



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:59 AM UTC

PDB ID : 1U0N / pdb\_00001u0n  
Title : The ternary von Willebrand Factor A1-glycoprotein Ibalphabotrocetin complex  
Authors : Fukuda, K.; Liddington, R.C.  
Deposited on : 2004-07-13  
Resolution : 2.95 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)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

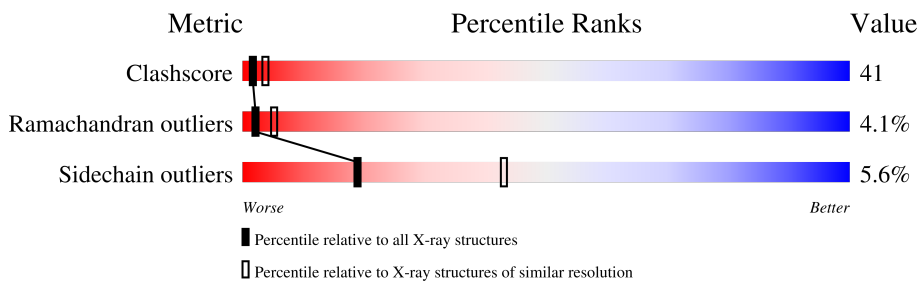
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 1157 (2.98-2.94)                                      |
| Ramachandran outliers | 187476                      | 1101 (2.98-2.94)                                      |
| Sidechain outliers    | 187428                      | 1101 (2.98-2.94)                                      |

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  $\leq 5\%$

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain                                          |
|-----|-------|--------|-----------------------------------------------------------|
| 1   | A     | 208    | <div> <div>39%</div> <div>53%</div> <div>8%</div> </div>  |
| 2   | B     | 133    | <div> <div>49%</div> <div>42%</div> <div>8%</div> </div>  |
| 3   | C     | 125    | <div> <div>37%</div> <div>55%</div> <div>7%</div> </div>  |
| 4   | D     | 265    | <div> <div>34%</div> <div>56%</div> <div>10%</div> </div> |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5864 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 Von Willebrand factor.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 208      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1664  | 1062 | 293 | 303 | 6 |         |         |       |

- Molecule 2 is a protein called Botrocetin.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 133      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1066  | 679 | 175 | 204 | 8 |         |         |       |

- Molecule 3 is a protein called Botrocetin.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 3   | C     | 125      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1060  | 682 | 166 | 202 | 10 |         |         |       |

- Molecule 4 is a protein called Platelet glycoprotein Ib.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | D     | 265      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2074  | 1334 | 344 | 387 | 9 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| D     | 21      | GLN      | ASN    | engineered mutation | UNP P07359 |
| D     | 159     | GLN      | ASN    | engineered mutation | UNP P07359 |

### 3 Residue-property plots

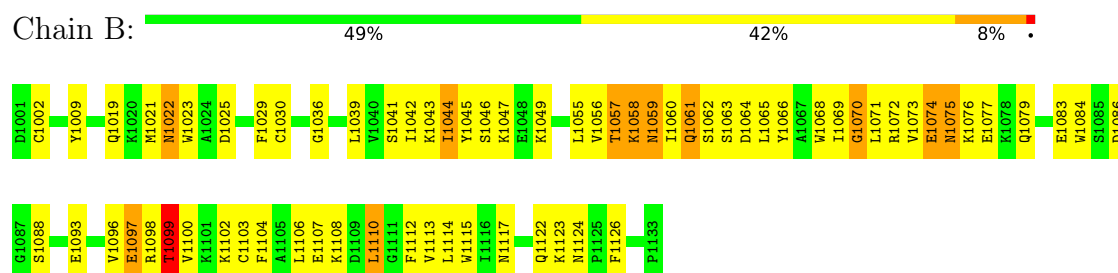
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

#### • Molecule 1: Von Willebrand factor



#### • Molecule 2: Botrocetin



#### • Molecule 3: Botrocetin



#### • Molecule 4: Platelet glycoprotein Ib



|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| C209 | N210 | C211 | E212 | I213 | I214 | Y215 | F216 | R217 | L220 | Q221 | D222 | N223 | N226 | V227 | W230 | K231 | Q232 | G233 | V234 | D235 | V236 | K237 | A238 | M239 | V243 | A244 | S245 | V246 | Q247 | C248 | D249 | N250 | S251 | D252 | K253 | F254 | P255 | V256 | Y259 | P260 | G261 | K262 | F265 |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| H1   | P2   | I3   | C4   | E5   | V6   | S7   | K8   | V9   |      | H12  | L13  | E14  | V15  | N16  | C17  | D18  | K19  | R20  | Q21  | L22  |      | L25  | P26  |      | L29  | P30  | K31  | D32  | T33  | T34  | I35  |      | L38  | S39  |      | L42  | L43  | Y44  |      | S47  | L48  | A49  | T50  | L51  | M52  | P53  | Y54  | T55  |      | R56  | L57  | T58  | Q59  | L60  | N61  | L62  | D63  | R64  | C65  | E66  |
| L67  | T68  | K69  | L70  | Q71  | V72  | D73  | G74  | T75  |      | V78  | L79  | G80  | T81  | L82  | D83  | L84  | S85  | H86  |      | L89  |      | L92  | P93  | L94  | L95  | G96  | Q97  | T98  | L99  | P100 | A101 | L102 | T103 | V104 | L105 | D106 | V107 |      | N110 | R111 |      | L115 | P116 | L117 | G118 | A119 | L120 | R121 |      | G122 | L123 | G124 | E125 | L126 | Q127 | E128 | L129 | Y130 | L131 | K132 |
|      | E135 | L136 | K137 | T138 | L139 | P140 |      | L143 | L144 | T145 | P146 |      | L150 | E151 | K152 | L153 | S154 | L155 | A156 | M157 | N158 | Q159 | L160 | T161 |      | P164 | A165 | G166 | L167 | L168 |      | E172 | M173 | L174 | D175 | T176 | L177 | L178 | L179 | Q180 | E181 | N182 | S183 |      | F192 | G193 | S194 | H195 | L196 | L197 | P198 | F199 | A200 | F201 | L202 | H203 |      | W207 | L208 |      |

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                           | Source    |
|----------------------------------------------------------|-------------------------------------------------|-----------|
| Space group                                              | P 41 21 2                                       | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 108.31Å 108.31Å 221.97Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 6.00 – 2.95                                     | Depositor |
| % Data completeness<br>(in resolution range)             | 94.5 (6.00-2.95)                                | Depositor |
| $R_{merge}$                                              | 0.10                                            | Depositor |
| $R_{sym}$                                                | (Not available)                                 | Depositor |
| Refinement program                                       | CNS 1.0                                         | Depositor |
| R, $R_{free}$                                            | 0.213 , 0.276                                   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 5864                                            | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 48.0                                            | wwPDB-VP  |

## 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     | 0.54         | 1/1696 (0.1%) | 1.07        | 8/2290 (0.3%)  |
| 2   | B     | 0.48         | 0/1094        | 1.01        | 7/1476 (0.5%)  |
| 3   | C     | 0.42         | 0/1098        | 0.85        | 2/1490 (0.1%)  |
| 4   | D     | 0.45         | 0/2121        | 1.00        | 11/2895 (0.4%) |
| All | All   | 0.48         | 1/6009 (0.0%) | 1.00        | 28/8151 (0.3%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 704 | PRO  | C-N   | -5.43 | 1.25        | 1.33     |

All (28) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | D     | 155  | LEU  | N-CA-C  | -7.51 | 102.35      | 112.26   |
| 1   | A     | 558  | TYR  | N-CA-C  | 7.24  | 121.32      | 109.24   |
| 4   | D     | 110  | ASN  | N-CA-C  | -7.13 | 98.90       | 108.74   |
| 4   | D     | 97   | GLN  | N-CA-C  | 6.65  | 118.33      | 111.14   |
| 1   | A     | 546  | ILE  | N-CA-C  | 6.61  | 118.05      | 107.73   |
| 4   | D     | 215  | TYR  | N-CA-C  | -6.05 | 104.76      | 111.71   |
| 4   | D     | 194  | SER  | N-CA-C  | -5.89 | 105.40      | 112.59   |
| 1   | A     | 519  | LEU  | N-CA-C  | 5.84  | 118.19      | 108.20   |
| 4   | D     | 44   | TYR  | N-CA-C  | -5.80 | 106.16      | 113.18   |
| 2   | B     | 1002 | CYS  | N-CA-C  | 5.72  | 117.28      | 110.07   |
| 4   | D     | 12   | HIS  | N-CA-C  | 5.67  | 118.96      | 109.95   |
| 2   | B     | 1070 | GLY  | N-CA-C  | 5.66  | 120.95      | 113.37   |
| 4   | D     | 38   | LEU  | N-CA-C  | -5.64 | 105.71      | 112.59   |
| 3   | C     | 2067 | GLY  | N-CA-C  | 5.54  | 126.32      | 113.18   |
| 4   | D     | 251  | SER  | CB-CA-C | -5.52 | 109.72      | 117.23   |
| 2   | B     | 1063 | SER  | N-CA-C  | -5.51 | 105.92      | 113.30   |
| 2   | B     | 1036 | GLY  | N-CA-C  | -5.43 | 107.77      | 115.43   |
| 1   | A     | 703  | PRO  | N-CA-C  | 5.43  | 117.32      | 110.70   |
| 4   | D     | 259  | TYR  | CA-C-N  | 5.35  | 125.42      | 119.32   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4   | D     | 259  | TYR  | C-N-CA | 5.35  | 125.42      | 119.32   |
| 1   | A     | 590  | GLN  | N-CA-C | -5.32 | 105.37      | 111.07   |
| 2   | B     | 1042 | ILE  | N-CA-C | 5.27  | 115.17      | 107.37   |
| 2   | B     | 1002 | CYS  | CA-C-N | 5.27  | 125.56      | 119.93   |
| 2   | B     | 1002 | CYS  | C-N-CA | 5.27  | 125.56      | 119.93   |
| 1   | A     | 538  | VAL  | N-CA-C | -5.22 | 105.44      | 110.72   |
| 1   | A     | 688  | ASP  | N-CA-C | 5.17  | 117.31      | 111.11   |
| 3   | C     | 2020 | TRP  | N-CA-C | 5.15  | 117.12      | 108.73   |
| 1   | A     | 599  | LYS  | N-CA-C | -5.08 | 105.64      | 111.07   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1664  | 0        | 1708     | 157     | 0            |
| 2   | B     | 1066  | 0        | 1009     | 85      | 0            |
| 3   | C     | 1060  | 0        | 937      | 105     | 0            |
| 4   | D     | 2074  | 0        | 2112     | 193     | 0            |
| All | All   | 5864  | 0        | 5766     | 479     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (479) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:75:THR:HA    | 4:D:98:THR:HG23   | 1.43                     | 1.01              |
| 4:D:47:SER:HA    | 4:D:71:GLN:HB2    | 1.39                     | 1.00              |
| 2:B:1074:GLU:HB2 | 3:C:2078:GLU:HG2  | 1.42                     | 1.00              |
| 4:D:232:GLN:NE2  | 4:D:233:GLY:H     | 1.59                     | 0.99              |
| 4:D:232:GLN:HE21 | 4:D:233:GLY:N     | 1.60                     | 0.99              |
| 4:D:84:LEU:HB2   | 4:D:107:VAL:HG12  | 1.49                     | 0.94              |
| 1:A:632:ARG:HH11 | 3:C:2114:THR:HG21 | 1.33                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:227:VAL:HG21  | 4:D:243:VAL:HG23  | 1.52                     | 0.91              |
| 4:D:6:VAL:HG22    | 4:D:15:VAL:HG22   | 1.54                     | 0.90              |
| 4:D:35:ILE:HG22   | 4:D:59:GLN:HB3    | 1.55                     | 0.89              |
| 4:D:232:GLN:HE21  | 4:D:233:GLY:H     | 0.92                     | 0.89              |
| 1:A:628:GLN:HE21  | 3:C:2092:LEU:HD21 | 1.37                     | 0.89              |
| 2:B:1022:ASN:HD22 | 2:B:1022:ASN:H    | 1.19                     | 0.88              |
| 4:D:227:VAL:HG11  | 4:D:243:VAL:HA    | 1.57                     | 0.86              |
| 2:B:1009:TYR:OH   | 2:B:1047:LYS:HB3  | 1.75                     | 0.86              |
| 4:D:154:SER:HA    | 4:D:178:LEU:HB2   | 1.57                     | 0.86              |
| 3:C:2059:LEU:HD12 | 3:C:2059:LEU:H    | 1.40                     | 0.86              |
| 2:B:1075:ASN:N    | 2:B:1075:ASN:HD22 | 1.71                     | 0.85              |
| 4:D:201:PHE:HZ    | 4:D:239:MET:HE2   | 1.43                     | 0.83              |
| 4:D:12:HIS:HA     | 4:D:34:THR:HG21   | 1.60                     | 0.83              |
| 4:D:201:PHE:CZ    | 4:D:239:MET:HE2   | 2.16                     | 0.81              |
| 1:A:552:ARG:HG3   | 1:A:611:ARG:NH2   | 1.96                     | 0.80              |
| 4:D:209:CYS:HA    | 4:D:213:ILE:HG21  | 1.64                     | 0.80              |
| 2:B:1022:ASN:H    | 2:B:1022:ASN:ND2  | 1.80                     | 0.80              |
| 1:A:546:ILE:HD11  | 1:A:577:LEU:HD13  | 1.64                     | 0.80              |
| 3:C:2061:GLY:HA2  | 3:C:2102:LYS:HE3  | 1.63                     | 0.79              |
| 4:D:104:VAL:HG12  | 4:D:128:GLU:HB2   | 1.64                     | 0.79              |
| 4:D:80:GLY:HA2    | 4:D:102:LEU:HA    | 1.65                     | 0.79              |
| 4:D:58:THR:HA     | 4:D:79:LEU:HA     | 1.65                     | 0.78              |
| 3:C:2012:HIS:CE1  | 3:C:2124:GLN:HB3  | 2.20                     | 0.77              |
| 4:D:233:GLY:O     | 4:D:234:VAL:HG12  | 1.85                     | 0.77              |
| 1:A:604:GLN:NE2   | 4:D:239:MET:HE1   | 2.00                     | 0.77              |
| 1:A:663:ARG:NH1   | 1:A:667:LYS:HD2   | 2.00                     | 0.76              |
| 1:A:549:LYS:HB2   | 4:D:9:VAL:HG21    | 1.67                     | 0.75              |
| 1:A:663:ARG:HH11  | 1:A:667:LYS:HD2   | 1.52                     | 0.75              |
| 4:D:103:THR:HA    | 4:D:126:LEU:HA    | 1.69                     | 0.75              |
| 1:A:660:LYS:O     | 1:A:664:LEU:HD13  | 1.86                     | 0.74              |
| 2:B:1099:THR:HG21 | 3:C:2110:ILE:H    | 1.51                     | 0.74              |
| 1:A:546:ILE:HG23  | 1:A:574:PRO:HG3   | 1.69                     | 0.73              |
| 4:D:253:LYS:HG2   | 4:D:254:PHE:CE2   | 2.24                     | 0.73              |
| 1:A:552:ARG:HG3   | 1:A:611:ARG:HH21  | 1.51                     | 0.73              |
| 4:D:196:LEU:O     | 4:D:198:PRO:HD3   | 1.89                     | 0.72              |
| 3:C:2012:HIS:ND1  | 3:C:2124:GLN:HB3  | 2.04                     | 0.72              |
| 1:A:703:PRO:HB2   | 1:A:705:THR:N     | 2.04                     | 0.71              |
| 1:A:663:ARG:HH22  | 3:C:2089:ASP:HA   | 1.55                     | 0.71              |
| 2:B:1075:ASN:HD21 | 3:C:2076:ARG:H    | 1.38                     | 0.70              |
| 1:A:666:GLU:HA    | 1:A:672:ASN:O     | 1.92                     | 0.70              |
| 1:A:648:VAL:HB    | 1:A:672:ASN:HD21  | 1.57                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:664:LEU:HD21  | 3:C:2091:TYR:HB2  | 1.74                     | 0.69              |
| 2:B:1044:ILE:HG13 | 3:C:2090:TYR:CE2  | 2.28                     | 0.69              |
| 4:D:145:THR:HB    | 4:D:146:PRO:HD3   | 1.75                     | 0.69              |
| 4:D:95:LEU:HD13   | 4:D:99:LEU:HD12   | 1.73                     | 0.68              |
| 4:D:39:SER:HB3    | 4:D:63:ASP:OD1    | 1.92                     | 0.68              |
| 4:D:58:THR:HG22   | 4:D:78:VAL:O      | 1.93                     | 0.68              |
| 4:D:227:VAL:CG1   | 4:D:243:VAL:HA    | 2.23                     | 0.68              |
| 1:A:616:ARG:HH21  | 1:A:645:LYS:HB2   | 1.58                     | 0.68              |
| 4:D:8:LYS:HG2     | 4:D:13:LEU:CD1    | 2.24                     | 0.68              |
| 4:D:44:TYR:HA     | 4:D:66:GLU:O      | 1.94                     | 0.67              |
| 1:A:703:PRO:HG2   | 1:A:704:PRO:HA    | 1.77                     | 0.67              |
| 1:A:703:PRO:HB2   | 1:A:704:PRO:C     | 2.20                     | 0.67              |
| 4:D:60:LEU:HD23   | 4:D:82:LEU:CD1    | 2.25                     | 0.67              |
| 1:A:604:GLN:HE21  | 4:D:239:MET:HE1   | 1.59                     | 0.67              |
| 1:A:701:ALA:C     | 1:A:703:PRO:HD2   | 2.21                     | 0.66              |
| 4:D:111:ARG:HG2   | 4:D:135:GLU:OE2   | 1.94                     | 0.66              |
| 3:C:2091:TYR:CE2  | 3:C:2092:LEU:HD12 | 2.29                     | 0.66              |
| 3:C:2105:ASN:OD1  | 3:C:2107:LYS:HB2  | 1.95                     | 0.66              |
| 4:D:247:GLN:HA    | 4:D:256:VAL:HG23  | 1.76                     | 0.66              |
| 1:A:546:ILE:HD11  | 1:A:577:LEU:CD1   | 2.27                     | 0.66              |
| 2:B:1060:ILE:O    | 2:B:1061:GLN:C    | 2.39                     | 0.65              |
| 2:B:1075:ASN:N    | 2:B:1075:ASN:ND2  | 2.43                     | 0.64              |
| 2:B:1075:ASN:HD22 | 2:B:1075:ASN:H    | 1.44                     | 0.64              |
| 1:A:663:ARG:CZ    | 1:A:667:LYS:HZ3   | 2.10                     | 0.64              |
| 3:C:2049:ASP:O    | 3:C:2052:ARG:HB3  | 1.97                     | 0.64              |
| 1:A:629:ARG:HG3   | 1:A:629:ARG:HH11  | 1.63                     | 0.64              |
| 3:C:2059:LEU:HD12 | 3:C:2059:LEU:N    | 2.11                     | 0.64              |
| 4:D:81:THR:HA     | 4:D:104:VAL:HG23  | 1.80                     | 0.64              |
| 1:A:554:ALA:HA    | 1:A:566:ILE:HG22  | 1.80                     | 0.63              |
| 1:A:663:ARG:HD2   | 1:A:664:LEU:HD12  | 1.78                     | 0.63              |
| 4:D:175:ASP:HA    | 4:D:198:PRO:HD2   | 1.80                     | 0.63              |
| 4:D:217:ARG:O     | 4:D:221:GLN:HG3   | 1.99                     | 0.63              |
| 4:D:223:ASN:HB3   | 4:D:226:ASN:HD22  | 1.63                     | 0.63              |
| 2:B:1019:GLN:CD   | 2:B:1021:MET:HE3  | 2.23                     | 0.63              |
| 4:D:49:ALA:O      | 4:D:52:MET:HG3    | 1.99                     | 0.62              |
| 1:A:628:GLN:HE21  | 3:C:2092:LEU:CD2  | 2.10                     | 0.62              |
| 1:A:499:ILE:HD11  | 1:A:574:PRO:HD3   | 1.82                     | 0.62              |
| 1:A:580:ILE:HG23  | 4:D:235:ASP:OD2   | 1.99                     | 0.62              |
| 3:C:2023:TRP:CE2  | 3:C:2069:SER:HB3  | 2.33                     | 0.62              |
| 4:D:116:PRO:O     | 4:D:119:ALA:HB2   | 2.00                     | 0.62              |
| 2:B:1047:LYS:O    | 2:B:1047:LYS:HD3  | 2.00                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1044:ILE:HG13 | 3:C:2090:TYR:HE2  | 1.64                     | 0.61              |
| 2:B:1096:VAL:O    | 2:B:1099:THR:HB   | 2.00                     | 0.61              |
| 1:A:664:LEU:HD21  | 3:C:2091:TYR:CB   | 2.31                     | 0.61              |
| 4:D:64:ARG:HA     | 4:D:86:HIS:O      | 2.00                     | 0.61              |
| 1:A:648:VAL:HB    | 1:A:672:ASN:ND2   | 2.15                     | 0.61              |
| 4:D:248:CYS:O     | 4:D:249:ASP:HB2   | 2.01                     | 0.61              |
| 4:D:253:LYS:HE3   | 4:D:254:PHE:CE1   | 2.36                     | 0.61              |
| 2:B:1084:TRP:HE3  | 3:C:2067:GLY:HA3  | 1.66                     | 0.61              |
| 1:A:636:ARG:HG2   | 2:B:1114:LEU:CD1  | 2.31                     | 0.61              |
| 3:C:2059:LEU:H    | 3:C:2059:LEU:CD1  | 2.13                     | 0.61              |
| 1:A:629:ARG:HG3   | 1:A:629:ARG:NH1   | 2.16                     | 0.61              |
| 1:A:628:GLN:NE2   | 3:C:2092:LEU:HD21 | 2.13                     | 0.60              |
| 1:A:621:LEU:HD23  | 1:A:651:VAL:HB    | 1.84                     | 0.60              |
| 2:B:1021:MET:HA   | 2:B:1123:LYS:NZ   | 2.17                     | 0.60              |
| 2:B:1099:THR:HG23 | 3:C:2110:ILE:HB   | 1.84                     | 0.60              |
| 1:A:499:ILE:HD13  | 1:A:499:ILE:C     | 2.26                     | 0.60              |
| 1:A:529:GLU:HB3   | 1:A:680:VAL:HG11  | 1.84                     | 0.60              |
| 3:C:2012:HIS:HD1  | 3:C:2124:GLN:HB3  | 1.64                     | 0.60              |
| 4:D:84:LEU:HB2    | 4:D:107:VAL:CG1   | 2.27                     | 0.60              |
| 4:D:120:LEU:HB3   | 4:D:123:LEU:HD12  | 1.84                     | 0.60              |
| 1:A:499:ILE:HA    | 1:A:573:ARG:NH2   | 2.16                     | 0.60              |
| 1:A:576:GLU:OE2   | 1:A:576:GLU:HA    | 2.01                     | 0.59              |
| 3:C:2037:ALA:HB2  | 3:C:2123:PHE:HB3  | 1.84                     | 0.59              |
| 1:A:513:LEU:HD12  | 1:A:514:ASP:N     | 2.17                     | 0.59              |
| 4:D:209:CYS:HB3   | 4:D:259:TYR:CD1   | 2.37                     | 0.59              |
| 1:A:511:ARG:NH1   | 1:A:696:ASP:HA    | 2.17                     | 0.59              |
| 4:D:259:TYR:CE2   | 4:D:261:GLY:HA2   | 2.37                     | 0.59              |
| 1:A:702:PRO:N     | 1:A:703:PRO:HD2   | 2.17                     | 0.59              |
| 1:A:549:LYS:CB    | 4:D:9:VAL:HG21    | 2.32                     | 0.59              |
| 4:D:4:CYS:HB3     | 4:D:16:ASN:O      | 2.02                     | 0.59              |
| 4:D:230:TRP:HH2   | 4:D:237:LYS:HD3   | 1.67                     | 0.59              |
| 4:D:55:THR:O      | 4:D:56:ARG:HB2    | 2.03                     | 0.58              |
| 3:C:2097:GLU:C    | 3:C:2113:CYS:SG   | 2.87                     | 0.58              |
| 4:D:25:LEU:HD11   | 4:D:29:LEU:CD1    | 2.33                     | 0.58              |
| 1:A:499:ILE:HD11  | 1:A:574:PRO:CD    | 2.34                     | 0.58              |
| 4:D:161:THR:HA    | 4:D:183:SER:O     | 2.04                     | 0.58              |
| 2:B:1065:LEU:HA   | 2:B:1108:LYS:HB2  | 1.83                     | 0.58              |
| 4:D:49:ALA:C      | 4:D:51:LEU:H      | 2.12                     | 0.58              |
| 2:B:1022:ASN:HD21 | 2:B:1025:ASP:CG   | 2.12                     | 0.57              |
| 1:A:703:PRO:HG2   | 1:A:704:PRO:C     | 2.29                     | 0.57              |
| 4:D:213:ILE:HG12  | 4:D:213:ILE:O     | 2.04                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:155:LEU:HB2   | 4:D:179:LEU:HD23  | 1.84                     | 0.57              |
| 4:D:253:LYS:HE3   | 4:D:254:PHE:CD1   | 2.39                     | 0.57              |
| 1:A:677:LEU:N     | 1:A:677:LEU:HD12  | 2.20                     | 0.57              |
| 1:A:573:ARG:HB2   | 1:A:573:ARG:HH11  | 1.69                     | 0.57              |
| 1:A:608:LYS:HD2   | 4:D:128:GLU:OE2   | 2.03                     | 0.57              |
| 2:B:1096:VAL:HG23 | 3:C:2108:TRP:O    | 2.05                     | 0.57              |
| 3:C:2056:SER:O    | 3:C:2057:GLU:HB2  | 2.03                     | 0.57              |
| 4:D:193:GLY:HA3   | 4:D:195:HIS:CE1   | 2.39                     | 0.57              |
| 4:D:47:SER:OG     | 4:D:71:GLN:HG3    | 2.05                     | 0.57              |
| 1:A:636:ARG:HG2   | 2:B:1114:LEU:HD13 | 1.87                     | 0.57              |
| 2:B:1099:THR:CG2  | 3:C:2110:ILE:HB   | 2.34                     | 0.57              |
| 4:D:52:MET:SD     | 4:D:75:THR:N      | 2.75                     | 0.57              |
| 1:A:663:ARG:HH22  | 3:C:2089:ASP:CA   | 2.18                     | 0.56              |
| 4:D:249:ASP:O     | 4:D:250:ASN:O     | 2.23                     | 0.56              |
| 3:C:2065:TRP:HB2  | 3:C:2119:PHE:HB3  | 1.86                     | 0.56              |
| 1:A:522:SER:HB3   | 1:A:592:ALA:HB2   | 1.88                     | 0.55              |
| 4:D:144:LEU:HD11  | 4:D:153:LEU:HD22  | 1.89                     | 0.55              |
| 4:D:14:GLU:HG3    | 4:D:35:ILE:CG1    | 2.35                     | 0.55              |
| 4:D:34:THR:HA     | 4:D:56:ARG:O      | 2.05                     | 0.55              |
| 4:D:6:VAL:HG21    | 4:D:30:PRO:HG2    | 1.88                     | 0.55              |
| 2:B:1084:TRP:CG   | 3:C:2041:SER:HB2  | 2.42                     | 0.55              |
| 2:B:1041:SER:HA   | 3:C:2079:TRP:CZ3  | 2.42                     | 0.55              |
| 2:B:1086:ASP:HA   | 3:C:2038:HIS:CD2  | 2.42                     | 0.55              |
| 3:C:2086:ASP:C    | 3:C:2086:ASP:OD2  | 2.50                     | 0.55              |
| 1:A:664:LEU:O     | 1:A:668:GLN:HG2   | 2.07                     | 0.54              |
| 2:B:1023:TRP:CZ3  | 2:B:1072:ARG:HD2  | 2.43                     | 0.54              |
| 2:B:1100:VAL:HG12 | 2:B:1102:LYS:HG3  | 1.88                     | 0.54              |
| 3:C:2046:GLU:CD   | 3:C:2046:GLU:H    | 2.15                     | 0.54              |
| 4:D:253:LYS:HG2   | 4:D:254:PHE:CD2   | 2.42                     | 0.54              |
| 1:A:571:ARG:NH1   | 4:D:14:GLU:CD     | 2.66                     | 0.54              |
| 2:B:1075:ASN:ND2  | 2:B:1075:ASN:H    | 2.04                     | 0.54              |
| 4:D:25:LEU:HD11   | 4:D:29:LEU:HD12   | 1.90                     | 0.54              |
| 2:B:1093:GLU:HA   | 3:C:2108:TRP:CH2  | 2.43                     | 0.54              |
| 3:C:2006:TRP:CD2  | 3:C:2015:ARG:HB2  | 2.43                     | 0.54              |
| 4:D:207:TRP:HB2   | 4:D:248:CYS:HA    | 1.90                     | 0.54              |
| 1:A:543:ARG:HG3   | 1:A:543:ARG:HH11  | 1.73                     | 0.54              |
| 4:D:209:CYS:SG    | 4:D:213:ILE:HD13  | 2.47                     | 0.53              |
| 1:A:663:ARG:CD    | 1:A:664:LEU:HD12  | 2.37                     | 0.53              |
| 4:D:67:LEU:HD23   | 4:D:89:LEU:HD21   | 1.91                     | 0.53              |
| 4:D:34:THR:OG1    | 4:D:35:ILE:HD13   | 2.08                     | 0.53              |
| 1:A:676:VAL:C     | 1:A:677:LEU:HD12  | 2.33                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:135:GLU:HA    | 4:D:159:GLN:NE2   | 2.23                     | 0.53              |
| 1:A:538:VAL:HG13  | 1:A:578:ARG:HG2   | 1.90                     | 0.53              |
| 4:D:172:GLU:C     | 4:D:173:ASN:OD1   | 2.52                     | 0.53              |
| 1:A:501:GLU:OE2   | 1:A:573:ARG:HD3   | 2.08                     | 0.53              |
| 3:C:2097:GLU:HB3  | 3:C:2111:ILE:O    | 2.08                     | 0.53              |
| 4:D:92:LEU:HD12   | 4:D:93:PRO:HD2    | 1.91                     | 0.53              |
| 1:A:647:ILE:HD12  | 1:A:647:ILE:H     | 1.74                     | 0.53              |
| 4:D:128:GLU:HG2   | 4:D:152:LYS:CG    | 2.39                     | 0.53              |
| 4:D:202:LEU:HB2   | 4:D:246:VAL:HG22  | 1.90                     | 0.53              |
| 1:A:628:GLN:HE22  | 3:C:2096:TYR:HE2  | 1.56                     | 0.53              |
| 4:D:137:LYS:O     | 4:D:160:LEU:HA    | 2.09                     | 0.53              |
| 4:D:164:PRO:O     | 4:D:167:LEU:N     | 2.42                     | 0.53              |
| 1:A:581:ALA:O     | 1:A:584:VAL:HG23  | 2.09                     | 0.52              |
| 4:D:220:LEU:HD11  | 4:D:246:VAL:HG11  | 1.90                     | 0.52              |
| 1:A:636:ARG:NH2   | 2:B:1107:GLU:OE1  | 2.34                     | 0.52              |
| 1:A:622:MET:HE1   | 1:A:658:ASN:HB3   | 1.90                     | 0.52              |
| 1:A:682:GLU:OE1   | 1:A:685:GLN:NE2   | 2.43                     | 0.52              |
| 1:A:703:PRO:HG2   | 1:A:704:PRO:CA    | 2.38                     | 0.52              |
| 1:A:622:MET:CE    | 1:A:658:ASN:HB3   | 2.39                     | 0.52              |
| 2:B:1044:ILE:HG22 | 2:B:1045:TYR:CG   | 2.44                     | 0.52              |
| 3:C:2015:ARG:HG2  | 3:C:2015:ARG:HH11 | 1.74                     | 0.52              |
| 1:A:522:SER:C     | 1:A:524:ARG:H     | 2.17                     | 0.52              |
| 4:D:140:PRO:HG2   | 4:D:143:LEU:HB2   | 1.91                     | 0.52              |
| 1:A:664:LEU:HD21  | 3:C:2091:TYR:CG   | 2.45                     | 0.52              |
| 1:A:556:VAL:HA    | 1:A:563:HIS:O     | 2.09                     | 0.52              |
| 3:C:2042:PHE:HE2  | 3:C:2051:VAL:HG21 | 1.75                     | 0.52              |
| 4:D:102:LEU:HD23  | 4:D:123:LEU:HD22  | 1.92                     | 0.52              |
| 1:A:505:HIS:HE1   | 1:A:542:GLU:OE1   | 1.94                     | 0.51              |
| 2:B:1069:ILE:HG12 | 2:B:1104:PHE:O    | 2.09                     | 0.51              |
| 4:D:125:GLU:O     | 4:D:127:GLN:HG3   | 2.10                     | 0.51              |
| 4:D:202:LEU:HD13  | 4:D:216:PHE:CZ    | 2.45                     | 0.51              |
| 1:A:628:GLN:NE2   | 3:C:2096:TYR:CE2  | 2.77                     | 0.51              |
| 4:D:49:ALA:HB2    | 4:D:73:ASP:O      | 2.10                     | 0.51              |
| 4:D:197:LEU:HD23  | 4:D:200:ALA:HB2   | 1.91                     | 0.51              |
| 4:D:210:ASN:O     | 4:D:259:TYR:CE2   | 2.64                     | 0.51              |
| 2:B:1030:CYS:SG   | 2:B:1039:LEU:HD23 | 2.50                     | 0.51              |
| 2:B:1075:ASN:ND2  | 3:C:2076:ARG:H    | 2.05                     | 0.51              |
| 4:D:233:GLY:C     | 4:D:235:ASP:H     | 2.17                     | 0.51              |
| 4:D:52:MET:C      | 4:D:54:TYR:H      | 2.19                     | 0.51              |
| 4:D:180:GLN:HG3   | 4:D:203:HIS:CE1   | 2.46                     | 0.51              |
| 1:A:599:LYS:HE2   | 4:D:199:PHE:CE1   | 2.46                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:42:LEU:O      | 4:D:43:LEU:C      | 2.53                     | 0.51              |
| 1:A:638:VAL:HG11  | 1:A:668:GLN:HG3   | 1.93                     | 0.51              |
| 2:B:1021:MET:HA   | 2:B:1123:LYS:HZ2  | 1.76                     | 0.51              |
| 4:D:120:LEU:CB    | 4:D:123:LEU:HD12  | 2.41                     | 0.51              |
| 1:A:533:LEU:O     | 1:A:536:PHE:HB3   | 2.11                     | 0.50              |
| 4:D:1:HIS:ND1     | 4:D:2:PRO:HD2     | 2.27                     | 0.50              |
| 1:A:628:GLN:NE2   | 3:C:2096:TYR:HE2  | 2.09                     | 0.50              |
| 4:D:47:SER:HB2    | 4:D:50:THR:HG23   | 1.92                     | 0.50              |
| 4:D:102:LEU:HD21  | 4:D:105:LEU:HD13  | 1.93                     | 0.50              |
| 3:C:2116:PHE:HB2  | 4:D:221:GLN:HB3   | 1.92                     | 0.50              |
| 1:A:557:GLU:OE2   | 1:A:559:HIS:ND1   | 2.44                     | 0.50              |
| 3:C:2076:ARG:HG3  | 3:C:2076:ARG:NH1  | 2.27                     | 0.50              |
| 1:A:522:SER:C     | 1:A:588:GLY:HA2   | 2.36                     | 0.50              |
| 1:A:665:ILE:CG2   | 1:A:672:ASN:HD22  | 2.24                     | 0.50              |
| 2:B:1079:GLN:HB2  | 3:C:2071:VAL:HB   | 1.92                     | 0.50              |
| 2:B:1061:GLN:O    | 2:B:1062:SER:OG   | 2.20                     | 0.50              |
| 2:B:1073:VAL:HG13 | 3:C:2075:CYS:HB3  | 1.94                     | 0.50              |
| 3:C:2009:TYR:HB3  | 3:C:2014:TYR:CE1  | 2.46                     | 0.50              |
| 4:D:178:LEU:HD23  | 4:D:201:PHE:CD1   | 2.46                     | 0.50              |
| 4:D:132:LYS:HE3   | 4:D:157:ASN:OD1   | 2.12                     | 0.50              |
| 4:D:247:GLN:OE1   | 4:D:253:LYS:N     | 2.44                     | 0.50              |
| 4:D:233:GLY:O     | 4:D:235:ASP:N     | 2.39                     | 0.50              |
| 1:A:527:GLU:HA    | 1:A:586:TYR:CD1   | 2.47                     | 0.49              |
| 2:B:1108:LYS:HA   | 2:B:1112:PHE:CZ   | 2.47                     | 0.49              |
| 2:B:1075:ASN:HD21 | 3:C:2076:ARG:N    | 2.05                     | 0.49              |
| 3:C:2009:TYR:HB2  | 3:C:2050:PHE:CD2  | 2.48                     | 0.49              |
| 4:D:35:ILE:HD13   | 4:D:35:ILE:H      | 1.76                     | 0.49              |
| 1:A:609:ILE:O     | 1:A:609:ILE:HG22  | 2.11                     | 0.49              |
| 4:D:197:LEU:O     | 4:D:226:ASN:HB3   | 2.12                     | 0.49              |
| 1:A:501:GLU:OE1   | 1:A:573:ARG:HG2   | 2.12                     | 0.49              |
| 2:B:1049:LYS:HD2  | 2:B:1113:VAL:HG13 | 1.93                     | 0.49              |
| 1:A:565:TYR:CD2   | 4:D:236:VAL:HG22  | 2.48                     | 0.49              |
| 2:B:1086:ASP:C    | 2:B:1086:ASP:OD1  | 2.55                     | 0.49              |
| 3:C:2076:ARG:HG3  | 3:C:2076:ARG:HH11 | 1.77                     | 0.49              |
| 1:A:616:ARG:HH11  | 1:A:616:ARG:HG3   | 1.76                     | 0.49              |
| 4:D:6:VAL:HG22    | 4:D:15:VAL:CG2    | 2.36                     | 0.49              |
| 4:D:164:PRO:O     | 4:D:165:ALA:C     | 2.55                     | 0.49              |
| 2:B:1098:ARG:HG3  | 2:B:1098:ARG:O    | 2.13                     | 0.48              |
| 2:B:1108:LYS:HA   | 2:B:1112:PHE:CE1  | 2.48                     | 0.48              |
| 3:C:2065:TRP:HA   | 3:C:2065:TRP:CE3  | 2.47                     | 0.48              |
| 1:A:632:ARG:HH11  | 3:C:2114:THR:CG2  | 2.15                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:D:121:ARG:HA    | 4:D:146:PRO:HG2  | 1.96                     | 0.48              |
| 4:D:208:LEU:HG    | 4:D:210:ASN:ND2  | 2.28                     | 0.48              |
| 1:A:565:TYR:CE2   | 4:D:236:VAL:HG22 | 2.48                     | 0.48              |
| 1:A:579:ARG:HH11  | 1:A:579:ARG:HG2  | 1.77                     | 0.48              |
| 4:D:95:LEU:HD12   | 4:D:105:LEU:CD1  | 2.43                     | 0.48              |
| 1:A:530:PHE:O     | 1:A:534:LYS:HG3  | 2.13                     | 0.48              |
| 2:B:1126:PHE:CD1  | 2:B:1126:PHE:N   | 2.79                     | 0.48              |
| 3:C:2018:LYS:O    | 3:C:2018:LYS:HG3 | 2.12                     | 0.48              |
| 2:B:1039:LEU:HB2  | 2:B:1070:GLY:HA2 | 1.95                     | 0.48              |
| 3:C:2029:PHE:O    | 3:C:2033:GLN:HG2 | 2.14                     | 0.48              |
| 2:B:1084:TRP:HD1  | 2:B:1088:SER:O   | 1.96                     | 0.48              |
| 1:A:663:ARG:CZ    | 1:A:667:LYS:NZ   | 2.77                     | 0.48              |
| 3:C:2016:PHE:HE1  | 3:C:2118:ASN:HB3 | 1.78                     | 0.48              |
| 4:D:35:ILE:HD13   | 4:D:35:ILE:N     | 2.28                     | 0.48              |
| 4:D:94:LEU:N      | 4:D:94:LEU:HD22  | 2.28                     | 0.48              |
| 1:A:703:PRO:CB    | 1:A:704:PRO:C    | 2.86                     | 0.48              |
| 2:B:1060:ILE:HD11 | 2:B:1064:ASP:HB2 | 1.96                     | 0.48              |
| 1:A:616:ARG:NH2   | 1:A:645:LYS:HB2  | 2.26                     | 0.48              |
| 4:D:14:GLU:CB     | 4:D:35:ILE:HD11  | 2.44                     | 0.48              |
| 1:A:512:LEU:HB2   | 1:A:699:PRO:HG2  | 1.96                     | 0.47              |
| 1:A:535:ALA:O     | 1:A:539:ASP:HB2  | 2.14                     | 0.47              |
| 1:A:604:GLN:HE21  | 4:D:239:MET:CE   | 2.26                     | 0.47              |
| 2:B:1107:GLU:O    | 2:B:1112:PHE:HA  | 2.13                     | 0.47              |
| 4:D:17:CYS:O      | 4:D:20:ARG:HB2   | 2.14                     | 0.47              |
| 4:D:38:LEU:HB2    | 4:D:62:LEU:HD23  | 1.96                     | 0.47              |
| 1:A:616:ARG:HG3   | 1:A:616:ARG:NH1  | 2.29                     | 0.47              |
| 1:A:657:ALA:O     | 1:A:659:LEU:HD22 | 2.13                     | 0.47              |
| 1:A:687:ARG:NH1   | 1:A:688:ASP:OD1  | 2.46                     | 0.47              |
| 3:C:2061:GLY:CA   | 3:C:2102:LYS:HE3 | 2.40                     | 0.47              |
| 4:D:202:LEU:HD13  | 4:D:216:PHE:HZ   | 1.80                     | 0.47              |
| 1:A:508:TYR:CE1   | 1:A:545:ARG:HA   | 2.50                     | 0.47              |
| 1:A:523:SER:N     | 1:A:588:GLY:HA2  | 2.29                     | 0.47              |
| 1:A:634:PHE:CZ    | 1:A:661:GLN:HB3  | 2.50                     | 0.47              |
| 2:B:1059:ASN:C    | 2:B:1061:GLN:N   | 2.72                     | 0.47              |
| 2:B:1071:LEU:HD11 | 3:C:2077:PHE:HB3 | 1.95                     | 0.47              |
| 2:B:1110:LEU:HD12 | 2:B:1110:LEU:HA  | 1.67                     | 0.47              |
| 3:C:2002:CYS:SG   | 3:C:2007:SER:O   | 2.73                     | 0.47              |
| 1:A:522:SER:HA    | 1:A:589:SER:H    | 1.79                     | 0.47              |
| 1:A:663:ARG:HD2   | 1:A:663:ARG:C    | 2.40                     | 0.47              |
| 3:C:2014:TYR:HA   | 3:C:2121:CYS:O   | 2.15                     | 0.47              |
| 4:D:164:PRO:HB2   | 4:D:167:LEU:HB2  | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:519:LEU:HD12  | 1:A:519:LEU:N     | 2.30                     | 0.47              |
| 2:B:1096:VAL:O    | 2:B:1097:GLU:C    | 2.58                     | 0.47              |
| 1:A:522:SER:C     | 1:A:524:ARG:N     | 2.73                     | 0.47              |
| 4:D:254:PHE:CD2   | 4:D:254:PHE:N     | 2.82                     | 0.47              |
| 2:B:1122:GLN:HG2  | 2:B:1124:ASN:ND2  | 2.30                     | 0.46              |
| 3:C:2040:VAL:CG1  | 3:C:2066:ILE:HG22 | 2.45                     | 0.46              |
| 4:D:121:ARG:HA    | 4:D:146:PRO:CG    | 2.44                     | 0.46              |
| 1:A:593:SER:HB2   | 1:A:630:MET:HE1   | 1.96                     | 0.46              |
| 1:A:603:PHE:O     | 1:A:607:SER:HB3   | 2.16                     | 0.46              |
| 2:B:1023:TRP:CH2  | 2:B:1072:ARG:HD2  | 2.50                     | 0.46              |
| 3:C:2004:PRO:C    | 3:C:2006:TRP:H    | 2.24                     | 0.46              |
| 1:A:499:ILE:HG23  | 1:A:500:SER:N     | 2.31                     | 0.46              |
| 4:D:139:LEU:HD11  | 4:D:155:LEU:CD1   | 2.45                     | 0.46              |
| 1:A:647:ILE:HD12  | 1:A:647:ILE:N     | 2.30                     | 0.46              |
| 4:D:118:GLY:HA2   | 4:D:121:ARG:HB2   | 1.98                     | 0.46              |
| 1:A:532:VAL:HG11  | 1:A:680:VAL:HG23  | 1.97                     | 0.46              |
| 1:A:632:ARG:NH1   | 3:C:2114:THR:HG21 | 2.17                     | 0.46              |
| 4:D:1:HIS:HB3     | 4:D:4:CYS:O       | 2.16                     | 0.46              |
| 4:D:128:GLU:OE1   | 4:D:130:TYR:OH    | 2.27                     | 0.46              |
| 1:A:557:GLU:OE2   | 1:A:559:HIS:CE1   | 2.69                     | 0.46              |
| 2:B:1022:ASN:HD22 | 2:B:1022:ASN:N    | 1.99                     | 0.46              |
| 4:D:14:GLU:HG3    | 4:D:35:ILE:HG12   | 1.97                     | 0.46              |
| 4:D:197:LEU:CD2   | 4:D:200:ALA:HB2   | 2.45                     | 0.46              |
| 1:A:703:PRO:CG    | 1:A:704:PRO:C     | 2.88                     | 0.46              |
| 4:D:193:GLY:HA3   | 4:D:195:HIS:ND1   | 2.31                     | 0.46              |
| 1:A:532:VAL:HB    | 1:A:680:VAL:HB    | 1.97                     | 0.46              |
| 3:C:2023:TRP:CZ2  | 3:C:2069:SER:HB3  | 2.51                     | 0.46              |
| 3:C:2072:TRP:HA   | 3:C:2072:TRP:CE3  | 2.51                     | 0.46              |
| 4:D:139:LEU:HD11  | 4:D:155:LEU:HD13  | 1.97                     | 0.46              |
| 1:A:642:LYS:HE3   | 1:A:669:ALA:HB2   | 1.97                     | 0.46              |
| 3:C:2091:TYR:O    | 3:C:2092:LEU:C    | 2.59                     | 0.46              |
| 4:D:18:ASP:HB3    | 4:D:39:SER:OG     | 2.16                     | 0.46              |
| 1:A:642:LYS:HD2   | 1:A:669:ALA:HB2   | 1.98                     | 0.45              |
| 1:A:663:ARG:CD    | 1:A:663:ARG:C     | 2.89                     | 0.45              |
| 3:C:2006:TRP:NE1  | 3:C:2015:ARG:HH11 | 2.13                     | 0.45              |
| 4:D:49:ALA:O      | 4:D:51:LEU:N      | 2.49                     | 0.45              |
| 1:A:509:CYS:HB3   | 1:A:544:LEU:HD23  | 1.98                     | 0.45              |
| 4:D:120:LEU:HA    | 4:D:123:LEU:HD12  | 1.97                     | 0.45              |
| 4:D:56:ARG:HA     | 4:D:78:VAL:HG21   | 1.98                     | 0.45              |
| 1:A:501:GLU:OE2   | 1:A:575:SER:HB3   | 2.15                     | 0.45              |
| 2:B:1066:TYR:HA   | 2:B:1106:LEU:O    | 2.16                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:1077:GLU:N    | 2:B:1077:GLU:CD  | 2.74                     | 0.45              |
| 1:A:649:ILE:HD11  | 1:A:693:TYR:HE2  | 1.80                     | 0.45              |
| 1:A:702:PRO:N     | 1:A:703:PRO:CD   | 2.78                     | 0.45              |
| 2:B:1084:TRP:C    | 2:B:1086:ASP:H   | 2.23                     | 0.45              |
| 3:C:2097:GLU:HB3  | 3:C:2111:ILE:C   | 2.42                     | 0.45              |
| 4:D:107:VAL:HG23  | 4:D:131:LEU:HD23 | 1.99                     | 0.45              |
| 4:D:144:LEU:HD22  | 4:D:150:LEU:HD22 | 1.99                     | 0.45              |
| 1:A:531:GLU:O     | 1:A:532:VAL:C    | 2.60                     | 0.45              |
| 1:A:579:ARG:HG2   | 1:A:579:ARG:NH1  | 2.31                     | 0.45              |
| 1:A:665:ILE:HG22  | 1:A:672:ASN:HD22 | 1.82                     | 0.45              |
| 1:A:702:PRO:HG2   | 1:A:703:PRO:HD3  | 1.98                     | 0.45              |
| 4:D:202:LEU:HB2   | 4:D:246:VAL:CG2  | 2.46                     | 0.45              |
| 3:C:2039:LEU:CD2  | 3:C:2119:PHE:HB2 | 2.47                     | 0.45              |
| 3:C:2027:GLU:O    | 3:C:2028:GLU:C   | 2.60                     | 0.44              |
| 3:C:2086:ASP:O    | 3:C:2088:ASP:N   | 2.50                     | 0.44              |
| 4:D:42:LEU:O      | 4:D:44:TYR:N     | 2.49                     | 0.44              |
| 4:D:231:LYS:O     | 4:D:231:LYS:HD3  | 2.17                     | 0.44              |
| 1:A:537:VAL:O     | 1:A:541:MET:HG3  | 2.17                     | 0.44              |
| 4:D:49:ALA:HB1    | 4:D:52:MET:HE2   | 1.99                     | 0.44              |
| 4:D:52:MET:C      | 4:D:54:TYR:N     | 2.73                     | 0.44              |
| 4:D:245:SER:O     | 4:D:247:GLN:HG2  | 2.17                     | 0.44              |
| 2:B:1068:TRP:HB2  | 2:B:1126:PHE:HB3 | 1.98                     | 0.44              |
| 1:A:663:ARG:HH12  | 2:B:1045:TYR:HE2 | 1.66                     | 0.44              |
| 2:B:1074:GLU:HB3  | 3:C:2076:ARG:O   | 2.17                     | 0.44              |
| 2:B:1084:TRP:CD2  | 3:C:2041:SER:HB2 | 2.52                     | 0.44              |
| 2:B:1044:ILE:HG12 | 2:B:1115:TRP:CH2 | 2.53                     | 0.44              |
| 2:B:1056:VAL:O    | 2:B:1057:THR:C   | 2.61                     | 0.44              |
| 4:D:60:LEU:HD23   | 4:D:82:LEU:HD11  | 1.96                     | 0.44              |
| 4:D:101:ALA:O     | 4:D:103:THR:HG23 | 2.16                     | 0.44              |
| 4:D:127:GLN:HA    | 4:D:150:LEU:HA   | 2.00                     | 0.44              |
| 2:B:1065:LEU:O    | 2:B:1108:LYS:N   | 2.51                     | 0.44              |
| 4:D:25:LEU:HD11   | 4:D:29:LEU:HD11  | 1.99                     | 0.44              |
| 1:A:559:HIS:HA    | 1:A:592:ALA:HA   | 2.00                     | 0.44              |
| 4:D:18:ASP:HA     | 4:D:39:SER:O     | 2.18                     | 0.44              |
| 4:D:72:VAL:HG23   | 4:D:72:VAL:O     | 2.18                     | 0.44              |
| 4:D:94:LEU:N      | 4:D:94:LEU:CD2   | 2.80                     | 0.44              |
| 4:D:22:LEU:HD13   | 4:D:26:PRO:CG    | 2.47                     | 0.44              |
| 4:D:52:MET:N      | 4:D:53:PRO:CD    | 2.81                     | 0.44              |
| 1:A:498:ASP:OD2   | 1:A:499:ILE:HG22 | 2.19                     | 0.43              |
| 4:D:167:LEU:HD12  | 4:D:167:LEU:O    | 2.18                     | 0.43              |
| 2:B:1100:VAL:HG13 | 3:C:2072:TRP:HH2 | 1.82                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:2015:ARG:HG2  | 3:C:2015:ARG:NH1  | 2.33                     | 0.43              |
| 4:D:105:LEU:HD23  | 4:D:129:LEU:CD1   | 2.48                     | 0.43              |
| 4:D:177:LEU:HB3   | 4:D:197:LEU:HD21  | 1.99                     | 0.43              |
| 1:A:543:ARG:HG3   | 1:A:543:ARG:NH1   | 2.33                     | 0.43              |
| 1:A:574:PRO:O     | 1:A:578:ARG:HB2   | 2.19                     | 0.43              |
| 2:B:1041:SER:HA   | 3:C:2079:TRP:CE3  | 2.53                     | 0.43              |
| 1:A:546:ILE:CD1   | 1:A:577:LEU:CD1   | 2.95                     | 0.43              |
| 3:C:2009:TYR:HB2  | 3:C:2050:PHE:CE2  | 2.54                     | 0.43              |
| 4:D:70:LEU:HD23   | 4:D:93:PRO:CB     | 2.49                     | 0.43              |
| 1:A:687:ARG:HG2   | 1:A:688:ASP:N     | 2.34                     | 0.43              |
| 4:D:58:THR:HA     | 4:D:78:VAL:O      | 2.18                     | 0.43              |
| 4:D:120:LEU:CA    | 4:D:123:LEU:HD12  | 2.48                     | 0.43              |
| 4:D:132:LYS:HA    | 4:D:156:ALA:O     | 2.19                     | 0.43              |
| 4:D:192:PHE:O     | 4:D:195:HIS:ND1   | 2.51                     | 0.43              |
| 4:D:84:LEU:CB     | 4:D:107:VAL:HG12  | 2.34                     | 0.43              |
| 4:D:213:ILE:CD1   | 4:D:256:VAL:HG13  | 2.49                     | 0.43              |
| 3:C:2020:TRP:CE3  | 4:D:221:GLN:NE2   | 2.86                     | 0.43              |
| 4:D:13:LEU:HD23   | 4:D:32:ASP:C      | 2.44                     | 0.43              |
| 1:A:541:MET:HA    | 1:A:544:LEU:HD12  | 2.01                     | 0.43              |
| 2:B:1077:GLU:CD   | 2:B:1077:GLU:H    | 2.26                     | 0.43              |
| 1:A:507:PHE:CD1   | 1:A:507:PHE:C     | 2.97                     | 0.43              |
| 3:C:2050:PHE:CZ   | 3:C:2054:LEU:HD21 | 2.54                     | 0.43              |
| 3:C:2055:THR:O    | 3:C:2056:SER:C    | 2.62                     | 0.43              |
| 3:C:2066:ILE:O    | 3:C:2068:LEU:N    | 2.52                     | 0.43              |
| 3:C:2098:CYS:N    | 3:C:2113:CYS:SG   | 2.92                     | 0.43              |
| 4:D:210:ASN:OD1   | 4:D:211:CYS:N     | 2.52                     | 0.43              |
| 1:A:524:ARG:HA    | 1:A:524:ARG:HD2   | 1.65                     | 0.42              |
| 4:D:5:GLU:O       | 4:D:15:VAL:HA     | 2.18                     | 0.42              |
| 4:D:56:ARG:CA     | 4:D:78:VAL:HG21   | 2.49                     | 0.42              |
| 1:A:546:ILE:HD12  | 1:A:553:VAL:CG1   | 2.49                     | 0.42              |
| 2:B:1110:LEU:HD23 | 2:B:1114:LEU:HD11 | 2.00                     | 0.42              |
| 4:D:6:VAL:CG2     | 4:D:15:VAL:HG22   | 2.35                     | 0.42              |
| 4:D:81:THR:HA     | 4:D:104:VAL:CG2   | 2.48                     | 0.42              |
| 4:D:95:LEU:HD12   | 4:D:105:LEU:HD11  | 2.01                     | 0.42              |
| 4:D:144:LEU:CD1   | 4:D:153:LEU:HD22  | 2.49                     | 0.42              |
| 3:C:2009:TYR:HB3  | 3:C:2014:TYR:HE1  | 1.84                     | 0.42              |
| 4:D:95:LEU:HB3    | 4:D:99:LEU:HB2    | 2.01                     | 0.42              |
| 4:D:80:GLY:HA2    | 4:D:102:LEU:CA    | 2.41                     | 0.42              |
| 1:A:658:ASN:OD1   | 1:A:661:GLN:HG3   | 2.20                     | 0.42              |
| 4:D:47:SER:CA     | 4:D:71:GLN:HB2    | 2.29                     | 0.42              |
| 4:D:128:GLU:HG2   | 4:D:152:LYS:HG2   | 2.01                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:1043:LYS:HB3  | 2:B:1046:SER:OG  | 2.19                     | 0.42              |
| 3:C:2019:GLU:HB3  | 3:C:2021:MET:HE3 | 2.01                     | 0.42              |
| 4:D:14:GLU:CA     | 4:D:35:ILE:HD11  | 2.49                     | 0.42              |
| 4:D:135:GLU:O     | 4:D:137:LYS:HD2  | 2.19                     | 0.42              |
| 1:A:565:TYR:CE2   | 4:D:236:VAL:CG2  | 3.03                     | 0.42              |
| 1:A:703:PRO:HG2   | 1:A:704:PRO:O    | 2.20                     | 0.42              |
| 2:B:1029:PHE:CD1  | 2:B:1029:PHE:C   | 2.97                     | 0.42              |
| 4:D:34:THR:HG1    | 4:D:35:ILE:HD13  | 1.83                     | 0.42              |
| 1:A:663:ARG:NH2   | 3:C:2089:ASP:HA  | 2.30                     | 0.42              |
| 3:C:2016:PHE:CD1  | 3:C:2017:PHE:N   | 2.88                     | 0.42              |
| 1:A:619:LEU:HD12  | 1:A:619:LEU:HA   | 1.85                     | 0.42              |
| 2:B:1055:LEU:HD12 | 2:B:1055:LEU:HA  | 1.86                     | 0.42              |
| 3:C:2037:ALA:CB   | 3:C:2123:PHE:HB3 | 2.49                     | 0.42              |
| 4:D:167:LEU:HG    | 4:D:168:LEU:HD23 | 2.00                     | 0.42              |
| 1:A:500:SER:O     | 1:A:501:GLU:HB2  | 2.19                     | 0.42              |
| 1:A:686:GLN:O     | 1:A:690:ILE:HD13 | 2.20                     | 0.42              |
| 3:C:2124:GLN:HE21 | 3:C:2124:GLN:HB2 | 1.54                     | 0.41              |
| 1:A:559:HIS:HB3   | 1:A:589:SER:OG   | 2.20                     | 0.41              |
| 1:A:571:ARG:HH11  | 4:D:14:GLU:CD    | 2.28                     | 0.41              |
| 4:D:247:GLN:HB3   | 4:D:255:PRO:HA   | 2.03                     | 0.41              |
| 1:A:520:ASP:OD1   | 1:A:520:ASP:C    | 2.63                     | 0.41              |
| 1:A:541:MET:O     | 1:A:542:GLU:C    | 2.63                     | 0.41              |
| 3:C:2020:TRP:CD1  | 3:C:2020:TRP:N   | 2.88                     | 0.41              |
| 3:C:2053:SER:C    | 3:C:2055:THR:N   | 2.78                     | 0.41              |
| 1:A:499:ILE:HD11  | 1:A:573:ARG:HA   | 2.02                     | 0.41              |
| 1:A:644:LYS:O     | 1:A:645:LYS:HB2  | 2.21                     | 0.41              |
| 2:B:1075:ASN:HD21 | 3:C:2076:ARG:CB  | 2.33                     | 0.41              |
| 4:D:8:LYS:HG2     | 4:D:13:LEU:HD12  | 2.00                     | 0.41              |
| 4:D:14:GLU:HB2    | 4:D:35:ILE:HD11  | 2.00                     | 0.41              |
| 1:A:642:LYS:CE    | 1:A:669:ALA:HB2  | 2.50                     | 0.41              |
| 4:D:39:SER:CB     | 4:D:63:ASP:OD1   | 2.65                     | 0.41              |
| 4:D:180:GLN:O     | 4:D:181:GLU:HB2  | 2.21                     | 0.41              |
| 1:A:631:SER:HB2   | 3:C:2092:LEU:CD1 | 2.50                     | 0.41              |
| 4:D:80:GLY:CA     | 4:D:102:LEU:HA   | 2.42                     | 0.41              |
| 2:B:1021:MET:HA   | 2:B:1123:LYS:HZ3 | 1.85                     | 0.41              |
| 1:A:701:ALA:HB1   | 1:A:703:PRO:HD2  | 2.02                     | 0.41              |
| 2:B:1056:VAL:O    | 2:B:1059:ASN:N   | 2.53                     | 0.41              |
| 2:B:1056:VAL:O    | 2:B:1058:LYS:N   | 2.53                     | 0.41              |
| 3:C:2053:SER:C    | 3:C:2055:THR:H   | 2.28                     | 0.41              |
| 4:D:6:VAL:HG13    | 4:D:15:VAL:HG22  | 2.02                     | 0.41              |
| 1:A:606:PHE:CD1   | 1:A:616:ARG:HD2  | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1122:GLN:HE21 | 2:B:1122:GLN:HB2  | 1.62                     | 0.41              |
| 3:C:2040:VAL:HG21 | 3:C:2042:PHE:CE2  | 2.56                     | 0.41              |
| 3:C:2123:PHE:CD1  | 3:C:2123:PHE:C    | 2.99                     | 0.41              |
| 1:A:499:ILE:HG23  | 1:A:500:SER:H     | 1.86                     | 0.41              |
| 2:B:1070:GLY:O    | 3:C:2080:THR:HG23 | 2.21                     | 0.41              |
| 4:D:63:ASP:HA     | 4:D:85:SER:O      | 2.21                     | 0.41              |
| 4:D:92:LEU:HD22   | 4:D:115:LEU:HD22  | 2.03                     | 0.40              |
| 4:D:182:ASN:HB3   | 4:D:183:SER:H     | 1.80                     | 0.40              |
| 3:C:2029:PHE:O    | 3:C:2030:CYS:C    | 2.63                     | 0.40              |
| 1:A:498:ASP:O     | 1:A:499:ILE:C     | 2.64                     | 0.40              |
| 1:A:625:GLN:HG3   | 1:A:658:ASN:ND2   | 2.36                     | 0.40              |
| 2:B:1084:TRP:C    | 2:B:1086:ASP:N    | 2.79                     | 0.40              |
| 2:B:1103:CYS:O    | 2:B:1117:ASN:HA   | 2.22                     | 0.40              |
| 4:D:47:SER:O      | 4:D:48:LEU:C      | 2.64                     | 0.40              |
| 1:A:636:ARG:NH1   | 1:A:636:ARG:HG3   | 2.36                     | 0.40              |
| 1:A:690:ILE:HD12  | 1:A:690:ILE:N     | 2.36                     | 0.40              |
| 2:B:1093:GLU:HA   | 3:C:2108:TRP:CZ3  | 2.57                     | 0.40              |
| 2:B:1099:THR:CG2  | 3:C:2110:ILE:H    | 2.27                     | 0.40              |
| 3:C:2018:LYS:HD2  | 3:C:2118:ASN:OD1  | 2.20                     | 0.40              |
| 3:C:2044:SER:O    | 3:C:2047:GLU:HB3  | 2.22                     | 0.40              |
| 4:D:262:LYS:HB2   | 4:D:262:LYS:NZ    | 2.36                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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     | 206/208 (99%) | 183 (89%) | 19 (9%)  | 4 (2%)   | 6           | 17 |
| 2   | B     | 131/133 (98%) | 107 (82%) | 18 (14%) | 6 (5%)   | 2           | 4  |
| 3   | C     | 123/125 (98%) | 94 (76%)  | 20 (16%) | 9 (7%)   | 1           | 1  |
| 4   | D     | 263/265 (99%) | 216 (82%) | 36 (14%) | 11 (4%)  | 2           | 5  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles       |
|-----|-------|---------------|-----------|----------|----------|-------------------|
| All | All   | 723/731 (99%) | 600 (83%) | 93 (13%) | 30 (4%)  | <b>2</b> <b>5</b> |

All (30) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1061 | GLN  |
| 3   | C     | 2055 | THR  |
| 3   | C     | 2057 | GLU  |
| 3   | C     | 2067 | GLY  |
| 4   | D     | 43   | LEU  |
| 4   | D     | 56   | ARG  |
| 4   | D     | 195  | HIS  |
| 4   | D     | 250  | ASN  |
| 1   | A     | 703  | PRO  |
| 2   | B     | 1044 | ILE  |
| 2   | B     | 1057 | THR  |
| 3   | C     | 2056 | SER  |
| 3   | C     | 2087 | TYR  |
| 4   | D     | 50   | THR  |
| 4   | D     | 165  | ALA  |
| 1   | A     | 500  | SER  |
| 2   | B     | 1059 | ASN  |
| 4   | D     | 100  | PRO  |
| 4   | D     | 164  | PRO  |
| 4   | D     | 234  | VAL  |
| 1   | A     | 501  | GLU  |
| 2   | B     | 1097 | GLU  |
| 4   | D     | 157  | ASN  |
| 4   | D     | 249  | ASP  |
| 1   | A     | 670  | PRO  |
| 3   | C     | 2092 | LEU  |
| 2   | B     | 1099 | THR  |
| 3   | C     | 2042 | PHE  |
| 3   | C     | 2104 | THR  |
| 3   | C     | 2004 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A     | 185/186 (100%) | 172 (93%) | 13 (7%)  | 14          | 34 |
| 2   | B     | 118/119 (99%)  | 110 (93%) | 8 (7%)   | 14          | 35 |
| 3   | C     | 114/114 (100%) | 111 (97%) | 3 (3%)   | 40          | 65 |
| 4   | D     | 238/238 (100%) | 225 (94%) | 13 (6%)  | 19          | 43 |
| All | All   | 655/657 (100%) | 618 (94%) | 37 (6%)  | 19          | 43 |

All (37) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 499  | ILE  |
| 1   | A     | 513  | LEU  |
| 1   | A     | 559  | HIS  |
| 1   | A     | 562  | SER  |
| 1   | A     | 573  | ARG  |
| 1   | A     | 596  | GLU  |
| 1   | A     | 611  | ARG  |
| 1   | A     | 643  | LYS  |
| 1   | A     | 660  | LYS  |
| 1   | A     | 663  | ARG  |
| 1   | A     | 682  | GLU  |
| 1   | A     | 691  | VAL  |
| 1   | A     | 697  | LEU  |
| 2   | B     | 1022 | ASN  |
| 2   | B     | 1058 | LYS  |
| 2   | B     | 1074 | GLU  |
| 2   | B     | 1075 | ASN  |
| 2   | B     | 1076 | LYS  |
| 2   | B     | 1083 | GLU  |
| 2   | B     | 1099 | THR  |
| 2   | B     | 1110 | LEU  |
| 3   | C     | 2059 | LEU  |
| 3   | C     | 2093 | ILE  |
| 3   | C     | 2124 | GLN  |
| 4   | D     | 5    | GLU  |
| 4   | D     | 20   | ARG  |
| 4   | D     | 21   | GLN  |
| 4   | D     | 35   | ILE  |
| 4   | D     | 68   | THR  |
| 4   | D     | 75   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 79  | LEU  |
| 4   | D     | 94  | LEU  |
| 4   | D     | 137 | LYS  |
| 4   | D     | 143 | LEU  |
| 4   | D     | 232 | GLN  |
| 4   | D     | 248 | CYS  |
| 4   | D     | 262 | LYS  |

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

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 505  | HIS  |
| 1   | A     | 628  | GLN  |
| 1   | A     | 639  | GLN  |
| 1   | A     | 672  | ASN  |
| 1   | A     | 685  | GLN  |
| 2   | B     | 1012 | ASN  |
| 2   | B     | 1018 | GLN  |
| 2   | B     | 1022 | ASN  |
| 2   | B     | 1061 | GLN  |
| 2   | B     | 1075 | ASN  |
| 2   | B     | 1094 | ASN  |
| 3   | C     | 2124 | GLN  |
| 4   | D     | 16   | ASN  |
| 4   | D     | 61   | ASN  |
| 4   | D     | 86   | HIS  |
| 4   | D     | 88   | GLN  |
| 4   | D     | 159  | GLN  |
| 4   | D     | 226  | ASN  |
| 4   | D     | 232  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.