



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:28 PM UTC

PDB ID : 2D5H / pdb\_00002d5h  
Title : Crystal Structure of Recombinant Soybean Proglycinin A3B4 subunit, its Comparison with Mature Glycinin A3B4 subunit, Responsible for Hexamer Assembly  
Authors : Itoh, T.; Adachi, M.; Masuda, T.; Mikami, B.; Utsumi, S.  
Deposited on : 2005-11-01  
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                                                             |

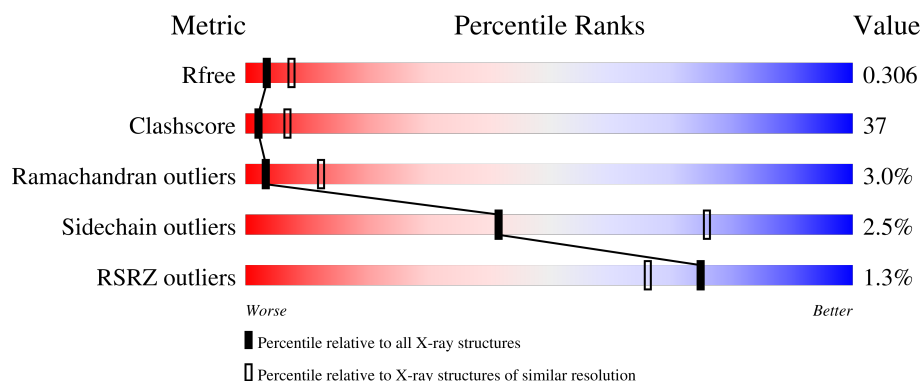
# 1 Overall quality at a glance

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     | 493    | <div> <div>31%</div> <div>41%</div> <div>24%</div> </div> |
| 1   | B     | 493    | <div> <div>32%</div> <div>41%</div> <div>25%</div> </div> |
| 1   | C     | 493    | <div> <div>26%</div> <div>45%</div> <div>25%</div> </div> |
| 1   | D     | 493    | <div> <div>35%</div> <div>39%</div> <div>24%</div> </div> |
| 1   | E     | 493    | <div> <div>39%</div> <div>37%</div> <div>23%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                               |
|-----|-------|--------|--------------------------------------------------------------------------------|
| 1   | F     | 493    | <div><div></div><div>35%</div><div>38%</div><div>• •</div><div>24%</div></div> |

## 2 Entry composition [i](#)

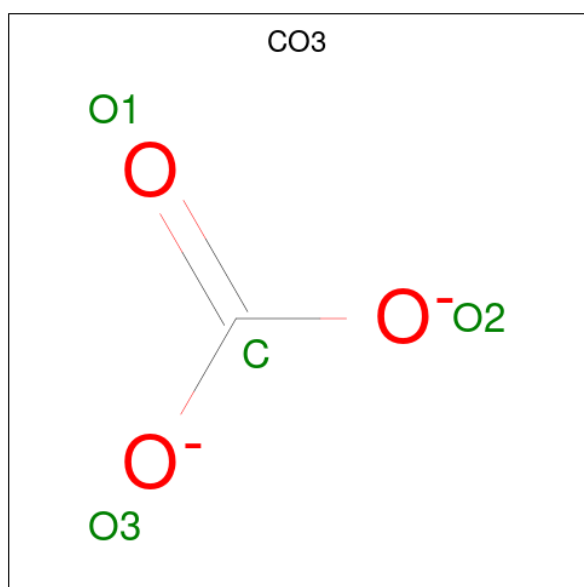
There are 3 unique types of molecules in this entry. The entry contains 17703 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 glycinin A3B4 subunit.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 374      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2937  | 1844 | 523 | 562 | 8 |         |         |       |
| 1   | B     | 372      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2920  | 1835 | 520 | 557 | 8 |         |         |       |
| 1   | C     | 370      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2905  | 1827 | 517 | 553 | 8 |         |         |       |
| 1   | D     | 377      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2967  | 1861 | 529 | 569 | 8 |         |         |       |
| 1   | E     | 380      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2981  | 1872 | 530 | 571 | 8 |         |         |       |
| 1   | F     | 377      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2963  | 1860 | 528 | 567 | 8 |         |         |       |

- Molecule 2 is CARBONATE ION (CCD ID: CO3) (formula: CO<sub>3</sub>).

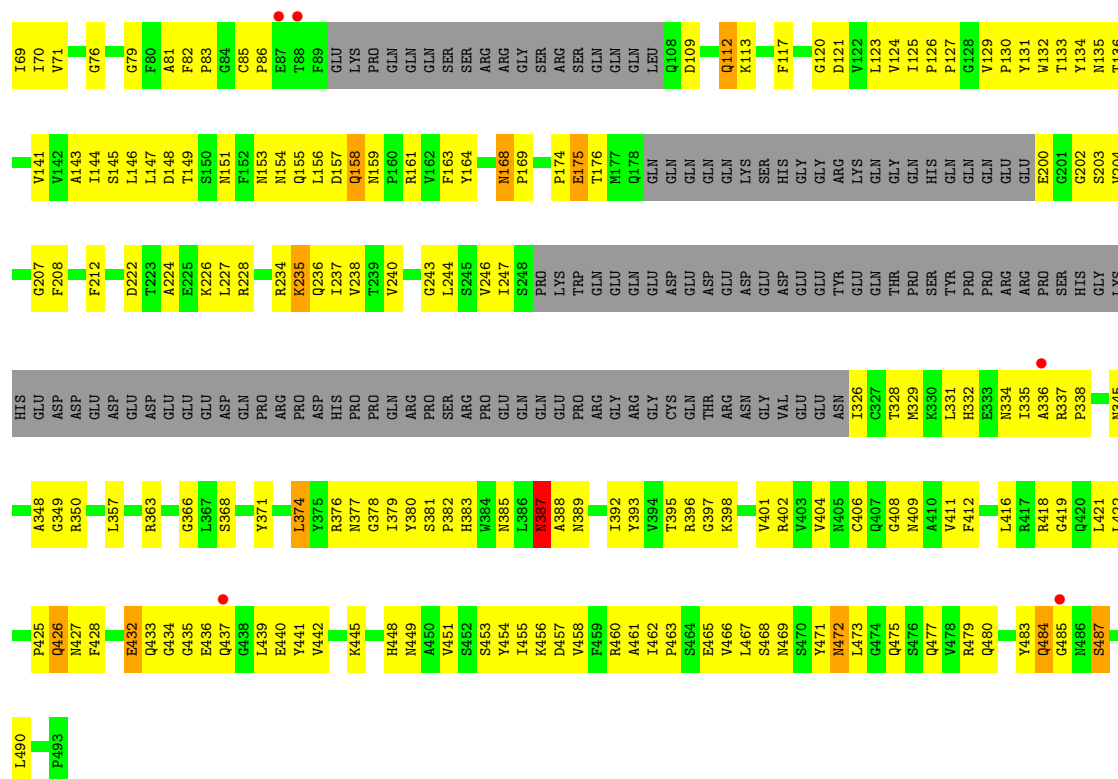


| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 2   | A     | 1        | Total C O<br>4 1 3 | 0       | 0       |
| 2   | B     | 1        | Total C O<br>4 1 3 | 0       | 0       |
| 2   | C     | 1        | Total C O<br>4 1 3 | 0       | 0       |
| 2   | D     | 1        | Total C O<br>4 1 3 | 0       | 0       |
| 2   | E     | 1        | Total C O<br>4 1 3 | 0       | 0       |
| 2   | F     | 1        | Total C O<br>4 1 3 | 0       | 0       |

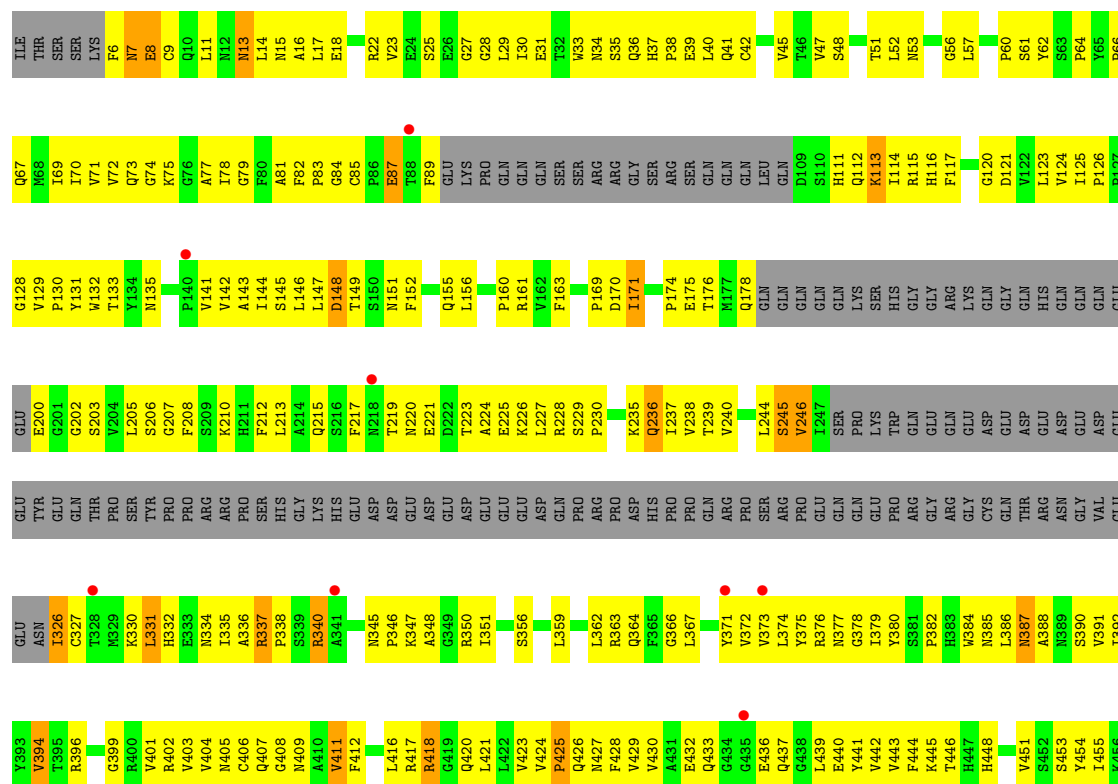
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | A     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | B     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | C     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | D     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | E     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | F     | 1        | Total Mg<br>1 1 | 0       | 0       |



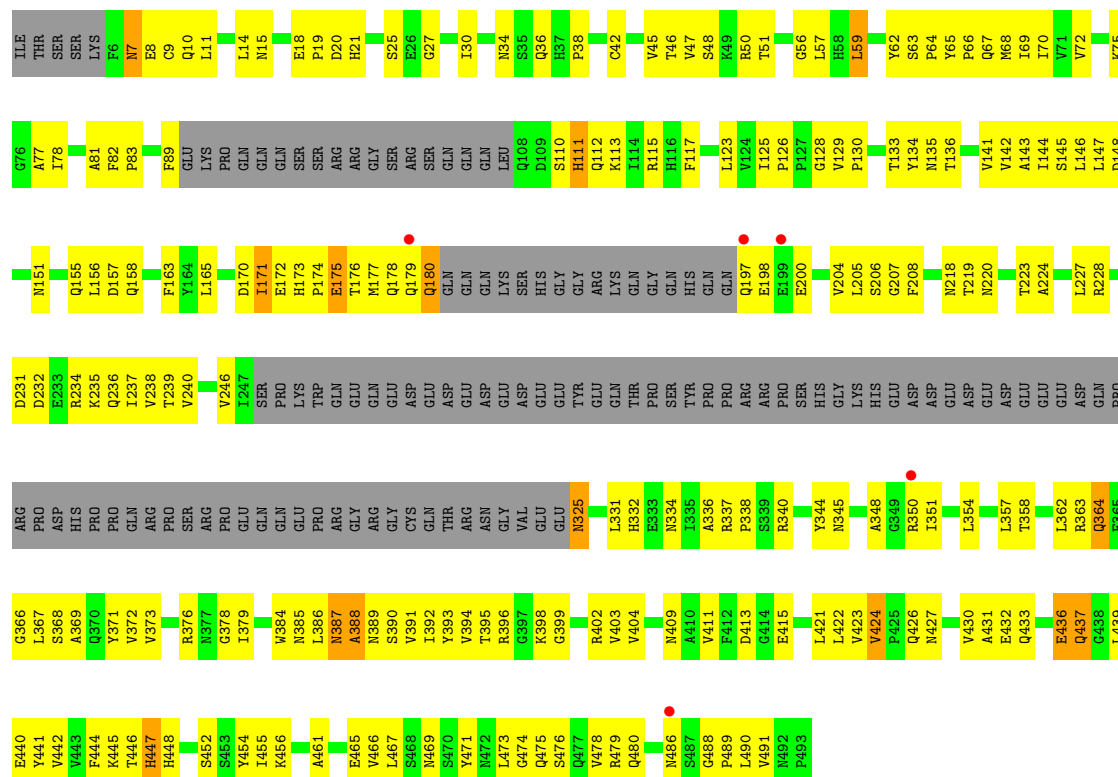


- Molecule 1: glycinin A3B4 subunit

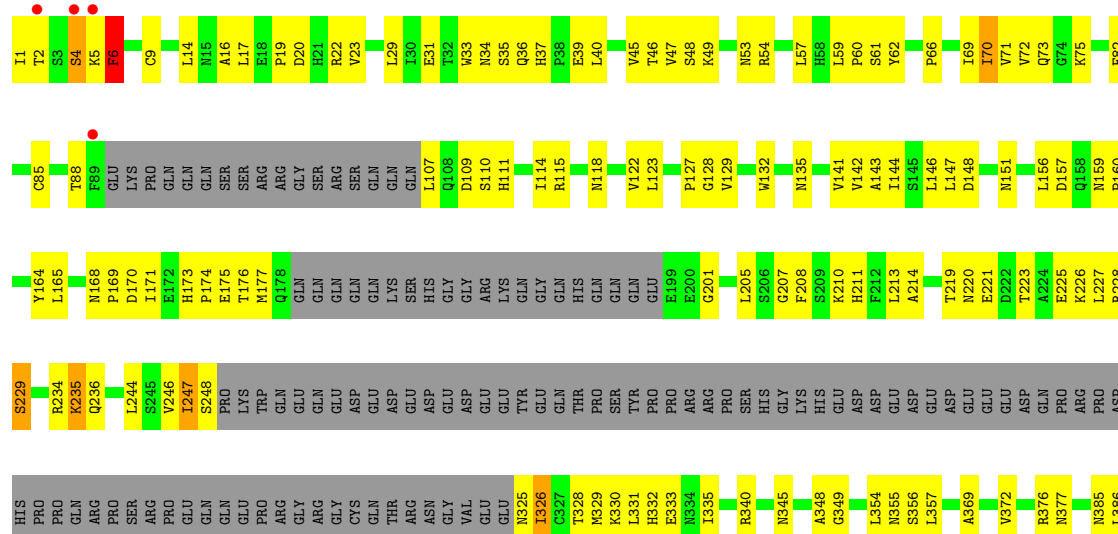


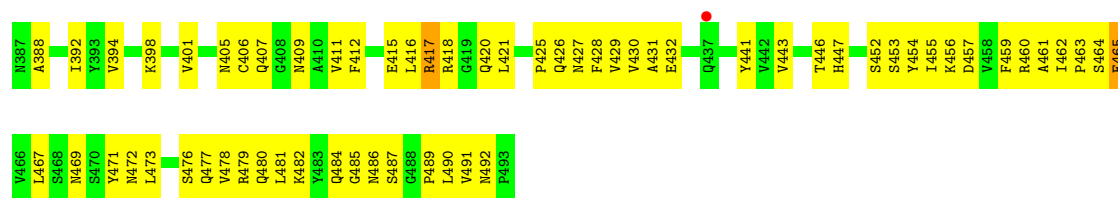


• Molecule 1: glycinin A3B4 subunit

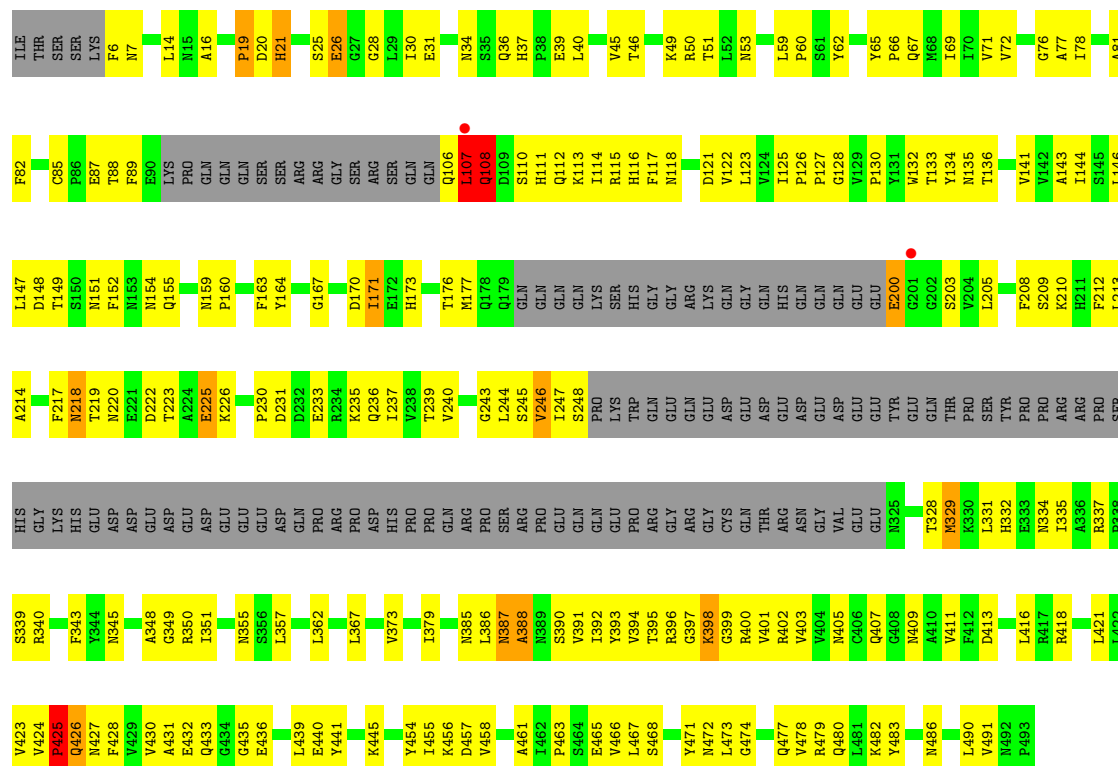


• Molecule 1: glycinin A3B4 subunit





• Molecule 1: glycinin A3B4 subunit



## 4 Data and refinement statistics

| Property                                                                | Value                                                                                                      | Source           |
|-------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 89.38Å 223.74Å 88.66Å<br>90.00° 119.85° 90.00°                                                             | Depositor        |
| Resolution (Å)                                                          | 15.00 – 2.80<br>15.00 – 2.80                                                                               | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 85.1 (15.00-2.80)<br>84.6 (15.00-2.80)                                                                     | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                                                                            | Depositor        |
| $R_{sym}$                                                               | 0.11                                                                                                       | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.79 (at 2.77Å)                                                                                            | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                                                                    | Depositor        |
| R, $R_{free}$                                                           | 0.248 , 0.325<br>0.231 , 0.306                                                                             | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 5961 reflections (9.43%)                                                                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 32.4                                                                                                       | Xtriage          |
| Anisotropy                                                              | 0.250                                                                                                      | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.26 , 26.8                                                                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$                                                | Xtriage          |
| Estimated twinning fraction                                             | 0.047 for -h-l,k,h<br>0.047 for l,k,-h-l<br>0.034 for -h-l,-k,l<br>0.035 for l,-k,h<br>0.034 for h,-k,-h-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.87                                                                                                       | EDS              |
| Total number of atoms                                                   | 17703                                                                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 28.0                                                                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CO3, CSD

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     | 0.29         | 0/2995      | 0.81        | 3/4068 (0.1%)   |
| 1   | B     | 0.28         | 0/2978      | 0.78        | 3/4045 (0.1%)   |
| 1   | C     | 0.29         | 0/2963      | 0.78        | 1/4025 (0.0%)   |
| 1   | D     | 0.30         | 0/3025      | 0.80        | 6/4108 (0.1%)   |
| 1   | E     | 0.32         | 0/3039      | 0.79        | 4/4127 (0.1%)   |
| 1   | F     | 0.31         | 0/3021      | 0.80        | 4/4103 (0.1%)   |
| All | All   | 0.30         | 0/18021     | 0.79        | 21/24476 (0.1%) |

There are no bond length outliers.

All (21) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 233 | GLU  | N-CA-C | -7.41 | 104.09      | 113.72   |
| 1   | D     | 387 | ASN  | N-CA-C | 6.83  | 119.62      | 110.88   |
| 1   | B     | 387 | ASN  | N-CA-C | 5.77  | 118.27      | 110.88   |
| 1   | B     | 168 | ASN  | CA-C-N | 5.41  | 125.87      | 120.14   |
| 1   | B     | 168 | ASN  | C-N-CA | 5.41  | 125.87      | 120.14   |
| 1   | F     | 173 | HIS  | CA-C-N | 5.31  | 125.39      | 119.87   |
| 1   | F     | 173 | HIS  | C-N-CA | 5.31  | 125.39      | 119.87   |
| 1   | C     | 7   | ASN  | N-CA-C | -5.30 | 105.13      | 113.02   |
| 1   | D     | 59  | LEU  | CA-C-N | 5.13  | 125.13      | 119.90   |
| 1   | D     | 59  | LEU  | C-N-CA | 5.13  | 125.13      | 119.90   |
| 1   | F     | 379 | ILE  | N-CA-C | 5.12  | 115.50      | 108.12   |
| 1   | E     | 229 | SER  | CA-C-N | 5.09  | 124.58      | 119.19   |
| 1   | E     | 229 | SER  | C-N-CA | 5.09  | 124.58      | 119.19   |
| 1   | F     | 16  | ALA  | N-CA-C | -5.08 | 101.47      | 109.25   |
| 1   | D     | 388 | ALA  | N-CA-C | 5.08  | 116.56      | 108.79   |
| 1   | E     | 168 | ASN  | CA-C-N | 5.03  | 124.96      | 119.78   |
| 1   | E     | 168 | ASN  | C-N-CA | 5.03  | 124.96      | 119.78   |
| 1   | A     | 125 | ILE  | CA-C-N | 5.00  | 123.31      | 119.66   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | A     | 125 | ILE  | C-N-CA | 5.00 | 123.31      | 119.66   |
| 1   | D     | 424 | VAL  | CA-C-N | 5.00 | 124.99      | 119.89   |
| 1   | D     | 424 | VAL  | C-N-CA | 5.00 | 124.99      | 119.89   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2937  | 0        | 2841     | 254     | 0            |
| 1   | B     | 2920  | 0        | 2830     | 260     | 0            |
| 1   | C     | 2905  | 0        | 2817     | 279     | 0            |
| 1   | D     | 2967  | 0        | 2867     | 206     | 0            |
| 1   | E     | 2981  | 0        | 2897     | 198     | 0            |
| 1   | F     | 2963  | 0        | 2868     | 223     | 0            |
| 2   | A     | 4     | 0        | 0        | 0       | 0            |
| 2   | B     | 4     | 0        | 0        | 1       | 0            |
| 2   | C     | 4     | 0        | 0        | 0       | 0            |
| 2   | D     | 4     | 0        | 0        | 0       | 0            |
| 2   | E     | 4     | 0        | 0        | 0       | 0            |
| 2   | F     | 4     | 0        | 0        | 0       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | E     | 1     | 0        | 0        | 0       | 0            |
| 3   | F     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 17703 | 0        | 17120    | 1301    | 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 37.

All (1301) 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:C:334:ASN:HD22 | 1:C:337:ARG:HG2  | 1.17                     | 1.08              |
| 1:F:159:ASN:HD22 | 1:F:176:THR:HG22 | 1.20                     | 1.06              |
| 1:F:115:ARG:HH22 | 1:F:331:LEU:HD12 | 1.20                     | 1.04              |
| 1:E:247:ILE:HG12 | 1:E:248:SER:H    | 1.19                     | 1.04              |
| 1:A:326:ILE:HA   | 1:A:329:MET:HE3  | 1.43                     | 0.99              |
| 1:B:159:ASN:HD22 | 1:B:176:THR:HG22 | 1.29                     | 0.98              |
| 1:C:81:ALA:HB3   | 1:C:130:PRO:HG2  | 1.46                     | 0.98              |
| 1:B:156:LEU:HB3  | 1:B:161:ARG:HH21 | 1.27                     | 0.98              |
| 1:D:36:GLN:HE21  | 1:D:175:GLU:HB2  | 1.30                     | 0.95              |
| 1:B:123:LEU:HD23 | 1:B:332:HIS:HB3  | 1.48                     | 0.94              |
| 1:A:340:ARG:HB3  | 1:A:340:ARG:NH1  | 1.83                     | 0.93              |
| 1:A:426:GLN:HE22 | 1:C:155:GLN:H    | 1.17                     | 0.92              |
| 1:F:34:ASN:HD21  | 1:F:36:GLN:HB2   | 1.34                     | 0.92              |
| 1:E:247:ILE:HD13 | 1:E:247:ILE:H    | 1.35                     | 0.91              |
| 1:F:334:ASN:ND2  | 1:F:337:ARG:HG2  | 1.86                     | 0.91              |
| 1:A:60:PRO:HG3   | 1:A:132:TRP:HB3  | 1.51                     | 0.90              |
| 1:A:340:ARG:HB3  | 1:A:340:ARG:HH11 | 1.34                     | 0.87              |
| 1:D:364:GLN:H    | 1:D:364:GLN:HE21 | 1.19                     | 0.86              |
| 1:E:376:ARG:HH11 | 1:E:376:ARG:HB3  | 1.41                     | 0.85              |
| 1:E:486:ASN:HD21 | 1:E:491:VAL:HG22 | 1.40                     | 0.85              |
| 1:A:334:ASN:ND2  | 1:A:337:ARG:HG2  | 1.92                     | 0.85              |
| 1:D:115:ARG:H    | 1:D:115:ARG:HD2  | 1.41                     | 0.85              |
| 1:C:124:VAL:H    | 1:C:331:LEU:HD12 | 1.42                     | 0.84              |
| 1:A:36:GLN:HE21  | 1:A:175:GLU:HB2  | 1.40                     | 0.84              |
| 1:A:340:ARG:NH1  | 1:A:350:ARG:HD2  | 1.92                     | 0.83              |
| 1:F:334:ASN:HD22 | 1:F:337:ARG:HG2  | 1.43                     | 0.83              |
| 1:D:384:TRP:HE1  | 1:D:386:LEU:HD12 | 1.44                     | 0.83              |
| 1:B:14:LEU:HD13  | 1:B:411:VAL:HB   | 1.60                     | 0.82              |
| 1:D:456:LYS:HE2  | 1:F:217:PHE:HA   | 1.60                     | 0.82              |
| 1:A:373:VAL:HG22 | 1:A:440:GLU:HG3  | 1.60                     | 0.82              |
| 1:C:124:VAL:HB   | 1:C:331:LEU:HD11 | 1.62                     | 0.82              |
| 1:C:338:PRO:HG3  | 1:C:350:ARG:HH11 | 1.43                     | 0.82              |
| 1:F:171:ILE:HD12 | 1:F:171:ILE:H    | 1.45                     | 0.81              |
| 1:D:72:VAL:HG22  | 1:D:142:VAL:O    | 1.78                     | 0.81              |
| 1:E:465:GLU:CD   | 1:E:465:GLU:H    | 1.85                     | 0.81              |
| 1:F:486:ASN:HD21 | 1:F:491:VAL:HG22 | 1.44                     | 0.81              |
| 1:C:373:VAL:HG22 | 1:C:440:GLU:HG3  | 1.60                     | 0.81              |
| 1:B:480:GLN:NE2  | 1:B:484:GLN:HE21 | 1.78                     | 0.80              |
| 1:F:328:THR:HG23 | 1:F:329:MET:H    | 1.45                     | 0.80              |
| 1:A:372:VAL:HB   | 1:A:441:TYR:HE2  | 1.48                     | 0.79              |
| 1:D:486:ASN:HD21 | 1:D:491:VAL:HG22 | 1.45                     | 0.79              |
| 1:C:477:GLN:O    | 1:C:480:GLN:HB3  | 1.82                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:83:PRO:HB3   | 1:E:453:SER:HB2  | 1.63                     | 0.79              |
| 1:E:405:ASN:HD22 | 1:E:411:VAL:HG13 | 1.47                     | 0.79              |
| 1:D:334:ASN:HD22 | 1:D:337:ARG:HB2  | 1.46                     | 0.79              |
| 1:C:462:ILE:HB   | 1:C:467:LEU:HD11 | 1.63                     | 0.78              |
| 1:F:50:ARG:HH22  | 1:F:67:GLN:HE22  | 1.30                     | 0.78              |
| 1:A:224:ALA:HA   | 1:A:227:LEU:HD12 | 1.66                     | 0.78              |
| 1:C:52:LEU:HD23  | 1:C:237:ILE:HD13 | 1.66                     | 0.77              |
| 1:E:73:GLN:HB3   | 1:E:142:VAL:HG12 | 1.65                     | 0.77              |
| 1:B:396:ARG:HH11 | 1:B:440:GLU:HG3  | 1.49                     | 0.77              |
| 1:E:460:ARG:NH2  | 1:E:487:SER:HB2  | 2.00                     | 0.77              |
| 1:A:334:ASN:HD21 | 1:A:337:ARG:H    | 1.31                     | 0.77              |
| 1:D:45:VAL:HG12  | 1:D:148:ASP:HA   | 1.67                     | 0.77              |
| 1:C:210:LYS:HD3  | 1:C:225:GLU:HG2  | 1.64                     | 0.77              |
| 1:D:46:THR:HG23  | 1:D:147:LEU:HD12 | 1.67                     | 0.77              |
| 1:E:247:ILE:HG12 | 1:E:248:SER:N    | 1.98                     | 0.76              |
| 1:C:392:ILE:HG12 | 1:C:443:VAL:HG22 | 1.65                     | 0.76              |
| 1:C:367:LEU:HD23 | 1:C:446:THR:HA   | 1.67                     | 0.76              |
| 1:D:34:ASN:ND2   | 1:D:36:GLN:HB2   | 2.01                     | 0.76              |
| 1:B:112:GLN:HE21 | 1:C:461:ALA:HB1  | 1.51                     | 0.76              |
| 1:A:388:ALA:HA   | 1:C:155:GLN:OE1  | 1.86                     | 0.75              |
| 1:E:376:ARG:HB3  | 1:E:376:ARG:NH1  | 2.01                     | 0.75              |
| 1:F:50:ARG:NH2   | 1:F:67:GLN:HE22  | 1.83                     | 0.75              |
| 1:F:107:LEU:H    | 1:F:107:LEU:HD22 | 1.51                     | 0.75              |
| 1:A:159:ASN:HD22 | 1:A:176:THR:HA   | 1.52                     | 0.75              |
| 1:A:372:VAL:HB   | 1:A:441:TYR:CE2  | 2.22                     | 0.75              |
| 1:F:486:ASN:ND2  | 1:F:491:VAL:HG22 | 2.01                     | 0.75              |
| 1:B:387:ASN:HD22 | 1:B:387:ASN:H    | 1.35                     | 0.75              |
| 1:B:135:ASN:ND2  | 1:B:141:VAL:HG23 | 2.01                     | 0.74              |
| 1:C:89:PHE:HB2   | 1:C:113:LYS:HA   | 1.70                     | 0.74              |
| 1:B:477:GLN:O    | 1:B:480:GLN:HB3  | 1.88                     | 0.74              |
| 1:E:235:LYS:HA   | 1:E:235:LYS:HE3  | 1.69                     | 0.74              |
| 1:E:486:ASN:ND2  | 1:E:491:VAL:HG22 | 2.02                     | 0.73              |
| 1:F:85:CYS:HB2   | 1:F:112:GLN:HE22 | 1.52                     | 0.73              |
| 1:F:399:GLY:HA3  | 1:F:439:LEU:HD22 | 1.70                     | 0.73              |
| 1:B:156:LEU:HD13 | 1:B:161:ARG:HE   | 1.54                     | 0.73              |
| 1:D:246:VAL:HG11 | 1:E:463:PRO:HB3  | 1.69                     | 0.73              |
| 1:C:391:VAL:HG23 | 1:C:444:PHE:HB2  | 1.70                     | 0.72              |
| 1:F:135:ASN:ND2  | 1:F:141:VAL:HG23 | 2.04                     | 0.72              |
| 1:F:240:VAL:HG11 | 1:F:244:LEU:HD12 | 1.72                     | 0.72              |
| 1:C:363:ARG:HE   | 1:C:448:HIS:CD2  | 2.07                     | 0.72              |
| 1:F:334:ASN:ND2  | 1:F:337:ARG:H    | 1.88                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:64:PRO:HG3   | 1:B:156:LEU:HD12 | 1.71                     | 0.72              |
| 1:C:390:SER:HB2  | 1:C:424:VAL:HB   | 1.71                     | 0.71              |
| 1:D:403:VAL:HG22 | 1:D:430:VAL:HG23 | 1.70                     | 0.71              |
| 1:B:480:GLN:HA   | 1:B:484:GLN:NE2  | 2.05                     | 0.71              |
| 1:F:400:ARG:HB3  | 1:F:433:GLN:HB3  | 1.73                     | 0.71              |
| 1:A:463:PRO:HB2  | 1:A:466:VAL:HG23 | 1.70                     | 0.71              |
| 1:B:14:LEU:C     | 1:B:15:ASN:HD22  | 1.99                     | 0.71              |
| 1:A:366:GLY:HA2  | 1:A:448:HIS:HB3  | 1.73                     | 0.71              |
| 1:D:364:GLN:H    | 1:D:364:GLN:NE2  | 1.88                     | 0.71              |
| 1:F:85:CYS:HB2   | 1:F:112:GLN:NE2  | 2.06                     | 0.71              |
| 1:A:455:ILE:HD13 | 1:C:205:LEU:HD21 | 1.72                     | 0.71              |
| 1:D:465:GLU:OE1  | 1:F:246:VAL:HG23 | 1.91                     | 0.71              |
| 1:B:156:LEU:HB3  | 1:B:161:ARG:NH2  | 2.05                     | 0.70              |
| 1:C:124:VAL:H    | 1:C:331:LEU:CD1  | 2.03                     | 0.70              |
| 1:D:240:VAL:HG13 | 1:E:469:ASN:HD21 | 1.57                     | 0.70              |
| 1:D:390:SER:HB2  | 1:D:424:VAL:HB   | 1.74                     | 0.70              |
| 1:C:60:PRO:HG3   | 1:C:132:TRP:HB3  | 1.73                     | 0.70              |
| 1:D:338:PRO:HG3  | 1:D:350:ARG:HH11 | 1.56                     | 0.70              |
| 1:D:384:TRP:NE1  | 1:D:386:LEU:HD12 | 2.07                     | 0.70              |
| 1:A:46:THR:HG23  | 1:A:147:LEU:HD12 | 1.74                     | 0.69              |
| 1:B:401:VAL:HG21 | 1:B:416:LEU:HD22 | 1.74                     | 0.69              |
| 1:B:113:LYS:H    | 1:B:113:LYS:HD2  | 1.55                     | 0.69              |
| 1:C:391:VAL:CG2  | 1:C:444:PHE:HB2  | 2.23                     | 0.69              |
| 1:E:326:ILE:HD13 | 1:E:326:ILE:O    | 1.91                     | 0.69              |
| 1:A:480:GLN:O    | 1:A:484:GLN:HB2  | 1.93                     | 0.69              |
| 1:E:37:HIS:HB2   | 1:E:40:LEU:HD23  | 1.74                     | 0.69              |
| 1:B:83:PRO:HB3   | 1:C:453:SER:HB2  | 1.75                     | 0.69              |
| 1:B:123:LEU:HD23 | 1:B:332:HIS:CB   | 2.22                     | 0.69              |
| 1:D:50:ARG:HH12  | 1:D:67:GLN:HE22  | 1.39                     | 0.69              |
| 1:D:391:VAL:HG22 | 1:D:421:LEU:HD11 | 1.74                     | 0.69              |
| 1:E:16:ALA:HB1   | 1:E:420:GLN:HE21 | 1.56                     | 0.69              |
| 1:A:221:GLU:O    | 1:A:225:GLU:HB2  | 1.92                     | 0.69              |
| 1:B:126:PRO:HB2  | 1:B:129:VAL:HG21 | 1.75                     | 0.69              |
| 1:B:374:LEU:HD11 | 1:B:378:GLY:C    | 2.18                     | 0.69              |
| 1:C:67:GLN:HB2   | 1:C:125:ILE:HB   | 1.74                     | 0.69              |
| 1:C:480:GLN:NE2  | 1:C:484:GLN:HG3  | 2.08                     | 0.69              |
| 1:A:453:SER:OG   | 1:C:83:PRO:HB3   | 1.93                     | 0.69              |
| 1:B:244:LEU:HB2  | 1:B:247:ILE:HD13 | 1.75                     | 0.68              |
| 1:B:385:ASN:HD21 | 1:B:445:LYS:NZ   | 1.90                     | 0.68              |
| 1:A:159:ASN:HB3  | 1:A:176:THR:HG22 | 1.75                     | 0.68              |
| 1:B:155:GLN:OE1  | 1:C:388:ALA:HA   | 1.92                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:460:ARG:HH22 | 1:E:487:SER:HB2  | 1.56                     | 0.68              |
| 1:F:46:THR:HG23  | 1:F:147:LEU:HD12 | 1.76                     | 0.68              |
| 1:F:123:LEU:HD23 | 1:F:332:HIS:HB3  | 1.73                     | 0.68              |
| 1:C:70:ILE:HD12  | 1:C:442:VAL:HG21 | 1.74                     | 0.68              |
| 1:A:357:LEU:H    | 1:A:357:LEU:HD12 | 1.57                     | 0.68              |
| 1:D:394:VAL:HA   | 1:D:441:TYR:HB3  | 1.76                     | 0.68              |
| 1:A:367:LEU:O    | 1:A:448:HIS:HA   | 1.93                     | 0.68              |
| 1:A:409:ASN:N    | 1:A:409:ASN:HD22 | 1.92                     | 0.68              |
| 1:E:385:ASN:HD22 | 1:E:452:SER:HB3  | 1.59                     | 0.68              |
| 1:B:368:SER:OG   | 1:B:445:LYS:HB2  | 1.94                     | 0.68              |
| 1:D:67:GLN:HB2   | 1:D:125:ILE:HB   | 1.75                     | 0.68              |
| 1:A:14:LEU:HD13  | 1:A:411:VAL:HB   | 1.75                     | 0.67              |
| 1:A:112:GLN:HE21 | 1:B:461:ALA:HB1  | 1.59                     | 0.67              |
| 1:B:467:LEU:HD22 | 1:B:467:LEU:H    | 1.59                     | 0.67              |
| 1:B:240:VAL:HG21 | 1:B:244:LEU:HD11 | 1.75                     | 0.67              |
| 1:E:345:ASN:HB3  | 1:E:348:ALA:HB3  | 1.77                     | 0.67              |
| 1:F:66:PRO:HG3   | 1:F:151:ASN:ND2  | 2.10                     | 0.67              |
| 1:D:364:GLN:HE21 | 1:D:364:GLN:N    | 1.90                     | 0.66              |
| 1:A:155:GLN:OE1  | 1:B:388:ALA:HA   | 1.94                     | 0.66              |
| 1:A:374:LEU:HD12 | 1:A:439:LEU:HD23 | 1.76                     | 0.66              |
| 1:C:403:VAL:O    | 1:C:411:VAL:HG22 | 1.95                     | 0.66              |
| 1:B:120:GLY:O    | 1:B:335:ILE:HG22 | 1.96                     | 0.66              |
| 1:B:159:ASN:ND2  | 1:B:176:THR:HG22 | 2.07                     | 0.66              |
| 1:C:169:PRO:HA   | 1:C:236:GLN:OE1  | 1.95                     | 0.66              |
| 1:C:463:PRO:O    | 1:C:467:LEU:HD13 | 1.95                     | 0.66              |
| 1:B:387:ASN:HD21 | 1:B:451:VAL:H    | 1.43                     | 0.66              |
| 1:C:69:ILE:HG12  | 1:C:145:SER:OG   | 1.95                     | 0.66              |
| 1:B:40:LEU:HD21  | 1:B:46:THR:HA    | 1.77                     | 0.66              |
| 1:D:334:ASN:ND2  | 1:D:337:ARG:HB2  | 2.09                     | 0.66              |
| 1:B:26:GLU:OE1   | 1:B:234:ARG:HG2  | 1.94                     | 0.66              |
| 1:C:121:ASP:HA   | 1:C:334:ASN:HA   | 1.78                     | 0.66              |
| 1:E:75:LYS:HB3   | 1:E:118:ASN:HA   | 1.77                     | 0.66              |
| 1:F:159:ASN:ND2  | 1:F:176:THR:HG22 | 2.03                     | 0.66              |
| 1:E:425:PRO:HB2  | 1:E:428:PHE:CD2  | 2.31                     | 0.66              |
| 1:C:56:GLY:H     | 1:C:135:ASN:HB3  | 1.61                     | 0.65              |
| 1:D:396:ARG:HB3  | 1:D:440:GLU:HB2  | 1.77                     | 0.65              |
| 1:A:481:LEU:HD22 | 1:C:217:PHE:HB3  | 1.77                     | 0.65              |
| 1:C:229:SER:N    | 1:C:230:PRO:HD3  | 2.10                     | 0.65              |
| 1:A:31:GLU:OE1   | 1:A:49:LYS:HD2   | 1.95                     | 0.65              |
| 1:F:30:ILE:HG12  | 1:F:50:ARG:HG3   | 1.78                     | 0.65              |
| 1:F:115:ARG:NH2  | 1:F:331:LEU:HD12 | 2.02                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:401:VAL:HG22 | 1:F:432:GLU:HG3  | 1.77                     | 0.65              |
| 1:A:426:GLN:NE2  | 1:C:155:GLN:H    | 1.92                     | 0.65              |
| 1:E:169:PRO:HB3  | 1:E:236:GLN:HB3  | 1.77                     | 0.65              |
| 1:A:454:TYR:CE1  | 1:A:457:ASP:HB2  | 2.30                     | 0.65              |
| 1:A:10:GLN:HA    | 1:C:161:ARG:HH22 | 1.61                     | 0.65              |
| 1:A:400:ARG:HG2  | 1:A:402:ARG:NH2  | 2.11                     | 0.65              |
| 1:E:148:ASP:OD2  | 1:E:151:ASN:HB2  | 1.97                     | 0.65              |
| 1:A:205:LEU:HD21 | 1:B:455:ILE:HD13 | 1.79                     | 0.65              |
| 1:B:387:ASN:C    | 1:B:426:GLN:HE21 | 2.04                     | 0.65              |
| 1:B:393:TYR:HB3  | 1:B:442:VAL:CG1  | 2.28                     | 0.65              |
| 1:F:14:LEU:HD13  | 1:F:411:VAL:HB   | 1.77                     | 0.65              |
| 1:C:382:PRO:HB2  | 1:C:455:ILE:HD12 | 1.78                     | 0.64              |
| 1:D:240:VAL:HG13 | 1:E:469:ASN:ND2  | 2.12                     | 0.64              |
| 1:E:208:PHE:HB2  | 1:E:213:LEU:HD21 | 1.79                     | 0.64              |
| 1:C:394:VAL:HG11 | 1:C:416:LEU:HG   | 1.79                     | 0.64              |
| 1:A:463:PRO:HG3  | 1:C:111:HIS:ND1  | 2.13                     | 0.64              |
| 1:E:244:LEU:HB3  | 1:E:247:ILE:HD11 | 1.77                     | 0.64              |
| 1:C:51:THR:HG23  | 1:C:142:VAL:HG22 | 1.78                     | 0.64              |
| 1:F:19:PRO:HB3   | 1:F:31:GLU:HB3   | 1.78                     | 0.64              |
| 1:B:22:ARG:HB3   | 1:B:22:ARG:HH11  | 1.62                     | 0.64              |
| 1:B:463:PRO:HB2  | 1:B:466:VAL:HG23 | 1.78                     | 0.64              |
| 1:A:334:ASN:ND2  | 1:A:337:ARG:H    | 1.96                     | 0.64              |
| 1:B:66:PRO:N     | 1:B:127:PRO:HG3  | 2.12                     | 0.64              |
| 1:D:176:THR:O    | 1:D:177:MET:HE2  | 1.98                     | 0.64              |
| 1:A:342:ASP:HB2  | 1:A:351:ILE:O    | 1.97                     | 0.64              |
| 1:B:22:ARG:NH2   | 1:B:29:LEU:HD21  | 2.13                     | 0.64              |
| 1:C:208:PHE:HB2  | 1:C:213:LEU:HD21 | 1.80                     | 0.64              |
| 1:A:326:ILE:HD13 | 1:A:326:ILE:O    | 1.98                     | 0.63              |
| 1:B:475:GLN:NE2  | 1:B:479:ARG:HB2  | 2.13                     | 0.63              |
| 1:F:25:SER:HB3   | 1:F:235:LYS:HB2  | 1.81                     | 0.63              |
| 1:C:14:LEU:C     | 1:C:15:ASN:HD22  | 2.05                     | 0.63              |
| 1:C:124:VAL:HG21 | 1:C:362:LEU:HD23 | 1.81                     | 0.63              |
| 1:A:235:LYS:HB3  | 1:A:236:GLN:OE1  | 1.99                     | 0.63              |
| 1:A:480:GLN:HE21 | 1:A:480:GLN:HA   | 1.63                     | 0.63              |
| 1:E:329:MET:HE2  | 1:E:331:LEU:HD21 | 1.81                     | 0.63              |
| 1:F:81:ALA:HB3   | 1:F:130:PRO:HB2  | 1.79                     | 0.63              |
| 1:A:112:GLN:NE2  | 1:B:461:ALA:HB1  | 2.14                     | 0.63              |
| 1:B:456:LYS:HG2  | 1:B:460:ARG:NH2  | 2.13                     | 0.63              |
| 1:C:205:LEU:HD13 | 1:C:227:LEU:HB3  | 1.79                     | 0.63              |
| 1:D:224:ALA:HA   | 1:D:227:LEU:HD12 | 1.81                     | 0.63              |
| 1:D:455:ILE:HD13 | 1:F:205:LEU:HD21 | 1.81                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:65:TYR:C     | 1:B:127:PRO:HG3  | 2.23                     | 0.63              |
| 1:F:67:GLN:HE21  | 1:F:69:ILE:HD11  | 1.63                     | 0.63              |
| 1:B:388:ALA:O    | 1:B:426:GLN:HA   | 1.98                     | 0.63              |
| 1:A:363:ARG:HE   | 1:A:448:HIS:CD2  | 2.16                     | 0.63              |
| 1:D:391:VAL:CG1  | 1:D:444:PHE:HB2  | 2.28                     | 0.63              |
| 1:E:73:GLN:HE21  | 1:E:142:VAL:CG1  | 2.12                     | 0.63              |
| 1:A:392:ILE:HG12 | 1:A:443:VAL:HG22 | 1.79                     | 0.63              |
| 1:C:62:TYR:CE2   | 1:C:163:PHE:HB2  | 2.34                     | 0.63              |
| 1:D:398:LYS:HE3  | 1:D:415:GLU:HB3  | 1.80                     | 0.63              |
| 1:F:50:ARG:HH22  | 1:F:67:GLN:NE2   | 1.97                     | 0.62              |
| 1:C:326:ILE:HG23 | 1:C:327:CYS:N    | 2.14                     | 0.62              |
| 1:E:60:PRO:HG3   | 1:E:132:TRP:HB3  | 1.80                     | 0.62              |
| 1:F:14:LEU:HD23  | 1:F:423:VAL:O    | 2.00                     | 0.62              |
| 1:E:459:PHE:O    | 1:E:482:LYS:HE2  | 2.00                     | 0.62              |
| 1:A:340:ARG:HB2  | 1:A:352:SER:OG   | 1.99                     | 0.62              |
| 1:A:349:GLY:HA3  | 1:A:373:VAL:O    | 2.00                     | 0.62              |
| 1:A:471:TYR:HB3  | 1:C:226:LYS:O    | 1.99                     | 0.62              |
| 1:B:388:ALA:N    | 1:B:426:GLN:HE21 | 1.98                     | 0.62              |
| 1:D:14:LEU:HD13  | 1:D:411:VAL:HB   | 1.81                     | 0.62              |
| 1:E:330:LYS:HE3  | 1:E:332:HIS:O    | 2.00                     | 0.62              |
| 1:C:351:ILE:HG12 | 1:C:372:VAL:HG13 | 1.82                     | 0.62              |
| 1:D:70:ILE:HD12  | 1:D:442:VAL:HG21 | 1.81                     | 0.62              |
| 1:D:364:GLN:NE2  | 1:D:364:GLN:N    | 2.47                     | 0.62              |
| 1:A:57:LEU:HD12  | 1:A:133:THR:O    | 2.00                     | 0.61              |
| 1:C:223:THR:O    | 1:C:226:LYS:HB2  | 1.99                     | 0.61              |
| 1:D:379:ILE:HD11 | 1:F:212:PHE:CZ   | 2.35                     | 0.61              |
| 1:F:245:SER:C    | 1:F:247:ILE:H    | 2.08                     | 0.61              |
| 1:F:454:TYR:CE1  | 1:F:457:ASP:HB2  | 2.35                     | 0.61              |
| 1:B:113:LYS:HD2  | 1:B:113:LYS:N    | 2.14                     | 0.61              |
| 1:B:224:ALA:HA   | 1:B:227:LEU:HD12 | 1.82                     | 0.61              |
| 1:F:345:ASN:HB3  | 1:F:348:ALA:HB3  | 1.82                     | 0.61              |
| 1:C:27:GLY:HA2   | 1:C:239:THR:HG23 | 1.82                     | 0.61              |
| 1:D:366:GLY:HA2  | 1:D:448:HIS:H    | 1.65                     | 0.61              |
| 1:E:109:ASP:HA   | 1:F:483:TYR:OH   | 2.01                     | 0.61              |
| 1:B:46:THR:CG2   | 1:B:147:LEU:HB2  | 2.30                     | 0.61              |
| 1:B:136:THR:HG22 | 1:B:247:ILE:HG21 | 1.82                     | 0.61              |
| 1:E:144:ILE:N    | 1:E:144:ILE:HD12 | 2.16                     | 0.61              |
| 1:E:135:ASN:ND2  | 1:E:141:VAL:HG23 | 2.14                     | 0.61              |
| 1:C:64:PRO:HG3   | 1:C:156:LEU:HD12 | 1.83                     | 0.61              |
| 1:D:446:THR:O    | 1:D:447:HIS:HB2  | 1.99                     | 0.61              |
| 1:E:156:LEU:HD21 | 1:F:426:GLN:H    | 1.65                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:170:ASP:HB2  | 1:F:235:LYS:HD2  | 1.82                     | 0.61              |
| 1:D:437:GLN:H    | 1:D:437:GLN:NE2  | 1.99                     | 0.60              |
| 1:A:468:SER:OG   | 1:A:478:VAL:HG21 | 2.01                     | 0.60              |
| 1:E:176:THR:O    | 1:E:177:MET:HE2  | 2.00                     | 0.60              |
| 1:F:176:THR:C    | 1:F:177:MET:HE2  | 2.26                     | 0.60              |
| 1:B:31:GLU:HB2   | 1:B:49:LYS:HB3   | 1.83                     | 0.60              |
| 1:C:52:LEU:CD2   | 1:C:237:ILE:HD13 | 2.31                     | 0.60              |
| 1:A:234:ARG:CB   | 1:A:238:VAL:HG12 | 2.31                     | 0.60              |
| 1:A:471:TYR:CD2  | 1:C:227:LEU:HA   | 2.36                     | 0.60              |
| 1:B:454:TYR:CZ   | 1:B:457:ASP:HB2  | 2.36                     | 0.60              |
| 1:C:6:PHE:C      | 1:C:7:ASN:HD22   | 2.08                     | 0.60              |
| 1:D:351:ILE:HG23 | 1:D:372:VAL:HG22 | 1.82                     | 0.60              |
| 1:F:28:GLY:HA3   | 1:F:237:ILE:HG21 | 1.84                     | 0.60              |
| 1:B:148:ASP:OD2  | 1:B:151:ASN:HB2  | 2.01                     | 0.60              |
| 1:D:68:MET:HE1   | 1:D:368:SER:O    | 2.01                     | 0.60              |
| 1:D:126:PRO:HB2  | 1:D:129:VAL:HG21 | 1.82                     | 0.60              |
| 1:D:338:PRO:HG3  | 1:D:350:ARG:NH1  | 2.16                     | 0.60              |
| 1:C:114:ILE:HD12 | 1:C:132:TRP:HZ2  | 1.66                     | 0.60              |
| 1:C:326:ILE:HG23 | 1:C:327:CYS:H    | 1.65                     | 0.60              |
| 1:D:325:ASN:N    | 1:D:325:ASN:HD22 | 1.97                     | 0.60              |
| 1:A:409:ASN:N    | 1:A:409:ASN:ND2  | 2.49                     | 0.60              |
| 1:B:240:VAL:HG13 | 1:C:469:ASN:HD21 | 1.67                     | 0.60              |
| 1:D:489:PRO:O    | 1:D:491:VAL:HG23 | 2.02                     | 0.60              |
| 1:B:246:VAL:HG23 | 1:C:465:GLU:OE2  | 2.01                     | 0.60              |
| 1:E:17:LEU:HD22  | 1:E:37:HIS:ND1   | 2.17                     | 0.60              |
| 1:A:33:TRP:CE3   | 1:A:47:VAL:HB    | 2.37                     | 0.59              |
| 1:B:69:ILE:HG12  | 1:B:145:SER:HA   | 1.84                     | 0.59              |
| 1:A:407:GLN:HB2  | 1:A:409:ASN:HD21 | 1.67                     | 0.59              |
| 1:B:376:ARG:HD3  | 1:B:436:GLU:O    | 2.02                     | 0.59              |
| 1:D:34:ASN:HD21  | 1:D:36:GLN:HB2   | 1.66                     | 0.59              |
| 1:A:374:LEU:HB2  | 1:A:439:LEU:HB3  | 1.83                     | 0.59              |
| 1:A:395:THR:C    | 1:A:418:ARG:HG3  | 2.27                     | 0.59              |
| 1:B:240:VAL:HG13 | 1:C:469:ASN:ND2  | 2.17                     | 0.59              |
| 1:B:475:GLN:HE21 | 1:B:479:ARG:HB2  | 1.67                     | 0.59              |
| 1:A:34:ASN:HD22  | 1:A:35:SER:N     | 2.00                     | 0.59              |
| 1:C:213:LEU:HD12 | 1:C:217:PHE:HE1  | 1.66                     | 0.59              |
| 1:C:350:ARG:HH21 | 1:C:350:ARG:HG3  | 1.68                     | 0.59              |
| 1:C:363:ARG:HE   | 1:C:448:HIS:CG   | 2.21                     | 0.59              |
| 1:E:234:ARG:O    | 1:E:235:LYS:HB2  | 2.02                     | 0.59              |
| 1:D:392:ILE:O    | 1:D:421:LEU:HD12 | 2.02                     | 0.59              |
| 1:A:60:PRO:HA    | 1:A:131:TYR:O    | 2.03                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:123:LEU:HD23 | 1:A:332:HIS:HB3  | 1.83                     | 0.59              |
| 1:A:471:TYR:CE2  | 1:C:205:LEU:HD12 | 2.38                     | 0.59              |
| 1:B:326:ILE:HG13 | 1:B:329:MET:SD   | 2.43                     | 0.59              |
| 1:D:123:LEU:HD23 | 1:D:332:HIS:HB3  | 1.84                     | 0.58              |
| 1:F:395:THR:O    | 1:F:418:ARG:HG3  | 2.02                     | 0.58              |
| 1:C:399:GLY:HA3  | 1:C:439:LEU:HD22 | 1.86                     | 0.58              |
| 1:B:348:ALA:O    | 1:B:374:LEU:HD22 | 2.03                     | 0.58              |
| 1:F:107:LEU:H    | 1:F:107:LEU:CD2  | 2.16                     | 0.58              |
| 1:A:159:ASN:ND2  | 1:A:176:THR:HA   | 2.19                     | 0.58              |
| 1:B:338:PRO:HG3  | 1:B:350:ARG:HH21 | 1.68                     | 0.58              |
| 1:C:23:VAL:HG11  | 1:C:170:ASP:HB3  | 1.85                     | 0.58              |
| 1:C:326:ILE:HD13 | 1:C:326:ILE:C    | 2.28                     | 0.58              |
| 1:E:47:VAL:HG21  | 1:E:421:LEU:HD11 | 1.84                     | 0.58              |
| 1:F:387:ASN:O    | 1:F:388:ALA:HB2  | 2.04                     | 0.58              |
| 1:B:121:ASP:HA   | 1:B:334:ASN:HA   | 1.84                     | 0.58              |
| 1:C:8:GLU:O      | 1:C:42:CYS:HB2   | 2.03                     | 0.58              |
| 1:D:386:LEU:HG   | 1:F:128:GLY:HA3  | 1.84                     | 0.58              |
| 1:A:45:VAL:HG12  | 1:A:148:ASP:HA   | 1.86                     | 0.58              |
| 1:C:174:PRO:O    | 1:C:178:GLN:HG3  | 2.02                     | 0.58              |
| 1:E:62:TYR:HE2   | 1:F:427:ASN:HB3  | 1.67                     | 0.58              |
| 1:F:164:TYR:O    | 1:F:203:SER:HB2  | 2.04                     | 0.58              |
| 1:D:246:VAL:HG13 | 1:E:465:GLU:CD   | 2.28                     | 0.58              |
| 1:D:368:SER:HB3  | 1:D:445:LYS:HB2  | 1.85                     | 0.58              |
| 1:A:22:ARG:HH12  | 1:A:29:LEU:HD21  | 1.69                     | 0.57              |
| 1:A:378:GLY:O    | 1:A:433:GLN:HA   | 2.04                     | 0.57              |
| 1:B:393:TYR:HB3  | 1:B:442:VAL:HG12 | 1.85                     | 0.57              |
| 1:D:480:GLN:OE1  | 1:F:219:THR:HA   | 2.04                     | 0.57              |
| 1:B:387:ASN:HA   | 1:B:426:GLN:NE2  | 2.20                     | 0.57              |
| 1:D:135:ASN:ND2  | 1:D:141:VAL:HG23 | 2.19                     | 0.57              |
| 1:A:144:ILE:HD12 | 1:A:144:ILE:N    | 2.20                     | 0.57              |
| 1:A:354:LEU:HD12 | 1:A:358:THR:OG1  | 2.04                     | 0.57              |
| 1:B:387:ASN:HD22 | 1:B:387:ASN:N    | 1.98                     | 0.57              |
| 1:C:338:PRO:CG   | 1:C:350:ARG:HH11 | 2.17                     | 0.57              |
| 1:B:34:ASN:HD22  | 1:B:35:SER:N     | 2.03                     | 0.57              |
| 1:B:124:VAL:HG12 | 1:B:331:LEU:O    | 2.05                     | 0.57              |
| 1:F:71:VAL:HG21  | 1:F:117:PHE:CD2  | 2.39                     | 0.57              |
| 1:F:456:LYS:NZ   | 1:F:486:ASN:HD21 | 2.02                     | 0.57              |
| 1:A:71:VAL:HG21  | 1:A:117:PHE:CD2  | 2.40                     | 0.57              |
| 1:A:463:PRO:HB2  | 1:A:466:VAL:CG2  | 2.35                     | 0.57              |
| 1:B:134:TYR:OH   | 1:B:243:GLY:HA2  | 2.05                     | 0.57              |
| 1:C:345:ASN:HD22 | 1:C:348:ALA:HB3  | 1.68                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:73:GLN:HE21  | 1:E:142:VAL:HG12 | 1.69                     | 0.57              |
| 1:F:219:THR:OG1  | 1:F:223:THR:HB   | 2.04                     | 0.57              |
| 1:A:22:ARG:NH1   | 1:A:22:ARG:HB2   | 2.19                     | 0.57              |
| 1:D:175:GLU:O    | 1:D:178:GLN:HG3  | 2.05                     | 0.57              |
| 1:C:386:LEU:HD12 | 1:C:386:LEU:H    | 1.70                     | 0.57              |
| 1:D:83:PRO:HB3   | 1:E:453:SER:CB   | 2.34                     | 0.57              |
| 1:A:234:ARG:HB2  | 1:A:238:VAL:HG12 | 1.86                     | 0.57              |
| 1:A:357:LEU:H    | 1:A:357:LEU:CD1  | 2.17                     | 0.57              |
| 1:D:379:ILE:HG13 | 1:D:433:GLN:HB2  | 1.87                     | 0.57              |
| 1:F:6:PHE:C      | 1:F:7:ASN:HD22   | 2.13                     | 0.57              |
| 1:B:168:ASN:ND2  | 1:B:202:GLY:HA2  | 2.20                     | 0.57              |
| 1:E:20:ASP:OD2   | 1:E:34:ASN:HB2   | 2.05                     | 0.57              |
| 1:B:22:ARG:HB3   | 1:B:22:ARG:NH1   | 2.20                     | 0.56              |
| 1:C:337:ARG:HA   | 1:C:337:ARG:HH21 | 1.69                     | 0.56              |
| 1:E:17:LEU:HD13  | 1:E:37:HIS:ND1   | 2.20                     | 0.56              |
| 1:C:170:ASP:H    | 1:C:236:GLN:CD   | 2.13                     | 0.56              |
| 1:C:174:PRO:C    | 1:C:178:GLN:HE21 | 2.13                     | 0.56              |
| 1:D:14:LEU:HD23  | 1:D:423:VAL:O    | 2.05                     | 0.56              |
| 1:D:34:ASN:OD1   | 1:D:175:GLU:HB3  | 2.06                     | 0.56              |
| 1:D:144:ILE:HG13 | 1:D:393:TYR:CE2  | 2.40                     | 0.56              |
| 1:D:391:VAL:HG13 | 1:D:391:VAL:O    | 2.05                     | 0.56              |
| 1:D:427:ASN:HB3  | 1:F:62:TYR:HE2   | 1.70                     | 0.56              |
| 1:E:430:VAL:HG22 | 1:E:431:ALA:N    | 2.21                     | 0.56              |
| 1:D:170:ASP:O    | 1:D:172:GLU:N    | 2.38                     | 0.56              |
| 1:A:396:ARG:HG2  | 1:A:396:ARG:HH11 | 1.71                     | 0.56              |
| 1:B:28:GLY:HA3   | 1:B:237:ILE:HG21 | 1.87                     | 0.56              |
| 1:D:47:VAL:HG13  | 1:D:145:SER:O    | 2.05                     | 0.56              |
| 1:C:124:VAL:CB   | 1:C:331:LEU:HD11 | 2.34                     | 0.56              |
| 1:C:123:LEU:HD23 | 1:C:331:LEU:O    | 2.06                     | 0.56              |
| 1:E:333:GLU:HG3  | 1:E:340:ARG:HH12 | 1.69                     | 0.56              |
| 1:F:51:THR:HA    | 1:F:141:VAL:O    | 2.05                     | 0.56              |
| 1:F:477:GLN:O    | 1:F:480:GLN:HB3  | 2.06                     | 0.56              |
| 1:C:66:PRO:HG3   | 1:C:151:ASN:ND2  | 2.21                     | 0.56              |
| 1:C:69:ILE:HG12  | 1:C:145:SER:CB   | 2.36                     | 0.56              |
| 1:D:36:GLN:HE22  | 1:D:178:GLN:NE2  | 2.04                     | 0.56              |
| 1:E:417:ARG:HG3  | 1:E:420:GLN:OE1  | 2.05                     | 0.56              |
| 1:A:204:VAL:O    | 1:B:404:VAL:HG11 | 2.06                     | 0.56              |
| 1:D:345:ASN:HB3  | 1:D:348:ALA:HB3  | 1.88                     | 0.56              |
| 1:C:371:TYR:HE1  | 1:C:440:GLU:HG2  | 1.69                     | 0.55              |
| 1:C:394:VAL:HG21 | 1:C:417:ARG:O    | 2.05                     | 0.55              |
| 1:F:67:GLN:HG2   | 1:F:125:ILE:HB   | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:385:ASN:HD21 | 1:A:445:LYS:CE   | 2.20                     | 0.55              |
| 1:B:61:SER:O     | 1:B:130:PRO:HA   | 2.06                     | 0.55              |
| 1:B:144:ILE:N    | 1:B:144:ILE:HD12 | 2.22                     | 0.55              |
| 1:C:394:VAL:O    | 1:C:418:ARG:HA   | 2.05                     | 0.55              |
| 1:D:234:ARG:O    | 1:D:235:LYS:HB2  | 2.06                     | 0.55              |
| 1:E:226:LYS:HB2  | 1:F:473:LEU:HD21 | 1.88                     | 0.55              |
| 1:F:214:ALA:HB1  | 1:F:219:THR:O    | 2.06                     | 0.55              |
| 1:C:47:VAL:HG12  | 1:C:48:SER:N     | 2.22                     | 0.55              |
| 1:D:173:HIS:HB3  | 1:D:175:GLU:OE1  | 2.06                     | 0.55              |
| 1:C:126:PRO:HB2  | 1:C:129:VAL:HG21 | 1.89                     | 0.55              |
| 1:C:417:ARG:HG2  | 1:C:417:ARG:HH11 | 1.71                     | 0.55              |
| 1:A:373:VAL:HG22 | 1:A:440:GLU:CG   | 2.35                     | 0.55              |
| 1:B:349:GLY:O    | 1:B:490:LEU:HD13 | 2.06                     | 0.55              |
| 1:B:408:GLY:C    | 1:B:409:ASN:HD22 | 2.14                     | 0.55              |
| 1:D:466:VAL:HG22 | 1:F:244:LEU:HD21 | 1.89                     | 0.55              |
| 1:A:26:GLU:OE1   | 1:A:234:ARG:HG2  | 2.06                     | 0.55              |
| 1:C:71:VAL:HG21  | 1:C:117:PHE:CD2  | 2.42                     | 0.55              |
| 1:E:73:GLN:HB3   | 1:E:142:VAL:CG1  | 2.36                     | 0.55              |
| 1:A:214:ALA:HB1  | 1:A:219:THR:O    | 2.07                     | 0.55              |
| 1:B:82:PHE:HZ    | 1:B:331:LEU:HD11 | 1.71                     | 0.55              |
| 1:C:61:SER:O     | 1:C:130:PRO:HA   | 2.06                     | 0.55              |
| 1:C:144:ILE:HD12 | 1:C:144:ILE:N    | 2.21                     | 0.55              |
| 1:D:14:LEU:C     | 1:D:15:ASN:HD22  | 2.15                     | 0.55              |
| 1:F:246:VAL:HG12 | 1:F:246:VAL:O    | 2.06                     | 0.55              |
| 1:A:390:SER:HB2  | 1:A:424:VAL:HB   | 1.88                     | 0.55              |
| 1:F:214:ALA:HA   | 1:F:219:THR:HG22 | 1.88                     | 0.55              |
| 1:A:409:ASN:ND2  | 1:A:409:ASN:H    | 2.03                     | 0.55              |
| 1:E:70:ILE:HG23  | 1:E:70:ILE:O     | 2.05                     | 0.55              |
| 1:E:333:GLU:CG   | 1:E:340:ARG:HH12 | 2.19                     | 0.55              |
| 1:F:349:GLY:O    | 1:F:490:LEU:HD13 | 2.07                     | 0.55              |
| 1:A:23:VAL:HB    | 1:A:30:ILE:HB    | 1.89                     | 0.55              |
| 1:A:357:LEU:HD12 | 1:A:357:LEU:N    | 2.22                     | 0.55              |
| 1:B:345:ASN:CG   | 1:B:348:ALA:HB3  | 2.31                     | 0.55              |
| 1:A:22:ARG:HA    | 1:A:30:ILE:O     | 2.07                     | 0.54              |
| 1:B:34:ASN:HD22  | 1:B:35:SER:H     | 1.55                     | 0.54              |
| 1:E:2:THR:HA     | 1:E:5:LYS:NZ     | 2.22                     | 0.54              |
| 1:B:471:TYR:O    | 1:B:472:ASN:HB2  | 2.06                     | 0.54              |
| 1:B:479:ARG:HE   | 1:B:483:TYR:HD2  | 1.53                     | 0.54              |
| 1:C:9:CYS:C      | 1:C:11:LEU:H     | 2.16                     | 0.54              |
| 1:E:244:LEU:HD21 | 1:F:466:VAL:CG2  | 2.37                     | 0.54              |
| 1:E:405:ASN:HD22 | 1:E:411:VAL:CG1  | 2.18                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:208:PHE:HB2  | 1:F:213:LEU:HD21 | 1.88                     | 0.54              |
| 1:A:350:ARG:NH1  | 1:A:373:VAL:HG21 | 2.22                     | 0.54              |
| 1:C:143:ALA:C    | 1:C:144:ILE:HD12 | 2.32                     | 0.54              |
| 1:D:156:LEU:HA   | 1:E:9:CYS:SG     | 2.46                     | 0.54              |
| 1:E:208:PHE:CD1  | 1:F:402:ARG:HD3  | 2.43                     | 0.54              |
| 1:F:235:LYS:HB3  | 1:F:236:GLN:OE1  | 2.08                     | 0.54              |
| 1:C:30:ILE:HD12  | 1:C:236:GLN:HG3  | 1.90                     | 0.54              |
| 1:F:25:SER:OG    | 1:F:237:ILE:HB   | 2.07                     | 0.54              |
| 1:A:358:THR:O    | 1:A:360:PRO:HD3  | 2.07                     | 0.54              |
| 1:B:65:TYR:CE2   | 1:B:147:LEU:HB3  | 2.43                     | 0.54              |
| 1:B:387:ASN:HA   | 1:B:426:GLN:HE21 | 1.72                     | 0.54              |
| 1:C:206:SER:HA   | 1:C:228:ARG:HG2  | 1.90                     | 0.54              |
| 1:C:403:VAL:HG22 | 1:C:430:VAL:HG23 | 1.89                     | 0.54              |
| 1:F:218:ASN:HD22 | 1:F:218:ASN:N    | 2.04                     | 0.54              |
| 1:A:340:ARG:CZ   | 1:A:350:ARG:HD2  | 2.37                     | 0.54              |
| 1:A:407:GLN:HB2  | 1:A:409:ASN:ND2  | 2.22                     | 0.54              |
| 1:C:11:LEU:HD21  | 1:C:38:PRO:HB3   | 1.89                     | 0.54              |
| 1:C:135:ASN:ND2  | 1:C:141:VAL:HG23 | 2.22                     | 0.54              |
| 1:E:36:GLN:HE21  | 1:E:175:GLU:HB2  | 1.73                     | 0.54              |
| 1:E:478:VAL:O    | 1:E:482:LYS:HB2  | 2.08                     | 0.54              |
| 1:A:46:THR:HG23  | 1:A:147:LEU:HB2  | 1.90                     | 0.54              |
| 1:A:400:ARG:HG2  | 1:A:402:ARG:HH22 | 1.72                     | 0.54              |
| 1:B:67:GLN:HE21  | 1:B:147:LEU:CD2  | 2.20                     | 0.54              |
| 1:C:396:ARG:HD2  | 1:C:396:ARG:C    | 2.33                     | 0.54              |
| 1:D:69:ILE:CG2   | 1:D:143:ALA:HB1  | 2.38                     | 0.54              |
| 1:A:325:ASN:HA   | 1:A:328:THR:HG22 | 1.89                     | 0.54              |
| 1:C:60:PRO:HA    | 1:C:131:TYR:O    | 2.08                     | 0.54              |
| 1:C:210:LYS:HD3  | 1:C:225:GLU:CG   | 2.35                     | 0.54              |
| 1:D:466:VAL:HG22 | 1:F:244:LEU:CD2  | 2.38                     | 0.54              |
| 1:F:25:SER:CB    | 1:F:235:LYS:HB2  | 2.38                     | 0.54              |
| 1:F:334:ASN:HB3  | 1:F:340:ARG:NH1  | 2.22                     | 0.54              |
| 1:A:25:SER:OG    | 1:A:237:ILE:HB   | 2.08                     | 0.54              |
| 1:B:35:SER:OG    | 1:B:175:GLU:HG3  | 2.08                     | 0.54              |
| 1:C:386:LEU:HD12 | 1:C:386:LEU:N    | 2.23                     | 0.54              |
| 1:A:124:VAL:O    | 1:A:126:PRO:HD3  | 2.08                     | 0.54              |
| 1:A:351:ILE:HG12 | 1:A:372:VAL:HG22 | 1.89                     | 0.54              |
| 1:A:480:GLN:CD   | 1:A:484:GLN:HG3  | 2.32                     | 0.54              |
| 1:B:46:THR:HG23  | 1:B:147:LEU:HB2  | 1.90                     | 0.54              |
| 1:A:350:ARG:HH12 | 1:A:373:VAL:HG21 | 1.73                     | 0.53              |
| 1:E:57:LEU:HD13  | 1:E:57:LEU:C     | 2.33                     | 0.53              |
| 1:E:376:ARG:HH11 | 1:E:376:ARG:CB   | 2.18                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:402:ARG:NH2  | 1:F:413:ASP:OD1  | 2.41                     | 0.53              |
| 1:A:163:PHE:CZ   | 1:B:406:CSD:HB2  | 2.43                     | 0.53              |
| 1:A:491:VAL:HG12 | 1:A:492:ASN:N    | 2.23                     | 0.53              |
| 1:D:50:ARG:HH12  | 1:D:67:GLN:NE2   | 2.05                     | 0.53              |
| 1:F:34:ASN:ND2   | 1:F:36:GLN:HB2   | 2.14                     | 0.53              |
| 1:A:122:VAL:O    | 1:A:332:HIS:HA   | 2.08                     | 0.53              |
| 1:B:385:ASN:HD21 | 1:B:445:LYS:HZ2  | 1.54                     | 0.53              |
| 1:D:394:VAL:HA   | 1:D:441:TYR:CB   | 2.38                     | 0.53              |
| 1:F:343:PHE:HB2  | 1:F:351:ILE:HB   | 1.89                     | 0.53              |
| 1:D:180:GLN:NE2  | 1:D:180:GLN:N    | 2.56                     | 0.53              |
| 1:D:218:ASN:OD1  | 1:E:485:GLY:HA3  | 2.08                     | 0.53              |
| 1:E:16:ALA:HB1   | 1:E:420:GLN:NE2  | 2.22                     | 0.53              |
| 1:A:15:ASN:HB2   | 1:A:39:GLU:OE2   | 2.09                     | 0.53              |
| 1:A:391:VAL:CG1  | 1:A:421:LEU:HD11 | 2.37                     | 0.53              |
| 1:D:115:ARG:HD2  | 1:D:115:ARG:N    | 2.20                     | 0.53              |
| 1:D:171:ILE:HG12 | 1:D:198:GLU:O    | 2.08                     | 0.53              |
| 1:A:465:GLU:OE2  | 1:C:245:SER:HB2  | 2.09                     | 0.53              |
| 1:A:493:PRO:HB3  | 1:C:215:GLN:OE1  | 2.08                     | 0.53              |
| 1:B:425:PRO:HB2  | 1:B:428:PHE:CD2  | 2.44                     | 0.53              |
| 1:D:9:CYS:C      | 1:D:11:LEU:H     | 2.16                     | 0.53              |
| 1:D:36:GLN:NE2   | 1:D:175:GLU:HB2  | 2.12                     | 0.53              |
| 1:F:170:ASP:HA   | 1:F:200:GLU:HA   | 1.89                     | 0.53              |
| 1:B:462:ILE:HG22 | 1:B:466:VAL:HB   | 1.91                     | 0.53              |
| 1:E:325:ASN:HA   | 1:E:328:THR:HG22 | 1.90                     | 0.53              |
| 1:E:335:ILE:HG12 | 1:E:335:ILE:O    | 2.09                     | 0.53              |
| 1:F:171:ILE:HD13 | 1:F:200:GLU:N    | 2.24                     | 0.53              |
| 1:A:391:VAL:HG12 | 1:A:421:LEU:HD11 | 1.90                     | 0.53              |
| 1:D:27:GLY:HA3   | 1:D:239:THR:HG23 | 1.90                     | 0.53              |
| 1:E:39:GLU:N     | 1:E:39:GLU:OE1   | 2.39                     | 0.53              |
| 1:E:170:ASP:OD2  | 1:E:235:LYS:HE2  | 2.09                     | 0.53              |
| 1:F:20:ASP:O     | 1:F:21:HIS:HB2   | 2.08                     | 0.53              |
| 1:B:396:ARG:HA   | 1:B:418:ARG:HG3  | 1.91                     | 0.53              |
| 1:C:454:TYR:CE1  | 1:C:457:ASP:HB2  | 2.44                     | 0.53              |
| 1:D:430:VAL:HG22 | 1:D:431:ALA:N    | 2.24                     | 0.53              |
| 1:B:69:ILE:CG2   | 1:B:143:ALA:HB1  | 2.39                     | 0.53              |
| 1:C:87:GLU:HG3   | 1:C:112:GLN:N    | 2.24                     | 0.53              |
| 1:F:405:ASN:OD1  | 1:F:407:GLN:HG3  | 2.08                     | 0.53              |
| 1:B:31:GLU:OE1   | 1:B:49:LYS:HD3   | 2.08                     | 0.52              |
| 1:E:247:ILE:H    | 1:E:247:ILE:CD1  | 2.16                     | 0.52              |
| 1:E:376:ARG:O    | 1:E:377:ASN:HB2  | 2.10                     | 0.52              |
| 1:A:70:ILE:O     | 1:A:70:ILE:HG23  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:87:GLU:O     | 1:A:88:THR:C     | 2.53                     | 0.52              |
| 1:A:461:ALA:HA   | 1:C:87:GLU:CG    | 2.39                     | 0.52              |
| 1:C:372:VAL:HB   | 1:C:441:TYR:CZ   | 2.44                     | 0.52              |
| 1:F:107:LEU:HD22 | 1:F:107:LEU:N    | 2.20                     | 0.52              |
| 1:A:386:LEU:HD13 | 1:A:452:SER:HA   | 1.90                     | 0.52              |
| 1:B:15:ASN:HD22  | 1:B:15:ASN:N     | 2.05                     | 0.52              |
| 1:B:379:ILE:HG12 | 1:B:433:GLN:HG3  | 1.91                     | 0.52              |
| 1:C:34:ASN:HD22  | 1:C:35:SER:N     | 2.07                     | 0.52              |
| 1:C:146:LEU:HB2  | 1:C:444:PHE:CD1  | 2.43                     | 0.52              |
| 1:E:40:LEU:HD12  | 1:E:45:VAL:O     | 2.10                     | 0.52              |
| 1:E:329:MET:HE2  | 1:E:331:LEU:CD2  | 2.39                     | 0.52              |
| 1:F:244:LEU:O    | 1:F:247:ILE:HD13 | 2.09                     | 0.52              |
| 1:A:387:ASN:HD21 | 1:A:451:VAL:H    | 1.57                     | 0.52              |
| 1:B:69:ILE:HA    | 1:B:144:ILE:O    | 2.09                     | 0.52              |
| 1:B:81:ALA:HA    | 1:B:112:GLN:NE2  | 2.24                     | 0.52              |
| 1:B:240:VAL:HG11 | 1:B:244:LEU:CD1  | 2.39                     | 0.52              |
| 1:B:396:ARG:HD3  | 1:B:396:ARG:C    | 2.34                     | 0.52              |
| 1:C:213:LEU:HD22 | 1:C:213:LEU:H    | 1.75                     | 0.52              |
| 1:C:240:VAL:HG11 | 1:C:244:LEU:HD13 | 1.91                     | 0.52              |
| 1:C:345:ASN:HD22 | 1:C:348:ALA:CB   | 2.23                     | 0.52              |
| 1:B:335:ILE:HG23 | 1:B:336:ALA:N    | 2.25                     | 0.52              |
| 1:C:394:VAL:CG1  | 1:C:416:LEU:HG   | 2.39                     | 0.52              |
| 1:D:62:TYR:HE2   | 1:E:427:ASN:HB3  | 1.74                     | 0.52              |
| 1:E:57:LEU:HD12  | 1:E:59:LEU:HD23  | 1.91                     | 0.52              |
| 1:A:61:SER:O     | 1:A:130:PRO:HA   | 2.10                     | 0.52              |
| 1:A:351:ILE:HG13 | 1:A:490:LEU:HD11 | 1.91                     | 0.52              |
| 1:E:235:LYS:HE3  | 1:E:235:LYS:CA   | 2.40                     | 0.52              |
| 1:E:244:LEU:HD11 | 1:F:465:GLU:HB3  | 1.91                     | 0.52              |
| 1:F:152:PHE:H    | 1:F:152:PHE:HD1  | 1.56                     | 0.52              |
| 1:B:76:GLY:HA2   | 1:B:136:THR:H    | 1.75                     | 0.52              |
| 1:B:85:CYS:HB3   | 1:B:113:LYS:NZ   | 2.24                     | 0.52              |
| 1:D:59:LEU:HG    | 1:D:236:GLN:O    | 2.10                     | 0.52              |
| 1:A:334:ASN:HD21 | 1:A:337:ARG:HG2  | 1.71                     | 0.52              |
| 1:A:395:THR:O    | 1:A:418:ARG:HG3  | 2.09                     | 0.52              |
| 1:B:480:GLN:O    | 1:B:484:GLN:HB2  | 2.10                     | 0.52              |
| 1:A:34:ASN:HD22  | 1:A:35:SER:H     | 1.56                     | 0.52              |
| 1:C:406:CSD:C    | 1:C:408:GLY:H    | 2.23                     | 0.52              |
| 1:C:425:PRO:HB2  | 1:C:428:PHE:CG   | 2.45                     | 0.52              |
| 1:F:170:ASP:O    | 1:F:171:ILE:C    | 2.52                     | 0.51              |
| 1:F:357:LEU:N    | 1:F:357:LEU:HD12 | 2.25                     | 0.51              |
| 1:F:391:VAL:CG1  | 1:F:421:LEU:HD11 | 2.40                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:204:VAL:HB   | 1:C:429:VAL:HG21 | 1.93                     | 0.51              |
| 1:B:335:ILE:HD11 | 1:B:371:TYR:N    | 2.25                     | 0.51              |
| 1:D:21:HIS:HE1   | 1:D:197:GLN:HG3  | 1.75                     | 0.51              |
| 1:F:46:THR:CG2   | 1:F:147:LEU:HB2  | 2.41                     | 0.51              |
| 1:C:392:ILE:O    | 1:C:421:LEU:HD12 | 2.11                     | 0.51              |
| 1:E:128:GLY:O    | 1:F:386:LEU:HG   | 2.09                     | 0.51              |
| 1:E:462:ILE:HB   | 1:E:467:LEU:HD21 | 1.92                     | 0.51              |
| 1:F:170:ASP:H    | 1:F:236:GLN:HE22 | 1.58                     | 0.51              |
| 1:C:25:SER:HB3   | 1:C:28:GLY:O     | 2.11                     | 0.51              |
| 1:A:22:ARG:CB    | 1:A:22:ARG:HH11  | 2.24                     | 0.51              |
| 1:A:23:VAL:O     | 1:A:29:LEU:HD12  | 2.11                     | 0.51              |
| 1:B:174:PRO:C    | 1:B:176:THR:H    | 2.18                     | 0.51              |
| 1:C:225:GLU:OE1  | 1:C:225:GLU:HA   | 2.11                     | 0.51              |
| 1:C:378:GLY:O    | 1:C:433:GLN:HA   | 2.11                     | 0.51              |
| 1:E:62:TYR:CE2   | 1:F:427:ASN:HB3  | 2.44                     | 0.51              |
| 1:E:210:LYS:HG3  | 1:E:221:GLU:OE2  | 2.10                     | 0.51              |
| 1:F:106:GLN:HE21 | 1:F:106:GLN:HA   | 1.76                     | 0.51              |
| 1:A:14:LEU:HD23  | 1:A:423:VAL:O    | 2.10                     | 0.51              |
| 1:A:18:GLU:CA    | 1:A:33:TRP:HE1   | 2.24                     | 0.51              |
| 1:B:240:VAL:HG11 | 1:B:244:LEU:HD12 | 1.92                     | 0.51              |
| 1:B:357:LEU:HD23 | 1:B:449:ASN:ND2  | 2.25                     | 0.51              |
| 1:D:57:LEU:HD12  | 1:D:133:THR:O    | 2.11                     | 0.51              |
| 1:D:126:PRO:HB2  | 1:D:129:VAL:CG2  | 2.40                     | 0.51              |
| 1:D:469:ASN:ND2  | 1:F:240:VAL:HG13 | 2.26                     | 0.51              |
| 1:E:421:LEU:C    | 1:E:421:LEU:HD23 | 2.35                     | 0.51              |
| 1:A:69:ILE:HG22  | 1:A:143:ALA:HB1  | 1.93                     | 0.51              |
| 1:A:462:ILE:HG22 | 1:A:466:VAL:HB   | 1.91                     | 0.51              |
| 1:A:480:GLN:HA   | 1:A:480:GLN:NE2  | 2.24                     | 0.51              |
| 1:E:227:LEU:HA   | 1:F:471:TYR:HD2  | 1.75                     | 0.51              |
| 1:B:164:TYR:CD1  | 1:B:169:PRO:HG3  | 2.45                     | 0.51              |
| 1:C:223:THR:O    | 1:C:227:LEU:HD22 | 2.11                     | 0.51              |
| 1:A:166:ALA:HB2  | 1:B:471:TYR:CZ   | 2.45                     | 0.51              |
| 1:A:344:TYR:CE1  | 1:F:233:GLU:HB2  | 2.46                     | 0.51              |
| 1:C:27:GLY:HA3   | 1:C:237:ILE:HG22 | 1.92                     | 0.51              |
| 1:D:206:SER:C    | 1:D:208:PHE:H    | 2.19                     | 0.51              |
| 1:B:57:LEU:C     | 1:B:57:LEU:HD23  | 2.36                     | 0.51              |
| 1:C:72:VAL:HG23  | 1:C:73:GLN:N     | 2.26                     | 0.51              |
| 1:F:430:VAL:HG22 | 1:F:431:ALA:N    | 2.25                     | 0.51              |
| 1:A:475:GLN:CG   | 1:A:479:ARG:HH12 | 2.23                     | 0.50              |
| 1:C:338:PRO:HG3  | 1:C:350:ARG:NH1  | 2.21                     | 0.50              |
| 1:D:475:GLN:O    | 1:D:479:ARG:HG2  | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:403:VAL:HG22 | 1:F:430:VAL:HG23 | 1.92                     | 0.50              |
| 1:A:76:GLY:HA2   | 1:A:136:THR:H    | 1.76                     | 0.50              |
| 1:B:200:GLU:N    | 1:B:200:GLU:OE1  | 2.44                     | 0.50              |
| 1:B:234:ARG:O    | 1:B:235:LYS:HB2  | 2.10                     | 0.50              |
| 1:F:40:LEU:N     | 1:F:40:LEU:HD12  | 2.26                     | 0.50              |
| 1:F:144:ILE:HD12 | 1:F:144:ILE:N    | 2.26                     | 0.50              |
| 1:A:134:TYR:OH   | 1:A:243:GLY:HA2  | 2.12                     | 0.50              |
| 1:A:229:SER:C    | 1:A:231:ASP:H    | 2.20                     | 0.50              |
| 1:A:460:ARG:O    | 1:C:87:GLU:HG2   | 2.11                     | 0.50              |
| 1:B:136:THR:CG2  | 1:B:247:ILE:HG21 | 2.41                     | 0.50              |
| 1:C:221:GLU:O    | 1:C:224:ALA:HB3  | 2.12                     | 0.50              |
| 1:D:115:ARG:H    | 1:D:115:ARG:CD   | 2.17                     | 0.50              |
| 1:E:326:ILE:HD13 | 1:E:326:ILE:C    | 2.36                     | 0.50              |
| 1:F:114:ILE:HD12 | 1:F:132:TRP:HZ2  | 1.74                     | 0.50              |
| 1:F:220:ASN:OD1  | 1:F:222:ASP:HB2  | 2.11                     | 0.50              |
| 1:D:8:GLU:O      | 1:D:42:CYS:HB2   | 2.11                     | 0.50              |
| 1:D:427:ASN:HB2  | 1:F:163:PHE:CZ   | 2.47                     | 0.50              |
| 1:E:369:ALA:HA   | 1:E:443:VAL:O    | 2.12                     | 0.50              |
| 1:B:134:TYR:CZ   | 1:B:244:LEU:HD13 | 2.46                     | 0.50              |
| 1:B:376:ARG:C    | 1:B:378:GLY:H    | 2.18                     | 0.50              |
| 1:B:404:VAL:HA   | 1:B:409:ASN:O    | 2.12                     | 0.50              |
| 1:C:79:GLY:HA3   | 1:C:132:TRP:CE2  | 2.47                     | 0.50              |
| 1:C:213:LEU:HD12 | 1:C:217:PHE:CE1  | 2.46                     | 0.50              |
| 1:C:418:ARG:HH21 | 1:C:418:ARG:HG3  | 1.76                     | 0.50              |
| 1:D:473:LEU:HD21 | 1:F:226:LYS:HB2  | 1.94                     | 0.50              |
| 1:E:157:ASP:OD2  | 1:E:159:ASN:HB2  | 2.11                     | 0.50              |
| 1:F:435:GLY:O    | 1:F:436:GLU:C    | 2.54                     | 0.50              |
| 1:A:23:VAL:HG11  | 1:A:236:GLN:NE2  | 2.27                     | 0.50              |
| 1:B:326:ILE:O    | 1:B:329:MET:HG2  | 2.11                     | 0.50              |
| 1:F:236:GLN:OE1  | 1:F:236:GLN:N    | 2.39                     | 0.50              |
| 1:F:474:GLY:O    | 1:F:478:VAL:HG23 | 2.11                     | 0.50              |
| 1:B:34:ASN:HD21  | 1:B:175:GLU:HB3  | 1.76                     | 0.50              |
| 1:C:36:GLN:HE21  | 1:C:175:GLU:HB2  | 1.76                     | 0.50              |
| 1:C:57:LEU:HD22  | 1:C:240:VAL:HG22 | 1.94                     | 0.50              |
| 1:C:114:ILE:HD12 | 1:C:132:TRP:CZ2  | 2.47                     | 0.50              |
| 1:C:479:ARG:HH11 | 1:C:479:ARG:HG2  | 1.77                     | 0.50              |
| 1:E:326:ILE:O    | 1:E:329:MET:HG2  | 2.12                     | 0.50              |
| 1:F:176:THR:O    | 1:F:177:MET:HE2  | 2.12                     | 0.50              |
| 1:F:385:ASN:HD21 | 1:F:445:LYS:CE   | 2.25                     | 0.50              |
| 1:A:379:ILE:HB   | 1:A:491:VAL:O    | 2.12                     | 0.50              |
| 1:C:146:LEU:HD13 | 1:C:146:LEU:C    | 2.37                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:112:GLN:HE21 | 1:E:461:ALA:HB1  | 1.76                     | 0.50              |
| 1:D:389:ASN:ND2  | 1:F:155:GLN:HB3  | 2.27                     | 0.50              |
| 1:E:476:SER:O    | 1:E:479:ARG:HB2  | 2.11                     | 0.50              |
| 1:F:65:TYR:CE1   | 1:F:149:THR:HG22 | 2.47                     | 0.50              |
| 1:A:226:LYS:HE3  | 1:A:231:ASP:OD1  | 2.11                     | 0.50              |
| 1:B:61:SER:HB3   | 1:B:164:TYR:CD2  | 2.47                     | 0.50              |
| 1:B:244:LEU:HD12 | 1:B:244:LEU:N    | 2.27                     | 0.50              |
| 1:D:66:PRO:HG3   | 1:D:151:ASN:ND2  | 2.26                     | 0.50              |
| 1:E:372:VAL:HB   | 1:E:441:TYR:CE1  | 2.47                     | 0.50              |
| 1:E:471:TYR:O    | 1:E:472:ASN:C    | 2.55                     | 0.50              |
| 1:B:67:GLN:O     | 1:B:124:VAL:HA   | 2.12                     | 0.49              |
| 1:B:396:ARG:HA   | 1:B:418:ARG:CG   | 2.42                     | 0.49              |
| 1:C:228:ARG:HB3  | 1:C:230:PRO:HG3  | 1.94                     | 0.49              |
| 1:C:336:ALA:O    | 1:C:337:ARG:C    | 2.55                     | 0.49              |
| 1:D:402:ARG:HG3  | 1:D:402:ARG:HH11 | 1.76                     | 0.49              |
| 1:A:331:LEU:O    | 1:A:359:LEU:HD21 | 2.12                     | 0.49              |
| 1:F:50:ARG:NH2   | 1:F:67:GLN:NE2   | 2.57                     | 0.49              |
| 1:B:17:LEU:HB2   | 1:B:421:LEU:HB3  | 1.94                     | 0.49              |
| 1:B:70:ILE:CG2   | 1:B:144:ILE:HB   | 2.42                     | 0.49              |
| 1:B:392:ILE:HG23 | 1:B:441:TYR:HD2  | 1.78                     | 0.49              |
| 1:D:204:VAL:HB   | 1:E:429:VAL:HG21 | 1.94                     | 0.49              |
| 1:D:404:VAL:HG13 | 1:D:409:ASN:O    | 2.13                     | 0.49              |
| 1:E:205:LEU:HD21 | 1:F:455:ILE:HD13 | 1.93                     | 0.49              |
| 1:A:124:VAL:HG11 | 1:A:365:PHE:CD2  | 2.47                     | 0.49              |
| 1:F:59:LEU:HD13  | 1:F:167:GLY:HA3  | 1.94                     | 0.49              |
| 1:F:386:LEU:N    | 1:F:386:LEU:HD12 | 2.27                     | 0.49              |
| 1:B:25:SER:OG    | 1:B:237:ILE:HB   | 2.13                     | 0.49              |
| 1:B:374:LEU:HD11 | 1:B:378:GLY:O    | 2.12                     | 0.49              |
| 1:C:377:ASN:O    | 1:C:433:GLN:HG3  | 2.13                     | 0.49              |
| 1:C:386:LEU:HD13 | 1:C:451:VAL:HG23 | 1.93                     | 0.49              |
| 1:E:146:LEU:HD13 | 1:E:146:LEU:C    | 2.37                     | 0.49              |
| 1:E:247:ILE:HD13 | 1:E:247:ILE:N    | 2.17                     | 0.49              |
| 1:A:247:ILE:HD12 | 1:A:247:ILE:N    | 2.27                     | 0.49              |
| 1:B:33:TRP:CE3   | 1:B:47:VAL:HB    | 2.46                     | 0.49              |
| 1:B:34:ASN:HA    | 1:B:175:GLU:OE2  | 2.13                     | 0.49              |
| 1:B:109:ASP:HA   | 1:C:483:TYR:OH   | 2.12                     | 0.49              |
| 1:D:34:ASN:C     | 1:D:36:GLN:H     | 2.20                     | 0.49              |
| 1:D:146:LEU:HB2  | 1:D:444:PHE:CD2  | 2.48                     | 0.49              |
| 1:E:349:GLY:O    | 1:E:490:LEU:HD13 | 2.11                     | 0.49              |
| 1:A:462:ILE:HB   | 1:A:467:LEU:HD21 | 1.95                     | 0.49              |
| 1:B:144:ILE:HG12 | 1:B:393:TYR:CD2  | 2.48                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:363:ARG:HA   | 1:B:448:HIS:CB   | 2.43                     | 0.49              |
| 1:C:77:ALA:HB2   | 1:C:116:HIS:ND1  | 2.28                     | 0.49              |
| 1:D:68:MET:HB2   | 1:D:367:LEU:HD13 | 1.94                     | 0.49              |
| 1:E:88:THR:O     | 1:E:110:SER:HA   | 2.13                     | 0.49              |
| 1:A:155:GLN:HB3  | 1:B:389:ASN:ND2  | 2.28                     | 0.49              |
| 1:A:329:MET:O    | 1:A:329:MET:HG3  | 2.11                     | 0.49              |
| 1:B:396:ARG:HA   | 1:B:418:ARG:CD   | 2.43                     | 0.49              |
| 1:B:402:ARG:HG3  | 1:B:402:ARG:HH11 | 1.78                     | 0.49              |
| 1:C:34:ASN:HD22  | 1:C:35:SER:H     | 1.59                     | 0.49              |
| 1:C:376:ARG:NH1  | 1:C:376:ARG:HB2  | 2.28                     | 0.49              |
| 1:F:46:THR:CG2   | 1:F:147:LEU:HD12 | 2.42                     | 0.49              |
| 1:A:72:VAL:HG22  | 1:A:142:VAL:O    | 2.13                     | 0.49              |
| 1:C:236:GLN:OE1  | 1:C:236:GLN:N    | 2.46                     | 0.49              |
| 1:C:385:ASN:HD21 | 1:C:445:LYS:CE   | 2.26                     | 0.49              |
| 1:C:404:VAL:HA   | 1:C:409:ASN:O    | 2.13                     | 0.49              |
| 1:E:46:THR:HG23  | 1:E:147:LEU:HD12 | 1.94                     | 0.49              |
| 1:A:59:LEU:HG    | 1:A:236:GLN:O    | 2.13                     | 0.49              |
| 1:A:71:VAL:HG21  | 1:A:117:PHE:HD2  | 1.78                     | 0.49              |
| 1:A:166:ALA:HB2  | 1:B:471:TYR:CE2  | 2.48                     | 0.49              |
| 1:D:357:LEU:HD12 | 1:D:357:LEU:N    | 2.27                     | 0.49              |
| 1:F:45:VAL:HG21  | 1:F:146:LEU:HD21 | 1.94                     | 0.49              |
| 1:F:401:VAL:HG21 | 1:F:416:LEU:HD23 | 1.95                     | 0.49              |
| 1:A:471:TYR:HE2  | 1:C:205:LEU:HD12 | 1.79                     | 0.48              |
| 1:F:394:VAL:HG21 | 1:F:416:LEU:HG   | 1.94                     | 0.48              |
| 1:F:409:ASN:N    | 1:F:409:ASN:HD22 | 2.11                     | 0.48              |
| 1:A:46:THR:CG2   | 1:A:147:LEU:HB2  | 2.43                     | 0.48              |
| 1:A:159:ASN:HB3  | 1:A:176:THR:CG2  | 2.41                     | 0.48              |
| 1:B:227:LEU:HD21 | 1:C:481:LEU:HD11 | 1.96                     | 0.48              |
| 1:B:385:ASN:HD21 | 1:B:445:LYS:HZ3  | 1.60                     | 0.48              |
| 1:C:376:ARG:HB2  | 1:C:376:ARG:HH11 | 1.77                     | 0.48              |
| 1:F:31:GLU:OE1   | 1:F:49:LYS:HD2   | 2.12                     | 0.48              |
| 1:F:400:ARG:O    | 1:F:432:GLU:HA   | 2.13                     | 0.48              |
| 1:A:13:ASN:C     | 1:A:14:LEU:HD12  | 2.38                     | 0.48              |
| 1:A:234:ARG:HB3  | 1:A:238:VAL:HG12 | 1.95                     | 0.48              |
| 1:A:240:VAL:HG13 | 1:B:469:ASN:ND2  | 2.29                     | 0.48              |
| 1:A:475:GLN:HG2  | 1:A:479:ARG:HH22 | 1.78                     | 0.48              |
| 1:A:481:LEU:CD2  | 1:C:217:PHE:HB3  | 2.42                     | 0.48              |
| 1:B:67:GLN:HB2   | 1:B:125:ILE:HB   | 1.95                     | 0.48              |
| 1:B:383:HIS:HB3  | 1:B:454:TYR:HB3  | 1.96                     | 0.48              |
| 1:E:22:ARG:HH11  | 1:E:22:ARG:HB3   | 1.77                     | 0.48              |
| 1:E:398:LYS:HE2  | 1:E:415:GLU:OE1  | 2.12                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:218:ASN:N    | 1:F:218:ASN:ND2  | 2.61                     | 0.48              |
| 1:F:328:THR:HG23 | 1:F:329:MET:N    | 2.22                     | 0.48              |
| 1:A:459:PHE:O    | 1:A:482:LYS:HE2  | 2.13                     | 0.48              |
| 1:D:82:PHE:HZ    | 1:D:331:LEU:HD11 | 1.78                     | 0.48              |
| 1:D:469:ASN:HD21 | 1:F:240:VAL:HG13 | 1.78                     | 0.48              |
| 1:E:244:LEU:CD1  | 1:F:465:GLU:HB3  | 2.42                     | 0.48              |
| 1:F:134:TYR:CE1  | 1:F:244:LEU:HD13 | 2.49                     | 0.48              |
| 1:A:337:ARG:HG3  | 1:A:337:ARG:HH11 | 1.78                     | 0.48              |
| 1:A:475:GLN:HG2  | 1:A:479:ARG:HH12 | 1.78                     | 0.48              |
| 1:B:326:ILE:C    | 1:B:328:THR:H    | 2.21                     | 0.48              |
| 1:D:47:VAL:HG12  | 1:D:48:SER:N     | 2.28                     | 0.48              |
| 1:E:1:ILE:HD11   | 1:F:155:GLN:HA   | 1.95                     | 0.48              |
| 1:F:65:TYR:HE1   | 1:F:160:PRO:HA   | 1.79                     | 0.48              |
| 1:F:123:LEU:HD23 | 1:F:332:HIS:CB   | 2.40                     | 0.48              |
| 1:C:350:ARG:HG3  | 1:C:350:ARG:NH2  | 2.27                     | 0.48              |
| 1:E:486:ASN:HD21 | 1:E:491:VAL:CG2  | 2.20                     | 0.48              |
| 1:A:12:ASN:O     | 1:A:411:VAL:HG12 | 2.14                     | 0.48              |
| 1:A:454:TYR:HD1  | 1:A:456:LYS:HB2  | 1.77                     | 0.48              |
| 1:B:65:TYR:OH    | 1:B:147:LEU:HD13 | 2.13                     | 0.48              |
| 1:B:70:ILE:HG22  | 1:B:144:ILE:HB   | 1.96                     | 0.48              |
| 1:A:469:ASN:ND2  | 1:C:240:VAL:HG13 | 2.29                     | 0.48              |
| 1:C:40:LEU:HD12  | 1:C:45:VAL:HG23  | 1.94                     | 0.48              |
| 1:C:57:LEU:HD22  | 1:C:240:VAL:CG2  | 2.43                     | 0.48              |
| 1:D:7:ASN:ND2    | 1:D:10:GLN:HB2   | 2.29                     | 0.48              |
| 1:E:480:GLN:HG3  | 1:E:481:LEU:N    | 2.29                     | 0.48              |
| 1:F:39:GLU:CD    | 1:F:39:GLU:H     | 2.22                     | 0.48              |
| 1:B:374:LEU:HD12 | 1:B:434:GLY:HA3  | 1.95                     | 0.48              |
| 1:B:387:ASN:CA   | 1:B:426:GLN:HE21 | 2.27                     | 0.48              |
| 1:D:205:LEU:HD21 | 1:E:455:ILE:HD13 | 1.96                     | 0.48              |
| 1:D:325:ASN:N    | 1:D:325:ASN:ND2  | 2.62                     | 0.48              |
| 1:F:337:ARG:HH21 | 1:F:337:ARG:HG3  | 1.78                     | 0.48              |
| 1:A:348:ALA:O    | 1:A:374:LEU:HA   | 2.14                     | 0.48              |
| 1:D:21:HIS:CE1   | 1:D:197:GLN:HG3  | 2.49                     | 0.48              |
| 1:D:51:THR:HA    | 1:D:141:VAL:O    | 2.14                     | 0.48              |
| 1:B:335:ILE:CD1  | 1:B:371:TYR:HB2  | 2.44                     | 0.47              |
| 1:F:395:THR:C    | 1:F:418:ARG:HG3  | 2.39                     | 0.47              |
| 1:A:175:GLU:HG2  | 1:A:176:THR:N    | 2.29                     | 0.47              |
| 1:B:460:ARG:NH1  | 1:B:487:SER:HA   | 2.29                     | 0.47              |
| 1:C:62:TYR:HD1   | 1:C:130:PRO:HB3  | 1.78                     | 0.47              |
| 1:C:425:PRO:HB2  | 1:C:428:PHE:CD2  | 2.48                     | 0.47              |
| 1:C:464:SER:HB3  | 1:C:475:GLN:HE22 | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:23:VAL:O     | 1:E:29:LEU:HD12  | 2.14                     | 0.47              |
| 1:A:392:ILE:O    | 1:A:421:LEU:HD12 | 2.15                     | 0.47              |
| 1:A:402:ARG:NH1  | 1:C:212:PHE:HE2  | 2.12                     | 0.47              |
| 1:C:111:HIS:CD2  | 1:C:111:HIS:H    | 2.32                     | 0.47              |
| 1:C:392:ILE:HG23 | 1:C:441:TYR:CD2  | 2.50                     | 0.47              |
| 1:C:396:ARG:HG3  | 1:C:396:ARG:HH11 | 1.79                     | 0.47              |
| 1:E:5:LYS:HB3    | 1:E:6:PHE:H      | 1.51                     | 0.47              |
| 1:E:75:LYS:CB    | 1:E:118:ASN:HA   | 2.42                     | 0.47              |
| 1:F:170:ASP:H    | 1:F:236:GLN:NE2  | 2.12                     | 0.47              |
| 1:A:337:ARG:C    | 1:A:339:SER:H    | 2.23                     | 0.47              |
| 1:A:467:LEU:HD12 | 1:A:471:TYR:HE1  | 1.79                     | 0.47              |
| 1:C:170:ASP:HB2  | 1:C:235:LYS:HD2  | 1.95                     | 0.47              |
| 1:C:362:LEU:HD22 | 1:C:367:LEU:O    | 2.14                     | 0.47              |
| 1:E:61:SER:HB3   | 1:E:164:TYR:CD2  | 2.49                     | 0.47              |
| 1:E:236:GLN:H    | 1:E:236:GLN:CD   | 2.20                     | 0.47              |
| 1:E:392:ILE:HG23 | 1:E:441:TYR:CD2  | 2.49                     | 0.47              |
| 1:E:405:ASN:OD1  | 1:E:407:GLN:HB2  | 2.14                     | 0.47              |
| 1:D:476:SER:O    | 1:D:479:ARG:HB2  | 2.15                     | 0.47              |
| 1:F:480:GLN:HA   | 1:F:480:GLN:HE21 | 1.78                     | 0.47              |
| 1:A:351:ILE:HG23 | 1:A:372:VAL:HG22 | 1.96                     | 0.47              |
| 1:B:425:PRO:O    | 1:B:428:PHE:HB2  | 2.15                     | 0.47              |
| 1:C:385:ASN:HD21 | 1:C:445:LYS:HE2  | 1.79                     | 0.47              |
| 1:E:394:VAL:HA   | 1:E:441:TYR:HB3  | 1.97                     | 0.47              |
| 1:A:394:VAL:HB   | 1:A:418:ARG:HA   | 1.96                     | 0.47              |
| 1:B:387:ASN:H    | 1:B:387:ASN:ND2  | 2.07                     | 0.47              |
| 1:C:112:GLN:O    | 1:C:114:ILE:N    | 2.47                     | 0.47              |
| 1:D:110:SER:O    | 1:D:111:HIS:HB3  | 2.15                     | 0.47              |
| 1:D:128:GLY:O    | 1:E:386:LEU:HG   | 2.15                     | 0.47              |
| 1:E:123:LEU:HD23 | 1:E:332:HIS:HB3  | 1.97                     | 0.47              |
| 1:E:205:LEU:C    | 1:E:207:GLY:H    | 2.22                     | 0.47              |
| 1:E:246:VAL:HG23 | 1:F:465:GLU:CD   | 2.40                     | 0.47              |
| 1:E:340:ARG:NH2  | 1:E:354:LEU:HD13 | 2.29                     | 0.47              |
| 1:A:47:VAL:HG12  | 1:A:48:SER:N     | 2.30                     | 0.47              |
| 1:A:83:PRO:HB3   | 1:B:453:SER:OG   | 2.13                     | 0.47              |
| 1:A:146:LEU:HD13 | 1:A:146:LEU:C    | 2.40                     | 0.47              |
| 1:A:380:TYR:HB3  | 1:A:432:GLU:H    | 1.80                     | 0.47              |
| 1:B:426:GLN:HG2  | 1:B:427:ASN:N    | 2.29                     | 0.47              |
| 1:C:148:ASP:CG   | 1:C:151:ASN:HB2  | 2.40                     | 0.47              |
| 1:D:56:GLY:O     | 1:D:134:TYR:HA   | 2.15                     | 0.47              |
| 1:D:219:THR:OG1  | 1:D:220:ASN:N    | 2.44                     | 0.47              |
| 1:E:228:ARG:O    | 1:E:229:SER:C    | 2.57                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:394:VAL:HG21 | 1:E:416:LEU:HG   | 1.96                     | 0.47              |
| 1:F:148:ASP:OD2  | 1:F:151:ASN:HB2  | 2.14                     | 0.47              |
| 1:F:334:ASN:HD22 | 1:F:337:ARG:H    | 1.59                     | 0.47              |
| 1:A:144:ILE:HG12 | 1:A:393:TYR:CE2  | 2.50                     | 0.47              |
| 1:A:210:LYS:HD3  | 1:A:225:GLU:HG2  | 1.97                     | 0.47              |
| 1:B:159:ASN:HD22 | 1:B:176:THR:CG2  | 2.12                     | 0.47              |
| 1:B:387:ASN:N    | 1:B:387:ASN:ND2  | 2.63                     | 0.47              |
| 1:B:388:ALA:H    | 1:B:426:GLN:HG3  | 1.80                     | 0.47              |
| 1:B:473:LEU:HB3  | 1:B:477:GLN:HB2  | 1.96                     | 0.47              |
| 1:C:6:PHE:CD2    | 1:C:6:PHE:N      | 2.81                     | 0.47              |
| 1:C:401:VAL:HG13 | 1:C:432:GLU:HG3  | 1.97                     | 0.47              |
| 1:F:40:LEU:HD12  | 1:F:40:LEU:H     | 1.80                     | 0.47              |
| 1:F:454:TYR:HD1  | 1:F:456:LYS:HB3  | 1.80                     | 0.47              |
| 1:B:60:PRO:HG3   | 1:B:132:TRP:HB3  | 1.97                     | 0.47              |
| 1:B:437:GLN:HA   | 1:B:437:GLN:NE2  | 2.30                     | 0.47              |
| 1:C:22:ARG:NH1   | 1:C:31:GLU:HG2   | 2.29                     | 0.47              |
| 1:C:340:ARG:H    | 1:C:340:ARG:HD2  | 1.80                     | 0.47              |
| 1:D:7:ASN:CG     | 1:D:10:GLN:HB2   | 2.40                     | 0.47              |
| 1:E:107:LEU:HA   | 1:F:479:ARG:HH21 | 1.79                     | 0.47              |
| 1:E:228:ARG:HB3  | 1:E:228:ARG:NH1  | 2.30                     | 0.47              |
| 1:E:489:PRO:O    | 1:E:491:VAL:HG23 | 2.15                     | 0.47              |
| 1:A:22:ARG:NH2   | 1:A:29:LEU:HD11  | 2.31                     | 0.46              |
| 1:A:363:ARG:O    | 1:A:363:ARG:CZ   | 2.64                     | 0.46              |
| 1:B:134:TYR:CE2  | 1:B:244:LEU:HD13 | 2.51                     | 0.46              |
| 1:F:392:ILE:HG23 | 1:F:441:TYR:CD2  | 2.51                     | 0.46              |
| 1:A:396:ARG:HG2  | 1:A:396:ARG:NH1  | 2.29                     | 0.46              |
| 1:B:398:LYS:N    | 1:B:439:LEU:HD13 | 2.30                     | 0.46              |
| 1:D:223:THR:OG1  | 1:E:477:GLN:NE2  | 2.48                     | 0.46              |
| 1:E:223:THR:O    | 1:E:227:LEU:HG   | 2.15                     | 0.46              |
| 1:A:387:ASN:C    | 1:A:387:ASN:HD22 | 2.24                     | 0.46              |
| 1:B:33:TRP:CD2   | 1:B:421:LEU:HD22 | 2.51                     | 0.46              |
| 1:B:371:TYR:OH   | 1:B:440:GLU:HB3  | 2.15                     | 0.46              |
| 1:B:382:PRO:HB2  | 1:B:455:ILE:HD12 | 1.98                     | 0.46              |
| 1:D:78:ILE:O     | 1:D:78:ILE:HG23  | 2.14                     | 0.46              |
| 1:D:336:ALA:HA   | 1:D:371:TYR:HD1  | 1.80                     | 0.46              |
| 1:D:392:ILE:N    | 1:D:422:LEU:O    | 2.42                     | 0.46              |
| 1:E:19:PRO:HG3   | 1:E:33:TRP:CZ2   | 2.50                     | 0.46              |
| 1:E:211:HIS:O    | 1:E:214:ALA:HB3  | 2.15                     | 0.46              |
| 1:A:326:ILE:HD13 | 1:A:326:ILE:C    | 2.41                     | 0.46              |
| 1:C:114:ILE:HG22 | 1:C:115:ARG:N    | 2.29                     | 0.46              |
| 1:C:394:VAL:HG22 | 1:C:420:GLN:O    | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:336:ALA:HA   | 1:D:371:TYR:CD1  | 2.50                     | 0.46              |
| 1:E:244:LEU:HD21 | 1:F:466:VAL:HG22 | 1.98                     | 0.46              |
| 1:D:388:ALA:HA   | 1:F:155:GLN:OE1  | 2.16                     | 0.46              |
| 1:E:418:ARG:HG2  | 1:E:418:ARG:HH21 | 1.81                     | 0.46              |
| 1:A:50:ARG:HH22  | 1:A:67:GLN:HE22  | 1.64                     | 0.46              |
| 1:B:15:ASN:N     | 1:B:15:ASN:ND2   | 2.63                     | 0.46              |
| 1:B:338:PRO:HG3  | 1:B:350:ARG:NH2  | 2.30                     | 0.46              |
| 1:C:225:GLU:OE1  | 1:C:228:ARG:HD3  | 2.15                     | 0.46              |
| 1:B:20:ASP:O     | 1:B:21:HIS:HB2   | 2.16                     | 0.46              |
| 1:B:46:THR:HG23  | 1:B:147:LEU:HD12 | 1.96                     | 0.46              |
| 1:C:84:GLY:O     | 1:C:85:CYS:C     | 2.58                     | 0.46              |
| 1:D:8:GLU:OE2    | 1:D:8:GLU:N      | 2.48                     | 0.46              |
| 1:D:171:ILE:HG21 | 1:D:174:PRO:HA   | 1.97                     | 0.46              |
| 1:D:235:LYS:HD2  | 1:D:235:LYS:N    | 2.31                     | 0.46              |
| 1:E:70:ILE:HD13  | 1:E:70:ILE:C     | 2.41                     | 0.46              |
| 1:F:171:ILE:HD12 | 1:F:171:ILE:N    | 2.23                     | 0.46              |
| 1:A:463:PRO:HA   | 1:C:111:HIS:HB3  | 1.98                     | 0.46              |
| 1:D:175:GLU:C    | 1:D:177:MET:H    | 2.23                     | 0.46              |
| 1:D:336:ALA:O    | 1:D:338:PRO:HD3  | 2.16                     | 0.46              |
| 1:A:461:ALA:HA   | 1:C:87:GLU:CD    | 2.41                     | 0.46              |
| 1:C:376:ARG:HG3  | 1:C:376:ARG:O    | 2.15                     | 0.46              |
| 1:D:36:GLN:NE2   | 1:D:178:GLN:NE2  | 2.64                     | 0.46              |
| 1:D:70:ILE:HG22  | 1:D:144:ILE:O    | 2.16                     | 0.46              |
| 1:D:391:VAL:CG2  | 1:D:421:LEU:HD11 | 2.43                     | 0.46              |
| 1:D:398:LYS:HE3  | 1:D:415:GLU:CB   | 2.46                     | 0.46              |
| 1:F:108:GLN:N    | 1:F:108:GLN:OE1  | 2.49                     | 0.46              |
| 1:F:108:GLN:O    | 1:F:108:GLN:HG2  | 2.16                     | 0.46              |
| 1:A:71:VAL:O     | 1:A:119:GLU:HA   | 2.15                     | 0.45              |
| 1:B:387:ASN:O    | 1:B:388:ALA:HB2  | 2.16                     | 0.45              |
| 1:B:425:PRO:HB2  | 1:B:428:PHE:CG   | 2.51                     | 0.45              |
| 1:B:460:ARG:CZ   | 1:B:487:SER:HA   | 2.46                     | 0.45              |
| 1:C:14:LEU:C     | 1:C:15:ASN:ND2   | 2.72                     | 0.45              |
| 1:C:57:LEU:HD12  | 1:C:133:THR:O    | 2.16                     | 0.45              |
| 1:C:74:GLY:HA3   | 1:C:141:VAL:HG22 | 1.97                     | 0.45              |
| 1:C:75:LYS:N     | 1:C:141:VAL:HG22 | 2.32                     | 0.45              |
| 1:C:169:PRO:HD2  | 1:C:202:GLY:HA2  | 1.98                     | 0.45              |
| 1:C:213:LEU:HD22 | 1:C:213:LEU:N    | 2.30                     | 0.45              |
| 1:C:351:ILE:CG2  | 1:C:372:VAL:HG22 | 2.46                     | 0.45              |
| 1:D:455:ILE:CD1  | 1:F:205:LEU:HD21 | 2.45                     | 0.45              |
| 1:E:201:GLY:HA2  | 1:F:407:GLN:O    | 2.16                     | 0.45              |
| 1:E:388:ALA:HB2  | 1:E:447:HIS:HB2  | 1.97                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:471:TYR:HB2  | 1:E:473:LEU:HG   | 1.97                     | 0.45              |
| 1:F:240:VAL:HG21 | 1:F:244:LEU:HD11 | 1.98                     | 0.45              |
| 1:F:328:THR:O    | 1:F:329:MET:C    | 2.59                     | 0.45              |
| 1:A:163:PHE:CE1  | 1:B:406:CSD:HB2  | 2.52                     | 0.45              |
| 1:A:340:ARG:NE   | 1:A:350:ARG:HB2  | 2.31                     | 0.45              |
| 1:D:157:ASP:HB2  | 1:E:5:LYS:O      | 2.16                     | 0.45              |
| 1:F:159:ASN:HB3  | 1:F:176:THR:CG2  | 2.45                     | 0.45              |
| 1:F:479:ARG:HG2  | 1:F:479:ARG:HH11 | 1.81                     | 0.45              |
| 1:B:228:ARG:HB3  | 1:B:228:ARG:NH1  | 2.31                     | 0.45              |
| 1:C:417:ARG:HG2  | 1:C:417:ARG:NH1  | 2.31                     | 0.45              |
| 1:A:54:ARG:HG3   | 1:A:54:ARG:HH11  | 1.82                     | 0.45              |
| 1:A:340:ARG:HH11 | 1:A:340:ARG:CB   | 2.17                     | 0.45              |
| 1:A:384:TRP:O    | 1:A:452:SER:HB2  | 2.17                     | 0.45              |
| 1:A:402:ARG:HG2  | 1:A:413:ASP:CG   | 2.42                     | 0.45              |
| 1:C:148:ASP:OD2  | 1:C:367:LEU:HD21 | 2.17                     | 0.45              |
| 1:C:418:ARG:HG3  | 1:C:418:ARG:NH2  | 2.32                     | 0.45              |
| 1:D:63:SER:C     | 1:D:65:TYR:H     | 2.23                     | 0.45              |
| 1:F:76:GLY:HA2   | 1:F:136:THR:HG23 | 1.98                     | 0.45              |
| 1:F:222:ASP:O    | 1:F:226:LYS:HG2  | 2.16                     | 0.45              |
| 1:A:7:ASN:N      | 1:A:7:ASN:HD22   | 2.14                     | 0.45              |
| 1:A:155:GLN:HB3  | 1:B:389:ASN:HD21 | 1.81                     | 0.45              |
| 1:A:402:ARG:O    | 1:A:430:VAL:HG23 | 2.15                     | 0.45              |
| 1:B:15:ASN:H     | 1:B:39:GLU:CD    | 2.23                     | 0.45              |
| 1:C:471:TYR:CB   | 1:C:473:LEU:HD13 | 2.47                     | 0.45              |
| 1:E:246:VAL:HG11 | 1:F:463:PRO:HB3  | 1.98                     | 0.45              |
| 1:F:343:PHE:O    | 1:F:350:ARG:HA   | 2.17                     | 0.45              |
| 1:A:446:THR:O    | 1:A:447:HIS:HB2  | 2.17                     | 0.45              |
| 1:B:454:TYR:CE1  | 1:B:457:ASP:HB2  | 2.52                     | 0.45              |
| 1:B:480:GLN:O    | 1:B:484:GLN:N    | 2.49                     | 0.45              |
| 1:C:67:GLN:HE21  | 1:C:147:LEU:HD22 | 1.80                     | 0.45              |
| 1:C:391:VAL:HG23 | 1:C:391:VAL:O    | 2.17                     | 0.45              |
| 1:D:81:ALA:HB3   | 1:D:130:PRO:HB2  | 1.98                     | 0.45              |
| 1:E:480:GLN:O    | 1:E:484:GLN:HB2  | 2.17                     | 0.45              |
| 1:C:22:ARG:NH1   | 1:C:22:ARG:HB3   | 2.32                     | 0.45              |
| 1:C:338:PRO:HB3  | 1:C:350:ARG:HE   | 1.81                     | 0.45              |
| 1:D:363:ARG:HD2  | 1:D:448:HIS:CD2  | 2.52                     | 0.45              |
| 1:E:355:ASN:OD1  | 1:E:357:LEU:HB2  | 2.16                     | 0.45              |
| 1:A:232:ASP:CG   | 1:A:234:ARG:HH21 | 2.24                     | 0.45              |
| 1:B:8:GLU:O      | 1:B:42:CYS:HB2   | 2.16                     | 0.45              |
| 1:B:70:ILE:HG23  | 1:B:70:ILE:O     | 2.17                     | 0.45              |
| 1:B:247:ILE:N    | 1:B:247:ILE:HD12 | 2.32                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:34:ASN:HB3   | 1:F:37:HIS:CD2   | 2.52                     | 0.45              |
| 1:F:72:VAL:HG11  | 1:F:144:ILE:HD13 | 1.99                     | 0.45              |
| 1:F:349:GLY:HA3  | 1:F:373:VAL:O    | 2.17                     | 0.45              |
| 1:F:424:VAL:O    | 1:F:425:PRO:O    | 2.35                     | 0.45              |
| 1:B:401:VAL:HB   | 1:B:412:PHE:HE1  | 1.81                     | 0.45              |
| 1:D:46:THR:HG23  | 1:D:147:LEU:HB2  | 1.99                     | 0.45              |
| 1:D:471:TYR:HB2  | 1:D:473:LEU:HG   | 1.99                     | 0.45              |
| 1:F:143:ALA:C    | 1:F:144:ILE:HD12 | 2.42                     | 0.45              |
| 1:F:144:ILE:HG12 | 1:F:393:TYR:CE2  | 2.52                     | 0.45              |
| 1:A:246:VAL:HG23 | 1:B:465:GLU:OE2  | 2.17                     | 0.45              |
| 1:B:71:VAL:HG21  | 1:B:117:PHE:HD2  | 1.81                     | 0.45              |
| 1:D:30:ILE:HD12  | 1:D:236:GLN:HG3  | 1.97                     | 0.45              |
| 1:E:114:ILE:HD12 | 1:E:132:TRP:CZ2  | 2.52                     | 0.45              |
| 1:A:325:ASN:HA   | 1:A:328:THR:CG2  | 2.47                     | 0.44              |
| 1:B:126:PRO:HB2  | 1:B:129:VAL:CG2  | 2.44                     | 0.44              |
| 1:D:18:GLU:O     | 1:D:19:PRO:C     | 2.60                     | 0.44              |
| 1:D:373:VAL:HG13 | 1:D:440:GLU:HG2  | 1.99                     | 0.44              |
| 1:D:461:ALA:O    | 1:F:111:HIS:HB2  | 2.17                     | 0.44              |
| 1:E:165:LEU:HD13 | 1:F:458:VAL:HG11 | 1.99                     | 0.44              |
| 1:F:77:ALA:HB2   | 1:F:116:HIS:CE1  | 2.52                     | 0.44              |
| 1:A:336:ALA:O    | 1:A:337:ARG:C    | 2.58                     | 0.44              |
| 1:B:6:PHE:CD1    | 1:B:6:PHE:N      | 2.84                     | 0.44              |
| 1:B:46:THR:HG22  | 1:B:147:LEU:HB2  | 1.98                     | 0.44              |
| 1:B:124:VAL:HG13 | 1:B:331:LEU:HD22 | 1.99                     | 0.44              |
| 1:B:379:ILE:HD11 | 1:B:433:GLN:NE2  | 2.32                     | 0.44              |
| 1:C:39:GLU:HB3   | 1:C:423:VAL:HG21 | 2.00                     | 0.44              |
| 1:C:337:ARG:HH21 | 1:C:337:ARG:CA   | 2.29                     | 0.44              |
| 1:C:404:VAL:CG1  | 1:C:408:GLY:HA2  | 2.46                     | 0.44              |
| 1:F:334:ASN:ND2  | 1:F:337:ARG:N    | 2.61                     | 0.44              |
| 1:A:240:VAL:HG11 | 1:A:244:LEU:HD12 | 1.99                     | 0.44              |
| 1:A:385:ASN:HD21 | 1:A:445:LYS:HE2  | 1.82                     | 0.44              |
| 1:D:171:ILE:HG21 | 1:D:177:MET:HG3  | 1.99                     | 0.44              |
| 1:D:402:ARG:HG2  | 1:D:413:ASP:OD1  | 2.17                     | 0.44              |
| 1:B:401:VAL:HG11 | 1:B:422:LEU:CD2  | 2.48                     | 0.44              |
| 1:C:67:GLN:O     | 1:C:124:VAL:HA   | 2.16                     | 0.44              |
| 1:C:120:GLY:O    | 1:C:335:ILE:HG22 | 2.18                     | 0.44              |
| 1:C:147:LEU:O    | 1:C:149:THR:N    | 2.49                     | 0.44              |
| 1:D:240:VAL:HG22 | 1:E:469:ASN:ND2  | 2.33                     | 0.44              |
| 1:D:403:VAL:O    | 1:D:411:VAL:HG22 | 2.18                     | 0.44              |
| 1:E:47:VAL:HG12  | 1:E:48:SER:N     | 2.33                     | 0.44              |
| 1:A:65:TYR:HD1   | 1:A:154:ASN:HD22 | 1.66                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:363:ARG:NE   | 1:A:448:HIS:CD2  | 2.86                     | 0.44              |
| 1:C:387:ASN:O    | 1:C:388:ALA:HB2  | 2.17                     | 0.44              |
| 1:D:354:LEU:HD12 | 1:D:358:THR:OG1  | 2.18                     | 0.44              |
| 1:E:235:LYS:HB3  | 1:E:236:GLN:OE1  | 2.18                     | 0.44              |
| 1:A:224:ALA:HA   | 1:A:227:LEU:CD1  | 2.43                     | 0.44              |
| 1:A:491:VAL:HG12 | 1:A:492:ASN:H    | 1.82                     | 0.44              |
| 1:B:158:GLN:OE1  | 1:B:158:GLN:N    | 2.50                     | 0.44              |
| 1:C:23:VAL:O     | 1:C:29:LEU:HD12  | 2.16                     | 0.44              |
| 1:C:356:SER:HA   | 1:C:359:LEU:O    | 2.18                     | 0.44              |
| 1:D:15:ASN:HD22  | 1:D:15:ASN:N     | 2.16                     | 0.44              |
| 1:D:340:ARG:O    | 1:D:340:ARG:HG2  | 2.18                     | 0.44              |
| 1:D:474:GLY:O    | 1:D:478:VAL:HG22 | 2.17                     | 0.44              |
| 1:F:89:PHE:CE1   | 1:F:110:SER:HB3  | 2.52                     | 0.44              |
| 1:B:26:GLU:CD    | 1:B:234:ARG:HG2  | 2.43                     | 0.44              |
| 1:D:200:GLU:O    | 1:D:200:GLU:HG3  | 2.18                     | 0.44              |
| 1:D:218:ASN:N    | 1:D:218:ASN:HD22 | 2.15                     | 0.44              |
| 1:D:436:GLU:OE1  | 1:D:436:GLU:HA   | 2.18                     | 0.44              |
| 1:F:247:ILE:HG22 | 1:F:248:SER:N    | 2.32                     | 0.44              |
| 1:F:425:PRO:HG2  | 1:F:428:PHE:CE1  | 2.52                     | 0.44              |
| 1:A:28:GLY:HA3   | 1:A:237:ILE:HG21 | 2.00                     | 0.44              |
| 1:B:65:TYR:CE1   | 1:B:149:THR:HG22 | 2.53                     | 0.44              |
| 1:C:82:PHE:CE1   | 1:C:129:VAL:HG11 | 2.52                     | 0.44              |
| 1:C:200:GLU:N    | 1:C:200:GLU:OE1  | 2.50                     | 0.44              |
| 1:C:228:ARG:C    | 1:C:230:PRO:HD3  | 2.43                     | 0.44              |
| 1:C:345:ASN:C    | 1:C:347:LYS:H    | 2.24                     | 0.44              |
| 1:D:11:LEU:HD22  | 1:D:38:PRO:HB3   | 1.99                     | 0.44              |
| 1:D:228:ARG:HB3  | 1:D:228:ARG:CZ   | 2.48                     | 0.44              |
| 1:D:461:ALA:HA   | 1:F:87:GLU:OE1   | 2.17                     | 0.44              |
| 1:D:465:GLU:CD   | 1:F:245:SER:H    | 2.26                     | 0.44              |
| 1:E:176:THR:C    | 1:E:177:MET:HE2  | 2.43                     | 0.44              |
| 1:E:328:THR:O    | 1:E:329:MET:C    | 2.60                     | 0.44              |
| 1:F:113:LYS:HD3  | 1:F:115:ARG:HE   | 1.82                     | 0.44              |
| 1:A:69:ILE:CG2   | 1:A:143:ALA:HB1  | 2.47                     | 0.44              |
| 1:B:22:ARG:HH22  | 1:B:29:LEU:HD21  | 1.83                     | 0.44              |
| 1:B:328:THR:O    | 1:B:329:MET:C    | 2.61                     | 0.44              |
| 1:B:436:GLU:OE1  | 1:B:436:GLU:HA   | 2.18                     | 0.44              |
| 1:C:405:ASN:HD22 | 1:C:411:VAL:CG1  | 2.31                     | 0.44              |
| 1:D:148:ASP:OD2  | 1:D:151:ASN:HB2  | 2.18                     | 0.44              |
| 1:D:163:PHE:CD2  | 1:E:406:CSD:HB2  | 2.52                     | 0.44              |
| 1:F:456:LYS:NZ   | 1:F:486:ASN:ND2  | 2.65                     | 0.44              |
| 1:A:22:ARG:CZ    | 1:A:29:LEU:HD11  | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:7:ASN:ND2    | 1:B:10:GLN:NE2   | 2.66                     | 0.43              |
| 1:B:234:ARG:HB3  | 1:B:238:VAL:HG12 | 1.99                     | 0.43              |
| 1:C:160:PRO:O    | 1:C:176:THR:HG21 | 2.18                     | 0.43              |
| 1:C:384:TRP:HH2  | 1:C:458:VAL:HG21 | 1.83                     | 0.43              |
| 1:D:146:LEU:HD21 | 1:D:391:VAL:HG11 | 2.00                     | 0.43              |
| 1:F:398:LYS:CB   | 1:F:398:LYS:NZ   | 2.82                     | 0.43              |
| 1:B:226:LYS:C    | 1:B:228:ARG:H    | 2.25                     | 0.43              |
| 1:D:456:LYS:HE2  | 1:F:217:PHE:CA   | 2.42                     | 0.43              |
| 1:E:210:LYS:CB   | 1:E:225:GLU:HG2  | 2.47                     | 0.43              |
| 1:F:25:SER:O     | 1:F:26:GLU:C     | 2.62                     | 0.43              |
| 1:F:78:ILE:HG13  | 1:F:133:THR:HG22 | 2.00                     | 0.43              |
| 1:A:18:GLU:HA    | 1:A:33:TRP:HE1   | 1.83                     | 0.43              |
| 1:A:22:ARG:NH1   | 1:A:22:ARG:CB    | 2.81                     | 0.43              |
| 1:A:65:TYR:CE1   | 1:A:149:THR:HG22 | 2.53                     | 0.43              |
| 1:B:124:VAL:HG13 | 1:B:124:VAL:O    | 2.18                     | 0.43              |
| 1:B:357:LEU:N    | 1:B:357:LEU:HD22 | 2.33                     | 0.43              |
| 1:B:379:ILE:HG22 | 1:B:380:TYR:N    | 2.34                     | 0.43              |
| 1:B:395:THR:C    | 1:B:418:ARG:HG3  | 2.44                     | 0.43              |
| 1:C:6:PHE:C      | 1:C:7:ASN:ND2    | 2.75                     | 0.43              |
| 1:C:16:ALA:HA    | 1:C:421:LEU:O    | 2.18                     | 0.43              |
| 1:C:38:PRO:HA    | 1:C:41:GLN:HB2   | 2.00                     | 0.43              |
| 1:C:340:ARG:HH11 | 1:C:340:ARG:HG2  | 1.83                     | 0.43              |
| 1:D:399:GLY:HA3  | 1:D:439:LEU:HD22 | 1.99                     | 0.43              |
| 1:E:114:ILE:HD12 | 1:E:132:TRP:HZ2  | 1.82                     | 0.43              |
| 1:E:478:VAL:O    | 1:E:478:VAL:HG12 | 2.18                     | 0.43              |
| 1:F:334:ASN:HB3  | 1:F:340:ARG:HH11 | 1.84                     | 0.43              |
| 1:B:228:ARG:HB3  | 1:B:228:ARG:CZ   | 2.49                     | 0.43              |
| 1:B:401:VAL:HA   | 1:B:432:GLU:HB3  | 2.01                     | 0.43              |
| 1:F:244:LEU:HD12 | 1:F:244:LEU:N    | 2.34                     | 0.43              |
| 1:F:348:ALA:CB   | 1:F:490:LEU:HB3  | 2.49                     | 0.43              |
| 1:F:373:VAL:HG13 | 1:F:440:GLU:HG2  | 1.98                     | 0.43              |
| 1:A:240:VAL:HG11 | 1:A:244:LEU:CD1  | 2.48                     | 0.43              |
| 1:B:47:VAL:HG12  | 1:B:48:SER:N     | 2.34                     | 0.43              |
| 1:B:335:ILE:HD11 | 1:B:371:TYR:H    | 1.84                     | 0.43              |
| 1:C:121:ASP:OD2  | 1:C:332:HIS:HE1  | 2.01                     | 0.43              |
| 1:C:471:TYR:HB2  | 1:C:473:LEU:HD13 | 1.99                     | 0.43              |
| 1:E:227:LEU:HA   | 1:F:471:TYR:CD2  | 2.53                     | 0.43              |
| 1:E:340:ARG:HH22 | 1:E:354:LEU:HD13 | 1.84                     | 0.43              |
| 1:F:53:ASN:N     | 1:F:53:ASN:HD22  | 2.16                     | 0.43              |
| 1:F:230:PRO:HG2  | 1:F:231:ASP:H    | 1.82                     | 0.43              |
| 1:A:345:ASN:HD22 | 1:A:486:ASN:ND2  | 2.16                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:425:PRO:O    | 1:A:426:GLN:C    | 2.62                     | 0.43              |
| 1:B:156:LEU:CD1  | 1:B:161:ARG:HE   | 2.29                     | 0.43              |
| 1:C:210:LYS:CD   | 1:C:225:GLU:HG2  | 2.42                     | 0.43              |
| 1:C:387:ASN:ND2  | 1:C:387:ASN:H    | 2.17                     | 0.43              |
| 1:C:478:VAL:C    | 1:C:480:GLN:N    | 2.77                     | 0.43              |
| 1:D:385:ASN:ND2  | 1:D:452:SER:HB3  | 2.33                     | 0.43              |
| 1:E:349:GLY:C    | 1:E:490:LEU:HD13 | 2.43                     | 0.43              |
| 1:F:46:THR:HG23  | 1:F:147:LEU:HB2  | 2.00                     | 0.43              |
| 1:A:64:PRO:O     | 1:A:154:ASN:HA   | 2.18                     | 0.43              |
| 1:A:386:LEU:HD13 | 1:A:452:SER:CA   | 2.48                     | 0.43              |
| 1:B:9:CYS:C      | 1:B:11:LEU:H     | 2.27                     | 0.43              |
| 1:B:71:VAL:HG21  | 1:B:117:PHE:CD2  | 2.52                     | 0.43              |
| 1:B:380:TYR:O    | 1:B:381:SER:C    | 2.61                     | 0.43              |
| 1:C:79:GLY:HA3   | 1:C:132:TRP:NE1  | 2.34                     | 0.43              |
| 1:C:210:LYS:HE2  | 1:C:221:GLU:OE2  | 2.18                     | 0.43              |
| 1:C:219:THR:OG1  | 1:C:220:ASN:N    | 2.51                     | 0.43              |
| 1:D:340:ARG:HG3  | 1:D:340:ARG:HH11 | 1.83                     | 0.43              |
| 1:D:391:VAL:HG12 | 1:D:444:PHE:HB2  | 1.98                     | 0.43              |
| 1:A:87:GLU:CD    | 1:A:87:GLU:N     | 2.76                     | 0.43              |
| 1:C:373:VAL:HG22 | 1:C:440:GLU:CG   | 2.41                     | 0.43              |
| 1:C:386:LEU:H    | 1:C:386:LEU:CD1  | 2.31                     | 0.43              |
| 1:D:338:PRO:C    | 1:D:340:ARG:H    | 2.27                     | 0.43              |
| 1:D:489:PRO:HG2  | 1:D:490:LEU:H    | 1.83                     | 0.43              |
| 1:F:146:LEU:HD13 | 1:F:146:LEU:C    | 2.44                     | 0.43              |
| 1:F:337:ARG:C    | 1:F:339:SER:H    | 2.27                     | 0.43              |
| 1:F:362:LEU:HB3  | 1:F:367:LEU:O    | 2.19                     | 0.43              |
| 1:A:64:PRO:HG2   | 1:A:65:TYR:CD1   | 2.54                     | 0.43              |
| 1:B:437:GLN:HA   | 1:B:437:GLN:HE21 | 1.83                     | 0.43              |
| 1:B:472:ASN:N    | 1:B:472:ASN:HD22 | 2.15                     | 0.43              |
| 1:C:78:ILE:HG12  | 1:C:79:GLY:N     | 2.34                     | 0.43              |
| 1:C:367:LEU:CD2  | 1:C:446:THR:HA   | 2.44                     | 0.43              |
| 1:D:236:GLN:H    | 1:D:236:GLN:CD   | 2.23                     | 0.43              |
| 1:E:417:ARG:HD2  | 1:E:417:ARG:C    | 2.43                     | 0.43              |
| 1:F:122:VAL:O    | 1:F:332:HIS:HA   | 2.19                     | 0.43              |
| 1:A:78:ILE:HG13  | 1:A:133:THR:HG22 | 2.00                     | 0.43              |
| 1:A:340:ARG:CD   | 1:A:350:ARG:HB2  | 2.49                     | 0.43              |
| 1:B:61:SER:HA    | 1:B:163:PHE:O    | 2.18                     | 0.43              |
| 1:C:34:ASN:HB3   | 1:C:37:HIS:CD2   | 2.53                     | 0.43              |
| 1:C:205:LEU:C    | 1:C:207:GLY:H    | 2.27                     | 0.43              |
| 1:C:387:ASN:C    | 1:C:387:ASN:HD22 | 2.26                     | 0.43              |
| 1:D:68:MET:CE    | 1:D:369:ALA:HB2  | 2.49                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:113:LYS:O    | 1:D:115:ARG:HD2  | 2.18                     | 0.43              |
| 1:D:454:TYR:HD1  | 1:D:456:LYS:HB2  | 1.83                     | 0.43              |
| 1:E:22:ARG:HH11  | 1:E:22:ARG:CB    | 2.32                     | 0.43              |
| 1:F:213:LEU:H    | 1:F:213:LEU:HD22 | 1.83                     | 0.43              |
| 1:B:47:VAL:HA    | 1:B:145:SER:O    | 2.19                     | 0.42              |
| 1:B:207:GLY:HA2  | 1:C:408:GLY:O    | 2.18                     | 0.42              |
| 1:C:170:ASP:O    | 1:C:171:ILE:C    | 2.62                     | 0.42              |
| 1:C:404:VAL:HG13 | 1:C:409:ASN:O    | 2.19                     | 0.42              |
| 1:D:228:ARG:HB3  | 1:D:228:ARG:NH1  | 2.34                     | 0.42              |
| 1:D:231:ASP:O    | 1:D:232:ASP:C    | 2.61                     | 0.42              |
| 1:E:82:PHE:HB2   | 1:E:85:CYS:SG    | 2.59                     | 0.42              |
| 1:E:175:GLU:OE1  | 1:E:175:GLU:N    | 2.50                     | 0.42              |
| 1:A:112:GLN:O    | 1:A:114:ILE:N    | 2.52                     | 0.42              |
| 1:A:233:GLU:O    | 1:A:235:LYS:HE3  | 2.19                     | 0.42              |
| 1:A:387:ASN:O    | 1:A:388:ALA:HB2  | 2.18                     | 0.42              |
| 1:A:408:GLY:HA2  | 1:C:203:SER:O    | 2.19                     | 0.42              |
| 1:B:79:GLY:O     | 1:B:131:TYR:HA   | 2.19                     | 0.42              |
| 1:B:86:PRO:O     | 1:B:113:LYS:HE3  | 2.19                     | 0.42              |
| 1:C:87:GLU:HA    | 1:C:112:GLN:HA   | 2.01                     | 0.42              |
| 1:C:471:TYR:O    | 1:C:472:ASN:HB2  | 2.19                     | 0.42              |
| 1:E:463:PRO:O    | 1:E:464:SER:C    | 2.61                     | 0.42              |
| 1:A:244:LEU:HD12 | 1:A:244:LEU:N    | 2.34                     | 0.42              |
| 1:A:441:TYR:HD2  | 1:A:441:TYR:O    | 2.01                     | 0.42              |
| 1:B:398:LYS:HA   | 1:B:416:LEU:O    | 2.19                     | 0.42              |
| 1:D:70:ILE:HG23  | 1:D:70:ILE:O     | 2.18                     | 0.42              |
| 1:E:171:ILE:HG21 | 1:E:174:PRO:HA   | 2.01                     | 0.42              |
| 1:E:376:ARG:O    | 1:E:377:ASN:CB   | 2.67                     | 0.42              |
| 1:F:337:ARG:C    | 1:F:339:SER:N    | 2.78                     | 0.42              |
| 1:B:169:PRO:HA   | 1:B:236:GLN:OE1  | 2.19                     | 0.42              |
| 1:B:366:GLY:HA2  | 1:B:448:HIS:H    | 1.84                     | 0.42              |
| 1:C:17:LEU:HD12  | 1:C:40:LEU:CD2   | 2.49                     | 0.42              |
| 1:C:348:ALA:O    | 1:C:374:LEU:HA   | 2.18                     | 0.42              |
| 1:E:22:ARG:CB    | 1:E:22:ARG:NH1   | 2.83                     | 0.42              |
| 1:E:73:GLN:HE21  | 1:E:142:VAL:HG11 | 1.84                     | 0.42              |
| 1:F:225:GLU:O    | 1:F:230:PRO:HD3  | 2.19                     | 0.42              |
| 1:A:7:ASN:N      | 1:A:7:ASN:ND2    | 2.66                     | 0.42              |
| 1:A:46:THR:CG2   | 1:A:147:LEU:HD12 | 2.43                     | 0.42              |
| 1:A:325:ASN:C    | 1:A:327:CYS:N    | 2.77                     | 0.42              |
| 1:A:454:TYR:CD2  | 1:A:489:PRO:HB3  | 2.55                     | 0.42              |
| 1:B:133:THR:HG21 | 2:B:502:CO3:O1   | 2.20                     | 0.42              |
| 1:B:396:ARG:HA   | 1:B:418:ARG:HD2  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:151:ASN:OD1  | 1:C:152:PHE:N    | 2.52                     | 0.42              |
| 1:C:245:SER:OG   | 1:C:246:VAL:N    | 2.51                     | 0.42              |
| 1:D:155:GLN:OE1  | 1:E:388:ALA:HA   | 2.20                     | 0.42              |
| 1:E:14:LEU:HD13  | 1:E:411:VAL:HB   | 2.01                     | 0.42              |
| 1:E:69:ILE:HB    | 1:E:123:LEU:HB2  | 2.00                     | 0.42              |
| 1:E:417:ARG:HG2  | 1:E:417:ARG:HH11 | 1.85                     | 0.42              |
| 1:B:146:LEU:C    | 1:B:146:LEU:HD13 | 2.45                     | 0.42              |
| 1:C:39:GLU:H     | 1:C:39:GLU:CD    | 2.28                     | 0.42              |
| 1:C:70:ILE:HG22  | 1:C:144:ILE:O    | 2.19                     | 0.42              |
| 1:C:72:VAL:HG23  | 1:C:73:GLN:H     | 1.84                     | 0.42              |
| 1:D:363:ARG:HG3  | 1:D:363:ARG:HH21 | 1.84                     | 0.42              |
| 1:E:72:VAL:HG23  | 1:E:142:VAL:HG13 | 2.01                     | 0.42              |
| 1:F:152:PHE:CD1  | 1:F:152:PHE:N    | 2.81                     | 0.42              |
| 1:F:246:VAL:C    | 1:F:247:ILE:HD12 | 2.44                     | 0.42              |
| 1:A:231:ASP:O    | 1:A:232:ASP:C    | 2.63                     | 0.42              |
| 1:A:474:GLY:O    | 1:A:475:GLN:C    | 2.63                     | 0.42              |
| 1:C:326:ILE:CG2  | 1:C:327:CYS:N    | 2.82                     | 0.42              |
| 1:C:405:ASN:OD1  | 1:C:406:CSD:N    | 2.53                     | 0.42              |
| 1:E:1:ILE:HD11   | 1:F:154:ASN:O    | 2.20                     | 0.42              |
| 1:E:75:LYS:HD2   | 1:E:75:LYS:C     | 2.45                     | 0.42              |
| 1:E:160:PRO:HB2  | 1:E:173:HIS:ND1  | 2.35                     | 0.42              |
| 1:A:18:GLU:C     | 1:A:33:TRP:NE1   | 2.78                     | 0.42              |
| 1:A:148:ASP:OD1  | 1:A:367:LEU:HD21 | 2.19                     | 0.42              |
| 1:C:13:ASN:C     | 1:C:14:LEU:HD12  | 2.45                     | 0.42              |
| 1:C:417:ARG:O    | 1:C:418:ARG:C    | 2.63                     | 0.42              |
| 1:D:350:ARG:HH21 | 1:D:350:ARG:HG3  | 1.85                     | 0.42              |
| 1:D:387:ASN:HA   | 1:D:426:GLN:NE2  | 2.35                     | 0.42              |
| 1:E:219:THR:OG1  | 1:E:220:ASN:N    | 2.51                     | 0.42              |
| 1:F:26:GLU:HG2   | 1:F:239:THR:OG1  | 2.20                     | 0.42              |
| 1:A:430:VAL:HG22 | 1:A:431:ALA:N    | 2.34                     | 0.42              |
| 1:B:60:PRO:HA    | 1:B:131:TYR:O    | 2.20                     | 0.42              |
| 1:B:222:ASP:O    | 1:B:226:LYS:HG2  | 2.20                     | 0.42              |
| 1:B:392:ILE:HG23 | 1:B:441:TYR:CD2  | 2.55                     | 0.42              |
| 1:C:7:ASN:O      | 1:C:9:CYS:N      | 2.53                     | 0.42              |
| 1:C:363:ARG:HH21 | 1:C:448:HIS:CD2  | 2.38                     | 0.42              |
| 1:C:394:VAL:HG21 | 1:C:417:ARG:C    | 2.45                     | 0.42              |
| 1:D:234:ARG:HB3  | 1:D:238:VAL:HG12 | 2.00                     | 0.42              |
| 1:E:72:VAL:HG22  | 1:E:142:VAL:O    | 2.20                     | 0.42              |
| 1:E:122:VAL:O    | 1:E:332:HIS:HA   | 2.20                     | 0.42              |
| 1:E:392:ILE:O    | 1:E:421:LEU:HA   | 2.20                     | 0.42              |
| 1:A:402:ARG:O    | 1:A:430:VAL:HA   | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:148:ASP:HB2  | 1:C:367:LEU:HD11 | 2.01                     | 0.42              |
| 1:C:345:ASN:O    | 1:C:347:LYS:N    | 2.53                     | 0.42              |
| 1:D:376:ARG:C    | 1:D:378:GLY:H    | 2.27                     | 0.42              |
| 1:F:134:TYR:CZ   | 1:F:244:LEU:HD13 | 2.55                     | 0.42              |
| 1:F:355:ASN:OD1  | 1:F:357:LEU:HB2  | 2.20                     | 0.42              |
| 1:A:80:PHE:CD1   | 1:A:80:PHE:N     | 2.87                     | 0.41              |
| 1:A:376:ARG:HH12 | 1:A:436:GLU:HG2  | 1.85                     | 0.41              |
| 1:C:47:VAL:HG12  | 1:C:48:SER:H     | 1.85                     | 0.41              |
| 1:C:120:GLY:C    | 1:C:334:ASN:OD1  | 2.62                     | 0.41              |
| 1:D:25:SER:OG    | 1:D:237:ILE:HB   | 2.20                     | 0.41              |
| 1:D:178:GLN:C    | 1:D:179:GLN:HG3  | 2.45                     | 0.41              |
| 1:D:402:ARG:HB2  | 1:F:208:PHE:HE1  | 1.84                     | 0.41              |
| 1:E:31:GLU:OE1   | 1:E:49:LYS:HD3   | 2.19                     | 0.41              |
| 1:E:111:HIS:HB2  | 1:F:461:ALA:O    | 2.19                     | 0.41              |
| 1:E:164:TYR:CD1  | 1:E:169:PRO:HG3  | 2.54                     | 0.41              |
| 1:F:72:VAL:CG1   | 1:F:144:ILE:HD13 | 2.50                     | 0.41              |
| 1:A:51:THR:HA    | 1:A:141:VAL:O    | 2.20                     | 0.41              |
| 1:A:426:GLN:HG2  | 1:A:427:ASN:N    | 2.36                     | 0.41              |
| 1:B:151:ASN:OD1  | 1:B:153:ASN:N    | 2.53                     | 0.41              |
| 1:B:397:GLY:HA3  | 1:B:439:LEU:HA   | 2.02                     | 0.41              |
| 1:C:67:GLN:O     | 1:C:125:ILE:N    | 2.53                     | 0.41              |
| 1:D:198:GLU:C    | 1:D:200:GLU:H    | 2.28                     | 0.41              |
| 1:F:467:LEU:HD12 | 1:F:467:LEU:HA   | 1.89                     | 0.41              |
| 1:A:12:ASN:O     | 1:A:411:VAL:HA   | 2.20                     | 0.41              |
| 1:B:337:ARG:HA   | 1:B:338:PRO:HD3  | 1.90                     | 0.41              |
| 1:B:479:ARG:NE   | 1:B:483:TYR:HD2  | 2.17                     | 0.41              |
| 1:D:11:LEU:HD11  | 1:D:38:PRO:O     | 2.21                     | 0.41              |
| 1:E:205:LEU:C    | 1:E:207:GLY:N    | 2.76                     | 0.41              |
| 1:A:386:LEU:CD1  | 1:A:452:SER:HA   | 2.50                     | 0.41              |
| 1:A:402:ARG:HH11 | 1:A:402:ARG:HG3  | 1.85                     | 0.41              |
| 1:B:228:ARG:NH1  | 1:B:228:ARG:CB   | 2.84                     | 0.41              |
| 1:C:337:ARG:HB2  | 1:C:340:ARG:HE   | 1.86                     | 0.41              |
| 1:C:437:GLN:HE21 | 1:C:437:GLN:HA   | 1.85                     | 0.41              |
| 1:D:34:ASN:C     | 1:D:36:GLN:N     | 2.78                     | 0.41              |
| 1:D:432:GLU:N    | 1:D:432:GLU:OE2  | 2.54                     | 0.41              |
| 1:D:437:GLN:H    | 1:D:437:GLN:CD   | 2.28                     | 0.41              |
| 1:E:46:THR:CG2   | 1:E:147:LEU:HD12 | 2.50                     | 0.41              |
| 1:F:398:LYS:NZ   | 1:F:398:LYS:HB2  | 2.36                     | 0.41              |
| 1:B:68:MET:HA    | 1:B:123:LEU:O    | 2.20                     | 0.41              |
| 1:B:79:GLY:HA3   | 1:B:132:TRP:CE2  | 2.56                     | 0.41              |
| 1:B:129:VAL:HA   | 1:B:130:PRO:HD3  | 1.91                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:156:LEU:CB   | 1:B:161:ARG:HH21 | 2.15                     | 0.41              |
| 1:B:234:ARG:CB   | 1:B:238:VAL:HG12 | 2.51                     | 0.41              |
| 1:C:480:GLN:CD   | 1:C:484:GLN:HG3  | 2.45                     | 0.41              |
| 1:E:2:THR:C      | 1:E:4:SER:H      | 2.28                     | 0.41              |
| 1:E:53:ASN:O     | 1:E:54:ARG:C     | 2.63                     | 0.41              |
| 1:E:71:VAL:HA    | 1:E:143:ALA:HB2  | 2.03                     | 0.41              |
| 1:F:209:SER:O    | 1:F:210:LYS:C    | 2.64                     | 0.41              |
| 1:F:396:ARG:HG2  | 1:F:397:GLY:N    | 2.36                     | 0.41              |
| 1:A:397:GLY:O    | 1:A:398:LYS:HB2  | 2.19                     | 0.41              |
| 1:A:455:ILE:CD1  | 1:C:205:LEU:HD21 | 2.48                     | 0.41              |
| 1:B:363:ARG:HA   | 1:B:448:HIS:HB2  | 2.02                     | 0.41              |
| 1:B:437:GLN:HE21 | 1:B:437:GLN:CA   | 2.33                     | 0.41              |
| 1:C:17:LEU:HD13  | 1:C:37:HIS:CD2   | 2.56                     | 0.41              |
| 1:C:56:GLY:N     | 1:C:135:ASN:HB3  | 2.32                     | 0.41              |
| 1:D:75:LYS:HG3   | 1:D:136:THR:OG1  | 2.21                     | 0.41              |
| 1:D:112:GLN:HE21 | 1:E:461:ALA:CB   | 2.32                     | 0.41              |
| 1:E:244:LEU:HD21 | 1:F:466:VAL:HG23 | 2.02                     | 0.41              |
| 1:F:88:THR:HG22  | 1:F:89:PHE:N     | 2.35                     | 0.41              |
| 1:F:89:PHE:CD1   | 1:F:110:SER:HB3  | 2.55                     | 0.41              |
| 1:F:335:ILE:O    | 1:F:335:ILE:HG12 | 2.21                     | 0.41              |
| 1:B:379:ILE:CG2  | 1:B:380:TYR:N    | 2.84                     | 0.41              |
| 1:C:70:ILE:O     | 1:C:70:ILE:HG23  | 2.19                     | 0.41              |
| 1:C:78:ILE:HB    | 1:C:133:THR:HG22 | 2.03                     | 0.41              |
| 1:C:89:PHE:HD1   | 1:C:114:ILE:H    | 1.67                     | 0.41              |
| 1:E:19:PRO:HB3   | 1:E:31:GLU:HB3   | 2.03                     | 0.41              |
| 1:E:412:PHE:CD1  | 1:E:412:PHE:C    | 2.99                     | 0.41              |
| 1:E:454:TYR:CZ   | 1:E:457:ASP:HB2  | 2.55                     | 0.41              |
| 1:F:59:LEU:HA    | 1:F:60:PRO:HD3   | 1.95                     | 0.41              |
| 1:B:412:PHE:CD1  | 1:B:412:PHE:C    | 2.98                     | 0.41              |
| 1:C:237:ILE:HG22 | 1:C:238:VAL:N    | 2.36                     | 0.41              |
| 1:D:362:LEU:HD13 | 1:D:367:LEU:O    | 2.20                     | 0.41              |
| 1:D:366:GLY:HA2  | 1:D:448:HIS:N    | 2.34                     | 0.41              |
| 1:D:437:GLN:NE2  | 1:D:437:GLN:N    | 2.67                     | 0.41              |
| 1:F:34:ASN:ND2   | 1:F:36:GLN:H     | 2.19                     | 0.41              |
| 1:F:82:PHE:HB3   | 1:F:85:CYS:SG    | 2.61                     | 0.41              |
| 1:F:390:SER:HB2  | 1:F:424:VAL:HB   | 2.02                     | 0.41              |
| 1:A:34:ASN:ND2   | 1:A:36:GLN:H     | 2.19                     | 0.41              |
| 1:A:80:PHE:HE2   | 1:A:125:ILE:HD13 | 1.86                     | 0.41              |
| 1:B:62:TYR:HE2   | 1:C:427:ASN:HB3  | 1.86                     | 0.41              |
| 1:B:208:PHE:CE2  | 1:C:382:PRO:HB3  | 2.56                     | 0.41              |
| 1:C:14:LEU:HD12  | 1:C:14:LEU:N     | 2.36                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:75:LYS:O     | 1:C:141:VAL:HG21 | 2.20                     | 0.41              |
| 1:C:337:ARG:NH2  | 1:C:337:ARG:HB3  | 2.36                     | 0.41              |
| 1:C:366:GLY:O    | 1:C:367:LEU:HG   | 2.20                     | 0.41              |
| 1:D:206:SER:O    | 1:D:208:PHE:N    | 2.54                     | 0.41              |
| 1:D:368:SER:HB2  | 1:D:447:HIS:O    | 2.21                     | 0.41              |
| 1:E:69:ILE:O     | 1:E:123:LEU:N    | 2.52                     | 0.41              |
| 1:F:332:HIS:CD2  | 1:F:332:HIS:C    | 2.99                     | 0.41              |
| 1:A:62:TYR:CE1   | 1:A:163:PHE:HB2  | 2.56                     | 0.41              |
| 1:A:338:PRO:C    | 1:A:340:ARG:H    | 2.29                     | 0.41              |
| 1:A:454:TYR:CD1  | 1:A:456:LYS:HB2  | 2.55                     | 0.41              |
| 1:B:164:TYR:O    | 1:B:203:SER:HB2  | 2.20                     | 0.41              |
| 1:B:456:LYS:HD2  | 1:B:485:GLY:CA   | 2.50                     | 0.41              |
| 1:C:36:GLN:HE21  | 1:C:175:GLU:CB   | 2.33                     | 0.41              |
| 1:D:82:PHE:CZ    | 1:D:331:LEU:HD11 | 2.56                     | 0.41              |
| 1:D:206:SER:C    | 1:D:208:PHE:N    | 2.78                     | 0.41              |
| 1:D:393:TYR:CE2  | 1:D:395:THR:HG22 | 2.56                     | 0.41              |
| 1:E:228:ARG:CB   | 1:E:228:ARG:HH11 | 2.34                     | 0.41              |
| 1:F:212:PHE:C    | 1:F:212:PHE:CD1  | 2.99                     | 0.41              |
| 1:A:54:ARG:HH11  | 1:A:138:ASP:HA   | 1.86                     | 0.40              |
| 1:B:33:TRP:O     | 1:B:34:ASN:C     | 2.63                     | 0.40              |
| 1:E:82:PHE:CE1   | 1:E:129:VAL:HG11 | 2.55                     | 0.40              |
| 1:F:126:PRO:HA   | 1:F:127:PRO:HD3  | 1.90                     | 0.40              |
| 1:A:19:PRO:HB3   | 1:A:31:GLU:HB3   | 2.02                     | 0.40              |
| 1:A:81:ALA:HB1   | 1:B:458:VAL:HG13 | 2.02                     | 0.40              |
| 1:A:480:GLN:HE21 | 1:A:480:GLN:CA   | 2.27                     | 0.40              |
| 1:B:212:PHE:HE2  | 1:C:379:ILE:HG21 | 1.86                     | 0.40              |
| 1:C:22:ARG:HB3   | 1:C:22:ARG:HH11  | 1.87                     | 0.40              |
| 1:C:405:ASN:ND2  | 1:C:409:ASN:HB2  | 2.36                     | 0.40              |
| 1:D:344:TYR:CD1  | 1:D:344:TYR:C    | 2.98                     | 0.40              |
| 1:F:348:ALA:HB1  | 1:F:490:LEU:HB3  | 2.02                     | 0.40              |
| 1:A:441:TYR:CD2  | 1:A:441:TYR:C    | 2.98                     | 0.40              |
| 1:B:50:ARG:HH12  | 1:B:67:GLN:NE2   | 2.20                     | 0.40              |
| 1:B:154:ASN:ND2  | 1:B:157:ASP:O    | 2.55                     | 0.40              |
| 1:C:18:GLU:HA    | 1:C:33:TRP:HE1   | 1.85                     | 0.40              |
| 1:C:124:VAL:HG21 | 1:C:362:LEU:CD2  | 2.49                     | 0.40              |
| 1:C:351:ILE:HD13 | 1:C:380:TYR:CE2  | 2.57                     | 0.40              |
| 1:C:387:ASN:HD22 | 1:C:387:ASN:N    | 2.19                     | 0.40              |
| 1:D:89:PHE:HD2   | 1:D:110:SER:HA   | 1.86                     | 0.40              |
| 1:D:165:LEU:HD23 | 1:D:204:VAL:HG21 | 2.02                     | 0.40              |
| 1:E:46:THR:HG22  | 1:E:147:LEU:HB2  | 2.03                     | 0.40              |
| 1:E:430:VAL:CG2  | 1:E:431:ALA:N    | 2.84                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:455:ILE:O    | 1:E:456:LYS:C    | 2.64                     | 0.40              |
| 1:F:46:THR:HG22  | 1:F:147:LEU:HB2  | 2.03                     | 0.40              |
| 1:F:118:ASN:N    | 1:F:121:ASP:OD2  | 2.51                     | 0.40              |
| 1:F:468:SER:O    | 1:F:472:ASN:N    | 2.54                     | 0.40              |
| 1:A:228:ARG:HB2  | 1:A:228:ARG:HH11 | 1.87                     | 0.40              |
| 1:A:386:LEU:HG   | 1:C:128:GLY:O    | 2.21                     | 0.40              |
| 1:A:472:ASN:O    | 1:C:226:LYS:HD2  | 2.21                     | 0.40              |
| 1:B:51:THR:HA    | 1:B:141:VAL:O    | 2.21                     | 0.40              |
| 1:B:66:PRO:HG2   | 1:B:148:ASP:HB3  | 2.02                     | 0.40              |
| 1:B:471:TYR:O    | 1:B:472:ASN:CB   | 2.68                     | 0.40              |
| 1:C:87:GLU:HG3   | 1:C:111:HIS:C    | 2.46                     | 0.40              |
| 1:C:402:ARG:HA   | 1:C:412:PHE:O    | 2.22                     | 0.40              |
| 1:D:77:ALA:O     | 1:D:117:PHE:HE1  | 2.04                     | 0.40              |
| 1:D:171:ILE:HG22 | 1:D:173:HIS:C    | 2.47                     | 0.40              |
| 1:E:401:VAL:HG22 | 1:E:432:GLU:HG3  | 2.04                     | 0.40              |
| 1:E:407:GLN:C    | 1:E:409:ASN:H    | 2.30                     | 0.40              |
| 1:E:491:VAL:HG12 | 1:E:492:ASN:N    | 2.36                     | 0.40              |
| 1:F:385:ASN:HD21 | 1:F:445:LYS:HZ3  | 1.70                     | 0.40              |
| 1:A:159:ASN:OD1  | 1:B:7:ASN:ND2    | 2.55                     | 0.40              |
| 1:A:227:LEU:HA   | 1:B:471:TYR:CD2  | 2.56                     | 0.40              |
| 1:A:333:GLU:HG3  | 1:A:334:ASN:N    | 2.36                     | 0.40              |
| 1:B:14:LEU:N     | 1:B:14:LEU:HD12  | 2.36                     | 0.40              |
| 1:B:368:SER:HG   | 1:B:445:LYS:HB2  | 1.86                     | 0.40              |
| 1:B:376:ARG:HA   | 1:B:435:GLY:O    | 2.21                     | 0.40              |
| 1:B:380:TYR:CZ   | 1:B:383:HIS:NE2  | 2.89                     | 0.40              |
| 1:E:66:PRO:N     | 1:E:127:PRO:HG3  | 2.35                     | 0.40              |
| 1:E:75:LYS:HD2   | 1:E:75:LYS:O     | 2.22                     | 0.40              |
| 1:E:115:ARG:HG2  | 1:E:115:ARG:HH21 | 1.87                     | 0.40              |
| 1:E:157:ASP:OD2  | 1:E:157:ASP:C    | 2.64                     | 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     | 365/493 (74%)   | 302 (83%)  | 54 (15%)  | 9 (2%)   | 4           | 16 |
| 1   | B     | 363/493 (74%)   | 297 (82%)  | 54 (15%)  | 12 (3%)  | 3           | 11 |
| 1   | C     | 361/493 (73%)   | 291 (81%)  | 51 (14%)  | 19 (5%)  | 1           | 5  |
| 1   | D     | 368/493 (75%)   | 307 (83%)  | 54 (15%)  | 7 (2%)   | 6           | 22 |
| 1   | E     | 371/493 (75%)   | 311 (84%)  | 54 (15%)  | 6 (2%)   | 7           | 27 |
| 1   | F     | 368/493 (75%)   | 311 (84%)  | 44 (12%)  | 13 (4%)  | 3           | 10 |
| All | All   | 2196/2958 (74%) | 1819 (83%) | 311 (14%) | 66 (3%)  | 3           | 12 |

All (66) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 426 | GLN  |
| 1   | B     | 426 | GLN  |
| 1   | C     | 245 | SER  |
| 1   | C     | 418 | ARG  |
| 1   | D     | 171 | ILE  |
| 1   | D     | 436 | GLU  |
| 1   | D     | 447 | HIS  |
| 1   | E     | 426 | GLN  |
| 1   | F     | 107 | LEU  |
| 1   | F     | 171 | ILE  |
| 1   | F     | 425 | PRO  |
| 1   | F     | 482 | LYS  |
| 1   | A     | 113 | LYS  |
| 1   | A     | 232 | ASP  |
| 1   | B     | 53  | ASN  |
| 1   | B     | 472 | ASN  |
| 1   | C     | 8   | GLU  |
| 1   | C     | 53  | ASN  |
| 1   | C     | 113 | LYS  |
| 1   | C     | 330 | LYS  |
| 1   | C     | 375 | TYR  |
| 1   | F     | 21  | HIS  |
| 1   | F     | 246 | VAL  |
| 1   | F     | 329 | MET  |
| 1   | F     | 388 | ALA  |
| 1   | A     | 398 | LYS  |
| 1   | A     | 447 | HIS  |
| 1   | A     | 475 | GLN  |
| 1   | B     | 175 | GLU  |
| 1   | C     | 171 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 346 | PRO  |
| 1   | C     | 407 | GLN  |
| 1   | C     | 482 | LYS  |
| 1   | D     | 207 | GLY  |
| 1   | E     | 6   | PHE  |
| 1   | E     | 446 | THR  |
| 1   | F     | 26  | GLU  |
| 1   | A     | 220 | ASN  |
| 1   | B     | 112 | GLN  |
| 1   | B     | 377 | ASN  |
| 1   | C     | 13  | ASN  |
| 1   | C     | 425 | PRO  |
| 1   | C     | 426 | GLN  |
| 1   | D     | 111 | HIS  |
| 1   | E     | 4   | SER  |
| 1   | E     | 35  | SER  |
| 1   | E     | 356 | SER  |
| 1   | F     | 108 | GLN  |
| 1   | F     | 243 | GLY  |
| 1   | F     | 426 | GLN  |
| 1   | A     | 88  | THR  |
| 1   | A     | 338 | PRO  |
| 1   | B     | 235 | LYS  |
| 1   | B     | 468 | SER  |
| 1   | B     | 487 | SER  |
| 1   | C     | 148 | ASP  |
| 1   | C     | 481 | LEU  |
| 1   | D     | 64  | PRO  |
| 1   | F     | 19  | PRO  |
| 1   | B     | 419 | GLY  |
| 1   | C     | 337 | ARG  |
| 1   | B     | 19  | PRO  |
| 1   | B     | 45  | VAL  |
| 1   | D     | 488 | GLY  |
| 1   | C     | 246 | VAL  |
| 1   | C     | 411 | VAL  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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     | 324/435 (74%)   | 314 (97%)  | 10 (3%)  | 35          | 70 |
| 1   | B     | 322/435 (74%)   | 317 (98%)  | 5 (2%)   | 55          | 83 |
| 1   | C     | 320/435 (74%)   | 311 (97%)  | 9 (3%)   | 38          | 73 |
| 1   | D     | 327/435 (75%)   | 318 (97%)  | 9 (3%)   | 38          | 73 |
| 1   | E     | 330/435 (76%)   | 323 (98%)  | 7 (2%)   | 47          | 79 |
| 1   | F     | 327/435 (75%)   | 319 (98%)  | 8 (2%)   | 43          | 77 |
| All | All   | 1950/2610 (75%) | 1902 (98%) | 48 (2%)  | 42          | 76 |

All (48) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 87  | GLU  |
| 1   | A     | 326 | ILE  |
| 1   | A     | 340 | ARG  |
| 1   | A     | 364 | GLN  |
| 1   | A     | 387 | ASN  |
| 1   | A     | 409 | ASN  |
| 1   | A     | 413 | ASP  |
| 1   | A     | 436 | GLU  |
| 1   | A     | 441 | TYR  |
| 1   | A     | 475 | GLN  |
| 1   | B     | 158 | GLN  |
| 1   | B     | 374 | LEU  |
| 1   | B     | 387 | ASN  |
| 1   | B     | 432 | GLU  |
| 1   | B     | 484 | GLN  |
| 1   | C     | 87  | GLU  |
| 1   | C     | 236 | GLN  |
| 1   | C     | 326 | ILE  |
| 1   | C     | 331 | LEU  |
| 1   | C     | 340 | ARG  |
| 1   | C     | 364 | GLN  |
| 1   | C     | 387 | ASN  |
| 1   | C     | 394 | VAL  |
| 1   | C     | 436 | GLU  |
| 1   | D     | 7   | ASN  |
| 1   | D     | 20  | ASP  |
| 1   | D     | 158 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 175 | GLU  |
| 1   | D     | 180 | GLN  |
| 1   | D     | 325 | ASN  |
| 1   | D     | 364 | GLN  |
| 1   | D     | 437 | GLN  |
| 1   | D     | 467 | LEU  |
| 1   | E     | 6   | PHE  |
| 1   | E     | 70  | ILE  |
| 1   | E     | 235 | LYS  |
| 1   | E     | 247 | ILE  |
| 1   | E     | 326 | ILE  |
| 1   | E     | 417 | ARG  |
| 1   | E     | 465 | GLU  |
| 1   | F     | 107 | LEU  |
| 1   | F     | 108 | GLN  |
| 1   | F     | 200 | GLU  |
| 1   | F     | 218 | ASN  |
| 1   | F     | 225 | GLU  |
| 1   | F     | 387 | ASN  |
| 1   | F     | 398 | LYS  |
| 1   | F     | 425 | PRO  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | ASN  |
| 1   | A     | 15  | ASN  |
| 1   | A     | 21  | HIS  |
| 1   | A     | 34  | ASN  |
| 1   | A     | 36  | GLN  |
| 1   | A     | 53  | ASN  |
| 1   | A     | 67  | GLN  |
| 1   | A     | 108 | GLN  |
| 1   | A     | 112 | GLN  |
| 1   | A     | 153 | ASN  |
| 1   | A     | 158 | GLN  |
| 1   | A     | 159 | ASN  |
| 1   | A     | 334 | ASN  |
| 1   | A     | 377 | ASN  |
| 1   | A     | 385 | ASN  |
| 1   | A     | 387 | ASN  |
| 1   | A     | 409 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 426 | GLN  |
| 1   | A     | 433 | GLN  |
| 1   | A     | 448 | HIS  |
| 1   | A     | 477 | GLN  |
| 1   | A     | 480 | GLN  |
| 1   | A     | 486 | ASN  |
| 1   | B     | 7   | ASN  |
| 1   | B     | 10  | GLN  |
| 1   | B     | 12  | ASN  |
| 1   | B     | 13  | ASN  |
| 1   | B     | 15  | ASN  |
| 1   | B     | 21  | HIS  |
| 1   | B     | 34  | ASN  |
| 1   | B     | 53  | ASN  |
| 1   | B     | 55  | ASN  |
| 1   | B     | 67  | GLN  |
| 1   | B     | 112 | GLN  |
| 1   | B     | 116 | HIS  |
| 1   | B     | 153 | ASN  |
| 1   | B     | 159 | ASN  |
| 1   | B     | 168 | ASN  |
| 1   | B     | 218 | ASN  |
| 1   | B     | 332 | HIS  |
| 1   | B     | 334 | ASN  |
| 1   | B     | 370 | GLN  |
| 1   | B     | 385 | ASN  |
| 1   | B     | 387 | ASN  |
| 1   | B     | 389 | ASN  |
| 1   | B     | 409 | ASN  |
| 1   | B     | 426 | GLN  |
| 1   | B     | 427 | ASN  |
| 1   | B     | 437 | GLN  |
| 1   | B     | 449 | ASN  |
| 1   | B     | 472 | ASN  |
| 1   | B     | 475 | GLN  |
| 1   | B     | 477 | GLN  |
| 1   | B     | 480 | GLN  |
| 1   | C     | 7   | ASN  |
| 1   | C     | 10  | GLN  |
| 1   | C     | 15  | ASN  |
| 1   | C     | 34  | ASN  |
| 1   | C     | 36  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 53  | ASN  |
| 1   | C     | 67  | GLN  |
| 1   | C     | 73  | GLN  |
| 1   | C     | 111 | HIS  |
| 1   | C     | 154 | ASN  |
| 1   | C     | 178 | GLN  |
| 1   | C     | 211 | HIS  |
| 1   | C     | 332 | HIS  |
| 1   | C     | 334 | ASN  |
| 1   | C     | 345 | ASN  |
| 1   | C     | 385 | ASN  |
| 1   | C     | 387 | ASN  |
| 1   | C     | 407 | GLN  |
| 1   | C     | 409 | ASN  |
| 1   | C     | 433 | GLN  |
| 1   | C     | 437 | GLN  |
| 1   | C     | 448 | HIS  |
| 1   | C     | 469 | ASN  |
| 1   | C     | 472 | ASN  |
| 1   | C     | 475 | GLN  |
| 1   | C     | 480 | GLN  |
| 1   | D     | 7   | ASN  |
| 1   | D     | 10  | GLN  |
| 1   | D     | 12  | ASN  |
| 1   | D     | 15  | ASN  |
| 1   | D     | 21  | HIS  |
| 1   | D     | 36  | GLN  |
| 1   | D     | 53  | ASN  |
| 1   | D     | 67  | GLN  |
| 1   | D     | 153 | ASN  |
| 1   | D     | 159 | ASN  |
| 1   | D     | 178 | GLN  |
| 1   | D     | 180 | GLN  |
| 1   | D     | 197 | GLN  |
| 1   | D     | 215 | GLN  |
| 1   | D     | 334 | ASN  |
| 1   | D     | 364 | GLN  |
| 1   | D     | 389 | ASN  |
| 1   | D     | 407 | GLN  |
| 1   | D     | 409 | ASN  |
| 1   | D     | 437 | GLN  |
| 1   | D     | 469 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 477 | GLN  |
| 1   | D     | 484 | GLN  |
| 1   | E     | 15  | ASN  |
| 1   | E     | 34  | ASN  |
| 1   | E     | 36  | GLN  |
| 1   | E     | 67  | GLN  |
| 1   | E     | 73  | GLN  |
| 1   | E     | 385 | ASN  |
| 1   | E     | 405 | ASN  |
| 1   | E     | 409 | ASN  |
| 1   | E     | 420 | GLN  |
| 1   | E     | 437 | GLN  |
| 1   | E     | 449 | ASN  |
| 1   | E     | 469 | ASN  |
| 1   | E     | 477 | GLN  |
| 1   | E     | 480 | GLN  |
| 1   | F     | 7   | ASN  |
| 1   | F     | 10  | GLN  |
| 1   | F     | 12  | ASN  |
| 1   | F     | 13  | ASN  |
| 1   | F     | 21  | HIS  |
| 1   | F     | 34  | ASN  |
| 1   | F     | 37  | HIS  |
| 1   | F     | 53  | ASN  |
| 1   | F     | 67  | GLN  |
| 1   | F     | 106 | GLN  |
| 1   | F     | 153 | ASN  |
| 1   | F     | 159 | ASN  |
| 1   | F     | 179 | GLN  |
| 1   | F     | 215 | GLN  |
| 1   | F     | 218 | ASN  |
| 1   | F     | 332 | HIS  |
| 1   | F     | 334 | ASN  |
| 1   | F     | 364 | GLN  |
| 1   | F     | 385 | ASN  |
| 1   | F     | 387 | ASN  |
| 1   | F     | 409 | ASN  |
| 1   | F     | 420 | GLN  |
| 1   | F     | 433 | GLN  |
| 1   | F     | 437 | GLN  |
| 1   | F     | 449 | ASN  |
| 1   | F     | 469 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 480 | GLN  |
| 1   | F     | 486 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 1   | CSD  | C     | 406 | 1    | 4,7,8        | 0.59 | 0           | 1,8,10      | 0.75 | 0           |
| 1   | CSD  | A     | 406 | 1    | 4,7,8        | 0.60 | 0           | 1,8,10      | 0.98 | 0           |
| 1   | CSD  | D     | 406 | 1    | 4,7,8        | 0.60 | 0           | 1,8,10      | 1.36 | 0           |
| 1   | CSD  | F     | 406 | 1    | 4,7,8        | 0.61 | 0           | 1,8,10      | 1.37 | 0           |
| 1   | CSD  | B     | 406 | 1    | 4,7,8        | 0.62 | 0           | 1,8,10      | 1.41 | 0           |
| 1   | CSD  | E     | 406 | 1    | 4,7,8        | 0.56 | 0           | 1,8,10      | 1.16 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1   | CSD  | C     | 406 | 1    | -       | 1/2/6/8  | -     |
| 1   | CSD  | A     | 406 | 1    | -       | 0/2/6/8  | -     |
| 1   | CSD  | D     | 406 | 1    | -       | 0/2/6/8  | -     |
| 1   | CSD  | F     | 406 | 1    | -       | 1/2/6/8  | -     |
| 1   | CSD  | B     | 406 | 1    | -       | 1/2/6/8  | -     |
| 1   | CSD  | E     | 406 | 1    | -       | 1/2/6/8  | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | E     | 406 | CSD  | CA-CB-SG-OD1 |
| 1   | F     | 406 | CSD  | CA-CB-SG-OD1 |
| 1   | B     | 406 | CSD  | CA-CB-SG-OD1 |
| 1   | C     | 406 | CSD  | CA-CB-SG-OD1 |

There are no ring outliers.

3 monomers are involved in 5 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | C     | 406 | CSD  | 2       | 0            |
| 1   | B     | 406 | CSD  | 2       | 0            |
| 1   | E     | 406 | CSD  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | CO3  | B     | 502 | -    | 3,3,3        | 0.76 | 0           | 2,3,3       | 0.18 | 0           |
| 2   | CO3  | E     | 505 | -    | 3,3,3        | 0.77 | 0           | 2,3,3       | 0.07 | 0           |
| 2   | CO3  | C     | 503 | -    | 3,3,3        | 0.68 | 0           | 2,3,3       | 0.15 | 0           |
| 2   | CO3  | D     | 504 | -    | 3,3,3        | 0.71 | 0           | 2,3,3       | 0.11 | 0           |
| 2   | CO3  | F     | 506 | -    | 3,3,3        | 0.72 | 0           | 2,3,3       | 0.14 | 0           |
| 2   | CO3  | A     | 501 | -    | 3,3,3        | 0.68 | 0           | 2,3,3       | 0.16 | 0           |

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.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | B     | 502 | CO3  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 373/493 (75%)   | 0.22   | 5 (1%) 75 66  | 13, 37, 54, 62        | 0     |
| 1   | B     | 371/493 (75%)   | 0.17   | 5 (1%) 75 66  | 6, 37, 56, 63         | 0     |
| 1   | C     | 369/493 (74%)   | 0.32   | 8 (2%) 62 52  | 7, 39, 54, 66         | 0     |
| 1   | D     | 376/493 (76%)   | -0.05  | 5 (1%) 75 66  | 6, 19, 46, 57         | 0     |
| 1   | E     | 379/493 (76%)   | -0.09  | 5 (1%) 75 66  | 6, 13, 43, 58         | 0     |
| 1   | F     | 376/493 (76%)   | -0.11  | 2 (0%) 87 82  | 6, 18, 45, 56         | 0     |
| All | All   | 2244/2958 (75%) | 0.08   | 30 (1%) 75 66 | 6, 28, 52, 66         | 0     |

All (30) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 340 | ARG  | 3.6  |
| 1   | E     | 4   | SER  | 3.5  |
| 1   | D     | 179 | GLN  | 3.4  |
| 1   | B     | 485 | GLY  | 3.3  |
| 1   | C     | 88  | THR  | 3.1  |
| 1   | F     | 107 | LEU  | 2.9  |
| 1   | C     | 435 | GLY  | 2.8  |
| 1   | B     | 88  | THR  | 2.7  |
| 1   | D     | 486 | ASN  | 2.6  |
| 1   | E     | 5   | LYS  | 2.6  |
| 1   | E     | 437 | GLN  | 2.6  |
| 1   | D     | 350 | ARG  | 2.6  |
| 1   | F     | 201 | GLY  | 2.5  |
| 1   | E     | 89  | PHE  | 2.4  |
| 1   | C     | 140 | PRO  | 2.3  |
| 1   | C     | 218 | ASN  | 2.3  |
| 1   | C     | 341 | ALA  | 2.3  |
| 1   | C     | 371 | TYR  | 2.3  |
| 1   | A     | 86  | PRO  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 8   | GLU  | 2.2  |
| 1   | B     | 87  | GLU  | 2.2  |
| 1   | B     | 437 | GLN  | 2.2  |
| 1   | D     | 197 | GLN  | 2.1  |
| 1   | C     | 328 | THR  | 2.1  |
| 1   | A     | 7   | ASN  | 2.1  |
| 1   | E     | 2   | THR  | 2.1  |
| 1   | B     | 336 | ALA  | 2.1  |
| 1   | D     | 199 | GLU  | 2.1  |
| 1   | A     | 434 | GLY  | 2.0  |
| 1   | C     | 373 | VAL  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 1   | CSD  | C     | 406 | 8/9   | 0.86 | 0.12 | 31,38,58,62                | 0     |
| 1   | CSD  | A     | 406 | 8/9   | 0.89 | 0.10 | 30,41,46,53                | 0     |
| 1   | CSD  | F     | 406 | 8/9   | 0.92 | 0.11 | 5,8,30,57                  | 0     |
| 1   | CSD  | B     | 406 | 8/9   | 0.93 | 0.07 | 39,44,63,73                | 0     |
| 1   | CSD  | E     | 406 | 8/9   | 0.94 | 0.09 | 5,7,45,53                  | 0     |
| 1   | CSD  | D     | 406 | 8/9   | 0.95 | 0.08 | 5,13,23,38                 | 0     |

## 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   | CO3  | A     | 501 | 4/4   | 0.73 | 0.19 | 14,35,39,41                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | CO3  | B     | 502 | 4/4   | 0.78 | 0.17 | 12,22,39,45                 | 0     |
| 2   | CO3  | E     | 505 | 4/4   | 0.80 | 0.12 | 5,5,10,17                   | 0     |
| 2   | CO3  | C     | 503 | 4/4   | 0.83 | 0.10 | 36,40,41,42                 | 0     |
| 2   | CO3  | F     | 506 | 4/4   | 0.83 | 0.11 | 5,5,18,21                   | 0     |
| 2   | CO3  | D     | 504 | 4/4   | 0.91 | 0.09 | 5,19,20,21                  | 0     |
| 3   | MG   | B     | 602 | 1/1   | 0.92 | 0.07 | 41,41,41,41                 | 0     |
| 3   | MG   | C     | 603 | 1/1   | 0.92 | 0.10 | 21,21,21,21                 | 0     |
| 3   | MG   | D     | 604 | 1/1   | 0.93 | 0.11 | 17,17,17,17                 | 0     |
| 3   | MG   | A     | 601 | 1/1   | 0.94 | 0.04 | 17,17,17,17                 | 0     |
| 3   | MG   | F     | 606 | 1/1   | 0.96 | 0.03 | 8,8,8,8                     | 0     |
| 3   | MG   | E     | 605 | 1/1   | 0.97 | 0.12 | 5,5,5,5                     | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.