0.12  | 5 (0%)    | 82 59 | 8, 28, 62, 105        | 0       |
| 1   | C     | 517/548 (94%)   | -0.10  | 4 (0%)    | 86 65 | 16, 40, 70, 100       | 0       |
| 1   | D     | 517/548 (94%)   | -0.02  | 8 (1%)    | 73 46 | 13, 41, 70, 102       | 0       |
| 1   | E     | 517/548 (94%)   | -0.06  | 6 (1%)    | 79 54 | 16, 41, 67, 108       | 0       |
| 1   | F     | 517/548 (94%)   | -0.08  | 8 (1%)    | 73 46 | 14, 34, 65, 109       | 0       |
| 1   | G     | 517/548 (94%)   | -0.08  | 6 (1%)    | 79 54 | 12, 35, 65, 98        | 0       |
| 1   | H     | 517/548 (94%)   | -0.14  | 5 (0%)    | 82 59 | 8, 29, 56, 96         | 0       |
| All | All   | 4136/4384 (94%) | -0.10  | 46 (1%)   | 80 56 | 8, 35, 66, 109        | 0       |

All (46) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 10  | VAL  | 10.7 |
| 1   | E     | 526 | ALA  | 10.3 |
| 1   | D     | 526 | ALA  | 9.3  |
| 1   | A     | 526 | ALA  | 8.2  |
| 1   | C     | 10  | VAL  | 7.0  |
| 1   | D     | 10  | VAL  | 6.5  |
| 1   | F     | 10  | VAL  | 6.3  |
| 1   | H     | 10  | VAL  | 6.1  |
| 1   | B     | 526 | ALA  | 5.9  |
| 1   | E     | 10  | VAL  | 5.8  |
| 1   | G     | 526 | ALA  | 5.0  |
| 1   | F     | 526 | ALA  | 5.0  |
| 1   | A     | 189 | LYS  | 4.6  |
| 1   | B     | 11  | ILE  | 4.6  |
| 1   | C     | 526 | ALA  | 4.6  |
| 1   | F     | 15  | GLY  | 4.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 167 | ALA  | 4.1  |
| 1   | D     | 525 | LYS  | 3.8  |
| 1   | D     | 166 | ASN  | 3.8  |
| 1   | G     | 167 | ALA  | 3.6  |
| 1   | E     | 525 | LYS  | 3.3  |
| 1   | D     | 15  | GLY  | 3.2  |
| 1   | E     | 189 | LYS  | 2.9  |
| 1   | B     | 17  | GLN  | 2.9  |
| 1   | H     | 189 | LYS  | 2.8  |
| 1   | F     | 167 | ALA  | 2.8  |
| 1   | G     | 10  | VAL  | 2.7  |
| 1   | D     | 14  | GLU  | 2.6  |
| 1   | H     | 166 | ASN  | 2.6  |
| 1   | F     | 11  | ILE  | 2.6  |
| 1   | C     | 525 | LYS  | 2.5  |
| 1   | H     | 167 | ALA  | 2.5  |
| 1   | G     | 166 | ASN  | 2.3  |
| 1   | H     | 15  | GLY  | 2.3  |
| 1   | A     | 167 | ALA  | 2.3  |
| 1   | F     | 189 | LYS  | 2.3  |
| 1   | A     | 15  | GLY  | 2.2  |
| 1   | E     | 15  | GLY  | 2.2  |
| 1   | F     | 166 | ASN  | 2.2  |
| 1   | C     | 11  | ILE  | 2.1  |
| 1   | B     | 167 | ALA  | 2.1  |
| 1   | F     | 525 | LYS  | 2.0  |
| 1   | D     | 11  | ILE  | 2.0  |
| 1   | E     | 11  | ILE  | 2.0  |
| 1   | G     | 17  | GLN  | 2.0  |
| 1   | G     | 525 | LYS  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands

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

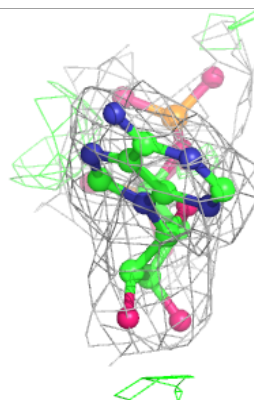
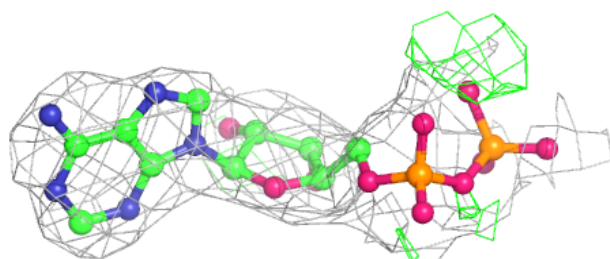
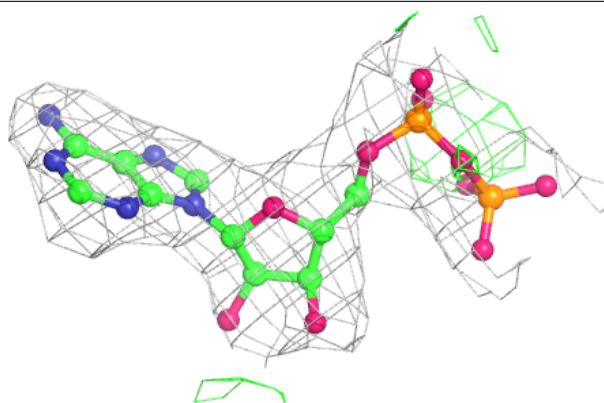
| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 2   | MG   | A     | 1527 | 1/1   | 0.84 | 0.18 | 15,15,15,15                | 0     |
| 2   | MG   | C     | 3527 | 1/1   | 0.88 | 0.16 | 18,18,18,18                | 0     |
| 2   | MG   | H     | 8527 | 1/1   | 0.91 | 0.21 | 25,25,25,25                | 0     |
| 3   | ADP  | F     | 6528 | 27/27 | 0.93 | 0.21 | 21,27,34,35                | 0     |
| 3   | ADP  | D     | 4528 | 27/27 | 0.94 | 0.20 | 32,37,44,45                | 0     |
| 2   | MG   | E     | 5527 | 1/1   | 0.94 | 0.20 | 14,14,14,14                | 0     |
| 3   | ADP  | G     | 7528 | 27/27 | 0.94 | 0.21 | 30,39,44,45                | 0     |
| 3   | ADP  | A     | 1528 | 27/27 | 0.95 | 0.20 | 21,33,39,41                | 0     |
| 3   | ADP  | E     | 5528 | 27/27 | 0.95 | 0.18 | 30,32,35,36                | 0     |
| 3   | ADP  | B     | 2528 | 27/27 | 0.95 | 0.19 | 17,24,28,29                | 0     |
| 3   | ADP  | C     | 3528 | 27/27 | 0.95 | 0.20 | 32,35,37,38                | 0     |
| 3   | ADP  | H     | 8528 | 27/27 | 0.95 | 0.21 | 26,28,31,32                | 0     |
| 2   | MG   | D     | 4527 | 1/1   | 0.97 | 0.17 | 17,17,17,17                | 0     |
| 2   | MG   | B     | 2527 | 1/1   | 0.97 | 0.21 | 10,10,10,10                | 0     |
| 2   | MG   | G     | 6527 | 1/1   | 0.97 | 0.16 | 16,16,16,16                | 0     |

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

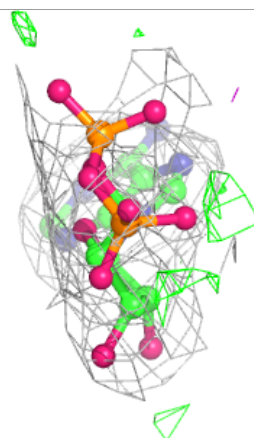
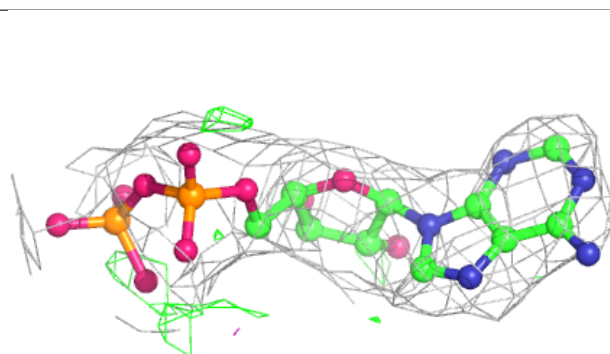
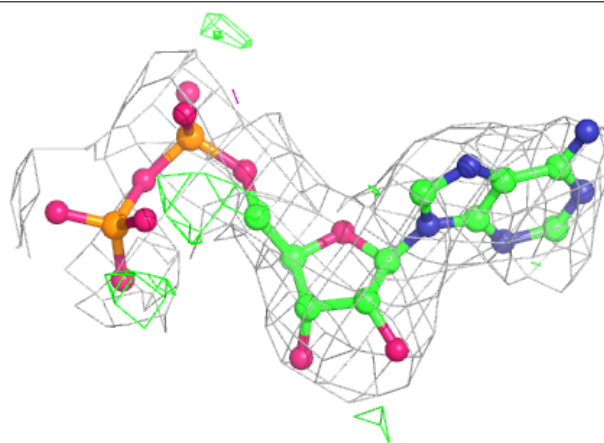


**Electron density around ADP F 6528:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

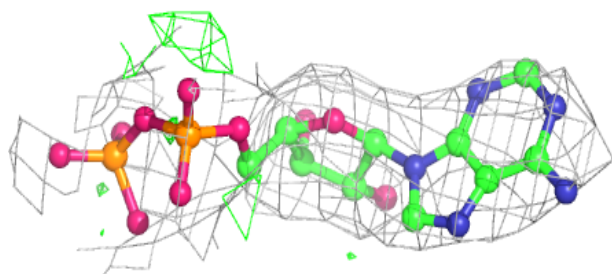
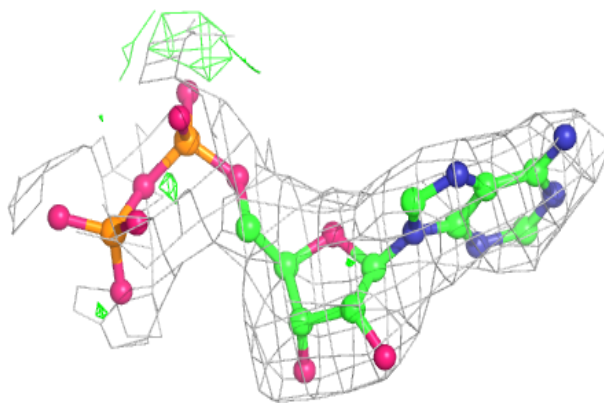
**Electron density around ADP D 4528:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

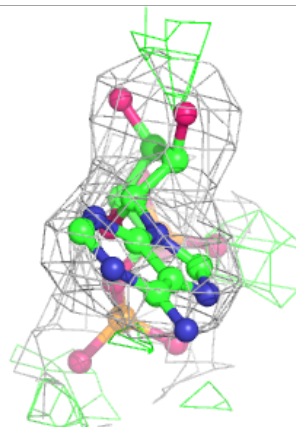
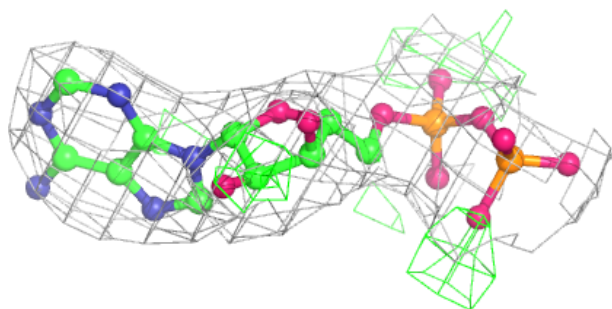
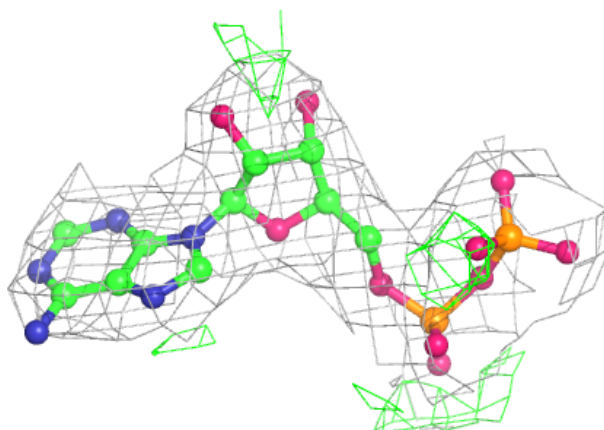


**Electron density around ADP G 7528:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

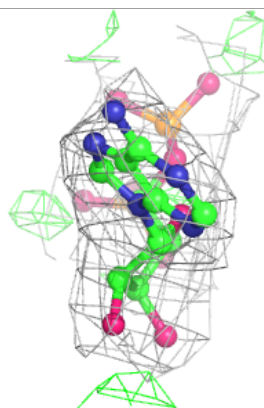
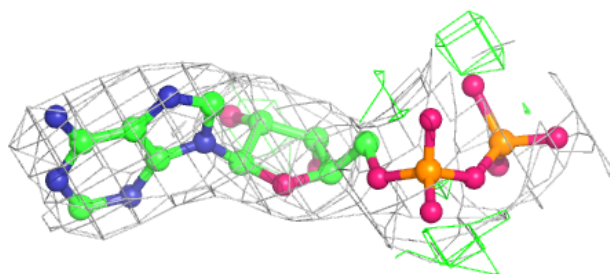
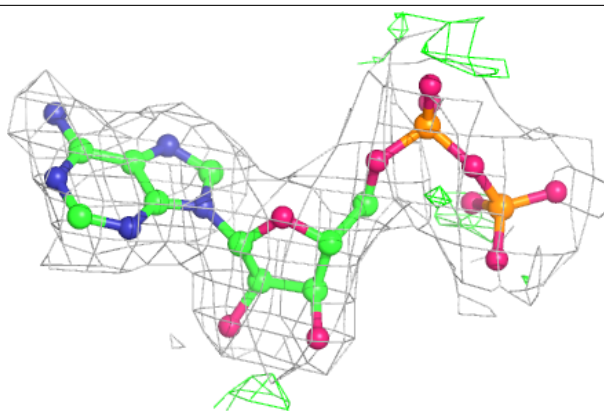
**Electron density around ADP A 1528:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

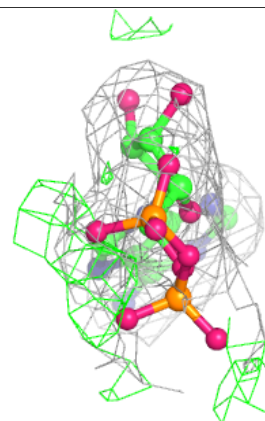
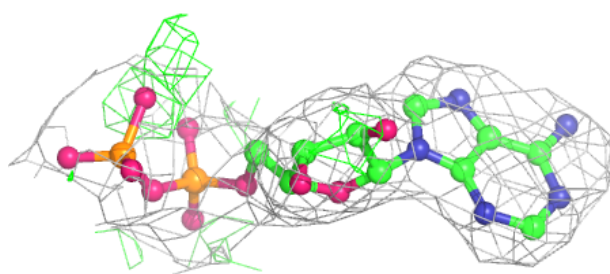
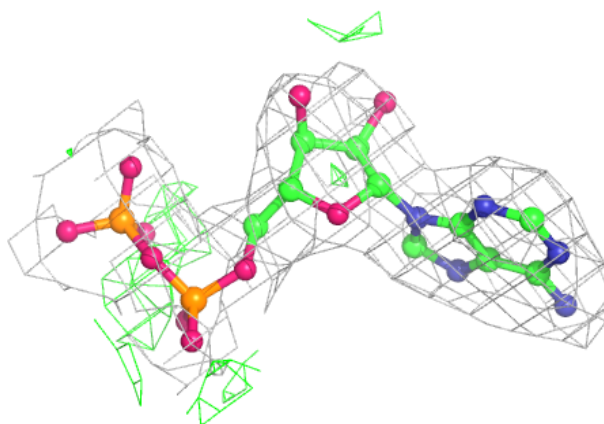


**Electron density around ADP E 5528:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

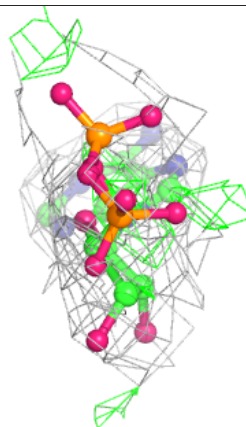
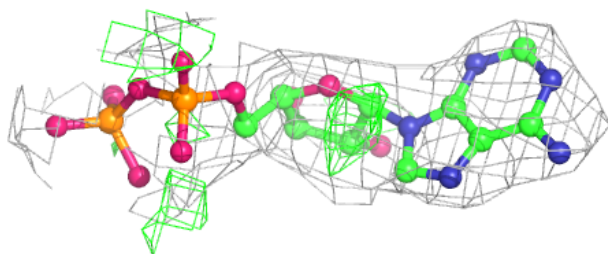
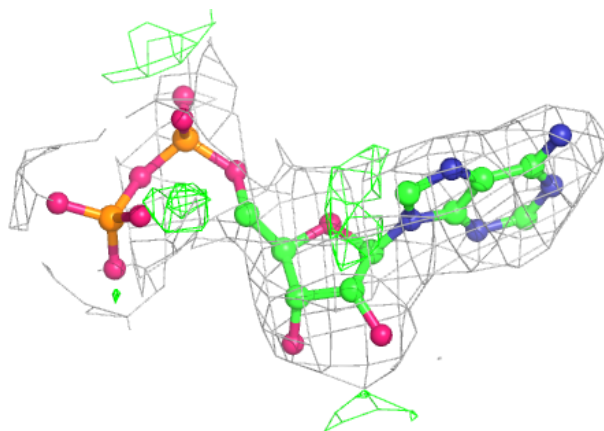
**Electron density around ADP B 2528:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

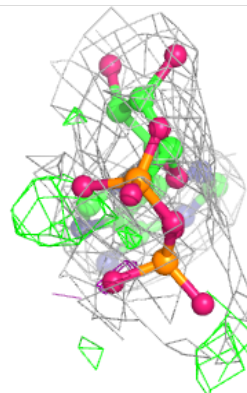
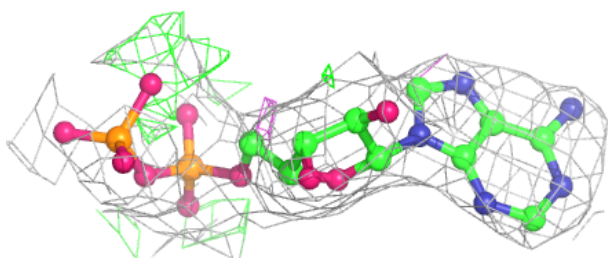
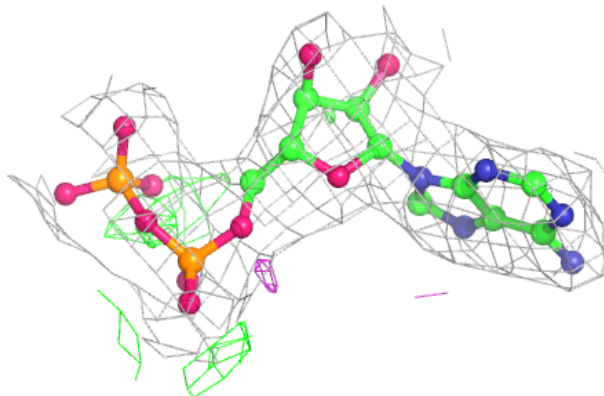


**Electron density around ADP C 3528:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ADP H 8528:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.