



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:29 PM UTC

PDB ID : 7DRI / pdb\_00007dri  
Title : Structure of SspE\_CTD\_41658  
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Deposited on : 2020-12-28  
Resolution : 2.72 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                                             |
| 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                                                             |

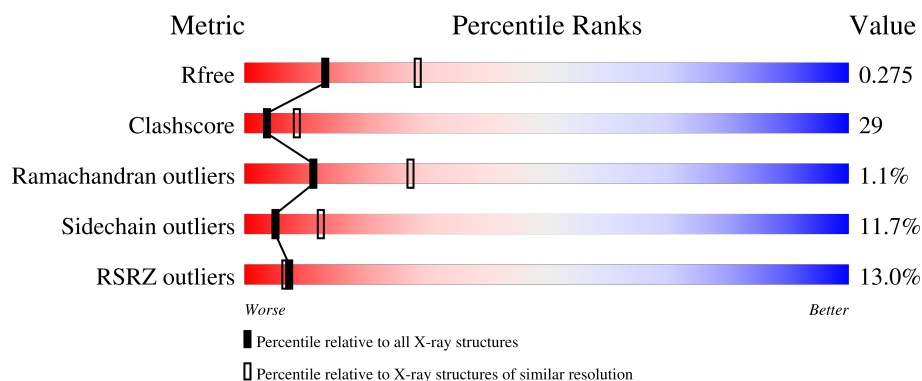
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.72 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                      | 4348 (2.74-2.70)                                      |
| Clashscore            | 190562                      | 4665 (2.74-2.70)                                      |
| Ramachandran outliers | 187476                      | 4584 (2.74-2.70)                                      |
| Sidechain outliers    | 187428                      | 4585 (2.74-2.70)                                      |
| RSRZ outliers         | 180081                      | 4348 (2.74-2.70)                                      |

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>11%</div> <div>61% 27% 6% . .</div> </div>  |
| 1   | B     | 493    | <div> <div>10%</div> <div>61% 27% 6% 5%</div> </div>   |
| 1   | C     | 493    | <div> <div>17%</div> <div>61% 26% 7% . 5%</div> </div> |
| 1   | D     | 493    | <div> <div>11%</div> <div>59% 29% 6% . 5%</div> </div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14108 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.

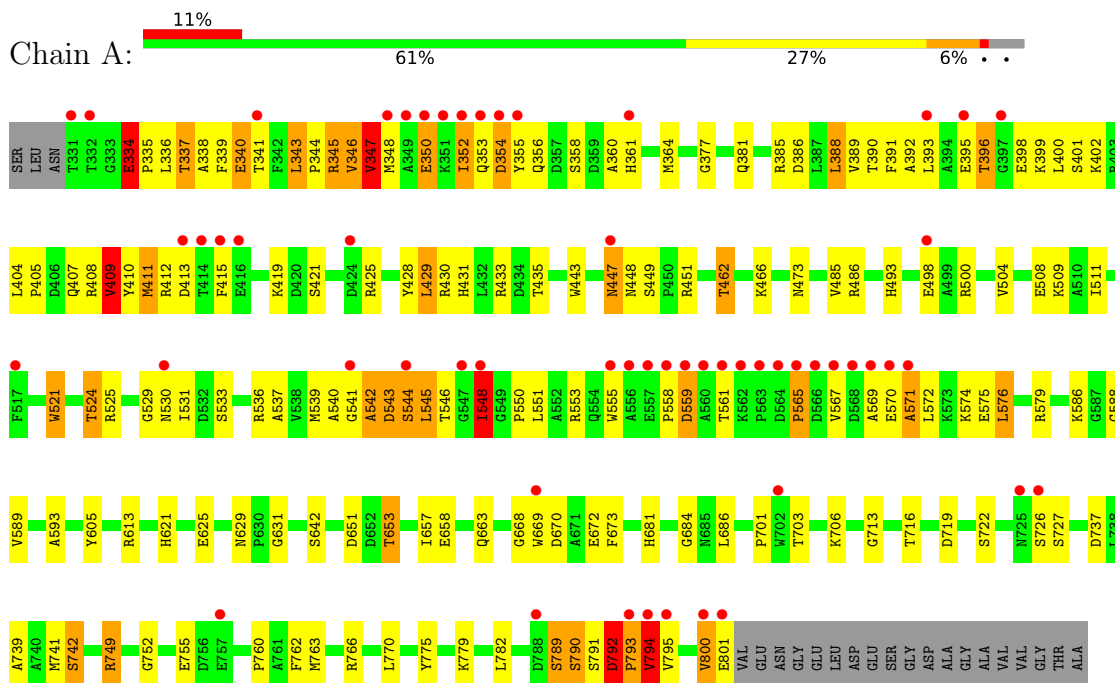
- Molecule 1 is a protein called DUF1524 domain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 471      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3564  | 2246 | 625 | 684 | 9 |         |         |       |
| 1   | B     | 466      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3530  | 2226 | 620 | 675 | 9 |         |         |       |
| 1   | C     | 468      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3524  | 2222 | 619 | 675 | 8 |         |         |       |
| 1   | D     | 467      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3490  | 2200 | 609 | 672 | 9 |         |         |       |

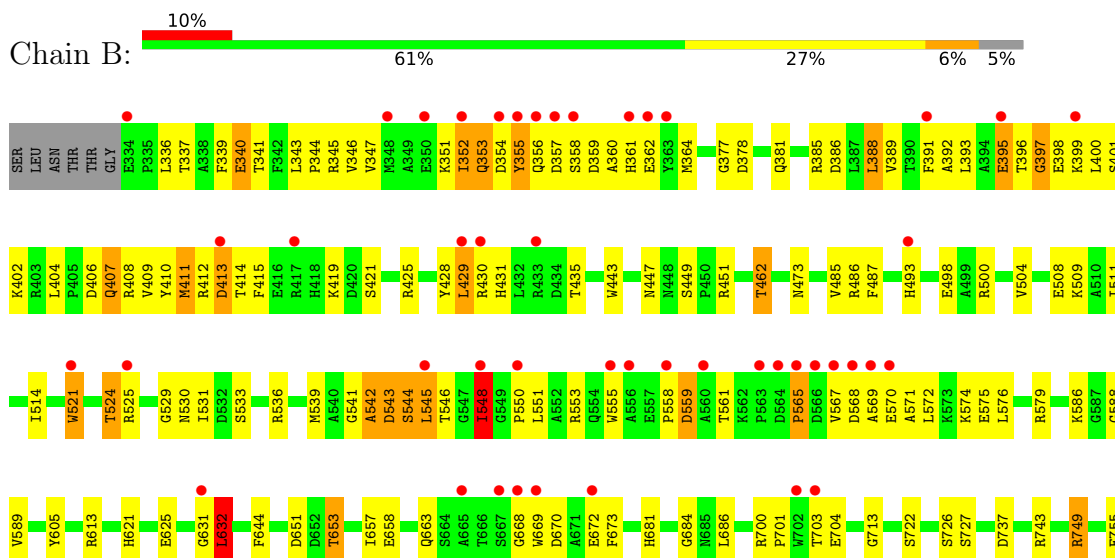
### 3 Residue-property plots

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

#### • Molecule 1: DUF1524 domain



#### • Molecule 1: DUF1524 domain





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 108.75Å 278.92Å 182.26Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 35.97 – 2.72<br>35.97 – 2.72                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.3 (35.97-2.72)<br>99.4 (35.97-2.72)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.12                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.61 (at 2.72Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0267                                             | Depositor        |
| R, $R_{free}$                                                           | 0.268 , 0.272<br>0.263 , 0.275                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3734 reflections (5.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 67.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.743                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 54.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 14108                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 81.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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

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     | 0.75         | 2/3640 (0.1%)   | 1.09        | 21/4955 (0.4%)  |
| 1   | B     | 0.71         | 1/3605 (0.0%)   | 0.99        | 9/4906 (0.2%)   |
| 1   | C     | 0.78         | 6/3598 (0.2%)   | 1.07        | 13/4900 (0.3%)  |
| 1   | D     | 0.71         | 2/3561 (0.1%)   | 1.03        | 13/4850 (0.3%)  |
| All | All   | 0.74         | 11/14404 (0.1%) | 1.05        | 56/19611 (0.3%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | C     | 0                   | 2                   |
| All | All   | 0                   | 3                   |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 795 | VAL  | C-O   | -8.44 | 1.14        | 1.24     |
| 1   | B     | 355 | TYR  | C-O   | -7.92 | 1.11        | 1.23     |
| 1   | A     | 354 | ASP  | C-O   | -7.91 | 1.16        | 1.24     |
| 1   | C     | 567 | VAL  | C-O   | -6.15 | 1.17        | 1.24     |
| 1   | D     | 800 | VAL  | C-O   | -5.97 | 1.17        | 1.24     |
| 1   | A     | 347 | VAL  | C-O   | -5.68 | 1.17        | 1.24     |
| 1   | C     | 343 | LEU  | C-O   | 5.57  | 1.30        | 1.24     |
| 1   | D     | 565 | PRO  | C-O   | -5.36 | 1.17        | 1.24     |
| 1   | C     | 353 | GLN  | CA-CB | -5.32 | 1.44        | 1.53     |
| 1   | C     | 794 | VAL  | C-O   | -5.23 | 1.18        | 1.24     |
| 1   | C     | 396 | THR  | C-O   | -5.12 | 1.17        | 1.24     |

All (56) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | C     | 353 | GLN  | N-CA-C  | 14.17  | 126.81      | 111.36   |
| 1   | A     | 792 | ASP  | C-N-CD  | -10.46 | 82.09       | 125.00   |
| 1   | C     | 797 | VAL  | N-CA-C  | 9.67   | 120.59      | 110.05   |
| 1   | C     | 788 | ASP  | N-CA-C  | -9.23  | 102.19      | 112.72   |
| 1   | B     | 353 | GLN  | N-CA-C  | -8.87  | 101.61      | 111.28   |
| 1   | A     | 352 | ILE  | N-CA-C  | 8.74   | 119.55      | 110.72   |
| 1   | D     | 794 | VAL  | N-CA-C  | 8.73   | 120.60      | 106.72   |
| 1   | C     | 793 | PRO  | N-CA-CB | 8.66   | 112.35      | 103.25   |
| 1   | A     | 565 | PRO  | N-CA-CB | 7.71   | 111.34      | 103.25   |
| 1   | A     | 792 | ASP  | CA-C-N  | 7.45   | 129.15      | 119.84   |
| 1   | A     | 792 | ASP  | C-N-CA  | 7.45   | 129.15      | 119.84   |
| 1   | B     | 565 | PRO  | N-CA-CB | 7.36   | 110.97      | 103.25   |
| 1   | A     | 794 | VAL  | N-CA-C  | 7.34   | 117.51      | 106.42   |
| 1   | C     | 365 | LYS  | N-CA-C  | -7.30  | 103.32      | 111.28   |
| 1   | D     | 360 | ALA  | N-CA-C  | -7.28  | 103.33      | 111.71   |
| 1   | D     | 789 | SER  | N-CA-C  | -7.27  | 103.98      | 112.92   |
| 1   | A     | 343 | LEU  | CA-C-N  | -7.03  | 111.30      | 119.32   |
| 1   | A     | 343 | LEU  | C-N-CA  | -7.03  | 111.30      | 119.32   |
| 1   | C     | 791 | SER  | N-CA-C  | -6.96  | 103.69      | 111.28   |
| 1   | A     | 790 | SER  | N-CA-C  | -6.95  | 100.15      | 110.23   |
| 1   | A     | 629 | ASN  | CA-C-N  | 6.93   | 127.22      | 119.32   |
| 1   | A     | 629 | ASN  | C-N-CA  | 6.93   | 127.22      | 119.32   |
| 1   | D     | 565 | PRO  | N-CA-CB | 6.88   | 110.59      | 103.23   |
| 1   | C     | 565 | PRO  | N-CA-CB | 6.84   | 110.44      | 103.25   |
| 1   | C     | 408 | ARG  | N-CA-C  | -6.65  | 104.03      | 111.28   |
| 1   | C     | 354 | ASP  | N-CA-C  | 6.45   | 119.75      | 107.75   |
| 1   | A     | 571 | ALA  | N-CA-C  | 6.39   | 121.18      | 112.68   |
| 1   | D     | 335 | PRO  | N-CA-CB | 6.21   | 109.77      | 103.25   |
| 1   | D     | 411 | MET  | N-CA-C  | -6.12  | 104.53      | 111.14   |
| 1   | A     | 447 | ASN  | N-CA-C  | 5.97   | 118.28      | 111.11   |
| 1   | D     | 409 | VAL  | N-CA-C  | 5.95   | 116.69      | 110.62   |
| 1   | B     | 793 | PRO  | N-CA-CB | 5.89   | 109.44      | 103.25   |
| 1   | A     | 548 | ILE  | N-CA-C  | 5.81   | 117.07      | 109.58   |
| 1   | B     | 397 | GLY  | N-CA-C  | -5.77  | 99.51       | 113.18   |
| 1   | A     | 572 | LEU  | N-CA-C  | 5.74   | 117.62      | 111.36   |
| 1   | C     | 346 | VAL  | N-CA-C  | 5.68   | 117.19      | 111.00   |
| 1   | B     | 632 | LEU  | N-CA-C  | 5.62   | 118.10      | 110.35   |
| 1   | D     | 548 | ILE  | N-CA-C  | 5.61   | 116.82      | 109.58   |
| 1   | D     | 793 | PRO  | N-CA-CB | 5.59   | 109.12      | 103.25   |
| 1   | A     | 408 | ARG  | CA-C-N  | 5.56   | 127.68      | 120.56   |
| 1   | A     | 408 | ARG  | C-N-CA  | 5.56   | 127.68      | 120.56   |
| 1   | B     | 548 | ILE  | N-CA-C  | 5.49   | 116.66      | 109.58   |
| 1   | C     | 334 | GLU  | CA-C-N  | 5.41   | 126.60      | 119.84   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | C     | 334 | GLU  | C-N-CA   | 5.41  | 126.60      | 119.84   |
| 1   | D     | 564 | ASP  | CA-C-N   | 5.34  | 124.53      | 118.97   |
| 1   | D     | 564 | ASP  | C-N-CA   | 5.34  | 124.53      | 118.97   |
| 1   | A     | 334 | GLU  | CA-C-N   | 5.26  | 126.42      | 119.84   |
| 1   | A     | 334 | GLU  | C-N-CA   | 5.26  | 126.42      | 119.84   |
| 1   | C     | 548 | ILE  | N-CA-C   | 5.21  | 117.13      | 109.63   |
| 1   | A     | 789 | SER  | CA-CB-OG | 5.19  | 121.49      | 111.10   |
| 1   | B     | 411 | MET  | N-CA-C   | -5.10 | 105.61      | 111.07   |
| 1   | D     | 565 | PRO  | N-CA-C   | 5.09  | 120.75      | 113.47   |
| 1   | D     | 416 | GLU  | N-CA-C   | -5.07 | 105.76      | 111.28   |
| 1   | A     | 409 | VAL  | CB-CA-C  | -5.03 | 105.44      | 112.02   |
| 1   | B     | 351 | LYS  | CB-CA-C  | -5.03 | 110.76      | 116.54   |
| 1   | B     | 788 | ASP  | N-CA-C   | -5.02 | 106.90      | 112.57   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 540 | ALA  | Peptide |
| 1   | C     | 540 | ALA  | Peptide |
| 1   | C     | 789 | SER  | Peptide |

## 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     | 3564  | 0        | 3439     | 219     | 0            |
| 1   | B     | 3530  | 0        | 3420     | 170     | 1            |
| 1   | C     | 3524  | 0        | 3394     | 204     | 0            |
| 1   | D     | 3490  | 0        | 3341     | 213     | 0            |
| All | All   | 14108 | 0        | 13594    | 801     | 1            |

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 29.

All (801) 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:A:790:SER:CB   | 1:A:794:VAL:CB   | 1.83                     | 1.53              |
| 1:A:340:GLU:HA   | 1:A:343:LEU:CD1  | 1.45                     | 1.43              |
| 1:A:790:SER:CB   | 1:A:794:VAL:HB   | 0.94                     | 1.42              |
| 1:C:795:VAL:HG23 | 1:C:796:LYS:CB   | 1.45                     | 1.42              |
| 1:C:795:VAL:HG23 | 1:C:796:LYS:CA   | 1.54                     | 1.37              |
| 1:C:795:VAL:CG2  | 1:C:796:LYS:HA   | 1.63                     | 1.29              |
| 1:A:541:GLY:HA2  | 1:A:542:ALA:CB   | 1.50                     | 1.27              |
| 1:C:354:ASP:O    | 1:C:357:ASP:HA   | 1.29                     | 1.27              |
| 1:A:792:ASP:CB   | 1:A:793:PRO:HD3  | 1.50                     | 1.26              |
| 1:A:340:GLU:O    | 1:A:344:PRO:HD2  | 1.38                     | 1.24              |
| 1:A:391:PHE:CE2  | 1:A:411:MET:HE1  | 1.72                     | 1.22              |
| 1:D:572:LEU:O    | 1:D:572:LEU:HD12 | 1.38                     | 1.22              |
| 1:A:541:GLY:CA   | 1:A:542:ALA:HB3  | 1.70                     | 1.22              |
| 1:A:792:ASP:HB2  | 1:A:793:PRO:CD   | 1.68                     | 1.22              |
| 1:D:399:LYS:HD2  | 1:D:399:LYS:O    | 1.41                     | 1.20              |
| 1:A:339:PHE:HE1  | 1:A:364:MET:CE   | 1.53                     | 1.20              |
| 1:C:541:GLY:HA2  | 1:C:542:ALA:CB   | 1.66                     | 1.20              |
| 1:C:354:ASP:O    | 1:C:356:GLN:HA   | 1.40                     | 1.19              |
| 1:A:334:GLU:HB2  | 1:A:335:PRO:CD   | 1.72                     | 1.19              |
| 1:A:339:PHE:CE1  | 1:A:364:MET:CE   | 2.27                     | 1.17              |
| 1:D:537:ALA:O    | 1:D:541:GLY:CA   | 1.92                     | 1.16              |
| 1:C:396:THR:HG23 | 1:C:410:TYR:OH   | 1.43                     | 1.16              |
| 1:C:795:VAL:CB   | 1:C:796:LYS:HA   | 1.73                     | 1.15              |
| 1:D:400:LEU:HD12 | 1:D:410:TYR:HD2  | 1.13                     | 1.12              |
| 1:A:354:ASP:CB   | 1:A:355:TYR:HA   | 1.80                     | 1.11              |
| 1:C:396:THR:CG2  | 1:C:410:TYR:OH   | 1.97                     | 1.11              |
| 1:A:345:ARG:HG3  | 1:A:345:ARG:HH11 | 1.04                     | 1.10              |
| 1:C:506:GLU:OE2  | 1:C:567:VAL:HG23 | 1.49                     | 1.10              |
| 1:A:339:PHE:CE1  | 1:A:364:MET:HE3  | 1.87                     | 1.09              |
| 1:A:345:ARG:HH11 | 1:A:345:ARG:CG   | 1.66                     | 1.09              |
| 1:A:405:PRO:O    | 1:A:409:VAL:HG23 | 1.53                     | 1.09              |
| 1:A:340:GLU:HA   | 1:A:343:LEU:HD12 | 1.36                     | 1.07              |
| 1:C:544:SER:OG   | 1:C:546:THR:O    | 1.70                     | 1.07              |
| 1:B:353:GLN:N    | 1:B:354:ASP:HA   | 1.65                     | 1.07              |
| 1:A:354:ASP:CB   | 1:A:355:TYR:CA   | 2.32                     | 1.06              |
| 1:C:541:GLY:CA   | 1:C:542:ALA:HB3  | 1.83                     | 1.06              |
| 1:D:791:SER:HA   | 1:D:794:VAL:CG2  | 1.86                     | 1.05              |
| 1:A:391:PHE:HE2  | 1:A:411:MET:HE1  | 1.08                     | 1.05              |
| 1:A:340:GLU:CA   | 1:A:343:LEU:CD1  | 2.34                     | 1.04              |
| 1:C:795:VAL:CG2  | 1:C:796:LYS:CA   | 2.27                     | 1.04              |
| 1:A:392:ALA:O    | 1:A:396:THR:O    | 1.74                     | 1.04              |
| 1:A:340:GLU:HA   | 1:A:343:LEU:HD13 | 1.34                     | 1.04              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:355:TYR:CB   | 1:C:358:SER:N    | 2.20                     | 1.04              |
| 1:A:396:THR:OG1  | 1:A:398:GLU:HG3  | 1.56                     | 1.04              |
| 1:A:334:GLU:CB   | 1:A:335:PRO:HD2  | 1.89                     | 1.02              |
| 1:D:789:SER:CB   | 1:D:792:ASP:O    | 2.08                     | 1.02              |
| 1:A:792:ASP:HB2  | 1:A:793:PRO:HD3  | 1.07                     | 1.01              |
| 1:A:350:GLU:OE2  | 1:A:353:GLN:N    | 1.94                     | 1.00              |
| 1:B:410:TYR:O    | 1:B:414:THR:HG22 | 1.61                     | 1.00              |
| 1:C:795:VAL:CG2  | 1:C:796:LYS:CB   | 2.39                     | 1.00              |
| 1:D:537:ALA:O    | 1:D:541:GLY:HA2  | 1.58                     | 1.00              |
| 1:D:789:SER:HB3  | 1:D:792:ASP:CB   | 1.92                     | 0.99              |
| 1:C:795:VAL:HB   | 1:C:796:LYS:HA   | 1.43                     | 0.99              |
| 1:C:632:LEU:HD13 | 1:C:769:VAL:HG21 | 1.45                     | 0.98              |
| 1:D:791:SER:HA   | 1:D:794:VAL:HG21 | 1.42                     | 0.98              |
| 1:C:548:ILE:HG13 | 1:C:571:ALA:HB1  | 1.42                     | 0.98              |
| 1:B:435:THR:HG22 | 1:B:485:VAL:HG11 | 1.43                     | 0.97              |
| 1:D:435:THR:HG22 | 1:D:485:VAL:HG11 | 1.44                     | 0.97              |
| 1:A:340:GLU:CA   | 1:A:343:LEU:HD12 | 1.92                     | 0.97              |
| 1:A:509:LYS:HD3  | 1:A:569:ALA:HB2  | 1.43                     | 0.97              |
| 1:C:435:THR:HG22 | 1:C:485:VAL:HG11 | 1.45                     | 0.97              |
| 1:A:354:ASP:CB   | 1:A:355:TYR:C    | 2.38                     | 0.97              |
| 1:B:393:LEU:N    | 1:B:398:GLU:CB   | 2.28                     | 0.97              |
| 1:A:435:THR:HG22 | 1:A:485:VAL:HG11 | 1.44                     | 0.96              |
| 1:B:353:GLN:CB   | 1:B:354:ASP:C    | 2.39                     | 0.96              |
| 1:C:430:ARG:HH12 | 1:C:493:HIS:HD2  | 1.13                     | 0.96              |
| 1:C:354:ASP:C    | 1:C:356:GLN:HA   | 1.89                     | 0.96              |
| 1:A:567:VAL:HG13 | 1:A:571:ALA:HB3  | 1.46                     | 0.96              |
| 1:D:738:LEU:HA   | 1:D:741:MET:CE   | 1.96                     | 0.96              |
| 1:A:537:ALA:O    | 1:A:541:GLY:CA   | 2.13                     | 0.96              |
| 1:A:716:THR:OG1  | 1:A:719:ASP:OD1  | 1.84                     | 0.96              |
| 1:B:352:ILE:HG23 | 1:B:354:ASP:N    | 1.81                     | 0.96              |
| 1:A:334:GLU:HB2  | 1:A:335:PRO:HD2  | 0.96                     | 0.95              |
| 1:A:405:PRO:O    | 1:A:409:VAL:CG2  | 2.15                     | 0.94              |
| 1:D:790:SER:O    | 1:D:791:SER:HB2  | 1.66                     | 0.94              |
| 1:B:359:ASP:HA   | 1:B:362:GLU:OE2  | 1.67                     | 0.94              |
| 1:B:544:SER:OG   | 1:B:546:THR:O    | 1.83                     | 0.94              |
| 1:B:430:ARG:HH12 | 1:B:493:HIS:HD2  | 1.12                     | 0.94              |
| 1:A:339:PHE:HE1  | 1:A:364:MET:HE1  | 1.31                     | 0.93              |
| 1:D:572:LEU:HD12 | 1:D:572:LEU:C    | 1.90                     | 0.93              |
| 1:B:359:ASP:HA   | 1:B:362:GLU:CD   | 1.93                     | 0.93              |
| 1:D:430:ARG:HH12 | 1:D:493:HIS:HD2  | 1.11                     | 0.93              |
| 1:B:353:GLN:N    | 1:B:354:ASP:CA   | 2.31                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:399:LYS:HD2  | 1:D:399:LYS:C    | 1.93                     | 0.93              |
| 1:C:388:LEU:HG   | 1:C:411:MET:HE3  | 1.50                     | 0.93              |
| 1:C:506:GLU:OE2  | 1:C:567:VAL:CG2  | 2.16                     | 0.93              |
| 1:D:400:LEU:HD12 | 1:D:410:TYR:CD2  | 2.04                     | 0.92              |
| 1:B:352:ILE:HG23 | 1:B:354:ASP:CA   | 1.99                     | 0.92              |
| 1:C:794:VAL:O    | 1:C:795:VAL:HG22 | 1.70                     | 0.92              |
| 1:C:391:PHE:CE2  | 1:C:395:GLU:OE1  | 2.22                     | 0.92              |
| 1:A:345:ARG:HG3  | 1:A:345:ARG:NH1  | 1.78                     | 0.92              |
| 1:C:537:ALA:O    | 1:C:541:GLY:CA   | 2.17                     | 0.91              |
| 1:C:399:LYS:O    | 1:C:399:LYS:HG3  | 1.66                     | 0.91              |
| 1:A:790:SER:CB   | 1:A:794:VAL:CG2  | 2.47                     | 0.91              |
| 1:D:352:ILE:N    | 1:D:353:GLN:CB   | 2.32                     | 0.91              |
| 1:A:339:PHE:CZ   | 1:A:364:MET:HE3  | 2.06                     | 0.91              |
| 1:D:548:ILE:HG13 | 1:D:571:ALA:HB1  | 1.52                     | 0.90              |
| 1:A:430:ARG:HH12 | 1:A:493:HIS:HD2  | 1.13                     | 0.90              |
| 1:D:392:ALA:O    | 1:D:396:THR:O    | 1.90                     | 0.90              |
| 1:C:799:ASP:O    | 1:C:800:VAL:HG23 | 1.72                     | 0.89              |
| 1:B:430:ARG:HH12 | 1:B:493:HIS:CD2  | 1.90                     | 0.89              |
| 1:A:544:SER:OG   | 1:A:546:THR:O    | 1.91                     | 0.88              |
| 1:B:336:LEU:HG   | 1:B:340:GLU:HG3  | 1.55                     | 0.88              |
| 1:D:544:SER:OG   | 1:D:546:THR:O    | 1.93                     | 0.87              |
| 1:D:396:THR:HG1  | 1:D:410:TYR:HH   | 1.20                     | 0.87              |
| 1:D:537:ALA:O    | 1:D:541:GLY:HA3  | 1.72                     | 0.87              |
| 1:D:391:PHE:O    | 1:D:395:GLU:HG2  | 1.73                     | 0.87              |
| 1:C:347:VAL:O    | 1:C:351:LYS:HA   | 1.72                     | 0.86              |
| 1:A:525:ARG:HH22 | 1:A:588:GLY:H    | 1.23                     | 0.86              |
| 1:C:391:PHE:CZ   | 1:C:395:GLU:OE1  | 2.28                     | 0.86              |
| 1:C:410:TYR:O    | 1:C:414:THR:HG22 | 1.75                     | 0.86              |
| 1:A:339:PHE:O    | 1:A:343:LEU:HD12 | 1.73                     | 0.86              |
| 1:A:334:GLU:CB   | 1:A:335:PRO:CD   | 2.45                     | 0.85              |
| 1:A:391:PHE:CZ   | 1:A:395:GLU:OE2  | 2.30                     | 0.85              |
| 1:D:789:SER:HB2  | 1:D:792:ASP:N    | 1.90                     | 0.85              |
| 1:C:354:ASP:O    | 1:C:357:ASP:CA   | 2.21                     | 0.85              |
| 1:A:537:ALA:O    | 1:A:541:GLY:HA3  | 1.74                     | 0.85              |
| 1:A:548:ILE:HG13 | 1:A:571:ALA:HB1  | 1.56                     | 0.85              |
| 1:A:790:SER:HA   | 1:A:791:SER:C    | 2.02                     | 0.84              |
| 1:B:541:GLY:O    | 1:B:542:ALA:HB3  | 1.77                     | 0.84              |
| 1:B:392:ALA:O    | 1:B:396:THR:O    | 1.96                     | 0.84              |
| 1:C:541:GLY:HA2  | 1:C:542:ALA:HB3  | 0.87                     | 0.84              |
| 1:B:525:ARG:HH22 | 1:B:588:GLY:H    | 1.24                     | 0.84              |
| 1:B:391:PHE:HD2  | 1:B:411:MET:HE1  | 1.43                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:406:ASP:O    | 1:B:409:VAL:HG23 | 1.78                     | 0.84              |
| 1:C:430:ARG:HH12 | 1:C:493:HIS:CD2  | 1.96                     | 0.83              |
| 1:D:540:ALA:O    | 1:D:550:PRO:HB3  | 1.79                     | 0.83              |
| 1:A:537:ALA:O    | 1:A:541:GLY:N    | 2.11                     | 0.83              |
| 1:D:430:ARG:HH12 | 1:D:493:HIS:CD2  | 1.96                     | 0.83              |
| 1:C:591:ASN:HD21 | 1:C:795:VAL:HG21 | 1.44                     | 0.82              |
| 1:D:738:LEU:HA   | 1:D:741:MET:HE2  | 1.59                     | 0.82              |
| 1:D:794:VAL:HG23 | 1:D:794:VAL:O    | 1.80                     | 0.82              |
| 1:A:430:ARG:HH12 | 1:A:493:HIS:CD2  | 1.97                     | 0.81              |
| 1:C:348:MET:O    | 1:C:351:LYS:CB   | 2.28                     | 0.81              |
| 1:B:700:ARG:NH2  | 1:B:704:GLU:OE2  | 2.14                     | 0.81              |
| 1:D:391:PHE:O    | 1:D:395:GLU:CG   | 2.29                     | 0.81              |
| 1:D:392:ALA:CB   | 1:D:410:TYR:HE2  | 1.94                     | 0.81              |
| 1:B:391:PHE:CD2  | 1:B:411:MET:HE1  | 2.16                     | 0.80              |
| 1:A:792:ASP:HB2  | 1:A:793:PRO:HD2  | 1.64                     | 0.80              |
| 1:C:354:ASP:O    | 1:C:356:GLN:CA   | 2.27                     | 0.80              |
| 1:D:791:SER:HA   | 1:D:794:VAL:HG22 | 1.64                     | 0.80              |
| 1:C:525:ARG:HH22 | 1:C:588:GLY:H    | 1.30                     | 0.79              |
| 1:D:525:ARG:NH2  | 1:D:588:GLY:H    | 1.81                     | 0.79              |
| 1:A:395:GLU:HG2  | 1:A:553:ARG:NH2  | 1.97                     | 0.79              |
| 1:B:541:GLY:O    | 1:B:542:ALA:CB   | 2.31                     | 0.79              |
| 1:D:525:ARG:HH22 | 1:D:588:GLY:H    | 1.29                     | 0.79              |
| 1:C:794:VAL:O    | 1:C:795:VAL:CG2  | 2.31                     | 0.78              |
| 1:A:343:LEU:HA   | 1:A:346:VAL:HG12 | 1.65                     | 0.78              |
| 1:C:672:GLU:HG3  | 1:C:760:PRO:HG2  | 1.64                     | 0.78              |
| 1:C:347:VAL:O    | 1:C:351:LYS:CA   | 2.32                     | 0.78              |
| 1:C:631:GLY:C    | 1:C:632:LEU:HD23 | 2.09                     | 0.78              |
| 1:A:350:GLU:C    | 1:A:350:GLU:OE1  | 2.27                     | 0.78              |
| 1:A:525:ARG:NH2  | 1:A:588:GLY:H    | 1.80                     | 0.78              |
| 1:C:399:LYS:O    | 1:C:399:LYS:CG   | 2.30                     | 0.78              |
| 1:A:350:GLU:OE1  | 1:A:350:GLU:CA   | 2.31                     | 0.77              |
| 1:C:525:ARG:NH2  | 1:C:588:GLY:H    | 1.82                     | 0.77              |
| 1:D:392:ALA:HB1  | 1:D:410:TYR:HE2  | 1.48                     | 0.77              |
| 1:C:521:TRP:CE3  | 1:C:531:ILE:HG12 | 2.18                     | 0.77              |
| 1:C:799:ASP:C    | 1:C:800:VAL:HG23 | 2.07                     | 0.77              |
| 1:B:525:ARG:NH2  | 1:B:588:GLY:H    | 1.83                     | 0.77              |
| 1:D:521:TRP:CE3  | 1:D:531:ILE:HG12 | 2.19                     | 0.77              |
| 1:D:789:SER:CB   | 1:D:792:ASP:CB   | 2.63                     | 0.77              |
| 1:D:570:GLU:HG2  | 1:D:574:LYS:HE2  | 1.67                     | 0.77              |
| 1:A:521:TRP:CE3  | 1:A:531:ILE:HG12 | 2.20                     | 0.77              |
| 1:B:631:GLY:HA3  | 1:B:762:PHE:HZ   | 1.50                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:355:TYR:CB   | 1:C:358:SER:CA   | 2.63                     | 0.76              |
| 1:B:356:GLN:O    | 1:B:358:SER:N    | 2.18                     | 0.76              |
| 1:B:353:GLN:H    | 1:B:354:ASP:HA   | 1.46                     | 0.76              |
| 1:A:346:VAL:HA   | 1:A:415:PHE:HE2  | 1.51                     | 0.76              |
| 1:B:352:ILE:HD13 | 1:B:354:ASP:CB   | 2.16                     | 0.76              |
| 1:B:521:TRP:CE3  | 1:B:531:ILE:HG12 | 2.20                     | 0.76              |
| 1:D:789:SER:O    | 1:D:792:ASP:CB   | 2.34                     | 0.76              |
| 1:B:353:GLN:CB   | 1:B:355:TYR:N    | 2.49                     | 0.76              |
| 1:C:354:ASP:C    | 1:C:356:GLN:CA   | 2.59                     | 0.75              |
| 1:A:343:LEU:HA   | 1:A:346:VAL:CG1  | 2.16                     | 0.75              |
| 1:A:355:TYR:O    | 1:A:358:SER:CB   | 2.35                     | 0.75              |
| 1:C:350:GLU:N    | 1:C:351:LYS:HA   | 2.00                     | 0.75              |
| 1:C:537:ALA:O    | 1:C:541:GLY:HA3  | 1.87                     | 0.75              |
| 1:C:355:TYR:CB   | 1:C:358:SER:CB   | 2.65                     | 0.74              |
| 1:B:392:ALA:C    | 1:B:398:GLU:CB   | 2.59                     | 0.74              |
| 1:C:799:ASP:O    | 1:C:800:VAL:CG2  | 2.35                     | 0.74              |
| 1:A:430:ARG:NH1  | 1:A:493:HIS:HD2  | 1.86                     | 0.74              |
| 1:A:722:SER:O    | 1:A:726:SER:HB2  | 1.87                     | 0.74              |
| 1:C:701:PRO:HB2  | 1:C:703:THR:HG22 | 1.69                     | 0.74              |
| 1:C:738:LEU:HA   | 1:C:741:MET:HE2  | 1.68                     | 0.74              |
| 1:A:672:GLU:HG3  | 1:A:760:PRO:HG2  | 1.69                     | 0.74              |
| 1:D:701:PRO:HB2  | 1:D:703:THR:HG22 | 1.68                     | 0.74              |
| 1:A:396:THR:OG1  | 1:A:398:GLU:CG   | 2.34                     | 0.74              |
| 1:B:700:ARG:NE   | 1:B:704:GLU:OE1  | 2.20                     | 0.73              |
| 1:B:406:ASP:O    | 1:B:409:VAL:CG2  | 2.36                     | 0.73              |
| 1:A:509:LYS:CD   | 1:A:569:ALA:HB2  | 2.18                     | 0.73              |
| 1:B:542:ALA:C    | 1:B:543:ASP:OD1  | 2.31                     | 0.73              |
| 1:C:567:VAL:O    | 1:C:571:ALA:HB3  | 1.89                     | 0.73              |
| 1:C:790:SER:CB   | 1:C:794:VAL:HA   | 2.18                     | 0.73              |
| 1:A:701:PRO:HB2  | 1:A:703:THR:HG22 | 1.70                     | 0.73              |
| 1:B:339:PHE:CE1  | 1:B:364:MET:CE   | 2.72                     | 0.73              |
| 1:C:334:GLU:H    | 1:C:334:GLU:CD   | 1.97                     | 0.73              |
| 1:A:486:ARG:HH21 | 1:A:553:ARG:HA   | 1.53                     | 0.73              |
| 1:C:548:ILE:HG13 | 1:C:571:ALA:CB   | 2.17                     | 0.72              |
| 1:D:410:TYR:O    | 1:D:414:THR:HG22 | 1.89                     | 0.72              |
| 1:D:339:PHE:CE1  | 1:D:364:MET:CE   | 2.73                     | 0.72              |
| 1:A:792:ASP:CB   | 1:A:793:PRO:CD   | 2.34                     | 0.72              |
| 1:B:486:ARG:HH21 | 1:B:553:ARG:HA   | 1.53                     | 0.72              |
| 1:D:385:ARG:NH1  | 1:D:402:LYS:HG2  | 2.04                     | 0.72              |
| 1:C:541:GLY:CA   | 1:C:542:ALA:CB   | 2.50                     | 0.72              |
| 1:A:706:LYS:HE3  | 1:A:752:GLY:O    | 1.89                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:672:GLU:HG3  | 1:B:760:PRO:HG2  | 1.70                     | 0.71              |
| 1:A:386:ASP:O    | 1:A:389:VAL:HG12 | 1.90                     | 0.71              |
| 1:B:631:GLY:HA3  | 1:B:762:PHE:CZ   | 2.24                     | 0.71              |
| 1:C:722:SER:O    | 1:C:726:SER:HB2  | 1.91                     | 0.71              |
| 1:D:672:GLU:HG3  | 1:D:760:PRO:HG2  | 1.70                     | 0.71              |
| 1:B:352:ILE:HG23 | 1:B:354:ASP:CB   | 2.19                     | 0.71              |
| 1:A:385:ARG:NH1  | 1:A:402:LYS:HG2  | 2.05                     | 0.71              |
| 1:C:347:VAL:HG13 | 1:C:351:LYS:O    | 1.91                     | 0.71              |
| 1:C:486:ARG:HH21 | 1:C:553:ARG:HA   | 1.56                     | 0.71              |
| 1:C:354:ASP:C    | 1:C:356:GLN:CB   | 2.63                     | 0.71              |
| 1:C:385:ARG:NH1  | 1:C:402:LYS:HG2  | 2.05                     | 0.71              |
| 1:D:789:SER:HB2  | 1:D:792:ASP:O    | 1.90                     | 0.70              |
| 1:D:572:LEU:C    | 1:D:572:LEU:CD1  | 2.64                     | 0.70              |
| 1:D:738:LEU:HD23 | 1:D:741:MET:HE1  | 1.73                     | 0.70              |
| 1:A:339:PHE:O    | 1:A:343:LEU:CD1  | 2.40                     | 0.70              |
| 1:A:350:GLU:OE1  | 1:A:350:GLU:HA   | 1.90                     | 0.70              |
| 1:B:386:ASP:O    | 1:B:389:VAL:HG12 | 1.92                     | 0.70              |
| 1:A:631:GLY:HA3  | 1:A:762:PHE:HZ   | 1.56                     | 0.70              |
| 1:C:355:TYR:CB   | 1:C:358:SER:H    | 2.01                     | 0.70              |
| 1:C:797:VAL:CG1  | 1:C:798:ASP:N    | 2.55                     | 0.70              |
| 1:B:789:SER:OG   | 1:B:794:VAL:HG23 | 1.92                     | 0.70              |
| 1:C:386:ASP:O    | 1:C:389:VAL:HG12 | 1.90                     | 0.69              |
| 1:A:391:PHE:HE2  | 1:A:411:MET:CE   | 1.96                     | 0.69              |
| 1:D:343:LEU:O    | 1:D:346:VAL:HG12 | 1.92                     | 0.69              |
| 1:D:410:TYR:O    | 1:D:410:TYR:HD1  | 1.75                     | 0.69              |
| 1:D:386:ASP:O    | 1:D:389:VAL:HG12 | 1.92                     | 0.69              |
| 1:B:567:VAL:O    | 1:B:571:ALA:HB3  | 1.91                     | 0.69              |
| 1:D:430:ARG:NH1  | 1:D:493:HIS:HD2  | 1.87                     | 0.69              |
| 1:D:486:ARG:HH21 | 1:D:553:ARG:HA   | 1.57                     | 0.69              |
| 1:A:541:GLY:HA2  | 1:A:542:ALA:HB3  | 0.73                     | 0.69              |
| 1:A:567:VAL:HG13 | 1:A:571:ALA:CB   | 2.23                     | 0.69              |
| 1:B:385:ARG:NH1  | 1:B:402:LYS:HG2  | 2.07                     | 0.68              |
| 1:D:400:LEU:CD1  | 1:D:410:TYR:HD2  | 2.00                     | 0.68              |
| 1:A:430:ARG:NH1  | 1:A:493:HIS:CD2  | 2.61                     | 0.68              |
| 1:C:430:ARG:NH1  | 1:C:493:HIS:CD2  | 2.61                     | 0.68              |
| 1:B:430:ARG:NH1  | 1:B:493:HIS:CD2  | 2.61                     | 0.68              |
| 1:C:430:ARG:NH1  | 1:C:493:HIS:HD2  | 1.87                     | 0.68              |
| 1:C:799:ASP:O    | 1:C:800:VAL:CB   | 2.41                     | 0.68              |
| 1:D:350:GLU:CB   | 1:D:351:LYS:HA   | 2.24                     | 0.68              |
| 1:D:392:ALA:CB   | 1:D:410:TYR:CE2  | 2.76                     | 0.68              |
| 1:B:632:LEU:HG   | 1:B:769:VAL:HG21 | 1.75                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:789:SER:HB3  | 1:D:792:ASP:O    | 1.90                     | 0.68              |
| 1:A:790:SER:CB   | 1:A:794:VAL:CA   | 2.71                     | 0.67              |
| 1:D:361:HIS:O    | 1:D:365:LYS:N    | 2.27                     | 0.67              |
| 1:C:632:LEU:CD1  | 1:C:769:VAL:HG21 | 2.22                     | 0.67              |
| 1:A:542:ALA:C    | 1:A:543:ASP:OD1  | 2.37                     | 0.67              |
| 1:A:340:GLU:HA   | 1:A:343:LEU:HD11 | 1.67                     | 0.67              |
| 1:A:354:ASP:CB   | 1:A:358:SER:H    | 2.08                     | 0.67              |
| 1:B:400:LEU:HD23 | 1:B:401:SER:O    | 1.94                     | 0.66              |
| 1:A:354:ASP:CB   | 1:A:358:SER:N    | 2.59                     | 0.66              |
| 1:D:405:PRO:O    | 1:D:409:VAL:CG2  | 2.43                     | 0.66              |
| 1:D:621:HIS:CE1  | 1:D:642:SER:HB3  | 2.30                     | 0.66              |
| 1:C:347:VAL:O    | 1:C:351:LYS:C    | 2.39                     | 0.66              |
| 1:C:797:VAL:HG13 | 1:C:798:ASP:N    | 2.10                     | 0.66              |
| 1:A:400:LEU:HD23 | 1:A:401:SER:O    | 1.95                     | 0.66              |
| 1:B:343:LEU:O    | 1:B:346:VAL:HG12 | 1.96                     | 0.66              |
| 1:B:632:LEU:HD13 | 1:B:632:LEU:N    | 2.11                     | 0.65              |
| 1:A:334:GLU:CA   | 1:A:334:GLU:OE1  | 2.42                     | 0.65              |
| 1:A:631:GLY:HA3  | 1:A:762:PHE:CZ   | 2.31                     | 0.65              |
| 1:D:430:ARG:NH1  | 1:D:493:HIS:CD2  | 2.62                     | 0.65              |
| 1:A:343:LEU:CA   | 1:A:346:VAL:HG12 | 2.27                     | 0.65              |
| 1:C:400:LEU:HD23 | 1:C:401:SER:O    | 1.97                     | 0.65              |
| 1:C:405:PRO:HA   | 1:C:408:ARG:HG3  | 1.77                     | 0.65              |
| 1:D:540:ALA:HB3  | 1:D:541:GLY:HA2  | 1.78                     | 0.65              |
| 1:B:548:ILE:HG13 | 1:B:571:ALA:HB1  | 1.79                     | 0.65              |
| 1:A:400:LEU:HD12 | 1:A:410:TYR:CG   | 2.32                     | 0.64              |
| 1:D:359:ASP:O    | 1:D:362:GLU:N    | 2.29                     | 0.64              |
| 1:D:405:PRO:O    | 1:D:409:VAL:HG22 | 1.97                     | 0.64              |
| 1:A:706:LYS:CE   | 1:A:752:GLY:O    | 2.45                     | 0.64              |
| 1:C:568:ASP:OD1  | 1:C:569:ALA:N    | 2.29                     | 0.64              |
| 1:C:336:LEU:HG   | 1:C:340:GLU:HG3  | 1.79                     | 0.64              |
| 1:D:391:PHE:CD2  | 1:D:395:GLU:OE2  | 2.27                     | 0.64              |
| 1:D:400:LEU:HD23 | 1:D:401:SER:O    | 1.97                     | 0.64              |
| 1:C:393:LEU:HA   | 1:C:397:GLY:HA2  | 1.80                     | 0.64              |
| 1:D:406:ASP:C    | 1:D:409:VAL:HG23 | 2.22                     | 0.64              |
| 1:D:789:SER:HB2  | 1:D:792:ASP:H    | 1.63                     | 0.63              |
| 1:A:356:GLN:CB   | 1:B:359:ASP:OD2  | 2.45                     | 0.63              |
| 1:A:410:TYR:CD1  | 1:A:410:TYR:C    | 2.77                     | 0.63              |
| 1:B:339:PHE:HE1  | 1:B:364:MET:CE   | 2.11                     | 0.63              |
| 1:D:487:PHE:CE2  | 1:D:568:ASP:HB3  | 2.32                     | 0.63              |
| 1:D:722:SER:O    | 1:D:726:SER:HB2  | 1.98                     | 0.63              |
| 1:A:345:ARG:CG   | 1:A:345:ARG:NH1  | 2.37                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:355:TYR:O    | 1:A:358:SER:N    | 2.29                     | 0.63              |
| 1:C:410:TYR:HA   | 1:C:413:ASP:HB2  | 1.79                     | 0.63              |
| 1:D:789:SER:C    | 1:D:792:ASP:H    | 2.07                     | 0.63              |
| 1:A:621:HIS:CE1  | 1:A:642:SER:HB3  | 2.33                     | 0.63              |
| 1:C:790:SER:O    | 1:C:794:VAL:N    | 2.32                     | 0.63              |
| 1:C:797:VAL:CG1  | 1:C:798:ASP:O    | 2.47                     | 0.63              |
| 1:A:593:ALA:HB3  | 1:A:794:VAL:HG21 | 1.81                     | 0.62              |
| 1:D:570:GLU:CG   | 1:D:574:LYS:HE2  | 2.29                     | 0.62              |
| 1:B:790:SER:O    | 1:B:792:ASP:N    | 2.32                     | 0.62              |
| 1:B:388:LEU:HG   | 1:B:411:MET:HE3  | 1.79                     | 0.62              |
| 1:B:570:GLU:CB   | 1:B:574:LYS:HE2  | 2.29                     | 0.62              |
| 1:C:388:LEU:HG   | 1:C:411:MET:CE   | 2.25                     | 0.62              |
| 1:D:410:TYR:CE1  | 1:D:414:THR:HG21 | 2.35                     | 0.62              |
| 1:D:632:LEU:HD13 | 1:D:769:VAL:HG21 | 1.80                     | 0.62              |
| 1:B:749:ARG:HH11 | 1:B:749:ARG:HB3  | 1.64                     | 0.62              |
| 1:C:396:THR:HG21 | 1:C:410:TYR:CE1  | 2.34                     | 0.62              |
| 1:A:343:LEU:O    | 1:A:346:VAL:CG1  | 2.48                     | 0.62              |
| 1:D:592:LEU:HD23 | 1:D:788:ASP:HB2  | 1.81                     | 0.62              |
| 1:A:340:GLU:O    | 1:A:344:PRO:CD   | 2.31                     | 0.62              |
| 1:A:791:SER:O    | 1:A:792:ASP:C    | 2.42                     | 0.61              |
| 1:D:791:SER:C    | 1:D:794:VAL:HG13 | 2.25                     | 0.61              |
| 1:C:537:ALA:O    | 1:C:541:GLY:N    | 2.33                     | 0.61              |
| 1:D:567:VAL:HG12 | 1:D:568:ASP:N    | 2.14                     | 0.61              |
| 1:A:334:GLU:OE1  | 1:A:334:GLU:N    | 2.33                     | 0.61              |
| 1:A:521:TRP:CH2  | 1:A:529:GLY:O    | 2.53                     | 0.61              |
| 1:B:521:TRP:CH2  | 1:B:529:GLY:O    | 2.53                     | 0.61              |
| 1:C:749:ARG:HH11 | 1:C:749:ARG:HB3  | 1.64                     | 0.61              |
| 1:A:794:VAL:HG13 | 1:A:794:VAL:O    | 2.00                     | 0.61              |
| 1:B:352:ILE:C    | 1:B:354:ASP:HA   | 2.26                     | 0.61              |
| 1:C:663:GLN:HE21 | 1:C:681:HIS:HE1  | 1.49                     | 0.61              |
| 1:D:462:THR:HG21 | 1:D:508:GLU:OE2  | 2.01                     | 0.61              |
| 1:A:539:MET:SD   | 1:A:551:LEU:HD22 | 2.40                     | 0.61              |
| 1:C:395:GLU:HG2  | 1:C:553:ARG:HH22 | 1.66                     | 0.60              |
| 1:A:340:GLU:C    | 1:A:343:LEU:HD12 | 2.25                     | 0.60              |
| 1:C:396:THR:CG2  | 1:C:410:TYR:CZ   | 2.84                     | 0.60              |
| 1:C:521:TRP:CH2  | 1:C:529:GLY:O    | 2.53                     | 0.60              |
| 1:C:790:SER:HA   | 1:C:793:PRO:C    | 2.26                     | 0.60              |
| 1:A:343:LEU:O    | 1:A:346:VAL:HG12 | 2.01                     | 0.60              |
| 1:C:550:PRO:HD3  | 1:C:555:TRP:CH2  | 2.36                     | 0.60              |
| 1:D:339:PHE:HE1  | 1:D:364:MET:CE   | 2.14                     | 0.60              |
| 1:C:521:TRP:HH2  | 1:C:529:GLY:O    | 1.85                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:407:GLN:O    | 1:B:409:VAL:O    | 2.19                     | 0.59              |
| 1:C:355:TYR:N    | 1:C:356:GLN:CA   | 2.65                     | 0.59              |
| 1:B:391:PHE:O    | 1:B:395:GLU:HG2  | 2.02                     | 0.59              |
| 1:C:539:MET:SD   | 1:C:551:LEU:HD22 | 2.41                     | 0.59              |
| 1:D:572:LEU:CD1  | 1:D:576:LEU:HD22 | 2.32                     | 0.59              |
| 1:A:558:PRO:O    | 1:A:559:ASP:HB3  | 2.02                     | 0.59              |
| 1:D:521:TRP:HH2  | 1:D:529:GLY:O    | 1.85                     | 0.59              |
| 1:D:794:VAL:CG2  | 1:D:794:VAL:O    | 2.50                     | 0.59              |
| 1:A:354:ASP:CB   | 1:A:355:TYR:O    | 2.50                     | 0.59              |
| 1:D:521:TRP:CH2  | 1:D:529:GLY:O    | 2.54                     | 0.59              |
| 1:A:749:ARG:HH11 | 1:A:749:ARG:HB3  | 1.67                     | 0.59              |
| 1:B:722:SER:O    | 1:B:726:SER:HB2  | 2.03                     | 0.59              |
| 1:D:789:SER:CB   | 1:D:792:ASP:CA   | 2.80                     | 0.59              |
| 1:C:395:GLU:HG2  | 1:C:553:ARG:NH2  | 2.16                     | 0.59              |
| 1:B:462:THR:HG21 | 1:B:508:GLU:OE2  | 2.02                     | 0.59              |
| 1:B:500:ARG:O    | 1:B:504:VAL:HG23 | 2.02                     | 0.59              |
| 1:B:521:TRP:HH2  | 1:B:529:GLY:O    | 1.84                     | 0.59              |
| 1:D:339:PHE:HE1  | 1:D:364:MET:HE1  | 1.68                     | 0.59              |
| 1:C:462:THR:HG21 | 1:C:508:GLU:OE2  | 2.02                     | 0.59              |
| 1:D:500:ARG:O    | 1:D:504:VAL:HG23 | 2.03                     | 0.58              |
| 1:D:789:SER:CB   | 1:D:792:ASP:C    | 2.75                     | 0.58              |
| 1:C:342:PHE:CZ   | 1:C:346:VAL:HG23 | 2.38                     | 0.58              |
| 1:C:405:PRO:O    | 1:C:409:VAL:HG23 | 2.03                     | 0.58              |
| 1:C:789:SER:O    | 1:C:792:ASP:N    | 2.35                     | 0.58              |
| 1:D:352:ILE:HA   | 1:D:353:GLN:C    | 2.28                     | 0.58              |
| 1:D:789:SER:HB2  | 1:D:792:ASP:CA   | 2.33                     | 0.58              |
| 1:D:399:LYS:C    | 1:D:399:LYS:CD   | 2.74                     | 0.58              |
| 1:D:548:ILE:HG13 | 1:D:571:ALA:CB   | 2.27                     | 0.58              |
| 1:D:663:GLN:HE21 | 1:D:681:HIS:HE1  | 1.51                     | 0.58              |
| 1:A:395:GLU:HG2  | 1:A:553:ARG:HH21 | 1.69                     | 0.58              |
| 1:A:508:GLU:HA   | 1:A:511:ILE:HG22 | 1.85                     | 0.58              |
| 1:D:539:MET:SD   | 1:D:551:LEU:HD22 | 2.44                     | 0.58              |
| 1:C:405:PRO:O    | 1:C:409:VAL:CG2  | 2.52                     | 0.58              |
| 1:B:558:PRO:O    | 1:B:559:ASP:HB3  | 2.03                     | 0.58              |
| 1:C:558:PRO:O    | 1:C:559:ASP:HB3  | 2.02                     | 0.58              |
| 1:A:391:PHE:CE1  | 1:A:395:GLU:OE2  | 2.56                     | 0.58              |
| 1:A:521:TRP:HH2  | 1:A:529:GLY:O    | 1.85                     | 0.58              |
| 1:B:393:LEU:CA   | 1:B:398:GLU:CB   | 2.81                     | 0.58              |
| 1:B:508:GLU:HA   | 1:B:511:ILE:HG22 | 1.86                     | 0.58              |
| 1:A:545:LEU:HD13 | 1:A:545:LEU:N    | 2.18                     | 0.57              |
| 1:A:508:GLU:O    | 1:A:511:ILE:HG22 | 2.04                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:749:ARG:HB3  | 1:D:749:ARG:HH11 | 1.69                     | 0.57              |
| 1:D:762:PHE:HD2  | 1:D:763:MET:CE   | 2.17                     | 0.57              |
| 1:C:500:ARG:O    | 1:C:504:VAL:HG23 | 2.04                     | 0.57              |
| 1:A:443:TRP:O    | 1:A:451:ARG:NH1  | 2.33                     | 0.57              |
| 1:A:462:THR:HG21 | 1:A:508:GLU:OE2  | 2.03                     | 0.57              |
| 1:B:410:TYR:HA   | 1:B:413:ASP:HB2  | 1.87                     | 0.57              |
| 1:D:391:PHE:O    | 1:D:395:GLU:HG3  | 2.05                     | 0.57              |
| 1:D:443:TRP:O    | 1:D:451:ARG:NH1  | 2.36                     | 0.57              |
| 1:D:791:SER:CA   | 1:D:794:VAL:HG22 | 2.33                     | 0.57              |
| 1:B:663:GLN:HE21 | 1:B:681:HIS:HE1  | 1.51                     | 0.57              |
| 1:B:795:VAL:HG22 | 1:B:797:VAL:HG23 | 1.86                     | 0.57              |
| 1:D:570:GLU:HB3  | 1:D:574:LYS:HE2  | 1.87                     | 0.57              |
| 1:B:508:GLU:O    | 1:B:511:ILE:HG22 | 2.03                     | 0.57              |
| 1:D:558:PRO:O    | 1:D:559:ASP:HB3  | 2.03                     | 0.57              |
| 1:C:591:ASN:HD21 | 1:C:795:VAL:CG2  | 2.17                     | 0.57              |
| 1:C:443:TRP:O    | 1:C:451:ARG:NH1  | 2.36                     | 0.57              |
| 1:D:704:GLU:HG2  | 1:D:729:PHE:CE2  | 2.39                     | 0.57              |
| 1:B:428:TYR:HD1  | 1:B:429:LEU:HD12 | 1.70                     | 0.57              |
| 1:D:508:GLU:O    | 1:D:511:ILE:HG22 | 2.04                     | 0.56              |
| 1:B:355:TYR:CB   | 1:B:361:HIS:CE1  | 2.89                     | 0.56              |
| 1:C:428:TYR:HD1  | 1:C:429:LEU:HD12 | 1.70                     | 0.56              |
| 1:C:508:GLU:HA   | 1:C:511:ILE:HG22 | 1.87                     | 0.56              |
| 1:C:545:LEU:N    | 1:C:545:LEU:HD13 | 2.20                     | 0.56              |
| 1:C:568:ASP:CG   | 1:C:569:ALA:N    | 2.63                     | 0.56              |
| 1:C:568:ASP:HA   | 1:C:572:LEU:H    | 1.70                     | 0.56              |
| 1:D:572:LEU:HD11 | 1:D:576:LEU:HD22 | 1.86                     | 0.56              |
| 1:B:762:PHE:HD2  | 1:B:763:MET:CE   | 2.18                     | 0.56              |
| 1:D:391:PHE:CD2  | 1:D:411:MET:HE1  | 2.41                     | 0.56              |
| 1:D:396:THR:OG1  | 1:D:410:TYR:OH   | 2.01                     | 0.56              |
| 1:D:508:GLU:HA   | 1:D:511:ILE:HG22 | 1.88                     | 0.56              |
| 1:A:431:HIS:O    | 1:A:435:THR:HG23 | 2.06                     | 0.56              |
| 1:A:447:ASN:C    | 1:A:447:ASN:HD22 | 2.12                     | 0.56              |
| 1:A:539:MET:SD   | 1:A:551:LEU:CD2  | 2.94                     | 0.56              |
| 1:C:794:VAL:C    | 1:C:795:VAL:HG22 | 2.29                     | 0.56              |
| 1:D:358:SER:O    | 1:D:361:HIS:CB   | 2.54                     | 0.56              |
| 1:A:348:MET:HE3  | 1:D:627:PRO:HB2  | 1.86                     | 0.56              |
| 1:A:391:PHE:CZ   | 1:A:395:GLU:CD   | 2.85                     | 0.56              |
| 1:C:797:VAL:HG13 | 1:C:798:ASP:O    | 2.06                     | 0.56              |
| 1:D:799:ASP:OD1  | 1:D:799:ASP:N    | 2.31                     | 0.56              |
| 1:D:545:LEU:HD13 | 1:D:545:LEU:N    | 2.21                     | 0.55              |
| 1:C:395:GLU:HG3  | 1:C:431:HIS:HD2  | 1.70                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:508:GLU:O    | 1:C:511:ILE:HG22 | 2.06                     | 0.55              |
| 1:A:343:LEU:C    | 1:A:346:VAL:HG12 | 2.32                     | 0.55              |
| 1:A:663:GLN:HE21 | 1:A:681:HIS:HE1  | 1.53                     | 0.55              |
| 1:A:447:ASN:O    | 1:A:447:ASN:ND2  | 2.37                     | 0.55              |
| 1:B:443:TRP:O    | 1:B:451:ARG:NH1  | 2.35                     | 0.55              |
| 1:C:631:GLY:O    | 1:C:632:LEU:HD23 | 2.07                     | 0.55              |
| 1:B:339:PHE:CZ   | 1:B:364:MET:HE3  | 2.41                     | 0.55              |
| 1:A:334:GLU:OE1  | 1:A:334:GLU:C    | 2.49                     | 0.55              |
| 1:C:670:ASP:OD2  | 1:C:672:GLU:HB2  | 2.06                     | 0.55              |
| 1:D:339:PHE:CZ   | 1:D:364:MET:HE3  | 2.41                     | 0.55              |
| 1:D:670:ASP:OD2  | 1:D:672:GLU:HB2  | 2.07                     | 0.55              |
| 1:B:670:ASP:OD2  | 1:B:672:GLU:HB2  | 2.07                     | 0.55              |
| 1:B:447:ASN:O    | 1:B:447:ASN:ND2  | 2.38                     | 0.54              |
| 1:D:789:SER:OG   | 1:D:792:ASP:O    | 2.25                     | 0.54              |
| 1:C:621:HIS:CE1  | 1:C:642:SER:HB3  | 2.42                     | 0.54              |
| 1:B:388:LEU:HG   | 1:B:411:MET:CE   | 2.37                     | 0.54              |
| 1:C:799:ASP:O    | 1:C:800:VAL:HB   | 2.05                     | 0.54              |
| 1:D:428:TYR:HD1  | 1:D:429:LEU:HD12 | 1.73                     | 0.54              |
| 1:B:339:PHE:CE1  | 1:B:364:MET:HE3  | 2.42                     | 0.54              |
| 1:B:539:MET:SD   | 1:B:551:LEU:HD22 | 2.47                     | 0.54              |
| 1:B:545:LEU:HD13 | 1:B:545:LEU:N    | 2.21                     | 0.54              |
| 1:D:613:ARG:HB2  | 1:D:657:ILE:HD11 | 1.90                     | 0.54              |
| 1:A:500:ARG:O    | 1:A:504:VAL:HG23 | 2.07                     | 0.54              |
| 1:C:407:GLN:O    | 1:C:409:VAL:O    | 2.26                     | 0.54              |
| 1:D:351:LYS:N    | 1:D:353:GLN:CB   | 2.71                     | 0.54              |
| 1:A:550:PRO:HD3  | 1:A:555:TRP:CH2  | 2.43                     | 0.54              |
| 1:B:340:GLU:O    | 1:B:344:PRO:HD2  | 2.08                     | 0.54              |
| 1:B:359:ASP:O    | 1:B:360:ALA:C    | 2.49                     | 0.54              |
| 1:A:346:VAL:HA   | 1:A:415:PHE:CE2  | 2.38                     | 0.54              |
| 1:A:377:GLY:O    | 1:A:381:GLN:HG2  | 2.08                     | 0.54              |
| 1:A:670:ASP:OD2  | 1:A:672:GLU:HB2  | 2.08                     | 0.54              |
| 1:C:342:PHE:CE2  | 1:C:346:VAL:HG23 | 2.44                     | 0.53              |
| 1:C:762:PHE:HD2  | 1:C:763:MET:CE   | 2.21                     | 0.53              |
| 1:D:340:GLU:O    | 1:D:344:PRO:HD2  | 2.08                     | 0.53              |
| 1:C:431:HIS:O    | 1:C:435:THR:HG23 | 2.08                     | 0.53              |
| 1:C:447:ASN:O    | 1:C:447:ASN:ND2  | 2.41                     | 0.53              |
| 1:B:431:HIS:O    | 1:B:435:THR:HG23 | 2.08                     | 0.53              |
| 1:D:431:HIS:O    | 1:D:435:THR:HG23 | 2.07                     | 0.53              |
| 1:A:352:ILE:O    | 1:D:637:LYS:HG2  | 2.09                     | 0.53              |
| 1:B:570:GLU:O    | 1:B:574:LYS:N    | 2.37                     | 0.53              |
| 1:B:550:PRO:HD3  | 1:B:555:TRP:CH2  | 2.44                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:509:LYS:NZ   | 1:A:569:ALA:HB1  | 2.24                     | 0.53              |
| 1:C:395:GLU:HG3  | 1:C:431:HIS:CD2  | 2.43                     | 0.53              |
| 1:D:550:PRO:HD3  | 1:D:555:TRP:CH2  | 2.43                     | 0.53              |
| 1:A:762:PHE:HD2  | 1:A:763:MET:CE   | 2.20                     | 0.53              |
| 1:C:568:ASP:OD1  | 1:C:569:ALA:HA   | 2.09                     | 0.53              |
| 1:D:447:ASN:ND2  | 1:D:447:ASN:O    | 2.39                     | 0.53              |
| 1:B:789:SER:HB2  | 1:B:792:ASP:O    | 2.09                     | 0.53              |
| 1:B:356:GLN:C    | 1:B:358:SER:N    | 2.60                     | 0.53              |
| 1:B:377:GLY:O    | 1:B:381:GLN:HG2  | 2.09                     | 0.53              |
| 1:B:524:THR:CG2  | 1:B:525:ARG:NH1  | 2.72                     | 0.53              |
| 1:A:411:MET:HE3  | 1:A:428:TYR:OH   | 2.09                     | 0.52              |
| 1:A:541:GLY:CA   | 1:A:542:ALA:CB   | 2.40                     | 0.52              |
| 1:B:341:THR:HG21 | 1:B:408:ARG:HD3  | 1.91                     | 0.52              |
| 1:D:406:ASP:O    | 1:D:409:VAL:HG23 | 2.09                     | 0.52              |
| 1:A:428:TYR:HD1  | 1:A:429:LEU:HD12 | 1.73                     | 0.52              |
| 1:C:568:ASP:OD1  | 1:C:569:ALA:CA   | 2.57                     | 0.52              |
| 1:A:339:PHE:C    | 1:A:343:LEU:HD12 | 2.33                     | 0.52              |
| 1:D:789:SER:HB2  | 1:D:792:ASP:C    | 2.34                     | 0.52              |
| 1:A:509:LYS:CE   | 1:A:569:ALA:CB   | 2.87                     | 0.52              |
| 1:A:486:ARG:NH2  | 1:A:553:ARG:HA   | 2.24                     | 0.52              |
| 1:C:790:SER:CA   | 1:C:794:VAL:HA   | 2.40                     | 0.52              |
| 1:A:672:GLU:HA   | 1:A:672:GLU:OE1  | 2.09                     | 0.52              |
| 1:D:509:LYS:HD3  | 1:D:569:ALA:HA   | 1.90                     | 0.52              |
| 1:A:593:ALA:CB   | 1:A:794:VAL:HG21 | 2.40                     | 0.52              |
| 1:C:428:TYR:HD1  | 1:C:429:LEU:CD1  | 2.22                     | 0.51              |
| 1:C:486:ARG:NH2  | 1:C:553:ARG:HA   | 2.25                     | 0.51              |
| 1:D:399:LYS:O    | 1:D:399:LYS:CD   | 2.35                     | 0.51              |
| 1:A:621:HIS:HE1  | 1:A:642:SER:HB3  | 1.75                     | 0.51              |
| 1:C:381:GLN:O    | 1:C:385:ARG:HG2  | 2.11                     | 0.51              |
| 1:B:713:GLY:O    | 1:B:749:ARG:HD2  | 2.09                     | 0.51              |
| 1:D:789:SER:CB   | 1:D:792:ASP:N    | 2.70                     | 0.51              |
| 1:A:360:ALA:CB   | 1:A:429:LEU:HD23 | 2.41                     | 0.51              |
| 1:B:428:TYR:CD1  | 1:B:429:LEU:HD12 | 2.45                     | 0.51              |
| 1:C:347:VAL:O    | 1:C:351:LYS:O    | 2.29                     | 0.51              |
| 1:D:342:PHE:CD1  | 1:D:411:MET:HB3  | 2.45                     | 0.51              |
| 1:C:428:TYR:CD1  | 1:C:429:LEU:HD12 | 2.44                     | 0.51              |
| 1:C:713:GLY:O    | 1:C:749:ARG:HD2  | 2.11                     | 0.51              |
| 1:D:392:ALA:HB2  | 1:D:410:TYR:CE2  | 2.45                     | 0.51              |
| 1:A:393:LEU:HD22 | 1:A:536:ARG:HG2  | 1.93                     | 0.51              |
| 1:A:605:TYR:HB2  | 1:A:686:LEU:HD11 | 1.93                     | 0.51              |
| 1:C:613:ARG:HB2  | 1:C:657:ILE:HD11 | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:713:GLY:O    | 1:A:749:ARG:HD2  | 2.11                     | 0.51              |
| 1:A:791:SER:O    | 1:A:793:PRO:N    | 2.44                     | 0.51              |
| 1:B:791:SER:N    | 1:B:794:VAL:HB   | 2.26                     | 0.51              |
| 1:C:443:TRP:O    | 1:C:473:ASN:ND2  | 2.44                     | 0.51              |
| 1:C:524:THR:CG2  | 1:C:525:ARG:NH1  | 2.74                     | 0.51              |
| 1:D:720:ALA:HB2  | 1:D:742:SER:OG   | 2.11                     | 0.51              |
| 1:A:428:TYR:HD1  | 1:A:429:LEU:CD1  | 2.24                     | 0.51              |
| 1:A:521:TRP:CZ3  | 1:A:525:ARG:HD3  | 2.46                     | 0.51              |
| 1:B:356:GLN:O    | 1:B:361:HIS:HB2  | 2.11                     | 0.51              |
| 1:D:377:GLY:O    | 1:D:381:GLN:HG2  | 2.11                     | 0.51              |
| 1:D:539:MET:SD   | 1:D:551:LEU:CD2  | 2.99                     | 0.51              |
| 1:A:334:GLU:CD   | 1:A:334:GLU:H    | 2.17                     | 0.51              |
| 1:D:410:TYR:CD1  | 1:D:410:TYR:C    | 2.88                     | 0.51              |
| 1:D:410:TYR:HE1  | 1:D:414:THR:HG21 | 1.74                     | 0.51              |
| 1:D:789:SER:HB3  | 1:D:792:ASP:CA   | 2.40                     | 0.50              |
| 1:A:354:ASP:CB   | 1:A:358:SER:CB   | 2.90                     | 0.50              |
| 1:C:355:TYR:N    | 1:C:356:GLN:HA   | 2.16                     | 0.50              |
| 1:C:364:MET:O    | 1:C:368:GLN:N    | 2.31                     | 0.50              |
| 1:D:400:LEU:CD1  | 1:D:410:TYR:CD2  | 2.85                     | 0.50              |
| 1:A:350:GLU:OE2  | 1:A:353:GLN:CA   | 2.60                     | 0.50              |
| 1:D:428:TYR:CD1  | 1:D:429:LEU:HD12 | 2.47                     | 0.50              |
| 1:D:672:GLU:HA   | 1:D:672:GLU:OE1  | 2.11                     | 0.50              |
| 1:D:713:GLY:O    | 1:D:749:ARG:HD2  | 2.11                     | 0.50              |
| 1:B:539:MET:SD   | 1:B:551:LEU:CD2  | 2.99                     | 0.50              |
| 1:C:410:TYR:CA   | 1:C:413:ASP:HB2  | 2.41                     | 0.50              |
| 1:A:428:TYR:CD1  | 1:A:429:LEU:HD12 | 2.47                     | 0.50              |
| 1:C:377:GLY:O    | 1:C:381:GLN:HG2  | 2.12                     | 0.50              |
| 1:B:352:ILE:CG2  | 1:B:354:ASP:N    | 2.67                     | 0.50              |
| 1:B:672:GLU:OE1  | 1:B:672:GLU:HA   | 2.12                     | 0.50              |
| 1:B:393:LEU:HD23 | 1:B:398:GLU:CB   | 2.41                     | 0.50              |
| 1:B:447:ASN:ND2  | 1:B:447:ASN:C    | 2.69                     | 0.50              |
| 1:D:789:SER:HB2  | 1:D:794:VAL:CG1  | 2.41                     | 0.50              |
| 1:A:339:PHE:CE1  | 1:A:364:MET:HE2  | 2.38                     | 0.50              |
| 1:C:632:LEU:HD23 | 1:C:632:LEU:N    | 2.22                     | 0.50              |
| 1:D:795:VAL:HB   | 1:D:797:VAL:HG23 | 1.94                     | 0.50              |
| 1:B:352:ILE:O    | 1:B:352:ILE:HG22 | 2.11                     | 0.49              |
| 1:D:447:ASN:ND2  | 1:D:447:ASN:C    | 2.70                     | 0.49              |
| 1:D:524:THR:CG2  | 1:D:525:ARG:NH1  | 2.75                     | 0.49              |
| 1:D:791:SER:CA   | 1:D:794:VAL:CG2  | 2.75                     | 0.49              |
| 1:A:613:ARG:HB2  | 1:A:657:ILE:HD11 | 1.94                     | 0.49              |
| 1:B:668:GLY:HA3  | 1:B:701:PRO:HB3  | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:340:GLU:O    | 1:C:344:PRO:HD2  | 2.11                     | 0.49              |
| 1:C:672:GLU:HA   | 1:C:672:GLU:OE1  | 2.11                     | 0.49              |
| 1:D:351:LYS:C    | 1:D:353:GLN:CB   | 2.84                     | 0.49              |
| 1:D:428:TYR:HD1  | 1:D:429:LEU:CD1  | 2.25                     | 0.49              |
| 1:A:350:GLU:C    | 1:A:350:GLU:CD   | 2.80                     | 0.49              |
| 1:A:396:THR:HG1  | 1:A:398:GLU:CD   | 2.20                     | 0.49              |
| 1:A:447:ASN:C    | 1:A:447:ASN:ND2  | 2.68                     | 0.49              |
| 1:C:521:TRP:CZ3  | 1:C:525:ARG:HD3  | 2.48                     | 0.49              |
| 1:B:339:PHE:HE1  | 1:B:364:MET:HE1  | 1.76                     | 0.49              |
| 1:D:486:ARG:NH2  | 1:D:553:ARG:HA   | 2.25                     | 0.49              |
| 1:A:794:VAL:O    | 1:A:794:VAL:CG1  | 2.59                     | 0.49              |
| 1:B:575:GLU:OE2  | 1:B:579:ARG:NE   | 2.45                     | 0.49              |
| 1:D:521:TRP:CZ3  | 1:D:525:ARG:HD3  | 2.48                     | 0.49              |
| 1:B:447:ASN:C    | 1:B:447:ASN:HD22 | 2.17                     | 0.49              |
| 1:C:355:TYR:N    | 1:C:356:GLN:CB   | 2.76                     | 0.49              |
| 1:D:391:PHE:HD2  | 1:D:411:MET:HE1  | 1.76                     | 0.49              |
| 1:B:621:HIS:HB2  | 1:B:644:PHE:HB2  | 1.94                     | 0.49              |
| 1:B:788:ASP:C    | 1:B:790:SER:N    | 2.68                     | 0.49              |
| 1:C:539:MET:SD   | 1:C:551:LEU:CD2  | 3.01                     | 0.49              |
| 1:A:524:THR:CG2  | 1:A:525:ARG:NH1  | 2.74                     | 0.49              |
| 1:B:396:THR:O    | 1:B:397:GLY:C    | 2.56                     | 0.49              |
| 1:A:381:GLN:O    | 1:A:385:ARG:HG2  | 2.13                     | 0.49              |
| 1:B:430:ARG:NH1  | 1:B:493:HIS:HD2  | 1.92                     | 0.49              |
| 1:C:797:VAL:HG13 | 1:C:798:ASP:H    | 1.78                     | 0.49              |
| 1:D:800:VAL:O    | 1:D:800:VAL:CG1  | 2.59                     | 0.49              |
| 1:B:356:GLN:O    | 1:B:358:SER:O    | 2.31                     | 0.49              |
| 1:C:787:SER:HB3  | 1:C:789:SER:OG   | 2.13                     | 0.48              |
| 1:A:337:THR:O    | 1:A:341:THR:HG23 | 2.12                     | 0.48              |
| 1:B:359:ASP:OD1  | 1:B:362:GLU:OE2  | 2.31                     | 0.48              |
| 1:B:393:LEU:HA   | 1:B:398:GLU:CB   | 2.43                     | 0.48              |
| 1:A:334:GLU:OE1  | 1:A:334:GLU:O    | 2.31                     | 0.48              |
| 1:A:395:GLU:HG2  | 1:A:553:ARG:HH22 | 1.75                     | 0.48              |
| 1:B:428:TYR:HD1  | 1:B:429:LEU:CD1  | 2.25                     | 0.48              |
| 1:C:739:ALA:O    | 1:C:742:SER:HB2  | 2.13                     | 0.48              |
| 1:A:339:PHE:CZ   | 1:A:364:MET:CE   | 2.81                     | 0.48              |
| 1:A:525:ARG:HH22 | 1:A:588:GLY:N    | 2.02                     | 0.48              |
| 1:D:447:ASN:C    | 1:D:447:ASN:HD22 | 2.18                     | 0.48              |
| 1:D:359:ASP:C    | 1:D:362:GLU:H    | 2.21                     | 0.48              |
| 1:D:628:ASP:O    | 1:D:630:PRO:HD3  | 2.14                     | 0.48              |
| 1:B:381:GLN:O    | 1:B:385:ARG:HG2  | 2.13                     | 0.48              |
| 1:B:521:TRP:CZ3  | 1:B:525:ARG:HD3  | 2.49                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:393:LEU:CA   | 1:D:396:THR:O    | 2.62                     | 0.48              |
| 1:A:343:LEU:HB2  | 1:A:344:PRO:CD   | 2.44                     | 0.48              |
| 1:A:509:LYS:CE   | 1:A:569:ALA:HB2  | 2.44                     | 0.48              |
| 1:A:775:TYR:O    | 1:A:779:LYS:HB2  | 2.13                     | 0.48              |
| 1:C:787:SER:C    | 1:C:789:SER:H    | 2.20                     | 0.48              |
| 1:B:393:LEU:HD22 | 1:B:536:ARG:HG2  | 1.96                     | 0.48              |
| 1:C:537:ALA:O    | 1:C:541:GLY:HA2  | 2.06                     | 0.48              |
| 1:D:339:PHE:CZ   | 1:D:343:LEU:HD11 | 2.49                     | 0.48              |
| 1:D:339:PHE:CZ   | 1:D:364:MET:CE   | 2.96                     | 0.48              |
| 1:D:352:ILE:H    | 1:D:353:GLN:CB   | 2.20                     | 0.48              |
| 1:B:673:PHE:HE1  | 1:B:763:MET:HG3  | 1.78                     | 0.48              |
| 1:C:447:ASN:HD22 | 1:C:447:ASN:C    | 2.20                     | 0.48              |
| 1:D:410:TYR:HD1  | 1:D:410:TYR:C    | 2.19                     | 0.48              |
| 1:D:443:TRP:O    | 1:D:473:ASN:ND2  | 2.47                     | 0.48              |
| 1:A:409:VAL:O    | 1:A:410:TYR:C    | 2.55                     | 0.47              |
| 1:B:486:ARG:NH2  | 1:B:553:ARG:HA   | 2.25                     | 0.47              |
| 1:D:537:ALA:O    | 1:D:541:GLY:C    | 2.55                     | 0.47              |
| 1:D:762:PHE:CD2  | 1:D:763:MET:HE2  | 2.49                     | 0.47              |
| 1:B:359:ASP:HA   | 1:B:362:GLU:OE1  | 2.14                     | 0.47              |
| 1:C:396:THR:CG2  | 1:C:410:TYR:CE1  | 2.97                     | 0.47              |
| 1:D:359:ASP:O    | 1:D:362:GLU:CB   | 2.63                     | 0.47              |
| 1:D:393:LEU:HA   | 1:D:396:THR:O    | 2.13                     | 0.47              |
| 1:A:347:VAL:HG23 | 1:A:361:HIS:NE2  | 2.29                     | 0.47              |
| 1:B:605:TYR:HB2  | 1:B:686:LEU:HD11 | 1.96                     | 0.47              |
| 1:D:525:ARG:HH22 | 1:D:588:GLY:N    | 2.05                     | 0.47              |
| 1:A:719:ASP:OD1  | 1:A:719:ASP:N    | 2.45                     | 0.47              |
| 1:C:524:THR:HG21 | 1:C:589:VAL:HG21 | 1.95                     | 0.47              |
| 1:A:340:GLU:H    | 1:A:340:GLU:HG2  | 1.42                     | 0.47              |
| 1:A:396:THR:OG1  | 1:A:398:GLU:OE2  | 2.31                     | 0.47              |
| 1:A:448:ASN:HB2  | 1:C:743:ARG:HB2  | 1.97                     | 0.47              |
| 1:A:668:GLY:HA3  | 1:A:701:PRO:HB3  | 1.96                     | 0.47              |
| 1:B:339:PHE:CZ   | 1:B:343:LEU:HD11 | 2.50                     | 0.47              |
| 1:B:524:THR:HG22 | 1:B:525:ARG:NH1  | 2.29                     | 0.47              |
| 1:C:409:VAL:O    | 1:C:410:TYR:HB3  | 2.14                     | 0.47              |
| 1:D:381:GLN:O    | 1:D:385:ARG:HG2  | 2.14                     | 0.47              |
| 1:D:605:TYR:HB2  | 1:D:686:LEU:HD11 | 1.95                     | 0.47              |
| 1:D:790:SER:O    | 1:D:791:SER:CB   | 2.44                     | 0.47              |
| 1:C:530:ASN:OD1  | 1:C:530:ASN:O    | 2.32                     | 0.47              |
| 1:C:567:VAL:O    | 1:C:567:VAL:HG13 | 2.14                     | 0.47              |
| 1:C:575:GLU:OE2  | 1:C:579:ARG:NE   | 2.47                     | 0.47              |
| 1:D:569:ALA:O    | 1:D:570:GLU:HG3  | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:399:LYS:O    | 1:A:399:LYS:HG2  | 2.14                     | 0.47              |
| 1:B:700:ARG:HH21 | 1:B:704:GLU:CD   | 2.21                     | 0.47              |
| 1:D:524:THR:HG21 | 1:D:589:VAL:HG21 | 1.96                     | 0.47              |
| 1:C:348:MET:C    | 1:C:351:LYS:CB   | 2.88                     | 0.47              |
| 1:D:416:GLU:O    | 1:D:418:HIS:N    | 2.48                     | 0.47              |
| 1:B:775:TYR:O    | 1:B:779:LYS:HB2  | 2.14                     | 0.46              |
| 1:A:651:ASP:OD1  | 1:A:653:THR:HG23 | 2.14                     | 0.46              |
| 1:C:447:ASN:ND2  | 1:C:447:ASN:C    | 2.70                     | 0.46              |
| 1:D:393:LEU:C    | 1:D:396:THR:O    | 2.57                     | 0.46              |
| 1:A:396:THR:O    | 1:A:398:GLU:N    | 2.47                     | 0.46              |
| 1:B:337:THR:HG22 | 1:B:381:GLN:NE2  | 2.30                     | 0.46              |
| 1:C:673:PHE:HE1  | 1:C:763:MET:HG3  | 1.81                     | 0.46              |
| 1:D:416:GLU:C    | 1:D:418:HIS:N    | 2.74                     | 0.46              |
| 1:D:572:LEU:HD11 | 1:D:576:LEU:HD13 | 1.96                     | 0.46              |
| 1:B:487:PHE:CE2  | 1:B:568:ASP:CB   | 2.99                     | 0.46              |
| 1:C:749:ARG:HH11 | 1:C:749:ARG:CB   | 2.27                     | 0.46              |
| 1:B:443:TRP:O    | 1:B:473:ASN:ND2  | 2.49                     | 0.46              |
| 1:C:775:TYR:CE1  | 1:C:779:LYS:HE2  | 2.50                     | 0.46              |
| 1:D:570:GLU:CB   | 1:D:574:LYS:HE2  | 2.45                     | 0.46              |
| 1:D:575:GLU:OE2  | 1:D:579:ARG:NE   | 2.46                     | 0.46              |
| 1:A:339:PHE:HZ   | 1:A:364:MET:HE3  | 1.75                     | 0.46              |
| 1:A:343:LEU:O    | 1:A:346:VAL:HG13 | 2.16                     | 0.46              |
| 1:C:396:THR:HG23 | 1:C:410:TYR:CZ   | 2.41                     | 0.46              |
| 1:D:393:LEU:HD22 | 1:D:536:ARG:HG2  | 1.98                     | 0.46              |
| 1:D:668:GLY:HA3  | 1:D:701:PRO:HB3  | 1.98                     | 0.46              |
| 1:B:743:ARG:HB2  | 1:D:448:ASN:HB2  | 1.98                     | 0.46              |
| 1:C:775:TYR:O    | 1:C:779:LYS:HB2  | 2.16                     | 0.46              |
| 1:D:398:GLU:O    | 1:D:399:LYS:HB3  | 2.16                     | 0.46              |
| 1:D:775:TYR:O    | 1:D:779:LYS:HB2  | 2.15                     | 0.46              |
| 1:B:409:VAL:O    | 1:B:410:TYR:HB3  | 2.16                     | 0.46              |
| 1:C:567:VAL:HG22 | 1:C:569:ALA:H    | 1.80                     | 0.46              |
| 1:D:548:ILE:HD13 | 1:D:548:ILE:HA   | 1.76                     | 0.46              |
| 1:A:530:ASN:OD1  | 1:A:530:ASN:O    | 2.34                     | 0.46              |
| 1:A:576:LEU:HB3  | 1:A:782:LEU:HD11 | 1.97                     | 0.46              |
| 1:B:388:LEU:O    | 1:B:391:PHE:HB3  | 2.16                     | 0.46              |
| 1:D:568:ASP:OD1  | 1:D:569:ALA:N    | 2.49                     | 0.46              |
| 1:A:339:PHE:CE1  | 1:A:364:MET:HE1  | 2.22                     | 0.46              |
| 1:B:392:ALA:CB   | 1:B:398:GLU:CB   | 2.93                     | 0.46              |
| 1:D:352:ILE:CA   | 1:D:353:GLN:CB   | 2.92                     | 0.46              |
| 1:A:749:ARG:HH11 | 1:A:749:ARG:CG   | 2.29                     | 0.45              |
| 1:C:524:THR:HG22 | 1:C:525:ARG:NH1  | 2.31                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:749:ARG:HH11 | 1:C:749:ARG:CG   | 2.29                     | 0.45              |
| 1:D:568:ASP:HA   | 1:D:572:LEU:H    | 1.81                     | 0.45              |
| 1:A:338:ALA:HB3  | 1:A:388:LEU:CD2  | 2.47                     | 0.45              |
| 1:A:386:ASP:O    | 1:A:390:THR:HG23 | 2.16                     | 0.45              |
| 1:A:443:TRP:O    | 1:A:473:ASN:ND2  | 2.49                     | 0.45              |
| 1:B:703:THR:CG2  | 1:B:704:GLU:N    | 2.80                     | 0.45              |
| 1:C:621:HIS:HE1  | 1:C:642:SER:HB3  | 1.82                     | 0.45              |
| 1:B:395:GLU:HB3  | 1:B:553:ARG:HH22 | 1.81                     | 0.45              |
| 1:B:762:PHE:CD2  | 1:B:763:MET:HE2  | 2.51                     | 0.45              |
| 1:D:487:PHE:CZ   | 1:D:568:ASP:HB3  | 2.51                     | 0.45              |
| 1:B:548:ILE:HD13 | 1:B:548:ILE:HA   | 1.76                     | 0.45              |
| 1:D:530:ASN:OD1  | 1:D:530:ASN:O    | 2.34                     | 0.45              |
| 1:C:396:THR:HG22 | 1:C:410:TYR:OH   | 2.08                     | 0.45              |
| 1:D:567:VAL:CG1  | 1:D:568:ASP:N    | 2.79                     | 0.45              |
| 1:D:749:ARG:HH11 | 1:D:749:ARG:CG   | 2.29                     | 0.45              |
| 1:A:334:GLU:N    | 1:A:334:GLU:CD   | 2.74                     | 0.45              |
| 1:A:430:ARG:HG2  | 1:A:433:ARG:NH1  | 2.32                     | 0.45              |
| 1:A:524:THR:HG22 | 1:A:525:ARG:NH1  | 2.31                     | 0.45              |
| 1:A:749:ARG:HH11 | 1:A:749:ARG:CB   | 2.30                     | 0.45              |
| 1:C:339:PHE:CZ   | 1:C:343:LEU:HD11 | 2.52                     | 0.45              |
| 1:B:509:LYS:HD3  | 1:B:569:ALA:HA   | 1.98                     | 0.45              |
| 1:C:790:SER:O    | 1:C:791:SER:C    | 2.55                     | 0.45              |
| 1:A:388:LEU:O    | 1:A:391:PHE:HB3  | 2.15                     | 0.44              |
| 1:C:539:MET:HA   | 1:C:551:LEU:HB3  | 1.99                     | 0.44              |
| 1:C:702:TRP:HH2  | 1:C:754:ARG:O    | 2.00                     | 0.44              |
| 1:D:351:LYS:H    | 1:D:353:GLN:CB   | 2.30                     | 0.44              |
| 1:A:345:ARG:HH11 | 1:A:345:ARG:HG2  | 1.71                     | 0.44              |
| 1:B:749:ARG:HH11 | 1:B:749:ARG:CG   | 2.31                     | 0.44              |
| 1:A:509:LYS:NZ   | 1:A:569:ALA:CB   | 2.80                     | 0.44              |
| 1:C:743:ARG:HG2  | 1:C:745:LEU:HG   | 1.99                     | 0.44              |
| 1:D:673:PHE:HE1  | 1:D:763:MET:HG3  | 1.83                     | 0.44              |
| 1:A:339:PHE:C    | 1:A:343:LEU:CD1  | 2.90                     | 0.44              |
| 1:B:345:ARG:HE   | 1:B:412:ARG:HG3  | 1.81                     | 0.44              |
| 1:B:356:GLN:C    | 1:B:358:SER:H    | 2.26                     | 0.44              |
| 1:A:775:TYR:CE1  | 1:A:779:LYS:HE2  | 2.53                     | 0.44              |
| 1:B:701:PRO:HB2  | 1:B:703:THR:HG22 | 2.00                     | 0.44              |
| 1:B:749:ARG:HH11 | 1:B:749:ARG:CB   | 2.28                     | 0.44              |
| 1:A:486:ARG:HA   | 1:A:486:ARG:HD2  | 1.84                     | 0.43              |
| 1:A:762:PHE:CD2  | 1:A:763:MET:HE2  | 2.53                     | 0.43              |
| 1:B:651:ASP:OD1  | 1:B:653:THR:HG23 | 2.17                     | 0.43              |
| 1:A:509:LYS:CE   | 1:A:569:ALA:HB1  | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:575:GLU:OE2  | 1:A:579:ARG:NE   | 2.51                     | 0.43              |
| 1:B:524:THR:HG22 | 1:B:525:ARG:HH11 | 1.83                     | 0.43              |
| 1:B:530:ASN:OD1  | 1:B:530:ASN:O    | 2.35                     | 0.43              |
| 1:D:388:LEU:O    | 1:D:391:PHE:HB3  | 2.18                     | 0.43              |
| 1:D:430:ARG:HG2  | 1:D:433:ARG:NH1  | 2.33                     | 0.43              |
| 1:B:353:GLN:CB   | 1:B:354:ASP:O    | 2.66                     | 0.43              |
| 1:C:790:SER:HA   | 1:C:794:VAL:HA   | 2.00                     | 0.43              |
| 1:A:739:ALA:O    | 1:A:742:SER:HB3  | 2.19                     | 0.43              |
| 1:C:356:GLN:HA   | 1:C:357:ASP:HA   | 1.80                     | 0.43              |
| 1:C:388:LEU:O    | 1:C:391:PHE:HB3  | 2.19                     | 0.43              |
| 1:C:795:VAL:HB   | 1:C:796:LYS:CA   | 2.30                     | 0.43              |
| 1:A:395:GLU:CG   | 1:A:553:ARG:HH22 | 2.31                     | 0.43              |
| 1:B:355:TYR:CB   | 1:B:361:HIS:ND1  | 2.82                     | 0.43              |
| 1:B:625:GLU:CD   | 1:B:625:GLU:H    | 2.27                     | 0.43              |
| 1:D:762:PHE:HD2  | 1:D:763:MET:HE2  | 1.82                     | 0.43              |
| 1:A:421:SER:O    | 1:A:425:ARG:NH1  | 2.52                     | 0.43              |
| 1:A:792:ASP:OD1  | 1:A:792:ASP:N    | 2.50                     | 0.43              |
| 1:B:524:THR:HG21 | 1:B:589:VAL:HG21 | 2.01                     | 0.43              |
| 1:A:625:GLU:CD   | 1:A:625:GLU:H    | 2.26                     | 0.43              |
| 1:C:365:LYS:O    | 1:C:369:GLY:N    | 2.47                     | 0.43              |
| 1:D:789:SER:O    | 1:D:792:ASP:N    | 2.49                     | 0.43              |
| 1:B:542:ALA:O    | 1:B:543:ASP:OD1  | 2.36                     | 0.43              |
| 1:C:430:ARG:HG2  | 1:C:433:ARG:NH1  | 2.34                     | 0.43              |
| 1:C:625:GLU:H    | 1:C:625:GLU:CD   | 2.26                     | 0.43              |
| 1:D:416:GLU:O    | 1:D:417:ARG:C    | 2.60                     | 0.43              |
| 1:D:621:HIS:HB2  | 1:D:644:PHE:HB2  | 2.00                     | 0.43              |
| 1:D:625:GLU:CD   | 1:D:625:GLU:H    | 2.27                     | 0.43              |
| 1:D:651:ASP:OD1  | 1:D:653:THR:HG23 | 2.18                     | 0.43              |
| 1:D:789:SER:HB3  | 1:D:792:ASP:C    | 2.40                     | 0.43              |
| 1:A:673:PHE:HE1  | 1:A:763:MET:HG3  | 1.83                     | 0.43              |
| 1:B:356:GLN:O    | 1:B:357:ASP:C    | 2.62                     | 0.43              |
| 1:B:421:SER:O    | 1:B:425:ARG:NH1  | 2.52                     | 0.43              |
| 1:C:525:ARG:HH22 | 1:C:588:GLY:N    | 2.07                     | 0.43              |
| 1:C:762:PHE:CD2  | 1:C:763:MET:HE2  | 2.54                     | 0.43              |
| 1:C:524:THR:HG22 | 1:C:525:ARG:HH11 | 1.83                     | 0.42              |
| 1:D:749:ARG:HH11 | 1:D:749:ARG:CB   | 2.31                     | 0.42              |
| 1:D:525:ARG:NH2  | 1:D:587:GLY:HA2  | 2.33                     | 0.42              |
| 1:B:486:ARG:HA   | 1:B:486:ARG:HD2  | 1.85                     | 0.42              |
| 1:B:545:LEU:HD12 | 1:B:545:LEU:HA   | 1.66                     | 0.42              |
| 1:A:684:GLY:O    | 1:A:766:ARG:HD3  | 2.19                     | 0.42              |
| 1:C:396:THR:HG21 | 1:C:410:TYR:HE1  | 1.79                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:524:THR:HG22 | 1:D:525:ARG:NH1  | 2.34                     | 0.42              |
| 1:B:339:PHE:CZ   | 1:B:364:MET:CE   | 3.02                     | 0.42              |
| 1:C:548:ILE:HD13 | 1:C:548:ILE:HA   | 1.81                     | 0.42              |
| 1:D:421:SER:O    | 1:D:425:ARG:NH1  | 2.52                     | 0.42              |
| 1:D:621:HIS:HE1  | 1:D:642:SER:HB3  | 1.76                     | 0.42              |
| 1:A:558:PRO:O    | 1:A:559:ASP:CB   | 2.67                     | 0.42              |
| 1:B:392:ALA:HA   | 1:B:410:TYR:OH   | 2.20                     | 0.42              |
| 1:C:342:PHE:CE2  | 1:C:346:VAL:CG2  | 3.02                     | 0.42              |
| 1:D:337:THR:HG23 | 1:D:340:GLU:CD   | 2.44                     | 0.42              |
| 1:D:567:VAL:HG12 | 1:D:568:ASP:H    | 1.83                     | 0.42              |
| 1:A:395:GLU:OE1  | 1:A:428:TYR:CE2  | 2.72                     | 0.42              |
| 1:A:790:SER:CA   | 1:A:791:SER:C    | 2.82                     | 0.42              |
| 1:A:800:VAL:O    | 1:A:801:GLU:CB   | 2.68                     | 0.42              |
| 1:B:410:TYR:CA   | 1:B:413:ASP:HB2  | 2.50                     | 0.42              |
| 1:A:396:THR:HG1  | 1:A:398:GLU:CG   | 2.32                     | 0.42              |
| 1:B:613:ARG:HB2  | 1:B:657:ILE:HD11 | 2.00                     | 0.42              |
| 1:B:632:LEU:N    | 1:B:632:LEU:CD1  | 2.78                     | 0.42              |
| 1:A:548:ILE:HD13 | 1:A:548:ILE:HA   | 1.78                     | 0.42              |
| 1:D:342:PHE:HD1  | 1:D:411:MET:HB3  | 1.84                     | 0.42              |
| 1:A:524:THR:HG21 | 1:A:589:VAL:HG21 | 2.02                     | 0.41              |
| 1:B:558:PRO:O    | 1:B:559:ASP:CB   | 2.68                     | 0.41              |
| 1:C:605:TYR:HB2  | 1:C:686:LEU:HD11 | 2.01                     | 0.41              |
| 1:B:391:PHE:O    | 1:B:395:GLU:CG   | 2.68                     | 0.41              |
| 1:C:345:ARG:HE   | 1:C:412:ARG:HG3  | 1.85                     | 0.41              |
| 1:D:792:ASP:N    | 1:D:794:VAL:HG13 | 2.34                     | 0.41              |
| 1:C:428:TYR:CD1  | 1:C:429:LEU:CD1  | 3.03                     | 0.41              |
| 1:C:486:ARG:HA   | 1:C:486:ARG:HD2  | 1.84                     | 0.41              |
| 1:B:700:ARG:NH2  | 1:B:704:GLU:CD   | 2.76                     | 0.41              |
| 1:C:334:GLU:HA   | 1:C:335:PRO:HD2  | 1.85                     | 0.41              |
| 1:C:734:THR:OG1  | 1:C:737:ASP:HB2  | 2.21                     | 0.41              |
| 1:C:487:PHE:CE2  | 1:C:568:ASP:HB3  | 2.55                     | 0.41              |
| 1:B:703:THR:HG23 | 1:B:704:GLU:N    | 2.35                     | 0.41              |
| 1:B:762:PHE:CD2  | 1:B:763:MET:CE   | 3.03                     | 0.41              |
| 1:C:421:SER:O    | 1:C:425:ARG:NH1  | 2.54                     | 0.41              |
| 1:C:567:VAL:O    | 1:C:567:VAL:CG1  | 2.69                     | 0.41              |
| 1:D:395:GLU:HG2  | 1:D:395:GLU:H    | 1.54                     | 0.41              |
| 1:A:360:ALA:HB1  | 1:A:429:LEU:HD23 | 2.03                     | 0.41              |
| 1:A:789:SER:O    | 1:A:790:SER:C    | 2.62                     | 0.41              |
| 1:B:548:ILE:HG13 | 1:B:571:ALA:CB   | 2.49                     | 0.41              |
| 1:C:396:THR:CG2  | 1:C:410:TYR:HH   | 2.23                     | 0.41              |
| 1:C:568:ASP:OD1  | 1:C:568:ASP:C    | 2.63                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:684:GLY:O    | 1:C:766:ARG:HD3  | 2.21                     | 0.41              |
| 1:A:524:THR:HG22 | 1:A:525:ARG:HH11 | 1.85                     | 0.41              |
| 1:B:360:ALA:CB   | 1:B:429:LEU:HD23 | 2.50                     | 0.41              |
| 1:C:509:LYS:HD3  | 1:C:569:ALA:HA   | 2.02                     | 0.41              |
| 1:D:800:VAL:O    | 1:D:800:VAL:HG12 | 2.20                     | 0.41              |
| 1:A:570:GLU:O    | 1:A:574:LYS:HD2  | 2.21                     | 0.41              |
| 1:C:404:LEU:O    | 1:C:408:ARG:HG2  | 2.21                     | 0.41              |
| 1:D:734:THR:OG1  | 1:D:737:ASP:HB2  | 2.21                     | 0.41              |
| 1:B:343:LEU:HA   | 1:B:346:VAL:HG12 | 2.03                     | 0.41              |
| 1:B:352:ILE:CD1  | 1:B:354:ASP:CB   | 2.93                     | 0.41              |
| 1:B:415:PHE:CE1  | 1:B:425:ARG:HB2  | 2.55                     | 0.41              |
| 1:D:347:VAL:HA   | 1:D:350:GLU:HB2  | 2.03                     | 0.41              |
| 1:D:350:GLU:HB3  | 1:D:351:LYS:HA   | 2.01                     | 0.41              |
| 1:D:339:PHE:HZ   | 1:D:364:MET:HE3  | 1.85                     | 0.40              |
| 1:B:631:GLY:C    | 1:B:632:LEU:HD13 | 2.46                     | 0.40              |
| 1:D:702:TRP:HH2  | 1:D:754:ARG:O    | 2.04                     | 0.40              |
| 1:B:428:TYR:CD1  | 1:B:428:TYR:C    | 2.99                     | 0.40              |
| 1:C:410:TYR:O    | 1:C:411:MET:C    | 2.63                     | 0.40              |
| 1:D:800:VAL:O    | 1:D:801:GLU:C    | 2.64                     | 0.40              |
| 1:B:684:GLY:O    | 1:B:766:ARG:HD3  | 2.21                     | 0.40              |
| 1:C:337:THR:HG22 | 1:C:381:GLN:NE2  | 2.36                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------------|--------------------------|-------------------|
| 1:B:378:ASP:OD2 | 1:B:792:ASP:CA[8_554] | 2.10                     | 0.10              |

## 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     | 469/493 (95%)   | 439 (94%)  | 26 (6%) | 4 (1%)   | 14          | 33 |
| 1   | B     | 464/493 (94%)   | 434 (94%)  | 22 (5%) | 8 (2%)   | 7           | 17 |
| 1   | C     | 466/493 (94%)   | 438 (94%)  | 22 (5%) | 6 (1%)   | 9           | 23 |
| 1   | D     | 463/493 (94%)   | 437 (94%)  | 23 (5%) | 3 (1%)   | 21          | 42 |
| All | All   | 1862/1972 (94%) | 1748 (94%) | 93 (5%) | 21 (1%)  | 11          | 27 |

All (21) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 559 | ASP  |
| 1   | A     | 793 | PRO  |
| 1   | B     | 559 | ASP  |
| 1   | B     | 793 | PRO  |
| 1   | C     | 559 | ASP  |
| 1   | C     | 565 | PRO  |
| 1   | C     | 793 | PRO  |
| 1   | D     | 559 | ASP  |
| 1   | D     | 793 | PRO  |
| 1   | B     | 790 | SER  |
| 1   | B     | 791 | SER  |
| 1   | C     | 542 | ALA  |
| 1   | A     | 542 | ALA  |
| 1   | B     | 542 | ALA  |
| 1   | B     | 565 | PRO  |
| 1   | C     | 335 | PRO  |
| 1   | A     | 565 | PRO  |
| 1   | B     | 789 | SER  |
| 1   | B     | 796 | LYS  |
| 1   | C     | 795 | VAL  |
| 1   | D     | 417 | ARG  |

### 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     | 355/392 (91%)   | 309 (87%)  | 46 (13%)  | 4           | 10 |
| 1   | B     | 353/392 (90%)   | 317 (90%)  | 36 (10%)  | 7           | 17 |
| 1   | C     | 348/392 (89%)   | 308 (88%)  | 40 (12%)  | 5           | 13 |
| 1   | D     | 342/392 (87%)   | 301 (88%)  | 41 (12%)  | 5           | 12 |
| All | All   | 1398/1568 (89%) | 1235 (88%) | 163 (12%) | 5           | 12 |

All (163) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 334 | GLU  |
| 1   | A     | 336 | LEU  |
| 1   | A     | 337 | THR  |
| 1   | A     | 340 | GLU  |
| 1   | A     | 345 | ARG  |
| 1   | A     | 346 | VAL  |
| 1   | A     | 347 | VAL  |
| 1   | A     | 350 | GLU  |
| 1   | A     | 388 | LEU  |
| 1   | A     | 396 | THR  |
| 1   | A     | 404 | LEU  |
| 1   | A     | 407 | GLN  |
| 1   | A     | 409 | VAL  |
| 1   | A     | 411 | MET  |
| 1   | A     | 412 | ARG  |
| 1   | A     | 413 | ASP  |
| 1   | A     | 419 | LYS  |
| 1   | A     | 429 | LEU  |
| 1   | A     | 449 | SER  |
| 1   | A     | 462 | THR  |
| 1   | A     | 466 | LYS  |
| 1   | A     | 498 | GLU  |
| 1   | A     | 521 | TRP  |
| 1   | A     | 524 | THR  |
| 1   | A     | 533 | SER  |
| 1   | A     | 543 | ASP  |
| 1   | A     | 544 | SER  |
| 1   | A     | 545 | LEU  |
| 1   | A     | 548 | ILE  |
| 1   | A     | 561 | THR  |
| 1   | A     | 576 | LEU  |
| 1   | A     | 586 | LYS  |
| 1   | A     | 653 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 658 | GLU  |
| 1   | A     | 669 | TRP  |
| 1   | A     | 727 | SER  |
| 1   | A     | 737 | ASP  |
| 1   | A     | 741 | MET  |
| 1   | A     | 742 | SER  |
| 1   | A     | 749 | ARG  |
| 1   | A     | 755 | GLU  |
| 1   | A     | 770 | LEU  |
| 1   | A     | 792 | ASP  |
| 1   | A     | 794 | VAL  |
| 1   | A     | 795 | VAL  |
| 1   | A     | 800 | VAL  |
| 1   | B     | 340 | GLU  |
| 1   | B     | 347 | VAL  |
| 1   | B     | 352 | ILE  |
| 1   | B     | 388 | LEU  |
| 1   | B     | 395 | GLU  |
| 1   | B     | 399 | LYS  |
| 1   | B     | 404 | LEU  |
| 1   | B     | 407 | GLN  |
| 1   | B     | 413 | ASP  |
| 1   | B     | 419 | LYS  |
| 1   | B     | 429 | LEU  |
| 1   | B     | 449 | SER  |
| 1   | B     | 462 | THR  |
| 1   | B     | 498 | GLU  |
| 1   | B     | 514 | ILE  |
| 1   | B     | 521 | TRP  |
| 1   | B     | 524 | THR  |
| 1   | B     | 533 | SER  |
| 1   | B     | 543 | ASP  |
| 1   | B     | 544 | SER  |
| 1   | B     | 545 | LEU  |
| 1   | B     | 548 | ILE  |
| 1   | B     | 561 | THR  |
| 1   | B     | 572 | LEU  |
| 1   | B     | 576 | LEU  |
| 1   | B     | 586 | LYS  |
| 1   | B     | 632 | LEU  |
| 1   | B     | 653 | THR  |
| 1   | B     | 658 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 669 | TRP  |
| 1   | B     | 727 | SER  |
| 1   | B     | 737 | ASP  |
| 1   | B     | 749 | ARG  |
| 1   | B     | 755 | GLU  |
| 1   | B     | 770 | LEU  |
| 1   | B     | 794 | VAL  |
| 1   | C     | 334 | GLU  |
| 1   | C     | 336 | LEU  |
| 1   | C     | 337 | THR  |
| 1   | C     | 340 | GLU  |
| 1   | C     | 346 | VAL  |
| 1   | C     | 347 | VAL  |
| 1   | C     | 364 | MET  |
| 1   | C     | 388 | LEU  |
| 1   | C     | 396 | THR  |
| 1   | C     | 404 | LEU  |
| 1   | C     | 407 | GLN  |
| 1   | C     | 408 | ARG  |
| 1   | C     | 409 | VAL  |
| 1   | C     | 411 | MET  |
| 1   | C     | 413 | ASP  |
| 1   | C     | 419 | LYS  |
| 1   | C     | 429 | LEU  |
| 1   | C     | 449 | SER  |
| 1   | C     | 462 | THR  |
| 1   | C     | 498 | GLU  |
| 1   | C     | 521 | TRP  |
| 1   | C     | 524 | THR  |
| 1   | C     | 533 | SER  |
| 1   | C     | 538 | VAL  |
| 1   | C     | 544 | SER  |
| 1   | C     | 545 | LEU  |
| 1   | C     | 548 | ILE  |
| 1   | C     | 561 | THR  |
| 1   | C     | 576 | LEU  |
| 1   | C     | 586 | LYS  |
| 1   | C     | 632 | LEU  |
| 1   | C     | 658 | GLU  |
| 1   | C     | 669 | TRP  |
| 1   | C     | 727 | SER  |
| 1   | C     | 737 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 742 | SER  |
| 1   | C     | 749 | ARG  |
| 1   | C     | 755 | GLU  |
| 1   | C     | 794 | VAL  |
| 1   | C     | 799 | ASP  |
| 1   | D     | 337 | THR  |
| 1   | D     | 340 | GLU  |
| 1   | D     | 347 | VAL  |
| 1   | D     | 350 | GLU  |
| 1   | D     | 388 | LEU  |
| 1   | D     | 395 | GLU  |
| 1   | D     | 399 | LYS  |
| 1   | D     | 404 | LEU  |
| 1   | D     | 409 | VAL  |
| 1   | D     | 413 | ASP  |
| 1   | D     | 429 | LEU  |
| 1   | D     | 449 | SER  |
| 1   | D     | 462 | THR  |
| 1   | D     | 466 | LYS  |
| 1   | D     | 498 | GLU  |
| 1   | D     | 514 | ILE  |
| 1   | D     | 521 | TRP  |
| 1   | D     | 524 | THR  |
| 1   | D     | 533 | SER  |
| 1   | D     | 543 | ASP  |
| 1   | D     | 544 | SER  |
| 1   | D     | 545 | LEU  |
| 1   | D     | 548 | ILE  |
| 1   | D     | 561 | THR  |
| 1   | D     | 572 | LEU  |
| 1   | D     | 576 | LEU  |
| 1   | D     | 586 | LYS  |
| 1   | D     | 624 | ILE  |
| 1   | D     | 642 | SER  |
| 1   | D     | 653 | THR  |
| 1   | D     | 658 | GLU  |
| 1   | D     | 669 | TRP  |
| 1   | D     | 727 | SER  |
| 1   | D     | 737 | ASP  |
| 1   | D     | 749 | ARG  |
| 1   | D     | 755 | GLU  |
| 1   | D     | 787 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 791 | SER  |
| 1   | D     | 795 | VAL  |
| 1   | D     | 799 | ASP  |
| 1   | D     | 800 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 381 | GLN  |
| 1   | A     | 493 | HIS  |
| 1   | A     | 663 | GLN  |
| 1   | A     | 681 | HIS  |
| 1   | B     | 381 | GLN  |
| 1   | B     | 447 | ASN  |
| 1   | B     | 493 | HIS  |
| 1   | B     | 530 | ASN  |
| 1   | B     | 654 | HIS  |
| 1   | B     | 663 | GLN  |
| 1   | B     | 681 | HIS  |
| 1   | C     | 368 | GLN  |
| 1   | C     | 431 | HIS  |
| 1   | C     | 447 | ASN  |
| 1   | C     | 448 | ASN  |
| 1   | C     | 493 | HIS  |
| 1   | C     | 530 | ASN  |
| 1   | C     | 654 | HIS  |
| 1   | C     | 663 | GLN  |
| 1   | C     | 681 | HIS  |
| 1   | D     | 447 | ASN  |
| 1   | D     | 448 | ASN  |
| 1   | D     | 493 | HIS  |
| 1   | D     | 530 | ASN  |
| 1   | D     | 654 | HIS  |
| 1   | D     | 663 | GLN  |
| 1   | D     | 681 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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     | 471/493 (95%)   | 0.77   | 56 (11%) <b>9</b> <b>8</b>   | 43, 69, 108, 160      | 0     |
| 1   | B     | 466/493 (94%)   | 0.83   | 50 (10%) <b>11</b> <b>10</b> | 58, 81, 129, 154      | 0     |
| 1   | C     | 468/493 (94%)   | 1.11   | 86 (18%) <b>3</b> <b>3</b>   | 51, 76, 126, 158      | 0     |
| 1   | D     | 467/493 (94%)   | 0.80   | 52 (11%) <b>10</b> <b>9</b>  | 53, 80, 130, 172      | 0     |
| All | All   | 1872/1972 (94%) | 0.88   | 244 (13%) <b>7</b> <b>7</b>  | 43, 77, 125, 172      | 0     |

All (244) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 668 | GLY  | 7.6  |
| 1   | A     | 352 | ILE  | 7.2  |
| 1   | C     | 357 | ASP  | 6.6  |
| 1   | A     | 563 | PRO  | 6.6  |
| 1   | C     | 667 | SER  | 6.1  |
| 1   | A     | 570 | GLU  | 6.0  |
| 1   | C     | 566 | ASP  | 5.8  |
| 1   | C     | 354 | ASP  | 5.4  |
| 1   | A     | 795 | VAL  | 5.2  |
| 1   | C     | 794 | VAL  | 5.1  |
| 1   | D     | 571 | ALA  | 5.0  |
| 1   | C     | 792 | ASP  | 4.8  |
| 1   | A     | 395 | GLU  | 4.7  |
| 1   | D     | 555 | TRP  | 4.7  |
| 1   | C     | 352 | ILE  | 4.6  |
| 1   | D     | 564 | ASP  | 4.6  |
| 1   | D     | 567 | VAL  | 4.6  |
| 1   | A     | 560 | ALA  | 4.6  |
| 1   | C     | 556 | ALA  | 4.5  |
| 1   | A     | 558 | PRO  | 4.5  |
| 1   | A     | 353 | GLN  | 4.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 351 | LYS  | 4.4  |
| 1   | C     | 702 | TRP  | 4.4  |
| 1   | B     | 395 | GLU  | 4.3  |
| 1   | C     | 344 | PRO  | 4.3  |
| 1   | C     | 447 | ASN  | 4.2  |
| 1   | B     | 352 | ILE  | 4.2  |
| 1   | B     | 631 | GLY  | 4.1  |
| 1   | C     | 564 | ASP  | 4.1  |
| 1   | D     | 800 | VAL  | 4.1  |
| 1   | D     | 669 | TRP  | 4.0  |
| 1   | D     | 801 | GLU  | 4.0  |
| 1   | D     | 790 | SER  | 4.0  |
| 1   | A     | 361 | HIS  | 4.0  |
| 1   | D     | 540 | ALA  | 4.0  |
| 1   | A     | 555 | TRP  | 4.0  |
| 1   | C     | 785 | GLU  | 3.9  |
| 1   | B     | 563 | PRO  | 3.9  |
| 1   | D     | 566 | ASP  | 3.9  |
| 1   | D     | 563 | PRO  | 3.9  |
| 1   | A     | 564 | ASP  | 3.9  |
| 1   | B     | 569 | ALA  | 3.8  |
| 1   | C     | 653 | THR  | 3.8  |
| 1   | B     | 348 | MET  | 3.8  |
| 1   | A     | 569 | ALA  | 3.8  |
| 1   | C     | 353 | GLN  | 3.8  |
| 1   | B     | 669 | TRP  | 3.8  |
| 1   | C     | 391 | PHE  | 3.7  |
| 1   | A     | 561 | THR  | 3.7  |
| 1   | A     | 541 | GLY  | 3.7  |
| 1   | A     | 414 | THR  | 3.6  |
| 1   | A     | 725 | ASN  | 3.6  |
| 1   | C     | 425 | ARG  | 3.6  |
| 1   | C     | 714 | ALA  | 3.6  |
| 1   | D     | 565 | PRO  | 3.6  |
| 1   | C     | 429 | LEU  | 3.6  |
| 1   | A     | 415 | PHE  | 3.5  |
| 1   | B     | 702 | TRP  | 3.5  |
| 1   | B     | 391 | PHE  | 3.5  |
| 1   | B     | 355 | TYR  | 3.5  |
| 1   | C     | 569 | ALA  | 3.5  |
| 1   | C     | 395 | GLU  | 3.5  |
| 1   | B     | 545 | LEU  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 346 | VAL  | 3.5  |
| 1   | A     | 566 | ASP  | 3.4  |
| 1   | B     | 567 | VAL  | 3.4  |
| 1   | A     | 547 | GLY  | 3.4  |
| 1   | B     | 413 | ASP  | 3.4  |
| 1   | C     | 338 | ALA  | 3.4  |
| 1   | C     | 797 | VAL  | 3.4  |
| 1   | C     | 560 | ALA  | 3.4  |
| 1   | D     | 333 | GLY  | 3.4  |
| 1   | B     | 356 | GLN  | 3.4  |
| 1   | C     | 800 | VAL  | 3.4  |
| 1   | D     | 793 | PRO  | 3.3  |
| 1   | A     | 416 | GLU  | 3.3  |
| 1   | B     | 558 | PRO  | 3.3  |
| 1   | A     | 800 | VAL  | 3.3  |
| 1   | C     | 669 | TRP  | 3.3  |
| 1   | B     | 667 | SER  | 3.3  |
| 1   | B     | 564 | ASP  | 3.3  |
| 1   | A     | 332 | THR  | 3.2  |
| 1   | C     | 345 | ARG  | 3.2  |
| 1   | B     | 357 | ASP  | 3.2  |
| 1   | B     | 361 | HIS  | 3.2  |
| 1   | B     | 363 | TYR  | 3.2  |
| 1   | A     | 424 | ASP  | 3.1  |
| 1   | B     | 568 | ASP  | 3.1  |
| 1   | C     | 563 | PRO  | 3.1  |
| 1   | A     | 726 | SER  | 3.1  |
| 1   | C     | 393 | LEU  | 3.1  |
| 1   | B     | 362 | GLU  | 3.1  |
| 1   | A     | 571 | ALA  | 3.1  |
| 1   | C     | 349 | ALA  | 3.1  |
| 1   | A     | 669 | TRP  | 3.1  |
| 1   | C     | 561 | THR  | 3.0  |
| 1   | D     | 560 | ALA  | 3.0  |
| 1   | C     | 793 | PRO  | 3.0  |
| 1   | B     | 566 | ASP  | 3.0  |
| 1   | D     | 429 | LEU  | 2.9  |
| 1   | D     | 556 | ALA  | 2.9  |
| 1   | B     | 429 | LEU  | 2.9  |
| 1   | A     | 567 | VAL  | 2.9  |
| 1   | D     | 389 | VAL  | 2.9  |
| 1   | A     | 557 | GLU  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 416 | GLU  | 2.8  |
| 1   | C     | 672 | GLU  | 2.8  |
| 1   | C     | 420 | ASP  | 2.8  |
| 1   | C     | 597 | ALA  | 2.8  |
| 1   | C     | 347 | VAL  | 2.8  |
| 1   | A     | 757 | GLU  | 2.8  |
| 1   | D     | 548 | ILE  | 2.8  |
| 1   | C     | 355 | TYR  | 2.8  |
| 1   | A     | 559 | ASP  | 2.8  |
| 1   | C     | 795 | VAL  | 2.8  |
| 1   | D     | 569 | ALA  | 2.8  |
| 1   | A     | 793 | PRO  | 2.8  |
| 1   | B     | 430 | ARG  | 2.8  |
| 1   | B     | 548 | ILE  | 2.8  |
| 1   | C     | 350 | GLU  | 2.8  |
| 1   | D     | 353 | GLN  | 2.7  |
| 1   | C     | 565 | PRO  | 2.7  |
| 1   | A     | 447 | ASN  | 2.7  |
| 1   | A     | 517 | PHE  | 2.7  |
| 1   | B     | 703 | THR  | 2.7  |
| 1   | B     | 550 | PRO  | 2.7  |
| 1   | B     | 493 | HIS  | 2.7  |
| 1   | B     | 433 | ARG  | 2.7  |
| 1   | B     | 555 | TRP  | 2.7  |
| 1   | B     | 672 | GLU  | 2.7  |
| 1   | C     | 383 | ALA  | 2.7  |
| 1   | B     | 354 | ASP  | 2.7  |
| 1   | C     | 390 | THR  | 2.7  |
| 1   | C     | 400 | LEU  | 2.7  |
| 1   | D     | 374 | PHE  | 2.7  |
| 1   | A     | 498 | GLU  | 2.6  |
| 1   | D     | 390 | THR  | 2.6  |
| 1   | D     | 391 | PHE  | 2.6  |
| 1   | A     | 562 | LYS  | 2.6  |
| 1   | B     | 570 | GLU  | 2.6  |
| 1   | A     | 565 | PRO  | 2.6  |
| 1   | D     | 568 | ASP  | 2.6  |
| 1   | D     | 397 | GLY  | 2.6  |
| 1   | A     | 331 | THR  | 2.5  |
| 1   | C     | 535 | TYR  | 2.5  |
| 1   | D     | 794 | VAL  | 2.5  |
| 1   | B     | 665 | ALA  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 665 | ALA  | 2.5  |
| 1   | A     | 801 | GLU  | 2.5  |
| 1   | B     | 757 | GLU  | 2.5  |
| 1   | C     | 658 | GLU  | 2.5  |
| 1   | A     | 354 | ASP  | 2.5  |
| 1   | B     | 334 | GLU  | 2.5  |
| 1   | C     | 405 | PRO  | 2.5  |
| 1   | C     | 367 | VAL  | 2.5  |
| 1   | D     | 347 | VAL  | 2.5  |
| 1   | A     | 349 | ALA  | 2.5  |
| 1   | B     | 796 | LYS  | 2.4  |
| 1   | C     | 555 | TRP  | 2.4  |
| 1   | D     | 798 | ASP  | 2.4  |
| 1   | C     | 675 | SER  | 2.4  |
| 1   | D     | 493 | HIS  | 2.4  |
| 1   | A     | 413 | ASP  | 2.4  |
| 1   | A     | 702 | TRP  | 2.4  |
| 1   | C     | 413 | ASP  | 2.4  |
| 1   | C     | 336 | LEU  | 2.4  |
| 1   | C     | 570 | GLU  | 2.4  |
| 1   | D     | 570 | GLU  | 2.4  |
| 1   | C     | 397 | GLY  | 2.4  |
| 1   | A     | 350 | GLU  | 2.4  |
| 1   | C     | 726 | SER  | 2.4  |
| 1   | C     | 791 | SER  | 2.4  |
| 1   | B     | 799 | ASP  | 2.4  |
| 1   | D     | 359 | ASP  | 2.4  |
| 1   | D     | 558 | PRO  | 2.4  |
| 1   | B     | 560 | ALA  | 2.4  |
| 1   | C     | 415 | PHE  | 2.4  |
| 1   | A     | 355 | TYR  | 2.3  |
| 1   | C     | 343 | LEU  | 2.3  |
| 1   | C     | 428 | TYR  | 2.3  |
| 1   | D     | 395 | GLU  | 2.3  |
| 1   | A     | 556 | ALA  | 2.3  |
| 1   | D     | 581 | SER  | 2.3  |
| 1   | B     | 521 | TRP  | 2.3  |
| 1   | C     | 558 | PRO  | 2.3  |
| 1   | D     | 335 | PRO  | 2.3  |
| 1   | D     | 342 | PHE  | 2.3  |
| 1   | B     | 350 | GLU  | 2.3  |
| 1   | C     | 699 | SER  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 376 | VAL  | 2.3  |
| 1   | C     | 414 | THR  | 2.3  |
| 1   | D     | 414 | THR  | 2.3  |
| 1   | C     | 568 | ASP  | 2.3  |
| 1   | C     | 548 | ILE  | 2.2  |
| 1   | A     | 348 | MET  | 2.2  |
| 1   | D     | 396 | THR  | 2.2  |
| 1   | C     | 522 | ARG  | 2.2  |
| 1   | C     | 335 | PRO  | 2.2  |
| 1   | C     | 550 | PRO  | 2.2  |
| 1   | D     | 547 | GLY  | 2.2  |
| 1   | C     | 567 | VAL  | 2.2  |
| 1   | C     | 486 | ARG  | 2.2  |
| 1   | A     | 397 | GLY  | 2.2  |
| 1   | C     | 670 | ASP  | 2.2  |
| 1   | D     | 792 | ASP  | 2.2  |
| 1   | A     | 393 | LEU  | 2.2  |
| 1   | B     | 556 | ALA  | 2.2  |
| 1   | D     | 349 | ALA  | 2.2  |
| 1   | B     | 399 | LYS  | 2.2  |
| 1   | C     | 369 | GLY  | 2.2  |
| 1   | A     | 788 | ASP  | 2.2  |
| 1   | C     | 348 | MET  | 2.2  |
| 1   | C     | 339 | PHE  | 2.2  |
| 1   | D     | 416 | GLU  | 2.1  |
| 1   | A     | 341 | THR  | 2.1  |
| 1   | C     | 379 | ARG  | 2.1  |
| 1   | A     | 568 | ASP  | 2.1  |
| 1   | A     | 544 | SER  | 2.1  |
| 1   | B     | 781 | TRP  | 2.1  |
| 1   | C     | 396 | THR  | 2.1  |
| 1   | B     | 565 | PRO  | 2.1  |
| 1   | D     | 407 | GLN  | 2.1  |
| 1   | C     | 545 | LEU  | 2.1  |
| 1   | D     | 709 | TYR  | 2.1  |
| 1   | B     | 358 | SER  | 2.1  |
| 1   | D     | 415 | PHE  | 2.1  |
| 1   | D     | 438 | PHE  | 2.1  |
| 1   | D     | 422 | ALA  | 2.1  |
| 1   | B     | 525 | ARG  | 2.1  |
| 1   | C     | 371 | LEU  | 2.1  |
| 1   | D     | 588 | GLY  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 794 | VAL  | 2.1  |
| 1   | C     | 412 | ARG  | 2.1  |
| 1   | B     | 668 | GLY  | 2.1  |
| 1   | C     | 411 | MET  | 2.0  |
| 1   | A     | 530 | ASN  | 2.0  |
| 1   | A     | 548 | ILE  | 2.0  |
| 1   | B     | 417 | ARG  | 2.0  |
| 1   | D     | 339 | PHE  | 2.0  |
| 1   | C     | 399 | LYS  | 2.0  |
| 1   | C     | 422 | ALA  | 2.0  |
| 1   | C     | 790 | SER  | 2.0  |
| 1   | D     | 561 | THR  | 2.0  |
| 1   | C     | 553 | ARG  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.