



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 21, 2017 – 04:07 AM EDT

PDB ID : 4AAQ  
EMDB ID: : EMD-1998  
Title : ATP-triggered molecular mechanics of the chaperonin GroEL  
Authors : Clare, D.K.; Vasishtan, D.; Stagg, S.; Quispe, J.; Farr, G.W.; Topf, M.; Horwich, A.L.; Saibil, H.R.  
Deposited on : unknown  
Resolution : 8.00 Å(reported)  
Based on PDB ID : 1OEL

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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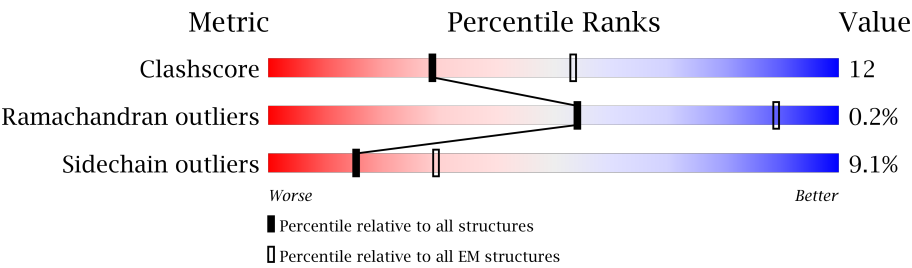
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 8.00 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) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 125131                      | 1336                        |
| Ramachandran outliers | 121729                      | 1120                        |
| Sidechain outliers    | 121581                      | 1026                        |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 548    | 61% 27% 7% . .   |
| 1   | B     | 548    | 60% 27% 7% . .   |
| 1   | C     | 548    | 61% 26% 7% . .   |
| 1   | D     | 548    | 60% 27% 8% . .   |
| 1   | E     | 548    | 61% 27% 7% . .   |
| 1   | F     | 548    | 61% 27% 7% . .   |
| 1   | G     | 548    | 60% 27% 8% . .   |
| 1   | H     | 548    | 78% 14% . . .    |
| 1   | I     | 548    | 78% 14% . . .    |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | J     | 548    |  78%14% . . . |
| 1   | K     | 548    |  79%14% . . . |
| 1   | L     | 548    |  78%14% . . . |
| 1   | M     | 548    |  78%14% . . . |
| 1   | N     | 548    |  78%14% . . . |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3   | PO4  | A     | 1526 | -         | -        | X       | -                |
| 3   | PO4  | B     | 1526 | -         | -        | X       | -                |
| 3   | PO4  | C     | 1527 | -         | -        | X       | -                |
| 3   | PO4  | D     | 1526 | -         | -        | X       | -                |
| 3   | PO4  | E     | 1526 | -         | -        | X       | -                |
| 3   | PO4  | F     | 1525 | -         | -        | X       | -                |
| 3   | PO4  | G     | 1525 | -         | -        | X       | -                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 54159 atoms, of which 84 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60 KDA CHAPERONIN.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3846  | 2391 | 665 | 770 | 20 |         |       |
| 1   | B     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3846  | 2391 | 665 | 770 | 20 |         |       |
| 1   | C     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3846  | 2391 | 665 | 770 | 20 |         |       |
| 1   | D     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3846  | 2391 | 665 | 770 | 20 |         |       |
| 1   | E     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3846  | 2391 | 665 | 770 | 20 |         |       |
| 1   | F     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3846  | 2391 | 665 | 770 | 20 |         |       |
| 1   | G     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3846  | 2391 | 665 | 770 | 20 |         |       |
| 1   | H     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3846  | 2391 | 665 | 770 | 20 |         |       |
| 1   | I     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3846  | 2391 | 665 | 770 | 20 |         |       |
| 1   | J     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3846  | 2391 | 665 | 770 | 20 |         |       |
| 1   | K     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3846  | 2391 | 665 | 770 | 20 |         |       |
| 1   | L     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3846  | 2391 | 665 | 770 | 20 |         |       |
| 1   | M     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3846  | 2391 | 665 | 770 | 20 |         |       |
| 1   | N     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3846  | 2391 | 665 | 770 | 20 |         |       |

There are 14 discrepancies between the modelled and reference sequences:

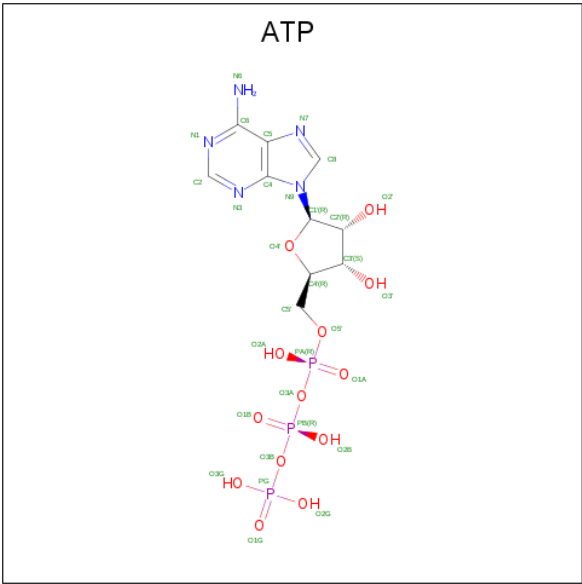
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| B     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| C     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| D     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| E     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| F     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| G     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| H     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| I     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| J     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| K     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| L     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| M     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| N     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms |    |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|----|---|---------|
| 2   | A     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 43    | 10 | 12 | 5 | 13 | 3 |         |
| 2   | B     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 43    | 10 | 12 | 5 | 13 | 3 |         |
| 2   | C     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 43    | 10 | 12 | 5 | 13 | 3 |         |
| 2   | D     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 43    | 10 | 12 | 5 | 13 | 3 |         |
| 2   | E     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 43    | 10 | 12 | 5 | 13 | 3 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|----|---|---------|
| 2   | F     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 43    | 10 | 12 | 5 | 13 | 3 |         |
| 2   | G     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 43    | 10 | 12 | 5 | 13 | 3 |         |

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 3   | A     | 1        | Total | P | 0       |
|     |       |          | 1     | 1 |         |
| 3   | B     | 1        | Total | P | 0       |
|     |       |          | 1     | 1 |         |
| 3   | C     | 1        | Total | P | 0       |
|     |       |          | 1     | 1 |         |
| 3   | D     | 1        | Total | P | 0       |
|     |       |          | 1     | 1 |         |
| 3   | E     | 1        | Total | P | 0       |
|     |       |          | 1     | 1 |         |
| 3   | F     | 1        | Total | P | 0       |
|     |       |          | 1     | 1 |         |
| 3   | G     | 1        | Total | P | 0       |
|     |       |          | 1     | 1 |         |

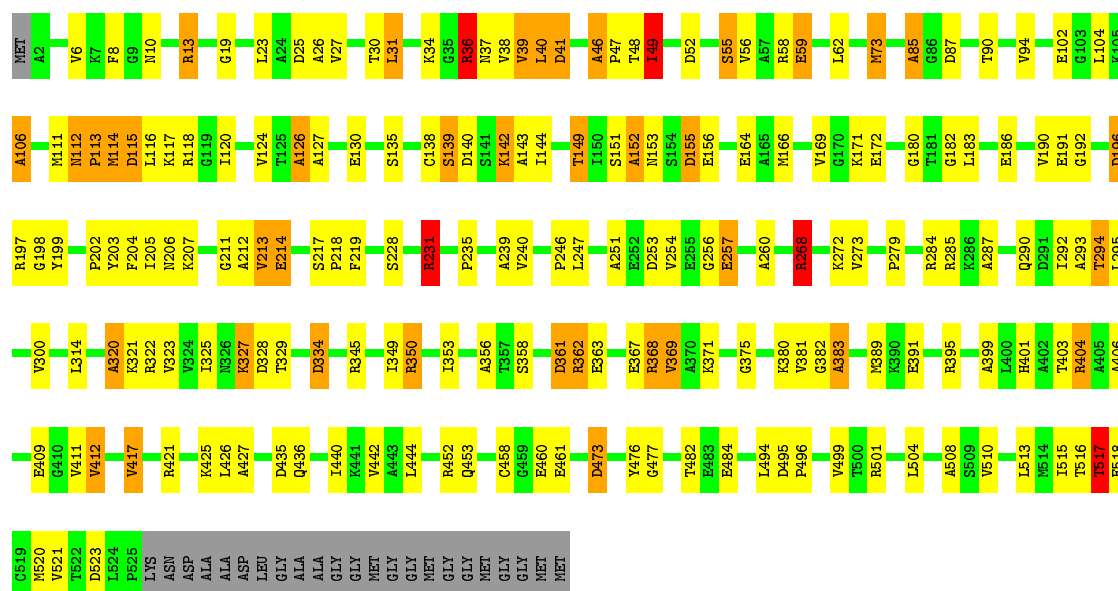
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 4   | G     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | D     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | E     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | B     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | C     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | A     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | F     | 1        | Total<br>1 | Mg<br>1 | 0       |



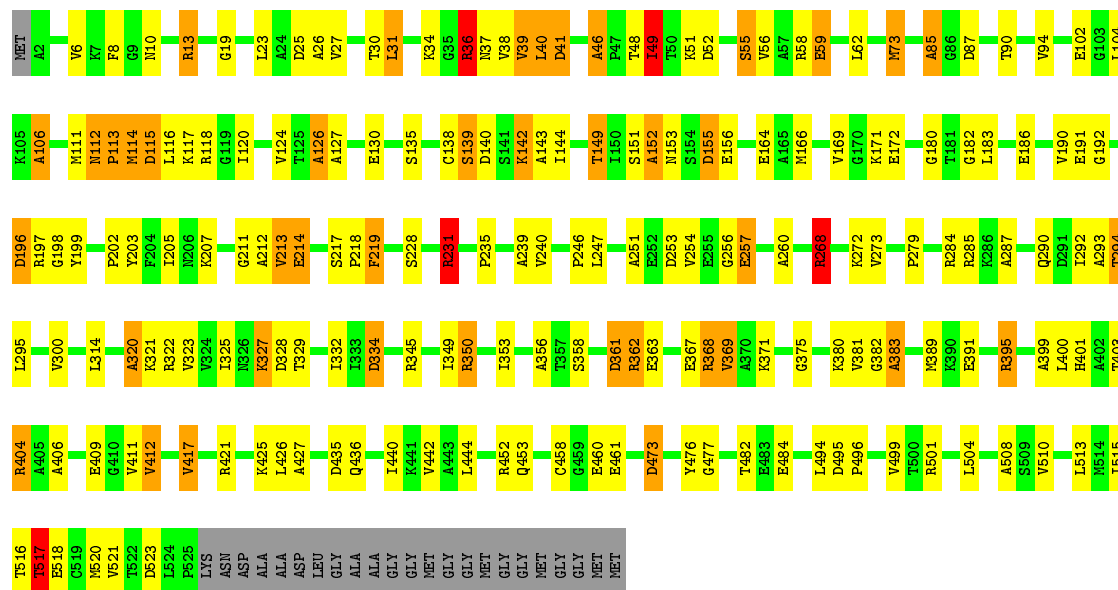






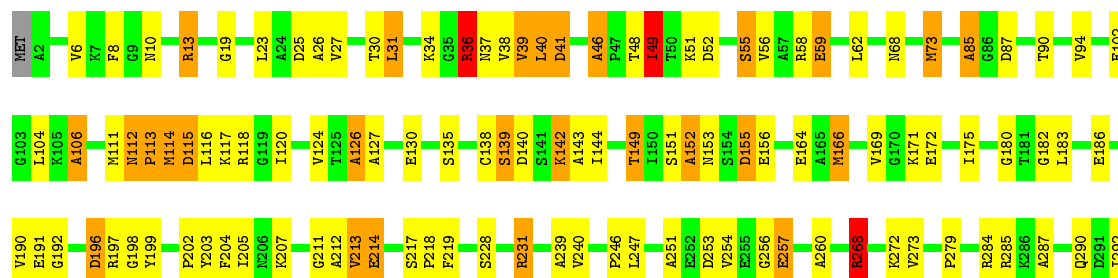
### • Molecule 1: 60 KDA CHAPERONIN

Chain F: 61% 27% 7% . . .



### • Molecule 1: 60 KDA CHAPERONIN

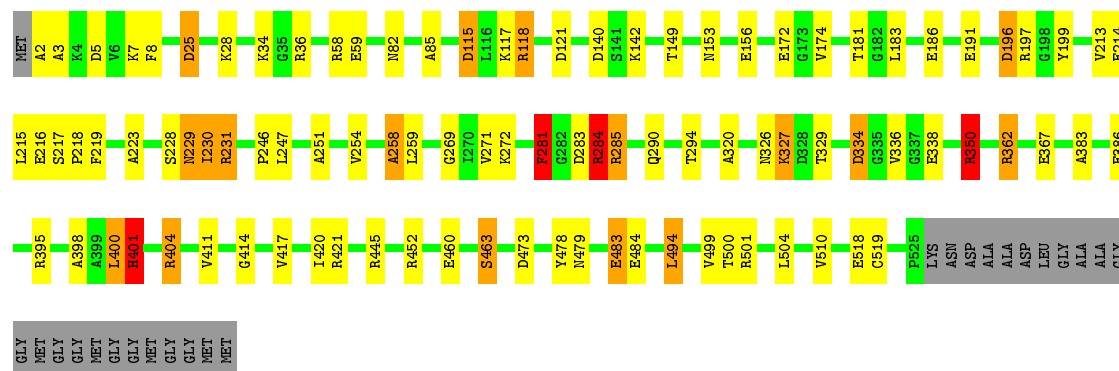
Chain G: 60% 27% 8% . . .







Chain N:  78% 14% . . .



## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| Reconstruction method                | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, C7                       | Depositor |
| Number of particles used             | 5500                            | Depositor |
| Resolution determination method      | Not provided                    | Depositor |
| CTF correction method                | EACH PARTICLE WAS PHASE FLIPPED | Depositor |
| Microscope                           | FEI TECNAI F20                  | Depositor |
| Voltage (kV)                         | 120                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 15                              | Depositor |
| Minimum defocus (nm)                 | 700                             | Depositor |
| Maximum defocus (nm)                 | 3500                            | Depositor |
| Magnification                        | 148500                          | Depositor |
| Image detector                       | GATAN ULTRASCAN 4000 (4k x 4k)  | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ATP

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         | $\# Z  > 2$     | RMSZ        | $\# Z  > 2$      |
| 1   | A     | 1.79         | 4/3873 (0.1%)   | 1.57        | 89/5229 (1.7%)   |
| 1   | B     | 1.79         | 4/3873 (0.1%)   | 1.57        | 90/5229 (1.7%)   |
| 1   | C     | 1.79         | 4/3873 (0.1%)   | 1.57        | 87/5229 (1.7%)   |
| 1   | D     | 1.79         | 4/3873 (0.1%)   | 1.57        | 89/5229 (1.7%)   |
| 1   | E     | 1.80         | 4/3873 (0.1%)   | 1.57        | 89/5229 (1.7%)   |
| 1   | F     | 1.79         | 4/3873 (0.1%)   | 1.57        | 89/5229 (1.7%)   |
| 1   | G     | 1.79         | 4/3873 (0.1%)   | 1.57        | 89/5229 (1.7%)   |
| 1   | H     | 0.70         | 2/3873 (0.1%)   | 1.09        | 22/5229 (0.4%)   |
| 1   | I     | 0.68         | 2/3873 (0.1%)   | 1.09        | 22/5229 (0.4%)   |
| 1   | J     | 0.74         | 2/3873 (0.1%)   | 1.11        | 24/5229 (0.5%)   |
| 1   | K     | 0.69         | 1/3873 (0.0%)   | 1.10        | 23/5229 (0.4%)   |
| 1   | L     | 0.74         | 1/3873 (0.0%)   | 1.12        | 28/5229 (0.5%)   |
| 1   | M     | 0.68         | 1/3873 (0.0%)   | 1.12        | 27/5229 (0.5%)   |
| 1   | N     | 0.81         | 2/3873 (0.1%)   | 1.10        | 23/5229 (0.4%)   |
| All | All   | 1.37         | 39/54222 (0.1%) | 1.36        | 791/73206 (1.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 9                   |
| 1   | B     | 0                   | 9                   |
| 1   | C     | 0                   | 10                  |
| 1   | D     | 0                   | 10                  |
| 1   | E     | 0                   | 9                   |
| 1   | F     | 0                   | 10                  |
| 1   | G     | 0                   | 9                   |
| 1   | H     | 0                   | 10                  |
| 1   | I     | 0                   | 10                  |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | J     | 0                   | 10                  |
| 1   | K     | 0                   | 10                  |
| 1   | L     | 0                   | 11                  |
| 1   | M     | 0                   | 10                  |
| 1   | N     | 0                   | 11                  |
| All | All   | 0                   | 138                 |

All (39) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | E     | 36  | ARG  | CZ-NH1 | 91.40  | 2.51        | 1.33     |
| 1   | G     | 36  | ARG  | CZ-NH1 | 91.28  | 2.51        | 1.33     |
| 1   | B     | 36  | ARG  | CZ-NH1 | 91.26  | 2.51        | 1.33     |
| 1   | F     | 36  | ARG  | CZ-NH1 | 91.25  | 2.51        | 1.33     |
| 1   | D     | 36  | ARG  | CZ-NH1 | 91.20  | 2.51        | 1.33     |
| 1   | C     | 36  | ARG  | CZ-NH1 | 91.16  | 2.51        | 1.33     |
| 1   | A     | 36  | ARG  | CZ-NH1 | 91.00  | 2.51        | 1.33     |
| 1   | N     | 400 | LEU  | C-N    | 21.68  | 1.83        | 1.34     |
| 1   | L     | 400 | LEU  | C-N    | 19.10  | 1.77        | 1.34     |
| 1   | N     | 401 | HIS  | C-N    | -18.91 | 0.90        | 1.34     |
| 1   | J     | 400 | LEU  | C-N    | 16.74  | 1.72        | 1.34     |
| 1   | H     | 401 | HIS  | C-N    | 11.32  | 1.60        | 1.34     |
| 1   | A     | 401 | HIS  | C-N    | 10.23  | 1.57        | 1.34     |
| 1   | K     | 401 | HIS  | C-N    | -10.22 | 1.10        | 1.34     |
| 1   | G     | 401 | HIS  | C-N    | 10.10  | 1.57        | 1.34     |
| 1   | B     | 401 | HIS  | C-N    | 10.02  | 1.57        | 1.34     |
| 1   | F     | 401 | HIS  | C-N    | 9.94   | 1.56        | 1.34     |
| 1   | C     | 401 | HIS  | C-N    | 9.72   | 1.56        | 1.34     |
| 1   | E     | 401 | HIS  | C-N    | 9.57   | 1.56        | 1.34     |
| 1   | D     | 401 | HIS  | C-N    | 9.54   | 1.55        | 1.34     |
| 1   | F     | 36  | ARG  | CD-NE  | 9.10   | 1.61        | 1.46     |
| 1   | C     | 36  | ARG  | CD-NE  | 9.09   | 1.61        | 1.46     |
| 1   | A     | 36  | ARG  | CD-NE  | 9.04   | 1.61        | 1.46     |
| 1   | B     | 36  | ARG  | CD-NE  | 9.02   | 1.61        | 1.46     |
| 1   | D     | 36  | ARG  | CD-NE  | 9.00   | 1.61        | 1.46     |
| 1   | E     | 36  | ARG  | CD-NE  | 9.00   | 1.61        | 1.46     |
| 1   | G     | 36  | ARG  | CD-NE  | 8.96   | 1.61        | 1.46     |
| 1   | J     | 401 | HIS  | C-N    | -8.68  | 1.14        | 1.34     |
| 1   | I     | 401 | HIS  | C-N    | 5.77   | 1.47        | 1.34     |
| 1   | H     | 400 | LEU  | C-N    | 5.70   | 1.47        | 1.34     |
| 1   | I     | 400 | LEU  | C-N    | 5.62   | 1.47        | 1.34     |
| 1   | M     | 400 | LEU  | C-N    | 5.23   | 1.46        | 1.34     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | F     | 517 | THR  | CA-CB | 5.14 | 1.66        | 1.53     |
| 1   | G     | 517 | THR  | CA-CB | 5.13 | 1.66        | 1.53     |
| 1   | C     | 517 | THR  | CA-CB | 5.11 | 1.66        | 1.53     |
| 1   | A     | 517 | THR  | CA-CB | 5.11 | 1.66        | 1.53     |
| 1   | E     | 517 | THR  | CA-CB | 5.11 | 1.66        | 1.53     |
| 1   | B     | 517 | THR  | CA-CB | 5.09 | 1.66        | 1.53     |
| 1   | D     | 517 | THR  | CA-CB | 5.09 | 1.66        | 1.53     |

All (791) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | F     | 36  | ARG  | NE-CZ-NH1  | 22.64  | 131.62      | 120.30   |
| 1   | D     | 36  | ARG  | NE-CZ-NH1  | 22.58  | 131.59      | 120.30   |
| 1   | G     | 36  | ARG  | NE-CZ-NH1  | 22.57  | 131.58      | 120.30   |
| 1   | C     | 36  | ARG  | NE-CZ-NH1  | 22.51  | 131.56      | 120.30   |
| 1   | A     | 36  | ARG  | NE-CZ-NH1  | 22.48  | 131.54      | 120.30   |
| 1   | B     | 36  | ARG  | NE-CZ-NH1  | 22.45  | 131.52      | 120.30   |
| 1   | E     | 36  | ARG  | NE-CZ-NH1  | 22.44  | 131.52      | 120.30   |
| 1   | E     | 36  | ARG  | NH1-CZ-NH2 | -13.84 | 104.18      | 119.40   |
| 1   | B     | 36  | ARG  | CD-NE-CZ   | 13.81  | 142.94      | 123.60   |
| 1   | F     | 36  | ARG  | NH1-CZ-NH2 | -13.79 | 104.23      | 119.40   |
| 1   | G     | 36  | ARG  | NH1-CZ-NH2 | -13.78 | 104.24      | 119.40   |
| 1   | G     | 36  | ARG  | CD-NE-CZ   | 13.77  | 142.87      | 123.60   |
| 1   | A     | 36  | ARG  | CD-NE-CZ   | 13.76  | 142.86      | 123.60   |
| 1   | D     | 36  | ARG  | NH1-CZ-NH2 | -13.75 | 104.28      | 119.40   |
| 1   | D     | 36  | ARG  | CD-NE-CZ   | 13.74  | 142.84      | 123.60   |
| 1   | A     | 36  | ARG  | NH1-CZ-NH2 | -13.74 | 104.28      | 119.40   |
| 1   | B     | 36  | ARG  | NH1-CZ-NH2 | -13.74 | 104.29      | 119.40   |
| 1   | F     | 36  | ARG  | CD-NE-CZ   | 13.73  | 142.83      | 123.60   |
| 1   | E     | 36  | ARG  | CD-NE-CZ   | 13.72  | 142.81      | 123.60   |
| 1   | C     | 36  | ARG  | CD-NE-CZ   | 13.71  | 142.80      | 123.60   |
| 1   | C     | 36  | ARG  | NH1-CZ-NH2 | -13.71 | 104.32      | 119.40   |
| 1   | M     | 401 | HIS  | O-C-N      | 12.36  | 142.48      | 122.70   |
| 1   | A     | 383 | ALA  | N-CA-CB    | 11.87  | 126.72      | 110.10   |
| 1   | C     | 383 | ALA  | N-CA-CB    | 11.85  | 126.69      | 110.10   |
| 1   | F     | 383 | ALA  | N-CA-CB    | 11.85  | 126.69      | 110.10   |
| 1   | E     | 383 | ALA  | N-CA-CB    | 11.84  | 126.68      | 110.10   |
| 1   | G     | 383 | ALA  | N-CA-CB    | 11.81  | 126.64      | 110.10   |
| 1   | D     | 383 | ALA  | N-CA-CB    | 11.79  | 126.60      | 110.10   |
| 1   | B     | 383 | ALA  | N-CA-CB    | 11.78  | 126.60      | 110.10   |
| 1   | B     | 114 | MET  | N-CA-CB    | 11.71  | 131.69      | 110.60   |
| 1   | D     | 114 | MET  | N-CA-CB    | 11.70  | 131.66      | 110.60   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | A     | 114 | MET  | N-CA-CB   | 11.69  | 131.64      | 110.60   |
| 1   | F     | 114 | MET  | N-CA-CB   | 11.68  | 131.62      | 110.60   |
| 1   | C     | 114 | MET  | N-CA-CB   | 11.67  | 131.61      | 110.60   |
| 1   | G     | 114 | MET  | N-CA-CB   | 11.67  | 131.61      | 110.60   |
| 1   | E     | 114 | MET  | N-CA-CB   | 11.67  | 131.60      | 110.60   |
| 1   | C     | 46  | ALA  | N-CA-CB   | -11.17 | 94.46       | 110.10   |
| 1   | A     | 46  | ALA  | N-CA-CB   | -11.15 | 94.49       | 110.10   |
| 1   | B     | 46  | ALA  | N-CA-CB   | -11.15 | 94.49       | 110.10   |
| 1   | G     | 46  | ALA  | N-CA-CB   | -11.15 | 94.49       | 110.10   |
| 1   | F     | 46  | ALA  | N-CA-CB   | -11.14 | 94.51       | 110.10   |
| 1   | E     | 46  | ALA  | N-CA-CB   | -11.13 | 94.51       | 110.10   |
| 1   | D     | 46  | ALA  | N-CA-CB   | -11.12 | 94.53       | 110.10   |
| 1   | L     | 401 | HIS  | O-C-N     | -11.05 | 105.02      | 122.70   |
| 1   | C     | 49  | ILE  | CB-CA-C   | -10.33 | 90.94       | 111.60   |
| 1   | D     | 49  | ILE  | CB-CA-C   | -10.33 | 90.94       | 111.60   |
| 1   | F     | 49  | ILE  | CB-CA-C   | -10.32 | 90.95       | 111.60   |
| 1   | B     | 49  | ILE  | CB-CA-C   | -10.32 | 90.96       | 111.60   |
| 1   | E     | 49  | ILE  | CB-CA-C   | -10.32 | 90.96       | 111.60   |
| 1   | A     | 49  | ILE  | CB-CA-C   | -10.31 | 90.97       | 111.60   |
| 1   | G     | 49  | ILE  | CB-CA-C   | -10.31 | 90.98       | 111.60   |
| 1   | C     | 36  | ARG  | NE-CZ-NH2 | -10.05 | 115.27      | 120.30   |
| 1   | D     | 36  | ARG  | NE-CZ-NH2 | -9.95  | 115.32      | 120.30   |
| 1   | F     | 36  | ARG  | NE-CZ-NH2 | -9.89  | 115.36      | 120.30   |
| 1   | A     | 36  | ARG  | NE-CZ-NH2 | -9.88  | 115.36      | 120.30   |
| 1   | G     | 36  | ARG  | NE-CZ-NH2 | -9.81  | 115.40      | 120.30   |
| 1   | B     | 36  | ARG  | NE-CZ-NH2 | -9.72  | 115.44      | 120.30   |
| 1   | E     | 36  | ARG  | NE-CZ-NH2 | -9.68  | 115.46      | 120.30   |
| 1   | M     | 401 | HIS  | CA-C-N    | -9.26  | 96.83       | 117.20   |
| 1   | D     | 36  | ARG  | CB-CA-C   | 9.17   | 128.73      | 110.40   |
| 1   | C     | 36  | ARG  | CB-CA-C   | 9.15   | 128.70      | 110.40   |
| 1   | A     | 36  | ARG  | CB-CA-C   | 9.14   | 128.68      | 110.40   |
| 1   | F     | 36  | ARG  | CB-CA-C   | 9.14   | 128.68      | 110.40   |
| 1   | G     | 36  | ARG  | CB-CA-C   | 9.13   | 128.67      | 110.40   |
| 1   | E     | 36  | ARG  | CB-CA-C   | 9.13   | 128.66      | 110.40   |
| 1   | B     | 36  | ARG  | CB-CA-C   | 9.12   | 128.64      | 110.40   |
| 1   | C     | 231 | ARG  | NE-CZ-NH1 | 8.95   | 124.78      | 120.30   |
| 1   | G     | 231 | ARG  | NE-CZ-NH1 | 8.93   | 124.76      | 120.30   |
| 1   | F     | 231 | ARG  | NE-CZ-NH1 | 8.91   | 124.76      | 120.30   |
| 1   | B     | 231 | ARG  | NE-CZ-NH1 | 8.84   | 124.72      | 120.30   |
| 1   | D     | 231 | ARG  | NE-CZ-NH1 | 8.83   | 124.71      | 120.30   |
| 1   | E     | 112 | ASN  | N-CA-CB   | -8.82  | 94.72       | 110.60   |
| 1   | E     | 231 | ARG  | NE-CZ-NH1 | 8.81   | 124.70      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | D     | 112 | ASN  | N-CA-CB   | -8.80 | 94.75       | 110.60   |
| 1   | B     | 112 | ASN  | N-CA-CB   | -8.79 | 94.77       | 110.60   |
| 1   | A     | 112 | ASN  | N-CA-CB   | -8.79 | 94.78       | 110.60   |
| 1   | C     | 112 | ASN  | N-CA-CB   | -8.79 | 94.78       | 110.60   |
| 1   | F     | 112 | ASN  | N-CA-CB   | -8.78 | 94.79       | 110.60   |
| 1   | G     | 112 | ASN  | N-CA-CB   | -8.77 | 94.82       | 110.60   |
| 1   | A     | 231 | ARG  | NE-CZ-NH1 | 8.75  | 124.68      | 120.30   |
| 1   | C     | 517 | THR  | CA-CB-OG1 | 8.71  | 127.30      | 109.00   |
| 1   | K     | 452 | ARG  | NE-CZ-NH1 | 8.68  | 124.64      | 120.30   |
| 1   | B     | 517 | THR  | CA-CB-OG1 | 8.67  | 127.20      | 109.00   |
| 1   | F     | 517 | THR  | CA-CB-OG1 | 8.66  | 127.19      | 109.00   |
| 1   | D     | 517 | THR  | CA-CB-OG1 | 8.66  | 127.18      | 109.00   |
| 1   | G     | 517 | THR  | CA-CB-OG1 | 8.66  | 127.18      | 109.00   |
| 1   | A     | 517 | THR  | CA-CB-OG1 | 8.64  | 127.16      | 109.00   |
| 1   | E     | 517 | THR  | CA-CB-OG1 | 8.64  | 127.15      | 109.00   |
| 1   | A     | 41  | ASP  | N-CA-CB   | 8.60  | 126.07      | 110.60   |
| 1   | E     | 41  | ASP  | N-CA-CB   | 8.59  | 126.06      | 110.60   |
| 1   | B     | 41  | ASP  | N-CA-CB   | 8.59  | 126.05      | 110.60   |
| 1   | F     | 41  | ASP  | N-CA-CB   | 8.57  | 126.03      | 110.60   |
| 1   | C     | 41  | ASP  | N-CA-CB   | 8.57  | 126.02      | 110.60   |
| 1   | N     | 452 | ARG  | NE-CZ-NH1 | 8.56  | 124.58      | 120.30   |
| 1   | G     | 41  | ASP  | N-CA-CB   | 8.55  | 126.00      | 110.60   |
| 1   | M     | 452 | ARG  | NE-CZ-NH1 | 8.55  | 124.57      | 120.30   |
| 1   | J     | 452 | ARG  | NE-CZ-NH1 | 8.54  | 124.57      | 120.30   |
| 1   | D     | 41  | ASP  | N-CA-CB   | 8.53  | 125.96      | 110.60   |
| 1   | B     | 152 | ALA  | CB-CA-C   | 8.53  | 122.89      | 110.10   |
| 1   | F     | 152 | ALA  | CB-CA-C   | 8.52  | 122.88      | 110.10   |
| 1   | H     | 452 | ARG  | NE-CZ-NH1 | 8.51  | 124.56      | 120.30   |
| 1   | I     | 452 | ARG  | NE-CZ-NH1 | 8.50  | 124.55      | 120.30   |
| 1   | D     | 152 | ALA  | CB-CA-C   | 8.50  | 122.85      | 110.10   |
| 1   | L     | 231 | ARG  | NE-CZ-NH1 | 8.49  | 124.55      | 120.30   |
| 1   | K     | 58  | ARG  | NE-CZ-NH1 | 8.49  | 124.54      | 120.30   |
| 1   | C     | 152 | ALA  | CB-CA-C   | 8.48  | 122.82      | 110.10   |
| 1   | G     | 152 | ALA  | CB-CA-C   | 8.48  | 122.81      | 110.10   |
| 1   | E     | 152 | ALA  | CB-CA-C   | 8.46  | 122.79      | 110.10   |
| 1   | D     | 461 | GLU  | CB-CA-C   | 8.46  | 127.31      | 110.40   |
| 1   | A     | 461 | GLU  | CB-CA-C   | 8.45  | 127.30      | 110.40   |
| 1   | A     | 152 | ALA  | CB-CA-C   | 8.45  | 122.77      | 110.10   |
| 1   | F     | 461 | GLU  | CB-CA-C   | 8.45  | 127.30      | 110.40   |
| 1   | L     | 452 | ARG  | NE-CZ-NH1 | 8.44  | 124.52      | 120.30   |
| 1   | C     | 461 | GLU  | CB-CA-C   | 8.44  | 127.28      | 110.40   |
| 1   | B     | 461 | GLU  | CB-CA-C   | 8.43  | 127.27      | 110.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | J     | 58  | ARG  | NE-CZ-NH1 | 8.43  | 124.52      | 120.30   |
| 1   | E     | 461 | GLU  | CB-CA-C   | 8.43  | 127.25      | 110.40   |
| 1   | G     | 461 | GLU  | CB-CA-C   | 8.42  | 127.23      | 110.40   |
| 1   | H     | 58  | ARG  | NE-CZ-NH1 | 8.37  | 124.49      | 120.30   |
| 1   | M     | 231 | ARG  | NE-CZ-NH1 | 8.37  | 124.49      | 120.30   |
| 1   | M     | 58  | ARG  | NE-CZ-NH1 | 8.36  | 124.48      | 120.30   |
| 1   | I     | 58  | ARG  | NE-CZ-NH1 | 8.35  | 124.48      | 120.30   |
| 1   | H     | 231 | ARG  | NE-CZ-NH1 | 8.34  | 124.47      | 120.30   |
| 1   | K     | 231 | ARG  | NE-CZ-NH1 | 8.33  | 124.46      | 120.30   |
| 1   | L     | 58  | ARG  | NE-CZ-NH1 | 8.33  | 124.46      | 120.30   |
| 1   | J     | 36  | ARG  | NE-CZ-NH1 | 8.32  | 124.46      | 120.30   |
| 1   | I     | 231 | ARG  | NE-CZ-NH1 | 8.30  | 124.45      | 120.30   |
| 1   | N     | 58  | ARG  | NE-CZ-NH1 | 8.28  | 124.44      | 120.30   |
| 1   | J     | 231 | ARG  | NE-CZ-NH1 | 8.20  | 124.40      | 120.30   |
| 1   | N     | 231 | ARG  | NE-CZ-NH1 | 8.18  | 124.39      | 120.30   |
| 1   | M     | 36  | ARG  | NE-CZ-NH1 | 8.16  | 124.38      | 120.30   |
| 1   | B     | 473 | ASP  | N-CA-CB   | 8.15  | 125.28      | 110.60   |
| 1   | G     | 473 | ASP  | N-CA-CB   | 8.15  | 125.27      | 110.60   |
| 1   | D     | 473 | ASP  | N-CA-CB   | 8.14  | 125.25      | 110.60   |
| 1   | E     | 473 | ASP  | N-CA-CB   | 8.14  | 125.25      | 110.60   |
| 1   | H     | 36  | ARG  | NE-CZ-NH1 | 8.14  | 124.37      | 120.30   |
| 1   | F     | 473 | ASP  | N-CA-CB   | 8.13  | 125.24      | 110.60   |
| 1   | B     | 153 | ASN  | CB-CA-C   | 8.13  | 126.67      | 110.40   |
| 1   | C     | 153 | ASN  | CB-CA-C   | 8.13  | 126.66      | 110.40   |
| 1   | I     | 36  | ARG  | NE-CZ-NH1 | 8.13  | 124.36      | 120.30   |
| 1   | C     | 473 | ASP  | N-CA-CB   | 8.12  | 125.22      | 110.60   |
| 1   | A     | 231 | ARG  | CB-CA-C   | -8.12 | 94.17       | 110.40   |
| 1   | A     | 473 | ASP  | N-CA-CB   | 8.12  | 125.21      | 110.60   |
| 1   | D     | 153 | ASN  | CB-CA-C   | 8.12  | 126.63      | 110.40   |
| 1   | K     | 36  | ARG  | NE-CZ-NH1 | 8.12  | 124.36      | 120.30   |
| 1   | G     | 153 | ASN  | CB-CA-C   | 8.11  | 126.62      | 110.40   |
| 1   | E     | 153 | ASN  | CB-CA-C   | 8.11  | 126.62      | 110.40   |
| 1   | A     | 153 | ASN  | CB-CA-C   | 8.11  | 126.61      | 110.40   |
| 1   | D     | 231 | ARG  | CB-CA-C   | -8.11 | 94.19       | 110.40   |
| 1   | E     | 231 | ARG  | CB-CA-C   | -8.10 | 94.21       | 110.40   |
| 1   | L     | 36  | ARG  | NE-CZ-NH1 | 8.09  | 124.35      | 120.30   |
| 1   | C     | 231 | ARG  | CB-CA-C   | -8.09 | 94.23       | 110.40   |
| 1   | F     | 153 | ASN  | CB-CA-C   | 8.09  | 126.58      | 110.40   |
| 1   | F     | 231 | ARG  | CB-CA-C   | -8.09 | 94.22       | 110.40   |
| 1   | G     | 231 | ARG  | CB-CA-C   | -8.08 | 94.24       | 110.40   |
| 1   | N     | 36  | ARG  | NE-CZ-NH1 | 8.07  | 124.33      | 120.30   |
| 1   | B     | 231 | ARG  | CB-CA-C   | -8.06 | 94.28       | 110.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | G     | 112 | ASN  | CB-CA-C   | 8.02  | 126.44      | 110.40   |
| 1   | C     | 112 | ASN  | CB-CA-C   | 8.02  | 126.43      | 110.40   |
| 1   | A     | 112 | ASN  | CB-CA-C   | 8.01  | 126.42      | 110.40   |
| 1   | D     | 112 | ASN  | CB-CA-C   | 8.00  | 126.41      | 110.40   |
| 1   | B     | 112 | ASN  | CB-CA-C   | 8.00  | 126.40      | 110.40   |
| 1   | E     | 112 | ASN  | CB-CA-C   | 8.00  | 126.40      | 110.40   |
| 1   | F     | 112 | ASN  | CB-CA-C   | 8.00  | 126.39      | 110.40   |
| 1   | F     | 391 | GLU  | CB-CA-C   | -7.94 | 94.51       | 110.40   |
| 1   | A     | 391 | GLU  | CB-CA-C   | -7.94 | 94.53       | 110.40   |
| 1   | E     | 391 | GLU  | CB-CA-C   | -7.91 | 94.57       | 110.40   |
| 1   | C     | 391 | GLU  | CB-CA-C   | -7.91 | 94.58       | 110.40   |
| 1   | D     | 391 | GLU  | CB-CA-C   | -7.91 | 94.58       | 110.40   |
| 1   | B     | 391 | GLU  | CB-CA-C   | -7.91 | 94.58       | 110.40   |
| 1   | G     | 391 | GLU  | CB-CA-C   | -7.90 | 94.59       | 110.40   |
| 1   | G     | 73  | MET  | CB-CA-C   | -7.89 | 94.62       | 110.40   |
| 1   | J     | 401 | HIS  | O-C-N     | 7.88  | 135.32      | 122.70   |
| 1   | E     | 73  | MET  | CB-CA-C   | -7.86 | 94.67       | 110.40   |
| 1   | D     | 73  | MET  | CB-CA-C   | -7.86 | 94.69       | 110.40   |
| 1   | F     | 73  | MET  | CB-CA-C   | -7.85 | 94.70       | 110.40   |
| 1   | B     | 73  | MET  | CB-CA-C   | -7.84 | 94.71       | 110.40   |
| 1   | C     | 73  | MET  | CB-CA-C   | -7.84 | 94.72       | 110.40   |
| 1   | B     | 39  | VAL  | CB-CA-C   | 7.83  | 126.28      | 111.40   |
| 1   | A     | 73  | MET  | CB-CA-C   | -7.83 | 94.75       | 110.40   |
| 1   | E     | 39  | VAL  | CB-CA-C   | 7.81  | 126.24      | 111.40   |
| 1   | F     | 39  | VAL  | CB-CA-C   | 7.79  | 126.20      | 111.40   |
| 1   | A     | 39  | VAL  | CB-CA-C   | 7.77  | 126.16      | 111.40   |
| 1   | C     | 39  | VAL  | CB-CA-C   | 7.77  | 126.16      | 111.40   |
| 1   | G     | 39  | VAL  | CB-CA-C   | 7.75  | 126.12      | 111.40   |
| 1   | D     | 39  | VAL  | CB-CA-C   | 7.74  | 126.10      | 111.40   |
| 1   | J     | 401 | HIS  | CA-C-N    | -7.63 | 100.42      | 117.20   |
| 1   | G     | 404 | ARG  | NE-CZ-NH2 | -7.54 | 116.53      | 120.30   |
| 1   | A     | 404 | ARG  | NE-CZ-NH2 | -7.49 | 116.55      | 120.30   |
| 1   | M     | 400 | LEU  | O-C-N     | -7.49 | 110.72      | 122.70   |
| 1   | C     | 404 | ARG  | NE-CZ-NH2 | -7.46 | 116.57      | 120.30   |
| 1   | D     | 404 | ARG  | NE-CZ-NH2 | -7.45 | 116.58      | 120.30   |
| 1   | E     | 404 | ARG  | NE-CZ-NH2 | -7.43 | 116.58      | 120.30   |
| 1   | L     | 400 | LEU  | O-C-N     | 7.43  | 134.59      | 122.70   |
| 1   | B     | 404 | ARG  | NE-CZ-NH2 | -7.37 | 116.61      | 120.30   |
| 1   | F     | 52  | ASP  | CB-CA-C   | 7.25  | 124.89      | 110.40   |
| 1   | F     | 404 | ARG  | NE-CZ-NH2 | -7.24 | 116.68      | 120.30   |
| 1   | G     | 52  | ASP  | CB-CA-C   | 7.23  | 124.86      | 110.40   |
| 1   | C     | 52  | ASP  | CB-CA-C   | 7.22  | 124.84      | 110.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 52  | ASP  | CB-CA-C   | 7.21  | 124.82      | 110.40   |
| 1   | N     | 367 | GLU  | CB-CA-C   | -7.20 | 96.00       | 110.40   |
| 1   | J     | 367 | GLU  | CB-CA-C   | -7.19 | 96.02       | 110.40   |
| 1   | B     | 52  | ASP  | CB-CA-C   | 7.19  | 124.78      | 110.40   |
| 1   | D     | 52  | ASP  | CB-CA-C   | 7.19  | 124.78      | 110.40   |
| 1   | E     | 52  | ASP  | CB-CA-C   | 7.19  | 124.78      | 110.40   |
| 1   | L     | 367 | GLU  | CB-CA-C   | -7.18 | 96.04       | 110.40   |
| 1   | H     | 367 | GLU  | CB-CA-C   | -7.18 | 96.04       | 110.40   |
| 1   | I     | 367 | GLU  | CB-CA-C   | -7.17 | 96.05       | 110.40   |
| 1   | M     | 367 | GLU  | CB-CA-C   | -7.17 | 96.05       | 110.40   |
| 1   | K     | 367 | GLU  | CB-CA-C   | -7.17 | 96.06       | 110.40   |
| 1   | M     | 401 | HIS  | C-N-CA    | -7.12 | 103.89      | 121.70   |
| 1   | L     | 362 | ARG  | NE-CZ-NH1 | 7.11  | 123.86      | 120.30   |
| 1   | M     | 362 | ARG  | NE-CZ-NH1 | 7.07  | 123.83      | 120.30   |
| 1   | J     | 362 | ARG  | NE-CZ-NH1 | 7.06  | 123.83      | 120.30   |
| 1   | K     | 362 | ARG  | NE-CZ-NH1 | 7.04  | 123.82      | 120.30   |
| 1   | H     | 362 | ARG  | NE-CZ-NH1 | 7.04  | 123.82      | 120.30   |
| 1   | F     | 118 | ARG  | NE-CZ-NH1 | 7.03  | 123.81      | 120.30   |
| 1   | N     | 362 | ARG  | NE-CZ-NH1 | 7.02  | 123.81      | 120.30   |
| 1   | I     | 362 | ARG  | NE-CZ-NH1 | 7.02  | 123.81      | 120.30   |
| 1   | D     | 118 | ARG  | NE-CZ-NH1 | 6.97  | 123.79      | 120.30   |
| 1   | B     | 115 | ASP  | N-CA-CB   | 6.96  | 123.12      | 110.60   |
| 1   | A     | 115 | ASP  | N-CA-CB   | 6.95  | 123.12      | 110.60   |
| 1   | A     | 118 | ARG  | NE-CZ-NH1 | 6.95  | 123.78      | 120.30   |
| 1   | C     | 118 | ARG  | NE-CZ-NH1 | 6.95  | 123.77      | 120.30   |
| 1   | G     | 115 | ASP  | N-CA-CB   | 6.95  | 123.10      | 110.60   |
| 1   | D     | 115 | ASP  | N-CA-CB   | 6.93  | 123.08      | 110.60   |
| 1   | E     | 115 | ASP  | N-CA-CB   | 6.93  | 123.08      | 110.60   |
| 1   | L     | 401 | HIS  | CA-C-N    | 6.92  | 132.43      | 117.20   |
| 1   | C     | 115 | ASP  | N-CA-CB   | 6.91  | 123.04      | 110.60   |
| 1   | F     | 115 | ASP  | N-CA-CB   | 6.90  | 123.02      | 110.60   |
| 1   | A     | 294 | THR  | CA-CB-CG2 | -6.89 | 102.76      | 112.40   |
| 1   | E     | 118 | ARG  | NE-CZ-NH1 | 6.88  | 123.74      | 120.30   |
| 1   | C     | 87  | ASP  | CB-CG-OD2 | 6.88  | 124.49      | 118.30   |
| 1   | F     | 294 | THR  | CA-CB-CG2 | -6.88 | 102.77      | 112.40   |
| 1   | C     | 46  | ALA  | CB-CA-C   | -6.87 | 99.80       | 110.10   |
| 1   | D     | 87  | ASP  | CB-CG-OD2 | 6.86  | 124.48      | 118.30   |
| 1   | B     | 294 | THR  | CA-CB-CG2 | -6.86 | 102.80      | 112.40   |
| 1   | G     | 118 | ARG  | NE-CZ-NH1 | 6.86  | 123.73      | 120.30   |
| 1   | G     | 294 | THR  | CA-CB-CG2 | -6.86 | 102.80      | 112.40   |
| 1   | G     | 46  | ALA  | CB-CA-C   | -6.86 | 99.82       | 110.10   |
| 1   | G     | 87  | ASP  | CB-CG-OD2 | 6.86  | 124.47      | 118.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | C     | 294 | THR  | CA-CB-CG2 | -6.85 | 102.81      | 112.40   |
| 1   | D     | 46  | ALA  | CB-CA-C   | -6.85 | 99.82       | 110.10   |
| 1   | E     | 294 | THR  | CA-CB-CG2 | -6.85 | 102.81      | 112.40   |
| 1   | D     | 294 | THR  | CA-CB-CG2 | -6.85 | 102.81      | 112.40   |
| 1   | E     | 87  | ASP  | CB-CG-OD2 | 6.84  | 124.46      | 118.30   |
| 1   | B     | 46  | ALA  | CB-CA-C   | -6.83 | 99.86       | 110.10   |
| 1   | A     | 46  | ALA  | CB-CA-C   | -6.83 | 99.86       | 110.10   |
| 1   | F     | 46  | ALA  | CB-CA-C   | -6.83 | 99.86       | 110.10   |
| 1   | E     | 46  | ALA  | CB-CA-C   | -6.82 | 99.87       | 110.10   |
| 1   | A     | 87  | ASP  | CB-CG-OD2 | 6.82  | 124.44      | 118.30   |
| 1   | C     | 231 | ARG  | CA-CB-CG  | 6.80  | 128.35      | 113.40   |
| 1   | D     | 39  | VAL  | CA-CB-CG1 | 6.79  | 121.08      | 110.90   |
| 1   | B     | 87  | ASP  | CB-CG-OD2 | 6.79  | 124.41      | 118.30   |
| 1   | B     | 231 | ARG  | CA-CB-CG  | 6.79  | 128.33      | 113.40   |
| 1   | G     | 231 | ARG  | CA-CB-CG  | 6.78  | 128.32      | 113.40   |
| 1   | A     | 231 | ARG  | CA-CB-CG  | 6.78  | 128.32      | 113.40   |
| 1   | C     | 39  | VAL  | CA-CB-CG1 | 6.78  | 121.07      | 110.90   |
| 1   | G     | 39  | VAL  | CA-CB-CG1 | 6.78  | 121.07      | 110.90   |
| 1   | F     | 87  | ASP  | CB-CG-OD2 | 6.77  | 124.40      | 118.30   |
| 1   | D     | 231 | ARG  | CA-CB-CG  | 6.77  | 128.30      | 113.40   |
| 1   | B     | 39  | VAL  | CA-CB-CG1 | 6.76  | 121.05      | 110.90   |
| 1   | F     | 231 | ARG  | CA-CB-CG  | 6.76  | 128.28      | 113.40   |
| 1   | A     | 39  | VAL  | CA-CB-CG1 | 6.76  | 121.05      | 110.90   |
| 1   | E     | 39  | VAL  | CA-CB-CG1 | 6.76  | 121.03      | 110.90   |
| 1   | E     | 231 | ARG  | CA-CB-CG  | 6.75  | 128.25      | 113.40   |
| 1   | F     | 39  | VAL  | CA-CB-CG1 | 6.74  | 121.01      | 110.90   |
| 1   | B     | 139 | SER  | CB-CA-C   | 6.72  | 122.86      | 110.10   |
| 1   | E     | 139 | SER  | CB-CA-C   | 6.71  | 122.85      | 110.10   |
| 1   | B     | 118 | ARG  | NE-CZ-NH1 | 6.71  | 123.66      | 120.30   |
| 1   | A     | 517 | THR  | N-CA-CB   | 6.71  | 123.04      | 110.30   |
| 1   | L     | 401 | HIS  | C-N-CA    | 6.71  | 138.47      | 121.70   |
| 1   | F     | 139 | SER  | CB-CA-C   | 6.69  | 122.81      | 110.10   |
| 1   | G     | 139 | SER  | CB-CA-C   | 6.69  | 122.80      | 110.10   |
| 1   | E     | 517 | THR  | N-CA-CB   | 6.68  | 123.00      | 110.30   |
| 1   | A     | 139 | SER  | CB-CA-C   | 6.68  | 122.80      | 110.10   |
| 1   | D     | 139 | SER  | CB-CA-C   | 6.67  | 122.78      | 110.10   |
| 1   | F     | 517 | THR  | N-CA-CB   | 6.67  | 122.98      | 110.30   |
| 1   | D     | 517 | THR  | N-CA-CB   | 6.67  | 122.98      | 110.30   |
| 1   | B     | 517 | THR  | N-CA-CB   | 6.66  | 122.96      | 110.30   |
| 1   | G     | 517 | THR  | N-CA-CB   | 6.66  | 122.95      | 110.30   |
| 1   | C     | 517 | THR  | N-CA-CB   | 6.64  | 122.92      | 110.30   |
| 1   | C     | 139 | SER  | CB-CA-C   | 6.64  | 122.71      | 110.10   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | E     | 285 | ARG  | CB-CA-C   | -6.60 | 97.20       | 110.40   |
| 1   | A     | 285 | ARG  | CB-CA-C   | -6.59 | 97.22       | 110.40   |
| 1   | G     | 285 | ARG  | CB-CA-C   | -6.59 | 97.22       | 110.40   |
| 1   | D     | 285 | ARG  | CB-CA-C   | -6.58 | 97.25       | 110.40   |
| 1   | F     | 285 | ARG  | CB-CA-C   | -6.57 | 97.27       | 110.40   |
| 1   | C     | 285 | ARG  | CB-CA-C   | -6.56 | 97.28       | 110.40   |
| 1   | B     | 285 | ARG  | CB-CA-C   | -6.56 | 97.28       | 110.40   |
| 1   | D     | 322 | ARG  | NE-CZ-NH2 | -6.55 | 117.03      | 120.30   |
| 1   | C     | 140 | ASP  | N-CA-CB   | -6.54 | 98.82       | 110.60   |
| 1   | D     | 140 | ASP  | N-CA-CB   | -6.54 | 98.82       | 110.60   |
| 1   | E     | 140 | ASP  | N-CA-CB   | -6.54 | 98.83       | 110.60   |
| 1   | A     | 140 | ASP  | N-CA-CB   | -6.54 | 98.83       | 110.60   |
| 1   | B     | 140 | ASP  | N-CA-CB   | -6.54 | 98.83       | 110.60   |
| 1   | J     | 473 | ASP  | N-CA-CB   | 6.53  | 122.35      | 110.60   |
| 1   | N     | 473 | ASP  | N-CA-CB   | 6.52  | 122.34      | 110.60   |
| 1   | F     | 140 | ASP  | N-CA-CB   | -6.52 | 98.86       | 110.60   |
| 1   | G     | 140 | ASP  | N-CA-CB   | -6.52 | 98.87       | 110.60   |
| 1   | C     | 425 | LYS  | CB-CA-C   | 6.51  | 123.42      | 110.40   |
| 1   | E     | 371 | LYS  | CB-CA-C   | 6.51  | 123.41      | 110.40   |
| 1   | I     | 473 | ASP  | N-CA-CB   | 6.51  | 122.31      | 110.60   |
| 1   | F     | 425 | LYS  | CB-CA-C   | 6.50  | 123.41      | 110.40   |
| 1   | G     | 425 | LYS  | CB-CA-C   | 6.50  | 123.41      | 110.40   |
| 1   | N     | 404 | ARG  | NE-CZ-NH1 | 6.50  | 123.55      | 120.30   |
| 1   | K     | 473 | ASP  | N-CA-CB   | 6.50  | 122.30      | 110.60   |
| 1   | A     | 425 | LYS  | CB-CA-C   | 6.50  | 123.39      | 110.40   |
| 1   | B     | 425 | LYS  | CB-CA-C   | 6.50  | 123.39      | 110.40   |
| 1   | L     | 118 | ARG  | NE-CZ-NH1 | 6.50  | 123.55      | 120.30   |
| 1   | B     | 371 | LYS  | CB-CA-C   | 6.50  | 123.39      | 110.40   |
| 1   | M     | 118 | ARG  | NE-CZ-NH1 | 6.50  | 123.55      | 120.30   |
| 1   | N     | 118 | ARG  | NE-CZ-NH1 | 6.49  | 123.55      | 120.30   |
| 1   | E     | 425 | LYS  | CB-CA-C   | 6.49  | 123.38      | 110.40   |
| 1   | H     | 501 | ARG  | NE-CZ-NH1 | 6.49  | 123.55      | 120.30   |
| 1   | C     | 371 | LYS  | CB-CA-C   | 6.49  | 123.38      | 110.40   |
| 1   | J     | 501 | ARG  | NE-CZ-NH1 | 6.49  | 123.54      | 120.30   |
| 1   | M     | 473 | ASP  | N-CA-CB   | 6.48  | 122.27      | 110.60   |
| 1   | H     | 473 | ASP  | N-CA-CB   | 6.48  | 122.27      | 110.60   |
| 1   | G     | 322 | ARG  | NE-CZ-NH2 | -6.48 | 117.06      | 120.30   |
| 1   | D     | 425 | LYS  | CB-CA-C   | 6.47  | 123.34      | 110.40   |
| 1   | L     | 473 | ASP  | N-CA-CB   | 6.47  | 122.24      | 110.60   |
| 1   | C     | 322 | ARG  | NE-CZ-NH2 | -6.46 | 117.07      | 120.30   |
| 1   | A     | 371 | LYS  | CB-CA-C   | 6.46  | 123.31      | 110.40   |
| 1   | F     | 322 | ARG  | NE-CZ-NH2 | -6.45 | 117.07      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | I     | 118 | ARG  | NE-CZ-NH1 | 6.45  | 123.52      | 120.30   |
| 1   | K     | 118 | ARG  | NE-CZ-NH1 | 6.44  | 123.52      | 120.30   |
| 1   | M     | 501 | ARG  | NE-CZ-NH1 | 6.43  | 123.52      | 120.30   |
| 1   | K     | 350 | ARG  | NE-CZ-NH1 | 6.43  | 123.52      | 120.30   |
| 1   | D     | 371 | LYS  | CB-CA-C   | 6.43  | 123.26      | 110.40   |
| 1   | G     | 371 | LYS  | CB-CA-C   | 6.42  | 123.25      | 110.40   |
| 1   | H     | 118 | ARG  | NE-CZ-NH1 | 6.42  | 123.51      | 120.30   |
| 1   | F     | 371 | LYS  | CB-CA-C   | 6.42  | 123.24      | 110.40   |
| 1   | K     | 501 | ARG  | NE-CZ-NH1 | 6.41  | 123.51      | 120.30   |
| 1   | A     | 322 | ARG  | NE-CZ-NH2 | -6.40 | 117.10      | 120.30   |
| 1   | B     | 52  | ASP  | N-CA-CB   | 6.39  | 122.11      | 110.60   |
| 1   | C     | 52  | ASP  | N-CA-CB   | 6.39  | 122.11      | 110.60   |
| 1   | J     | 118 | ARG  | NE-CZ-NH1 | 6.39  | 123.50      | 120.30   |
| 1   | E     | 52  | ASP  | N-CA-CB   | 6.39  | 122.10      | 110.60   |
| 1   | A     | 52  | ASP  | N-CA-CB   | 6.39  | 122.10      | 110.60   |
| 1   | N     | 501 | ARG  | NE-CZ-NH1 | 6.39  | 123.49      | 120.30   |
| 1   | F     | 52  | ASP  | N-CA-CB   | 6.37  | 122.06      | 110.60   |
| 1   | D     | 52  | ASP  | N-CA-CB   | 6.37  | 122.06      | 110.60   |
| 1   | G     | 52  | ASP  | N-CA-CB   | 6.37  | 122.06      | 110.60   |
| 1   | H     | 350 | ARG  | NE-CZ-NH1 | 6.36  | 123.48      | 120.30   |
| 1   | I     | 350 | ARG  | NE-CZ-NH1 | 6.34  | 123.47      | 120.30   |
| 1   | B     | 322 | ARG  | NE-CZ-NH2 | -6.34 | 117.13      | 120.30   |
| 1   | L     | 395 | ARG  | NE-CZ-NH1 | 6.34  | 123.47      | 120.30   |
| 1   | L     | 350 | ARG  | NE-CZ-NH1 | 6.33  | 123.46      | 120.30   |
| 1   | L     | 501 | ARG  | NE-CZ-NH1 | 6.32  | 123.46      | 120.30   |
| 1   | E     | 322 | ARG  | NE-CZ-NH2 | -6.31 | 117.14      | 120.30   |
| 1   | I     | 501 | ARG  | NE-CZ-NH1 | 6.29  | 123.45      | 120.30   |
| 1   | I     | 395 | ARG  | NE-CZ-NH1 | 6.28  | 123.44      | 120.30   |
| 1   | A     | 482 | THR  | N-CA-CB   | 6.25  | 122.18      | 110.30   |
| 1   | M     | 350 | ARG  | NE-CZ-NH1 | 6.25  | 123.42      | 120.30   |
| 1   | J     | 350 | ARG  | NE-CZ-NH1 | 6.24  | 123.42      | 120.30   |
| 1   | C     | 482 | THR  | N-CA-CB   | 6.24  | 122.15      | 110.30   |
| 1   | K     | 395 | ARG  | NE-CZ-NH1 | 6.23  | 123.42      | 120.30   |
| 1   | N     | 350 | ARG  | NE-CZ-NH1 | 6.22  | 123.41      | 120.30   |
| 1   | F     | 362 | ARG  | NE-CZ-NH1 | 6.21  | 123.40      | 120.30   |
| 1   | E     | 510 | VAL  | CB-CA-C   | -6.21 | 99.61       | 111.40   |
| 1   | D     | 482 | THR  | N-CA-CB   | 6.20  | 122.09      | 110.30   |
| 1   | C     | 510 | VAL  | CB-CA-C   | -6.20 | 99.63       | 111.40   |
| 1   | H     | 395 | ARG  | NE-CZ-NH1 | 6.19  | 123.40      | 120.30   |
| 1   | B     | 482 | THR  | N-CA-CB   | 6.19  | 122.07      | 110.30   |
| 1   | G     | 482 | THR  | N-CA-CB   | 6.19  | 122.07      | 110.30   |
| 1   | A     | 510 | VAL  | CB-CA-C   | -6.19 | 99.64       | 111.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | E     | 482 | THR  | N-CA-CB   | 6.19  | 122.06      | 110.30   |
| 1   | F     | 510 | VAL  | CB-CA-C   | -6.19 | 99.64       | 111.40   |
| 1   | M     | 395 | ARG  | NE-CZ-NH1 | 6.19  | 123.39      | 120.30   |
| 1   | D     | 510 | VAL  | CB-CA-C   | -6.19 | 99.65       | 111.40   |
| 1   | B     | 510 | VAL  | CB-CA-C   | -6.18 | 99.65       | 111.40   |
| 1   | F     | 482 | THR  | N-CA-CB   | 6.18  | 122.04      | 110.30   |
| 1   | J     | 395 | ARG  | NE-CZ-NH1 | 6.18  | 123.39      | 120.30   |
| 1   | G     | 362 | ARG  | NE-CZ-NH1 | 6.16  | 123.38      | 120.30   |
| 1   | G     | 510 | VAL  | CB-CA-C   | -6.16 | 99.70       | 111.40   |
| 1   | J     | 404 | ARG  | NE-CZ-NH1 | 6.16  | 123.38      | 120.30   |
| 1   | E     | 362 | ARG  | NE-CZ-NH1 | 6.15  | 123.37      | 120.30   |
| 1   | L     | 404 | ARG  | NE-CZ-NH1 | 6.15  | 123.37      | 120.30   |
| 1   | D     | 362 | ARG  | NE-CZ-NH1 | 6.13  | 123.37      | 120.30   |
| 1   | N     | 395 | ARG  | NE-CZ-NH1 | 6.12  | 123.36      | 120.30   |
| 1   | C     | 362 | ARG  | NE-CZ-NH1 | 6.11  | 123.35      | 120.30   |
| 1   | A     | 362 | ARG  | NE-CZ-NH1 | 6.10  | 123.35      | 120.30   |
| 1   | F     | 85  | ALA  | N-CA-CB   | -6.02 | 101.67      | 110.10   |
| 1   | L     | 196 | ASP  | N-CA-CB   | -6.02 | 99.76       | 110.60   |
| 1   | C     | 435 | ASP  | CB-CG-OD2 | -6.01 | 112.89      | 118.30   |
| 1   | M     | 5   | ASP  | N-CA-CB   | 6.01  | 121.42      | 110.60   |
| 1   | H     | 284 | ARG  | NE-CZ-NH1 | 6.01  | 123.30      | 120.30   |
| 1   | I     | 5   | ASP  | N-CA-CB   | 6.01  | 121.41      | 110.60   |
| 1   | E     | 435 | ASP  | CB-CG-OD2 | -6.00 | 112.90      | 118.30   |
| 1   | M     | 196 | ASP  | N-CA-CB   | -6.00 | 99.80       | 110.60   |
| 1   | N     | 196 | ASP  | N-CA-CB   | -6.00 | 99.80       | 110.60   |
| 1   | J     | 196 | ASP  | N-CA-CB   | -6.00 | 99.80       | 110.60   |
| 1   | N     | 5   | ASP  | N-CA-CB   | 6.00  | 121.40      | 110.60   |
| 1   | I     | 196 | ASP  | N-CA-CB   | -6.00 | 99.81       | 110.60   |
| 1   | K     | 196 | ASP  | N-CA-CB   | -5.99 | 99.83       | 110.60   |
| 1   | J     | 5   | ASP  | N-CA-CB   | 5.98  | 121.37      | 110.60   |
| 1   | L     | 5   | ASP  | N-CA-CB   | 5.98  | 121.37      | 110.60   |
| 1   | D     | 435 | ASP  | CB-CG-OD2 | -5.98 | 112.92      | 118.30   |
| 1   | E     | 85  | ALA  | N-CA-CB   | -5.98 | 101.73      | 110.10   |
| 1   | G     | 435 | ASP  | CB-CG-OD2 | -5.98 | 112.92      | 118.30   |
| 1   | H     | 196 | ASP  | N-CA-CB   | -5.98 | 99.83       | 110.60   |
| 1   | C     | 85  | ALA  | N-CA-CB   | -5.97 | 101.74      | 110.10   |
| 1   | D     | 40  | LEU  | N-CA-CB   | -5.97 | 98.46       | 110.40   |
| 1   | G     | 85  | ALA  | N-CA-CB   | -5.97 | 101.74      | 110.10   |
| 1   | B     | 85  | ALA  | N-CA-CB   | -5.97 | 101.75      | 110.10   |
| 1   | K     | 5   | ASP  | N-CA-CB   | 5.96  | 121.33      | 110.60   |
| 1   | D     | 85  | ALA  | N-CA-CB   | -5.96 | 101.75      | 110.10   |
| 1   | N     | 284 | ARG  | NE-CZ-NH1 | 5.96  | 123.28      | 120.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | H     | 5   | ASP  | N-CA-CB    | 5.96  | 121.33      | 110.60   |
| 1   | A     | 85  | ALA  | N-CA-CB    | -5.96 | 101.76      | 110.10   |
| 1   | G     | 40  | LEU  | N-CA-CB    | -5.95 | 98.49       | 110.40   |
| 1   | A     | 435 | ASP  | CB-CG-OD2  | -5.95 | 112.95      | 118.30   |
| 1   | B     | 362 | ARG  | NE-CZ-NH1  | 5.94  | 123.27      | 120.30   |
| 1   | I     | 284 | ARG  | NE-CZ-NH1  | 5.94  | 123.27      | 120.30   |
| 1   | A     | 40  | LEU  | N-CA-CB    | -5.93 | 98.53       | 110.40   |
| 1   | B     | 435 | ASP  | CB-CG-OD2  | -5.93 | 112.96      | 118.30   |
| 1   | F     | 40  | LEU  | N-CA-CB    | -5.93 | 98.53       | 110.40   |
| 1   | F     | 435 | ASP  | CB-CG-OD2  | -5.93 | 112.96      | 118.30   |
| 1   | E     | 40  | LEU  | N-CA-CB    | -5.93 | 98.55       | 110.40   |
| 1   | C     | 40  | LEU  | N-CA-CB    | -5.92 | 98.55       | 110.40   |
| 1   | B     | 40  | LEU  | N-CA-CB    | -5.92 | 98.56       | 110.40   |
| 1   | M     | 284 | ARG  | NE-CZ-NH1  | 5.91  | 123.25      | 120.30   |
| 1   | D     | 391 | GLU  | CA-CB-CG   | 5.85  | 126.27      | 113.40   |
| 1   | E     | 391 | GLU  | CA-CB-CG   | 5.85  | 126.27      | 113.40   |
| 1   | B     | 391 | GLU  | CA-CB-CG   | 5.85  | 126.27      | 113.40   |
| 1   | G     | 391 | GLU  | CA-CB-CG   | 5.84  | 126.26      | 113.40   |
| 1   | N     | 285 | ARG  | NE-CZ-NH1  | 5.84  | 123.22      | 120.30   |
| 1   | K     | 284 | ARG  | NE-CZ-NH1  | 5.84  | 123.22      | 120.30   |
| 1   | M     | 285 | ARG  | NE-CZ-NH1  | 5.84  | 123.22      | 120.30   |
| 1   | E     | 367 | GLU  | CB-CA-C    | -5.83 | 98.73       | 110.40   |
| 1   | D     | 367 | GLU  | CB-CA-C    | -5.83 | 98.73       | 110.40   |
| 1   | F     | 391 | GLU  | CA-CB-CG   | 5.83  | 126.22      | 113.40   |
| 1   | A     | 391 | GLU  | CA-CB-CG   | 5.83  | 126.21      | 113.40   |
| 1   | L     | 284 | ARG  | NE-CZ-NH1  | 5.83  | 123.21      | 120.30   |
| 1   | A     | 417 | VAL  | CA-CB-CG2  | -5.82 | 102.17      | 110.90   |
| 1   | B     | 367 | GLU  | CB-CA-C    | -5.82 | 98.76       | 110.40   |
| 1   | C     | 391 | GLU  | CA-CB-CG   | 5.82  | 126.20      | 113.40   |
| 1   | A     | 367 | GLU  | CB-CA-C    | -5.82 | 98.77       | 110.40   |
| 1   | C     | 367 | GLU  | CB-CA-C    | -5.81 | 98.77       | 110.40   |
| 1   | F     | 367 | GLU  | CB-CA-C    | -5.80 | 98.79       | 110.40   |
| 1   | G     | 367 | GLU  | CB-CA-C    | -5.80 | 98.79       | 110.40   |
| 1   | K     | 404 | ARG  | NE-CZ-NH1  | 5.80  | 123.20      | 120.30   |
| 1   | F     | 87  | ASP  | OD1-CG-OD2 | -5.80 | 112.28      | 123.30   |
| 1   | E     | 417 | VAL  | CA-CB-CG2  | -5.80 | 102.20      | 110.90   |
| 1   | G     | 417 | VAL  | CA-CB-CG2  | -5.79 | 102.21      | 110.90   |
| 1   | B     | 417 | VAL  | CA-CB-CG2  | -5.79 | 102.21      | 110.90   |
| 1   | C     | 417 | VAL  | CA-CB-CG2  | -5.79 | 102.21      | 110.90   |
| 1   | D     | 87  | ASP  | OD1-CG-OD2 | -5.79 | 112.30      | 123.30   |
| 1   | E     | 87  | ASP  | OD1-CG-OD2 | -5.79 | 112.30      | 123.30   |
| 1   | B     | 87  | ASP  | OD1-CG-OD2 | -5.78 | 112.32      | 123.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 417 | VAL  | CA-CB-CG2  | -5.78 | 102.23      | 110.90   |
| 1   | A     | 87  | ASP  | OD1-CG-OD2 | -5.78 | 112.32      | 123.30   |
| 1   | C     | 87  | ASP  | OD1-CG-OD2 | -5.77 | 112.33      | 123.30   |
| 1   | F     | 417 | VAL  | CA-CB-CG2  | -5.77 | 102.24      | 110.90   |
| 1   | G     | 87  | ASP  | OD1-CG-OD2 | -5.77 | 112.34      | 123.30   |
| 1   | J     | 284 | ARG  | NE-CZ-NH1  | 5.77  | 123.18      | 120.30   |
| 1   | E     | 149 | THR  | N-CA-CB    | 5.76  | 121.25      | 110.30   |
| 1   | D     | 149 | THR  | N-CA-CB    | 5.75  | 121.23      | 110.30   |
| 1   | I     | 285 | ARG  | NE-CZ-NH1  | 5.75  | 123.18      | 120.30   |
| 1   | G     | 149 | THR  | N-CA-CB    | 5.75  | 121.22      | 110.30   |
| 1   | K     | 115 | ASP  | CB-CA-C    | 5.75  | 121.90      | 110.40   |
| 1   | K     | 285 | ARG  | NE-CZ-NH1  | 5.75  | 123.17      | 120.30   |
| 1   | F     | 149 | THR  | N-CA-CB    | 5.75  | 121.22      | 110.30   |
| 1   | H     | 285 | ARG  | NE-CZ-NH1  | 5.74  | 123.17      | 120.30   |
| 1   | L     | 285 | ARG  | NE-CZ-NH1  | 5.73  | 123.16      | 120.30   |
| 1   | C     | 149 | THR  | N-CA-CB    | 5.71  | 121.16      | 110.30   |
| 1   | J     | 285 | ARG  | NE-CZ-NH1  | 5.71  | 123.16      | 120.30   |
| 1   | A     | 149 | THR  | N-CA-CB    | 5.71  | 121.15      | 110.30   |
| 1   | L     | 115 | ASP  | CB-CA-C    | 5.71  | 121.82      | 110.40   |
| 1   | B     | 149 | THR  | N-CA-CB    | 5.71  | 121.14      | 110.30   |
| 1   | C     | 39  | VAL  | CG1-CB-CG2 | 5.71  | 120.03      | 110.90   |
| 1   | B     | 39  | VAL  | CG1-CB-CG2 | 5.70  | 120.02      | 110.90   |
| 1   | L     | 400 | LEU  | CA-C-N     | -5.70 | 104.66      | 117.20   |
| 1   | I     | 115 | ASP  | CB-CA-C    | 5.70  | 121.80      | 110.40   |
| 1   | N     | 115 | ASP  | CB-CA-C    | 5.70  | 121.79      | 110.40   |
| 1   | E     | 452 | ARG  | NE-CZ-NH1  | 5.69  | 123.15      | 120.30   |
| 1   | E     | 39  | VAL  | CG1-CB-CG2 | 5.69  | 120.00      | 110.90   |
| 1   | J     | 115 | ASP  | CB-CA-C    | 5.68  | 121.77      | 110.40   |
| 1   | F     | 39  | VAL  | CG1-CB-CG2 | 5.68  | 119.99      | 110.90   |
| 1   | D     | 452 | ARG  | NE-CZ-NH1  | 5.68  | 123.14      | 120.30   |
| 1   | M     | 115 | ASP  | CB-CA-C    | 5.68  | 121.76      | 110.40   |
| 1   | D     | 353 | ILE  | CB-CA-C    | -5.68 | 100.25      | 111.60   |
| 1   | A     | 353 | ILE  | CB-CA-C    | -5.67 | 100.25      | 111.60   |
| 1   | E     | 412 | VAL  | CB-CA-C    | -5.67 | 100.62      | 111.40   |
| 1   | A     | 452 | ARG  | NE-CZ-NH1  | 5.67  | 123.14      | 120.30   |
| 1   | F     | 353 | ILE  | CB-CA-C    | -5.67 | 100.26      | 111.60   |
| 1   | H     | 115 | ASP  | CB-CA-C    | 5.67  | 121.74      | 110.40   |
| 1   | C     | 353 | ILE  | CB-CA-C    | -5.67 | 100.26      | 111.60   |
| 1   | G     | 39  | VAL  | CG1-CB-CG2 | 5.67  | 119.97      | 110.90   |
| 1   | C     | 412 | VAL  | CB-CA-C    | -5.66 | 100.64      | 111.40   |
| 1   | B     | 353 | ILE  | CB-CA-C    | -5.66 | 100.28      | 111.60   |
| 1   | D     | 412 | VAL  | CB-CA-C    | -5.66 | 100.65      | 111.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | G     | 353 | ILE  | CB-CA-C    | -5.66 | 100.28      | 111.60   |
| 1   | F     | 412 | VAL  | CB-CA-C    | -5.66 | 100.65      | 111.40   |
| 1   | G     | 412 | VAL  | CB-CA-C    | -5.66 | 100.65      | 111.40   |
| 1   | E     | 353 | ILE  | CB-CA-C    | -5.65 | 100.30      | 111.60   |
| 1   | B     | 412 | VAL  | CB-CA-C    | -5.65 | 100.66      | 111.40   |
| 1   | C     | 452 | ARG  | NE-CZ-NH1  | 5.64  | 123.12      | 120.30   |
| 1   | D     | 39  | VAL  | CG1-CB-CG2 | 5.64  | 119.92      | 110.90   |
| 1   | A     | 39  | VAL  | CG1-CB-CG2 | 5.64  | 119.92      | 110.90   |
| 1   | I     | 404 | ARG  | NE-CZ-NH1  | 5.63  | 123.12      | 120.30   |
| 1   | A     | 412 | VAL  | CB-CA-C    | -5.63 | 100.71      | 111.40   |
| 1   | E     | 231 | ARG  | NE-CZ-NH2  | -5.61 | 117.49      | 120.30   |
| 1   | C     | 231 | ARG  | NE-CZ-NH2  | -5.61 | 117.50      | 120.30   |
| 1   | B     | 231 | ARG  | NE-CZ-NH2  | -5.60 | 117.50      | 120.30   |
| 1   | G     | 452 | ARG  | NE-CZ-NH1  | 5.60  | 123.10      | 120.30   |
| 1   | G     | 126 | ALA  | CB-CA-C    | 5.60  | 118.50      | 110.10   |
| 1   | C     | 126 | ALA  | CB-CA-C    | 5.59  | 118.49      | 110.10   |
| 1   | B     | 400 | LEU  | O-C-N      | -5.59 | 113.76      | 122.70   |
| 1   | A     | 126 | ALA  | CB-CA-C    | 5.58  | 118.48      | 110.10   |
| 1   | H     | 463 | SER  | N-CA-CB    | -5.58 | 102.12      | 110.50   |
| 1   | F     | 126 | ALA  | CB-CA-C    | 5.58  | 118.47      | 110.10   |
| 1   | B     | 126 | ALA  | CB-CA-C    | 5.57  | 118.46      | 110.10   |
| 1   | J     | 463 | SER  | N-CA-CB    | -5.57 | 102.14      | 110.50   |
| 1   | G     | 231 | ARG  | NE-CZ-NH2  | -5.57 | 117.51      | 120.30   |
| 1   | F     | 452 | ARG  | NE-CZ-NH1  | 5.57  | 123.08      | 120.30   |
| 1   | M     | 463 | SER  | N-CA-CB    | -5.57 | 102.15      | 110.50   |
| 1   | E     | 126 | ALA  | CB-CA-C    | 5.57  | 118.45      | 110.10   |
| 1   | K     | 463 | SER  | N-CA-CB    | -5.57 | 102.15      | 110.50   |
| 1   | I     | 463 | SER  | N-CA-CB    | -5.56 | 102.15      | 110.50   |
| 1   | B     | 452 | ARG  | NE-CZ-NH1  | 5.56  | 123.08      | 120.30   |
| 1   | D     | 126 | ALA  | CB-CA-C    | 5.56  | 118.44      | 110.10   |
| 1   | L     | 463 | SER  | N-CA-CB    | -5.55 | 102.17      | 110.50   |
| 1   | A     | 400 | LEU  | O-C-N      | -5.55 | 113.82      | 122.70   |
| 1   | N     | 463 | SER  | N-CA-CB    | -5.53 | 102.20      | 110.50   |
| 1   | D     | 231 | ARG  | NE-CZ-NH2  | -5.50 | 117.55      | 120.30   |
| 1   | H     | 404 | ARG  | NE-CZ-NH1  | 5.49  | 123.05      | 120.30   |
| 1   | B     | 166 | MET  | CG-SD-CE   | -5.47 | 91.44       | 100.20   |
| 1   | F     | 166 | MET  | CG-SD-CE   | -5.47 | 91.44       | 100.20   |
| 1   | G     | 166 | MET  | CG-SD-CE   | -5.47 | 91.44       | 100.20   |
| 1   | M     | 404 | ARG  | NE-CZ-NH1  | 5.47  | 123.04      | 120.30   |
| 1   | A     | 166 | MET  | CG-SD-CE   | -5.46 | 91.46       | 100.20   |
| 1   | D     | 166 | MET  | CG-SD-CE   | -5.46 | 91.47       | 100.20   |
| 1   | F     | 231 | ARG  | NE-CZ-NH2  | -5.46 | 117.57      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | C     | 113 | PRO  | CA-N-CD   | -5.45 | 103.87      | 111.50   |
| 1   | C     | 166 | MET  | CG-SD-CE  | -5.45 | 91.48       | 100.20   |
| 1   | E     | 166 | MET  | CG-SD-CE  | -5.44 | 91.49       | 100.20   |
| 1   | E     | 113 | PRO  | CA-N-CD   | -5.43 | 103.89      | 111.50   |
| 1   | C     | 409 | GLU  | N-CA-CB   | 5.42  | 120.36      | 110.60   |
| 1   | F     | 517 | THR  | CB-CA-C   | -5.42 | 96.96       | 111.60   |
| 1   | G     | 400 | LEU  | O-C-N     | -5.42 | 114.03      | 122.70   |
| 1   | G     | 517 | THR  | CB-CA-C   | -5.42 | 96.96       | 111.60   |
| 1   | C     | 517 | THR  | CB-CA-C   | -5.42 | 96.97       | 111.60   |
| 1   | I     | 281 | PHE  | N-CA-CB   | 5.42  | 120.36      | 110.60   |
| 1   | H     | 281 | PHE  | N-CA-CB   | 5.42  | 120.36      | 110.60   |
| 1   | F     | 369 | VAL  | N-CA-CB   | 5.42  | 123.42      | 111.50   |
| 1   | B     | 517 | THR  | CB-CA-C   | -5.42 | 96.98       | 111.60   |
| 1   | A     | 435 | ASP  | CB-CA-C   | -5.41 | 99.57       | 110.40   |
| 1   | C     | 435 | ASP  | CB-CA-C   | -5.41 | 99.57       | 110.40   |
| 1   | G     | 435 | ASP  | CB-CA-C   | -5.41 | 99.58       | 110.40   |
| 1   | A     | 409 | GLU  | N-CA-CB   | 5.41  | 120.34      | 110.60   |
| 1   | E     | 435 | ASP  | CB-CA-C   | -5.41 | 99.58       | 110.40   |
| 1   | J     | 294 | THR  | CA-CB-CG2 | -5.41 | 104.83      | 112.40   |
| 1   | L     | 281 | PHE  | N-CA-CB   | 5.41  | 120.33      | 110.60   |
| 1   | M     | 281 | PHE  | N-CA-CB   | 5.41  | 120.33      | 110.60   |
| 1   | A     | 117 | LYS  | N-CA-CB   | 5.40  | 120.33      | 110.60   |
| 1   | A     | 369 | VAL  | N-CA-CB   | 5.40  | 123.39      | 111.50   |
| 1   | E     | 369 | VAL  | N-CA-CB   | 5.40  | 123.39      | 111.50   |
| 1   | A     | 517 | THR  | CB-CA-C   | -5.40 | 97.02       | 111.60   |
| 1   | F     | 435 | ASP  | CB-CA-C   | -5.40 | 99.60       | 110.40   |
| 1   | F     | 113 | PRO  | CA-N-CD   | -5.40 | 103.94      | 111.50   |
| 1   | J     | 281 | PHE  | N-CA-CB   | 5.40  | 120.32      | 110.60   |
| 1   | B     | 113 | PRO  | CA-N-CD   | -5.40 | 103.94      | 111.50   |
| 1   | G     | 369 | VAL  | N-CA-CB   | 5.40  | 123.38      | 111.50   |
| 1   | B     | 369 | VAL  | N-CA-CB   | 5.40  | 123.37      | 111.50   |
| 1   | D     | 409 | GLU  | N-CA-CB   | 5.39  | 120.31      | 110.60   |
| 1   | A     | 113 | PRO  | CA-N-CD   | -5.39 | 103.95      | 111.50   |
| 1   | B     | 59  | GLU  | CB-CA-C   | 5.39  | 121.18      | 110.40   |
| 1   | D     | 517 | THR  | CB-CA-C   | -5.39 | 97.04       | 111.60   |
| 1   | D     | 435 | ASP  | CB-CA-C   | -5.39 | 99.62       | 110.40   |
| 1   | B     | 435 | ASP  | CB-CA-C   | -5.39 | 99.62       | 110.40   |
| 1   | D     | 369 | VAL  | N-CA-CB   | 5.39  | 123.36      | 111.50   |
| 1   | E     | 117 | LYS  | N-CA-CB   | 5.39  | 120.30      | 110.60   |
| 1   | K     | 281 | PHE  | N-CA-CB   | 5.39  | 120.30      | 110.60   |
| 1   | E     | 409 | GLU  | N-CA-CB   | 5.39  | 120.30      | 110.60   |
| 1   | E     | 517 | THR  | CB-CA-C   | -5.39 | 97.06       | 111.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | I     | 294 | THR  | CA-CB-CG2 | -5.39 | 104.86      | 112.40   |
| 1   | K     | 294 | THR  | CA-CB-CG2 | -5.39 | 104.86      | 112.40   |
| 1   | N     | 294 | THR  | CA-CB-CG2 | -5.39 | 104.86      | 112.40   |
| 1   | C     | 117 | LYS  | N-CA-CB   | 5.38  | 120.29      | 110.60   |
| 1   | A     | 231 | ARG  | NE-CZ-NH2 | -5.38 | 117.61      | 120.30   |
| 1   | D     | 59  | GLU  | CB-CA-C   | 5.38  | 121.16      | 110.40   |
| 1   | L     | 294 | THR  | CA-CB-CG2 | -5.38 | 104.87      | 112.40   |
| 1   | C     | 369 | VAL  | N-CA-CB   | 5.37  | 123.32      | 111.50   |
| 1   | G     | 117 | LYS  | N-CA-CB   | 5.37  | 120.27      | 110.60   |
| 1   | B     | 117 | LYS  | N-CA-CB   | 5.37  | 120.27      | 110.60   |
| 1   | D     | 285 | ARG  | NE-CZ-NH1 | 5.37  | 122.98      | 120.30   |
| 1   | B     | 409 | GLU  | N-CA-CB   | 5.37  | 120.27      | 110.60   |
| 1   | D     | 117 | LYS  | N-CA-CB   | 5.37  | 120.26      | 110.60   |
| 1   | F     | 117 | LYS  | N-CA-CB   | 5.37  | 120.26      | 110.60   |
| 1   | G     | 59  | GLU  | CB-CA-C   | 5.36  | 121.12      | 110.40   |
| 1   | N     | 281 | PHE  | N-CA-CB   | 5.36  | 120.26      | 110.60   |
| 1   | F     | 409 | GLU  | N-CA-CB   | 5.36  | 120.25      | 110.60   |
| 1   | M     | 294 | THR  | CA-CB-CG2 | -5.36 | 104.90      | 112.40   |
| 1   | D     | 113 | PRO  | CA-N-CD   | -5.35 | 104.01      | 111.50   |
| 1   | F     | 59  | GLU  | CB-CA-C   | 5.35  | 121.09      | 110.40   |
| 1   | E     | 59  | GLU  | CB-CA-C   | 5.35  | 121.09      | 110.40   |
| 1   | G     | 113 | PRO  | CA-N-CD   | -5.35 | 104.02      | 111.50   |
| 1   | G     | 285 | ARG  | NE-CZ-NH1 | 5.34  | 122.97      | 120.30   |
| 1   | H     | 294 | THR  | CA-CB-CG2 | -5.34 | 104.92      | 112.40   |
| 1   | A     | 285 | ARG  | NE-CZ-NH1 | 5.34  | 122.97      | 120.30   |
| 1   | G     | 409 | GLU  | N-CA-CB   | 5.34  | 120.22      | 110.60   |
| 1   | C     | 59  | GLU  | CB-CA-C   | 5.34  | 121.07      | 110.40   |
| 1   | A     | 59  | GLU  | CB-CA-C   | 5.33  | 121.06      | 110.40   |
| 1   | B     | 58  | ARG  | NE-CZ-NH1 | 5.33  | 122.96      | 120.30   |
| 1   | B     | 257 | GLU  | N-CA-CB   | 5.32  | 120.18      | 110.60   |
| 1   | C     | 400 | LEU  | O-C-N     | -5.31 | 114.20      | 122.70   |
| 1   | F     | 257 | GLU  | N-CA-CB   | 5.31  | 120.16      | 110.60   |
| 1   | A     | 368 | ARG  | NE-CZ-NH1 | 5.31  | 122.95      | 120.30   |
| 1   | L     | 400 | LEU  | C-N-CA    | -5.30 | 108.44      | 121.70   |
| 1   | C     | 257 | GLU  | N-CA-CB   | 5.30  | 120.15      | 110.60   |
| 1   | F     | 196 | ASP  | N-CA-CB   | -5.30 | 101.05      | 110.60   |
| 1   | E     | 113 | PRO  | N-CA-CB   | 5.30  | 109.66      | 103.30   |
| 1   | E     | 257 | GLU  | N-CA-CB   | 5.29  | 120.13      | 110.60   |
| 1   | A     | 196 | ASP  | N-CA-CB   | -5.29 | 101.08      | 110.60   |
| 1   | D     | 196 | ASP  | N-CA-CB   | -5.29 | 101.08      | 110.60   |
| 1   | C     | 196 | ASP  | N-CA-CB   | -5.29 | 101.08      | 110.60   |
| 1   | B     | 473 | ASP  | CB-CA-C   | 5.29  | 120.97      | 110.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | F     | 140 | ASP  | CB-CG-OD1 | 5.29  | 123.06      | 118.30   |
| 1   | D     | 473 | ASP  | CB-CA-C   | 5.28  | 120.97      | 110.40   |
| 1   | G     | 58  | ARG  | NE-CZ-NH1 | 5.28  | 122.94      | 120.30   |
| 1   | D     | 257 | GLU  | N-CA-CB   | 5.28  | 120.11      | 110.60   |
| 1   | G     | 473 | ASP  | CB-CA-C   | 5.28  | 120.96      | 110.40   |
| 1   | C     | 58  | ARG  | NE-CZ-NH1 | 5.28  | 122.94      | 120.30   |
| 1   | A     | 140 | ASP  | CB-CG-OD1 | 5.28  | 123.05      | 118.30   |
| 1   | E     | 196 | ASP  | N-CA-CB   | -5.28 | 101.10      | 110.60   |
| 1   | B     | 196 | ASP  | N-CA-CB   | -5.28 | 101.10      | 110.60   |
| 1   | F     | 58  | ARG  | NE-CZ-NH1 | 5.27  | 122.94      | 120.30   |
| 1   | A     | 322 | ARG  | NE-CZ-NH1 | 5.27  | 122.94      | 120.30   |
| 1   | J     | 258 | ALA  | CB-CA-C   | 5.27  | 118.01      | 110.10   |
| 1   | C     | 113 | PRO  | N-CA-CB   | 5.27  | 109.62      | 103.30   |
| 1   | I     | 258 | ALA  | CB-CA-C   | 5.27  | 118.01      | 110.10   |
| 1   | E     | 473 | ASP  | CB-CA-C   | 5.27  | 120.94      | 110.40   |
| 1   | C     | 368 | ARG  | NE-CZ-NH1 | 5.27  | 122.93      | 120.30   |
| 1   | A     | 473 | ASP  | CB-CA-C   | 5.26  | 120.92      | 110.40   |
| 1   | F     | 473 | ASP  | CB-CA-C   | 5.26  | 120.92      | 110.40   |
| 1   | G     | 140 | ASP  | CB-CG-OD1 | 5.26  | 123.04      | 118.30   |
| 1   | J     | 401 | HIS  | C-N-CA    | -5.26 | 108.55      | 121.70   |
| 1   | A     | 106 | ALA  | CB-CA-C   | 5.26  | 117.99      | 110.10   |
| 1   | G     | 196 | ASP  | N-CA-CB   | -5.26 | 101.13      | 110.60   |
| 1   | N     | 258 | ALA  | CB-CA-C   | 5.26  | 117.99      | 110.10   |
| 1   | C     | 473 | ASP  | CB-CA-C   | 5.26  | 120.92      | 110.40   |
| 1   | B     | 140 | ASP  | CB-CG-OD1 | 5.25  | 123.03      | 118.30   |
| 1   | A     | 257 | GLU  | N-CA-CB   | 5.25  | 120.06      | 110.60   |
| 1   | E     | 106 | ALA  | CB-CA-C   | 5.25  | 117.98      | 110.10   |
| 1   | F     | 322 | ARG  | NE-CZ-NH1 | 5.25  | 122.92      | 120.30   |
| 1   | H     | 258 | ALA  | CB-CA-C   | 5.25  | 117.98      | 110.10   |
| 1   | M     | 258 | ALA  | CB-CA-C   | 5.25  | 117.97      | 110.10   |
| 1   | F     | 113 | PRO  | N-CA-CB   | 5.25  | 109.60      | 103.30   |
| 1   | K     | 258 | ALA  | CB-CA-C   | 5.25  | 117.97      | 110.10   |
| 1   | L     | 258 | ALA  | CB-CA-C   | 5.24  | 117.97      | 110.10   |
| 1   | F     | 106 | ALA  | CB-CA-C   | 5.24  | 117.96      | 110.10   |
| 1   | B     | 285 | ARG  | NE-CZ-NH1 | 5.24  | 122.92      | 120.30   |
| 1   | F     | 368 | ARG  | NE-CZ-NH1 | 5.24  | 122.92      | 120.30   |
| 1   | G     | 322 | ARG  | NE-CZ-NH1 | 5.23  | 122.92      | 120.30   |
| 1   | D     | 106 | ALA  | CB-CA-C   | 5.23  | 117.94      | 110.10   |
| 1   | G     | 257 | GLU  | N-CA-CB   | 5.23  | 120.02      | 110.60   |
| 1   | E     | 58  | ARG  | NE-CZ-NH1 | 5.23  | 122.91      | 120.30   |
| 1   | C     | 106 | ALA  | CB-CA-C   | 5.23  | 117.94      | 110.10   |
| 1   | E     | 285 | ARG  | NE-CZ-NH1 | 5.23  | 122.91      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | G     | 320 | ALA  | N-CA-CB   | 5.22  | 117.41      | 110.10   |
| 1   | G     | 368 | ARG  | NE-CZ-NH1 | 5.22  | 122.91      | 120.30   |
| 1   | D     | 58  | ARG  | NE-CZ-NH1 | 5.22  | 122.91      | 120.30   |
| 1   | G     | 106 | ALA  | CB-CA-C   | 5.22  | 117.93      | 110.10   |
| 1   | B     | 106 | ALA  | CB-CA-C   | 5.22  | 117.92      | 110.10   |
| 1   | D     | 113 | PRO  | N-CA-CB   | 5.22  | 109.56      | 103.30   |
| 1   | G     | 113 | PRO  | N-CA-CB   | 5.22  | 109.56      | 103.30   |
| 1   | G     | 268 | ARG  | NE-CZ-NH1 | 5.22  | 122.91      | 120.30   |
| 1   | B     | 368 | ARG  | NE-CZ-NH1 | 5.21  | 122.91      | 120.30   |
| 1   | F     | 320 | ALA  | N-CA-CB   | 5.21  | 117.40      | 110.10   |
| 1   | A     | 113 | PRO  | N-CA-CB   | 5.21  | 109.55      | 103.30   |
| 1   | C     | 322 | ARG  | NE-CZ-NH1 | 5.21  | 122.91      | 120.30   |
| 1   | C     | 320 | ALA  | N-CA-CB   | 5.21  | 117.39      | 110.10   |
| 1   | B     | 113 | PRO  | N-CA-CB   | 5.21  | 109.55      | 103.30   |
| 1   | C     | 140 | ASP  | CB-CG-OD1 | 5.20  | 122.98      | 118.30   |
| 1   | E     | 140 | ASP  | CB-CG-OD1 | 5.20  | 122.98      | 118.30   |
| 1   | A     | 320 | ALA  | N-CA-CB   | 5.20  | 117.38      | 110.10   |
| 1   | E     | 320 | ALA  | N-CA-CB   | 5.20  | 117.38      | 110.10   |
| 1   | F     | 285 | ARG  | NE-CZ-NH1 | 5.20  | 122.90      | 120.30   |
| 1   | B     | 320 | ALA  | N-CA-CB   | 5.20  | 117.38      | 110.10   |
| 1   | D     | 320 | ALA  | N-CA-CB   | 5.20  | 117.38      | 110.10   |
| 1   | B     | 268 | ARG  | NE-CZ-NH1 | 5.20  | 122.90      | 120.30   |
| 1   | D     | 140 | ASP  | CB-CG-OD1 | 5.19  | 122.97      | 118.30   |
| 1   | E     | 368 | ARG  | NE-CZ-NH1 | 5.19  | 122.89      | 120.30   |
| 1   | A     | 203 | TYR  | CB-CG-CD2 | -5.18 | 117.89      | 121.00   |
| 1   | D     | 322 | ARG  | NE-CZ-NH1 | 5.18  | 122.89      | 120.30   |
| 1   | F     | 400 | LEU  | O-C-N     | -5.18 | 114.41      | 122.70   |
| 1   | D     | 268 | ARG  | NE-CZ-NH1 | 5.17  | 122.88      | 120.30   |
| 1   | F     | 87  | ASP  | CB-CG-OD1 | 5.17  | 122.95      | 118.30   |
| 1   | F     | 268 | ARG  | NE-CZ-NH1 | 5.17  | 122.88      | 120.30   |
| 1   | F     | 284 | ARG  | CB-CA-C   | -5.15 | 100.10      | 110.40   |
| 1   | A     | 58  | ARG  | NE-CZ-NH1 | 5.15  | 122.88      | 120.30   |
| 1   | A     | 284 | ARG  | CB-CA-C   | -5.15 | 100.10      | 110.40   |
| 1   | C     | 203 | TYR  | CB-CG-CD2 | -5.15 | 117.91      | 121.00   |
| 1   | B     | 203 | TYR  | CB-CG-CD2 | -5.14 | 117.92      | 121.00   |
| 1   | C     | 285 | ARG  | NE-CZ-NH1 | 5.14  | 122.87      | 120.30   |
| 1   | D     | 140 | ASP  | CA-CB-CG  | 5.13  | 124.70      | 113.40   |
| 1   | F     | 140 | ASP  | CA-CB-CG  | 5.13  | 124.68      | 113.40   |
| 1   | G     | 284 | ARG  | CB-CA-C   | -5.13 | 100.14      | 110.40   |
| 1   | C     | 284 | ARG  | CB-CA-C   | -5.13 | 100.15      | 110.40   |
| 1   | B     | 284 | ARG  | CB-CA-C   | -5.12 | 100.15      | 110.40   |
| 1   | D     | 284 | ARG  | CB-CA-C   | -5.12 | 100.15      | 110.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 322 | ARG  | NE-CZ-NH1 | 5.12  | 122.86      | 120.30   |
| 1   | D     | 368 | ARG  | NE-CZ-NH1 | 5.12  | 122.86      | 120.30   |
| 1   | E     | 140 | ASP  | CA-CB-CG  | 5.12  | 124.66      | 113.40   |
| 1   | B     | 87  | ASP  | CB-CG-OD1 | 5.12  | 122.91      | 118.30   |
| 1   | C     | 140 | ASP  | CA-CB-CG  | 5.12  | 124.65      | 113.40   |
| 1   | M     | 285 | ARG  | NE-CZ-NH2 | -5.12 | 117.74      | 120.30   |
| 1   | E     | 284 | ARG  | CB-CA-C   | -5.11 | 100.18      | 110.40   |
| 1   | A     | 204 | PHE  | CB-CG-CD2 | -5.10 | 117.23      | 120.80   |
| 1   | B     | 140 | ASP  | CA-CB-CG  | 5.10  | 124.62      | 113.40   |
| 1   | E     | 322 | ARG  | NE-CZ-NH1 | 5.10  | 122.85      | 120.30   |
| 1   | G     | 140 | ASP  | CA-CB-CG  | 5.10  | 124.62      | 113.40   |
| 1   | A     | 87  | ASP  | CB-CG-OD1 | 5.10  | 122.89      | 118.30   |
| 1   | A     | 140 | ASP  | CA-CB-CG  | 5.10  | 124.61      | 113.40   |
| 1   | E     | 268 | ARG  | NE-CZ-NH1 | 5.08  | 122.84      | 120.30   |
| 1   | D     | 203 | TYR  | CB-CG-CD2 | -5.08 | 117.95      | 121.00   |
| 1   | E     | 87  | ASP  | CB-CG-OD1 | 5.08  | 122.87      | 118.30   |
| 1   | A     | 73  | MET  | CA-CB-CG  | 5.08  | 121.93      | 113.30   |
| 1   | C     | 268 | ARG  | NE-CZ-NH1 | 5.07  | 122.84      | 120.30   |
| 1   | D     | 73  | MET  | CA-CB-CG  | 5.07  | 121.92      | 113.30   |
| 1   | D     | 203 | TYR  | CB-CG-CD1 | 5.07  | 124.04      | 121.00   |
| 1   | E     | 73  | MET  | CA-CB-CG  | 5.07  | 121.92      | 113.30   |
| 1   | B     | 73  | MET  | CA-CB-CG  | 5.07  | 121.92      | 113.30   |
| 1   | D     | 369 | VAL  | CB-CA-C   | -5.07 | 101.77      | 111.40   |
| 1   | E     | 203 | TYR  | CB-CG-CD2 | -5.07 | 117.96      | 121.00   |
| 1   | B     | 204 | PHE  | CB-CG-CD2 | -5.06 | 117.25      | 120.80   |
| 1   | D     | 104 | LEU  | CB-CA-C   | 5.06  | 119.82      | 110.20   |
| 1   | F     | 203 | TYR  | CB-CG-CD2 | -5.06 | 117.96      | 121.00   |
| 1   | M     | 59  | GLU  | CB-CA-C   | 5.06  | 120.52      | 110.40   |
| 1   | C     | 361 | ASP  | CB-CA-C   | 5.06  | 120.52      | 110.40   |
| 1   | C     | 436 | GLN  | N-CA-CB   | 5.06  | 119.70      | 110.60   |
| 1   | E     | 369 | VAL  | CB-CA-C   | -5.06 | 101.79      | 111.40   |
| 1   | F     | 104 | LEU  | CB-CA-C   | 5.05  | 119.80      | 110.20   |
| 1   | K     | 285 | ARG  | NE-CZ-NH2 | -5.05 | 117.77      | 120.30   |
| 1   | B     | 436 | GLN  | N-CA-CB   | 5.05  | 119.69      | 110.60   |
| 1   | C     | 369 | VAL  | CB-CA-C   | -5.05 | 101.80      | 111.40   |
| 1   | F     | 73  | MET  | CA-CB-CG  | 5.05  | 121.89      | 113.30   |
| 1   | I     | 59  | GLU  | CB-CA-C   | 5.05  | 120.50      | 110.40   |
| 1   | B     | 361 | ASP  | CB-CA-C   | 5.05  | 120.50      | 110.40   |
| 1   | C     | 73  | MET  | CA-CB-CG  | 5.05  | 121.88      | 113.30   |
| 1   | G     | 73  | MET  | CA-CB-CG  | 5.05  | 121.88      | 113.30   |
| 1   | D     | 87  | ASP  | CB-CG-OD1 | 5.05  | 122.84      | 118.30   |
| 1   | G     | 361 | ASP  | CB-CA-C   | 5.05  | 120.49      | 110.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | F     | 369 | VAL  | CB-CA-C   | -5.04 | 101.81      | 111.40   |
| 1   | G     | 436 | GLN  | N-CA-CB   | 5.04  | 119.68      | 110.60   |
| 1   | A     | 436 | GLN  | N-CA-CB   | 5.04  | 119.67      | 110.60   |
| 1   | E     | 501 | ARG  | N-CA-CB   | -5.04 | 101.52      | 110.60   |
| 1   | A     | 361 | ASP  | CB-CA-C   | 5.04  | 120.48      | 110.40   |
| 1   | F     | 501 | ARG  | N-CA-CB   | -5.04 | 101.53      | 110.60   |
| 1   | C     | 501 | ARG  | N-CA-CB   | -5.04 | 101.53      | 110.60   |
| 1   | F     | 203 | TYR  | CB-CG-CD1 | 5.04  | 124.02      | 121.00   |
| 1   | B     | 369 | VAL  | CB-CA-C   | -5.04 | 101.83      | 111.40   |
| 1   | D     | 400 | LEU  | O-C-N     | -5.04 | 114.64      | 122.70   |
| 1   | E     | 436 | GLN  | N-CA-CB   | 5.04  | 119.67      | 110.60   |
| 1   | F     | 436 | GLN  | N-CA-CB   | 5.04  | 119.67      | 110.60   |
| 1   | G     | 203 | TYR  | CB-CG-CD2 | -5.04 | 117.98      | 121.00   |
| 1   | H     | 59  | GLU  | CB-CA-C   | 5.04  | 120.47      | 110.40   |
| 1   | F     | 361 | ASP  | CB-CA-C   | 5.03  | 120.47      | 110.40   |
| 1   | L     | 59  | GLU  | CB-CA-C   | 5.03  | 120.47      | 110.40   |
| 1   | D     | 361 | ASP  | CB-CA-C   | 5.03  | 120.47      | 110.40   |
| 1   | D     | 436 | GLN  | N-CA-CB   | 5.03  | 119.66      | 110.60   |
| 1   | E     | 203 | TYR  | CB-CG-CD1 | 5.03  | 124.02      | 121.00   |
| 1   | E     | 321 | LYS  | N-CA-CB   | 5.03  | 119.66      | 110.60   |
| 1   | A     | 104 | LEU  | CB-CA-C   | 5.03  | 119.76      | 110.20   |
| 1   | B     | 104 | LEU  | CB-CA-C   | 5.03  | 119.76      | 110.20   |
| 1   | G     | 204 | PHE  | CB-CG-CD2 | -5.03 | 117.28      | 120.80   |
| 1   | K     | 59  | GLU  | CB-CA-C   | 5.03  | 120.46      | 110.40   |
| 1   | B     | 501 | ARG  | N-CA-CB   | -5.03 | 101.55      | 110.60   |
| 1   | E     | 104 | LEU  | CB-CA-C   | 5.03  | 119.75      | 110.20   |
| 1   | G     | 87  | ASP  | CB-CG-OD1 | 5.03  | 122.83      | 118.30   |
| 1   | F     | 321 | LYS  | N-CA-CB   | 5.03  | 119.65      | 110.60   |
| 1   | N     | 59  | GLU  | CB-CA-C   | 5.02  | 120.45      | 110.40   |
| 1   | N     | 285 | ARG  | NE-CZ-NH2 | -5.02 | 117.79      | 120.30   |
| 1   | G     | 321 | LYS  | N-CA-CB   | 5.02  | 119.64      | 110.60   |
| 1   | A     | 321 | LYS  | N-CA-CB   | 5.02  | 119.64      | 110.60   |
| 1   | G     | 369 | VAL  | CB-CA-C   | -5.02 | 101.86      | 111.40   |
| 1   | B     | 203 | TYR  | CB-CG-CD1 | 5.01  | 124.01      | 121.00   |
| 1   | D     | 321 | LYS  | N-CA-CB   | 5.01  | 119.62      | 110.60   |
| 1   | E     | 361 | ASP  | CB-CA-C   | 5.01  | 120.43      | 110.40   |
| 1   | C     | 87  | ASP  | CB-CG-OD1 | 5.01  | 122.81      | 118.30   |
| 1   | G     | 104 | LEU  | CB-CA-C   | 5.01  | 119.72      | 110.20   |
| 1   | E     | 204 | PHE  | CB-CG-CD2 | -5.01 | 117.29      | 120.80   |
| 1   | A     | 369 | VAL  | CB-CA-C   | -5.01 | 101.89      | 111.40   |
| 1   | D     | 501 | ARG  | N-CA-CB   | -5.01 | 101.59      | 110.60   |
| 1   | G     | 501 | ARG  | N-CA-CB   | -5.01 | 101.59      | 110.60   |

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| Mol | Chain | Res | Type | Atoms     | Z    | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|-----------|------|------------------------|---------------------|
| 1   | A     | 203 | TYR  | CB-CG-CD1 | 5.00 | 124.00                 | 121.00              |
| 1   | A     | 268 | ARG  | NE-CZ-NH1 | 5.00 | 122.80                 | 120.30              |
| 1   | B     | 321 | LYS  | N-CA-CB   | 5.00 | 119.60                 | 110.60              |
| 1   | C     | 104 | LEU  | CB-CA-C   | 5.00 | 119.70                 | 110.20              |

There are no chirality outliers.

All (138) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 13  | ARG  | Sidechain |
| 1   | A     | 197 | ARG  | Sidechain |
| 1   | A     | 231 | ARG  | Sidechain |
| 1   | A     | 268 | ARG  | Sidechain |
| 1   | A     | 350 | ARG  | Sidechain |
| 1   | A     | 36  | ARG  | Sidechain |
| 1   | A     | 362 | ARG  | Sidechain |
| 1   | A     | 395 | ARG  | Sidechain |
| 1   | A     | 404 | ARG  | Sidechain |
| 1   | B     | 13  | ARG  | Sidechain |
| 1   | B     | 197 | ARG  | Sidechain |
| 1   | B     | 231 | ARG  | Sidechain |
| 1   | B     | 268 | ARG  | Sidechain |
| 1   | B     | 350 | ARG  | Sidechain |
| 1   | B     | 36  | ARG  | Sidechain |
| 1   | B     | 362 | ARG  | Sidechain |
| 1   | B     | 395 | ARG  | Sidechain |
| 1   | B     | 404 | ARG  | Sidechain |
| 1   | C     | 13  | ARG  | Sidechain |
| 1   | C     | 197 | ARG  | Sidechain |
| 1   | C     | 219 | PHE  | Sidechain |
| 1   | C     | 231 | ARG  | Sidechain |
| 1   | C     | 268 | ARG  | Sidechain |
| 1   | C     | 350 | ARG  | Sidechain |
| 1   | C     | 36  | ARG  | Sidechain |
| 1   | C     | 362 | ARG  | Sidechain |
| 1   | C     | 395 | ARG  | Sidechain |
| 1   | C     | 404 | ARG  | Sidechain |
| 1   | D     | 13  | ARG  | Sidechain |
| 1   | D     | 197 | ARG  | Sidechain |
| 1   | D     | 219 | PHE  | Sidechain |
| 1   | D     | 231 | ARG  | Sidechain |
| 1   | D     | 268 | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | D     | 350 | ARG  | Sidechain |
| 1   | D     | 36  | ARG  | Sidechain |
| 1   | D     | 362 | ARG  | Sidechain |
| 1   | D     | 395 | ARG  | Sidechain |
| 1   | D     | 404 | ARG  | Sidechain |
| 1   | E     | 13  | ARG  | Sidechain |
| 1   | E     | 197 | ARG  | Sidechain |
| 1   | E     | 231 | ARG  | Sidechain |
| 1   | E     | 268 | ARG  | Sidechain |
| 1   | E     | 350 | ARG  | Sidechain |
| 1   | E     | 36  | ARG  | Sidechain |
| 1   | E     | 362 | ARG  | Sidechain |
| 1   | E     | 395 | ARG  | Sidechain |
| 1   | E     | 404 | ARG  | Sidechain |
| 1   | F     | 13  | ARG  | Sidechain |
| 1   | F     | 197 | ARG  | Sidechain |
| 1   | F     | 219 | PHE  | Sidechain |
| 1   | F     | 231 | ARG  | Sidechain |
| 1   | F     | 268 | ARG  | Sidechain |
| 1   | F     | 350 | ARG  | Sidechain |
| 1   | F     | 36  | ARG  | Sidechain |
| 1   | F     | 362 | ARG  | Sidechain |
| 1   | F     | 395 | ARG  | Sidechain |
| 1   | F     | 404 | ARG  | Sidechain |
| 1   | G     | 13  | ARG  | Sidechain |
| 1   | G     | 197 | ARG  | Sidechain |
| 1   | G     | 231 | ARG  | Sidechain |
| 1   | G     | 268 | ARG  | Sidechain |
| 1   | G     | 350 | ARG  | Sidechain |
| 1   | G     | 36  | ARG  | Sidechain |
| 1   | G     | 362 | ARG  | Sidechain |
| 1   | G     | 395 | ARG  | Sidechain |
| 1   | G     | 404 | ARG  | Sidechain |
| 1   | H     | 118 | ARG  | Sidechain |
| 1   | H     | 197 | ARG  | Sidechain |
| 1   | H     | 231 | ARG  | Sidechain |
| 1   | H     | 284 | ARG  | Sidechain |
| 1   | H     | 285 | ARG  | Sidechain |
| 1   | H     | 350 | ARG  | Sidechain |
| 1   | H     | 362 | ARG  | Sidechain |
| 1   | H     | 421 | ARG  | Sidechain |
| 1   | H     | 445 | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | H     | 478 | TYR  | Sidechain |
| 1   | I     | 118 | ARG  | Sidechain |
| 1   | I     | 197 | ARG  | Sidechain |
| 1   | I     | 231 | ARG  | Sidechain |
| 1   | I     | 284 | ARG  | Sidechain |
| 1   | I     | 285 | ARG  | Sidechain |
| 1   | I     | 350 | ARG  | Sidechain |
| 1   | I     | 362 | ARG  | Sidechain |
| 1   | I     | 421 | ARG  | Sidechain |
| 1   | I     | 445 | ARG  | Sidechain |
| 1   | I     | 478 | TYR  | Sidechain |
| 1   | J     | 118 | ARG  | Sidechain |
| 1   | J     | 197 | ARG  | Sidechain |
| 1   | J     | 231 | ARG  | Sidechain |
| 1   | J     | 284 | ARG  | Sidechain |
| 1   | J     | 285 | ARG  | Sidechain |
| 1   | J     | 350 | ARG  | Sidechain |
| 1   | J     | 362 | ARG  | Sidechain |
| 1   | J     | 421 | ARG  | Sidechain |
| 1   | J     | 445 | ARG  | Sidechain |
| 1   | J     | 478 | TYR  | Sidechain |
| 1   | K     | 118 | ARG  | Sidechain |
| 1   | K     | 197 | ARG  | Sidechain |
| 1   | K     | 231 | ARG  | Sidechain |
| 1   | K     | 284 | ARG  | Sidechain |
| 1   | K     | 285 | ARG  | Sidechain |
| 1   | K     | 350 | ARG  | Sidechain |
| 1   | K     | 362 | ARG  | Sidechain |
| 1   | K     | 421 | ARG  | Sidechain |
| 1   | K     | 445 | ARG  | Sidechain |
| 1   | K     | 478 | TYR  | Sidechain |
| 1   | L     | 118 | ARG  | Sidechain |
| 1   | L     | 197 | ARG  | Sidechain |
| 1   | L     | 231 | ARG  | Sidechain |
| 1   | L     | 284 | ARG  | Sidechain |
| 1   | L     | 285 | ARG  | Sidechain |
| 1   | L     | 350 | ARG  | Sidechain |
| 1   | L     | 362 | ARG  | Sidechain |
| 1   | L     | 401 | HIS  | Mainchain |
| 1   | L     | 421 | ARG  | Sidechain |
| 1   | L     | 445 | ARG  | Sidechain |
| 1   | L     | 478 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | M     | 118 | ARG  | Sidechain |
| 1   | M     | 197 | ARG  | Sidechain |
| 1   | M     | 231 | ARG  | Sidechain |
| 1   | M     | 284 | ARG  | Sidechain |
| 1   | M     | 285 | ARG  | Sidechain |
| 1   | M     | 350 | ARG  | Sidechain |
| 1   | M     | 362 | ARG  | Sidechain |
| 1   | M     | 421 | ARG  | Sidechain |
| 1   | M     | 445 | ARG  | Sidechain |
| 1   | M     | 478 | TYR  | Sidechain |
| 1   | N     | 118 | ARG  | Sidechain |
| 1   | N     | 197 | ARG  | Sidechain |
| 1   | N     | 231 | ARG  | Sidechain |
| 1   | N     | 284 | ARG  | Sidechain |
| 1   | N     | 285 | ARG  | Sidechain |
| 1   | N     | 350 | ARG  | Sidechain |
| 1   | N     | 362 | ARG  | Sidechain |
| 1   | N     | 401 | HIS  | Mainchain |
| 1   | N     | 421 | ARG  | Sidechain |
| 1   | N     | 445 | ARG  | Sidechain |
| 1   | N     | 478 | TYR  | Sidechain |

## 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     | 3846  | 0        | 3970     | 203     | 0            |
| 1   | B     | 3846  | 0        | 3970     | 205     | 0            |
| 1   | C     | 3846  | 0        | 3970     | 205     | 0            |
| 1   | D     | 3846  | 0        | 3970     | 210     | 0            |
| 1   | E     | 3846  | 0        | 3970     | 209     | 0            |
| 1   | F     | 3846  | 0        | 3970     | 208     | 0            |
| 1   | G     | 3846  | 0        | 3970     | 207     | 0            |
| 1   | H     | 3846  | 0        | 3970     | 28      | 0            |
| 1   | I     | 3846  | 0        | 3970     | 28      | 0            |
| 1   | J     | 3846  | 0        | 3968     | 29      | 0            |
| 1   | K     | 3846  | 0        | 3969     | 27      | 0            |
| 1   | L     | 3846  | 0        | 3969     | 30      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | M     | 3846  | 0        | 3970     | 27      | 0            |
| 1   | N     | 3846  | 0        | 3968     | 32      | 0            |
| 2   | A     | 31    | 12       | 12       | 4       | 0            |
| 2   | B     | 31    | 12       | 12       | 3       | 0            |
| 2   | C     | 31    | 12       | 12       | 3       | 0            |
| 2   | D     | 31    | 12       | 12       | 3       | 0            |
| 2   | E     | 31    | 12       | 12       | 3       | 0            |
| 2   | F     | 31    | 12       | 12       | 4       | 0            |
| 2   | G     | 31    | 12       | 12       | 4       | 0            |
| 3   | A     | 1     | 0        | 0        | 5       | 0            |
| 3   | B     | 1     | 0        | 0        | 4       | 0            |
| 3   | C     | 1     | 0        | 0        | 4       | 0            |
| 3   | D     | 1     | 0        | 0        | 4       | 0            |
| 3   | E     | 1     | 0        | 0        | 4       | 0            |
| 3   | F     | 1     | 0        | 0        | 5       | 0            |
| 3   | G     | 1     | 0        | 0        | 5       | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | D     | 1     | 0        | 0        | 0       | 0            |
| 4   | E     | 1     | 0        | 0        | 0       | 0            |
| 4   | F     | 1     | 0        | 0        | 0       | 0            |
| 4   | G     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 54075 | 84       | 55658    | 1291    | 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 12.

All (1291) 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:J:400:LEU:C | 1:J:401:HIS:N  | 1.72                     | 1.43              |
| 1:A:115:ASP:H | 1:B:36:ARG:CZ  | 1.37                     | 1.37              |
| 1:C:115:ASP:H | 1:D:36:ARG:CZ  | 1.37                     | 1.37              |
| 1:D:115:ASP:H | 1:E:36:ARG:CZ  | 1.37                     | 1.36              |
| 1:A:116:LEU:H | 1:B:36:ARG:NH1 | 1.24                     | 1.36              |
| 1:C:116:LEU:H | 1:D:36:ARG:NH1 | 1.24                     | 1.36              |
| 1:B:115:ASP:H | 1:C:36:ARG:CZ  | 1.37                     | 1.36              |
| 1:F:115:ASP:H | 1:G:36:ARG:CZ  | 1.37                     | 1.35              |
| 1:L:400:LEU:C | 1:L:401:HIS:N  | 1.78                     | 1.35              |
| 1:A:36:ARG:CZ | 1:G:115:ASP:H  | 1.37                     | 1.35              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:E:115:ASP:H   | 1:F:36:ARG:CZ   | 1.37                     | 1.34              |
| 1:E:116:LEU:H   | 1:F:36:ARG:NH1  | 1.24                     | 1.33              |
| 1:F:116:LEU:H   | 1:G:36:ARG:NH1  | 1.24                     | 1.33              |
| 1:D:116:LEU:H   | 1:E:36:ARG:NH1  | 1.24                     | 1.33              |
| 1:B:116:LEU:H   | 1:C:36:ARG:NH1  | 1.24                     | 1.32              |
| 1:A:36:ARG:NH1  | 1:G:116:LEU:H   | 1.24                     | 1.32              |
| 1:N:400:LEU:C   | 1:N:401:HIS:N   | 1.83                     | 1.32              |
| 1:B:116:LEU:N   | 1:C:36:ARG:HH12 | 1.29                     | 1.30              |
| 1:D:116:LEU:N   | 1:E:36:ARG:HH12 | 1.29                     | 1.29              |
| 1:A:36:ARG:HH12 | 1:G:116:LEU:N   | 1.30                     | 1.29              |
| 1:C:116:LEU:N   | 1:D:36:ARG:HH12 | 1.30                     | 1.29              |
| 1:E:116:LEU:N   | 1:F:36:ARG:HH12 | 1.30                     | 1.28              |
| 1:A:116:LEU:N   | 1:B:36:ARG:HH12 | 1.30                     | 1.27              |
| 1:F:116:LEU:N   | 1:G:36:ARG:HH12 | 1.30                     | 1.26              |
| 1:A:112:ASN:O   | 1:B:36:ARG:NH1  | 1.85                     | 1.10              |
| 1:F:112:ASN:O   | 1:G:36:ARG:NH1  | 1.85                     | 1.10              |
| 1:C:112:ASN:O   | 1:D:36:ARG:NH1  | 1.85                     | 1.10              |
| 1:E:112:ASN:O   | 1:F:36:ARG:NH1  | 1.85                     | 1.09              |
| 1:B:112:ASN:O   | 1:C:36:ARG:NH1  | 1.85                     | 1.09              |
| 1:A:36:ARG:NH1  | 1:G:112:ASN:O   | 1.84                     | 1.08              |
| 1:D:112:ASN:O   | 1:E:36:ARG:NH1  | 1.85                     | 1.08              |
| 1:B:115:ASP:N   | 1:C:36:ARG:CZ   | 2.18                     | 1.07              |
| 1:C:113:PRO:C   | 1:D:36:ARG:HH11 | 1.59                     | 1.07              |
| 1:C:115:ASP:N   | 1:D:36:ARG:CZ   | 2.18                     | 1.07              |
| 1:D:113:PRO:C   | 1:E:36:ARG:HH11 | 1.59                     | 1.06              |
| 1:A:36:ARG:HH11 | 1:G:113:PRO:C   | 1.59                     | 1.06              |
| 1:F:113:PRO:C   | 1:G:36:ARG:HH11 | 1.59                     | 1.06              |
| 1:B:113:PRO:C   | 1:C:36:ARG:HH11 | 1.59                     | 1.06              |
| 1:A:113:PRO:C   | 1:B:36:ARG:HH11 | 1.59                     | 1.06              |
| 1:E:113:PRO:C   | 1:F:36:ARG:HH11 | 1.59                     | 1.06              |
| 1:A:115:ASP:N   | 1:B:36:ARG:CZ   | 2.18                     | 1.06              |
| 1:A:113:PRO:C   | 1:B:36:ARG:NH1  | 2.09                     | 1.06              |
| 1:A:36:ARG:CZ   | 1:G:115:ASP:N   | 2.18                     | 1.06              |
| 1:B:113:PRO:C   | 1:C:36:ARG:NH1  | 2.10                     | 1.06              |
| 1:A:36:ARG:NH1  | 1:G:113:PRO:C   | 2.10                     | 1.05              |
| 1:F:115:ASP:N   | 1:G:36:ARG:CZ   | 2.18                     | 1.05              |
| 1:D:115:ASP:N   | 1:E:36:ARG:CZ   | 2.18                     | 1.05              |
| 1:F:113:PRO:C   | 1:G:36:ARG:NH1  | 2.10                     | 1.05              |
| 1:C:113:PRO:C   | 1:D:36:ARG:NH1  | 2.10                     | 1.05              |
| 1:E:115:ASP:N   | 1:F:36:ARG:CZ   | 2.18                     | 1.05              |
| 1:E:113:PRO:C   | 1:F:36:ARG:NH1  | 2.10                     | 1.05              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:115:ASP:N   | 1:E:36:ARG:NH1  | 2.05                     | 1.05              |
| 1:C:115:ASP:N   | 1:D:36:ARG:NH1  | 2.05                     | 1.05              |
| 1:D:113:PRO:C   | 1:E:36:ARG:NH1  | 2.10                     | 1.04              |
| 1:B:115:ASP:N   | 1:C:36:ARG:NH1  | 2.05                     | 1.04              |
| 1:E:115:ASP:N   | 1:F:36:ARG:NH1  | 2.05                     | 1.04              |
| 1:F:115:ASP:N   | 1:G:36:ARG:NH1  | 2.05                     | 1.03              |
| 1:A:36:ARG:NH1  | 1:G:115:ASP:N   | 2.05                     | 1.03              |
| 1:A:115:ASP:N   | 1:B:36:ARG:NH1  | 2.05                     | 1.02              |
| 1:B:112:ASN:O   | 1:C:36:ARG:CZ   | 2.08                     | 1.02              |
| 1:D:112:ASN:O   | 1:E:36:ARG:CZ   | 2.08                     | 1.01              |
| 1:A:36:ARG:CZ   | 1:G:112:ASN:O   | 2.08                     | 1.01              |
| 1:F:112:ASN:O   | 1:G:36:ARG:CZ   | 2.08                     | 1.01              |
| 1:C:112:ASN:O   | 1:D:36:ARG:CZ   | 2.08                     | 1.01              |
| 1:E:112:ASN:O   | 1:F:36:ARG:CZ   | 2.08                     | 1.01              |
| 1:A:112:ASN:O   | 1:B:36:ARG:CZ   | 2.08                     | 1.00              |
| 1:D:27:VAL:HG12 | 1:D:90:THR:HG23 | 1.51                     | 0.93              |
| 1:C:27:VAL:HG12 | 1:C:90:THR:HG23 | 1.50                     | 0.92              |
| 1:E:27:VAL:HG12 | 1:E:90:THR:HG23 | 1.51                     | 0.92              |
| 1:A:27:VAL:HG12 | 1:A:90:THR:HG23 | 1.51                     | 0.91              |
| 1:F:27:VAL:HG12 | 1:F:90:THR:HG23 | 1.50                     | 0.91              |
| 1:G:27:VAL:HG12 | 1:G:90:THR:HG23 | 1.51                     | 0.91              |
| 1:B:27:VAL:HG12 | 1:B:90:THR:HG23 | 1.50                     | 0.90              |
| 1:E:114:MET:N   | 1:F:36:ARG:CZ   | 2.38                     | 0.87              |
| 1:D:114:MET:N   | 1:E:36:ARG:CZ   | 2.38                     | 0.87              |
| 1:A:36:ARG:CZ   | 1:G:114:MET:N   | 2.38                     | 0.87              |
| 1:F:114:MET:N   | 1:G:36:ARG:CZ   | 2.38                     | 0.87              |
| 1:C:114:MET:N   | 1:D:36:ARG:CZ   | 2.38                     | 0.86              |
| 1:B:114:MET:N   | 1:C:36:ARG:CZ   | 2.38                     | 0.86              |
| 1:A:114:MET:N   | 1:B:36:ARG:CZ   | 2.38                     | 0.86              |
| 1:A:49:ILE:HD11 | 1:G:513:LEU:HA  | 1.61                     | 0.83              |
| 1:F:513:LEU:HA  | 1:G:49:ILE:HD11 | 1.61                     | 0.83              |
| 1:E:513:LEU:HA  | 1:F:49:ILE:HD11 | 1.61                     | 0.83              |
| 1:A:513:LEU:HA  | 1:B:49:ILE:HD11 | 1.61                     | 0.82              |
| 1:D:513:LEU:HA  | 1:E:49:ILE:HD11 | 1.61                     | 0.82              |
| 1:C:513:LEU:HA  | 1:D:49:ILE:HD11 | 1.61                     | 0.82              |
| 1:B:513:LEU:HA  | 1:C:49:ILE:HD11 | 1.61                     | 0.82              |
| 1:C:112:ASN:C   | 1:D:36:ARG:CZ   | 2.49                     | 0.81              |
| 1:E:112:ASN:C   | 1:F:36:ARG:CZ   | 2.49                     | 0.81              |
| 1:A:112:ASN:C   | 1:B:36:ARG:CZ   | 2.49                     | 0.81              |
| 1:A:36:ARG:CZ   | 1:G:112:ASN:C   | 2.49                     | 0.81              |
| 1:F:112:ASN:C   | 1:G:36:ARG:CZ   | 2.49                     | 0.81              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:112:ASN:C   | 1:E:36:ARG:CZ    | 2.49                     | 0.80              |
| 1:A:183:LEU:O   | 1:A:382:GLY:HA3  | 1.82                     | 0.80              |
| 1:B:183:LEU:O   | 1:B:382:GLY:HA3  | 1.82                     | 0.80              |
| 1:C:183:LEU:O   | 1:C:382:GLY:HA3  | 1.82                     | 0.80              |
| 1:F:183:LEU:O   | 1:F:382:GLY:HA3  | 1.82                     | 0.80              |
| 1:D:183:LEU:O   | 1:D:382:GLY:HA3  | 1.82                     | 0.80              |
| 1:B:112:ASN:C   | 1:C:36:ARG:CZ    | 2.49                     | 0.79              |
| 1:B:114:MET:H   | 1:C:36:ARG:NE    | 1.80                     | 0.79              |
| 1:G:183:LEU:O   | 1:G:382:GLY:HA3  | 1.82                     | 0.79              |
| 1:D:114:MET:H   | 1:E:36:ARG:NE    | 1.80                     | 0.79              |
| 1:E:114:MET:H   | 1:F:36:ARG:NE    | 1.81                     | 0.79              |
| 1:E:116:LEU:N   | 1:F:36:ARG:NH1   | 2.05                     | 0.79              |
| 1:E:183:LEU:O   | 1:E:382:GLY:HA3  | 1.82                     | 0.79              |
| 1:A:36:ARG:NE   | 1:G:114:MET:H    | 1.80                     | 0.79              |
| 1:A:113:PRO:CA  | 1:B:36:ARG:HH11  | 1.96                     | 0.79              |
| 1:C:114:MET:H   | 1:D:36:ARG:NE    | 1.80                     | 0.78              |
| 1:A:114:MET:H   | 1:B:36:ARG:NE    | 1.80                     | 0.78              |
| 1:F:114:MET:H   | 1:G:36:ARG:NE    | 1.80                     | 0.78              |
| 1:E:199:TYR:CD2 | 1:E:205:ILE:HD11 | 2.19                     | 0.78              |
| 1:F:199:TYR:CD2 | 1:F:205:ILE:HD11 | 2.19                     | 0.78              |
| 1:A:199:TYR:CD2 | 1:A:205:ILE:HD11 | 2.19                     | 0.78              |
| 1:A:135:SER:HA  | 1:A:412:VAL:HG12 | 1.66                     | 0.78              |
| 1:B:199:TYR:CD2 | 1:B:205:ILE:HD11 | 2.19                     | 0.78              |
| 1:C:113:PRO:CA  | 1:D:36:ARG:HH11  | 1.96                     | 0.78              |
| 1:E:115:ASP:HB2 | 1:F:36:ARG:HH22  | 1.49                     | 0.78              |
| 1:G:199:TYR:CD2 | 1:G:205:ILE:HD11 | 2.19                     | 0.78              |
| 1:D:115:ASP:HB2 | 1:E:36:ARG:HH22  | 1.49                     | 0.78              |
| 1:D:113:PRO:CA  | 1:E:36:ARG:HH11  | 1.96                     | 0.78              |
| 1:F:113:PRO:CA  | 1:G:36:ARG:HH11  | 1.96                     | 0.78              |
| 1:F:115:ASP:HB2 | 1:G:36:ARG:HH22  | 1.49                     | 0.78              |
| 1:B:135:SER:HA  | 1:B:412:VAL:HG12 | 1.66                     | 0.78              |
| 1:D:199:TYR:CD2 | 1:D:205:ILE:HD11 | 2.19                     | 0.77              |
| 1:G:135:SER:HA  | 1:G:412:VAL:HG12 | 1.66                     | 0.77              |
| 1:B:113:PRO:CA  | 1:C:36:ARG:HH11  | 1.96                     | 0.77              |
| 1:A:36:ARG:HH22 | 1:G:115:ASP:HB2  | 1.49                     | 0.77              |
| 1:A:36:ARG:HH11 | 1:G:113:PRO:CA   | 1.96                     | 0.77              |
| 1:C:135:SER:HA  | 1:C:412:VAL:HG12 | 1.66                     | 0.77              |
| 1:C:199:TYR:CD2 | 1:C:205:ILE:HD11 | 2.19                     | 0.77              |
| 1:E:113:PRO:CA  | 1:F:36:ARG:HH11  | 1.96                     | 0.77              |
| 1:D:198:GLY:HA2 | 1:D:327:LYS:O    | 1.86                     | 0.76              |
| 1:F:198:GLY:HA2 | 1:F:327:LYS:O    | 1.86                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:115:ASP:HB2  | 1:C:36:ARG:HH22  | 1.49                     | 0.76              |
| 1:F:135:SER:HA   | 1:F:412:VAL:HG12 | 1.66                     | 0.76              |
| 1:G:198:GLY:HA2  | 1:G:327:LYS:O    | 1.86                     | 0.76              |
| 1:C:115:ASP:HB2  | 1:D:36:ARG:HH22  | 1.49                     | 0.76              |
| 1:D:135:SER:HA   | 1:D:412:VAL:HG12 | 1.66                     | 0.76              |
| 1:C:198:GLY:HA2  | 1:C:327:LYS:O    | 1.86                     | 0.75              |
| 1:D:115:ASP:H    | 1:E:36:ARG:NH1   | 1.84                     | 0.75              |
| 1:D:116:LEU:N    | 1:E:36:ARG:NH1   | 2.05                     | 0.75              |
| 1:E:135:SER:HA   | 1:E:412:VAL:HG12 | 1.66                     | 0.75              |
| 1:A:115:ASP:HB2  | 1:B:36:ARG:HH22  | 1.49                     | 0.75              |
| 1:A:198:GLY:HA2  | 1:A:327:LYS:O    | 1.86                     | 0.75              |
| 1:C:115:ASP:H    | 1:D:36:ARG:NH1   | 1.84                     | 0.75              |
| 1:B:115:ASP:H    | 1:C:36:ARG:NH1   | 1.84                     | 0.75              |
| 1:B:198:GLY:HA2  | 1:B:327:LYS:O    | 1.86                     | 0.74              |
| 1:E:198:GLY:HA2  | 1:E:327:LYS:O    | 1.86                     | 0.74              |
| 1:A:36:ARG:CZ    | 1:A:36:ARG:NH1   | 2.51                     | 0.74              |
| 1:A:30:THR:HG22  | 1:A:38:VAL:HG21  | 1.69                     | 0.74              |
| 1:B:521:VAL:HG21 | 1:C:59:GLU:HB3   | 1.70                     | 0.74              |
| 1:G:36:ARG:CZ    | 1:G:36:ARG:NH1   | 2.51                     | 0.74              |
| 1:D:30:THR:HG22  | 1:D:38:VAL:HG21  | 1.69                     | 0.74              |
| 1:F:521:VAL:HG21 | 1:G:59:GLU:HB3   | 1.70                     | 0.73              |
| 1:A:36:ARG:NH1   | 1:G:115:ASP:H    | 1.84                     | 0.73              |
| 1:G:30:THR:HG22  | 1:G:38:VAL:HG21  | 1.69                     | 0.73              |
| 1:A:115:ASP:H    | 1:B:36:ARG:NH1   | 1.84                     | 0.73              |
| 1:D:36:ARG:NH1   | 1:D:36:ARG:CZ    | 2.51                     | 0.73              |
| 1:C:521:VAL:HG21 | 1:D:59:GLU:HB3   | 1.70                     | 0.73              |
| 1:F:36:ARG:NH1   | 1:F:36:ARG:CZ    | 2.51                     | 0.73              |
| 1:E:30:THR:HG22  | 1:E:38:VAL:HG21  | 1.69                     | 0.73              |
| 1:A:36:ARG:NH1   | 1:G:116:LEU:N    | 2.05                     | 0.73              |
| 1:B:36:ARG:NH1   | 1:B:36:ARG:CZ    | 2.51                     | 0.73              |
| 1:B:30:THR:HG22  | 1:B:38:VAL:HG21  | 1.69                     | 0.73              |
| 1:C:30:THR:HG22  | 1:C:38:VAL:HG21  | 1.69                     | 0.73              |
| 1:E:521:VAL:HG21 | 1:F:59:GLU:HB3   | 1.70                     | 0.73              |
| 1:A:521:VAL:HG21 | 1:B:59:GLU:HB3   | 1.70                     | 0.73              |
| 1:C:36:ARG:CZ    | 1:C:36:ARG:NH1   | 2.51                     | 0.73              |
| 1:D:521:VAL:HG21 | 1:E:59:GLU:HB3   | 1.70                     | 0.72              |
| 1:F:30:THR:HG22  | 1:F:38:VAL:HG21  | 1.69                     | 0.72              |
| 3:E:1526:PO4:P   | 2:E:1527:ATP:O1G | 2.48                     | 0.72              |
| 3:G:1525:PO4:P   | 2:G:1527:ATP:O1G | 2.48                     | 0.72              |
| 1:A:59:GLU:HB3   | 1:G:521:VAL:HG21 | 1.70                     | 0.72              |
| 1:E:36:ARG:NH1   | 1:E:36:ARG:CZ    | 2.51                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:115:ASP:H    | 1:G:36:ARG:NH1   | 1.84                     | 0.72              |
| 3:F:1525:PO4:P   | 2:F:1527:ATP:O1G | 2.48                     | 0.72              |
| 2:D:1525:ATP:O1G | 3:D:1526:PO4:P   | 2.48                     | 0.72              |
| 2:C:1526:ATP:O1G | 3:C:1527:PO4:P   | 2.48                     | 0.71              |
| 2:A:1525:ATP:O1G | 3:A:1526:PO4:P   | 2.48                     | 0.71              |
| 1:L:181:THR:O    | 1:M:283:ASP:N    | 2.24                     | 0.71              |
| 1:M:181:THR:O    | 1:N:283:ASP:N    | 2.24                     | 0.71              |
| 1:E:115:ASP:H    | 1:F:36:ARG:NH2   | 1.86                     | 0.71              |
| 1:E:115:ASP:H    | 1:F:36:ARG:NH1   | 1.84                     | 0.71              |
| 2:B:1525:ATP:O1G | 3:B:1526:PO4:P   | 2.48                     | 0.71              |
| 2:B:1525:ATP:O1A | 3:B:1526:PO4:P   | 2.49                     | 0.71              |
| 1:D:115:ASP:H    | 1:E:36:ARG:NH2   | 1.86                     | 0.71              |
| 2:D:1525:ATP:O1A | 3:D:1526:PO4:P   | 2.49                     | 0.71              |
| 1:I:181:THR:O    | 1:J:283:ASP:N    | 2.23                     | 0.70              |
| 1:F:115:ASP:H    | 1:G:36:ARG:NH2   | 1.86                     | 0.70              |
| 3:E:1526:PO4:P   | 2:E:1527:ATP:O1A | 2.49                     | 0.70              |
| 1:J:181:THR:O    | 1:K:283:ASP:N    | 2.24                     | 0.70              |
| 3:G:1525:PO4:P   | 2:G:1527:ATP:O1A | 2.49                     | 0.70              |
| 2:C:1526:ATP:O1A | 3:C:1527:PO4:P   | 2.49                     | 0.70              |
| 3:F:1525:PO4:P   | 2:F:1527:ATP:O1A | 2.49                     | 0.70              |
| 1:K:181:THR:O    | 1:L:283:ASP:N    | 2.23                     | 0.70              |
| 2:A:1525:ATP:O1A | 3:A:1526:PO4:P   | 2.49                     | 0.70              |
| 1:D:191:GLU:O    | 1:D:334:ASP:HA   | 1.92                     | 0.70              |
| 1:C:115:ASP:H    | 1:D:36:ARG:NH2   | 1.86                     | 0.70              |
| 1:C:191:GLU:O    | 1:C:334:ASP:HA   | 1.92                     | 0.70              |
| 1:H:283:ASP:N    | 1:N:181:THR:O    | 2.24                     | 0.70              |
| 1:B:116:LEU:N    | 1:C:36:ARG:NH1   | 2.05                     | 0.69              |
| 1:E:191:GLU:O    | 1:E:334:ASP:HA   | 1.92                     | 0.69              |
| 1:A:36:ARG:NH2   | 1:G:115:ASP:H    | 1.86                     | 0.69              |
| 1:H:181:THR:O    | 1:I:283:ASP:N    | 2.24                     | 0.69              |
| 1:C:116:LEU:N    | 1:D:36:ARG:NH1   | 2.05                     | 0.69              |
| 1:B:115:ASP:H    | 1:C:36:ARG:NH2   | 1.86                     | 0.69              |
| 1:A:115:ASP:H    | 1:B:36:ARG:NH2   | 1.86                     | 0.69              |
| 1:F:191:GLU:O    | 1:F:334:ASP:HA   | 1.92                     | 0.69              |
| 1:B:191:GLU:O    | 1:B:334:ASP:HA   | 1.92                     | 0.69              |
| 1:G:191:GLU:O    | 1:G:334:ASP:HA   | 1.92                     | 0.69              |
| 1:A:191:GLU:O    | 1:A:334:ASP:HA   | 1.92                     | 0.68              |
| 1:E:517:THR:HB   | 1:F:39:VAL:HB    | 1.76                     | 0.68              |
| 1:B:114:MET:H    | 1:C:36:ARG:CZ    | 2.05                     | 0.68              |
| 1:F:517:THR:HB   | 1:G:39:VAL:HB    | 1.76                     | 0.68              |
| 1:D:517:THR:HB   | 1:E:39:VAL:HB    | 1.76                     | 0.68              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:114:MET:H   | 1:G:36:ARG:CZ    | 2.06                     | 0.68              |
| 1:A:6:VAL:HG22  | 1:A:521:VAL:HG22 | 1.76                     | 0.68              |
| 1:B:6:VAL:HG22  | 1:B:521:VAL:HG22 | 1.76                     | 0.68              |
| 1:F:116:LEU:N   | 1:G:36:ARG:NH1   | 2.05                     | 0.68              |
| 1:E:114:MET:H   | 1:F:36:ARG:CZ    | 2.05                     | 0.67              |
| 1:C:6:VAL:HG22  | 1:C:521:VAL:HG22 | 1.76                     | 0.67              |
| 1:A:36:ARG:CZ   | 1:G:114:MET:H    | 2.05                     | 0.67              |
| 1:B:517:THR:HB  | 1:C:39:VAL:HB    | 1.76                     | 0.67              |
| 1:G:6:VAL:HG22  | 1:G:521:VAL:HG22 | 1.76                     | 0.67              |
| 1:L:400:LEU:C   | 1:L:401:HIS:CA   | 2.63                     | 0.67              |
| 1:A:517:THR:HB  | 1:B:39:VAL:HB    | 1.76                     | 0.66              |
| 1:A:116:LEU:N   | 1:B:36:ARG:NH1   | 2.05                     | 0.66              |
| 1:B:180:GLY:HA2 | 1:B:380:LYS:HB3  | 1.78                     | 0.66              |
| 1:C:517:THR:HB  | 1:D:39:VAL:HB    | 1.76                     | 0.66              |
| 1:D:6:VAL:HG22  | 1:D:521:VAL:HG22 | 1.76                     | 0.66              |
| 1:F:6:VAL:HG22  | 1:F:521:VAL:HG22 | 1.76                     | 0.66              |
| 1:A:180:GLY:HA2 | 1:A:380:LYS:HB3  | 1.78                     | 0.66              |
| 1:G:180:GLY:HA2 | 1:G:380:LYS:HB3  | 1.78                     | 0.66              |
| 1:K:223:ALA:O   | 1:K:251:ALA:HA   | 1.96                     | 0.66              |
| 1:A:39:VAL:HB   | 1:G:517:THR:HB   | 1.76                     | 0.66              |
| 1:G:40:LEU:HD21 | 1:G:55:SER:HB3   | 1.78                     | 0.66              |
| 1:I:223:ALA:O   | 1:I:251:ALA:HA   | 1.96                     | 0.66              |
| 1:C:114:MET:H   | 1:D:36:ARG:CZ    | 2.05                     | 0.66              |
| 1:C:180:GLY:HA2 | 1:C:380:LYS:HB3  | 1.78                     | 0.66              |
| 1:E:6:VAL:HG22  | 1:E:521:VAL:HG22 | 1.76                     | 0.66              |
| 1:A:40:LEU:HD21 | 1:A:55:SER:HB3   | 1.78                     | 0.65              |
| 1:F:180:GLY:HA2 | 1:F:380:LYS:HB3  | 1.78                     | 0.65              |
| 1:F:73:MET:HA   | 1:G:46:ALA:CB    | 2.26                     | 0.65              |
| 1:D:114:MET:H   | 1:E:36:ARG:CZ    | 2.05                     | 0.65              |
| 1:D:180:GLY:HA2 | 1:D:380:LYS:HB3  | 1.78                     | 0.65              |
| 1:C:39:VAL:HG13 | 1:C:48:THR:O     | 1.97                     | 0.65              |
| 1:B:73:MET:HA   | 1:C:46:ALA:HB2   | 1.78                     | 0.65              |
| 1:M:223:ALA:O   | 1:M:251:ALA:HA   | 1.96                     | 0.65              |
| 1:B:73:MET:HA   | 1:C:46:ALA:CB    | 2.26                     | 0.65              |
| 1:E:180:GLY:HA2 | 1:E:380:LYS:HB3  | 1.78                     | 0.65              |
| 1:F:40:LEU:HD21 | 1:F:55:SER:HB3   | 1.78                     | 0.65              |
| 1:L:223:ALA:O   | 1:L:251:ALA:HA   | 1.96                     | 0.65              |
| 1:J:223:ALA:O   | 1:J:251:ALA:HA   | 1.96                     | 0.65              |
| 1:C:73:MET:HA   | 1:D:46:ALA:HB2   | 1.79                     | 0.65              |
| 1:F:39:VAL:HG13 | 1:F:48:THR:O     | 1.97                     | 0.65              |
| 1:G:39:VAL:HG13 | 1:G:48:THR:O     | 1.97                     | 0.65              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:27:VAL:HG12 | 1:A:90:THR:CG2  | 2.27                     | 0.65              |
| 1:B:40:LEU:HD21 | 1:B:55:SER:HB3  | 1.78                     | 0.65              |
| 1:A:46:ALA:CB   | 1:G:73:MET:HA   | 2.26                     | 0.65              |
| 1:A:73:MET:HA   | 1:B:46:ALA:CB   | 2.26                     | 0.65              |
| 1:D:73:MET:HA   | 1:E:46:ALA:CB   | 2.26                     | 0.65              |
| 1:E:73:MET:HA   | 1:F:46:ALA:CB   | 2.26                     | 0.65              |
| 1:N:223:ALA:O   | 1:N:251:ALA:HA  | 1.96                     | 0.65              |
| 1:A:73:MET:HA   | 1:B:46:ALA:HB2  | 1.79                     | 0.65              |
| 1:H:223:ALA:O   | 1:H:251:ALA:HA  | 1.96                     | 0.65              |
| 1:F:114:MET:HB2 | 1:G:36:ARG:HD2  | 1.79                     | 0.64              |
| 1:E:39:VAL:HG13 | 1:E:48:THR:O    | 1.97                     | 0.64              |
| 1:A:39:VAL:HG13 | 1:A:48:THR:O    | 1.97                     | 0.64              |
| 1:C:73:MET:HA   | 1:D:46:ALA:CB   | 2.26                     | 0.64              |
| 1:B:27:VAL:HG12 | 1:B:90:THR:CG2  | 2.27                     | 0.64              |
| 1:E:114:MET:HB2 | 1:F:36:ARG:HD2  | 1.79                     | 0.64              |
| 1:A:46:ALA:HB2  | 1:G:73:MET:HA   | 1.78                     | 0.64              |
| 1:D:40:LEU:HD21 | 1:D:55:SER:HB3  | 1.78                     | 0.64              |
| 1:A:36:ARG:HD2  | 1:G:114:MET:HB2 | 1.79                     | 0.64              |
| 1:D:73:MET:HA   | 1:E:46:ALA:HB2  | 1.79                     | 0.64              |
| 1:E:40:LEU:HD21 | 1:E:55:SER:HB3  | 1.78                     | 0.64              |
| 1:A:517:THR:CB  | 1:B:39:VAL:HB   | 2.28                     | 0.64              |
| 1:C:40:LEU:HD21 | 1:C:55:SER:HB3  | 1.78                     | 0.64              |
| 1:A:39:VAL:HB   | 1:G:517:THR:CB  | 2.28                     | 0.64              |
| 1:D:114:MET:HB2 | 1:E:36:ARG:HD2  | 1.79                     | 0.64              |
| 1:D:39:VAL:HG13 | 1:D:48:THR:O    | 1.97                     | 0.64              |
| 1:E:517:THR:CB  | 1:F:39:VAL:HB   | 2.28                     | 0.63              |
| 1:E:73:MET:HA   | 1:F:46:ALA:HB2  | 1.79                     | 0.63              |
| 1:F:73:MET:HA   | 1:G:46:ALA:HB2  | 1.79                     | 0.63              |
| 1:A:114:MET:HB2 | 1:B:36:ARG:HD2  | 1.79                     | 0.63              |
| 1:B:114:MET:HB2 | 1:C:36:ARG:HD2  | 1.79                     | 0.63              |
| 1:F:517:THR:CB  | 1:G:39:VAL:HB   | 2.28                     | 0.63              |
| 1:C:27:VAL:HG12 | 1:C:90:THR:CG2  | 2.27                     | 0.63              |
| 1:B:39:VAL:HG13 | 1:B:48:THR:O    | 1.97                     | 0.63              |
| 1:C:517:THR:HA  | 1:D:39:VAL:HG23 | 1.81                     | 0.63              |
| 1:C:114:MET:HB2 | 1:D:36:ARG:HD2  | 1.79                     | 0.63              |
| 1:A:114:MET:H   | 1:B:36:ARG:CD   | 2.12                     | 0.63              |
| 1:D:114:MET:H   | 1:E:36:ARG:CD   | 2.12                     | 0.63              |
| 1:A:39:VAL:HG23 | 1:G:517:THR:HA  | 1.81                     | 0.63              |
| 1:B:517:THR:HA  | 1:C:39:VAL:HG23 | 1.81                     | 0.63              |
| 1:E:114:MET:H   | 1:F:36:ARG:CD   | 2.12                     | 0.63              |
| 1:B:517:THR:CB  | 1:C:39:VAL:HB   | 2.29                     | 0.62              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:F:114:MET:H   | 1:G:36:ARG:CD   | 2.12                     | 0.62              |
| 1:A:517:THR:HA  | 1:B:39:VAL:HG23 | 1.81                     | 0.62              |
| 1:D:517:THR:CB  | 1:E:39:VAL:HB   | 2.28                     | 0.62              |
| 1:E:517:THR:HA  | 1:F:39:VAL:HG23 | 1.81                     | 0.62              |
| 1:F:517:THR:HA  | 1:G:39:VAL:HG23 | 1.81                     | 0.62              |
| 1:B:114:MET:H   | 1:C:36:ARG:CD   | 2.12                     | 0.62              |
| 1:B:31:LEU:HB3  | 1:B:90:THR:HG21 | 1.82                     | 0.62              |
| 1:C:114:MET:H   | 1:D:36:ARG:CD   | 2.12                     | 0.62              |
| 1:D:517:THR:HA  | 1:E:39:VAL:HG23 | 1.81                     | 0.62              |
| 1:A:114:MET:H   | 1:B:36:ARG:CZ   | 2.05                     | 0.62              |
| 1:A:521:VAL:H   | 1:B:41:ASP:HB3  | 1.65                     | 0.62              |
| 1:D:30:THR:HG21 | 1:D:56:VAL:HG21 | 1.82                     | 0.62              |
| 1:E:30:THR:HG21 | 1:E:56:VAL:HG21 | 1.82                     | 0.62              |
| 1:C:31:LEU:HB3  | 1:C:90:THR:HG21 | 1.82                     | 0.62              |
| 1:F:30:THR:HG21 | 1:F:56:VAL:HG21 | 1.82                     | 0.62              |
| 1:B:520:MET:HA  | 1:C:41:ASP:HB2  | 1.82                     | 0.62              |
| 1:C:517:THR:CB  | 1:D:39:VAL:HB   | 2.28                     | 0.62              |
| 1:D:521:VAL:H   | 1:E:41:ASP:HB3  | 1.65                     | 0.62              |
| 1:A:41:ASP:HB3  | 1:G:521:VAL:H   | 1.65                     | 0.62              |
| 1:B:521:VAL:H   | 1:C:41:ASP:HB3  | 1.65                     | 0.62              |
| 1:D:27:VAL:HG12 | 1:D:90:THR:CG2  | 2.27                     | 0.62              |
| 1:A:31:LEU:HB3  | 1:A:90:THR:HG21 | 1.82                     | 0.61              |
| 1:A:520:MET:HA  | 1:B:41:ASP:HB2  | 1.82                     | 0.61              |
| 1:G:30:THR:HG21 | 1:G:56:VAL:HG21 | 1.82                     | 0.61              |
| 1:D:520:MET:HA  | 1:E:41:ASP:HB2  | 1.82                     | 0.61              |
| 1:F:27:VAL:HG12 | 1:F:90:THR:CG2  | 2.27                     | 0.61              |
| 1:C:30:THR:HG21 | 1:C:56:VAL:HG21 | 1.82                     | 0.61              |
| 1:C:520:MET:HA  | 1:D:41:ASP:HB2  | 1.82                     | 0.61              |
| 1:E:520:MET:HA  | 1:F:41:ASP:HB2  | 1.82                     | 0.61              |
| 1:A:36:ARG:CD   | 1:G:114:MET:H   | 2.12                     | 0.61              |
| 1:D:31:LEU:HB3  | 1:D:90:THR:HG21 | 1.82                     | 0.61              |
| 1:E:214:GLU:HA  | 1:E:323:VAL:O   | 2.01                     | 0.61              |
| 1:A:30:THR:HG21 | 1:A:56:VAL:HG21 | 1.82                     | 0.61              |
| 1:D:214:GLU:HA  | 1:D:323:VAL:O   | 2.01                     | 0.61              |
| 1:F:521:VAL:H   | 1:G:41:ASP:HB3  | 1.65                     | 0.61              |
| 1:A:41:ASP:HB2  | 1:G:520:MET:HA  | 1.82                     | 0.61              |
| 1:G:214:GLU:HA  | 1:G:323:VAL:O   | 2.01                     | 0.61              |
| 1:F:520:MET:HA  | 1:G:41:ASP:HB2  | 1.82                     | 0.61              |
| 1:C:214:GLU:HA  | 1:C:323:VAL:O   | 2.01                     | 0.61              |
| 1:E:521:VAL:H   | 1:F:41:ASP:HB3  | 1.65                     | 0.61              |
| 1:G:31:LEU:HB3  | 1:G:90:THR:HG21 | 1.82                     | 0.61              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:214:GLU:HA   | 1:A:323:VAL:O   | 2.00                     | 0.61              |
| 1:F:214:GLU:HA   | 1:F:323:VAL:O   | 2.01                     | 0.61              |
| 1:F:31:LEU:HB3   | 1:F:90:THR:HG21 | 1.82                     | 0.61              |
| 1:A:36:ARG:NH1   | 1:G:114:MET:N   | 2.49                     | 0.61              |
| 1:B:214:GLU:HA   | 1:B:323:VAL:O   | 2.01                     | 0.60              |
| 1:C:521:VAL:H    | 1:D:41:ASP:HB3  | 1.65                     | 0.60              |
| 1:E:31:LEU:HB3   | 1:E:90:THR:HG21 | 1.82                     | 0.60              |
| 1:E:27:VAL:HG12  | 1:E:90:THR:CG2  | 2.27                     | 0.60              |
| 1:B:30:THR:HG21  | 1:B:56:VAL:HG21 | 1.82                     | 0.60              |
| 1:B:114:MET:N    | 1:C:36:ARG:NH1  | 2.49                     | 0.60              |
| 1:D:114:MET:N    | 1:E:36:ARG:NH1  | 2.50                     | 0.60              |
| 1:A:114:MET:N    | 1:B:36:ARG:NH1  | 2.49                     | 0.60              |
| 1:E:417:VAL:HG21 | 1:E:477:GLY:HA3 | 1.84                     | 0.60              |
| 1:E:114:MET:N    | 1:F:36:ARG:NH1  | 2.50                     | 0.60              |
| 1:F:417:VAL:HG21 | 1:F:477:GLY:HA3 | 1.84                     | 0.60              |
| 1:G:417:VAL:HG21 | 1:G:477:GLY:HA3 | 1.84                     | 0.60              |
| 1:C:114:MET:N    | 1:D:36:ARG:NH1  | 2.49                     | 0.60              |
| 1:G:40:LEU:HB3   | 1:G:59:GLU:HG3  | 1.84                     | 0.60              |
| 1:E:40:LEU:HB3   | 1:E:59:GLU:HG3  | 1.84                     | 0.59              |
| 1:G:27:VAL:HG12  | 1:G:90:THR:CG2  | 2.27                     | 0.59              |
| 1:D:417:VAL:HG21 | 1:D:477:GLY:HA3 | 1.84                     | 0.59              |
| 1:F:40:LEU:HB3   | 1:F:59:GLU:HG3  | 1.84                     | 0.59              |
| 1:A:40:LEU:HB3   | 1:A:59:GLU:HG3  | 1.84                     | 0.59              |
| 1:C:417:VAL:HG21 | 1:C:477:GLY:HA3 | 1.84                     | 0.59              |
| 1:A:417:VAL:HG21 | 1:A:477:GLY:HA3 | 1.84                     | 0.59              |
| 1:G:151:SER:HB3  | 1:G:399:ALA:HA  | 1.85                     | 0.59              |
| 1:B:417:VAL:HG21 | 1:B:477:GLY:HA3 | 1.84                     | 0.59              |
| 1:F:114:MET:N    | 1:G:36:ARG:NH1  | 2.49                     | 0.59              |
| 1:B:40:LEU:HB3   | 1:B:59:GLU:HG3  | 1.84                     | 0.59              |
| 1:D:40:LEU:HB3   | 1:D:59:GLU:HG3  | 1.84                     | 0.59              |
| 1:C:240:VAL:HG11 | 1:C:247:LEU:HB2 | 1.85                     | 0.58              |
| 1:L:400:LEU:CA   | 1:L:401:HIS:N   | 2.62                     | 0.58              |
| 1:D:240:VAL:HG11 | 1:D:247:LEU:HB2 | 1.85                     | 0.58              |
| 1:F:151:SER:HB3  | 1:F:399:ALA:HA  | 1.85                     | 0.58              |
| 1:A:36:ARG:HH12  | 1:G:116:LEU:H   | 0.62                     | 0.58              |
| 1:A:151:SER:HB3  | 1:A:399:ALA:HA  | 1.85                     | 0.58              |
| 1:A:217:SER:HA   | 1:A:320:ALA:O   | 2.04                     | 0.58              |
| 1:B:116:LEU:H    | 1:C:36:ARG:HH12 | 0.61                     | 0.58              |
| 1:A:115:ASP:CB   | 1:B:36:ARG:HH22 | 2.15                     | 0.58              |
| 1:B:217:SER:HA   | 1:B:320:ALA:O   | 2.04                     | 0.58              |
| 1:C:217:SER:HA   | 1:C:320:ALA:O   | 2.04                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:40:LEU:HB3   | 1:C:59:GLU:HG3   | 1.84                     | 0.58              |
| 1:G:217:SER:HA   | 1:G:320:ALA:O    | 2.04                     | 0.58              |
| 1:D:116:LEU:H    | 1:E:36:ARG:HH12  | 0.61                     | 0.58              |
| 1:E:151:SER:CB   | 1:E:399:ALA:HA   | 2.34                     | 0.58              |
| 1:F:192:GLY:O    | 1:F:375:GLY:HA2  | 2.04                     | 0.58              |
| 1:G:151:SER:CB   | 1:G:399:ALA:HA   | 2.34                     | 0.58              |
| 1:B:240:VAL:HG11 | 1:B:247:LEU:HB2  | 1.85                     | 0.58              |
| 1:D:151:SER:CB   | 1:D:399:ALA:HA   | 2.34                     | 0.58              |
| 1:E:151:SER:HB3  | 1:E:399:ALA:HA   | 1.85                     | 0.58              |
| 1:F:217:SER:HA   | 1:F:320:ALA:O    | 2.04                     | 0.58              |
| 1:A:151:SER:CB   | 1:A:399:ALA:HA   | 2.34                     | 0.58              |
| 1:E:116:LEU:H    | 1:F:36:ARG:HH12  | 0.62                     | 0.58              |
| 1:E:240:VAL:HG11 | 1:E:247:LEU:HB2  | 1.85                     | 0.58              |
| 1:G:192:GLY:O    | 1:G:375:GLY:HA2  | 2.04                     | 0.58              |
| 1:D:217:SER:HA   | 1:D:320:ALA:O    | 2.04                     | 0.57              |
| 1:E:217:SER:HA   | 1:E:320:ALA:O    | 2.04                     | 0.57              |
| 1:F:240:VAL:HG11 | 1:F:247:LEU:HB2  | 1.85                     | 0.57              |
| 1:G:240:VAL:HG11 | 1:G:247:LEU:HB2  | 1.85                     | 0.57              |
| 1:C:192:GLY:O    | 1:C:375:GLY:HA2  | 2.04                     | 0.57              |
| 1:D:192:GLY:O    | 1:D:375:GLY:HA2  | 2.04                     | 0.57              |
| 1:F:115:ASP:CB   | 1:G:36:ARG:HH22  | 2.15                     | 0.57              |
| 1:B:151:SER:HB3  | 1:B:399:ALA:HA   | 1.85                     | 0.57              |
| 1:G:127:ALA:HB2  | 1:G:426:LEU:HD11 | 1.86                     | 0.57              |
| 1:B:192:GLY:O    | 1:B:375:GLY:HA2  | 2.04                     | 0.57              |
| 1:C:151:SER:CB   | 1:C:399:ALA:HA   | 2.34                     | 0.57              |
| 1:A:192:GLY:O    | 1:A:375:GLY:HA2  | 2.04                     | 0.57              |
| 1:B:151:SER:CB   | 1:B:399:ALA:HA   | 2.34                     | 0.57              |
| 1:D:151:SER:HB3  | 1:D:399:ALA:HA   | 1.85                     | 0.57              |
| 1:E:115:ASP:CB   | 1:F:36:ARG:HH22  | 2.15                     | 0.57              |
| 1:E:192:GLY:O    | 1:E:375:GLY:HA2  | 2.04                     | 0.57              |
| 1:F:127:ALA:HB2  | 1:F:426:LEU:HD11 | 1.87                     | 0.57              |
| 1:D:127:ALA:HB2  | 1:D:426:LEU:HD11 | 1.86                     | 0.57              |
| 1:D:115:ASP:CB   | 1:E:36:ARG:HH22  | 2.15                     | 0.57              |
| 1:A:36:ARG:NH2   | 1:G:112:ASN:O    | 2.38                     | 0.57              |
| 1:J:85:ALA:HB1   | 1:J:499:VAL:HG12 | 1.86                     | 0.57              |
| 1:K:85:ALA:HB1   | 1:K:499:VAL:HG12 | 1.86                     | 0.57              |
| 1:A:240:VAL:HG11 | 1:A:247:LEU:HB2  | 1.85                     | 0.57              |
| 1:C:151:SER:HB3  | 1:C:399:ALA:HA   | 1.85                     | 0.57              |
| 1:F:151:SER:CB   | 1:F:399:ALA:HA   | 2.34                     | 0.57              |
| 1:E:127:ALA:HB2  | 1:E:426:LEU:HD11 | 1.87                     | 0.57              |
| 1:A:36:ARG:HH22  | 1:G:115:ASP:CB   | 2.15                     | 0.57              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:112:ASN:O   | 1:B:36:ARG:NH2   | 2.38                     | 0.57              |
| 1:F:39:VAL:HG21 | 1:F:49:ILE:CD1   | 2.35                     | 0.57              |
| 1:A:127:ALA:HB2 | 1:A:426:LEU:HD11 | 1.87                     | 0.56              |
| 1:D:212:ALA:HA  | 1:D:325:ILE:O    | 2.06                     | 0.56              |
| 1:E:112:ASN:O   | 1:F:36:ARG:NH2   | 2.38                     | 0.56              |
| 1:E:39:VAL:HG21 | 1:E:49:ILE:CD1   | 2.35                     | 0.56              |
| 1:K:229:ASN:HA  | 1:K:258:ALA:HB3  | 1.87                     | 0.56              |
| 1:E:212:ALA:HA  | 1:E:325:ILE:O    | 2.06                     | 0.56              |
| 1:M:229:ASN:HA  | 1:M:258:ALA:HB3  | 1.88                     | 0.56              |
| 1:M:85:ALA:HB1  | 1:M:499:VAL:HG12 | 1.86                     | 0.56              |
| 1:C:127:ALA:HB2 | 1:C:426:LEU:HD11 | 1.87                     | 0.56              |
| 1:F:212:ALA:HA  | 1:F:325:ILE:O    | 2.06                     | 0.56              |
| 1:H:85:ALA:HB1  | 1:H:499:VAL:HG12 | 1.86                     | 0.56              |
| 1:L:229:ASN:HA  | 1:L:258:ALA:HB3  | 1.88                     | 0.56              |
| 1:L:85:ALA:HB1  | 1:L:499:VAL:HG12 | 1.86                     | 0.56              |
| 1:N:229:ASN:HA  | 1:N:258:ALA:HB3  | 1.88                     | 0.56              |
| 1:E:152:ALA:HB1 | 1:E:155:ASP:HB2  | 1.87                     | 0.56              |
| 1:F:113:PRO:O   | 1:G:36:ARG:NH1   | 2.39                     | 0.56              |
| 1:F:112:ASN:O   | 1:G:36:ARG:NH2   | 2.38                     | 0.56              |
| 1:I:85:ALA:HB1  | 1:I:499:VAL:HG12 | 1.86                     | 0.56              |
| 1:B:39:VAL:HG21 | 1:B:49:ILE:CD1   | 2.35                     | 0.56              |
| 1:B:112:ASN:O   | 1:C:36:ARG:NH2   | 2.38                     | 0.56              |
| 1:D:152:ALA:HB1 | 1:D:155:ASP:HB2  | 1.87                     | 0.56              |
| 1:C:112:ASN:O   | 1:D:36:ARG:NH2   | 2.38                     | 0.56              |
| 1:G:152:ALA:HB1 | 1:G:155:ASP:HB2  | 1.87                     | 0.56              |
| 1:J:229:ASN:HA  | 1:J:258:ALA:HB3  | 1.87                     | 0.56              |
| 1:N:85:ALA:HB1  | 1:N:499:VAL:HG12 | 1.86                     | 0.56              |
| 1:A:152:ALA:HB1 | 1:A:155:ASP:HB2  | 1.87                     | 0.56              |
| 1:B:127:ALA:HB2 | 1:B:426:LEU:HD11 | 1.86                     | 0.56              |
| 1:A:113:PRO:O   | 1:B:36:ARG:NH1   | 2.39                     | 0.56              |
| 1:B:115:ASP:CB  | 1:C:36:ARG:HH22  | 2.15                     | 0.56              |
| 1:C:115:ASP:CB  | 1:D:36:ARG:HH22  | 2.15                     | 0.56              |
| 1:D:39:VAL:HG21 | 1:D:49:ILE:CD1   | 2.35                     | 0.56              |
| 1:A:212:ALA:HA  | 1:A:325:ILE:O    | 2.06                     | 0.56              |
| 1:B:212:ALA:HA  | 1:B:325:ILE:O    | 2.05                     | 0.56              |
| 1:B:115:ASP:C   | 1:C:36:ARG:HH12  | 2.07                     | 0.56              |
| 1:C:113:PRO:O   | 1:D:36:ARG:NH1   | 2.39                     | 0.56              |
| 1:D:112:ASN:C   | 1:E:36:ARG:NE    | 2.59                     | 0.56              |
| 1:A:39:VAL:HG21 | 1:A:49:ILE:CD1   | 2.35                     | 0.56              |
| 1:B:152:ALA:HB1 | 1:B:155:ASP:HB2  | 1.87                     | 0.56              |
| 1:C:112:ASN:C   | 1:D:36:ARG:NE    | 2.59                     | 0.56              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:113:PRO:O   | 1:C:36:ARG:NH1  | 2.39                     | 0.56              |
| 1:G:39:VAL:HG21 | 1:G:49:ILE:CD1  | 2.35                     | 0.56              |
| 1:B:112:ASN:C   | 1:C:36:ARG:NE   | 2.59                     | 0.56              |
| 1:C:152:ALA:HB1 | 1:C:155:ASP:HB2 | 1.87                     | 0.56              |
| 1:C:212:ALA:HA  | 1:C:325:ILE:O   | 2.05                     | 0.56              |
| 1:F:112:ASN:C   | 1:G:36:ARG:NE   | 2.59                     | 0.56              |
| 1:A:36:ARG:NE   | 1:G:112:ASN:C   | 2.59                     | 0.55              |
| 1:A:36:ARG:NH1  | 1:G:113:PRO:O   | 2.39                     | 0.55              |
| 1:E:113:PRO:O   | 1:F:36:ARG:NH1  | 2.39                     | 0.55              |
| 1:H:229:ASN:HA  | 1:H:258:ALA:HB3 | 1.88                     | 0.55              |
| 1:C:39:VAL:HG21 | 1:C:49:ILE:CD1  | 2.35                     | 0.55              |
| 1:D:112:ASN:O   | 1:E:36:ARG:NH2  | 2.38                     | 0.55              |
| 1:C:186:GLU:H   | 1:C:380:LYS:HB2 | 1.72                     | 0.55              |
| 1:F:152:ALA:HB1 | 1:F:155:ASP:HB2 | 1.87                     | 0.55              |
| 1:G:212:ALA:HA  | 1:G:325:ILE:O   | 2.06                     | 0.55              |
| 1:A:112:ASN:C   | 1:B:36:ARG:NE   | 2.59                     | 0.55              |
| 1:C:116:LEU:H   | 1:D:36:ARG:HH12 | 0.62                     | 0.55              |
| 1:A:26:ALA:O    | 1:A:30:THR:HG23 | 2.07                     | 0.55              |
| 1:B:114:MET:CB  | 1:C:36:ARG:HD2  | 2.36                     | 0.55              |
| 1:C:115:ASP:C   | 1:D:36:ARG:HH12 | 2.07                     | 0.55              |
| 1:D:114:MET:CB  | 1:E:36:ARG:HD2  | 2.36                     | 0.55              |
| 1:D:246:PRO:HB3 | 1:D:272:LYS:HB2 | 1.89                     | 0.55              |
| 1:C:114:MET:CB  | 1:D:36:ARG:HD2  | 2.37                     | 0.55              |
| 1:E:112:ASN:C   | 1:F:36:ARG:NE   | 2.59                     | 0.55              |
| 1:E:246:PRO:HB3 | 1:E:272:LYS:HB2 | 1.89                     | 0.55              |
| 1:A:114:MET:CB  | 1:B:36:ARG:HD2  | 2.36                     | 0.55              |
| 1:I:229:ASN:HA  | 1:I:258:ALA:HB3 | 1.88                     | 0.55              |
| 1:F:246:PRO:HB3 | 1:F:272:LYS:HB2 | 1.89                     | 0.55              |
| 1:G:26:ALA:O    | 1:G:30:THR:HG23 | 2.07                     | 0.55              |
| 1:G:246:PRO:HB3 | 1:G:272:LYS:HB2 | 1.89                     | 0.55              |
| 1:A:186:GLU:H   | 1:A:380:LYS:HB2 | 1.72                     | 0.54              |
| 1:E:186:GLU:H   | 1:E:380:LYS:HB2 | 1.72                     | 0.54              |
| 1:E:114:MET:CB  | 1:F:36:ARG:HD2  | 2.37                     | 0.54              |
| 1:H:25:ASP:CG   | 1:H:28:LYS:HZ3  | 2.11                     | 0.54              |
| 1:B:26:ALA:O    | 1:B:30:THR:HG23 | 2.07                     | 0.54              |
| 1:C:26:ALA:O    | 1:C:30:THR:HG23 | 2.07                     | 0.54              |
| 1:D:26:ALA:O    | 1:D:30:THR:HG23 | 2.07                     | 0.54              |
| 1:D:39:VAL:HG21 | 1:D:49:ILE:HG12 | 1.89                     | 0.54              |
| 1:N:398:ALA:O   | 1:N:401:HIS:N   | 2.41                     | 0.54              |
| 1:A:246:PRO:HB3 | 1:A:272:LYS:HB2 | 1.89                     | 0.54              |
| 1:G:186:GLU:H   | 1:G:380:LYS:HB2 | 1.72                     | 0.54              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:C:39:VAL:HG21  | 1:C:49:ILE:HG12 | 1.89                     | 0.54              |
| 1:F:114:MET:CB   | 1:G:36:ARG:HD2  | 2.36                     | 0.54              |
| 1:B:186:GLU:H    | 1:B:380:LYS:HB2 | 1.72                     | 0.54              |
| 1:C:218:PRO:HG2  | 1:C:320:ALA:HB3 | 1.90                     | 0.54              |
| 1:D:40:LEU:HD11  | 1:D:55:SER:HB3  | 1.90                     | 0.54              |
| 1:G:39:VAL:HG21  | 1:G:49:ILE:HG12 | 1.89                     | 0.54              |
| 1:A:36:ARG:HD2   | 1:G:114:MET:CB  | 2.36                     | 0.54              |
| 1:C:246:PRO:HB3  | 1:C:272:LYS:HB2 | 1.89                     | 0.54              |
| 1:E:26:ALA:O     | 1:E:30:THR:HG23 | 2.07                     | 0.54              |
| 1:F:26:ALA:O     | 1:F:30:THR:HG23 | 2.07                     | 0.54              |
| 1:F:39:VAL:HG21  | 1:F:49:ILE:HG12 | 1.89                     | 0.54              |
| 1:J:25:ASP:CG    | 1:J:28:LYS:HZ3  | 2.11                     | 0.54              |
| 1:N:25:ASP:CG    | 1:N:28:LYS:HZ3  | 2.11                     | 0.54              |
| 1:A:218:PRO:HG2  | 1:A:320:ALA:HB3 | 1.90                     | 0.54              |
| 1:G:218:PRO:HG2  | 1:G:320:ALA:HB3 | 1.90                     | 0.54              |
| 1:B:218:PRO:HG2  | 1:B:320:ALA:HB3 | 1.90                     | 0.54              |
| 1:B:39:VAL:HG21  | 1:B:49:ILE:HG12 | 1.89                     | 0.54              |
| 1:E:39:VAL:HG21  | 1:E:49:ILE:HG12 | 1.89                     | 0.54              |
| 1:F:186:GLU:H    | 1:F:380:LYS:HB2 | 1.72                     | 0.54              |
| 1:B:246:PRO:HB3  | 1:B:272:LYS:HB2 | 1.89                     | 0.54              |
| 1:C:40:LEU:HD11  | 1:C:55:SER:HB3  | 1.90                     | 0.54              |
| 1:E:40:LEU:HD11  | 1:E:55:SER:HB3  | 1.90                     | 0.54              |
| 1:E:115:ASP:C    | 1:F:36:ARG:HH12 | 2.07                     | 0.54              |
| 1:F:40:LEU:HD11  | 1:F:55:SER:HB3  | 1.90                     | 0.54              |
| 1:B:205:ILE:HD12 | 1:B:211:GLY:O   | 2.09                     | 0.53              |
| 1:B:40:LEU:HD11  | 1:B:55:SER:HB3  | 1.90                     | 0.53              |
| 1:C:205:ILE:HD12 | 1:C:211:GLY:O   | 2.09                     | 0.53              |
| 1:D:218:PRO:HG2  | 1:D:320:ALA:HB3 | 1.90                     | 0.53              |
| 1:D:186:GLU:H    | 1:D:380:LYS:HB2 | 1.72                     | 0.53              |
| 1:E:31:LEU:CB    | 1:E:90:THR:HG21 | 2.39                     | 0.53              |
| 1:D:113:PRO:O    | 1:E:36:ARG:NH1  | 2.39                     | 0.53              |
| 1:L:25:ASP:CG    | 1:L:28:LYS:HZ3  | 2.11                     | 0.53              |
| 1:D:31:LEU:CB    | 1:D:90:THR:HG21 | 2.39                     | 0.53              |
| 1:F:218:PRO:HG2  | 1:F:320:ALA:HB3 | 1.90                     | 0.53              |
| 1:G:39:VAL:HG13  | 1:G:48:THR:C    | 2.29                     | 0.53              |
| 1:I:25:ASP:CG    | 1:I:28:LYS:HZ3  | 2.12                     | 0.53              |
| 1:A:205:ILE:HD12 | 1:A:211:GLY:O   | 2.08                     | 0.53              |
| 1:C:31:LEU:CB    | 1:C:90:THR:HG21 | 2.39                     | 0.53              |
| 1:D:205:ILE:HD12 | 1:D:211:GLY:O   | 2.09                     | 0.53              |
| 1:D:39:VAL:HG13  | 1:D:48:THR:C    | 2.29                     | 0.53              |
| 1:A:39:VAL:HG21  | 1:A:49:ILE:HG12 | 1.89                     | 0.53              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:F:205:ILE:HD12 | 1:F:211:GLY:O   | 2.09                     | 0.53              |
| 1:F:31:LEU:CB    | 1:F:90:THR:HG21 | 2.39                     | 0.53              |
| 1:G:40:LEU:HD11  | 1:G:55:SER:HB3  | 1.90                     | 0.53              |
| 1:K:25:ASP:CG    | 1:K:28:LYS:HZ3  | 2.12                     | 0.53              |
| 1:C:113:PRO:CA   | 1:D:36:ARG:NH1  | 2.66                     | 0.53              |
| 1:E:39:VAL:HG13  | 1:E:48:THR:C    | 2.29                     | 0.53              |
| 1:F:113:PRO:HA   | 1:G:36:ARG:HH11 | 1.73                     | 0.53              |
| 1:A:39:VAL:HG13  | 1:A:48:THR:C    | 2.29                     | 0.53              |
| 1:B:239:ALA:HB1  | 1:B:314:LEU:HG  | 1.91                     | 0.53              |
| 1:B:31:LEU:CB    | 1:B:90:THR:HG21 | 2.39                     | 0.53              |
| 1:F:112:ASN:CB   | 1:G:36:ARG:HE   | 2.22                     | 0.53              |
| 1:A:36:ARG:HE    | 1:G:112:ASN:CB  | 2.22                     | 0.52              |
| 1:B:411:VAL:HB   | 1:B:494:LEU:HB3 | 1.92                     | 0.52              |
| 1:C:239:ALA:HB1  | 1:C:314:LEU:HG  | 1.91                     | 0.52              |
| 1:E:218:PRO:HG2  | 1:E:320:ALA:HB3 | 1.90                     | 0.52              |
| 1:G:31:LEU:CB    | 1:G:90:THR:HG21 | 2.39                     | 0.52              |
| 1:A:239:ALA:HB1  | 1:A:314:LEU:HG  | 1.91                     | 0.52              |
| 1:B:144:ILE:HG23 | 1:B:403:THR:CG2 | 2.40                     | 0.52              |
| 1:C:144:ILE:HG23 | 1:C:403:THR:CG2 | 2.40                     | 0.52              |
| 1:G:411:VAL:HB   | 1:G:494:LEU:HB3 | 1.92                     | 0.52              |
| 1:A:36:ARG:HH11  | 1:G:113:PRO:HA  | 1.73                     | 0.52              |
| 1:A:40:LEU:HD11  | 1:A:55:SER:HB3  | 1.90                     | 0.52              |
| 1:A:112:ASN:CB   | 1:B:36:ARG:HE   | 2.23                     | 0.52              |
| 1:E:113:PRO:HA   | 1:F:36:ARG:HH11 | 1.73                     | 0.52              |
| 1:A:144:ILE:HG23 | 1:A:403:THR:CG2 | 2.40                     | 0.52              |
| 1:C:142:LYS:H    | 1:C:142:LYS:HD2 | 1.75                     | 0.52              |
| 1:D:247:LEU:O    | 1:D:273:VAL:HA  | 2.10                     | 0.52              |
| 1:F:411:VAL:HB   | 1:F:494:LEU:HB3 | 1.92                     | 0.52              |
| 1:A:247:LEU:O    | 1:A:273:VAL:HA  | 2.10                     | 0.52              |
| 1:C:39:VAL:HG13  | 1:C:48:THR:C    | 2.29                     | 0.52              |
| 1:F:39:VAL:HG13  | 1:F:48:THR:C    | 2.29                     | 0.52              |
| 1:G:142:LYS:H    | 1:G:142:LYS:HD2 | 1.75                     | 0.52              |
| 1:E:205:ILE:HD12 | 1:E:211:GLY:O   | 2.09                     | 0.52              |
| 1:A:31:LEU:CB    | 1:A:90:THR:HG21 | 2.39                     | 0.52              |
| 1:B:142:LYS:H    | 1:B:142:LYS:HD2 | 1.75                     | 0.52              |
| 1:C:247:LEU:O    | 1:C:273:VAL:HA  | 2.10                     | 0.52              |
| 1:E:142:LYS:HD2  | 1:E:142:LYS:H   | 1.75                     | 0.52              |
| 1:G:247:LEU:O    | 1:G:273:VAL:HA  | 2.10                     | 0.52              |
| 1:G:239:ALA:HB1  | 1:G:314:LEU:HG  | 1.92                     | 0.52              |
| 1:B:247:LEU:O    | 1:B:273:VAL:HA  | 2.10                     | 0.52              |
| 1:B:39:VAL:HG13  | 1:B:48:THR:C    | 2.29                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:142:LYS:HD2  | 1:D:142:LYS:H    | 1.75                     | 0.52              |
| 1:F:247:LEU:O    | 1:F:273:VAL:HA   | 2.10                     | 0.52              |
| 1:G:205:ILE:HD12 | 1:G:211:GLY:O    | 2.09                     | 0.52              |
| 1:A:142:LYS:HD2  | 1:A:142:LYS:H    | 1.75                     | 0.52              |
| 2:A:1525:ATP:O3B | 3:A:1526:PO4:P   | 2.68                     | 0.52              |
| 2:C:1526:ATP:O3B | 3:C:1527:PO4:P   | 2.68                     | 0.52              |
| 1:C:411:VAL:HB   | 1:C:494:LEU:HB3  | 1.92                     | 0.52              |
| 1:D:144:ILE:HG23 | 1:D:403:THR:CG2  | 2.40                     | 0.52              |
| 1:E:13:ARG:HG2   | 1:E:13:ARG:HH11  | 1.75                     | 0.52              |
| 1:E:247:LEU:O    | 1:E:273:VAL:HA   | 2.10                     | 0.52              |
| 1:A:113:PRO:HA   | 1:B:36:ARG:HH11  | 1.73                     | 0.52              |
| 3:E:1526:PO4:P   | 2:E:1527:ATP:O3B | 2.68                     | 0.52              |
| 1:E:112:ASN:CB   | 1:F:36:ARG:HE    | 2.22                     | 0.52              |
| 1:D:13:ARG:HH11  | 1:D:13:ARG:HG2   | 1.75                     | 0.51              |
| 1:D:113:PRO:HA   | 1:E:36:ARG:HH11  | 1.73                     | 0.51              |
| 1:F:239:ALA:HB1  | 1:F:314:LEU:HG   | 1.91                     | 0.51              |
| 1:G:144:ILE:HG23 | 1:G:403:THR:CG2  | 2.40                     | 0.51              |
| 1:A:13:ARG:HH11  | 1:A:13:ARG:HG2   | 1.75                     | 0.51              |
| 1:A:411:VAL:HB   | 1:A:494:LEU:HB3  | 1.91                     | 0.51              |
| 1:B:113:PRO:HA   | 1:C:36:ARG:HH11  | 1.73                     | 0.51              |
| 1:D:106:ALA:HB3  | 1:D:116:LEU:HD21 | 1.92                     | 0.51              |
| 1:D:239:ALA:HB1  | 1:D:314:LEU:HG   | 1.91                     | 0.51              |
| 1:F:251:ALA:HB3  | 1:F:254:VAL:HG23 | 1.93                     | 0.51              |
| 1:F:113:PRO:CA   | 1:G:36:ARG:NH1   | 2.66                     | 0.51              |
| 1:A:149:THR:HA   | 1:A:152:ALA:HB3  | 1.92                     | 0.51              |
| 1:B:251:ALA:HB3  | 1:B:254:VAL:HG23 | 1.92                     | 0.51              |
| 1:D:251:ALA:HB3  | 1:D:254:VAL:HG23 | 1.92                     | 0.51              |
| 1:E:106:ALA:HB3  | 1:E:116:LEU:HD21 | 1.93                     | 0.51              |
| 1:F:13:ARG:HG2   | 1:F:13:ARG:HH11  | 1.75                     | 0.51              |
| 3:F:1525:PO4:P   | 2:F:1527:ATP:O3B | 2.68                     | 0.51              |
| 1:C:13:ARG:HH11  | 1:C:13:ARG:HG2   | 1.75                     | 0.51              |
| 1:B:112:ASN:CB   | 1:C:36:ARG:HE    | 2.22                     | 0.51              |
| 1:C:112:ASN:CB   | 1:D:36:ARG:HE    | 2.22                     | 0.51              |
| 2:B:1525:ATP:O3B | 3:B:1526:PO4:P   | 2.68                     | 0.51              |
| 1:C:113:PRO:HA   | 1:D:36:ARG:HH11  | 1.74                     | 0.51              |
| 1:E:251:ALA:HB3  | 1:E:254:VAL:HG23 | 1.93                     | 0.51              |
| 1:D:112:ASN:CB   | 1:E:36:ARG:HE    | 2.22                     | 0.51              |
| 1:E:144:ILE:HG23 | 1:E:403:THR:CG2  | 2.40                     | 0.51              |
| 1:F:106:ALA:HB3  | 1:F:116:LEU:HD21 | 1.93                     | 0.51              |
| 1:A:106:ALA:HB3  | 1:A:116:LEU:HD21 | 1.93                     | 0.51              |
| 1:A:36:ARG:HH12  | 1:G:115:ASP:C    | 2.07                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:149:THR:HA   | 1:B:152:ALA:HB3  | 1.93                     | 0.51              |
| 1:E:239:ALA:HB1  | 1:E:314:LEU:HG   | 1.91                     | 0.51              |
| 1:G:106:ALA:HB3  | 1:G:116:LEU:HD21 | 1.93                     | 0.51              |
| 3:G:1525:PO4:P   | 2:G:1527:ATP:O3B | 2.68                     | 0.51              |
| 1:G:251:ALA:HB3  | 1:G:254:VAL:HG23 | 1.92                     | 0.51              |
| 1:M:25:ASP:CG    | 1:M:28:LYS:HZ3   | 2.13                     | 0.51              |
| 1:E:213:VAL:HG13 | 1:E:325:ILE:HB   | 1.93                     | 0.51              |
| 1:E:411:VAL:HB   | 1:E:494:LEU:HB3  | 1.92                     | 0.51              |
| 1:F:144:ILE:HG23 | 1:F:403:THR:CG2  | 2.40                     | 0.51              |
| 1:B:106:ALA:HB3  | 1:B:116:LEU:HD21 | 1.93                     | 0.51              |
| 2:D:1525:ATP:O3B | 3:D:1526:PO4:P   | 2.68                     | 0.51              |
| 1:D:411:VAL:HB   | 1:D:494:LEU:HB3  | 1.92                     | 0.51              |
| 1:E:39:VAL:CG2   | 1:E:49:ILE:HD13  | 2.41                     | 0.51              |
| 1:F:142:LYS:H    | 1:F:142:LYS:HD2  | 1.75                     | 0.51              |
| 1:A:39:VAL:CG2   | 1:A:49:ILE:HD13  | 2.41                     | 0.50              |
| 1:C:213:VAL:HG13 | 1:C:325:ILE:HB   | 1.94                     | 0.50              |
| 1:D:39:VAL:CG2   | 1:D:49:ILE:HD13  | 2.41                     | 0.50              |
| 1:F:39:VAL:CG2   | 1:F:49:ILE:HD13  | 2.41                     | 0.50              |
| 1:G:39:VAL:CG2   | 1:G:49:ILE:HD13  | 2.42                     | 0.50              |
| 1:B:213:VAL:HG13 | 1:B:325:ILE:HB   | 1.93                     | 0.50              |
| 1:E:34:LYS:HE2   | 1:E:458:CYS:HA   | 1.93                     | 0.50              |
| 1:F:213:VAL:HG13 | 1:F:325:ILE:HB   | 1.93                     | 0.50              |
| 1:F:34:LYS:HE2   | 1:F:458:CYS:HA   | 1.94                     | 0.50              |
| 1:G:149:THR:HA   | 1:G:152:ALA:HB3  | 1.93                     | 0.50              |
| 1:B:39:VAL:CG2   | 1:B:49:ILE:HD13  | 2.41                     | 0.50              |
| 1:C:106:ALA:HB3  | 1:C:116:LEU:HD21 | 1.92                     | 0.50              |
| 1:C:39:VAL:CG2   | 1:C:49:ILE:HD13  | 2.42                     | 0.50              |
| 1:D:213:VAL:HG13 | 1:D:325:ILE:HB   | 1.94                     | 0.50              |
| 1:G:34:LYS:HE2   | 1:G:458:CYS:HA   | 1.94                     | 0.50              |
| 1:C:149:THR:HA   | 1:C:152:ALA:HB3  | 1.93                     | 0.50              |
| 1:E:149:THR:HA   | 1:E:152:ALA:HB3  | 1.93                     | 0.50              |
| 1:D:113:PRO:CA   | 1:E:36:ARG:NH1   | 2.66                     | 0.50              |
| 1:N:400:LEU:C    | 1:N:401:HIS:CA   | 2.77                     | 0.50              |
| 1:A:213:VAL:HG13 | 1:A:325:ILE:HB   | 1.94                     | 0.49              |
| 1:E:113:PRO:CA   | 1:F:36:ARG:NH1   | 2.66                     | 0.49              |
| 1:G:213:VAL:HG13 | 1:G:325:ILE:HB   | 1.93                     | 0.49              |
| 1:A:34:LYS:HE2   | 1:A:458:CYS:HA   | 1.94                     | 0.49              |
| 1:F:149:THR:HA   | 1:F:152:ALA:HB3  | 1.93                     | 0.49              |
| 1:D:149:THR:HA   | 1:D:152:ALA:HB3  | 1.93                     | 0.49              |
| 1:D:34:LYS:HE2   | 1:D:458:CYS:HA   | 1.94                     | 0.49              |
| 1:G:13:ARG:HH11  | 1:G:13:ARG:HG2   | 1.75                     | 0.49              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:13:ARG:HH11 | 1:B:13:ARG:HG2   | 1.75                     | 0.49              |
| 1:C:251:ALA:HB3 | 1:C:254:VAL:HG23 | 1.93                     | 0.49              |
| 1:E:172:GLU:H   | 1:E:172:GLU:CD   | 2.16                     | 0.49              |
| 1:E:138:CYS:HA  | 1:E:411:VAL:HG22 | 1.94                     | 0.49              |
| 1:G:6:VAL:HG13  | 1:G:521:VAL:HG22 | 1.95                     | 0.49              |
| 1:F:138:CYS:HA  | 1:F:411:VAL:HG22 | 1.95                     | 0.49              |
| 1:F:6:VAL:HG13  | 1:F:521:VAL:HG22 | 1.95                     | 0.49              |
| 1:A:251:ALA:HB3 | 1:A:254:VAL:HG23 | 1.93                     | 0.49              |
| 1:A:36:ARG:NH1  | 1:G:113:PRO:CA   | 2.66                     | 0.49              |
| 1:F:114:MET:CA  | 1:G:36:ARG:CZ    | 2.91                     | 0.49              |
| 1:A:6:VAL:HG13  | 1:A:521:VAL:HG22 | 1.95                     | 0.49              |
| 1:B:114:MET:CA  | 1:C:36:ARG:CZ    | 2.91                     | 0.49              |
| 1:A:36:ARG:CZ   | 1:G:114:MET:CA   | 2.91                     | 0.49              |
| 1:F:39:VAL:HG21 | 1:F:49:ILE:HD13  | 1.95                     | 0.49              |
| 1:G:39:VAL:HG21 | 1:G:49:ILE:HD13  | 1.95                     | 0.49              |
| 1:C:106:ALA:CB  | 1:C:116:LEU:HD21 | 2.43                     | 0.48              |
| 1:E:517:THR:HA  | 1:F:39:VAL:CG2   | 2.43                     | 0.48              |
| 1:G:138:CYS:HA  | 1:G:411:VAL:HG22 | 1.94                     | 0.48              |
| 1:A:39:VAL:HG21 | 1:A:49:ILE:HD13  | 1.95                     | 0.48              |
| 1:A:114:MET:CA  | 1:B:36:ARG:CZ    | 2.91                     | 0.48              |
| 1:B:39:VAL:HG21 | 1:B:49:ILE:HD13  | 1.95                     | 0.48              |
| 1:B:6:VAL:HG13  | 1:B:521:VAL:HG22 | 1.95                     | 0.48              |
| 1:C:34:LYS:HE2  | 1:C:458:CYS:HA   | 1.94                     | 0.48              |
| 1:D:517:THR:HA  | 1:E:39:VAL:CG2   | 2.43                     | 0.48              |
| 1:B:34:LYS:HE2  | 1:B:458:CYS:HA   | 1.94                     | 0.48              |
| 1:E:39:VAL:HG21 | 1:E:49:ILE:HD13  | 1.95                     | 0.48              |
| 1:E:6:VAL:HG13  | 1:E:521:VAL:HG22 | 1.95                     | 0.48              |
| 1:B:106:ALA:CB  | 1:B:116:LEU:HD21 | 2.43                     | 0.48              |
| 1:B:27:VAL:CG1  | 1:B:90:THR:HG23  | 2.35                     | 0.48              |
| 1:B:517:THR:HA  | 1:C:39:VAL:CG2   | 2.43                     | 0.48              |
| 1:C:39:VAL:HG21 | 1:C:49:ILE:HD13  | 1.95                     | 0.48              |
| 1:D:106:ALA:CB  | 1:D:116:LEU:HD21 | 2.43                     | 0.48              |
| 1:B:30:THR:CG2  | 1:B:38:VAL:HG21  | 2.42                     | 0.48              |
| 1:B:138:CYS:HA  | 1:B:411:VAL:HG22 | 1.95                     | 0.48              |
| 1:D:172:GLU:CD  | 1:D:172:GLU:H    | 2.16                     | 0.48              |
| 1:C:517:THR:HA  | 1:D:39:VAL:CG2   | 2.43                     | 0.48              |
| 1:D:39:VAL:HG21 | 1:D:49:ILE:HD13  | 1.95                     | 0.48              |
| 1:A:39:VAL:CG2  | 1:G:517:THR:HA   | 2.43                     | 0.48              |
| 1:C:138:CYS:HA  | 1:C:411:VAL:HG22 | 1.94                     | 0.48              |
| 1:F:106:ALA:CB  | 1:F:116:LEU:HD21 | 2.43                     | 0.48              |
| 1:F:116:LEU:H   | 1:G:36:ARG:HH12  | 0.62                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:106:ALA:CB   | 1:G:116:LEU:HD21 | 2.43                     | 0.48              |
| 1:C:112:ASN:CG   | 1:D:36:ARG:HE    | 2.18                     | 0.48              |
| 1:D:114:MET:CA   | 1:E:36:ARG:CZ    | 2.91                     | 0.48              |
| 1:F:517:THR:HA   | 1:G:39:VAL:CG2   | 2.43                     | 0.48              |
| 1:B:39:VAL:HG21  | 1:B:49:ILE:CG1   | 2.44                     | 0.48              |
| 1:C:6:VAL:HG13   | 1:C:521:VAL:HG22 | 1.95                     | 0.48              |
| 1:D:112:ASN:CG   | 1:E:36:ARG:HE    | 2.18                     | 0.48              |
| 1:B:172:GLU:CD   | 1:B:172:GLU:H    | 2.16                     | 0.47              |
| 1:B:112:ASN:CG   | 1:C:36:ARG:HE    | 2.18                     | 0.47              |
| 1:D:115:ASP:CA   | 1:E:36:ARG:NH1   | 2.77                     | 0.47              |
| 1:A:138:CYS:HA   | 1:A:411:VAL:HG22 | 1.94                     | 0.47              |
| 1:A:172:GLU:H    | 1:A:172:GLU:CD   | 2.16                     | 0.47              |
| 1:C:114:MET:CA   | 1:D:36:ARG:CZ    | 2.91                     | 0.47              |
| 1:C:39:VAL:HG21  | 1:C:49:ILE:CG1   | 2.44                     | 0.47              |
| 1:E:112:ASN:CG   | 1:F:36:ARG:HE    | 2.17                     | 0.47              |
| 1:F:115:ASP:CA   | 1:G:36:ARG:NH1   | 2.77                     | 0.47              |
| 1:A:112:ASN:CG   | 1:B:36:ARG:HE    | 2.18                     | 0.47              |
| 1:L:326:ASN:HD22 | 1:L:327:LYS:HD2  | 1.80                     | 0.47              |
| 1:A:240:VAL:HG21 | 1:A:247:LEU:HD13 | 1.97                     | 0.47              |
| 1:D:144:ILE:HG23 | 1:D:403:THR:HG21 | 1.97                     | 0.47              |
| 1:D:6:VAL:HG13   | 1:D:521:VAL:HG22 | 1.95                     | 0.47              |
| 1:E:106:ALA:CB   | 1:E:116:LEU:HD21 | 2.43                     | 0.47              |
| 1:E:114:MET:CA   | 1:F:36:ARG:CZ    | 2.91                     | 0.47              |
| 1:A:113:PRO:CA   | 1:B:36:ARG:NH1   | 2.66                     | 0.47              |
| 1:D:138:CYS:HA   | 1:D:411:VAL:HG22 | 1.95                     | 0.47              |
| 1:E:144:ILE:HG23 | 1:E:403:THR:HG21 | 1.97                     | 0.47              |
| 1:H:326:ASN:HD22 | 1:H:327:LYS:HD2  | 1.80                     | 0.47              |
| 1:A:106:ALA:CB   | 1:A:116:LEU:HD21 | 2.43                     | 0.47              |
| 1:A:36:ARG:HE    | 1:G:112:ASN:CG   | 2.17                     | 0.47              |
| 1:J:326:ASN:HD22 | 1:J:327:LYS:HD2  | 1.80                     | 0.47              |
| 1:A:196:ASP:HA   | 1:A:329:THR:HA   | 1.97                     | 0.47              |
| 1:B:240:VAL:HG21 | 1:B:247:LEU:HD13 | 1.97                     | 0.47              |
| 1:B:114:MET:C    | 1:C:36:ARG:NH1   | 2.67                     | 0.47              |
| 1:C:27:VAL:CG1   | 1:C:90:THR:HG23  | 2.35                     | 0.47              |
| 1:D:115:ASP:C    | 1:E:36:ARG:HH12  | 2.06                     | 0.47              |
| 1:F:112:ASN:CG   | 1:G:36:ARG:HE    | 2.18                     | 0.47              |
| 1:G:196:ASP:HA   | 1:G:329:THR:HA   | 1.97                     | 0.47              |
| 1:F:115:ASP:C    | 1:G:36:ARG:HH12  | 2.07                     | 0.47              |
| 1:J:320:ALA:HA   | 1:J:334:ASP:O    | 2.15                     | 0.47              |
| 1:M:320:ALA:HA   | 1:M:334:ASP:O    | 2.15                     | 0.47              |
| 1:N:326:ASN:HD22 | 1:N:327:LYS:HD2  | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:196:ASP:HA   | 1:C:329:THR:HA   | 1.97                     | 0.47              |
| 1:G:172:GLU:H    | 1:G:172:GLU:CD   | 2.16                     | 0.47              |
| 1:I:326:ASN:HD22 | 1:I:327:LYS:HD2  | 1.80                     | 0.47              |
| 1:K:320:ALA:HA   | 1:K:334:ASP:O    | 2.15                     | 0.47              |
| 1:C:144:ILE:HG23 | 1:C:403:THR:HG21 | 1.97                     | 0.47              |
| 1:E:427:ALA:HA   | 1:E:444:LEU:CD1  | 2.45                     | 0.47              |
| 1:M:326:ASN:HD22 | 1:M:327:LYS:HD2  | 1.80                     | 0.47              |
| 1:A:30:THR:CG2   | 1:A:38:VAL:HG21  | 2.42                     | 0.47              |
| 1:B:196:ASP:HA   | 1:B:329:THR:HA   | 1.97                     | 0.47              |
| 1:F:144:ILE:HG23 | 1:F:403:THR:HG21 | 1.97                     | 0.47              |
| 1:I:320:ALA:HA   | 1:I:334:ASP:O    | 2.15                     | 0.47              |
| 1:L:320:ALA:HA   | 1:L:334:ASP:O    | 2.15                     | 0.47              |
| 1:N:320:ALA:HA   | 1:N:334:ASP:O    | 2.15                     | 0.47              |
| 1:A:124:VAL:HG21 | 1:A:508:ALA:CB   | 2.45                     | 0.47              |
| 1:F:172:GLU:H    | 1:F:172:GLU:CD   | 2.16                     | 0.47              |
| 1:F:196:ASP:HA   | 1:F:329:THR:HA   | 1.97                     | 0.47              |
| 1:G:240:VAL:HG21 | 1:G:247:LEU:HD13 | 1.97                     | 0.47              |
| 1:G:39:VAL:HG21  | 1:G:49:ILE:CG1   | 2.44                     | 0.47              |
| 1:H:320:ALA:HA   | 1:H:334:ASP:O    | 2.15                     | 0.47              |
| 1:D:356:ALA:HB1  | 1:D:361:ASP:HB2  | 1.97                     | 0.46              |
| 1:D:427:ALA:HA   | 1:D:444:LEU:CD1  | 2.45                     | 0.46              |
| 1:E:356:ALA:HB1  | 1:E:361:ASP:HB2  | 1.97                     | 0.46              |
| 1:E:39:VAL:HG21  | 1:E:49:ILE:CG1   | 2.44                     | 0.46              |
| 1:G:144:ILE:HG23 | 1:G:403:THR:HG21 | 1.97                     | 0.46              |
| 1:N:479:ASN:O    | 1:N:483:GLU:N    | 2.49                     | 0.46              |
| 1:B:124:VAL:HG21 | 1:B:508:ALA:CB   | 2.46                     | 0.46              |
| 1:C:124:VAL:HG21 | 1:C:508:ALA:CB   | 2.46                     | 0.46              |
| 1:G:356:ALA:HB1  | 1:G:361:ASP:HB2  | 1.97                     | 0.46              |
| 1:K:183:LEU:HA   | 1:K:383:ALA:O    | 2.15                     | 0.46              |
| 1:L:183:LEU:HA   | 1:L:383:ALA:O    | 2.15                     | 0.46              |
| 1:A:144:ILE:HG23 | 1:A:403:THR:HG21 | 1.97                     | 0.46              |
| 1:A:152:ALA:HB1  | 1:A:155:ASP:CB   | 2.45                     | 0.46              |
| 1:A:356:ALA:HB1  | 1:A:361:ASP:HB2  | 1.97                     | 0.46              |
| 1:F:356:ALA:HB1  | 1:F:361:ASP:HB2  | 1.97                     | 0.46              |
| 1:G:124:VAL:HG21 | 1:G:508:ALA:CB   | 2.46                     | 0.46              |
| 1:H:183:LEU:HA   | 1:H:383:ALA:O    | 2.15                     | 0.46              |
| 1:A:120:ILE:O    | 1:A:124:VAL:HG23 | 2.16                     | 0.46              |
| 1:A:39:VAL:HG21  | 1:A:49:ILE:CG1   | 2.44                     | 0.46              |
| 1:B:120:ILE:O    | 1:B:124:VAL:HG23 | 2.16                     | 0.46              |
| 1:B:427:ALA:HA   | 1:B:444:LEU:CD1  | 2.45                     | 0.46              |
| 1:D:39:VAL:HG21  | 1:D:49:ILE:CG1   | 2.44                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:120:ILE:O    | 1:E:124:VAL:HG23 | 2.16                     | 0.46              |
| 1:G:152:ALA:HB1  | 1:G:155:ASP:CB   | 2.46                     | 0.46              |
| 1:F:114:MET:C    | 1:G:36:ARG:NH1   | 2.67                     | 0.46              |
| 1:J:183:LEU:HA   | 1:J:383:ALA:O    | 2.15                     | 0.46              |
| 1:M:183:LEU:HA   | 1:M:383:ALA:O    | 2.16                     | 0.46              |
| 1:B:356:ALA:HB1  | 1:B:361:ASP:HB2  | 1.98                     | 0.46              |
| 1:C:356:ALA:HB1  | 1:C:361:ASP:HB2  | 1.97                     | 0.46              |
| 1:D:124:VAL:HG21 | 1:D:508:ALA:CB   | 2.45                     | 0.46              |
| 1:D:196:ASP:HA   | 1:D:329:THR:HA   | 1.97                     | 0.46              |
| 1:D:517:THR:HA   | 1:E:39:VAL:CB    | 2.46                     | 0.46              |
| 1:G:120:ILE:O    | 1:G:124:VAL:HG23 | 2.16                     | 0.46              |
| 1:K:326:ASN:HD22 | 1:K:327:LYS:HD2  | 1.80                     | 0.46              |
| 1:B:113:PRO:CA   | 1:C:36:ARG:NH1   | 2.66                     | 0.46              |
| 1:C:172:GLU:H    | 1:C:172:GLU:CD   | 2.16                     | 0.46              |
| 1:D:139:SER:HB3  | 1:D:143:ALA:HB2  | 1.98                     | 0.46              |
| 1:D:383:ALA:HB3  | 1:D:389:MET:HB2  | 1.98                     | 0.46              |
| 1:F:120:ILE:O    | 1:F:124:VAL:HG23 | 2.16                     | 0.46              |
| 1:B:152:ALA:HB1  | 1:B:155:ASP:CB   | 2.45                     | 0.46              |
| 1:C:240:VAL:HG21 | 1:C:247:LEU:HD13 | 1.97                     | 0.46              |
| 1:C:383:ALA:HB3  | 1:C:389:MET:HB2  | 1.98                     | 0.46              |
| 1:E:517:THR:HA   | 1:F:39:VAL:CB    | 2.46                     | 0.46              |
| 1:F:39:VAL:HG21  | 1:F:49:ILE:CG1   | 2.44                     | 0.46              |
| 1:J:246:PRO:HB3  | 1:J:272:LYS:HB2  | 1.98                     | 0.46              |
| 1:K:414:GLY:N    | 1:K:494:LEU:HA   | 2.31                     | 0.46              |
| 1:M:479:ASN:O    | 1:M:483:GLU:N    | 2.48                     | 0.46              |
| 1:N:183:LEU:HA   | 1:N:383:ALA:O    | 2.16                     | 0.46              |
| 1:B:144:ILE:HG23 | 1:B:403:THR:HG21 | 1.97                     | 0.46              |
| 1:C:427:ALA:HA   | 1:C:444:LEU:CD1  | 2.45                     | 0.46              |
| 1:E:124:VAL:HG21 | 1:E:508:ALA:CB   | 2.45                     | 0.46              |
| 1:E:139:SER:HB3  | 1:E:143:ALA:HB2  | 1.98                     | 0.46              |
| 1:H:246:PRO:HB3  | 1:H:272:LYS:HB2  | 1.98                     | 0.46              |
| 1:I:246:PRO:HB3  | 1:I:272:LYS:HB2  | 1.98                     | 0.46              |
| 1:B:383:ALA:HB3  | 1:B:389:MET:HB2  | 1.98                     | 0.46              |
| 1:A:517:THR:HA   | 1:B:39:VAL:CB    | 2.46                     | 0.46              |
| 1:C:111:MET:O    | 1:C:113:PRO:HD3  | 2.16                     | 0.46              |
| 1:D:27:VAL:CG1   | 1:D:90:THR:HG23  | 2.35                     | 0.46              |
| 1:E:196:ASP:HA   | 1:E:329:THR:HA   | 1.97                     | 0.46              |
| 1:F:152:ALA:HB1  | 1:F:155:ASP:CB   | 2.45                     | 0.46              |
| 1:F:240:VAL:HG21 | 1:F:247:LEU:HD13 | 1.97                     | 0.46              |
| 1:F:517:THR:HA   | 1:G:39:VAL:CB    | 2.46                     | 0.46              |
| 1:G:427:ALA:HA   | 1:G:444:LEU:CD1  | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:246:PRO:HB3  | 1:K:272:LYS:HB2  | 1.98                     | 0.46              |
| 1:A:36:ARG:NH1   | 1:G:114:MET:C    | 2.67                     | 0.46              |
| 1:A:36:ARG:NH1   | 1:G:115:ASP:CA   | 2.77                     | 0.46              |
| 1:A:115:ASP:CA   | 1:B:36:ARG:NH1   | 2.77                     | 0.46              |
| 1:A:517:THR:HA   | 1:B:39:VAL:CG2   | 2.43                     | 0.46              |
| 1:C:114:MET:C    | 1:D:36:ARG:NH1   | 2.67                     | 0.46              |
| 1:C:115:ASP:CA   | 1:D:36:ARG:NH1   | 2.77                     | 0.46              |
| 1:C:517:THR:HA   | 1:D:39:VAL:CB    | 2.46                     | 0.46              |
| 1:F:124:VAL:HG21 | 1:F:508:ALA:CB   | 2.46                     | 0.46              |
| 1:G:287:ALA:HB1  | 1:G:368:ARG:CZ   | 2.46                     | 0.46              |
| 1:A:39:VAL:CB    | 1:G:517:THR:HA   | 2.46                     | 0.46              |
| 1:M:246:PRO:HB3  | 1:M:272:LYS:HB2  | 1.98                     | 0.46              |
| 1:N:246:PRO:HB3  | 1:N:272:LYS:HB2  | 1.98                     | 0.46              |
| 1:C:139:SER:HB3  | 1:C:143:ALA:HB2  | 1.98                     | 0.45              |
| 1:C:427:ALA:HA   | 1:C:444:LEU:HD11 | 1.98                     | 0.45              |
| 1:D:120:ILE:O    | 1:D:124:VAL:HG23 | 2.16                     | 0.45              |
| 1:F:111:MET:O    | 1:F:113:PRO:HD3  | 2.17                     | 0.45              |
| 1:F:13:ARG:HH21  | 1:F:518:GLU:CD   | 2.20                     | 0.45              |
| 1:L:246:PRO:HB3  | 1:L:272:LYS:HB2  | 1.98                     | 0.45              |
| 1:A:427:ALA:HA   | 1:A:444:LEU:CD1  | 2.45                     | 0.45              |
| 1:B:427:ALA:HA   | 1:B:444:LEU:HD11 | 1.99                     | 0.45              |
| 1:C:31:LEU:HA    | 3:C:1527:PO4:P   | 2.56                     | 0.45              |
| 1:C:287:ALA:HB1  | 1:C:368:ARG:CZ   | 2.46                     | 0.45              |
| 1:D:114:MET:C    | 1:E:36:ARG:NH1   | 2.67                     | 0.45              |
| 1:F:287:ALA:HB1  | 1:F:368:ARG:CZ   | 2.47                     | 0.45              |
| 1:F:427:ALA:HA   | 1:F:444:LEU:CD1  | 2.45                     | 0.45              |
| 1:G:111:MET:O    | 1:G:113:PRO:HD3  | 2.16                     | 0.45              |
| 1:G:30:THR:CG2   | 1:G:38:VAL:HG21  | 2.42                     | 0.45              |
| 1:I:414:GLY:N    | 1:I:494:LEU:HA   | 2.32                     | 0.45              |
| 1:N:414:GLY:N    | 1:N:494:LEU:HA   | 2.31                     | 0.45              |
| 1:A:287:ALA:HB1  | 1:A:368:ARG:CZ   | 2.46                     | 0.45              |
| 1:B:139:SER:HB3  | 1:B:143:ALA:HB2  | 1.98                     | 0.45              |
| 1:B:287:ALA:HB1  | 1:B:368:ARG:CZ   | 2.47                     | 0.45              |
| 1:F:427:ALA:HA   | 1:F:444:LEU:HD11 | 1.99                     | 0.45              |
| 1:H:414:GLY:N    | 1:H:494:LEU:HA   | 2.31                     | 0.45              |
| 1:M:414:GLY:N    | 1:M:494:LEU:HA   | 2.31                     | 0.45              |
| 1:A:13:ARG:HH21  | 1:A:518:GLU:CD   | 2.20                     | 0.45              |
| 1:A:31:LEU:HA    | 3:A:1526:PO4:P   | 2.57                     | 0.45              |
| 1:C:120:ILE:O    | 1:C:124:VAL:HG23 | 2.16                     | 0.45              |
| 1:D:111:MET:O    | 1:D:113:PRO:HD3  | 2.16                     | 0.45              |
| 1:D:13:ARG:HH21  | 1:D:518:GLU:CD   | 2.20                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:287:ALA:HB1  | 1:D:368:ARG:CZ   | 2.47                     | 0.45              |
| 1:D:427:ALA:HA   | 1:D:444:LEU:HD11 | 1.99                     | 0.45              |
| 1:E:287:ALA:HB1  | 1:E:368:ARG:CZ   | 2.46                     | 0.45              |
| 1:E:427:ALA:HA   | 1:E:444:LEU:HD11 | 1.99                     | 0.45              |
| 1:G:31:LEU:HA    | 3:G:1525:PO4:P   | 2.57                     | 0.45              |
| 1:J:149:THR:CG2  | 1:J:156:GLU:HA   | 2.47                     | 0.45              |
| 1:J:479:ASN:O    | 1:J:483:GLU:N    | 2.48                     | 0.45              |
| 1:L:149:THR:CG2  | 1:L:156:GLU:HA   | 2.47                     | 0.45              |
| 1:A:112:ASN:HA   | 1:A:113:PRO:HD2  | 1.74                     | 0.45              |
| 1:A:111:MET:O    | 1:A:113:PRO:HD3  | 2.16                     | 0.45              |
| 1:A:127:ALA:CB   | 1:A:426:LEU:HD11 | 2.47                     | 0.45              |
| 1:A:427:ALA:HA   | 1:A:444:LEU:HD11 | 1.99                     | 0.45              |
| 1:C:349:ILE:HG22 | 1:C:369:VAL:HG13 | 1.98                     | 0.45              |
| 1:B:115:ASP:CA   | 1:C:36:ARG:NH1   | 2.77                     | 0.45              |
| 1:F:383:ALA:HB3  | 1:F:389:MET:HB2  | 1.98                     | 0.45              |
| 1:K:149:THR:CG2  | 1:K:156:GLU:HA   | 2.47                     | 0.45              |
| 1:M:217:SER:HA   | 1:M:320:ALA:O    | 2.17                     | 0.45              |
| 1:M:284:ARG:HG3  | 1:M:284:ARG:HH11 | 1.81                     | 0.45              |
| 1:A:383:ALA:HB3  | 1:A:389:MET:HB2  | 1.98                     | 0.45              |
| 1:F:139:SER:HB3  | 1:F:143:ALA:HB2  | 1.98                     | 0.45              |
| 1:E:115:ASP:CA   | 1:F:36:ARG:NH1   | 2.77                     | 0.45              |
| 1:G:127:ALA:CB   | 1:G:426:LEU:HD11 | 2.46                     | 0.45              |
| 1:G:383:ALA:HB3  | 1:G:389:MET:HB2  | 1.98                     | 0.45              |
| 1:G:427:ALA:HA   | 1:G:444:LEU:HD11 | 1.99                     | 0.45              |
| 1:I:284:ARG:HH11 | 1:I:284:ARG:HG3  | 1.81                     | 0.45              |
| 1:I:479:ASN:O    | 1:I:483:GLU:N    | 2.48                     | 0.45              |
| 1:B:31:LEU:HA    | 3:B:1526:PO4:P   | 2.56                     | 0.45              |
| 1:C:13:ARG:HH21  | 1:C:518:GLU:CD   | 2.20                     | 0.45              |
| 1:D:31:LEU:HA    | 3:D:1526:PO4:P   | 2.56                     | 0.45              |
| 1:D:152:ALA:HB1  | 1:D:155:ASP:CB   | 2.46                     | 0.45              |
| 1:I:149:THR:CG2  | 1:I:156:GLU:HA   | 2.46                     | 0.45              |
| 1:I:183:LEU:HA   | 1:I:383:ALA:O    | 2.15                     | 0.45              |
| 1:J:284:ARG:HH11 | 1:J:284:ARG:HG3  | 1.81                     | 0.45              |
| 1:K:479:ASN:O    | 1:K:483:GLU:N    | 2.49                     | 0.45              |
| 1:N:217:SER:HA   | 1:N:320:ALA:O    | 2.17                     | 0.45              |
| 1:N:284:ARG:HH11 | 1:N:284:ARG:HG3  | 1.81                     | 0.45              |
| 1:A:114:MET:C    | 1:B:36:ARG:NH1   | 2.67                     | 0.45              |
| 1:E:13:ARG:HH21  | 1:E:518:GLU:CD   | 2.20                     | 0.45              |
| 1:E:152:ALA:HB1  | 1:E:155:ASP:CB   | 2.45                     | 0.45              |
| 1:E:127:ALA:CB   | 1:E:426:LEU:HD11 | 2.47                     | 0.45              |
| 1:F:30:THR:CG2   | 1:F:38:VAL:HG21  | 2.42                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:406:ALA:HB2  | 1:F:496:PRO:HG3  | 1.99                     | 0.45              |
| 1:H:149:THR:CG2  | 1:H:156:GLU:HA   | 2.46                     | 0.45              |
| 1:I:217:SER:HA   | 1:I:320:ALA:O    | 2.17                     | 0.45              |
| 1:B:349:ILE:HG22 | 1:B:369:VAL:HG13 | 1.99                     | 0.45              |
| 1:C:152:ALA:HB1  | 1:C:155:ASP:CB   | 2.45                     | 0.45              |
| 1:D:240:VAL:HG21 | 1:D:247:LEU:HD13 | 1.97                     | 0.45              |
| 1:D:349:ILE:HG22 | 1:D:369:VAL:HG13 | 1.99                     | 0.45              |
| 1:J:217:SER:HA   | 1:J:320:ALA:O    | 2.17                     | 0.45              |
| 1:B:127:ALA:CB   | 1:B:426:LEU:HD11 | 2.46                     | 0.45              |
| 1:G:406:ALA:HB2  | 1:G:496:PRO:HG3  | 1.99                     | 0.45              |
| 1:K:284:ARG:HG3  | 1:K:284:ARG:HH11 | 1.81                     | 0.45              |
| 1:A:139:SER:HB3  | 1:A:143:ALA:HB2  | 1.98                     | 0.44              |
| 1:B:111:MET:O    | 1:B:113:PRO:HD3  | 2.17                     | 0.44              |
| 1:B:517:THR:HA   | 1:C:39:VAL:CB    | 2.46                     | 0.44              |
| 1:E:240:VAL:HG21 | 1:E:247:LEU:HD13 | 1.97                     | 0.44              |
| 1:A:349:ILE:HG22 | 1:A:369:VAL:HG13 | 1.99                     | 0.44              |
| 1:F:256:GLY:O    | 1:F:260:ALA:HB3  | 2.18                     | 0.44              |
| 1:H:217:SER:HA   | 1:H:320:ALA:O    | 2.17                     | 0.44              |
| 1:J:414:GLY:N    | 1:J:494:LEU:HA   | 2.31                     | 0.44              |
| 1:L:414:GLY:N    | 1:L:494:LEU:HA   | 2.31                     | 0.44              |
| 1:M:149:THR:CG2  | 1:M:156:GLU:HA   | 2.46                     | 0.44              |
| 1:A:256:GLY:O    | 1:A:260:ALA:HB3  | 2.18                     | 0.44              |
| 1:E:349:ILE:HG22 | 1:E:369:VAL:HG13 | 1.98                     | 0.44              |
| 1:E:417:VAL:HG13 | 1:E:476:TYR:O    | 2.18                     | 0.44              |
| 1:J:191:GLU:O    | 1:J:334:ASP:HA   | 2.18                     | 0.44              |
| 1:N:149:THR:CG2  | 1:N:156:GLU:HA   | 2.47                     | 0.44              |
| 1:B:440:ILE:O    | 1:B:444:LEU:HG   | 2.18                     | 0.44              |
| 1:D:521:VAL:HG21 | 1:E:59:GLU:CB    | 2.46                     | 0.44              |
| 1:E:27:VAL:CG1   | 1:E:90:THR:HG23  | 2.35                     | 0.44              |
| 1:H:8:PHE:HA     | 1:H:518:GLU:O    | 2.18                     | 0.44              |
| 1:K:230:ILE:HG23 | 1:K:259:LEU:HD12 | 2.00                     | 0.44              |
| 1:L:8:PHE:HA     | 1:L:518:GLU:O    | 2.18                     | 0.44              |
| 1:M:417:VAL:HA   | 1:M:420:ILE:HG22 | 2.00                     | 0.44              |
| 1:N:417:VAL:HA   | 1:N:420:ILE:HG22 | 2.00                     | 0.44              |
| 1:B:115:ASP:CA   | 1:C:36:ARG:HH12  | 2.30                     | 0.44              |
| 1:C:440:ILE:O    | 1:C:444:LEU:HG   | 2.18                     | 0.44              |
| 1:D:256:GLY:O    | 1:D:260:ALA:HB3  | 2.18                     | 0.44              |
| 1:E:111:MET:O    | 1:E:113:PRO:HD3  | 2.17                     | 0.44              |
| 1:F:127:ALA:CB   | 1:F:426:LEU:HD11 | 2.46                     | 0.44              |
| 1:F:349:ILE:HG22 | 1:F:369:VAL:HG13 | 1.98                     | 0.44              |
| 1:F:417:VAL:HG13 | 1:F:476:TYR:O    | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:139:SER:HB3  | 1:G:143:ALA:HB2  | 1.98                     | 0.44              |
| 1:G:13:ARG:HH21  | 1:G:518:GLU:CD   | 2.20                     | 0.44              |
| 1:G:417:VAL:HG13 | 1:G:476:TYR:O    | 2.18                     | 0.44              |
| 1:F:521:VAL:N    | 1:G:41:ASP:HB3   | 2.32                     | 0.44              |
| 1:H:284:ARG:HG3  | 1:H:284:ARG:HH11 | 1.81                     | 0.44              |
| 1:H:479:ASN:O    | 1:H:483:GLU:N    | 2.48                     | 0.44              |
| 1:L:230:ILE:HG23 | 1:L:259:LEU:HD12 | 2.00                     | 0.44              |
| 1:L:284:ARG:HG3  | 1:L:284:ARG:HH11 | 1.81                     | 0.44              |
| 1:M:8:PHE:HA     | 1:M:518:GLU:O    | 2.18                     | 0.44              |
| 1:N:230:ILE:HG23 | 1:N:259:LEU:HD12 | 2.00                     | 0.44              |
| 1:N:8:PHE:HA     | 1:N:518:GLU:O    | 2.18                     | 0.44              |
| 1:A:440:ILE:O    | 1:A:444:LEU:HG   | 2.18                     | 0.44              |
| 1:B:412:VAL:HG22 | 1:B:495:ASP:O    | 2.18                     | 0.44              |
| 1:D:417:VAL:HG13 | 1:D:476:TYR:O    | 2.18                     | 0.44              |
| 1:E:406:ALA:HB2  | 1:E:496:PRO:HG3  | 1.99                     | 0.44              |
| 1:E:90:THR:HG22  | 1:E:94:VAL:HG23  | 2.00                     | 0.44              |
| 1:F:31:LEU:HA    | 3:F:1525:PO4:P   | 2.56                     | 0.44              |
| 1:G:349:ILE:HG22 | 1:G:369:VAL:HG13 | 1.99                     | 0.44              |
| 1:I:191:GLU:O    | 1:I:334:ASP:HA   | 2.18                     | 0.44              |
| 1:K:8:PHE:HA     | 1:K:518:GLU:O    | 2.18                     | 0.44              |
| 1:A:412:VAL:HG22 | 1:A:495:ASP:O    | 2.18                     | 0.44              |
| 1:A:90:THR:HG22  | 1:A:94:VAL:HG23  | 2.00                     | 0.44              |
| 1:A:115:ASP:CA   | 1:B:36:ARG:HH12  | 2.31                     | 0.44              |
| 1:B:13:ARG:HH21  | 1:B:518:GLU:CD   | 2.20                     | 0.44              |
| 1:B:90:THR:HG22  | 1:B:94:VAL:HG23  | 2.00                     | 0.44              |
| 1:D:279:PRO:HG3  | 1:D:292:ILE:HD11 | 2.00                     | 0.44              |
| 1:D:127:ALA:CB   | 1:D:426:LEU:HD11 | 2.47                     | 0.44              |
| 1:E:31:LEU:HA    | 3:E:1526:PO4:P   | 2.57                     | 0.44              |
| 1:E:30:THR:CG2   | 1:E:38:VAL:HG21  | 2.42                     | 0.44              |
| 1:F:440:ILE:O    | 1:F:444:LEU:HG   | 2.18                     | 0.44              |
| 1:I:386:GLU:HA   | 1:J:281:PHE:CG   | 2.53                     | 0.44              |
| 1:I:8:PHE:HA     | 1:I:518:GLU:O    | 2.18                     | 0.44              |
| 1:J:8:PHE:HA     | 1:J:518:GLU:O    | 2.18                     | 0.44              |
| 1:L:479:ASN:O    | 1:L:483:GLU:N    | 2.48                     | 0.44              |
| 1:A:36:ARG:HH12  | 1:G:115:ASP:CA   | 2.30                     | 0.44              |
| 1:C:279:PRO:HG3  | 1:C:292:ILE:HD11 | 2.00                     | 0.44              |
| 1:D:90:THR:HG22  | 1:D:94:VAL:HG23  | 2.00                     | 0.44              |
| 1:E:383:ALA:HB3  | 1:E:389:MET:HB2  | 1.98                     | 0.44              |
| 1:E:412:VAL:HG22 | 1:E:495:ASP:O    | 2.18                     | 0.44              |
| 1:H:230:ILE:HG23 | 1:H:259:LEU:HD12 | 2.00                     | 0.44              |
| 1:H:386:GLU:HA   | 1:I:281:PHE:CG   | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:230:ILE:HG23 | 1:J:259:LEU:HD12 | 2.00                     | 0.44              |
| 1:K:217:SER:HA   | 1:K:320:ALA:O    | 2.17                     | 0.44              |
| 1:L:217:SER:HA   | 1:L:320:ALA:O    | 2.17                     | 0.44              |
| 1:A:115:ASP:C    | 1:B:36:ARG:HH12  | 2.07                     | 0.44              |
| 1:B:417:VAL:HG13 | 1:B:476:TYR:O    | 2.18                     | 0.44              |
| 1:C:412:VAL:HG22 | 1:C:495:ASP:O    | 2.18                     | 0.44              |
| 1:C:521:VAL:HG21 | 1:D:59:GLU:CB    | 2.45                     | 0.44              |
| 1:E:440:ILE:O    | 1:E:444:LEU:HG   | 2.18                     | 0.44              |
| 1:F:412:VAL:HG22 | 1:F:495:ASP:O    | 2.18                     | 0.44              |
| 1:M:230:ILE:HG23 | 1:M:259:LEU:HD12 | 2.00                     | 0.44              |
| 1:C:417:VAL:HG13 | 1:C:476:TYR:O    | 2.18                     | 0.43              |
| 1:D:412:VAL:HG22 | 1:D:495:ASP:O    | 2.18                     | 0.43              |
| 1:G:412:VAL:HG22 | 1:G:495:ASP:O    | 2.18                     | 0.43              |
| 1:J:386:GLU:HA   | 1:K:281:PHE:CG   | 2.53                     | 0.43              |
| 1:L:386:GLU:HA   | 1:M:281:PHE:CG   | 2.53                     | 0.43              |
| 1:A:417:VAL:HG13 | 1:A:476:TYR:O    | 2.18                     | 0.43              |
| 1:C:115:ASP:CA   | 1:D:36:ARG:HH12  | 2.31                     | 0.43              |
| 1:E:256:GLY:O    | 1:E:260:ALA:HB3  | 2.18                     | 0.43              |
| 1:E:279:PRO:HG3  | 1:E:292:ILE:HD11 | 2.00                     | 0.43              |
| 1:F:90:THR:HG22  | 1:F:94:VAL:HG23  | 2.00                     | 0.43              |
| 1:K:191:GLU:O    | 1:K:334:ASP:HA   | 2.18                     | 0.43              |
| 1:L:215:LEU:O    | 1:L:218:PRO:HD3  | 2.18                     | 0.43              |
| 1:L:417:VAL:HA   | 1:L:420:ILE:HG22 | 2.00                     | 0.43              |
| 1:H:281:PHE:CG   | 1:N:386:GLU:HA   | 2.53                     | 0.43              |
| 1:C:256:GLY:O    | 1:C:260:ALA:HB3  | 2.18                     | 0.43              |
| 1:B:521:VAL:N    | 1:C:41:ASP:HB3   | 2.31                     | 0.43              |
| 1:E:293:ALA:HB2  | 1:E:300:VAL:CG2  | 2.49                     | 0.43              |
| 1:D:520:MET:CA   | 1:E:41:ASP:HB2   | 2.48                     | 0.43              |
| 1:H:117:LYS:HZ2  | 1:H:121:ASP:CG   | 2.21                     | 0.43              |
| 1:B:279:PRO:HG3  | 1:B:292:ILE:HD11 | 2.00                     | 0.43              |
| 1:B:520:MET:CA   | 1:C:41:ASP:HB2   | 2.48                     | 0.43              |
| 1:C:406:ALA:HB2  | 1:C:496:PRO:HG3  | 1.99                     | 0.43              |
| 1:C:90:THR:HG22  | 1:C:94:VAL:HG23  | 2.00                     | 0.43              |
| 1:F:293:ALA:HB2  | 1:F:300:VAL:CG2  | 2.49                     | 0.43              |
| 1:G:256:GLY:O    | 1:G:260:ALA:HB3  | 2.18                     | 0.43              |
| 1:F:115:ASP:CA   | 1:G:36:ARG:HH12  | 2.30                     | 0.43              |
| 1:I:230:ILE:HG23 | 1:I:259:LEU:HD12 | 2.00                     | 0.43              |
| 1:M:7:LYS:O      | 1:M:519:CYS:HA   | 2.18                     | 0.43              |
| 1:A:406:ALA:HB2  | 1:A:496:PRO:HG3  | 1.99                     | 0.43              |
| 1:C:520:MET:CA   | 1:D:41:ASP:HB2   | 2.48                     | 0.43              |
| 1:D:40:LEU:HD11  | 1:D:55:SER:CB    | 2.48                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:191:GLU:O   | 1:H:334:ASP:HA   | 2.18                     | 0.43              |
| 1:J:7:LYS:O     | 1:J:519:CYS:HA   | 2.18                     | 0.43              |
| 1:M:215:LEU:O   | 1:M:218:PRO:HD3  | 2.18                     | 0.43              |
| 1:A:10:ASN:HA   | 1:A:13:ARG:HD2   | 2.01                     | 0.43              |
| 1:A:41:ASP:HB3  | 1:G:521:VAL:N    | 2.32                     | 0.43              |
| 1:B:202:PRO:O   | 1:B:205:ILE:HB   | 2.19                     | 0.43              |
| 1:B:256:GLY:O   | 1:B:260:ALA:HB3  | 2.18                     | 0.43              |
| 1:B:406:ALA:HB2 | 1:B:496:PRO:HG3  | 1.99                     | 0.43              |
| 1:C:10:ASN:HA   | 1:C:13:ARG:HD2   | 2.01                     | 0.43              |
| 1:C:180:GLY:HA3 | 1:C:381:VAL:O    | 2.19                     | 0.43              |
| 1:B:513:LEU:CA  | 1:C:49:ILE:HD11  | 2.43                     | 0.43              |
| 1:F:10:ASN:HA   | 1:F:13:ARG:HD2   | 2.01                     | 0.43              |
| 1:F:279:PRO:HG3 | 1:F:292:ILE:HD11 | 2.00                     | 0.43              |
| 1:F:13:ARG:NH1  | 1:F:515:ILE:O    | 2.49                     | 0.43              |
| 1:G:293:ALA:HB2 | 1:G:300:VAL:CG2  | 2.49                     | 0.43              |
| 1:G:40:LEU:HD11 | 1:G:55:SER:CB    | 2.48                     | 0.43              |
| 1:G:440:ILE:O   | 1:G:444:LEU:HG   | 2.18                     | 0.43              |
| 1:H:417:VAL:HA  | 1:H:420:ILE:HG22 | 2.00                     | 0.43              |
| 1:K:215:LEU:O   | 1:K:218:PRO:HD3  | 2.18                     | 0.43              |
| 1:A:293:ALA:HB2 | 1:A:300:VAL:CG2  | 2.49                     | 0.43              |
| 1:B:10:ASN:HA   | 1:B:13:ARG:HD2   | 2.01                     | 0.43              |
| 1:C:182:GLY:O   | 1:C:382:GLY:HA2  | 2.19                     | 0.43              |
| 1:D:115:ASP:CA  | 1:E:36:ARG:HH12  | 2.30                     | 0.43              |
| 1:E:40:LEU:HD11 | 1:E:55:SER:CB    | 2.48                     | 0.43              |
| 1:F:180:GLY:HA3 | 1:F:381:VAL:O    | 2.19                     | 0.43              |
| 1:I:215:LEU:O   | 1:I:218:PRO:HD3  | 2.18                     | 0.43              |
| 1:I:417:VAL:HA  | 1:I:420:ILE:HG22 | 2.00                     | 0.43              |
| 1:J:117:LYS:HZ2 | 1:J:121:ASP:CG   | 2.22                     | 0.43              |
| 1:M:117:LYS:HZ2 | 1:M:121:ASP:CG   | 2.21                     | 0.43              |
| 1:M:191:GLU:O   | 1:M:334:ASP:HA   | 2.18                     | 0.43              |
| 1:M:386:GLU:HA  | 1:N:281:PHE:CG   | 2.53                     | 0.43              |
| 1:A:40:LEU:HD11 | 1:A:55:SER:CB    | 2.48                     | 0.43              |
| 1:D:293:ALA:HB2 | 1:D:300:VAL:CG2  | 2.49                     | 0.43              |
| 1:D:182:GLY:O   | 1:D:382:GLY:HA2  | 2.18                     | 0.43              |
| 1:E:10:ASN:HA   | 1:E:13:ARG:HD2   | 2.01                     | 0.43              |
| 1:E:114:MET:C   | 1:F:36:ARG:NH1   | 2.67                     | 0.43              |
| 1:F:40:LEU:HD11 | 1:F:55:SER:CB    | 2.48                     | 0.43              |
| 1:G:90:THR:HG22 | 1:G:94:VAL:HG23  | 2.00                     | 0.43              |
| 1:H:215:LEU:O   | 1:H:218:PRO:HD3  | 2.18                     | 0.43              |
| 1:H:7:LYS:O     | 1:H:519:CYS:HA   | 2.18                     | 0.43              |
| 1:M:219:PHE:O   | 1:M:247:LEU:HD12 | 2.19                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:N:215:LEU:O   | 1:N:218:PRO:HD3  | 2.18                     | 0.43              |
| 1:N:7:LYS:O     | 1:N:519:CYS:HA   | 2.18                     | 0.43              |
| 1:A:279:PRO:HG3 | 1:A:292:ILE:HD11 | 2.00                     | 0.43              |
| 1:B:180:GLY:HA3 | 1:B:381:VAL:O    | 2.19                     | 0.43              |
| 1:B:30:THR:HG22 | 1:B:38:VAL:CG2   | 2.45                     | 0.43              |
| 1:A:520:MET:CA  | 1:B:41:ASP:HB2   | 2.48                     | 0.43              |
| 1:C:202:PRO:O   | 1:C:205:ILE:HB   | 2.19                     | 0.43              |
| 1:D:30:THR:CG2  | 1:D:38:VAL:HG21  | 2.42                     | 0.43              |
| 1:C:521:VAL:N   | 1:D:41:ASP:HB3   | 2.32                     | 0.43              |
| 1:D:440:ILE:O   | 1:D:444:LEU:HG   | 2.18                     | 0.43              |
| 1:E:115:ASP:CA  | 1:F:36:ARG:HH12  | 2.31                     | 0.43              |
| 1:F:39:VAL:HG13 | 1:F:49:ILE:HA    | 2.01                     | 0.43              |
| 1:I:219:PHE:O   | 1:I:247:LEU:HD12 | 2.19                     | 0.43              |
| 1:L:219:PHE:O   | 1:L:247:LEU:HD12 | 2.19                     | 0.43              |
| 1:L:7:LYS:O     | 1:L:519:CYS:HA   | 2.18                     | 0.43              |
| 1:A:30:THR:HG22 | 1:A:38:VAL:CG2   | 2.45                     | 0.43              |
| 1:A:41:ASP:HB2  | 1:G:520:MET:CA   | 2.48                     | 0.43              |
| 1:A:513:LEU:CA  | 1:B:49:ILE:HD11  | 2.43                     | 0.43              |
| 1:C:40:LEU:HD11 | 1:C:55:SER:CB    | 2.48                     | 0.43              |
| 1:D:10:ASN:HA   | 1:D:13:ARG:HD2   | 2.01                     | 0.43              |
| 1:C:513:LEU:CA  | 1:D:49:ILE:HD11  | 2.43                     | 0.43              |
| 1:E:180:GLY:HA3 | 1:E:381:VAL:O    | 2.19                     | 0.43              |
| 1:E:39:VAL:HG13 | 1:E:49:ILE:HA    | 2.01                     | 0.43              |
| 1:F:182:GLY:O   | 1:F:382:GLY:HA2  | 2.19                     | 0.43              |
| 1:G:10:ASN:HA   | 1:G:13:ARG:HD2   | 2.01                     | 0.43              |
| 1:G:182:GLY:O   | 1:G:382:GLY:HA2  | 2.19                     | 0.43              |
| 1:G:13:ARG:NH1  | 1:G:515:ILE:O    | 2.49                     | 0.43              |
| 1:J:417:VAL:HA  | 1:J:420:ILE:HG22 | 2.00                     | 0.43              |
| 1:K:417:VAL:HA  | 1:K:420:ILE:HG22 | 2.00                     | 0.43              |
| 1:A:202:PRO:O   | 1:A:205:ILE:HB   | 2.19                     | 0.42              |
| 1:B:293:ALA:HB2 | 1:B:300:VAL:CG2  | 2.49                     | 0.42              |
| 1:B:182:GLY:O   | 1:B:382:GLY:HA2  | 2.19                     | 0.42              |
| 1:C:112:ASN:HA  | 1:C:113:PRO:HD2  | 1.74                     | 0.42              |
| 1:C:127:ALA:CB  | 1:C:426:LEU:HD11 | 2.47                     | 0.42              |
| 1:D:23:LEU:O    | 1:D:27:VAL:HG23  | 2.19                     | 0.42              |
| 1:D:406:ALA:HB2 | 1:D:496:PRO:HG3  | 1.99                     | 0.42              |
| 1:D:521:VAL:N   | 1:E:41:ASP:HB3   | 2.32                     | 0.42              |
| 1:F:112:ASN:HA  | 1:F:113:PRO:HD2  | 1.74                     | 0.42              |
| 1:G:279:PRO:HG3 | 1:G:292:ILE:HD11 | 2.00                     | 0.42              |
| 1:K:386:GLU:HA  | 1:L:281:PHE:CG   | 2.54                     | 0.42              |
| 1:L:191:GLU:O   | 1:L:334:ASP:HA   | 2.18                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:219:PHE:O    | 1:N:247:LEU:HD12 | 2.19                     | 0.42              |
| 1:A:73:MET:HA    | 1:B:46:ALA:HB1   | 2.01                     | 0.42              |
| 1:D:39:VAL:HG13  | 1:D:49:ILE:HA    | 2.01                     | 0.42              |
| 1:G:180:GLY:HA3  | 1:G:381:VAL:O    | 2.19                     | 0.42              |
| 1:H:219:PHE:O    | 1:H:247:LEU:HD12 | 2.19                     | 0.42              |
| 1:A:27:VAL:CG1   | 1:A:90:THR:HG23  | 2.35                     | 0.42              |
| 1:E:182:GLY:O    | 1:E:382:GLY:HA2  | 2.19                     | 0.42              |
| 1:F:73:MET:HA    | 1:G:46:ALA:HB1   | 2.01                     | 0.42              |
| 1:G:23:LEU:O     | 1:G:27:VAL:HG23  | 2.19                     | 0.42              |
| 1:J:219:PHE:O    | 1:J:247:LEU:HD12 | 2.19                     | 0.42              |
| 1:K:219:PHE:O    | 1:K:247:LEU:HD12 | 2.19                     | 0.42              |
| 1:N:271:VAL:HG12 | 1:N:272:LYS:H    | 1.85                     | 0.42              |
| 1:A:182:GLY:O    | 1:A:382:GLY:HA2  | 2.19                     | 0.42              |
| 1:A:517:THR:HA   | 1:B:39:VAL:HB    | 2.02                     | 0.42              |
| 1:A:19:GLY:HA2   | 1:A:62:LEU:CD1   | 2.50                     | 0.42              |
| 1:C:30:THR:HG22  | 1:C:38:VAL:CG2   | 2.45                     | 0.42              |
| 1:E:23:LEU:O     | 1:E:27:VAL:HG23  | 2.19                     | 0.42              |
| 1:E:521:VAL:N    | 1:F:41:ASP:HB3   | 2.32                     | 0.42              |
| 1:H:271:VAL:HG12 | 1:H:272:LYS:H    | 1.85                     | 0.42              |
| 1:I:117:LYS:HZ2  | 1:I:121:ASP:CG   | 2.22                     | 0.42              |
| 1:I:271:VAL:HG12 | 1:I:272:LYS:H    | 1.85                     | 0.42              |
| 1:J:215:LEU:O    | 1:J:218:PRO:HD3  | 2.18                     | 0.42              |
| 1:N:400:LEU:CA   | 1:N:401:HIS:N    | 2.76                     | 0.42              |
| 1:D:180:GLY:HA3  | 1:D:381:VAL:O    | 2.19                     | 0.42              |
| 1:F:294:THR:HG21 | 1:F:345:ARG:HG3  | 2.01                     | 0.42              |
| 1:E:520:MET:CA   | 1:F:41:ASP:HB2   | 2.48                     | 0.42              |
| 1:G:19:GLY:HA2   | 1:G:62:LEU:CD1   | 2.50                     | 0.42              |
| 1:A:46:ALA:HB1   | 1:G:73:MET:HA    | 2.01                     | 0.42              |
| 1:M:271:VAL:HG12 | 1:M:272:LYS:H    | 1.85                     | 0.42              |
| 1:A:23:LEU:O     | 1:A:27:VAL:HG23  | 2.19                     | 0.42              |
| 1:A:13:ARG:NH1   | 1:A:515:ILE:O    | 2.49                     | 0.42              |
| 1:C:39:VAL:HG13  | 1:C:49:ILE:HA    | 2.01                     | 0.42              |
| 1:E:112:ASN:HA   | 1:E:113:PRO:HD2  | 1.74                     | 0.42              |
| 1:G:39:VAL:HG13  | 1:G:49:ILE:HA    | 2.01                     | 0.42              |
| 1:A:39:VAL:HB    | 1:G:517:THR:HA   | 2.02                     | 0.42              |
| 1:I:7:LYS:O      | 1:I:519:CYS:HA   | 2.18                     | 0.42              |
| 1:J:271:VAL:HG12 | 1:J:272:LYS:H    | 1.85                     | 0.42              |
| 1:K:117:LYS:HZ2  | 1:K:121:ASP:CG   | 2.21                     | 0.42              |
| 1:N:117:LYS:HZ2  | 1:N:121:ASP:CG   | 2.23                     | 0.42              |
| 1:B:73:MET:HA    | 1:C:46:ALA:HB1   | 2.01                     | 0.42              |
| 1:C:23:LEU:O     | 1:C:27:VAL:HG23  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:513:LEU:CA   | 1:E:49:ILE:HD11  | 2.43                     | 0.42              |
| 1:E:19:GLY:HA2   | 1:E:62:LEU:CD1   | 2.49                     | 0.42              |
| 1:E:73:MET:HA    | 1:F:46:ALA:HB1   | 2.01                     | 0.42              |
| 1:F:27:VAL:CG1   | 1:F:90:THR:HG23  | 2.35                     | 0.42              |
| 1:G:294:THR:HG21 | 1:G:345:ARG:HG3  | 2.01                     | 0.42              |
| 1:B:23:LEU:O     | 1:B:27:VAL:HG23  | 2.19                     | 0.42              |
| 1:B:40:LEU:HD11  | 1:B:55:SER:CB    | 2.48                     | 0.42              |
| 1:C:30:THR:CG2   | 1:C:38:VAL:HG21  | 2.42                     | 0.42              |
| 1:D:30:THR:HG22  | 1:D:38:VAL:CG2   | 2.45                     | 0.42              |
| 1:D:46:ALA:HA    | 1:D:47:PRO:HD2   | 1.85                     | 0.42              |
| 1:E:294:THR:HG21 | 1:E:345:ARG:HG3  | 2.02                     | 0.42              |
| 1:F:19:GLY:HA2   | 1:F:62:LEU:CD1   | 2.50                     | 0.42              |
| 1:F:520:MET:CA   | 1:G:41:ASP:HB2   | 2.48                     | 0.42              |
| 1:L:271:VAL:HG12 | 1:L:272:LYS:H    | 1.85                     | 0.42              |
| 1:N:191:GLU:O    | 1:N:334:ASP:HA   | 2.18                     | 0.42              |
| 1:A:521:VAL:N    | 1:B:41:ASP:HB3   | 2.32                     | 0.42              |
| 1:C:19:GLY:HA2   | 1:C:62:LEU:CD1   | 2.50                     | 0.42              |
| 1:F:202:PRO:O    | 1:F:205:ILE:HB   | 2.19                     | 0.42              |
| 1:K:7:LYS:O      | 1:K:519:CYS:HA   | 2.18                     | 0.42              |
| 1:A:180:GLY:HA3  | 1:A:381:VAL:O    | 2.19                     | 0.42              |
| 1:A:383:ALA:HB3  | 1:A:389:MET:N    | 2.35                     | 0.42              |
| 1:B:39:VAL:HG13  | 1:B:49:ILE:HA    | 2.01                     | 0.42              |
| 1:E:30:THR:HG22  | 1:E:38:VAL:CG2   | 2.45                     | 0.42              |
| 1:F:30:THR:HG22  | 1:F:38:VAL:CG2   | 2.45                     | 0.42              |
| 1:F:517:THR:HA   | 1:G:39:VAL:HB    | 2.02                     | 0.42              |
| 1:G:30:THR:HG22  | 1:G:38:VAL:CG2   | 2.45                     | 0.42              |
| 1:L:117:LYS:HZ2  | 1:L:121:ASP:CG   | 2.22                     | 0.42              |
| 1:A:39:VAL:HG13  | 1:A:49:ILE:HA    | 2.01                     | 0.41              |
| 1:C:293:ALA:HB2  | 1:C:300:VAL:CG2  | 2.49                     | 0.41              |
| 1:C:34:LYS:HZ1   | 1:C:483:GLU:CD   | 2.23                     | 0.41              |
| 1:D:73:MET:HA    | 1:E:46:ALA:HB1   | 2.01                     | 0.41              |
| 1:E:202:PRO:O    | 1:E:205:ILE:HB   | 2.19                     | 0.41              |
| 1:K:254:VAL:CG1  | 1:K:259:LEU:HD23 | 2.50                     | 0.41              |
| 1:B:517:THR:HA   | 1:C:39:VAL:HB    | 2.02                     | 0.41              |
| 1:D:19:GLY:HA2   | 1:D:62:LEU:CD1   | 2.50                     | 0.41              |
| 1:D:294:THR:HG21 | 1:D:345:ARG:HG3  | 2.02                     | 0.41              |
| 1:E:102:GLU:HB2  | 1:E:442:VAL:HG13 | 2.02                     | 0.41              |
| 1:G:112:ASN:HA   | 1:G:113:PRO:HD2  | 1.74                     | 0.41              |
| 1:G:383:ALA:HB3  | 1:G:389:MET:N    | 2.35                     | 0.41              |
| 1:J:254:VAL:CG1  | 1:J:259:LEU:HD23 | 2.50                     | 0.41              |
| 1:A:49:ILE:HD11  | 1:G:513:LEU:CA   | 2.43                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:323:VAL:HG22 | 1:B:332:ILE:HA   | 2.03                     | 0.41              |
| 1:C:294:THR:HG21 | 1:C:345:ARG:HG3  | 2.01                     | 0.41              |
| 1:C:73:MET:HA    | 1:D:46:ALA:HB1   | 2.01                     | 0.41              |
| 1:F:126:ALA:HB3  | 1:F:426:LEU:HD22 | 2.03                     | 0.41              |
| 1:F:23:LEU:O     | 1:F:27:VAL:HG23  | 2.19                     | 0.41              |
| 1:N:254:VAL:CG1  | 1:N:259:LEU:HD23 | 2.50                     | 0.41              |
| 1:A:323:VAL:HG22 | 1:A:332:ILE:HA   | 2.03                     | 0.41              |
| 1:B:19:GLY:HA2   | 1:B:62:LEU:CD1   | 2.50                     | 0.41              |
| 1:C:383:ALA:HB3  | 1:C:389:MET:N    | 2.35                     | 0.41              |
| 1:G:126:ALA:HB3  | 1:G:426:LEU:HD22 | 2.03                     | 0.41              |
| 1:L:2:ALA:O      | 1:L:3:ALA:C      | 2.59                     | 0.41              |
| 1:A:294:THR:HG21 | 1:A:345:ARG:HG3  | 2.01                     | 0.41              |
| 1:D:202:PRO:O    | 1:D:205:ILE:HB   | 2.19                     | 0.41              |
| 1:D:13:ARG:NH1   | 1:D:515:ILE:O    | 2.49                     | 0.41              |
| 1:I:254:VAL:CG1  | 1:I:259:LEU:HD23 | 2.50                     | 0.41              |
| 1:N:2:ALA:O      | 1:N:3:ALA:C      | 2.59                     | 0.41              |
| 1:A:268:ARG:CZ   | 1:A:268:ARG:HA   | 2.51                     | 0.41              |
| 1:E:126:ALA:HB3  | 1:E:426:LEU:HD22 | 2.03                     | 0.41              |
| 1:E:205:ILE:HG23 | 1:E:211:GLY:HA2  | 2.03                     | 0.41              |
| 1:E:517:THR:HA   | 1:F:39:VAL:HB    | 2.02                     | 0.41              |
| 1:E:513:LEU:CA   | 1:F:49:ILE:HD11  | 2.43                     | 0.41              |
| 1:H:2:ALA:O      | 1:H:3:ALA:C      | 2.59                     | 0.41              |
| 1:M:254:VAL:CG1  | 1:M:259:LEU:HD23 | 2.50                     | 0.41              |
| 1:A:126:ALA:HB3  | 1:A:426:LEU:HD22 | 2.03                     | 0.41              |
| 1:A:102:GLU:HB2  | 1:A:442:VAL:HG13 | 2.02                     | 0.41              |
| 1:C:135:SER:CA   | 1:C:412:VAL:HG12 | 2.45                     | 0.41              |
| 1:D:517:THR:HA   | 1:E:39:VAL:HB    | 2.02                     | 0.41              |
| 1:G:202:PRO:O    | 1:G:205:ILE:HB   | 2.19                     | 0.41              |
| 1:G:323:VAL:HG22 | 1:G:332:ILE:HA   | 2.03                     | 0.41              |
| 1:B:294:THR:HG21 | 1:B:345:ARG:HG3  | 2.01                     | 0.41              |
| 1:B:383:ALA:HB3  | 1:B:389:MET:N    | 2.35                     | 0.41              |
| 1:C:323:VAL:HG22 | 1:C:332:ILE:HA   | 2.03                     | 0.41              |
| 1:D:383:ALA:HB3  | 1:D:389:MET:N    | 2.35                     | 0.41              |
| 1:F:102:GLU:HB2  | 1:F:442:VAL:HG13 | 2.02                     | 0.41              |
| 1:B:268:ARG:CZ   | 1:B:268:ARG:HA   | 2.51                     | 0.41              |
| 1:B:13:ARG:NH1   | 1:B:515:ILE:O    | 2.49                     | 0.41              |
| 1:E:46:ALA:HA    | 1:E:47:PRO:HD2   | 1.84                     | 0.41              |
| 1:F:383:ALA:HB3  | 1:F:389:MET:N    | 2.35                     | 0.41              |
| 1:F:85:ALA:HB1   | 1:F:499:VAL:HA   | 2.03                     | 0.41              |
| 1:F:513:LEU:CA   | 1:G:49:ILE:HD11  | 2.43                     | 0.41              |
| 1:K:271:VAL:HG12 | 1:K:272:LYS:H    | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:102:GLU:HB2  | 1:D:442:VAL:HG13 | 2.02                     | 0.41              |
| 1:J:2:ALA:O      | 1:J:3:ALA:C      | 2.59                     | 0.41              |
| 1:C:152:ALA:HB1  | 1:C:155:ASP:CA   | 2.51                     | 0.41              |
| 1:D:112:ASN:HA   | 1:D:113:PRO:HD2  | 1.74                     | 0.41              |
| 1:F:205:ILE:HG23 | 1:F:211:GLY:HA2  | 2.03                     | 0.41              |
| 1:F:51:LYS:HB2   | 1:F:395:ARG:HD3  | 2.03                     | 0.41              |
| 1:G:268:ARG:HA   | 1:G:268:ARG:CZ   | 2.51                     | 0.41              |
| 1:G:27:VAL:CG1   | 1:G:90:THR:HG23  | 2.35                     | 0.41              |
| 1:B:102:GLU:HB2  | 1:B:442:VAL:HG13 | 2.02                     | 0.40              |
| 1:B:152:ALA:HB1  | 1:B:155:ASP:CA   | 2.51                     | 0.40              |
| 1:B:126:ALA:HB3  | 1:B:426:LEU:HD22 | 2.03                     | 0.40              |
| 1:G:102:GLU:HB2  | 1:G:442:VAL:HG13 | 2.02                     | 0.40              |
| 1:D:152:ALA:HB1  | 1:D:155:ASP:CA   | 2.51                     | 0.40              |
| 1:D:461:GLU:HA   | 1:D:462:PRO:HD2  | 1.83                     | 0.40              |
| 1:E:383:ALA:HB3  | 1:E:389:MET:N    | 2.35                     | 0.40              |
| 1:E:13:ARG:NH1   | 1:E:515:ILE:O    | 2.49                     | 0.40              |
| 3:G:1525:PO4:P   | 2:G:1527:ATP:PG  | 3.20                     | 0.40              |
| 1:I:2:ALA:O      | 1:I:3:ALA:C      | 2.59                     | 0.40              |
| 1:A:152:ALA:HB1  | 1:A:155:ASP:CA   | 2.51                     | 0.40              |
| 1:B:34:LYS:HZ1   | 1:B:483:GLU:CD   | 2.24                     | 0.40              |
| 1:D:126:ALA:HB3  | 1:D:426:LEU:HD22 | 2.03                     | 0.40              |
| 1:D:206:ASN:HB2  | 1:D:213:VAL:CB   | 2.52                     | 0.40              |
| 1:D:205:ILE:HG23 | 1:D:211:GLY:HA2  | 2.03                     | 0.40              |
| 1:D:323:VAL:HG22 | 1:D:332:ILE:HA   | 2.03                     | 0.40              |
| 1:E:206:ASN:HB2  | 1:E:213:VAL:CB   | 2.51                     | 0.40              |
| 1:E:85:ALA:HB1   | 1:E:499:VAL:HA   | 2.04                     | 0.40              |
| 3:F:1525:PO4:P   | 2:F:1527:ATP:PG  | 3.20                     | 0.40              |
| 1:F:231:ARG:O    | 1:F:235:PRO:HD2  | 2.22                     | 0.40              |
| 1:G:205:ILE:HG23 | 1:G:211:GLY:HA2  | 2.03                     | 0.40              |
| 1:H:254:VAL:CG1  | 1:H:259:LEU:HD23 | 2.50                     | 0.40              |
| 2:A:1525:ATP:PG  | 3:A:1526:PO4:P   | 3.20                     | 0.40              |
| 1:B:13:ARG:CG    | 1:B:13:ARG:HH11  | 2.34                     | 0.40              |
| 1:B:85:ALA:HB1   | 1:B:499:VAL:HA   | 2.04                     | 0.40              |
| 1:C:166:MET:HA   | 1:C:175:ILE:HD11 | 2.04                     | 0.40              |
| 1:C:268:ARG:CZ   | 1:C:268:ARG:HA   | 2.51                     | 0.40              |
| 1:C:517:THR:HA   | 1:D:39:VAL:HB    | 2.02                     | 0.40              |
| 1:D:85:ALA:HB1   | 1:D:499:VAL:HA   | 2.03                     | 0.40              |
| 1:D:517:THR:CA   | 1:E:39:VAL:HB    | 2.52                     | 0.40              |
| 1:F:152:ALA:HB1  | 1:F:155:ASP:CA   | 2.51                     | 0.40              |
| 1:F:323:VAL:HG22 | 1:F:332:ILE:HA   | 2.03                     | 0.40              |
| 1:G:166:MET:HA   | 1:G:175:ILE:HD11 | 2.04                     | 0.40              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:G:62:LEU:HB2 | 1:G:68:ASN:HA   | 2.04                     | 0.40              |
| 1:A:62:LEU:HB2 | 1:A:68:ASN:HA   | 2.04                     | 0.40              |
| 1:B:62:LEU:HB2 | 1:B:68:ASN:HA   | 2.04                     | 0.40              |
| 1:C:85:ALA:HB1 | 1:C:499:VAL:HA  | 2.04                     | 0.40              |
| 1:E:231:ARG:O  | 1:E:235:PRO:HD2 | 2.22                     | 0.40              |
| 1:E:268:ARG:CZ | 1:E:268:ARG:HA  | 2.51                     | 0.40              |
| 1:F:268:ARG:HA | 1:F:268:ARG:NE  | 2.37                     | 0.40              |
| 1:E:517:THR:CA | 1:F:39:VAL:HB   | 2.52                     | 0.40              |
| 1:G:51:LYS:HB2 | 1:G:395:ARG:HD3 | 2.03                     | 0.40              |
| 1:G:85:ALA:HB1 | 1:G:499:VAL:HA  | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 522/548 (95%) | 517 (99%) | 5 (1%)  | 0        | 100         | 100 |
| 1   | B     | 522/548 (95%) | 517 (99%) | 5 (1%)  | 0        | 100         | 100 |
| 1   | C     | 522/548 (95%) | 517 (99%) | 5 (1%)  | 0        | 100         | 100 |
| 1   | D     | 522/548 (95%) | 517 (99%) | 5 (1%)  | 0        | 100         | 100 |
| 1   | E     | 522/548 (95%) | 517 (99%) | 5 (1%)  | 0        | 100         | 100 |
| 1   | F     | 522/548 (95%) | 517 (99%) | 5 (1%)  | 0        | 100         | 100 |
| 1   | G     | 522/548 (95%) | 517 (99%) | 5 (1%)  | 0        | 100         | 100 |
| 1   | H     | 522/548 (95%) | 498 (95%) | 22 (4%) | 2 (0%)   | 38          | 77  |
| 1   | I     | 522/548 (95%) | 498 (95%) | 22 (4%) | 2 (0%)   | 38          | 77  |
| 1   | J     | 522/548 (95%) | 498 (95%) | 22 (4%) | 2 (0%)   | 38          | 77  |
| 1   | K     | 522/548 (95%) | 498 (95%) | 22 (4%) | 2 (0%)   | 38          | 77  |
| 1   | L     | 522/548 (95%) | 498 (95%) | 22 (4%) | 2 (0%)   | 38          | 77  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | M     | 522/548 (95%)   | 498 (95%)  | 22 (4%)  | 2 (0%)   | 38          | 77 |
| 1   | N     | 522/548 (95%)   | 498 (95%)  | 22 (4%)  | 2 (0%)   | 38          | 77 |
| All | All   | 7308/7672 (95%) | 7105 (97%) | 189 (3%) | 14 (0%)  | 54          | 84 |

All (14) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 269 | GLY  |
| 1   | I     | 269 | GLY  |
| 1   | J     | 269 | GLY  |
| 1   | K     | 269 | GLY  |
| 1   | L     | 269 | GLY  |
| 1   | M     | 269 | GLY  |
| 1   | N     | 269 | GLY  |
| 1   | H     | 336 | VAL  |
| 1   | I     | 336 | VAL  |
| 1   | J     | 336 | VAL  |
| 1   | K     | 336 | VAL  |
| 1   | L     | 336 | VAL  |
| 1   | M     | 336 | VAL  |
| 1   | N     | 336 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 402/414 (97%) | 364 (90%) | 38 (10%) | 10          | 36 |
| 1   | B     | 402/414 (97%) | 364 (90%) | 38 (10%) | 10          | 36 |
| 1   | C     | 402/414 (97%) | 364 (90%) | 38 (10%) | 10          | 36 |
| 1   | D     | 402/414 (97%) | 364 (90%) | 38 (10%) | 10          | 36 |
| 1   | E     | 402/414 (97%) | 364 (90%) | 38 (10%) | 10          | 36 |
| 1   | F     | 402/414 (97%) | 364 (90%) | 38 (10%) | 10          | 36 |
| 1   | G     | 402/414 (97%) | 364 (90%) | 38 (10%) | 10          | 36 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | H     | 402/414 (97%)   | 367 (91%)  | 35 (9%)  | 12          | 40 |
| 1   | I     | 402/414 (97%)   | 367 (91%)  | 35 (9%)  | 12          | 40 |
| 1   | J     | 402/414 (97%)   | 367 (91%)  | 35 (9%)  | 12          | 40 |
| 1   | K     | 402/414 (97%)   | 367 (91%)  | 35 (9%)  | 12          | 40 |
| 1   | L     | 402/414 (97%)   | 366 (91%)  | 36 (9%)  | 11          | 38 |
| 1   | M     | 402/414 (97%)   | 367 (91%)  | 35 (9%)  | 12          | 40 |
| 1   | N     | 402/414 (97%)   | 367 (91%)  | 35 (9%)  | 12          | 40 |
| All | All   | 5628/5796 (97%) | 5116 (91%) | 512 (9%) | 15          | 38 |

All (512) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 8   | PHE  |
| 1   | A     | 25  | ASP  |
| 1   | A     | 31  | LEU  |
| 1   | A     | 37  | ASN  |
| 1   | A     | 49  | ILE  |
| 1   | A     | 55  | SER  |
| 1   | A     | 130 | GLU  |
| 1   | A     | 142 | LYS  |
| 1   | A     | 155 | ASP  |
| 1   | A     | 156 | GLU  |
| 1   | A     | 164 | GLU  |
| 1   | A     | 169 | VAL  |
| 1   | A     | 171 | LYS  |
| 1   | A     | 190 | VAL  |
| 1   | A     | 207 | LYS  |
| 1   | A     | 213 | VAL  |
| 1   | A     | 214 | GLU  |
| 1   | A     | 219 | PHE  |
| 1   | A     | 228 | SER  |
| 1   | A     | 253 | ASP  |
| 1   | A     | 257 | GLU  |
| 1   | A     | 290 | GLN  |
| 1   | A     | 295 | LEU  |
| 1   | A     | 327 | LYS  |
| 1   | A     | 328 | ASP  |
| 1   | A     | 334 | ASP  |
| 1   | A     | 350 | ARG  |
| 1   | A     | 358 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 363 | GLU  |
| 1   | A     | 421 | ARG  |
| 1   | A     | 453 | GLN  |
| 1   | A     | 460 | GLU  |
| 1   | A     | 473 | ASP  |
| 1   | A     | 484 | GLU  |
| 1   | A     | 504 | LEU  |
| 1   | A     | 516 | THR  |
| 1   | A     | 517 | THR  |
| 1   | A     | 523 | ASP  |
| 1   | B     | 8   | PHE  |
| 1   | B     | 25  | ASP  |
| 1   | B     | 31  | LEU  |
| 1   | B     | 37  | ASN  |
| 1   | B     | 49  | ILE  |
| 1   | B     | 55  | SER  |
| 1   | B     | 130 | GLU  |
| 1   | B     | 142 | LYS  |
| 1   | B     | 155 | ASP  |
| 1   | B     | 156 | GLU  |
| 1   | B     | 164 | GLU  |
| 1   | B     | 169 | VAL  |
| 1   | B     | 171 | LYS  |
| 1   | B     | 190 | VAL  |
| 1   | B     | 207 | LYS  |
| 1   | B     | 213 | VAL  |
| 1   | B     | 214 | GLU  |
| 1   | B     | 219 | PHE  |
| 1   | B     | 228 | SER  |
| 1   | B     | 253 | ASP  |
| 1   | B     | 257 | GLU  |
| 1   | B     | 290 | GLN  |
| 1   | B     | 295 | LEU  |
| 1   | B     | 327 | LYS  |
| 1   | B     | 328 | ASP  |
| 1   | B     | 334 | ASP  |
| 1   | B     | 350 | ARG  |
| 1   | B     | 358 | SER  |
| 1   | B     | 363 | GLU  |
| 1   | B     | 421 | ARG  |
| 1   | B     | 453 | GLN  |
| 1   | B     | 460 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 473 | ASP  |
| 1   | B     | 484 | GLU  |
| 1   | B     | 504 | LEU  |
| 1   | B     | 516 | THR  |
| 1   | B     | 517 | THR  |
| 1   | B     | 523 | ASP  |
| 1   | C     | 8   | PHE  |
| 1   | C     | 25  | ASP  |
| 1   | C     | 31  | LEU  |
| 1   | C     | 37  | ASN  |
| 1   | C     | 49  | ILE  |
| 1   | C     | 55  | SER  |
| 1   | C     | 130 | GLU  |
| 1   | C     | 142 | LYS  |
| 1   | C     | 155 | ASP  |
| 1   | C     | 156 | GLU  |
| 1   | C     | 164 | GLU  |
| 1   | C     | 169 | VAL  |
| 1   | C     | 171 | LYS  |
| 1   | C     | 190 | VAL  |
| 1   | C     | 207 | LYS  |
| 1   | C     | 213 | VAL  |
| 1   | C     | 214 | GLU  |
| 1   | C     | 219 | PHE  |
| 1   | C     | 228 | SER  |
| 1   | C     | 253 | ASP  |
| 1   | C     | 257 | GLU  |
| 1   | C     | 290 | GLN  |
| 1   | C     | 295 | LEU  |
| 1   | C     | 327 | LYS  |
| 1   | C     | 328 | ASP  |
| 1   | C     | 334 | ASP  |
| 1   | C     | 350 | ARG  |
| 1   | C     | 358 | SER  |
| 1   | C     | 363 | GLU  |
| 1   | C     | 421 | ARG  |
| 1   | C     | 453 | GLN  |
| 1   | C     | 460 | GLU  |
| 1   | C     | 473 | ASP  |
| 1   | C     | 484 | GLU  |
| 1   | C     | 504 | LEU  |
| 1   | C     | 516 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 517 | THR  |
| 1   | C     | 523 | ASP  |
| 1   | D     | 8   | PHE  |
| 1   | D     | 25  | ASP  |
| 1   | D     | 31  | LEU  |
| 1   | D     | 37  | ASN  |
| 1   | D     | 49  | ILE  |
| 1   | D     | 55  | SER  |
| 1   | D     | 130 | GLU  |
| 1   | D     | 142 | LYS  |
| 1   | D     | 155 | ASP  |
| 1   | D     | 156 | GLU  |
| 1   | D     | 164 | GLU  |
| 1   | D     | 169 | VAL  |
| 1   | D     | 171 | LYS  |
| 1   | D     | 190 | VAL  |
| 1   | D     | 207 | LYS  |
| 1   | D     | 213 | VAL  |
| 1   | D     | 214 | GLU  |
| 1   | D     | 219 | PHE  |
| 1   | D     | 228 | SER  |
| 1   | D     | 253 | ASP  |
| 1   | D     | 257 | GLU  |
| 1   | D     | 290 | GLN  |
| 1   | D     | 295 | LEU  |
| 1   | D     | 327 | LYS  |
| 1   | D     | 328 | ASP  |
| 1   | D     | 334 | ASP  |
| 1   | D     | 350 | ARG  |
| 1   | D     | 358 | SER  |
| 1   | D     | 363 | GLU  |
| 1   | D     | 421 | ARG  |
| 1   | D     | 453 | GLN  |
| 1   | D     | 460 | GLU  |
| 1   | D     | 473 | ASP  |
| 1   | D     | 484 | GLU  |
| 1   | D     | 504 | LEU  |
| 1   | D     | 516 | THR  |
| 1   | D     | 517 | THR  |
| 1   | D     | 523 | ASP  |
| 1   | E     | 8   | PHE  |
| 1   | E     | 25  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 31  | LEU  |
| 1   | E     | 37  | ASN  |
| 1   | E     | 49  | ILE  |
| 1   | E     | 55  | SER  |
| 1   | E     | 130 | GLU  |
| 1   | E     | 142 | LYS  |
| 1   | E     | 155 | ASP  |
| 1   | E     | 156 | GLU  |
| 1   | E     | 164 | GLU  |
| 1   | E     | 169 | VAL  |
| 1   | E     | 171 | LYS  |
| 1   | E     | 190 | VAL  |
| 1   | E     | 207 | LYS  |
| 1   | E     | 213 | VAL  |
| 1   | E     | 214 | GLU  |
| 1   | E     | 219 | PHE  |
| 1   | E     | 228 | SER  |
| 1   | E     | 253 | ASP  |
| 1   | E     | 257 | GLU  |
| 1   | E     | 290 | GLN  |
| 1   | E     | 295 | LEU  |
| 1   | E     | 327 | LYS  |
| 1   | E     | 328 | ASP  |
| 1   | E     | 334 | ASP  |
| 1   | E     | 350 | ARG  |
| 1   | E     | 358 | SER  |
| 1   | E     | 363 | GLU  |
| 1   | E     | 421 | ARG  |
| 1   | E     | 453 | GLN  |
| 1   | E     | 460 | GLU  |
| 1   | E     | 473 | ASP  |
| 1   | E     | 484 | GLU  |
| 1   | E     | 504 | LEU  |
| 1   | E     | 516 | THR  |
| 1   | E     | 517 | THR  |
| 1   | E     | 523 | ASP  |
| 1   | F     | 8   | PHE  |
| 1   | F     | 25  | ASP  |
| 1   | F     | 31  | LEU  |
| 1   | F     | 37  | ASN  |
| 1   | F     | 49  | ILE  |
| 1   | F     | 55  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 130 | GLU  |
| 1   | F     | 142 | LYS  |
| 1   | F     | 155 | ASP  |
| 1   | F     | 156 | GLU  |
| 1   | F     | 164 | GLU  |
| 1   | F     | 169 | VAL  |
| 1   | F     | 171 | LYS  |
| 1   | F     | 190 | VAL  |
| 1   | F     | 207 | LYS  |
| 1   | F     | 213 | VAL  |
| 1   | F     | 214 | GLU  |
| 1   | F     | 219 | PHE  |
| 1   | F     | 228 | SER  |
| 1   | F     | 253 | ASP  |
| 1   | F     | 257 | GLU  |
| 1   | F     | 290 | GLN  |
| 1   | F     | 295 | LEU  |
| 1   | F     | 327 | LYS  |
| 1   | F     | 328 | ASP  |
| 1   | F     | 334 | ASP  |
| 1   | F     | 350 | ARG  |
| 1   | F     | 358 | SER  |
| 1   | F     | 363 | GLU  |
| 1   | F     | 421 | ARG  |
| 1   | F     | 453 | GLN  |
| 1   | F     | 460 | GLU  |
| 1   | F     | 473 | ASP  |
| 1   | F     | 484 | GLU  |
| 1   | F     | 504 | LEU  |
| 1   | F     | 516 | THR  |
| 1   | F     | 517 | THR  |
| 1   | F     | 523 | ASP  |
| 1   | G     | 8   | PHE  |
| 1   | G     | 25  | ASP  |
| 1   | G     | 31  | LEU  |
| 1   | G     | 37  | ASN  |
| 1   | G     | 49  | ILE  |
| 1   | G     | 55  | SER  |
| 1   | G     | 130 | GLU  |
| 1   | G     | 142 | LYS  |
| 1   | G     | 155 | ASP  |
| 1   | G     | 156 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 164 | GLU  |
| 1   | G     | 169 | VAL  |
| 1   | G     | 171 | LYS  |
| 1   | G     | 190 | VAL  |
| 1   | G     | 207 | LYS  |
| 1   | G     | 213 | VAL  |
| 1   | G     | 214 | GLU  |
| 1   | G     | 219 | PHE  |
| 1   | G     | 228 | SER  |
| 1   | G     | 253 | ASP  |
| 1   | G     | 257 | GLU  |
| 1   | G     | 290 | GLN  |
| 1   | G     | 295 | LEU  |
| 1   | G     | 327 | LYS  |
| 1   | G     | 328 | ASP  |
| 1   | G     | 334 | ASP  |
| 1   | G     | 350 | ARG  |
| 1   | G     | 358 | SER  |
| 1   | G     | 363 | GLU  |
| 1   | G     | 421 | ARG  |
| 1   | G     | 453 | GLN  |
| 1   | G     | 460 | GLU  |
| 1   | G     | 473 | ASP  |
| 1   | G     | 484 | GLU  |
| 1   | G     | 504 | LEU  |
| 1   | G     | 516 | THR  |
| 1   | G     | 517 | THR  |
| 1   | G     | 523 | ASP  |
| 1   | H     | 25  | ASP  |
| 1   | H     | 34  | LYS  |
| 1   | H     | 82  | ASN  |
| 1   | H     | 115 | ASP  |
| 1   | H     | 140 | ASP  |
| 1   | H     | 142 | LYS  |
| 1   | H     | 153 | ASN  |
| 1   | H     | 172 | GLU  |
| 1   | H     | 174 | VAL  |
| 1   | H     | 186 | GLU  |
| 1   | H     | 196 | ASP  |
| 1   | H     | 199 | TYR  |
| 1   | H     | 213 | VAL  |
| 1   | H     | 214 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 216 | GLU  |
| 1   | H     | 228 | SER  |
| 1   | H     | 229 | ASN  |
| 1   | H     | 230 | ILE  |
| 1   | H     | 281 | PHE  |
| 1   | H     | 290 | GLN  |
| 1   | H     | 327 | LYS  |
| 1   | H     | 329 | THR  |
| 1   | H     | 334 | ASP  |
| 1   | H     | 338 | GLU  |
| 1   | H     | 350 | ARG  |
| 1   | H     | 404 | ARG  |
| 1   | H     | 411 | VAL  |
| 1   | H     | 460 | GLU  |
| 1   | H     | 463 | SER  |
| 1   | H     | 483 | GLU  |
| 1   | H     | 484 | GLU  |
| 1   | H     | 494 | LEU  |
| 1   | H     | 500 | THR  |
| 1   | H     | 504 | LEU  |
| 1   | H     | 510 | VAL  |
| 1   | I     | 25  | ASP  |
| 1   | I     | 34  | LYS  |
| 1   | I     | 82  | ASN  |
| 1   | I     | 115 | ASP  |
| 1   | I     | 140 | ASP  |
| 1   | I     | 142 | LYS  |
| 1   | I     | 153 | ASN  |
| 1   | I     | 172 | GLU  |
| 1   | I     | 174 | VAL  |
| 1   | I     | 186 | GLU  |
| 1   | I     | 196 | ASP  |
| 1   | I     | 199 | TYR  |
| 1   | I     | 213 | VAL  |
| 1   | I     | 214 | GLU  |
| 1   | I     | 216 | GLU  |
| 1   | I     | 228 | SER  |
| 1   | I     | 229 | ASN  |
| 1   | I     | 230 | ILE  |
| 1   | I     | 281 | PHE  |
| 1   | I     | 290 | GLN  |
| 1   | I     | 327 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 329 | THR  |
| 1   | I     | 334 | ASP  |
| 1   | I     | 338 | GLU  |
| 1   | I     | 350 | ARG  |
| 1   | I     | 404 | ARG  |
| 1   | I     | 411 | VAL  |
| 1   | I     | 460 | GLU  |
| 1   | I     | 463 | SER  |
| 1   | I     | 483 | GLU  |
| 1   | I     | 484 | GLU  |
| 1   | I     | 494 | LEU  |
| 1   | I     | 500 | THR  |
| 1   | I     | 504 | LEU  |
| 1   | I     | 510 | VAL  |
| 1   | J     | 25  | ASP  |
| 1   | J     | 34  | LYS  |
| 1   | J     | 82  | ASN  |
| 1   | J     | 115 | ASP  |
| 1   | J     | 140 | ASP  |
| 1   | J     | 142 | LYS  |
| 1   | J     | 153 | ASN  |
| 1   | J     | 172 | GLU  |
| 1   | J     | 174 | VAL  |
| 1   | J     | 186 | GLU  |
| 1   | J     | 196 | ASP  |
| 1   | J     | 199 | TYR  |
| 1   | J     | 213 | VAL  |
| 1   | J     | 214 | GLU  |
| 1   | J     | 216 | GLU  |
| 1   | J     | 228 | SER  |
| 1   | J     | 229 | ASN  |
| 1   | J     | 230 | ILE  |
| 1   | J     | 281 | PHE  |
| 1   | J     | 290 | GLN  |
| 1   | J     | 327 | LYS  |
| 1   | J     | 329 | THR  |
| 1   | J     | 334 | ASP  |
| 1   | J     | 338 | GLU  |
| 1   | J     | 350 | ARG  |
| 1   | J     | 404 | ARG  |
| 1   | J     | 411 | VAL  |
| 1   | J     | 460 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 463 | SER  |
| 1   | J     | 483 | GLU  |
| 1   | J     | 484 | GLU  |
| 1   | J     | 494 | LEU  |
| 1   | J     | 500 | THR  |
| 1   | J     | 504 | LEU  |
| 1   | J     | 510 | VAL  |
| 1   | K     | 25  | ASP  |
| 1   | K     | 34  | LYS  |
| 1   | K     | 82  | ASN  |
| 1   | K     | 115 | ASP  |
| 1   | K     | 140 | ASP  |
| 1   | K     | 142 | LYS  |
| 1   | K     | 153 | ASN  |
| 1   | K     | 172 | GLU  |
| 1   | K     | 174 | VAL  |
| 1   | K     | 186 | GLU  |
| 1   | K     | 196 | ASP  |
| 1   | K     | 199 | TYR  |
| 1   | K     | 213 | VAL  |
| 1   | K     | 214 | GLU  |
| 1   | K     | 216 | GLU  |
| 1   | K     | 228 | SER  |
| 1   | K     | 229 | ASN  |
| 1   | K     | 230 | ILE  |
| 1   | K     | 281 | PHE  |
| 1   | K     | 290 | GLN  |
| 1   | K     | 327 | LYS  |
| 1   | K     | 329 | THR  |
| 1   | K     | 334 | ASP  |
| 1   | K     | 338 | GLU  |
| 1   | K     | 350 | ARG  |
| 1   | K     | 404 | ARG  |
| 1   | K     | 411 | VAL  |
| 1   | K     | 460 | GLU  |
| 1   | K     | 463 | SER  |
| 1   | K     | 483 | GLU  |
| 1   | K     | 484 | GLU  |
| 1   | K     | 494 | LEU  |
| 1   | K     | 500 | THR  |
| 1   | K     | 504 | LEU  |
| 1   | K     | 510 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 25  | ASP  |
| 1   | L     | 34  | LYS  |
| 1   | L     | 82  | ASN  |
| 1   | L     | 115 | ASP  |
| 1   | L     | 140 | ASP  |
| 1   | L     | 142 | LYS  |
| 1   | L     | 153 | ASN  |
| 1   | L     | 172 | GLU  |
| 1   | L     | 174 | VAL  |
| 1   | L     | 186 | GLU  |
| 1   | L     | 187 | LEU  |
| 1   | L     | 196 | ASP  |
| 1   | L     | 199 | TYR  |
| 1   | L     | 213 | VAL  |
| 1   | L     | 214 | GLU  |
| 1   | L     | 216 | GLU  |
| 1   | L     | 228 | SER  |
| 1   | L     | 229 | ASN  |
| 1   | L     | 230 | ILE  |
| 1   | L     | 281 | PHE  |
| 1   | L     | 290 | GLN  |
| 1   | L     | 327 | LYS  |
| 1   | L     | 329 | THR  |
| 1   | L     | 334 | ASP  |
| 1   | L     | 338 | GLU  |
| 1   | L     | 350 | ARG  |
| 1   | L     | 404 | ARG  |
| 1   | L     | 411 | VAL  |
| 1   | L     | 460 | GLU  |
| 1   | L     | 463 | SER  |
| 1   | L     | 483 | GLU  |
| 1   | L     | 484 | GLU  |
| 1   | L     | 494 | LEU  |
| 1   | L     | 500 | THR  |
| 1   | L     | 504 | LEU  |
| 1   | L     | 510 | VAL  |
| 1   | M     | 25  | ASP  |
| 1   | M     | 34  | LYS  |
| 1   | M     | 82  | ASN  |
| 1   | M     | 115 | ASP  |
| 1   | M     | 140 | ASP  |
| 1   | M     | 142 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 153 | ASN  |
| 1   | M     | 172 | GLU  |
| 1   | M     | 174 | VAL  |
| 1   | M     | 186 | GLU  |
| 1   | M     | 196 | ASP  |
| 1   | M     | 199 | TYR  |
| 1   | M     | 213 | VAL  |
| 1   | M     | 214 | GLU  |
| 1   | M     | 216 | GLU  |
| 1   | M     | 228 | SER  |
| 1   | M     | 229 | ASN  |
| 1   | M     | 230 | ILE  |
| 1   | M     | 281 | PHE  |
| 1   | M     | 290 | GLN  |
| 1   | M     | 327 | LYS  |
| 1   | M     | 329 | THR  |
| 1   | M     | 334 | ASP  |
| 1   | M     | 338 | GLU  |
| 1   | M     | 350 | ARG  |
| 1   | M     | 404 | ARG  |
| 1   | M     | 411 | VAL  |
| 1   | M     | 460 | GLU  |
| 1   | M     | 463 | SER  |
| 1   | M     | 483 | GLU  |
| 1   | M     | 484 | GLU  |
| 1   | M     | 494 | LEU  |
| 1   | M     | 500 | THR  |
| 1   | M     | 504 | LEU  |
| 1   | M     | 510 | VAL  |
| 1   | N     | 25  | ASP  |
| 1   | N     | 34  | LYS  |
| 1   | N     | 82  | ASN  |
| 1   | N     | 115 | ASP  |
| 1   | N     | 140 | ASP  |
| 1   | N     | 142 | LYS  |
| 1   | N     | 153 | ASN  |
| 1   | N     | 172 | GLU  |
| 1   | N     | 174 | VAL  |
| 1   | N     | 186 | GLU  |
| 1   | N     | 196 | ASP  |
| 1   | N     | 199 | TYR  |
| 1   | N     | 213 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 214 | GLU  |
| 1   | N     | 216 | GLU  |
| 1   | N     | 228 | SER  |
| 1   | N     | 229 | ASN  |
| 1   | N     | 230 | ILE  |
| 1   | N     | 281 | PHE  |
| 1   | N     | 290 | GLN  |
| 1   | N     | 327 | LYS  |
| 1   | N     | 329 | THR  |
| 1   | N     | 334 | ASP  |
| 1   | N     | 338 | GLU  |
| 1   | N     | 350 | ARG  |
| 1   | N     | 404 | ARG  |
| 1   | N     | 411 | VAL  |
| 1   | N     | 460 | GLU  |
| 1   | N     | 463 | SER  |
| 1   | N     | 483 | GLU  |
| 1   | N     | 484 | GLU  |
| 1   | N     | 494 | LEU  |
| 1   | N     | 500 | THR  |
| 1   | N     | 504 | LEU  |
| 1   | N     | 510 | VAL  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 366 | GLN  |
| 1   | B     | 366 | GLN  |
| 1   | C     | 366 | GLN  |
| 1   | D     | 366 | GLN  |
| 1   | E     | 366 | GLN  |
| 1   | F     | 366 | GLN  |
| 1   | G     | 366 | GLN  |
| 1   | H     | 68  | ASN  |
| 1   | H     | 326 | ASN  |
| 1   | I     | 68  | ASN  |
| 1   | I     | 326 | ASN  |
| 1   | J     | 68  | ASN  |
| 1   | J     | 326 | ASN  |
| 1   | K     | 68  | ASN  |
| 1   | K     | 326 | ASN  |
| 1   | L     | 68  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 326 | ASN  |
| 1   | M     | 68  | ASN  |
| 1   | M     | 326 | ASN  |
| 1   | N     | 68  | ASN  |
| 1   | N     | 326 | ASN  |

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 7 are modelled with single atom and 7 are monoatomic - leaving 7 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$ |
| 2   | ATP  | A     | 1525 | 4    | 27,33,33     | 0.94 | 1 (3%)      | 25,52,52    | 1.31 | 3 (12%)     |
| 2   | ATP  | B     | 1525 | 4    | 27,33,33     | 0.95 | 1 (3%)      | 25,52,52    | 1.31 | 3 (12%)     |
| 2   | ATP  | C     | 1526 | 4    | 27,33,33     | 0.95 | 1 (3%)      | 25,52,52    | 1.31 | 3 (12%)     |
| 2   | ATP  | D     | 1525 | 4    | 27,33,33     | 0.96 | 1 (3%)      | 25,52,52    | 1.32 | 3 (12%)     |
| 2   | ATP  | E     | 1527 | 4    | 27,33,33     | 0.96 | 1 (3%)      | 25,52,52    | 1.32 | 3 (12%)     |
| 2   | ATP  | F     | 1527 | 4    | 27,33,33     | 0.95 | 1 (3%)      | 25,52,52    | 1.32 | 4 (16%)     |
| 2   | ATP  | G     | 1527 | 4    | 27,33,33     | 0.95 | 1 (3%)      | 25,52,52    | 1.31 | 3 (12%)     |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | ATP  | A     | 1525 | 4    | -       | 0/18/38/38 | 0/3/3/3 |
| 2   | ATP  | B     | 1525 | 4    | -       | 0/18/38/38 | 0/3/3/3 |
| 2   | ATP  | C     | 1526 | 4    | -       | 0/18/38/38 | 0/3/3/3 |
| 2   | ATP  | D     | 1525 | 4    | -       | 0/18/38/38 | 0/3/3/3 |
| 2   | ATP  | E     | 1527 | 4    | -       | 0/18/38/38 | 0/3/3/3 |
| 2   | ATP  | F     | 1527 | 4    | -       | 0/18/38/38 | 0/3/3/3 |
| 2   | ATP  | G     | 1527 | 4    | -       | 0/18/38/38 | 0/3/3/3 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | E     | 1527 | ATP  | C2'-C1' | -3.34 | 1.48        | 1.53     |
| 2   | C     | 1526 | ATP  | C2'-C1' | -3.33 | 1.48        | 1.53     |
| 2   | D     | 1525 | ATP  | C2'-C1' | -3.32 | 1.48        | 1.53     |
| 2   | G     | 1527 | ATP  | C2'-C1' | -3.29 | 1.48        | 1.53     |
| 2   | B     | 1525 | ATP  | C2'-C1' | -3.29 | 1.48        | 1.53     |
| 2   | F     | 1527 | ATP  | C2'-C1' | -3.29 | 1.48        | 1.53     |
| 2   | A     | 1525 | ATP  | C2'-C1' | -3.24 | 1.48        | 1.53     |

All (22) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | E     | 1527 | ATP  | C4'-O4'-C1' | -2.62 | 106.98      | 109.77   |
| 2   | D     | 1525 | ATP  | C4'-O4'-C1' | -2.61 | 106.99      | 109.77   |
| 2   | B     | 1525 | ATP  | C4'-O4'-C1' | -2.59 | 107.02      | 109.77   |
| 2   | C     | 1526 | ATP  | C4'-O4'-C1' | -2.59 | 107.02      | 109.77   |
| 2   | F     | 1527 | ATP  | C4'-O4'-C1' | -2.59 | 107.02      | 109.77   |
| 2   | A     | 1525 | ATP  | C4'-O4'-C1' | -2.58 | 107.03      | 109.77   |
| 2   | G     | 1527 | ATP  | C4'-O4'-C1' | -2.56 | 107.05      | 109.77   |
| 2   | F     | 1527 | ATP  | O3B-PG-O1G  | -2.26 | 97.52       | 111.44   |
| 2   | B     | 1525 | ATP  | O3B-PG-O1G  | -2.25 | 97.59       | 111.44   |
| 2   | C     | 1526 | ATP  | O3B-PG-O1G  | -2.25 | 97.59       | 111.44   |
| 2   | E     | 1527 | ATP  | O3B-PG-O1G  | -2.25 | 97.60       | 111.44   |
| 2   | D     | 1525 | ATP  | O3B-PG-O1G  | -2.25 | 97.61       | 111.44   |
| 2   | A     | 1525 | ATP  | O3B-PG-O1G  | -2.25 | 97.62       | 111.44   |
| 2   | G     | 1527 | ATP  | O3B-PG-O1G  | -2.25 | 97.63       | 111.44   |
| 2   | F     | 1527 | ATP  | C4-C5-N7    | 2.04  | 111.38      | 109.41   |
| 2   | G     | 1527 | ATP  | O3G-PG-O2G  | 2.15  | 116.30      | 107.61   |

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| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 2   | A     | 1525 | ATP  | O3G-PG-O2G | 2.16 | 116.33      | 107.61   |
| 2   | D     | 1525 | ATP  | O3G-PG-O2G | 2.17 | 116.36      | 107.61   |
| 2   | E     | 1527 | ATP  | O3G-PG-O2G | 2.17 | 116.36      | 107.61   |
| 2   | C     | 1526 | ATP  | O3G-PG-O2G | 2.17 | 116.37      | 107.61   |
| 2   | B     | 1525 | ATP  | O3G-PG-O2G | 2.18 | 116.40      | 107.61   |
| 2   | F     | 1527 | ATP  | O3G-PG-O2G | 2.19 | 116.43      | 107.61   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 24 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | A     | 1525 | ATP  | 4       | 0            |
| 2   | B     | 1525 | ATP  | 3       | 0            |
| 2   | C     | 1526 | ATP  | 3       | 0            |
| 2   | D     | 1525 | ATP  | 3       | 0            |
| 2   | E     | 1527 | ATP  | 3       | 0            |
| 2   | F     | 1527 | ATP  | 4       | 0            |
| 2   | G     | 1527 | ATP  | 4       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | J     | 2                |
| 1   | N     | 2                |
| 1   | L     | 1                |
| 1   | K     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | N     | 400:LEU   | C      | 401:HIS   | N      | 1.83         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | L     | 400:LEU   | C      | 401:HIS   | N      | 1.78         |
| 1     | J     | 400:LEU   | C      | 401:HIS   | N      | 1.72         |
| 1     | J     | 401:HIS   | C      | 402:ALA   | N      | 1.14         |
| 1     | K     | 401:HIS   | C      | 402:ALA   | N      | 1.10         |
| 1     | N     | 401:HIS   | C      | 402:ALA   | N      | 0.90         |