



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:53 AM UTC

PDB ID : 3F79 / pdb\_00003f79  
Title : Structure of pseudo-centered cell crystal form of the C-terminal phosphatase domain of *P. aeruginosa* RssB  
Authors : Levchenko, I.; Grant, R.A.; Sauer, R.T.; Baker, T.A.  
Deposited on : 2008-11-07  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

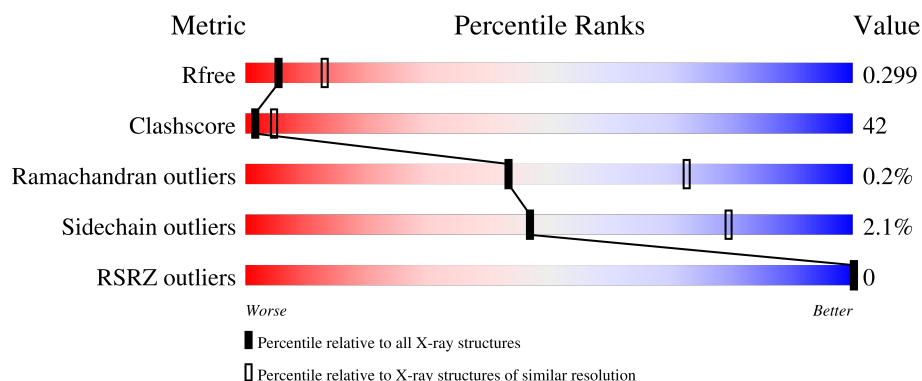
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3866 (2.80-2.80)                                      |
| Clashscore            | 190562                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |
| Sidechain outliers    | 187428                      | 4198 (2.80-2.80)                                      |
| RSRZ outliers         | 180081                      | 3869 (2.80-2.80)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 255    |                  |
| 1   | B     | 255    |                  |
| 1   | C     | 255    |                  |
| 1   | D     | 255    |                  |
| 1   | E     | 255    |                  |

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| Mol | Chain | Length | Quality of chain                                                                                                                                                                                                                                                       |
|-----|-------|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1   | F     | 255    |  A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (53%), yellow (38%), and grey (8%). The percentages are labeled below the bar. |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10386 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Probable two-component response regulator.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 223      | Total | C    | N   | O   | Se | 12      | 0       | 0     |
|     |       |          | 1659  | 1065 | 276 | 312 | 6  |         |         |       |
| 1   | B     | 229      | Total | C    | N   | O   | Se | 5       | 0       | 0     |
|     |       |          | 1738  | 1111 | 295 | 326 | 6  |         |         |       |
| 1   | C     | 229      | Total | C    | N   | O   | Se | 5       | 0       | 0     |
|     |       |          | 1728  | 1112 | 286 | 325 | 5  |         |         |       |
| 1   | D     | 230      | Total | C    | N   | O   | Se | 0       | 0       | 0     |
|     |       |          | 1719  | 1105 | 284 | 324 | 6  |         |         |       |
| 1   | E     | 236      | Total | C    | N   | O   | Se | 13      | 0       | 0     |
|     |       |          | 1778  | 1133 | 302 | 337 | 6  |         |         |       |
| 1   | F     | 235      | Total | C    | N   | O   | Se | 12      | 0       | 0     |
|     |       |          | 1757  | 1125 | 300 | 327 | 5  |         |         |       |

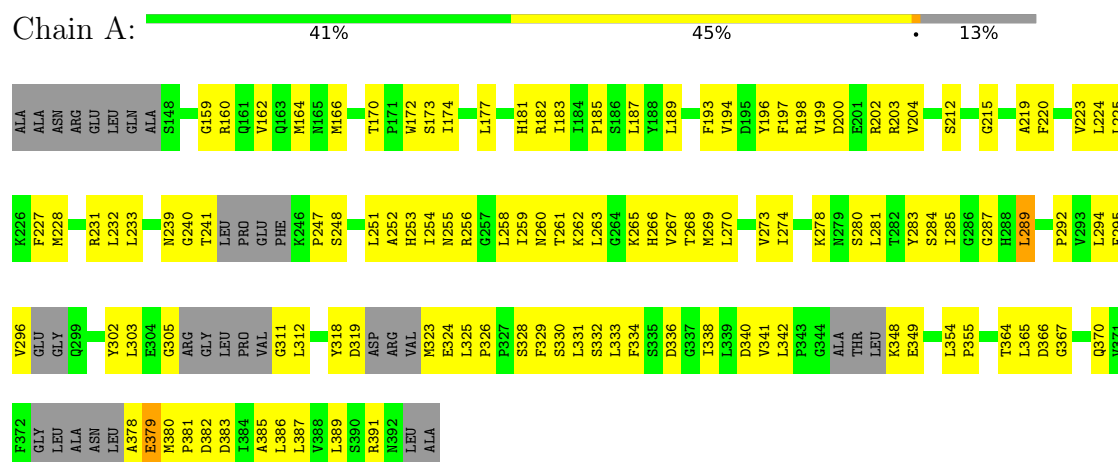
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

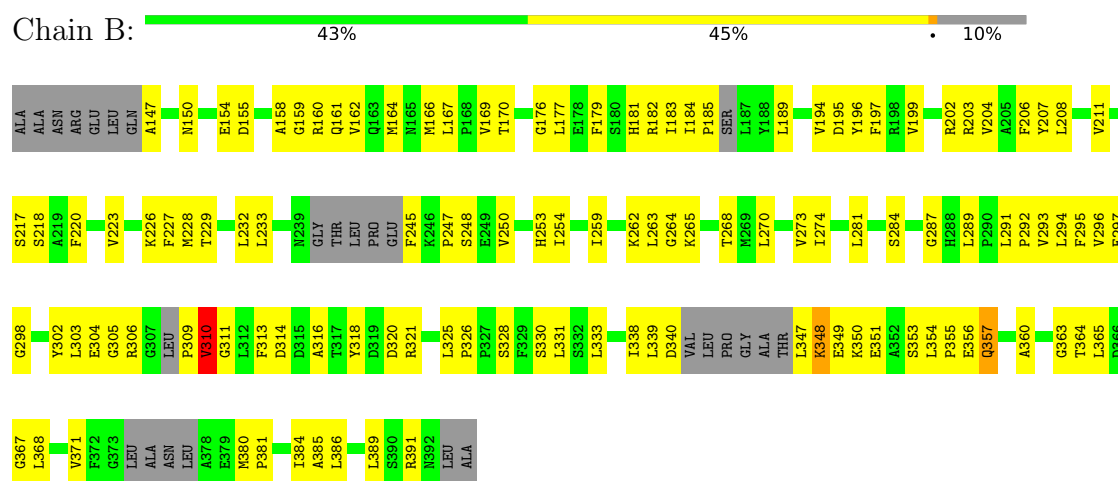
### 3 Residue-property plots

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

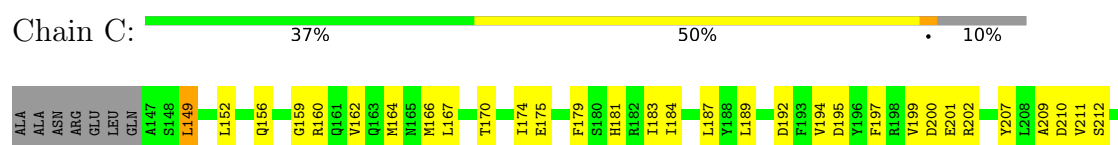
- Molecule 1: Probable two-component response regulator

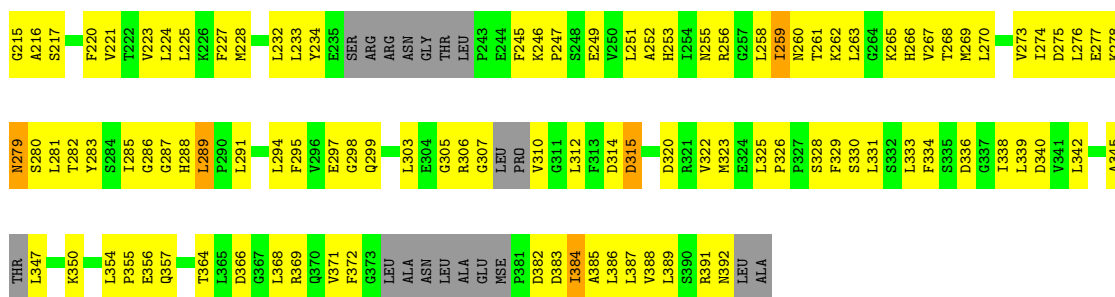


- Molecule 1: Probable two-component response regulator



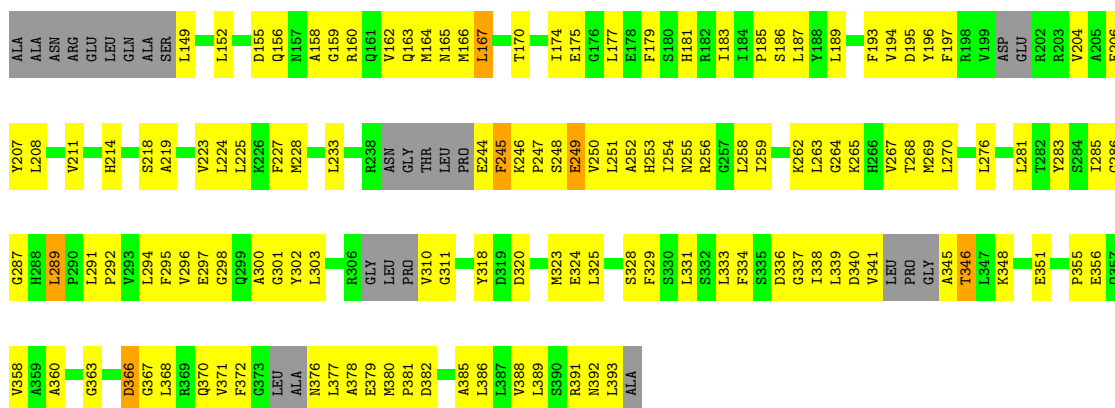
- Molecule 1: Probable two-component response regulator





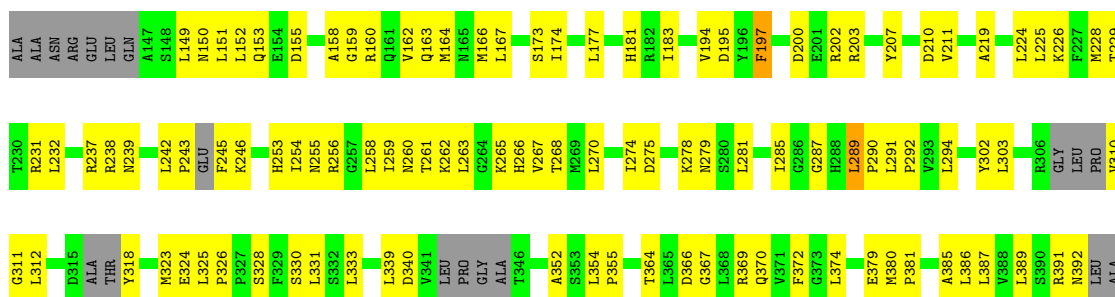
- Molecule 1: Probable two-component response regulator

Chain D: 39% 49% 10%



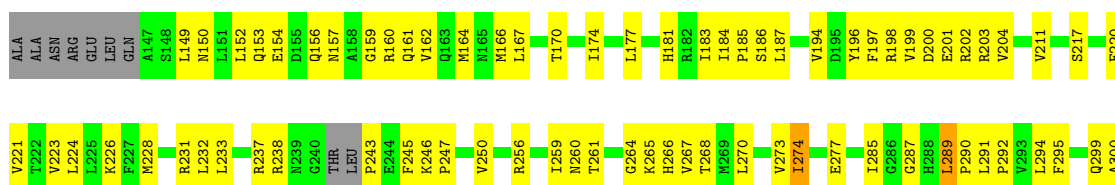
- Molecule 1: Probable two-component response regulator

Chain E: 51% 40% 7%



- Molecule 1: Probable two-component response regulator

Chain F: 53% 38% 8%



|      |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |     |
|------|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|-----|
| R306 | GLY | P309 | V310 | G311 | L312 | L325 | S328 | F329 | S330 | L331 | S332 | L333 | F334 | S335 | D336 | G337 | I338 | L339 | D340 | V341 | L342 | L354 | P355 | D366 | Q370 | V371 | F372 | GLY | LEU | ALA | ASN | LEU | ALA | GLU | MSF | P381 | I384 | A385 | L386 | L389 | S390 | R391 | N392 | L393 | ALA |
|------|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|-----|

## 4 Data and refinement statistics

| Property                                                                | Value                                                          | Source           |
|-------------------------------------------------------------------------|----------------------------------------------------------------|------------------|
| Space group                                                             | P 31                                                           | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 124.87Å 124.87Å 92.90Å<br>90.00° 90.00° 120.00°                | Depositor        |
| Resolution (Å)                                                          | 15.00 – 2.80<br>15.00 – 2.80                                   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.4 (15.00-2.80)<br>99.5 (15.00-2.80)                         | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                           | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.85 (at 2.81Å)                                                | Xtriage          |
| Refinement program                                                      | PHENIX                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.243 , 0.297<br>0.243 , 0.299                                 | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1983 reflections (4.98%)                                       | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 56.8                                                           | Xtriage          |
| Anisotropy                                                              | 0.597                                                          | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 73.1                                                    | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$    | Xtriage          |
| Estimated twinning fraction                                             | 0.047 for -h,-k,l<br>0.048 for h,-h-k,-l<br>0.477 for -k,-h,-l | Xtriage          |
| Reported twinning fraction                                              | 0.498 for -k,-h,-l                                             | Depositor        |
| Outliers                                                                | 0 of 39804 reflections                                         | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.97                                                           | EDS              |
| Total number of atoms                                                   | 10386                                                          | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 91.0                                                           | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.0149e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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



## 5 Model quality [i](#)

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

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

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

| Mol | Chain | Bond lengths |             | Bond angles |                |
|-----|-------|--------------|-------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$    |
| 1   | A     | 0.27         | 0/1682      | 0.73        | 1/2271 (0.0%)  |
| 1   | B     | 0.29         | 0/1762      | 0.73        | 0/2371         |
| 1   | C     | 0.28         | 0/1756      | 0.77        | 1/2374 (0.0%)  |
| 1   | D     | 0.31         | 0/1740      | 0.74        | 1/2349 (0.0%)  |
| 1   | E     | 0.28         | 0/1800      | 0.73        | 0/2429         |
| 1   | F     | 0.29         | 0/1785      | 0.73        | 0/2413         |
| All | All   | 0.29         | 0/10525     | 0.74        | 3/14207 (0.0%) |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 379 | GLU  | CB-CA-C | -6.44 | 109.16      | 116.63   |
| 1   | C     | 279 | ASN  | N-CA-C  | -5.58 | 106.42      | 113.23   |
| 1   | D     | 245 | PHE  | N-CA-C  | -5.43 | 105.36      | 111.28   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1659  | 0        | 1613     | 130     | 0            |
| 1   | B     | 1738  | 0        | 1706     | 167     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | C     | 1728  | 0        | 1687     | 199     | 0            |
| 1   | D     | 1719  | 0        | 1680     | 192     | 0            |
| 1   | E     | 1778  | 0        | 1758     | 123     | 0            |
| 1   | F     | 1757  | 0        | 1713     | 124     | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 2     | 0        | 0        | 0       | 0            |
| 2   | E     | 1     | 0        | 0        | 0       | 0            |
| 2   | F     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 10386 | 0        | 10157    | 860     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (860) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:246:LYS:CB   | 1:D:249:GLU:HB3  | 1.35                     | 1.51              |
| 1:D:246:LYS:HB2  | 1:D:249:GLU:CB   | 1.39                     | 1.49              |
| 1:D:380:MSE:SE   | 1:D:381:PRO:HD2  | 1.85                     | 1.26              |
| 1:B:356:GLU:HG3  | 1:B:357:GLN:NE2  | 1.56                     | 1.20              |
| 1:D:175:GLU:O    | 1:D:391:ARG:NH2  | 1.73                     | 1.19              |
| 1:C:256:ARG:HA   | 1:C:259:ILE:HD12 | 1.24                     | 1.19              |
| 1:C:255:ASN:O    | 1:C:259:ILE:HG13 | 1.41                     | 1.18              |
| 1:D:247:PRO:HB2  | 1:D:320:ASP:OD2  | 1.38                     | 1.18              |
| 1:B:338:ILE:HD12 | 1:B:351:GLU:HG2  | 1.24                     | 1.13              |
| 1:D:295:PHE:CD1  | 1:D:300:ALA:HB2  | 1.87                     | 1.09              |
| 1:B:353:SER:O    | 1:B:357:GLN:NE2  | 1.85                     | 1.09              |
| 1:B:357:GLN:HE21 | 1:B:357:GLN:N    | 1.50                     | 1.08              |
| 1:B:356:GLU:CG   | 1:B:357:GLN:HE22 | 1.68                     | 1.06              |
| 1:B:338:ILE:HD12 | 1:B:351:GLU:CG   | 1.85                     | 1.06              |
| 1:C:268:THR:HG23 | 1:C:287:GLY:HA3  | 1.35                     | 1.06              |
| 1:C:160:ARG:HG3  | 1:C:164:MSE:HE2  | 1.32                     | 1.05              |
| 1:D:270:LEU:HD23 | 1:D:285:ILE:HD13 | 1.39                     | 1.04              |
| 1:B:268:THR:OG1  | 1:B:287:GLY:HA3  | 1.58                     | 1.03              |
| 1:A:380:MSE:HB3  | 1:A:381:PRO:HA   | 1.40                     | 1.03              |
| 1:A:220:PHE:HA   | 1:B:220:PHE:CE2  | 1.96                     | 1.00              |
| 1:D:268:THR:HG23 | 1:D:287:GLY:HA3  | 1.42                     | 0.98              |
| 1:A:294:LEU:HD23 | 1:A:331:LEU:HD13 | 1.43                     | 0.98              |
| 1:E:263:LEU:HD22 | 1:F:162:VAL:CG2  | 1.94                     | 0.98              |
| 1:B:203:ARG:NH2  | 1:B:245:PHE:HD2  | 1.61                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:357:GLN:NE2  | 1:B:357:GLN:N    | 2.12                     | 0.97              |
| 1:E:149:LEU:HA   | 1:F:149:LEU:HD13 | 1.45                     | 0.97              |
| 1:B:270:LEU:HD11 | 1:B:333:LEU:HD13 | 1.46                     | 0.96              |
| 1:B:356:GLU:CG   | 1:B:357:GLN:NE2  | 2.27                     | 0.96              |
| 1:C:256:ARG:HA   | 1:C:259:ILE:CD1  | 1.96                     | 0.96              |
| 1:D:339:LEU:HD23 | 1:D:380:MSE:SE   | 2.15                     | 0.95              |
| 1:D:248:SER:HB2  | 1:D:318:TYR:CB   | 1.95                     | 0.95              |
| 1:B:338:ILE:CD1  | 1:B:351:GLU:HG2  | 1.97                     | 0.94              |
| 1:C:234:TYR:CE2  | 1:D:256:ARG:NH2  | 2.35                     | 0.94              |
| 1:B:305:GLY:CA   | 1:B:321:ARG:HH12 | 1.81                     | 0.94              |
| 1:D:380:MSE:SE   | 1:D:381:PRO:CD   | 2.66                     | 0.94              |
| 1:A:219:ALA:O    | 1:B:220:PHE:HE2  | 1.50                     | 0.93              |
| 1:C:234:TYR:HE2  | 1:D:256:ARG:NH2  | 1.65                     | 0.93              |
| 1:F:166:MSE:HE1  | 1:F:223:VAL:HA   | 1.47                     | 0.92              |
| 1:B:357:GLN:HE21 | 1:B:357:GLN:H    | 0.97                     | 0.92              |
| 1:C:156:GLN:HG3  | 1:D:152:LEU:HD11 | 1.53                     | 0.91              |
| 1:D:295:PHE:HD1  | 1:D:300:ALA:HB2  | 1.21                     | 0.91              |
| 1:D:338:ILE:HG21 | 1:D:351:GLU:HG3  | 1.53                     | 0.90              |
| 1:D:377:LEU:HD23 | 1:D:379:GLU:H    | 1.34                     | 0.90              |
| 1:C:339:LEU:HD22 | 1:C:345:ALA:HA   | 1.52                     | 0.90              |
| 1:B:203:ARG:NH2  | 1:B:245:PHE:CD2  | 2.40                     | 0.90              |
| 1:C:263:LEU:HD13 | 1:C:263:LEU:O    | 1.72                     | 0.89              |
| 1:D:248:SER:HB2  | 1:D:318:TYR:HB3  | 1.50                     | 0.89              |
| 1:D:329:PHE:N    | 1:D:391:ARG:O    | 2.04                     | 0.89              |
| 1:C:227:PHE:HE2  | 1:D:227:PHE:CE2  | 1.90                     | 0.89              |
| 1:C:263:LEU:HG   | 1:D:165:ASN:HB3  | 1.52                     | 0.89              |
| 1:C:285:ILE:HD13 | 1:C:291:LEU:HD22 | 1.53                     | 0.89              |
| 1:E:152:LEU:HD12 | 1:F:149:LEU:HD11 | 1.54                     | 0.89              |
| 1:B:356:GLU:HG2  | 1:B:357:GLN:HE22 | 1.37                     | 0.88              |
| 1:B:270:LEU:HD21 | 1:B:333:LEU:HB3  | 1.55                     | 0.87              |
| 1:C:263:LEU:CD2  | 1:D:165:ASN:HD22 | 1.86                     | 0.87              |
| 1:B:270:LEU:HD12 | 1:B:270:LEU:O    | 1.74                     | 0.86              |
| 1:C:255:ASN:OD1  | 1:C:259:ILE:HD11 | 1.75                     | 0.85              |
| 1:A:294:LEU:HB3  | 1:A:329:PHE:HZ   | 1.40                     | 0.85              |
| 1:D:263:LEU:HB3  | 1:D:265:LYS:HG2  | 1.58                     | 0.85              |
| 1:B:357:GLN:NE2  | 1:B:357:GLN:H    | 1.71                     | 0.84              |
| 1:C:160:ARG:CG   | 1:C:164:MSE:HE2  | 2.07                     | 0.84              |
| 1:C:283:TYR:HE2  | 1:C:323:MSE:HB2  | 1.43                     | 0.84              |
| 1:E:239:ASN:HB2  | 1:E:245:PHE:HB2  | 1.60                     | 0.84              |
| 1:F:198:ARG:HH21 | 1:F:201:GLU:HG3  | 1.43                     | 0.84              |
| 1:A:219:ALA:O    | 1:B:220:PHE:CE2  | 2.30                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:356:GLU:HG3  | 1:B:357:GLN:CD   | 2.02                     | 0.83              |
| 1:A:183:ILE:HD11 | 1:A:194:VAL:HG12 | 1.59                     | 0.83              |
| 1:E:166:MSE:HE2  | 1:E:226:LYS:HB3  | 1.59                     | 0.82              |
| 1:F:204:VAL:HB   | 1:F:274:ILE:HG22 | 1.60                     | 0.82              |
| 1:B:306:ARG:HH22 | 1:D:298:GLY:HA3  | 1.43                     | 0.82              |
| 1:D:296:VAL:HG12 | 1:D:297:GLU:HG2  | 1.58                     | 0.82              |
| 1:B:305:GLY:HA3  | 1:B:321:ARG:HH12 | 1.44                     | 0.82              |
| 1:C:326:PRO:HD2  | 1:C:329:PHE:HD1  | 1.45                     | 0.81              |
| 1:F:268:THR:HG23 | 1:F:287:GLY:HA3  | 1.61                     | 0.81              |
| 1:B:150:ASN:O    | 1:B:154:GLU:HG3  | 1.81                     | 0.80              |
| 1:C:183:ILE:HD11 | 1:C:194:VAL:HG12 | 1.63                     | 0.80              |
| 1:D:194:VAL:HG12 | 1:D:208:LEU:CD1  | 2.11                     | 0.80              |
| 1:F:183:ILE:HD11 | 1:F:194:VAL:HG12 | 1.63                     | 0.80              |
| 1:F:202:ARG:NH1  | 1:F:277:GLU:HB2  | 1.97                     | 0.80              |
| 1:D:363:GLY:N    | 1:D:368:LEU:HD23 | 1.97                     | 0.80              |
| 1:D:341:VAL:O    | 1:D:372:PHE:HE2  | 1.64                     | 0.80              |
| 1:A:365:LEU:HG   | 1:A:367:GLY:H    | 1.47                     | 0.79              |
| 1:A:380:MSE:HB3  | 1:A:381:PRO:CA   | 2.11                     | 0.79              |
| 1:E:367:GLY:HA2  | 1:E:370:GLN:HE21 | 1.46                     | 0.79              |
| 1:A:294:LEU:HB3  | 1:A:329:PHE:CZ   | 2.17                     | 0.79              |
| 1:C:255:ASN:O    | 1:C:259:ILE:CG1  | 2.28                     | 0.79              |
| 1:C:338:ILE:HG22 | 1:C:339:LEU:N    | 1.95                     | 0.79              |
| 1:E:374:LEU:HD23 | 1:E:374:LEU:H    | 1.47                     | 0.79              |
| 1:D:338:ILE:CG2  | 1:D:351:GLU:HG3  | 2.12                     | 0.79              |
| 1:C:202:ARG:NH1  | 1:C:277:GLU:OE2  | 2.17                     | 0.78              |
| 1:D:246:LYS:CB   | 1:D:249:GLU:CB   | 2.23                     | 0.78              |
| 1:E:380:MSE:N    | 1:E:381:PRO:HA   | 1.98                     | 0.78              |
| 1:B:305:GLY:HA2  | 1:B:321:ARG:HH12 | 1.48                     | 0.78              |
| 1:D:366:ASP:O    | 1:D:370:GLN:HB3  | 1.84                     | 0.78              |
| 1:D:363:GLY:N    | 1:D:368:LEU:CD2  | 2.47                     | 0.77              |
| 1:E:195:ASP:CG   | 1:E:197:PHE:HE2  | 1.91                     | 0.77              |
| 1:C:247:PRO:O    | 1:C:251:LEU:HD13 | 1.85                     | 0.77              |
| 1:D:248:SER:HB2  | 1:D:318:TYR:HB2  | 1.67                     | 0.77              |
| 1:C:149:LEU:HA   | 1:C:152:LEU:HD12 | 1.66                     | 0.77              |
| 1:C:247:PRO:HG3  | 1:C:273:VAL:HG22 | 1.66                     | 0.77              |
| 1:D:194:VAL:CG1  | 1:D:208:LEU:HD13 | 2.15                     | 0.77              |
| 1:B:147:ALA:HB3  | 1:B:150:ASN:HB2  | 1.67                     | 0.76              |
| 1:E:149:LEU:HA   | 1:F:149:LEU:CD1  | 2.16                     | 0.76              |
| 1:D:194:VAL:CG1  | 1:D:208:LEU:CD1  | 2.63                     | 0.76              |
| 1:B:316:ALA:HB1  | 1:B:318:TYR:HD2  | 1.50                     | 0.76              |
| 1:E:263:LEU:HD22 | 1:F:162:VAL:HG22 | 1.67                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:363:GLY:H    | 1:D:368:LEU:CD2  | 1.97                     | 0.76              |
| 1:D:294:LEU:HD23 | 1:D:303:LEU:HD21 | 1.67                     | 0.76              |
| 1:D:295:PHE:CZ   | 1:D:360:ALA:HA   | 2.21                     | 0.76              |
| 1:E:149:LEU:HD12 | 1:E:150:ASN:N    | 2.01                     | 0.76              |
| 1:B:296:VAL:HG22 | 1:B:297:GLU:HG2  | 1.68                     | 0.75              |
| 1:D:255:ASN:HB2  | 1:D:318:TYR:OH   | 1.86                     | 0.75              |
| 1:D:378:ALA:HB3  | 1:D:379:GLU:OE1  | 1.87                     | 0.74              |
| 1:C:227:PHE:HE2  | 1:D:227:PHE:CD2  | 2.04                     | 0.74              |
| 1:C:329:PHE:HE2  | 1:C:331:LEU:HB2  | 1.52                     | 0.74              |
| 1:D:245:PHE:O    | 1:D:246:LYS:HD2  | 1.87                     | 0.74              |
| 1:C:342:LEU:HD12 | 1:C:354:LEU:HD21 | 1.68                     | 0.74              |
| 1:D:246:LYS:CG   | 1:D:249:GLU:HB3  | 2.16                     | 0.74              |
| 1:E:242:LEU:HB2  | 1:E:243:PRO:HD2  | 1.69                     | 0.74              |
| 1:A:240:GLY:O    | 1:A:241:THR:HG22 | 1.88                     | 0.73              |
| 1:B:202:ARG:HG2  | 1:B:203:ARG:HG3  | 1.70                     | 0.73              |
| 1:D:246:LYS:CG   | 1:D:249:GLU:CB   | 2.67                     | 0.73              |
| 1:D:251:LEU:HG   | 1:D:269:MSE:HE3  | 1.70                     | 0.73              |
| 1:A:270:LEU:HD11 | 1:A:289:LEU:HD21 | 1.68                     | 0.73              |
| 1:C:255:ASN:OD1  | 1:C:259:ILE:CD1  | 2.35                     | 0.73              |
| 1:B:287:GLY:HA2  | 1:B:310:VAL:HG12 | 1.70                     | 0.73              |
| 1:A:268:THR:HG23 | 1:A:287:GLY:HA3  | 1.70                     | 0.73              |
| 1:C:263:LEU:HD21 | 1:D:165:ASN:HD22 | 1.54                     | 0.73              |
| 1:D:338:ILE:O    | 1:D:338:ILE:HG22 | 1.87                     | 0.73              |
| 1:C:160:ARG:O    | 1:C:164:MSE:HG2  | 1.89                     | 0.73              |
| 1:A:262:LYS:HE3  | 1:B:162:VAL:CG2  | 2.20                     | 0.72              |
| 1:E:195:ASP:CG   | 1:E:197:PHE:CE2  | 2.67                     | 0.72              |
| 1:C:175:GLU:HG3  | 1:C:276:LEU:HD23 | 1.70                     | 0.72              |
| 1:B:159:GLY:O    | 1:B:162:VAL:HG12 | 1.90                     | 0.72              |
| 1:C:160:ARG:HE   | 1:C:164:MSE:HE3  | 1.54                     | 0.72              |
| 1:D:263:LEU:HD22 | 1:D:265:LYS:HD3  | 1.71                     | 0.72              |
| 1:E:270:LEU:HD13 | 1:E:333:LEU:HD22 | 1.71                     | 0.72              |
| 1:B:365:LEU:HG   | 1:B:367:GLY:H    | 1.55                     | 0.72              |
| 1:C:220:PHE:O    | 1:C:223:VAL:HG22 | 1.90                     | 0.71              |
| 1:F:292:PRO:HB2  | 1:F:331:LEU:HD11 | 1.71                     | 0.71              |
| 1:A:251:LEU:HD23 | 1:A:318:TYR:HB3  | 1.71                     | 0.71              |
| 1:E:379:GLU:C    | 1:E:381:PRO:HA   | 2.15                     | 0.71              |
| 1:B:197:PHE:CE1  | 1:B:229:THR:HG21 | 2.25                     | 0.71              |
| 1:E:268:THR:OG1  | 1:E:287:GLY:HA3  | 1.90                     | 0.71              |
| 1:B:295:PHE:HB3  | 1:B:330:SER:HB3  | 1.72                     | 0.71              |
| 1:B:291:LEU:HD13 | 1:B:304:GLU:HG2  | 1.71                     | 0.71              |
| 1:C:179:PHE:CE1  | 1:C:389:LEU:HB3  | 2.25                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:167:LEU:HD13 | 1:D:183:ILE:HD12 | 1.71                     | 0.71              |
| 1:E:333:LEU:HD12 | 1:E:387:LEU:HD23 | 1.72                     | 0.71              |
| 1:C:227:PHE:CE2  | 1:D:227:PHE:CE2  | 2.76                     | 0.70              |
| 1:C:255:ASN:C    | 1:C:259:ILE:HG13 | 2.15                     | 0.70              |
| 1:D:341:VAL:O    | 1:D:372:PHE:CE2  | 2.45                     | 0.70              |
| 1:F:159:GLY:C    | 1:F:162:VAL:HG12 | 2.17                     | 0.70              |
| 1:F:289:LEU:HB2  | 1:F:290:PRO:HD2  | 1.73                     | 0.70              |
| 1:B:158:ALA:HA   | 1:B:161:GLN:HG2  | 1.74                     | 0.70              |
| 1:C:261:THR:HG23 | 1:C:261:THR:O    | 1.92                     | 0.70              |
| 1:F:197:PHE:CD2  | 1:F:233:LEU:HD11 | 2.27                     | 0.70              |
| 1:A:219:ALA:C    | 1:B:220:PHE:CE2  | 2.71                     | 0.69              |
| 1:B:316:ALA:HB1  | 1:B:318:TYR:CD2  | 2.27                     | 0.69              |
| 1:C:294:LEU:HD22 | 1:C:329:PHE:HZ   | 1.56                     | 0.69              |
| 1:A:227:PHE:HD1  | 1:B:262:LYS:HE2  | 1.55                     | 0.69              |
| 1:E:152:LEU:HD22 | 1:F:156:GLN:HG3  | 1.75                     | 0.69              |
| 1:C:369:ARG:O    | 1:C:372:PHE:HB2  | 1.93                     | 0.69              |
| 1:D:295:PHE:HD1  | 1:D:300:ALA:CB   | 2.02                     | 0.69              |
| 1:A:284:SER:HB2  | 1:A:319:ASP:O    | 1.93                     | 0.69              |
| 1:D:380:MSE:CE   | 1:D:381:PRO:HD2  | 2.23                     | 0.68              |
| 1:F:238:ARG:H    | 1:F:238:ARG:HD2  | 1.59                     | 0.68              |
| 1:F:392:ASN:O    | 1:F:393:LEU:HB2  | 1.93                     | 0.68              |
| 1:B:166:MSE:HE2  | 1:B:226:LYS:HB3  | 1.74                     | 0.68              |
| 1:D:179:PHE:CE1  | 1:D:389:LEU:HD13 | 2.28                     | 0.68              |
| 1:F:237:ARG:HE   | 1:F:237:ARG:HA   | 1.58                     | 0.68              |
| 1:C:256:ARG:CA   | 1:C:259:ILE:HD12 | 2.15                     | 0.68              |
| 1:F:159:GLY:O    | 1:F:162:VAL:HG12 | 1.92                     | 0.68              |
| 1:C:149:LEU:CD1  | 1:D:149:LEU:HG   | 2.24                     | 0.68              |
| 1:F:166:MSE:CE   | 1:F:223:VAL:HA   | 2.20                     | 0.68              |
| 1:F:166:MSE:HE1  | 1:F:223:VAL:HG13 | 1.76                     | 0.68              |
| 1:A:160:ARG:O    | 1:A:164:MSE:HG2  | 1.94                     | 0.68              |
| 1:A:333:LEU:HD12 | 1:A:387:LEU:HD23 | 1.76                     | 0.68              |
| 1:B:294:LEU:HD23 | 1:B:303:LEU:HD21 | 1.74                     | 0.68              |
| 1:C:259:ILE:HD13 | 1:C:314:ASP:HA   | 1.76                     | 0.67              |
| 1:A:223:VAL:HG21 | 1:B:220:PHE:CD2  | 2.28                     | 0.67              |
| 1:B:259:ILE:HD13 | 1:B:314:ASP:HA   | 1.73                     | 0.67              |
| 1:D:366:ASP:O    | 1:D:370:GLN:CB   | 2.42                     | 0.67              |
| 1:C:194:VAL:HG23 | 1:C:387:LEU:HD12 | 1.75                     | 0.67              |
| 1:D:194:VAL:HG12 | 1:D:208:LEU:HD12 | 1.74                     | 0.67              |
| 1:C:283:TYR:OH   | 1:C:323:MSE:HE2  | 1.94                     | 0.67              |
| 1:C:354:LEU:N    | 1:C:355:PRO:HD2  | 2.08                     | 0.67              |
| 1:E:289:LEU:HB2  | 1:E:290:PRO:HD2  | 1.77                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:215:GLY:HA3  | 1:B:155:ASP:OD2  | 1.95                     | 0.67              |
| 1:B:170:THR:HG21 | 1:B:181:HIS:H    | 1.59                     | 0.67              |
| 1:C:263:LEU:CD2  | 1:D:165:ASN:ND2  | 2.58                     | 0.67              |
| 1:E:167:LEU:HD23 | 1:E:181:HIS:CD2  | 2.28                     | 0.67              |
| 1:A:274:ILE:HB   | 1:A:281:LEU:HD13 | 1.78                     | 0.66              |
| 1:B:160:ARG:HG2  | 1:B:164:MSE:HE2  | 1.77                     | 0.66              |
| 1:E:160:ARG:O    | 1:E:164:MSE:HG2  | 1.95                     | 0.66              |
| 1:F:259:ILE:HG23 | 1:F:260:ASN:OD1  | 1.95                     | 0.66              |
| 1:C:342:LEU:CD1  | 1:C:354:LEU:HD21 | 2.24                     | 0.66              |
| 1:B:348:LYS:HD2  | 1:B:349:GLU:HG3  | 1.78                     | 0.66              |
| 1:C:326:PRO:HD2  | 1:C:329:PHE:CD1  | 2.28                     | 0.66              |
| 1:A:225:LEU:HD11 | 1:A:267:VAL:HG11 | 1.77                     | 0.66              |
| 1:C:295:PHE:CD2  | 1:C:364:THR:HG21 | 2.30                     | 0.66              |
| 1:F:392:ASN:O    | 1:F:393:LEU:HD13 | 1.96                     | 0.66              |
| 1:B:348:LYS:HD3  | 1:B:348:LYS:C    | 2.21                     | 0.66              |
| 1:D:166:MSE:HG2  | 1:D:193:PHE:CZ   | 2.31                     | 0.66              |
| 1:A:162:VAL:HG22 | 1:B:263:LEU:HD22 | 1.78                     | 0.66              |
| 1:C:338:ILE:CG2  | 1:C:339:LEU:N    | 2.58                     | 0.66              |
| 1:C:200:ASP:C    | 1:C:201:GLU:HG3  | 2.19                     | 0.66              |
| 1:F:294:LEU:O    | 1:F:300:ALA:HA   | 1.96                     | 0.66              |
| 1:D:194:VAL:HG12 | 1:D:208:LEU:HD13 | 1.74                     | 0.65              |
| 1:D:264:GLY:HA3  | 1:E:323:MSE:HA   | 1.77                     | 0.65              |
| 1:C:160:ARG:NE   | 1:C:164:MSE:HE3  | 2.11                     | 0.65              |
| 1:D:329:PHE:CE1  | 1:D:391:ARG:HB3  | 2.32                     | 0.65              |
| 1:F:203:ARG:NH2  | 1:F:245:PHE:HB2  | 2.11                     | 0.65              |
| 1:C:221:VAL:O    | 1:C:225:LEU:HG   | 1.97                     | 0.65              |
| 1:E:263:LEU:CD2  | 1:F:162:VAL:HG22 | 2.26                     | 0.65              |
| 1:B:306:ARG:NH2  | 1:D:298:GLY:HA3  | 2.10                     | 0.65              |
| 1:E:275:ASP:HB3  | 1:E:278:LYS:HG2  | 1.79                     | 0.65              |
| 1:C:212:SER:OG   | 1:C:265:LYS:HD3  | 1.96                     | 0.65              |
| 1:C:283:TYR:CE2  | 1:C:323:MSE:HB2  | 2.31                     | 0.65              |
| 1:A:220:PHE:HA   | 1:B:220:PHE:CD2  | 2.32                     | 0.64              |
| 1:A:220:PHE:CA   | 1:B:220:PHE:CE2  | 2.78                     | 0.64              |
| 1:D:334:PHE:CD2  | 1:D:386:LEU:HD22 | 2.32                     | 0.64              |
| 1:F:237:ARG:HA   | 1:F:237:ARG:NE   | 2.12                     | 0.64              |
| 1:A:311:GLY:HA3  | 1:A:318:TYR:OH   | 1.98                     | 0.64              |
| 1:A:259:ILE:O    | 1:A:260:ASN:HB3  | 1.97                     | 0.64              |
| 1:C:199:VAL:O    | 1:C:200:ASP:HB3  | 1.96                     | 0.64              |
| 1:F:392:ASN:C    | 1:F:393:LEU:CD1  | 2.71                     | 0.64              |
| 1:A:303:LEU:HD12 | 1:A:303:LEU:O    | 1.97                     | 0.64              |
| 1:C:202:ARG:HD2  | 1:C:202:ARG:O    | 1.97                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:174:ILE:HD12 | 1:D:174:ILE:O    | 1.98                     | 0.64              |
| 1:F:166:MSE:HE1  | 1:F:223:VAL:CA   | 2.23                     | 0.64              |
| 1:E:200:ASP:OD1  | 1:E:202:ARG:HG2  | 1.98                     | 0.64              |
| 1:F:247:PRO:HG3  | 1:F:273:VAL:HG12 | 1.80                     | 0.64              |
| 1:B:183:ILE:HG22 | 1:B:385:ALA:HB1  | 1.79                     | 0.63              |
| 1:B:305:GLY:HA2  | 1:B:321:ARG:NH1  | 2.13                     | 0.63              |
| 1:C:202:ARG:HA   | 1:C:276:LEU:HB2  | 1.79                     | 0.63              |
| 1:F:266:HIS:CG   | 1:F:312:LEU:HD23 | 2.34                     | 0.63              |
| 1:E:195:ASP:OD1  | 1:E:197:PHE:CE2  | 2.52                     | 0.63              |
| 1:C:356:GLU:HG3  | 1:C:357:GLN:N    | 2.12                     | 0.63              |
| 1:E:367:GLY:HA2  | 1:E:370:GLN:NE2  | 2.12                     | 0.63              |
| 1:A:223:VAL:CG2  | 1:B:220:PHE:CD2  | 2.82                     | 0.63              |
| 1:C:295:PHE:CG   | 1:C:364:THR:HG21 | 2.34                     | 0.63              |
| 1:D:246:LYS:HG2  | 1:D:249:GLU:HG2  | 1.81                     | 0.63              |
| 1:E:255:ASN:O    | 1:E:259:ILE:HG23 | 1.98                     | 0.63              |
| 1:B:356:GLU:OE2  | 1:B:357:GLN:OE1  | 2.16                     | 0.62              |
| 1:C:266:HIS:HB3  | 1:C:312:LEU:HD21 | 1.80                     | 0.62              |
| 1:A:285:ILE:HD11 | 1:A:305:GLY:C    | 2.23                     | 0.62              |
| 1:B:348:LYS:HD3  | 1:B:348:LYS:O    | 1.99                     | 0.62              |
| 1:C:199:VAL:O    | 1:C:199:VAL:HG12 | 1.99                     | 0.62              |
| 1:D:295:PHE:CE1  | 1:D:360:ALA:HA   | 2.33                     | 0.62              |
| 1:F:161:GLN:HA   | 1:F:164:MSE:HG3  | 1.80                     | 0.62              |
| 1:C:263:LEU:HD23 | 1:D:165:ASN:ND2  | 2.14                     | 0.62              |
| 1:D:244:GLU:OE1  | 1:D:247:PRO:HD3  | 1.99                     | 0.62              |
| 1:A:278:LYS:HE2  | 1:A:280:SER:HB3  | 1.82                     | 0.62              |
| 1:F:338:ILE:HD12 | 1:F:355:PRO:HG3  | 1.81                     | 0.62              |
| 1:B:305:GLY:CA   | 1:B:321:ARG:NH1  | 2.60                     | 0.62              |
| 1:F:260:ASN:O    | 1:F:261:THR:OG1  | 2.15                     | 0.62              |
| 1:D:244:GLU:OE1  | 1:D:244:GLU:O    | 2.17                     | 0.62              |
| 1:B:195:ASP:HB3  | 1:B:207:TYR:CE1  | 2.34                     | 0.62              |
| 1:B:309:PRO:O    | 1:B:310:VAL:HG22 | 2.00                     | 0.61              |
| 1:B:197:PHE:CE1  | 1:B:229:THR:CG2  | 2.83                     | 0.61              |
| 1:C:156:GLN:HG2  | 1:D:156:GLN:HE21 | 1.65                     | 0.61              |
| 1:F:256:ARG:O    | 1:F:259:ILE:HG22 | 2.00                     | 0.61              |
| 1:A:227:PHE:CE2  | 1:B:227:PHE:HE2  | 2.19                     | 0.61              |
| 1:B:160:ARG:O    | 1:B:164:MSE:HG2  | 2.00                     | 0.61              |
| 1:C:212:SER:HB3  | 1:C:266:HIS:CE1  | 2.35                     | 0.61              |
| 1:B:228:MSE:HE1  | 1:B:253:HIS:O    | 1.99                     | 0.61              |
| 1:B:291:LEU:HB2  | 1:B:302:TYR:CD1  | 2.35                     | 0.61              |
| 1:C:303:LEU:HD13 | 1:C:323:MSE:HE3  | 1.83                     | 0.61              |
| 1:A:219:ALA:CB   | 1:B:220:PHE:HZ   | 2.14                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:267:VAL:HG12 | 1:A:269:MSE:HG3  | 1.81                     | 0.61              |
| 1:D:197:PHE:CD2  | 1:D:233:LEU:HD11 | 2.36                     | 0.61              |
| 1:D:256:ARG:O    | 1:D:259:ILE:HG22 | 1.99                     | 0.61              |
| 1:B:338:ILE:HD12 | 1:B:351:GLU:HG3  | 1.80                     | 0.61              |
| 1:C:247:PRO:HG2  | 1:C:282:THR:HG22 | 1.83                     | 0.61              |
| 1:C:391:ARG:O    | 1:C:392:ASN:HB3  | 2.01                     | 0.61              |
| 1:B:202:ARG:NH1  | 1:B:203:ARG:HD2  | 2.15                     | 0.61              |
| 1:D:248:SER:CB   | 1:D:318:TYR:HB3  | 2.26                     | 0.61              |
| 1:A:227:PHE:CD2  | 1:B:227:PHE:HE2  | 2.19                     | 0.60              |
| 1:D:179:PHE:CD1  | 1:D:389:LEU:HD13 | 2.36                     | 0.60              |
| 1:D:177:LEU:HD23 | 1:D:391:ARG:HB2  | 1.84                     | 0.60              |
| 1:D:281:LEU:HD22 | 1:D:323:MSE:HE2  | 1.83                     | 0.60              |
| 1:E:369:ARG:O    | 1:E:372:PHE:CD1  | 2.54                     | 0.60              |
| 1:D:392:ASN:OD1  | 1:D:393:LEU:N    | 2.34                     | 0.60              |
| 1:E:210:ASP:O    | 1:E:268:THR:HG22 | 2.01                     | 0.60              |
| 1:A:268:THR:HG21 | 1:A:289:LEU:HB3  | 1.83                     | 0.60              |
| 1:B:264:GLY:O    | 1:D:324:GLU:HG2  | 2.02                     | 0.60              |
| 1:C:255:ASN:CG   | 1:C:259:ILE:HD11 | 2.25                     | 0.60              |
| 1:C:149:LEU:HD12 | 1:D:149:LEU:HA   | 1.82                     | 0.60              |
| 1:A:219:ALA:C    | 1:B:220:PHE:HE2  | 2.10                     | 0.60              |
| 1:C:212:SER:CB   | 1:C:266:HIS:CE1  | 2.84                     | 0.60              |
| 1:A:170:THR:HG21 | 1:A:181:HIS:H    | 1.66                     | 0.60              |
| 1:A:240:GLY:O    | 1:A:241:THR:CG2  | 2.50                     | 0.60              |
| 1:E:263:LEU:HD22 | 1:F:162:VAL:HG23 | 1.84                     | 0.60              |
| 1:B:181:HIS:HB2  | 1:B:194:VAL:HG21 | 1.84                     | 0.60              |
| 1:B:294:LEU:HA   | 1:B:331:LEU:HA   | 1.84                     | 0.60              |
| 1:C:202:ARG:HD3  | 1:C:277:GLU:HB3  | 1.83                     | 0.60              |
| 1:E:149:LEU:CA   | 1:F:149:LEU:HD13 | 2.27                     | 0.59              |
| 1:C:245:PHE:CE2  | 1:C:273:VAL:HG11 | 2.37                     | 0.59              |
| 1:C:294:LEU:HD22 | 1:C:329:PHE:CZ   | 2.37                     | 0.59              |
| 1:F:295:PHE:HB3  | 1:F:330:SER:HB2  | 1.84                     | 0.59              |
| 1:C:322:VAL:HG12 | 1:C:323:MSE:H    | 1.67                     | 0.59              |
| 1:D:286:GLY:O    | 1:D:310:VAL:HG22 | 2.01                     | 0.59              |
| 1:D:367:GLY:O    | 1:D:371:VAL:HG12 | 2.01                     | 0.59              |
| 1:F:328:SER:HA   | 1:F:391:ARG:O    | 2.03                     | 0.59              |
| 1:F:392:ASN:O    | 1:F:393:LEU:CB   | 2.51                     | 0.59              |
| 1:C:220:PHE:HB3  | 1:D:223:VAL:HG21 | 1.85                     | 0.59              |
| 1:C:306:ARG:HG2  | 1:C:307:GLY:H    | 1.67                     | 0.59              |
| 1:D:166:MSE:HG2  | 1:D:193:PHE:HZ   | 1.67                     | 0.59              |
| 1:E:339:LEU:HD13 | 1:E:340:ASP:N    | 2.18                     | 0.59              |
| 1:F:392:ASN:C    | 1:F:393:LEU:HD12 | 2.28                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:293:VAL:HG22 | 1:B:302:TYR:CE1  | 2.38                     | 0.58              |
| 1:C:256:ARG:O    | 1:C:260:ASN:N    | 2.32                     | 0.58              |
| 1:D:167:LEU:HD23 | 1:D:167:LEU:N    | 2.18                     | 0.58              |
| 1:C:149:LEU:HD23 | 1:C:149:LEU:C    | 2.28                     | 0.58              |
| 1:D:291:LEU:HD12 | 1:D:302:TYR:HB3  | 1.85                     | 0.58              |
| 1:E:149:LEU:CA   | 1:F:149:LEU:HD22 | 2.33                     | 0.58              |
| 1:E:270:LEU:HG   | 1:E:289:LEU:HD21 | 1.85                     | 0.58              |
| 1:E:195:ASP:HB3  | 1:E:207:TYR:CE1  | 2.37                     | 0.58              |
| 1:E:292:PRO:HB2  | 1:E:331:LEU:HD11 | 1.85                     | 0.58              |
| 1:B:196:TYR:HB3  | 1:B:206:PHE:HB3  | 1.84                     | 0.58              |
| 1:A:240:GLY:O    | 1:A:241:THR:CB   | 2.50                     | 0.58              |
| 1:C:234:TYR:HE2  | 1:D:256:ARG:HH22 | 1.49                     | 0.58              |
| 1:C:333:LEU:HD12 | 1:C:387:LEU:HB3  | 1.85                     | 0.58              |
| 1:B:354:LEU:N    | 1:B:355:PRO:HD2  | 2.18                     | 0.58              |
| 1:C:256:ARG:CA   | 1:C:259:ILE:CD1  | 2.78                     | 0.58              |
| 1:A:270:LEU:CD1  | 1:A:289:LEU:HD21 | 2.34                     | 0.58              |
| 1:E:243:PRO:HG3  | 1:E:246:LYS:HG2  | 1.86                     | 0.58              |
| 1:A:219:ALA:HB1  | 1:B:220:PHE:HZ   | 1.69                     | 0.58              |
| 1:A:232:LEU:HD21 | 1:A:253:HIS:CE1  | 2.39                     | 0.58              |
| 1:A:232:LEU:HD21 | 1:A:253:HIS:NE2  | 2.19                     | 0.58              |
| 1:A:382:ASP:OD1  | 1:A:383:ASP:N    | 2.37                     | 0.58              |
| 1:D:295:PHE:CE1  | 1:D:360:ALA:CB   | 2.87                     | 0.58              |
| 1:B:274:ILE:HD11 | 1:B:281:LEU:HG   | 1.86                     | 0.57              |
| 1:B:294:LEU:CD2  | 1:B:303:LEU:HD21 | 2.33                     | 0.57              |
| 1:B:380:MSE:HE3  | 1:B:381:PRO:HD2  | 1.86                     | 0.57              |
| 1:B:270:LEU:HD13 | 1:B:333:LEU:HD22 | 1.86                     | 0.57              |
| 1:F:174:ILE:O    | 1:F:174:ILE:HD12 | 2.04                     | 0.57              |
| 1:F:197:PHE:CE2  | 1:F:233:LEU:HD11 | 2.39                     | 0.57              |
| 1:E:149:LEU:HB3  | 1:F:149:LEU:HB2  | 1.87                     | 0.57              |
| 1:A:228:MSE:HE2  | 1:A:253:HIS:CD2  | 2.39                     | 0.57              |
| 1:E:274:ILE:HG22 | 1:E:281:LEU:HA   | 1.87                     | 0.57              |
| 1:B:177:LEU:HG   | 1:B:389:LEU:HD11 | 1.85                     | 0.57              |
| 1:C:156:GLN:HG3  | 1:D:152:LEU:CD1  | 2.32                     | 0.57              |
| 1:F:166:MSE:HE2  | 1:F:226:LYS:HB3  | 1.86                     | 0.57              |
| 1:C:149:LEU:HD13 | 1:D:149:LEU:HG   | 1.87                     | 0.56              |
| 1:E:181:HIS:CB   | 1:E:194:VAL:HG11 | 2.35                     | 0.56              |
| 1:A:247:PRO:HG3  | 1:A:273:VAL:HG12 | 1.86                     | 0.56              |
| 1:B:247:PRO:O    | 1:B:250:VAL:N    | 2.35                     | 0.56              |
| 1:D:385:ALA:O    | 1:D:386:LEU:HD23 | 2.05                     | 0.56              |
| 1:F:211:VAL:HG11 | 1:F:221:VAL:HG21 | 1.88                     | 0.56              |
| 1:A:220:PHE:HB3  | 1:B:223:VAL:HG21 | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:183:ILE:HG12 | 1:E:385:ALA:HB1  | 1.86                     | 0.56              |
| 1:F:157:ASN:O    | 1:F:161:GLN:HG2  | 2.04                     | 0.56              |
| 1:D:194:VAL:CG1  | 1:D:208:LEU:HD12 | 2.34                     | 0.56              |
| 1:E:291:LEU:HB3  | 1:E:292:PRO:HD2  | 1.87                     | 0.56              |
| 1:F:238:ARG:HD2  | 1:F:238:ARG:N    | 2.20                     | 0.56              |
| 1:F:150:ASN:O    | 1:F:154:GLU:HG3  | 2.05                     | 0.56              |
| 1:C:194:VAL:CG2  | 1:C:387:LEU:HD12 | 2.34                     | 0.56              |
| 1:E:152:LEU:CD1  | 1:F:149:LEU:HD11 | 2.29                     | 0.56              |
| 1:B:183:ILE:HG22 | 1:B:385:ALA:CB   | 2.36                     | 0.56              |
| 1:C:328:SER:HA   | 1:C:392:ASN:HB3  | 1.86                     | 0.56              |
| 1:D:295:PHE:CZ   | 1:D:360:ALA:CA   | 2.89                     | 0.56              |
| 1:E:149:LEU:N    | 1:F:149:LEU:HD22 | 2.20                     | 0.56              |
| 1:B:295:PHE:CE1  | 1:B:360:ALA:HA   | 2.41                     | 0.56              |
| 1:C:289:LEU:HD23 | 1:C:334:PHE:O    | 2.06                     | 0.56              |
| 1:C:338:ILE:CG2  | 1:C:339:LEU:H    | 2.19                     | 0.56              |
| 1:C:263:LEU:O    | 1:C:263:LEU:CD1  | 2.51                     | 0.56              |
| 1:B:206:PHE:CE2  | 1:B:274:ILE:HD13 | 2.40                     | 0.55              |
| 1:D:379:GLU:OE1  | 1:D:379:GLU:N    | 2.39                     | 0.55              |
| 1:F:267:VAL:O    | 1:F:310:VAL:HB   | 2.06                     | 0.55              |
| 1:C:184:ILE:HB   | 1:C:384:ILE:HG23 | 1.88                     | 0.55              |
| 1:C:285:ILE:HD12 | 1:C:305:GLY:HA3  | 1.87                     | 0.55              |
| 1:E:256:ARG:O    | 1:E:259:ILE:HG13 | 2.06                     | 0.55              |
| 1:D:181:HIS:ND1  | 1:D:196:TYR:HE1  | 2.04                     | 0.55              |
| 1:F:392:ASN:O    | 1:F:393:LEU:CD1  | 2.53                     | 0.55              |
| 1:F:243:PRO:HD2  | 1:F:245:PHE:CZ   | 2.42                     | 0.55              |
| 1:F:246:LYS:O    | 1:F:250:VAL:HG23 | 2.07                     | 0.55              |
| 1:C:170:THR:HG21 | 1:C:181:HIS:H    | 1.71                     | 0.55              |
| 1:D:244:GLU:O    | 1:D:244:GLU:CD   | 2.49                     | 0.55              |
| 1:F:392:ASN:CG   | 1:F:393:LEU:HD12 | 2.31                     | 0.55              |
| 1:A:232:LEU:HD21 | 1:A:253:HIS:CD2  | 2.41                     | 0.55              |
| 1:C:368:LEU:O    | 1:C:371:VAL:HB   | 2.07                     | 0.55              |
| 1:D:251:LEU:HB3  | 1:D:318:TYR:CE1  | 2.41                     | 0.55              |
| 1:F:224:LEU:O    | 1:F:228:MSE:HG3  | 2.07                     | 0.55              |
| 1:F:334:PHE:HE2  | 1:F:386:LEU:HD22 | 1.71                     | 0.55              |
| 1:A:174:ILE:HD12 | 1:A:174:ILE:O    | 2.06                     | 0.55              |
| 1:C:338:ILE:HG22 | 1:C:339:LEU:H    | 1.71                     | 0.55              |
| 1:E:274:ILE:HG22 | 1:E:281:LEU:HG   | 1.89                     | 0.55              |
| 1:B:347:LEU:HG   | 1:B:350:LYS:HD3  | 1.89                     | 0.55              |
| 1:D:183:ILE:HD11 | 1:D:194:VAL:HG22 | 1.89                     | 0.55              |
| 1:D:270:LEU:CD2  | 1:D:285:ILE:HD13 | 2.26                     | 0.55              |
| 1:E:167:LEU:HD21 | 1:E:183:ILE:HD12 | 1.89                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:219:ALA:C    | 1:B:220:PHE:CZ   | 2.85                     | 0.55              |
| 1:D:225:LEU:HD11 | 1:D:267:VAL:HG11 | 1.88                     | 0.55              |
| 1:B:247:PRO:HD2  | 1:B:320:ASP:OD2  | 2.06                     | 0.54              |
| 1:B:330:SER:OG   | 1:B:364:THR:CG2  | 2.55                     | 0.54              |
| 1:C:279:ASN:O    | 1:C:325:LEU:HG   | 2.06                     | 0.54              |
| 1:F:392:ASN:CG   | 1:F:393:LEU:CD1  | 2.80                     | 0.54              |
| 1:D:224:LEU:O    | 1:D:228:MSE:HG3  | 2.06                     | 0.54              |
| 1:D:265:LYS:HD2  | 1:E:324:GLU:HG3  | 1.90                     | 0.54              |
| 1:D:295:PHE:CD1  | 1:D:300:ALA:CB   | 2.77                     | 0.54              |
| 1:C:195:ASP:HB3  | 1:C:207:TYR:CE1  | 2.42                     | 0.54              |
| 1:D:268:THR:CG2  | 1:D:289:LEU:HD12 | 2.37                     | 0.54              |
| 1:F:177:LEU:HB3  | 1:F:389:LEU:HD11 | 1.89                     | 0.54              |
| 1:C:338:ILE:C    | 1:C:339:LEU:HG   | 2.33                     | 0.54              |
| 1:D:206:PHE:CE2  | 1:D:333:LEU:HD11 | 2.43                     | 0.54              |
| 1:E:210:ASP:HB3  | 1:E:268:THR:HG23 | 1.90                     | 0.54              |
| 1:E:380:MSE:N    | 1:E:381:PRO:CA   | 2.69                     | 0.54              |
| 1:F:341:VAL:HG13 | 1:F:342:LEU:HD12 | 1.89                     | 0.54              |
| 1:A:247:PRO:HB2  | 1:A:284:SER:HB3  | 1.90                     | 0.54              |
| 1:B:159:GLY:C    | 1:B:162:VAL:HG12 | 2.32                     | 0.54              |
| 1:C:175:GLU:HG3  | 1:C:276:LEU:CD2  | 2.36                     | 0.54              |
| 1:C:270:LEU:HD23 | 1:C:285:ILE:HG23 | 1.89                     | 0.54              |
| 1:D:377:LEU:CD2  | 1:D:379:GLU:H    | 2.14                     | 0.54              |
| 1:E:159:GLY:O    | 1:E:162:VAL:HG22 | 2.07                     | 0.54              |
| 1:C:224:LEU:C    | 1:C:224:LEU:HD23 | 2.31                     | 0.54              |
| 1:D:300:ALA:HB3  | 1:D:356:GLU:O    | 2.08                     | 0.54              |
| 1:E:291:LEU:HD13 | 1:E:303:LEU:O    | 2.08                     | 0.54              |
| 1:E:294:LEU:HD12 | 1:E:294:LEU:O    | 2.08                     | 0.54              |
| 1:A:323:MSE:HG2  | 1:A:324:GLU:N    | 2.23                     | 0.54              |
| 1:A:331:LEU:HD12 | 1:A:332:SER:H    | 1.71                     | 0.54              |
| 1:C:328:SER:HA   | 1:C:391:ARG:O    | 2.08                     | 0.53              |
| 1:D:366:ASP:O    | 1:D:370:GLN:N    | 2.31                     | 0.53              |
| 1:B:292:PRO:HB2  | 1:B:331:LEU:HD11 | 1.89                     | 0.53              |
| 1:C:295:PHE:HB3  | 1:C:330:SER:OG   | 2.08                     | 0.53              |
| 1:C:387:LEU:C    | 1:C:387:LEU:HD23 | 2.34                     | 0.53              |
| 1:D:285:ILE:HD11 | 1:D:289:LEU:CD1  | 2.38                     | 0.53              |
| 1:D:363:GLY:CA   | 1:D:368:LEU:HD23 | 2.38                     | 0.53              |
| 1:B:167:LEU:HD13 | 1:B:181:HIS:CE1  | 2.43                     | 0.53              |
| 1:A:187:LEU:HD11 | 1:A:380:MSE:SE   | 2.58                     | 0.53              |
| 1:C:212:SER:HB2  | 1:C:266:HIS:CE1  | 2.44                     | 0.53              |
| 1:C:278:LYS:O    | 1:C:279:ASN:HB2  | 2.09                     | 0.53              |
| 1:B:199:VAL:HG22 | 1:B:233:LEU:HD21 | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:368:LEU:O    | 1:B:371:VAL:HG22 | 2.09                     | 0.53              |
| 1:C:200:ASP:O    | 1:C:201:GLU:CB   | 2.56                     | 0.53              |
| 1:E:163:GLN:O    | 1:E:167:LEU:HD13 | 2.09                     | 0.53              |
| 1:A:262:LYS:HE3  | 1:B:162:VAL:HG22 | 1.91                     | 0.53              |
| 1:D:393:LEU:O    | 1:D:393:LEU:HG   | 2.08                     | 0.53              |
| 1:C:224:LEU:HD21 | 1:C:228:MSE:SE   | 2.59                     | 0.52              |
| 1:D:263:LEU:HD23 | 1:D:263:LEU:O    | 2.08                     | 0.52              |
| 1:C:217:SER:HB3  | 1:D:158:ALA:HB1  | 1.91                     | 0.52              |
| 1:C:295:PHE:CE1  | 1:C:298:GLY:HA2  | 2.45                     | 0.52              |
| 1:E:232:LEU:HD11 | 1:E:253:HIS:CD2  | 2.45                     | 0.52              |
| 1:E:328:SER:HA   | 1:E:391:ARG:O    | 2.08                     | 0.52              |
| 1:E:354:LEU:N    | 1:E:355:PRO:CD   | 2.72                     | 0.52              |
| 1:F:334:PHE:HE2  | 1:F:386:LEU:CD2  | 2.21                     | 0.52              |
| 1:A:270:LEU:HD13 | 1:A:333:LEU:HD22 | 1.92                     | 0.52              |
| 1:A:292:PRO:HG2  | 1:A:303:LEU:HD21 | 1.90                     | 0.52              |
| 1:C:149:LEU:CD1  | 1:D:149:LEU:HA   | 2.39                     | 0.52              |
| 1:D:377:LEU:HD23 | 1:D:379:GLU:N    | 2.15                     | 0.52              |
| 1:F:183:ILE:HG12 | 1:F:385:ALA:HB1  | 1.91                     | 0.52              |
| 1:B:270:LEU:CD1  | 1:B:333:LEU:HD22 | 2.39                     | 0.52              |
| 1:B:330:SER:OG   | 1:B:364:THR:HG22 | 2.09                     | 0.52              |
| 1:F:285:ILE:HD13 | 1:F:291:LEU:CD2  | 2.40                     | 0.52              |
| 1:A:183:ILE:HG12 | 1:A:385:ALA:HB1  | 1.92                     | 0.52              |
| 1:C:281:LEU:HB2  | 1:C:325:LEU:HD21 | 1.92                     | 0.52              |
| 1:A:240:GLY:O    | 1:A:241:THR:HB   | 2.09                     | 0.52              |
| 1:B:386:LEU:HD12 | 1:B:386:LEU:C    | 2.35                     | 0.52              |
| 1:D:187:LEU:HD23 | 1:D:214:HIS:CD2  | 2.45                     | 0.52              |
| 1:B:203:ARG:HH22 | 1:B:245:PHE:HD2  | 1.56                     | 0.52              |
| 1:E:310:VAL:N    | 1:E:318:TYR:HE1  | 2.08                     | 0.52              |
| 1:C:295:PHE:HE1  | 1:C:298:GLY:HA2  | 1.75                     | 0.51              |
| 1:F:337:GLY:O    | 1:F:384:ILE:HD13 | 2.10                     | 0.51              |
| 1:B:247:PRO:O    | 1:B:248:SER:C    | 2.53                     | 0.51              |
| 1:F:243:PRO:HD2  | 1:F:245:PHE:CE2  | 2.45                     | 0.51              |
| 1:D:381:PRO:HG2  | 1:D:382:ASP:H    | 1.75                     | 0.51              |
| 1:E:177:LEU:HD22 | 1:E:389:LEU:HD11 | 1.91                     | 0.51              |
| 1:D:355:PRO:HA   | 1:D:358:VAL:HG12 | 1.91                     | 0.51              |
| 1:E:268:THR:OG1  | 1:E:289:LEU:HD12 | 2.10                     | 0.51              |
| 1:A:227:PHE:CD2  | 1:B:227:PHE:CE2  | 2.99                     | 0.51              |
| 1:A:254:ILE:HG21 | 1:A:269:MSE:HE1  | 1.91                     | 0.51              |
| 1:B:179:PHE:HE1  | 1:B:206:PHE:CD2  | 2.28                     | 0.51              |
| 1:A:200:ASP:OD1  | 1:A:202:ARG:HB2  | 2.10                     | 0.51              |
| 1:C:212:SER:OG   | 1:C:265:LYS:CD   | 2.59                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:215:GLY:HA3  | 1:D:155:ASP:OD1  | 2.10                     | 0.51              |
| 1:D:175:GLU:HB2  | 1:D:276:LEU:HD23 | 1.91                     | 0.51              |
| 1:B:250:VAL:O    | 1:B:254:ILE:HG12 | 2.11                     | 0.51              |
| 1:C:286:GLY:O    | 1:C:310:VAL:HB   | 2.11                     | 0.51              |
| 1:A:334:PHE:HE2  | 1:A:386:LEU:HD22 | 1.75                     | 0.51              |
| 1:D:181:HIS:HB2  | 1:D:194:VAL:HG21 | 1.93                     | 0.51              |
| 1:D:294:LEU:HA   | 1:D:331:LEU:HA   | 1.93                     | 0.51              |
| 1:E:167:LEU:HD23 | 1:E:181:HIS:NE2  | 2.25                     | 0.51              |
| 1:E:163:GLN:O    | 1:E:167:LEU:CD1  | 2.59                     | 0.51              |
| 1:A:340:ASP:OD2  | 1:A:354:LEU:HD23 | 2.11                     | 0.50              |
| 1:B:161:GLN:HG3  | 1:B:162:VAL:N    | 2.26                     | 0.50              |
| 1:B:206:PHE:CZ   | 1:B:274:ILE:HD13 | 2.47                     | 0.50              |
| 1:E:160:ARG:HG2  | 1:E:164:MSE:HE2  | 1.94                     | 0.50              |
| 1:B:166:MSE:HE1  | 1:B:223:VAL:HG13 | 1.93                     | 0.50              |
| 1:D:174:ILE:HG13 | 1:D:179:PHE:HE2  | 1.76                     | 0.50              |
| 1:A:295:PHE:CE1  | 1:A:364:THR:HB   | 2.46                     | 0.50              |
| 1:C:258:LEU:HD11 | 1:C:267:VAL:HG23 | 1.93                     | 0.50              |
| 1:A:227:PHE:CD1  | 1:B:262:LYS:HE2  | 2.43                     | 0.50              |
| 1:C:197:PHE:CE1  | 1:C:233:LEU:HD11 | 2.47                     | 0.50              |
| 1:C:329:PHE:CE2  | 1:C:331:LEU:HB2  | 2.40                     | 0.50              |
| 1:D:270:LEU:HD13 | 1:D:333:LEU:HD22 | 1.94                     | 0.50              |
| 1:A:182:ARG:NH1  | 1:A:370:GLN:HG2  | 2.27                     | 0.50              |
| 1:C:279:ASN:O    | 1:C:325:LEU:CG   | 2.59                     | 0.50              |
| 1:D:170:THR:HG21 | 1:D:181:HIS:H    | 1.77                     | 0.50              |
| 1:D:174:ILE:CG1  | 1:D:179:PHE:HE2  | 2.25                     | 0.50              |
| 1:E:294:LEU:HD12 | 1:E:294:LEU:C    | 2.37                     | 0.50              |
| 1:A:262:LYS:HD2  | 1:A:263:LEU:H    | 1.76                     | 0.50              |
| 1:D:262:LYS:C    | 1:D:264:GLY:H    | 2.20                     | 0.50              |
| 1:A:294:LEU:HD22 | 1:A:329:PHE:CZ   | 2.47                     | 0.50              |
| 1:E:183:ILE:HG12 | 1:E:385:ALA:CB   | 2.41                     | 0.50              |
| 1:A:324:GLU:OE1  | 1:A:324:GLU:HA   | 2.12                     | 0.49              |
| 1:B:294:LEU:HD23 | 1:B:303:LEU:HD11 | 1.94                     | 0.49              |
| 1:E:274:ILE:CG2  | 1:E:281:LEU:HG   | 2.42                     | 0.49              |
| 1:E:366:ASP:O    | 1:E:370:GLN:HG2  | 2.12                     | 0.49              |
| 1:C:179:PHE:HE1  | 1:C:389:LEU:HB3  | 1.76                     | 0.49              |
| 1:C:255:ASN:C    | 1:C:259:ILE:CG1  | 2.81                     | 0.49              |
| 1:E:197:PHE:CD2  | 1:E:197:PHE:N    | 2.79                     | 0.49              |
| 1:E:270:LEU:HD21 | 1:E:285:ILE:HD12 | 1.93                     | 0.49              |
| 1:D:255:ASN:OD1  | 1:D:311:GLY:HA2  | 2.12                     | 0.49              |
| 1:A:366:ASP:O    | 1:A:370:GLN:HG3  | 2.13                     | 0.49              |
| 1:B:211:VAL:HB   | 1:B:218:SER:HB2  | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:297:GLU:O    | 1:C:299:GLN:HG2  | 2.13                     | 0.49              |
| 1:C:322:VAL:HG12 | 1:C:323:MSE:N    | 2.26                     | 0.49              |
| 1:D:366:ASP:OD1  | 1:D:388:VAL:HB   | 2.13                     | 0.49              |
| 1:E:153:GLN:HG3  | 1:F:152:LEU:HD11 | 1.95                     | 0.49              |
| 1:B:217:SER:HB2  | 1:B:265:LYS:HZ1  | 1.77                     | 0.49              |
| 1:C:166:MSE:HE1  | 1:C:223:VAL:HB   | 1.95                     | 0.49              |
| 1:C:217:SER:HB3  | 1:D:158:ALA:C    | 2.37                     | 0.49              |
| 1:E:330:SER:HB3  | 1:E:364:THR:HG21 | 1.95                     | 0.49              |
| 1:B:197:PHE:HE1  | 1:B:229:THR:HG21 | 1.73                     | 0.49              |
| 1:B:263:LEU:HB2  | 1:B:265:LYS:HG2  | 1.94                     | 0.49              |
| 1:C:160:ARG:NE   | 1:C:164:MSE:CE   | 2.75                     | 0.49              |
| 1:E:340:ASP:OD1  | 1:E:340:ASP:C    | 2.56                     | 0.49              |
| 1:E:391:ARG:O    | 1:E:392:ASN:HB3  | 2.13                     | 0.49              |
| 1:F:291:LEU:HB3  | 1:F:292:PRO:HD2  | 1.95                     | 0.49              |
| 1:C:200:ASP:O    | 1:C:200:ASP:CG   | 2.55                     | 0.49              |
| 1:C:262:LYS:O    | 1:C:263:LEU:HB3  | 2.13                     | 0.49              |
| 1:C:275:ASP:HB3  | 1:C:278:LYS:CB   | 2.42                     | 0.49              |
| 1:C:294:LEU:CD2  | 1:C:303:LEU:HD21 | 2.43                     | 0.49              |
| 1:C:228:MSE:O    | 1:C:232:LEU:HD13 | 2.12                     | 0.49              |
| 1:A:199:VAL:HB   | 1:A:203:ARG:O    | 2.13                     | 0.49              |
| 1:C:216:ALA:N    | 1:D:155:ASP:OD1  | 2.42                     | 0.49              |
| 1:C:256:ARG:HA   | 1:C:259:ILE:CG1  | 2.43                     | 0.49              |
| 1:C:389:LEU:HD12 | 1:C:389:LEU:O    | 2.12                     | 0.49              |
| 1:D:206:PHE:HE2  | 1:D:333:LEU:HD11 | 1.77                     | 0.49              |
| 1:C:283:TYR:HE2  | 1:C:323:MSE:CB   | 2.22                     | 0.48              |
| 1:D:186:SER:O    | 1:D:187:LEU:HD13 | 2.13                     | 0.48              |
| 1:F:334:PHE:CD2  | 1:F:386:LEU:HB3  | 2.48                     | 0.48              |
| 1:A:172:TRP:HH2  | 1:A:198:ARG:HG3  | 1.76                     | 0.48              |
| 1:B:179:PHE:CE1  | 1:B:206:PHE:CD2  | 3.02                     | 0.48              |
| 1:C:340:ASP:OD2  | 1:C:384:ILE:HD12 | 2.14                     | 0.48              |
| 1:E:243:PRO:HG3  | 1:E:246:LYS:CG   | 2.42                     | 0.48              |
| 1:E:367:GLY:HA2  | 1:E:370:GLN:HG2  | 1.94                     | 0.48              |
| 1:F:228:MSE:O    | 1:F:232:LEU:HG   | 2.13                     | 0.48              |
| 1:F:268:THR:HG21 | 1:F:289:LEU:HB3  | 1.95                     | 0.48              |
| 1:C:201:GLU:O    | 1:C:202:ARG:HB3  | 2.14                     | 0.48              |
| 1:F:183:ILE:HG23 | 1:F:385:ALA:HB2  | 1.94                     | 0.48              |
| 1:B:328:SER:HA   | 1:B:391:ARG:O    | 2.13                     | 0.48              |
| 1:D:363:GLY:H    | 1:D:368:LEU:HD22 | 1.76                     | 0.48              |
| 1:E:158:ALA:HB1  | 1:F:217:SER:HB3  | 1.95                     | 0.48              |
| 1:E:242:LEU:HD23 | 1:E:242:LEU:H    | 1.79                     | 0.48              |
| 1:F:170:THR:HG22 | 1:F:196:TYR:OH   | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:256:ARG:C    | 1:F:259:ILE:HG22 | 2.38                     | 0.48              |
| 1:A:181:HIS:HD1  | 1:A:196:TYR:HE1  | 1.62                     | 0.48              |
| 1:B:270:LEU:HD11 | 1:B:333:LEU:CD1  | 2.31                     | 0.48              |
| 1:C:342:LEU:HD12 | 1:C:354:LEU:CD2  | 2.40                     | 0.48              |
| 1:D:249:GLU:HA   | 1:D:252:ALA:HB3  | 1.95                     | 0.48              |
| 1:D:341:VAL:C    | 1:D:372:PHE:CE2  | 2.92                     | 0.48              |
| 1:A:283:TYR:CE1  | 1:A:303:LEU:HD13 | 2.48                     | 0.48              |
| 1:C:209:ALA:HB2  | 1:C:269:MSE:HG2  | 1.95                     | 0.48              |
| 1:C:255:ASN:OD1  | 1:C:259:ILE:CG1  | 2.61                     | 0.48              |
| 1:D:197:PHE:CE2  | 1:D:233:LEU:HD11 | 2.48                     | 0.48              |
| 1:E:153:GLN:HG3  | 1:F:152:LEU:CD1  | 2.43                     | 0.48              |
| 1:E:292:PRO:HB3  | 1:E:333:LEU:HD23 | 1.94                     | 0.48              |
| 1:A:292:PRO:HD2  | 1:A:303:LEU:HG   | 1.96                     | 0.48              |
| 1:B:194:VAL:CG1  | 1:B:208:LEU:HD13 | 2.44                     | 0.48              |
| 1:B:348:LYS:C    | 1:B:348:LYS:CD   | 2.86                     | 0.48              |
| 1:A:365:LEU:HG   | 1:A:366:ASP:N    | 2.29                     | 0.48              |
| 1:B:339:LEU:O    | 1:B:340:ASP:C    | 2.55                     | 0.48              |
| 1:C:179:PHE:CD1  | 1:C:389:LEU:HB3  | 2.48                     | 0.48              |
| 1:E:211:VAL:HG22 | 1:E:267:VAL:HG22 | 1.95                     | 0.48              |
| 1:A:294:LEU:CB   | 1:A:329:PHE:HZ   | 2.17                     | 0.48              |
| 1:B:296:VAL:O    | 1:B:296:VAL:HG13 | 2.13                     | 0.48              |
| 1:C:246:LYS:HB2  | 1:C:249:GLU:HG3  | 1.95                     | 0.48              |
| 1:F:295:PHE:HA   | 1:F:299:GLN:O    | 2.13                     | 0.48              |
| 1:B:270:LEU:CD1  | 1:B:333:LEU:HD13 | 2.31                     | 0.48              |
| 1:E:181:HIS:HB2  | 1:E:194:VAL:HG11 | 1.96                     | 0.48              |
| 1:A:248:SER:HB3  | 1:A:319:ASP:O    | 2.14                     | 0.47              |
| 1:D:163:GLN:O    | 1:D:167:LEU:CD2  | 2.62                     | 0.47              |
| 1:B:363:GLY:N    | 1:B:368:LEU:HD22 | 2.28                     | 0.47              |
| 1:C:200:ASP:O    | 1:C:201:GLU:CG   | 2.62                     | 0.47              |
| 1:D:276:LEU:N    | 1:D:276:LEU:HD12 | 2.29                     | 0.47              |
| 1:E:210:ASP:HB3  | 1:E:268:THR:CG2  | 2.43                     | 0.47              |
| 1:A:261:THR:O    | 1:A:261:THR:HG22 | 2.14                     | 0.47              |
| 1:A:303:LEU:HD12 | 1:A:303:LEU:C    | 2.39                     | 0.47              |
| 1:A:354:LEU:N    | 1:A:355:PRO:CD   | 2.77                     | 0.47              |
| 1:B:294:LEU:HD12 | 1:B:294:LEU:C    | 2.39                     | 0.47              |
| 1:E:354:LEU:N    | 1:E:355:PRO:HD3  | 2.29                     | 0.47              |
| 1:A:197:PHE:CE2  | 1:A:233:LEU:HD11 | 2.49                     | 0.47              |
| 1:C:216:ALA:O    | 1:C:220:PHE:CD1  | 2.67                     | 0.47              |
| 1:C:279:ASN:C    | 1:C:325:LEU:HD12 | 2.39                     | 0.47              |
| 1:F:386:LEU:O    | 1:F:386:LEU:HD12 | 2.14                     | 0.47              |
| 1:C:184:ILE:HB   | 1:C:384:ILE:CG2  | 2.44                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:338:ILE:CG2  | 1:D:338:ILE:O    | 2.59                     | 0.47              |
| 1:F:289:LEU:HD23 | 1:F:334:PHE:O    | 2.14                     | 0.47              |
| 1:B:268:THR:HG1  | 1:B:287:GLY:HA3  | 1.75                     | 0.47              |
| 1:E:173:SER:HA   | 1:E:177:LEU:O    | 2.14                     | 0.47              |
| 1:E:225:LEU:O    | 1:E:229:THR:HG23 | 2.14                     | 0.47              |
| 1:E:294:LEU:HB3  | 1:E:331:LEU:HD13 | 1.96                     | 0.47              |
| 1:A:285:ILE:HD11 | 1:A:305:GLY:O    | 2.15                     | 0.47              |
| 1:A:302:TYR:CD1  | 1:A:302:TYR:C    | 2.92                     | 0.47              |
| 1:B:206:PHE:CZ   | 1:B:389:LEU:HD22 | 2.49                     | 0.47              |
| 1:C:174:ILE:HG13 | 1:C:175:GLU:HG2  | 1.95                     | 0.47              |
| 1:C:179:PHE:CE1  | 1:C:389:LEU:CB   | 2.96                     | 0.47              |
| 1:B:181:HIS:CB   | 1:B:194:VAL:HG21 | 2.45                     | 0.47              |
| 1:F:270:LEU:HD11 | 1:F:289:LEU:HD21 | 1.97                     | 0.47              |
| 1:E:224:LEU:O    | 1:E:228:MSE:HG3  | 2.14                     | 0.47              |
| 1:A:159:GLY:O    | 1:A:162:VAL:HG12 | 2.15                     | 0.47              |
| 1:D:211:VAL:HB   | 1:D:218:SER:HB2  | 1.97                     | 0.47              |
| 1:F:166:MSE:HE1  | 1:F:223:VAL:CG1  | 2.44                     | 0.47              |
| 1:F:198:ARG:NH2  | 1:F:201:GLU:HG3  | 2.22                     | 0.47              |
| 1:F:335:SER:HB2  | 1:F:384:ILE:HD12 | 1.96                     | 0.47              |
| 1:B:169:VAL:HG22 | 1:B:170:THR:N    | 2.30                     | 0.46              |
| 1:C:181:HIS:HB2  | 1:C:194:VAL:HG11 | 1.97                     | 0.46              |
| 1:C:391:ARG:O    | 1:C:392:ASN:CB   | 2.63                     | 0.46              |
| 1:E:228:MSE:HE2  | 1:E:253:HIS:CD2  | 2.50                     | 0.46              |
| 1:D:204:VAL:HG23 | 1:D:276:LEU:HD11 | 1.97                     | 0.46              |
| 1:F:329:PHE:HE1  | 1:F:391:ARG:HD2  | 1.80                     | 0.46              |
| 1:B:284:SER:HB2  | 1:B:320:ASP:HB3  | 1.97                     | 0.46              |
| 1:B:291:LEU:O    | 1:B:302:TYR:HE1  | 1.99                     | 0.46              |
| 1:C:192:ASP:OD1  | 1:C:210:ASP:OD1  | 2.33                     | 0.46              |
| 1:D:345:ALA:O    | 1:D:346:THR:HB   | 2.14                     | 0.46              |
| 1:F:338:ILE:HG23 | 1:F:339:LEU:N    | 2.31                     | 0.46              |
| 1:A:348:LYS:HG3  | 1:A:349:GLU:N    | 2.30                     | 0.46              |
| 1:A:177:LEU:HD23 | 1:A:391:ARG:HB2  | 1.98                     | 0.46              |
| 1:B:386:LEU:HD12 | 1:B:386:LEU:O    | 2.16                     | 0.46              |
| 1:C:294:LEU:HD13 | 1:C:329:PHE:CZ   | 2.51                     | 0.46              |
| 1:D:340:ASP:O    | 1:D:341:VAL:O    | 2.33                     | 0.46              |
| 1:C:262:LYS:O    | 1:C:263:LEU:CB   | 2.63                     | 0.46              |
| 1:D:163:GLN:O    | 1:D:167:LEU:HD21 | 2.16                     | 0.46              |
| 1:E:266:HIS:HB3  | 1:E:312:LEU:HB3  | 1.98                     | 0.46              |
| 1:F:160:ARG:HE   | 1:F:164:MSE:HE2  | 1.81                     | 0.46              |
| 1:D:175:GLU:HG3  | 1:D:276:LEU:CD2  | 2.46                     | 0.46              |
| 1:F:202:ARG:HH11 | 1:F:277:GLU:HB2  | 1.79                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:270:LEU:CD1  | 1:F:289:LEU:HD21 | 2.46                     | 0.46              |
| 1:F:274:ILE:HD11 | 1:F:325:LEU:HD11 | 1.98                     | 0.46              |
| 1:F:329:PHE:CE1  | 1:F:391:ARG:HD2  | 2.51                     | 0.46              |
| 1:F:354:LEU:N    | 1:F:355:PRO:CD   | 2.78                     | 0.46              |
| 1:B:177:LEU:CG   | 1:B:389:LEU:HD11 | 2.46                     | 0.46              |
| 1:C:224:LEU:HD22 | 1:C:225:LEU:HD23 | 1.98                     | 0.46              |
| 1:C:246:LYS:HB3  | 1:C:320:ASP:OD2  | 2.15                     | 0.46              |
| 1:D:159:GLY:HA2  | 1:D:162:VAL:HG12 | 1.97                     | 0.46              |
| 1:A:228:MSE:O    | 1:A:232:LEU:HG   | 2.16                     | 0.45              |
| 1:B:281:LEU:C    | 1:B:281:LEU:HD23 | 2.41                     | 0.45              |
| 1:D:270:LEU:HD11 | 1:D:289:LEU:HD21 | 1.97                     | 0.45              |
| 1:E:177:LEU:HD23 | 1:E:391:ARG:HB2  | 1.98                     | 0.45              |
| 1:B:268:THR:O    | 1:B:268:THR:HG23 | 2.16                     | 0.45              |
| 1:C:252:ALA:O    | 1:C:255:ASN:HB3  | 2.16                     | 0.45              |
| 1:C:336:ASP:HB3  | 1:C:382:ASP:OD2  | 2.16                     | 0.45              |
| 1:B:291:LEU:O    | 1:B:302:TYR:CE1  | 2.68                     | 0.45              |
| 1:C:197:PHE:CD1  | 1:C:233:LEU:HD11 | 2.52                     | 0.45              |
| 1:E:162:VAL:HG23 | 1:E:163:GLN:N    | 2.31                     | 0.45              |
| 1:E:237:ARG:O    | 1:E:238:ARG:HB2  | 2.15                     | 0.45              |
| 1:A:295:PHE:HB3  | 1:A:330:SER:HB2  | 1.99                     | 0.45              |
| 1:D:228:MSE:HE1  | 1:D:253:HIS:O    | 2.16                     | 0.45              |
| 1:B:183:ILE:HD12 | 1:B:183:ILE:O    | 2.16                     | 0.45              |
| 1:C:354:LEU:N    | 1:C:355:PRO:CD   | 2.80                     | 0.45              |
| 1:E:151:LEU:O    | 1:E:155:ASP:N    | 2.42                     | 0.45              |
| 1:A:228:MSE:HE2  | 1:A:253:HIS:HD2  | 1.81                     | 0.45              |
| 1:C:274:ILE:HG13 | 1:C:280:SER:O    | 2.16                     | 0.45              |
| 1:D:268:THR:HG23 | 1:D:289:LEU:HD12 | 1.98                     | 0.45              |
| 1:F:200:ASP:O    | 1:F:201:GLU:HB2  | 2.17                     | 0.45              |
| 1:A:379:GLU:HB3  | 1:A:380:MSE:H    | 1.55                     | 0.45              |
| 1:B:259:ILE:CD1  | 1:B:314:ASP:HA   | 2.43                     | 0.45              |
| 1:E:333:LEU:HB2  | 1:E:387:LEU:HB3  | 1.99                     | 0.45              |
| 1:F:170:THR:HG21 | 1:F:181:HIS:H    | 1.81                     | 0.45              |
| 1:F:366:ASP:O    | 1:F:370:GLN:HG3  | 2.16                     | 0.45              |
| 1:B:291:LEU:CD1  | 1:B:304:GLU:HG2  | 2.43                     | 0.45              |
| 1:C:216:ALA:O    | 1:C:220:PHE:HD1  | 2.00                     | 0.45              |
| 1:C:281:LEU:CB   | 1:C:325:LEU:HD21 | 2.47                     | 0.45              |
| 1:A:292:PRO:HB2  | 1:A:331:LEU:HD11 | 1.99                     | 0.45              |
| 1:C:294:LEU:HD21 | 1:C:303:LEU:HD21 | 1.99                     | 0.45              |
| 1:D:183:ILE:O    | 1:D:185:PRO:HD3  | 2.17                     | 0.45              |
| 1:F:161:GLN:HA   | 1:F:164:MSE:CG   | 2.47                     | 0.45              |
| 1:A:181:HIS:HB2  | 1:A:194:VAL:HG11 | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:380:MSE:CB   | 1:A:381:PRO:CA   | 2.87                     | 0.44              |
| 1:B:176:GLY:O    | 1:B:391:ARG:HG3  | 2.17                     | 0.44              |
| 1:C:156:GLN:OE1  | 1:C:189:LEU:HG   | 2.17                     | 0.44              |
| 1:C:192:ASP:OD1  | 1:C:383:ASP:HB2  | 2.17                     | 0.44              |
| 1:E:149:LEU:HB3  | 1:F:149:LEU:HD22 | 1.97                     | 0.44              |
| 1:D:292:PRO:HB2  | 1:D:331:LEU:HD11 | 1.99                     | 0.44              |
| 1:E:181:HIS:CG   | 1:E:194:VAL:HG11 | 2.52                     | 0.44              |
| 1:C:369:ARG:HA   | 1:C:372:PHE:CD2  | 2.52                     | 0.44              |
| 1:D:160:ARG:O    | 1:D:164:MSE:HG2  | 2.17                     | 0.44              |
| 1:E:174:ILE:HD12 | 1:E:174:ILE:O    | 2.17                     | 0.44              |
| 1:F:264:GLY:C    | 1:F:265:LYS:HD2  | 2.42                     | 0.44              |
| 1:A:224:LEU:O    | 1:A:228:MSE:HG3  | 2.18                     | 0.44              |
| 1:E:325:LEU:HA   | 1:E:326:PRO:HD3  | 1.87                     | 0.44              |
| 1:A:252:ALA:O    | 1:A:256:ARG:HG3  | 2.18                     | 0.44              |
| 1:A:340:ASP:O    | 1:A:342:LEU:HG   | 2.18                     | 0.44              |
| 1:D:250:VAL:O    | 1:D:254:ILE:HD13 | 2.17                     | 0.44              |
| 1:A:378:ALA:HB1  | 1:A:379:GLU:OE1  | 2.17                     | 0.44              |
| 1:C:387:LEU:HD23 | 1:C:388:VAL:N    | 2.32                     | 0.44              |
| 1:D:160:ARG:HE   | 1:D:164:MSE:HE2  | 1.82                     | 0.44              |
| 1:F:184:ILE:HB   | 1:F:384:ILE:CG2  | 2.48                     | 0.44              |
| 1:F:184:ILE:HB   | 1:F:384:ILE:HG23 | 2.00                     | 0.44              |
| 1:B:183:ILE:HD12 | 1:B:185:PRO:HD3  | 2.00                     | 0.44              |
| 1:B:292:PRO:HB3  | 1:B:333:LEU:HD23 | 2.00                     | 0.44              |
| 1:C:255:ASN:C    | 1:C:259:ILE:HD11 | 2.43                     | 0.44              |
| 1:F:186:SER:C    | 1:F:187:LEU:HD22 | 2.42                     | 0.44              |
| 1:D:207:TYR:HA   | 1:D:270:LEU:O    | 2.18                     | 0.44              |
| 1:B:182:ARG:CZ   | 1:B:184:ILE:HG12 | 2.48                     | 0.43              |
| 1:B:197:PHE:CZ   | 1:B:229:THR:CG2  | 3.01                     | 0.43              |
| 1:C:225:LEU:HD13 | 1:C:269:MSE:HE2  | 2.00                     | 0.43              |
| 1:D:246:LYS:HB2  | 1:D:249:GLU:CA   | 2.30                     | 0.43              |
| 1:D:294:LEU:CD2  | 1:D:303:LEU:HD21 | 2.44                     | 0.43              |
| 1:E:260:ASN:O    | 1:E:261:THR:HG22 | 2.18                     | 0.43              |
| 1:F:159:GLY:HA2  | 1:F:162:VAL:CG1  | 2.48                     | 0.43              |
| 1:B:158:ALA:CA   | 1:B:161:GLN:HG2  | 2.44                     | 0.43              |
| 1:E:254:ILE:O    | 1:E:258:LEU:HG   | 2.19                     | 0.43              |
| 1:F:203:ARG:NH1  | 1:F:245:PHE:HD2  | 2.16                     | 0.43              |
| 1:A:386:LEU:O    | 1:A:386:LEU:HD12 | 2.19                     | 0.43              |
| 1:D:281:LEU:C    | 1:D:281:LEU:HD23 | 2.43                     | 0.43              |
| 1:B:166:MSE:O    | 1:B:226:LYS:NZ   | 2.51                     | 0.43              |
| 1:C:386:LEU:HD12 | 1:C:386:LEU:O    | 2.18                     | 0.43              |
| 1:D:267:VAL:O    | 1:D:310:VAL:HG11 | 2.16                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:204:VAL:HB   | 1:A:274:ILE:HG23 | 2.00                     | 0.43              |
| 1:A:225:LEU:HD22 | 1:A:254:ILE:HD13 | 2.00                     | 0.43              |
| 1:D:167:LEU:CD2  | 1:D:193:PHE:CE1  | 3.02                     | 0.43              |
| 1:D:336:ASP:O    | 1:D:338:ILE:HG13 | 2.19                     | 0.43              |
| 1:A:324:GLU:OE1  | 1:A:324:GLU:CA   | 2.66                     | 0.43              |
| 1:B:351:GLU:HG3  | 1:B:351:GLU:O    | 2.18                     | 0.43              |
| 1:C:255:ASN:C    | 1:C:259:ILE:CD1  | 2.92                     | 0.43              |
| 1:D:189:LEU:HB3  | 1:D:219:ALA:HB2  | 2.00                     | 0.43              |
| 1:D:285:ILE:HD11 | 1:D:289:LEU:HD11 | 2.00                     | 0.43              |
| 1:E:203:ARG:HD3  | 1:E:239:ASN:HD21 | 1.84                     | 0.43              |
| 1:E:302:TYR:HE2  | 1:E:352:ALA:O    | 2.01                     | 0.43              |
| 1:B:232:LEU:HD21 | 1:B:253:HIS:ND1  | 2.34                     | 0.43              |
| 1:C:255:ASN:OD1  | 1:C:259:ILE:HG12 | 2.18                     | 0.43              |
| 1:D:195:ASP:HB3  | 1:D:207:TYR:CE1  | 2.53                     | 0.43              |
| 1:D:380:MSE:HE3  | 1:D:381:PRO:HD2  | 1.98                     | 0.43              |
| 1:F:392:ASN:ND2  | 1:F:393:LEU:CD1  | 2.82                     | 0.43              |
| 1:A:227:PHE:CE2  | 1:A:231:ARG:HD2  | 2.53                     | 0.43              |
| 1:B:167:LEU:HD13 | 1:B:181:HIS:NE2  | 2.34                     | 0.43              |
| 1:B:265:LYS:HD2  | 1:D:324:GLU:CG   | 2.49                     | 0.43              |
| 1:E:294:LEU:CD2  | 1:E:303:LEU:HD21 | 2.49                     | 0.43              |
| 1:C:159:GLY:C    | 1:C:189:LEU:HD21 | 2.44                     | 0.43              |
| 1:D:174:ILE:HD11 | 1:D:179:PHE:CZ   | 2.54                     | 0.43              |
| 1:D:179:PHE:CZ   | 1:D:204:VAL:HG11 | 2.54                     | 0.43              |
| 1:A:173:SER:HA   | 1:A:177:LEU:O    | 2.19                     | 0.43              |
| 1:A:239:ASN:OD1  | 1:A:239:ASN:O    | 2.37                     | 0.43              |
| 1:A:365:LEU:HD12 | 1:A:366:ASP:H    | 1.84                     | 0.43              |
| 1:B:159:GLY:O    | 1:B:162:VAL:CG1  | 2.63                     | 0.43              |
| 1:C:347:LEU:HG   | 1:C:350:LYS:HD2  | 2.00                     | 0.43              |
| 1:E:386:LEU:HD12 | 1:E:386:LEU:O    | 2.19                     | 0.43              |
| 1:B:273:VAL:C    | 1:B:274:ILE:HD12 | 2.44                     | 0.42              |
| 1:C:200:ASP:O    | 1:C:201:GLU:HG3  | 2.17                     | 0.42              |
| 1:D:281:LEU:HD21 | 1:D:283:TYR:HB3  | 2.00                     | 0.42              |
| 1:A:340:ASP:O    | 1:A:341:VAL:HG12 | 2.19                     | 0.42              |
| 1:C:288:HIS:O    | 1:C:288:HIS:ND1  | 2.48                     | 0.42              |
| 1:D:328:SER:HA   | 1:D:392:ASN:H    | 1.84                     | 0.42              |
| 1:E:207:TYR:C    | 1:E:207:TYR:CD2  | 2.96                     | 0.42              |
| 1:A:183:ILE:O    | 1:A:185:PRO:HD3  | 2.20                     | 0.42              |
| 1:A:296:VAL:O    | 1:A:296:VAL:HG13 | 2.19                     | 0.42              |
| 1:C:268:THR:HG21 | 1:C:289:LEU:HB3  | 2.01                     | 0.42              |
| 1:C:289:LEU:HD13 | 1:C:289:LEU:O    | 2.20                     | 0.42              |
| 1:F:159:GLY:O    | 1:F:162:VAL:CG1  | 2.62                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:162:VAL:CG2  | 1:B:263:LEU:HD22 | 2.45                     | 0.42              |
| 1:A:183:ILE:HG23 | 1:A:385:ALA:HB2  | 2.01                     | 0.42              |
| 1:A:312:LEU:C    | 1:A:312:LEU:HD12 | 2.45                     | 0.42              |
| 1:A:336:ASP:O    | 1:A:338:ILE:HD12 | 2.19                     | 0.42              |
| 1:C:227:PHE:CE2  | 1:D:227:PHE:CD2  | 2.95                     | 0.42              |
| 1:E:310:VAL:HG22 | 1:E:311:GLY:H    | 1.82                     | 0.42              |
| 1:F:159:GLY:CA   | 1:F:162:VAL:HG12 | 2.49                     | 0.42              |
| 1:B:330:SER:OG   | 1:B:364:THR:HG21 | 2.20                     | 0.42              |
| 1:C:160:ARG:CG   | 1:C:164:MSE:CE   | 2.89                     | 0.42              |
| 1:C:366:ASP:OD1  | 1:C:366:ASP:C    | 2.63                     | 0.42              |
| 1:D:295:PHE:CE1  | 1:D:360:ALA:CA   | 3.00                     | 0.42              |
| 1:D:339:LEU:HD12 | 1:D:340:ASP:N    | 2.35                     | 0.42              |
| 1:B:313:PHE:CD1  | 1:D:301:GLY:HA3  | 2.55                     | 0.42              |
| 1:D:254:ILE:O    | 1:D:258:LEU:HG   | 2.19                     | 0.42              |
| 1:E:152:LEU:CD1  | 1:F:153:GLN:HG2  | 2.50                     | 0.42              |
| 1:F:183:ILE:O    | 1:F:185:PRO:HD3  | 2.19                     | 0.42              |
| 1:C:217:SER:HB3  | 1:D:158:ALA:O    | 2.19                     | 0.42              |
| 1:D:372:PHE:CD2  | 1:D:372:PHE:O    | 2.71                     | 0.42              |
| 1:F:156:GLN:OE1  | 1:F:156:GLN:HA   | 2.19                     | 0.42              |
| 1:F:211:VAL:HG21 | 1:F:221:VAL:HB   | 2.02                     | 0.42              |
| 1:A:166:MSE:HE3  | 1:A:193:PHE:CE1  | 2.54                     | 0.42              |
| 1:A:247:PRO:HB2  | 1:A:284:SER:CB   | 2.50                     | 0.42              |
| 1:A:266:HIS:HB3  | 1:A:312:LEU:HB3  | 2.02                     | 0.42              |
| 1:A:328:SER:HA   | 1:A:391:ARG:O    | 2.19                     | 0.42              |
| 1:D:174:ILE:HD11 | 1:D:179:PHE:CE2  | 2.55                     | 0.42              |
| 1:D:181:HIS:CB   | 1:D:194:VAL:HG21 | 2.49                     | 0.42              |
| 1:A:294:LEU:HD22 | 1:A:329:PHE:HZ   | 1.84                     | 0.42              |
| 1:B:184:ILE:HB   | 1:B:384:ILE:HG23 | 2.02                     | 0.42              |
| 1:B:294:LEU:HB3  | 1:B:331:LEU:HD13 | 2.01                     | 0.42              |
| 1:E:151:LEU:O    | 1:E:155:ASP:HB2  | 2.19                     | 0.42              |
| 1:F:167:LEU:HD13 | 1:F:181:HIS:CE1  | 2.55                     | 0.42              |
| 1:F:392:ASN:ND2  | 1:F:393:LEU:HD12 | 2.34                     | 0.42              |
| 1:C:200:ASP:C    | 1:C:201:GLU:CG   | 2.88                     | 0.41              |
| 1:D:249:GLU:OE1  | 1:D:252:ALA:HB3  | 2.20                     | 0.41              |
| 1:E:310:VAL:HG22 | 1:E:311:GLY:N    | 2.34                     | 0.41              |
| 1:D:225:LEU:HD23 | 1:D:225:LEU:HA   | 1.84                     | 0.41              |
| 1:D:294:LEU:HB3  | 1:D:331:LEU:HD13 | 2.02                     | 0.41              |
| 1:E:263:LEU:CB   | 1:E:265:LYS:HG2  | 2.50                     | 0.41              |
| 1:E:279:ASN:ND2  | 1:E:325:LEU:O    | 2.51                     | 0.41              |
| 1:A:330:SER:HA   | 1:A:389:LEU:O    | 2.21                     | 0.41              |
| 1:C:211:VAL:HG22 | 1:C:267:VAL:HG22 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:232:LEU:HD11 | 1:C:253:HIS:CD2  | 2.55                     | 0.41              |
| 1:C:386:LEU:HD12 | 1:C:386:LEU:C    | 2.45                     | 0.41              |
| 1:E:374:LEU:H    | 1:E:374:LEU:CD2  | 2.24                     | 0.41              |
| 1:D:167:LEU:HD13 | 1:D:183:ILE:CD1  | 2.47                     | 0.41              |
| 1:D:252:ALA:HA   | 1:D:318:TYR:CE2  | 2.55                     | 0.41              |
| 1:D:295:PHE:CE1  | 1:D:300:ALA:HB2  | 2.44                     | 0.41              |
| 1:E:149:LEU:HD12 | 1:E:149:LEU:C    | 2.43                     | 0.41              |
| 1:A:325:LEU:HA   | 1:A:326:PRO:HD3  | 1.85                     | 0.41              |
| 1:B:309:PRO:C    | 1:B:311:GLY:H    | 2.29                     | 0.41              |
| 1:C:339:LEU:HD22 | 1:C:345:ALA:CA   | 2.37                     | 0.41              |
| 1:E:228:MSE:HE2  | 1:E:253:HIS:NE2  | 2.35                     | 0.41              |
| 1:D:291:LEU:HB2  | 1:D:302:TYR:CD1  | 2.56                     | 0.41              |
| 1:F:159:GLY:HA2  | 1:F:162:VAL:HG12 | 2.03                     | 0.41              |
| 1:B:159:GLY:HA3  | 1:B:189:LEU:HD21 | 2.02                     | 0.41              |
| 1:B:179:PHE:CZ   | 1:B:204:VAL:HG11 | 2.55                     | 0.41              |
| 1:B:380:MSE:CE   | 1:B:381:PRO:HD2  | 2.50                     | 0.41              |
| 1:C:224:LEU:O    | 1:C:228:MSE:HG3  | 2.21                     | 0.41              |
| 1:E:330:SER:CB   | 1:E:364:THR:HG21 | 2.50                     | 0.41              |
| 1:A:258:LEU:HD13 | 1:A:267:VAL:HG23 | 2.02                     | 0.41              |
| 1:B:325:LEU:HA   | 1:B:326:PRO:HD3  | 1.89                     | 0.41              |
| 1:C:167:LEU:HD13 | 1:C:181:HIS:NE2  | 2.35                     | 0.41              |
| 1:C:266:HIS:HB3  | 1:C:312:LEU:CD2  | 2.48                     | 0.41              |
| 1:E:152:LEU:HD23 | 1:E:152:LEU:HA   | 1.95                     | 0.41              |
| 1:F:160:ARG:O    | 1:F:164:MSE:HG2  | 2.21                     | 0.41              |
| 1:A:159:GLY:HA3  | 1:A:189:LEU:HD21 | 2.02                     | 0.41              |
| 1:A:240:GLY:C    | 1:A:241:THR:HG22 | 2.43                     | 0.41              |
| 1:B:295:PHE:CZ   | 1:B:298:GLY:HA2  | 2.56                     | 0.41              |
| 1:C:325:LEU:HA   | 1:C:326:PRO:HD3  | 1.77                     | 0.41              |
| 1:D:177:LEU:HD23 | 1:D:391:ARG:CB   | 2.50                     | 0.41              |
| 1:D:377:LEU:HD23 | 1:D:378:ALA:N    | 2.34                     | 0.41              |
| 1:E:242:LEU:O    | 1:E:243:PRO:C    | 2.64                     | 0.41              |
| 1:C:183:ILE:HG12 | 1:C:385:ALA:HB1  | 2.02                     | 0.40              |
| 1:C:315:ASP:N    | 1:C:315:ASP:OD1  | 2.53                     | 0.40              |
| 1:F:238:ARG:H    | 1:F:238:ARG:CD   | 2.31                     | 0.40              |
| 1:F:334:PHE:CE2  | 1:F:386:LEU:HD22 | 2.54                     | 0.40              |
| 1:C:200:ASP:O    | 1:C:201:GLU:HB2  | 2.21                     | 0.40              |
| 1:C:329:PHE:CD2  | 1:C:330:SER:N    | 2.89                     | 0.40              |
| 1:E:237:ARG:HA   | 1:E:237:ARG:HD3  | 1.79                     | 0.40              |
| 1:F:166:MSE:CE   | 1:F:223:VAL:HG13 | 2.49                     | 0.40              |
| 1:F:292:PRO:HB3  | 1:F:333:LEU:CD2  | 2.51                     | 0.40              |
| 1:C:225:LEU:HD21 | 1:C:267:VAL:HG21 | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:245:PHE:CD2  | 1:C:245:PHE:C    | 2.99                     | 0.40              |
| 1:D:289:LEU:HD22 | 1:D:289:LEU:C    | 2.46                     | 0.40              |
| 1:E:219:ALA:C    | 1:F:220:PHE:HE2  | 2.29                     | 0.40              |
| 1:F:256:ARG:HA   | 1:F:259:ILE:HG22 | 2.03                     | 0.40              |
| 1:A:255:ASN:O    | 1:A:259:ILE:HG22 | 2.21                     | 0.40              |
| 1:D:325:LEU:HD13 | 1:D:329:PHE:CE1  | 2.57                     | 0.40              |
| 1:E:231:ARG:NH2  | 1:F:231:ARG:NH2  | 2.69                     | 0.40              |
| 1:E:262:LYS:O    | 1:E:263:LEU:HB2  | 2.20                     | 0.40              |
| 1:F:203:ARG:HH12 | 1:F:245:PHE:HD2  | 1.67                     | 0.40              |
| 1:A:212:SER:OG   | 1:A:265:LYS:HA   | 2.22                     | 0.40              |
| 1:A:273:VAL:O    | 1:A:273:VAL:HG13 | 2.21                     | 0.40              |
| 1:B:177:LEU:CD1  | 1:B:391:ARG:HH11 | 2.34                     | 0.40              |
| 1:B:281:LEU:HD11 | 1:B:331:LEU:HD22 | 2.04                     | 0.40              |
| 1:C:294:LEU:HD13 | 1:C:329:PHE:CE1  | 2.57                     | 0.40              |
| 1:D:179:PHE:HB2  | 1:D:196:TYR:CE2  | 2.57                     | 0.40              |
| 1:F:199:VAL:O    | 1:F:200:ASP:HB3  | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | A     | 209/255 (82%)   | 193 (92%)  | 16 (8%) | 0        | 100         | 100 |
| 1   | B     | 217/255 (85%)   | 202 (93%)  | 14 (6%) | 1 (0%)   | 24          | 55  |
| 1   | C     | 219/255 (86%)   | 199 (91%)  | 20 (9%) | 0        | 100         | 100 |
| 1   | D     | 218/255 (86%)   | 202 (93%)  | 15 (7%) | 1 (0%)   | 24          | 55  |
| 1   | E     | 226/255 (89%)   | 211 (93%)  | 15 (7%) | 0        | 100         | 100 |
| 1   | F     | 227/255 (89%)   | 214 (94%)  | 13 (6%) | 0        | 100         | 100 |
| All | All   | 1316/1530 (86%) | 1221 (93%) | 93 (7%) | 2 (0%)   | 43          | 72  |



All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 310 | VAL  |
| 1   | D     | 337 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 173/206 (84%)   | 172 (99%)  | 1 (1%)   | 78          | 92 |
| 1   | B     | 182/206 (88%)   | 178 (98%)  | 4 (2%)   | 45          | 78 |
| 1   | C     | 181/206 (88%)   | 174 (96%)  | 7 (4%)   | 28          | 64 |
| 1   | D     | 179/206 (87%)   | 172 (96%)  | 7 (4%)   | 28          | 64 |
| 1   | E     | 189/206 (92%)   | 187 (99%)  | 2 (1%)   | 65          | 87 |
| 1   | F     | 181/206 (88%)   | 179 (99%)  | 2 (1%)   | 65          | 87 |
| All | All   | 1085/1236 (88%) | 1062 (98%) | 23 (2%)  | 47          | 79 |

All (23) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 289 | LEU  |
| 1   | B     | 289 | LEU  |
| 1   | B     | 310 | VAL  |
| 1   | B     | 348 | LYS  |
| 1   | B     | 357 | GLN  |
| 1   | C     | 149 | LEU  |
| 1   | C     | 162 | VAL  |
| 1   | C     | 187 | LEU  |
| 1   | C     | 259 | ILE  |
| 1   | C     | 289 | LEU  |
| 1   | C     | 315 | ASP  |
| 1   | C     | 384 | ILE  |
| 1   | D     | 167 | LEU  |
| 1   | D     | 249 | GLU  |
| 1   | D     | 289 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 346 | THR  |
| 1   | D     | 348 | LYS  |
| 1   | D     | 366 | ASP  |
| 1   | D     | 376 | ASN  |
| 1   | E     | 197 | PHE  |
| 1   | E     | 289 | LEU  |
| 1   | F     | 274 | ILE  |
| 1   | F     | 289 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 161 | GLN  |
| 1   | A     | 253 | HIS  |
| 1   | A     | 255 | ASN  |
| 1   | B     | 163 | GLN  |
| 1   | B     | 266 | HIS  |
| 1   | B     | 357 | GLN  |
| 1   | C     | 163 | GLN  |
| 1   | C     | 253 | HIS  |
| 1   | C     | 266 | HIS  |
| 1   | D     | 156 | GLN  |
| 1   | D     | 165 | ASN  |
| 1   | D     | 376 | ASN  |
| 1   | E     | 163 | GLN  |
| 1   | E     | 165 | ASN  |
| 1   | E     | 214 | HIS  |
| 1   | E     | 253 | HIS  |
| 1   | E     | 255 | ASN  |
| 1   | E     | 370 | GLN  |
| 1   | F     | 150 | 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2   | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------|-----------------------|-------|
| 1   | A     | 215/255 (84%)   | -1.14  | 0 100 100 | 41, 92, 166, 244      | 0     |
| 1   | B     | 222/255 (87%)   | -1.15  | 0 100 100 | 42, 86, 129, 224      | 0     |
| 1   | C     | 223/255 (87%)   | -1.15  | 0 100 100 | 43, 91, 141, 234      | 0     |
| 1   | D     | 224/255 (87%)   | -1.17  | 0 100 100 | 36, 88, 150, 275      | 0     |
| 1   | E     | 228/255 (89%)   | -1.21  | 0 100 100 | 39, 86, 146, 192      | 0     |
| 1   | F     | 228/255 (89%)   | -1.28  | 0 100 100 | 23, 80, 132, 226      | 0     |
| All | All   | 1340/1530 (87%) | -1.18  | 0 100 100 | 23, 88, 146, 275      | 0     |

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | MG   | D     | 6   | 1/1   | 0.98 | 0.08 | 78,78,78,78                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | MG   | C     | 5   | 1/1   | 0.99 | 0.02 | 50,50,50,50                 | 0     |
| 2   | MG   | B     | 1   | 1/1   | 0.99 | 0.02 | 61,61,61,61                 | 0     |
| 2   | MG   | F     | 3   | 1/1   | 0.99 | 0.03 | 47,47,47,47                 | 0     |
| 2   | MG   | F     | 4   | 1/1   | 0.99 | 0.06 | 94,94,94,94                 | 0     |
| 2   | MG   | D     | 7   | 1/1   | 1.00 | 0.02 | 40,40,40,40                 | 0     |
| 2   | MG   | E     | 2   | 1/1   | 1.00 | 0.02 | 39,39,39,39                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.