



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:40 AM UTC

PDB ID : 1WIIQ / pdb\_00001wiq  
Title : STRUCTURE OF T-CELL SURFACE GLYCOPROTEIN CD4, TRIGONAL CRYSTAL FORM  
Authors : Wu, H.; Kwong, P.D.; Hendrickson, W.A.  
Deposited on : 1996-12-18  
Resolution : 5.00 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

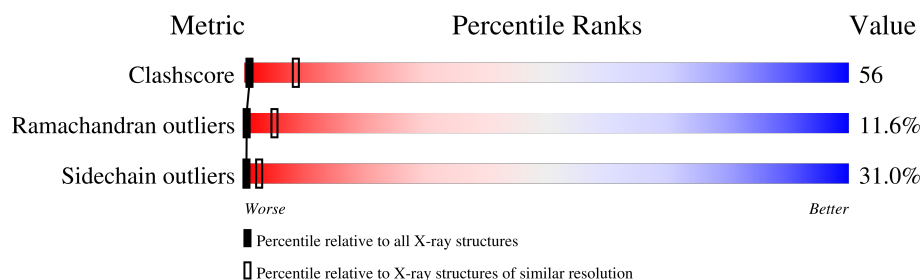
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.00 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 1040 (6.00-4.00)                                      |
| Ramachandran outliers | 187476                      | 1015 (6.06-3.92)                                      |
| Sidechain outliers    | 187428                      | 1136 (6.10-3.90)                                      |

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     | 363    | <div> <div></div> <div>20%</div> <div>47%</div> <div>28%</div> <div>5%</div> </div> |
| 1   | B     | 363    | <div> <div></div> <div>21%</div> <div>48%</div> <div>25%</div> <div>5%</div> </div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5624 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 T-CELL SURFACE GLYCOPROTEIN CD4.

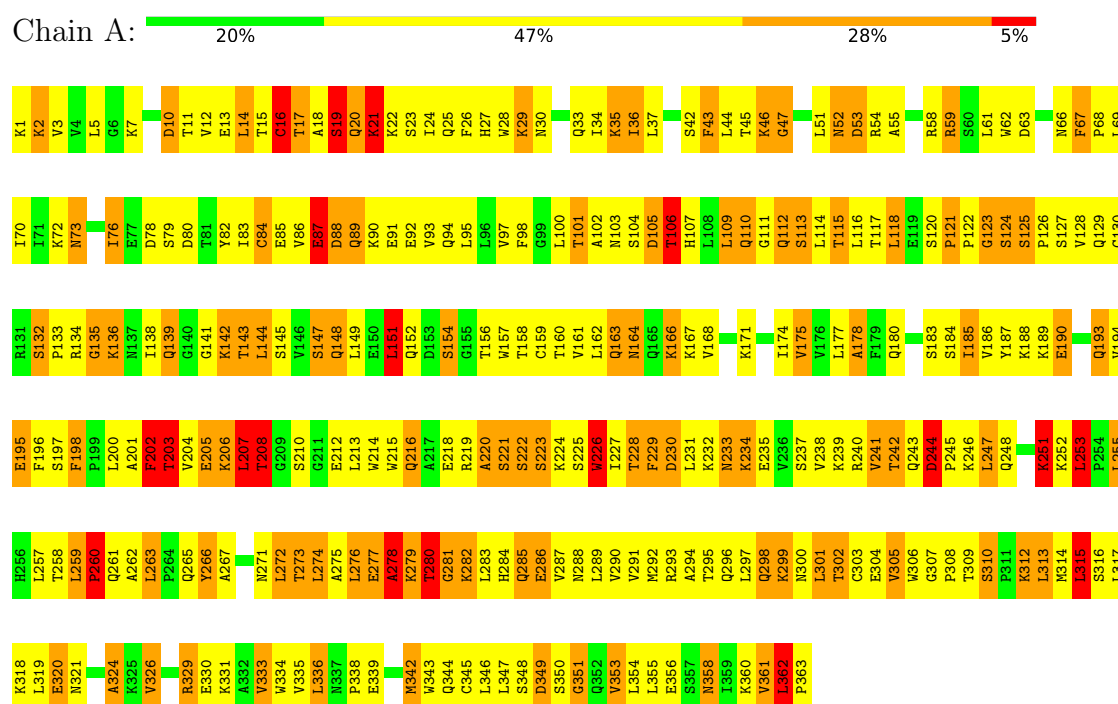
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 363      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2812  | 1784 | 479 | 539 | 10 |         |         |       |
| 1   | B     | 363      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2812  | 1784 | 479 | 539 | 10 |         |         |       |

### 3 Residue-property plots

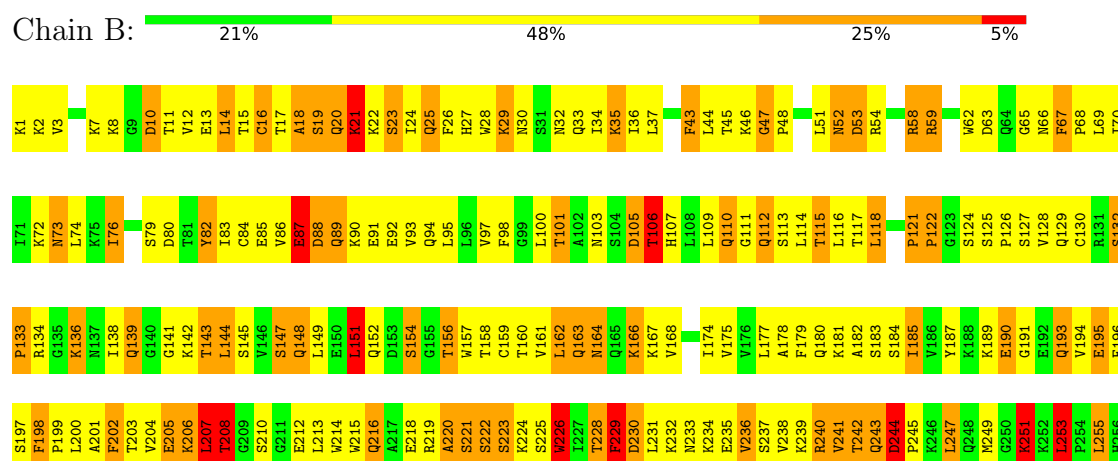
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: T-CELL SURFACE GLYCOPROTEIN CD4



#### • Molecule 1: T-CELL SURFACE GLYCOPROTEIN CD4



[illegible]

## 4 Data and refinement statistics

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

| Property                                                 | Value                                                       | Source    |
|----------------------------------------------------------|-------------------------------------------------------------|-----------|
| Space group                                              | P 31 2 1                                                    | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 126.00 Å   126.00 Å   205.00 Å<br>90.00°   90.00°   120.00° | Depositor |
| Resolution (Å)                                           | 8.00 – 5.00                                                 | Depositor |
| % Data completeness<br>(in resolution range)             | 67.3 (8.00-5.00)                                            | Depositor |
| $R_{merge}$                                              | (Not available)                                             | Depositor |
| $R_{sym}$                                                | (Not available)                                             | Depositor |
| Refinement program                                       | X-PLOR                                                      | Depositor |
| R, $R_{free}$                                            | 0.422 , 0.442                                               | Depositor |
| Estimated twinning fraction                              | No twinning to report.                                      | Xtriage   |
| Total number of atoms                                    | 5624                                                        | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 20.0                                                        | wwPDB-VP  |

## 5 Model quality [i](#)

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

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     | 0.88         | 4/2860 (0.1%) | 1.37        | 47/3868 (1.2%) |
| 1   | B     | 0.80         | 3/2860 (0.1%) | 1.35        | 40/3868 (1.0%) |
| All | All   | 0.84         | 7/5720 (0.1%) | 1.36        | 87/7736 (1.1%) |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 202 | PHE  | C-O   | -8.25 | 1.13        | 1.24     |
| 1   | B     | 202 | PHE  | C-O   | -7.50 | 1.14        | 1.24     |
| 1   | B     | 249 | MET  | SD-CE | -6.86 | 1.62        | 1.79     |
| 1   | A     | 260 | PRO  | C-O   | -6.73 | 1.15        | 1.24     |
| 1   | A     | 178 | ALA  | CA-CB | -6.65 | 1.42        | 1.53     |
| 1   | B     | 260 | PRO  | C-O   | -5.36 | 1.17        | 1.23     |
| 1   | A     | 207 | LEU  | CA-C  | 5.10  | 1.59        | 1.52     |

All (87) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 208 | THR  | N-CA-C | 12.48 | 133.62      | 113.89   |
| 1   | A     | 208 | THR  | N-CA-C | 11.86 | 131.40      | 113.61   |
| 1   | A     | 87  | GLU  | N-CA-C | 8.74  | 129.41      | 110.80   |
| 1   | B     | 87  | GLU  | N-CA-C | 8.61  | 129.15      | 110.80   |
| 1   | B     | 226 | TRP  | N-CA-C | 8.58  | 119.23      | 107.73   |
| 1   | B     | 301 | LEU  | N-CA-C | 8.50  | 121.94      | 109.69   |
| 1   | B     | 277 | GLU  | O-C-N  | 8.49  | 133.88      | 122.59   |
| 1   | A     | 226 | TRP  | N-CA-C | 8.48  | 119.09      | 107.73   |
| 1   | A     | 277 | GLU  | O-C-N  | 8.47  | 133.86      | 122.59   |
| 1   | B     | 67  | PHE  | CA-C-N | 8.04  | 127.97      | 119.85   |
| 1   | B     | 67  | PHE  | C-N-CA | 8.04  | 127.97      | 119.85   |
| 1   | B     | 362 | LEU  | N-CA-C | 7.98  | 127.45      | 109.81   |
| 1   | A     | 301 | LEU  | N-CA-C | 7.90  | 121.07      | 109.69   |
| 1   | A     | 202 | PHE  | N-CA-C | 7.44  | 126.65      | 110.80   |
| 1   | B     | 106 | THR  | N-CA-C | 7.24  | 126.22      | 110.80   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 106 | THR  | N-CA-C  | 7.12  | 125.97      | 110.80   |
| 1   | B     | 110 | GLN  | N-CA-C  | 7.11  | 119.92      | 110.53   |
| 1   | B     | 105 | ASP  | N-CA-C  | 7.10  | 125.92      | 110.80   |
| 1   | A     | 67  | PHE  | N-CA-C  | -6.98 | 98.63       | 109.79   |
| 1   | A     | 47  | GLY  | CA-C-N  | 6.76  | 126.39      | 119.56   |
| 1   | A     | 47  | GLY  | C-N-CA  | 6.76  | 126.39      | 119.56   |
| 1   | A     | 105 | ASP  | N-CA-C  | 6.70  | 125.08      | 110.80   |
| 1   | A     | 67  | PHE  | CA-C-N  | 6.67  | 126.59      | 119.85   |
| 1   | A     | 67  | PHE  | C-N-CA  | 6.67  | 126.59      | 119.85   |
| 1   | B     | 239 | LYS  | N-CA-C  | -6.58 | 104.03      | 111.07   |
| 1   | B     | 67  | PHE  | N-CA-C  | -6.58 | 99.27       | 109.79   |
| 1   | B     | 142 | LYS  | N-CA-C  | -6.54 | 105.28      | 113.20   |
| 1   | A     | 142 | LYS  | N-CA-C  | -6.54 | 105.41      | 113.19   |
| 1   | A     | 278 | ALA  | O-C-N   | 6.51  | 131.25      | 122.59   |
| 1   | B     | 315 | LEU  | N-CA-C  | -6.43 | 99.34       | 109.50   |
| 1   | B     | 278 | ALA  | O-C-N   | 6.41  | 131.11      | 122.59   |
| 1   | A     | 242 | THR  | N-CA-C  | -6.40 | 97.16       | 110.80   |
| 1   | A     | 244 | ASP  | CA-C-N  | -6.40 | 114.18      | 120.52   |
| 1   | A     | 244 | ASP  | C-N-CA  | -6.40 | 114.18      | 120.52   |
| 1   | A     | 251 | LYS  | N-CA-C  | -6.27 | 105.45      | 113.23   |
| 1   | A     | 253 | LEU  | N-CA-C  | 6.25  | 123.62      | 109.81   |
| 1   | B     | 261 | GLN  | N-CA-C  | 6.16  | 123.93      | 110.80   |
| 1   | A     | 362 | LEU  | N-CA-C  | 6.15  | 123.41      | 109.81   |
| 1   | A     | 203 | THR  | N-CA-C  | 6.13  | 123.86      | 110.80   |
| 1   | B     | 21  | LYS  | N-CA-C  | 6.10  | 123.80      | 110.80   |
| 1   | B     | 244 | ASP  | CA-C-N  | -6.09 | 114.47      | 120.98   |
| 1   | B     | 244 | ASP  | C-N-CA  | -6.09 | 114.47      | 120.98   |
| 1   | A     | 109 | LEU  | N-CA-C  | -6.08 | 101.00      | 110.17   |
| 1   | A     | 78  | ASP  | N-CA-C  | -6.03 | 105.97      | 113.38   |
| 1   | A     | 280 | THR  | O-C-N   | 6.00  | 130.57      | 122.59   |
| 1   | B     | 133 | PRO  | N-CA-C  | -5.99 | 106.38      | 113.86   |
| 1   | B     | 253 | LEU  | N-CA-C  | 5.97  | 123.00      | 109.81   |
| 1   | B     | 280 | THR  | O-C-N   | 5.90  | 130.44      | 122.59   |
| 1   | A     | 133 | PRO  | N-CA-C  | -5.80 | 106.60      | 113.86   |
| 1   | B     | 325 | LYS  | N-CA-C  | -5.75 | 106.09      | 113.23   |
| 1   | A     | 184 | SER  | N-CA-C  | -5.72 | 102.01      | 110.48   |
| 1   | A     | 21  | LYS  | N-CA-C  | 5.71  | 122.97      | 110.80   |
| 1   | A     | 315 | LEU  | N-CA-C  | -5.70 | 100.50      | 109.50   |
| 1   | B     | 298 | GLN  | N-CA-C  | -5.61 | 98.86       | 110.80   |
| 1   | A     | 208 | THR  | CB-CA-C | -5.60 | 100.25      | 109.99   |
| 1   | B     | 121 | PRO  | CA-C-N  | 5.60  | 126.84      | 119.84   |
| 1   | B     | 121 | PRO  | C-N-CA  | 5.60  | 126.84      | 119.84   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 340 | ALA  | N-CA-C  | 5.60  | 118.92      | 110.64   |
| 1   | A     | 263 | LEU  | CA-C-N  | 5.59  | 125.70      | 119.32   |
| 1   | A     | 263 | LEU  | C-N-CA  | 5.59  | 125.70      | 119.32   |
| 1   | A     | 239 | LYS  | N-CA-C  | -5.49 | 105.20      | 111.07   |
| 1   | A     | 358 | ASN  | N-CA-C  | 5.45  | 118.55      | 110.48   |
| 1   | B     | 193 | GLN  | N-CA-CB | 5.37  | 117.98      | 109.71   |
| 1   | A     | 101 | THR  | N-CA-C  | 5.36  | 117.40      | 108.99   |
| 1   | B     | 101 | THR  | N-CA-C  | 5.30  | 117.31      | 108.99   |
| 1   | A     | 121 | PRO  | CA-C-N  | 5.29  | 126.45      | 119.84   |
| 1   | A     | 121 | PRO  | C-N-CA  | 5.29  | 126.45      | 119.84   |
| 1   | A     | 123 | GLY  | N-CA-C  | 5.21  | 125.53      | 113.18   |
| 1   | B     | 47  | GLY  | CA-C-N  | 5.20  | 124.81      | 119.56   |
| 1   | B     | 47  | GLY  | C-N-CA  | 5.20  | 124.81      | 119.56   |
| 1   | A     | 252 | LYS  | N-CA-C  | 5.18  | 117.93      | 109.59   |
| 1   | B     | 251 | LYS  | N-CA-C  | -5.17 | 106.81      | 113.23   |
| 1   | A     | 324 | ALA  | N-CA-C  | 5.15  | 121.77      | 110.80   |
| 1   | B     | 260 | PRO  | N-CA-C  | -5.12 | 103.15      | 111.14   |
| 1   | B     | 304 | GLU  | N-CA-C  | 5.09  | 116.99      | 108.99   |
| 1   | A     | 353 | VAL  | N-CA-C  | 5.09  | 115.80      | 108.93   |
| 1   | A     | 361 | VAL  | CA-C-O  | -5.07 | 114.62      | 121.32   |
| 1   | B     | 184 | SER  | N-CA-C  | -5.07 | 102.25      | 110.32   |
| 1   | A     | 110 | GLN  | N-CA-C  | 5.07  | 116.83      | 110.24   |
| 1   | A     | 110 | GLN  | N-CA-CB | -5.06 | 101.83      | 109.92   |
| 1   | A     | 17  | THR  | N-CA-C  | -5.05 | 101.68      | 108.19   |
| 1   | B     | 263 | LEU  | CA-C-N  | 5.05  | 125.08      | 119.32   |
| 1   | B     | 263 | LEU  | C-N-CA  | 5.05  | 125.08      | 119.32   |
| 1   | A     | 281 | GLY  | N-CA-C  | -5.04 | 104.39      | 111.09   |
| 1   | A     | 135 | GLY  | N-CA-C  | 5.03  | 120.12      | 111.47   |
| 1   | B     | 229 | PHE  | N-CA-C  | 5.01  | 117.58      | 109.06   |
| 1   | B     | 281 | GLY  | N-CA-C  | -5.01 | 104.43      | 111.09   |

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     | 2812  | 0        | 2872     | 340     | 29           |
| 1   | B     | 2812  | 0        | 2870     | 309     | 32           |
| All | All   | 5624  | 0        | 5742     | 638     | 32           |

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 56.

All (638) 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:B:151:LEU:CD2  | 1:B:180:GLN:HA   | 1.55                     | 1.33              |
| 1:B:177:LEU:HD13 | 1:B:283:LEU:CD1  | 1.60                     | 1.31              |
| 1:B:151:LEU:HD21 | 1:B:180:GLN:CA   | 1.63                     | 1.28              |
| 1:B:178:ALA:CB   | 1:B:179:PHE:O    | 1.86                     | 1.19              |
| 1:A:109:LEU:HD13 | 1:A:280:THR:O    | 1.47                     | 1.13              |
| 1:A:276:LEU:HD23 | 1:A:276:LEU:N    | 1.63                     | 1.12              |
| 1:A:276:LEU:H    | 1:A:276:LEU:CD2  | 1.63                     | 1.11              |
| 1:A:245:PRO:HB3  | 1:A:266:TYR:HE2  | 1.09                     | 1.11              |
| 1:B:276:LEU:HD23 | 1:B:276:LEU:N    | 1.63                     | 1.11              |
| 1:B:276:LEU:H    | 1:B:276:LEU:CD2  | 1.63                     | 1.11              |
| 1:B:177:LEU:HD13 | 1:B:283:LEU:HD11 | 1.19                     | 1.09              |
| 1:A:234:LYS:HA   | 1:A:253:LEU:HG   | 1.35                     | 1.09              |
| 1:B:314:MET:SD   | 1:B:329:ARG:HG3  | 1.96                     | 1.05              |
| 1:B:234:LYS:HA   | 1:B:253:LEU:HG   | 1.39                     | 1.04              |
| 1:A:276:LEU:N    | 1:A:276:LEU:CD2  | 2.19                     | 1.02              |
| 1:A:107:HIS:ND1  | 1:A:278:ALA:HB1  | 1.74                     | 1.02              |
| 1:B:318:LYS:HE3  | 1:B:320:GLU:HA   | 1.38                     | 1.02              |
| 1:A:178:ALA:HA   | 1:A:283:LEU:CD2  | 1.88                     | 1.01              |
| 1:A:178:ALA:HA   | 1:A:283:LEU:HD21 | 1.42                     | 1.01              |
| 1:A:276:LEU:HD23 | 1:A:276:LEU:H    | 0.84                     | 1.01              |
| 1:B:276:LEU:N    | 1:B:276:LEU:CD2  | 2.19                     | 1.00              |
| 1:A:318:LYS:HE3  | 1:A:320:GLU:HA   | 1.41                     | 1.00              |
| 1:B:276:LEU:HD23 | 1:B:276:LEU:H    | 0.84                     | 0.98              |
| 1:A:309:THR:HB   | 1:A:313:LEU:HD11 | 1.46                     | 0.98              |
| 1:A:245:PRO:HB3  | 1:A:266:TYR:CE2  | 1.99                     | 0.97              |
| 1:A:107:HIS:ND1  | 1:A:278:ALA:CB   | 2.27                     | 0.96              |
| 1:A:314:MET:SD   | 1:A:329:ARG:HG3  | 2.05                     | 0.96              |
| 1:B:178:ALA:HB3  | 1:B:179:PHE:O    | 1.00                     | 0.95              |
| 1:A:178:ALA:O    | 1:A:200:LEU:HD22 | 1.68                     | 0.93              |
| 1:A:107:HIS:CG   | 1:A:278:ALA:CB   | 2.51                     | 0.93              |
| 1:A:109:LEU:HD13 | 1:A:280:THR:C    | 1.94                     | 0.92              |
| 1:A:218:GLU:HG2  | 1:A:219:ARG:HD2  | 1.51                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:107:HIS:CG   | 1:A:278:ALA:HB3  | 2.06                     | 0.91              |
| 1:B:177:LEU:HD11 | 1:B:200:LEU:CD1  | 2.00                     | 0.90              |
| 1:B:151:LEU:CD2  | 1:B:180:GLN:CA   | 2.36                     | 0.90              |
| 1:A:107:HIS:CB   | 1:A:278:ALA:HB3  | 2.01                     | 0.89              |
| 1:A:358:ASN:HB3  | 1:B:342:MET:HE3  | 1.52                     | 0.89              |
| 1:A:54:ARG:HD3   | 1:A:73:ASN:HB2   | 1.56                     | 0.87              |
| 1:A:320:GLU:HG3  | 1:B:358:ASN:OD1  | 1.74                     | 0.87              |
| 1:B:245:PRO:HG3  | 1:B:266:TYR:HE2  | 1.39                     | 0.87              |
| 1:B:177:LEU:HD13 | 1:B:283:LEU:HD13 | 1.57                     | 0.85              |
| 1:B:263:LEU:HB2  | 1:B:266:TYR:CE1  | 2.11                     | 0.84              |
| 1:B:37:LEU:HA    | 1:B:46:LYS:HA    | 1.59                     | 0.84              |
| 1:A:37:LEU:HA    | 1:A:46:LYS:HA    | 1.58                     | 0.84              |
| 1:B:218:GLU:HG2  | 1:B:219:ARG:HD2  | 1.59                     | 0.83              |
| 1:B:124:SER:HB3  | 1:B:163:GLN:HE22 | 1.42                     | 0.83              |
| 1:B:177:LEU:HD11 | 1:B:200:LEU:HD13 | 1.59                     | 0.83              |
| 1:A:109:LEU:CD1  | 1:A:280:THR:O    | 2.25                     | 0.83              |
| 1:B:313:LEU:HB3  | 1:B:348:SER:O    | 1.79                     | 0.83              |
| 1:A:245:PRO:CB   | 1:A:266:TYR:HE2  | 1.89                     | 0.82              |
| 1:A:111:GLY:O    | 1:A:148:GLN:HA   | 1.80                     | 0.82              |
| 1:B:319:LEU:CD1  | 1:B:321:ASN:HB2  | 2.10                     | 0.81              |
| 1:A:245:PRO:HG2  | 1:A:247:LEU:HD21 | 1.63                     | 0.81              |
| 1:A:213:LEU:HB2  | 1:A:272:LEU:HD12 | 1.63                     | 0.81              |
| 1:A:244:ASP:HB3  | 1:A:245:PRO:CD   | 2.12                     | 0.80              |
| 1:A:2:LYS:HB2    | 1:A:93:VAL:HG13  | 1.62                     | 0.80              |
| 1:A:315:LEU:HD21 | 1:A:345:CYS:SG   | 2.21                     | 0.80              |
| 1:B:130:CYS:HG   | 1:B:159:CYS:HG   | 1.27                     | 0.79              |
| 1:A:110:GLN:HE22 | 1:A:178:ALA:HB1  | 1.47                     | 0.79              |
| 1:A:59:ARG:O     | 1:A:62:TRP:HB2   | 1.82                     | 0.79              |
| 1:B:130:CYS:SG   | 1:B:144:LEU:HD11 | 2.23                     | 0.79              |
| 1:B:54:ARG:HD3   | 1:B:73:ASN:HB2   | 1.64                     | 0.79              |
| 1:B:177:LEU:CD1  | 1:B:283:LEU:HD11 | 2.10                     | 0.79              |
| 1:A:224:LYS:HA   | 1:A:226:TRP:CH2  | 2.17                     | 0.78              |
| 1:B:33:GLN:HA    | 1:B:33:GLN:OE1   | 1.82                     | 0.78              |
| 1:B:309:THR:HB   | 1:B:313:LEU:HD11 | 1.64                     | 0.78              |
| 1:B:160:THR:HG21 | 1:B:167:LYS:HE3  | 1.67                     | 0.77              |
| 1:B:177:LEU:CD1  | 1:B:283:LEU:CD1  | 2.55                     | 0.77              |
| 1:A:244:ASP:HB3  | 1:A:245:PRO:HD2  | 1.66                     | 0.77              |
| 1:B:76:ILE:HD12  | 1:B:76:ILE:H     | 1.50                     | 0.76              |
| 1:B:59:ARG:O     | 1:B:62:TRP:HB2   | 1.86                     | 0.76              |
| 1:A:76:ILE:HD12  | 1:A:76:ILE:H     | 1.49                     | 0.76              |
| 1:A:177:LEU:CD2  | 1:A:276:LEU:HD11 | 2.15                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:213:LEU:HB2  | 1:B:272:LEU:HD12 | 1.66                     | 0.76              |
| 1:B:245:PRO:HG3  | 1:B:266:TYR:CE2  | 2.20                     | 0.76              |
| 1:B:244:ASP:HB3  | 1:B:245:PRO:HD3  | 1.66                     | 0.75              |
| 1:A:160:THR:HG21 | 1:A:167:LYS:HE3  | 1.68                     | 0.75              |
| 1:A:29:LYS:HD3   | 1:A:33:GLN:OE1   | 1.87                     | 0.75              |
| 1:A:124:SER:HB2  | 1:A:163:GLN:HE22 | 1.52                     | 0.75              |
| 1:B:245:PRO:HG2  | 1:B:247:LEU:HD21 | 1.67                     | 0.74              |
| 1:B:162:LEU:HD23 | 1:B:163:GLN:N    | 2.01                     | 0.74              |
| 1:A:162:LEU:HD23 | 1:A:163:GLN:N    | 2.02                     | 0.74              |
| 1:A:110:GLN:NE2  | 1:A:178:ALA:HB1  | 2.03                     | 0.74              |
| 1:A:277:GLU:HG3  | 1:A:278:ALA:N    | 2.02                     | 0.74              |
| 1:A:292:MET:HE2  | 1:A:345:CYS:SG   | 2.28                     | 0.73              |
| 1:A:185:ILE:HG12 | 1:A:288:ASN:HB2  | 1.70                     | 0.73              |
| 1:B:224:LYS:HA   | 1:B:226:TRP:CH2  | 2.23                     | 0.73              |
| 1:B:214:TRP:CE3  | 1:B:226:TRP:CZ3  | 2.76                     | 0.73              |
| 1:B:151:LEU:HD22 | 1:B:179:PHE:O    | 1.87                     | 0.73              |
| 1:A:109:LEU:CD1  | 1:A:280:THR:C    | 2.60                     | 0.73              |
| 1:B:314:MET:SD   | 1:B:329:ARG:CG   | 2.75                     | 0.72              |
| 1:B:299:LYS:H    | 1:B:299:LYS:HD3  | 1.54                     | 0.72              |
| 1:B:109:LEU:CB   | 1:B:283:LEU:HA   | 2.19                     | 0.72              |
| 1:B:315:LEU:HD21 | 1:B:345:CYS:SG   | 2.30                     | 0.72              |
| 1:B:204:VAL:HG12 | 1:B:205:GLU:H    | 1.54                     | 0.72              |
| 1:B:277:GLU:HG3  | 1:B:278:ALA:N    | 2.02                     | 0.72              |
| 1:B:89:GLN:HG2   | 1:B:90:LYS:N     | 2.05                     | 0.71              |
| 1:A:210:SER:HB3  | 1:A:230:ASP:HA   | 1.73                     | 0.71              |
| 1:A:36:ILE:O     | 1:A:46:LYS:HG3   | 1.91                     | 0.71              |
| 1:B:245:PRO:HB3  | 1:B:266:TYR:CE2  | 2.26                     | 0.71              |
| 1:A:177:LEU:HD21 | 1:A:276:LEU:HD11 | 1.73                     | 0.70              |
| 1:A:310:SER:OG   | 1:A:312:LYS:HB2  | 1.92                     | 0.70              |
| 1:B:245:PRO:CG   | 1:B:266:TYR:HE2  | 2.05                     | 0.70              |
| 1:A:214:TRP:CE3  | 1:A:226:TRP:CZ3  | 2.80                     | 0.70              |
| 1:A:294:ALA:HA   | 1:A:303:CYS:SG   | 2.31                     | 0.70              |
| 1:A:193:GLN:HA   | 1:A:260:PRO:O    | 1.91                     | 0.69              |
| 1:B:1:LYS:HD2    | 1:B:92:GLU:HB2   | 1.74                     | 0.69              |
| 1:A:107:HIS:HB2  | 1:A:278:ALA:HB3  | 1.74                     | 0.69              |
| 1:B:213:LEU:HD12 | 1:B:271:ASN:O    | 1.92                     | 0.69              |
| 1:A:187:TYR:CE2  | 1:A:354:LEU:HD22 | 2.27                     | 0.69              |
| 1:B:187:TYR:CE2  | 1:B:354:LEU:HD22 | 2.28                     | 0.69              |
| 1:B:261:GLN:HE21 | 1:B:263:LEU:HD11 | 1.56                     | 0.68              |
| 1:A:224:LYS:HA   | 1:A:226:TRP:CZ2  | 2.28                     | 0.68              |
| 1:B:290:VAL:HG13 | 1:B:306:TRP:O    | 1.93                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:85:GLU:HG2   | 1:A:90:LYS:HG2   | 1.74                     | 0.68              |
| 1:B:109:LEU:HB2  | 1:B:283:LEU:HA   | 1.76                     | 0.68              |
| 1:A:177:LEU:HD23 | 1:A:178:ALA:N    | 2.09                     | 0.68              |
| 1:A:110:GLN:NE2  | 1:A:178:ALA:CB   | 2.57                     | 0.68              |
| 1:B:263:LEU:HB2  | 1:B:266:TYR:CD1  | 2.28                     | 0.67              |
| 1:A:130:CYS:HA   | 1:A:159:CYS:HA   | 1.75                     | 0.67              |
| 1:A:178:ALA:CA   | 1:A:283:LEU:CD2  | 2.68                     | 0.67              |
| 1:A:17:THR:HG22  | 1:A:18:ALA:H     | 1.59                     | 0.67              |
| 1:A:313:LEU:HB3  | 1:A:348:SER:O    | 1.94                     | 0.67              |
| 1:B:79:SER:HA    | 1:B:95:LEU:O     | 1.95                     | 0.67              |
| 1:B:205:GLU:CG   | 1:B:208:THR:HG21 | 2.24                     | 0.67              |
| 1:A:109:LEU:CD1  | 1:A:279:LYS:O    | 2.42                     | 0.67              |
| 1:B:319:LEU:HD12 | 1:B:321:ASN:HB2  | 1.77                     | 0.67              |
| 1:A:89:GLN:HG2   | 1:A:90:LYS:N     | 2.09                     | 0.67              |
| 1:B:35:LYS:O     | 1:B:47:GLY:HA3   | 1.94                     | 0.66              |
| 1:A:356:GLU:CD   | 1:B:320:GLU:HG2  | 2.21                     | 0.66              |
| 1:B:205:GLU:HG2  | 1:B:208:THR:HG21 | 1.76                     | 0.66              |
| 1:A:177:LEU:HD23 | 1:A:178:ALA:H    | 1.59                     | 0.66              |
| 1:A:1:LYS:HD2    | 1:A:92:GLU:HB2   | 1.76                     | 0.66              |
| 1:A:314:MET:SD   | 1:A:329:ARG:CG   | 2.83                     | 0.66              |
| 1:B:111:GLY:O    | 1:B:148:GLN:HA   | 1.95                     | 0.66              |
| 1:B:113:SER:HA   | 1:B:147:SER:O    | 1.95                     | 0.66              |
| 1:A:204:VAL:HG12 | 1:A:205:GLU:H    | 1.61                     | 0.66              |
| 1:A:27:HIS:CD2   | 1:A:85:GLU:HB2   | 2.30                     | 0.65              |
| 1:A:107:HIS:NE2  | 1:A:205:GLU:OE1  | 2.29                     | 0.65              |
| 1:A:223:SER:O    | 1:A:224:LYS:HB2  | 1.95                     | 0.65              |
| 1:B:21:LYS:O     | 1:B:21:LYS:HG2   | 1.97                     | 0.65              |
| 1:A:294:ALA:CA   | 1:A:303:CYS:SG   | 2.84                     | 0.65              |
| 1:A:234:LYS:HA   | 1:A:253:LEU:CG   | 2.22                     | 0.65              |
| 1:A:305:VAL:O    | 1:A:331:LYS:HE3  | 1.97                     | 0.65              |
| 1:B:43:PHE:CD1   | 1:B:43:PHE:N     | 2.64                     | 0.65              |
| 1:A:309:THR:HB   | 1:A:313:LEU:CD1  | 2.24                     | 0.64              |
| 1:A:318:LYS:HG3  | 1:A:320:GLU:H    | 1.62                     | 0.64              |
| 1:A:178:ALA:C    | 1:A:283:LEU:HD13 | 2.21                     | 0.64              |
| 1:A:245:PRO:HG2  | 1:A:247:LEU:CD2  | 2.26                     | 0.64              |
| 1:A:116:LEU:HB2  | 1:A:144:LEU:O    | 1.97                     | 0.64              |
| 1:A:261:GLN:HE21 | 1:A:263:LEU:HD11 | 1.63                     | 0.64              |
| 1:A:43:PHE:CD1   | 1:A:43:PHE:N     | 2.63                     | 0.64              |
| 1:A:208:THR:O    | 1:A:276:LEU:CB   | 2.46                     | 0.64              |
| 1:B:185:ILE:HG13 | 1:B:288:ASN:HB2  | 1.79                     | 0.64              |
| 1:A:196:PHE:HE2  | 1:A:259:LEU:HD12 | 1.64                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:318:LYS:HG3  | 1:B:320:GLU:H    | 1.64                     | 0.63              |
| 1:A:286:GLU:HG3  | 1:A:287:VAL:N    | 2.13                     | 0.63              |
| 1:A:2:LYS:HG3    | 1:A:92:GLU:O     | 1.98                     | 0.63              |
| 1:A:229:PHE:HE2  | 1:A:255:LEU:HD21 | 1.63                     | 0.63              |
| 1:A:162:LEU:HD23 | 1:A:162:LEU:C    | 2.24                     | 0.63              |
| 1:B:83:ILE:HA    | 1:B:91:GLU:O     | 1.99                     | 0.63              |
| 1:A:314:MET:SD   | 1:A:329:ARG:HD2  | 2.38                     | 0.63              |
| 1:A:178:ALA:HA   | 1:A:283:LEU:CD1  | 2.29                     | 0.62              |
| 1:A:319:LEU:CD1  | 1:A:321:ASN:HB2  | 2.29                     | 0.62              |
| 1:A:338:PRO:HB2  | 1:A:361:VAL:HG21 | 1.81                     | 0.62              |
| 1:A:59:ARG:HG2   | 1:A:62:TRP:CZ3   | 2.34                     | 0.62              |
| 1:A:98:PHE:HZ    | 1:A:163:GLN:HE21 | 1.46                     | 0.62              |
| 1:B:210:SER:HB3  | 1:B:230:ASP:HA   | 1.82                     | 0.62              |
| 1:B:305:VAL:O    | 1:B:331:LYS:HE3  | 2.00                     | 0.62              |
| 1:A:113:SER:HA   | 1:A:147:SER:O    | 1.99                     | 0.62              |
| 1:A:305:VAL:CG1  | 1:A:309:THR:HG21 | 2.30                     | 0.62              |
| 1:B:208:THR:O    | 1:B:276:LEU:CB   | 2.47                     | 0.62              |
| 1:B:310:SER:OG   | 1:B:312:LYS:HB2  | 2.00                     | 0.62              |
| 1:A:177:LEU:O    | 1:A:178:ALA:HB2  | 2.00                     | 0.61              |
| 1:B:36:ILE:O     | 1:B:46:LYS:HG3   | 2.00                     | 0.61              |
| 1:A:265:GLN:HG2  | 1:A:266:TYR:CE1  | 2.35                     | 0.61              |
| 1:A:347:LEU:HB3  | 1:A:355:LEU:HB2  | 1.81                     | 0.61              |
| 1:B:286:GLU:HG3  | 1:B:287:VAL:N    | 2.16                     | 0.61              |
| 1:B:362:LEU:HB2  | 1:B:363:PRO:HD3  | 1.82                     | 0.61              |
| 1:B:130:CYS:HA   | 1:B:159:CYS:HA   | 1.82                     | 0.61              |
| 1:B:177:LEU:HD23 | 1:B:179:PHE:HA   | 1.83                     | 0.61              |
| 1:B:224:LYS:HA   | 1:B:226:TRP:CZ2  | 2.35                     | 0.61              |
| 1:A:106:THR:HG22 | 1:A:107:HIS:ND1  | 2.16                     | 0.61              |
| 1:B:121:PRO:HG2  | 1:B:124:SER:HB2  | 1.81                     | 0.61              |
| 1:B:244:ASP:CB   | 1:B:245:PRO:HD3  | 2.31                     | 0.61              |
| 1:A:130:CYS:HG   | 1:A:159:CYS:HG   | 0.65                     | 0.60              |
| 1:B:106:THR:HG22 | 1:B:107:HIS:ND1  | 2.16                     | 0.60              |
| 1:B:151:LEU:HD11 | 1:B:180:GLN:NE2  | 2.16                     | 0.60              |
| 1:B:151:LEU:HD21 | 1:B:180:GLN:HA   | 0.71                     | 0.60              |
| 1:A:28:TRP:NE1   | 1:A:69:LEU:HB2   | 2.16                     | 0.60              |
| 1:A:83:ILE:HA    | 1:A:91:GLU:O     | 2.01                     | 0.60              |
| 1:A:109:LEU:HD11 | 1:A:279:LYS:O    | 2.02                     | 0.60              |
| 1:A:114:LEU:O    | 1:A:145:SER:HB3  | 2.02                     | 0.60              |
| 1:A:180:GLN:O    | 1:A:180:GLN:HG3  | 2.01                     | 0.60              |
| 1:B:24:ILE:HD12  | 1:B:87:GLU:HB2   | 1.83                     | 0.60              |
| 1:A:43:PHE:N     | 1:A:43:PHE:HD1   | 1.98                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:356:GLU:HG2  | 1:B:320:GLU:HG3  | 1.83                     | 0.60              |
| 1:B:245:PRO:HB3  | 1:B:266:TYR:HE2  | 1.64                     | 0.60              |
| 1:B:314:MET:SD   | 1:B:329:ARG:HD2  | 2.41                     | 0.60              |
| 1:A:178:ALA:CA   | 1:A:283:LEU:HD22 | 2.32                     | 0.60              |
| 1:A:21:LYS:HG2   | 1:A:21:LYS:O     | 2.02                     | 0.59              |
| 1:A:265:GLN:HG2  | 1:A:266:TYR:CD1  | 2.36                     | 0.59              |
| 1:B:277:GLU:CG   | 1:B:278:ALA:N    | 2.59                     | 0.59              |
| 1:A:178:ALA:CA   | 1:A:283:LEU:HD21 | 2.27                     | 0.59              |
| 1:A:344:GLN:NE2  | 1:B:344:GLN:OE1  | 2.33                     | 0.59              |
| 1:B:347:LEU:O    | 1:B:354:LEU:HB2  | 2.03                     | 0.59              |
| 1:A:37:LEU:HB2   | 1:A:45:THR:O     | 2.01                     | 0.59              |
| 1:B:241:VAL:HG12 | 1:B:242:THR:H    | 1.68                     | 0.59              |
| 1:A:28:TRP:CE2   | 1:A:69:LEU:HB2   | 2.37                     | 0.59              |
| 1:B:151:LEU:CD2  | 1:B:180:GLN:C    | 2.74                     | 0.59              |
| 1:A:277:GLU:CG   | 1:A:278:ALA:N    | 2.59                     | 0.59              |
| 1:A:319:LEU:HB3  | 1:A:343:TRP:CE2  | 2.38                     | 0.59              |
| 1:A:111:GLY:HA2  | 1:A:148:GLN:CB   | 2.32                     | 0.59              |
| 1:B:109:LEU:CB   | 1:B:283:LEU:CA   | 2.73                     | 0.59              |
| 1:B:245:PRO:HG2  | 1:B:247:LEU:CD2  | 2.32                     | 0.59              |
| 1:A:194:VAL:HB   | 1:A:259:LEU:HB3  | 1.83                     | 0.59              |
| 1:B:180:GLN:HB3  | 1:B:199:PRO:HG2  | 1.85                     | 0.59              |
| 1:B:223:SER:O    | 1:B:224:LYS:HB2  | 2.02                     | 0.59              |
| 1:A:229:PHE:CE2  | 1:A:255:LEU:HD21 | 2.38                     | 0.58              |
| 1:B:85:GLU:HG2   | 1:B:90:LYS:HG2   | 1.85                     | 0.58              |
| 1:B:124:SER:HB3  | 1:B:163:GLN:NE2  | 2.15                     | 0.58              |
| 1:B:263:LEU:HB2  | 1:B:266:TYR:HE1  | 1.66                     | 0.58              |
| 1:B:43:PHE:N     | 1:B:43:PHE:HD1   | 1.99                     | 0.58              |
| 1:B:229:PHE:HE2  | 1:B:255:LEU:HD21 | 1.67                     | 0.58              |
| 1:A:244:ASP:CB   | 1:A:245:PRO:HD2  | 2.34                     | 0.58              |
| 1:B:116:LEU:HB2  | 1:B:144:LEU:O    | 2.03                     | 0.58              |
| 1:A:177:LEU:HD22 | 1:A:276:LEU:HD11 | 1.85                     | 0.58              |
| 1:B:7:LYS:HB2    | 1:B:10:ASP:HB2   | 1.85                     | 0.58              |
| 1:B:245:PRO:CB   | 1:B:266:TYR:HE2  | 2.16                     | 0.58              |
| 1:B:347:LEU:HB3  | 1:B:355:LEU:HB2  | 1.86                     | 0.58              |
| 1:B:2:LYS:HD3    | 1:B:93:VAL:HG22  | 1.84                     | 0.58              |
| 1:A:7:LYS:HB2    | 1:A:10:ASP:HB2   | 1.84                     | 0.58              |
| 1:B:220:ALA:C    | 1:B:222:SER:H    | 2.12                     | 0.58              |
| 1:B:204:VAL:O    | 1:B:205:GLU:HB3  | 2.04                     | 0.58              |
| 1:B:305:VAL:HG12 | 1:B:309:THR:HG21 | 1.85                     | 0.58              |
| 1:B:205:GLU:HG3  | 1:B:208:THR:CG2  | 2.34                     | 0.57              |
| 1:B:296:GLN:HG2  | 1:B:298:GLN:O    | 2.05                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:17:THR:HG22  | 1:B:18:ALA:H     | 1.68                     | 0.57              |
| 1:A:62:TRP:HA    | 1:A:66:ASN:O     | 2.05                     | 0.57              |
| 1:A:356:GLU:CD   | 1:B:320:GLU:CG   | 2.77                     | 0.57              |
| 1:A:14:LEU:HB2   | 1:A:69:LEU:HB3   | 1.87                     | 0.57              |
| 1:A:315:LEU:HA   | 1:A:346:LEU:O    | 2.04                     | 0.57              |
| 1:B:231:LEU:HG   | 1:B:236:VAL:HG13 | 1.86                     | 0.57              |
| 1:A:89:GLN:HG2   | 1:A:90:LYS:H     | 1.69                     | 0.57              |
| 1:A:273:THR:HG23 | 1:A:284:HIS:CD2  | 2.40                     | 0.57              |
| 1:B:177:LEU:HD22 | 1:B:283:LEU:HD13 | 1.87                     | 0.57              |
| 1:B:194:VAL:HB   | 1:B:259:LEU:HB3  | 1.85                     | 0.56              |
| 1:A:79:SER:HA    | 1:A:95:LEU:O     | 2.06                     | 0.56              |
| 1:B:28:TRP:NE1   | 1:B:69:LEU:HB2   | 2.20                     | 0.56              |
| 1:B:112:GLN:OE1  | 1:B:282:LYS:O    | 2.24                     | 0.56              |
| 1:A:196:PHE:CE2  | 1:A:259:LEU:HD12 | 2.41                     | 0.56              |
| 1:A:266:TYR:CD1  | 1:A:266:TYR:N    | 2.74                     | 0.56              |
| 1:A:274:LEU:O    | 1:A:283:LEU:N    | 2.39                     | 0.56              |
| 1:A:342:MET:SD   | 1:A:360:LYS:HG2  | 2.45                     | 0.56              |
| 1:B:151:LEU:CD2  | 1:B:179:PHE:O    | 2.53                     | 0.56              |
| 1:A:109:LEU:HD22 | 1:A:281:GLY:CA   | 2.36                     | 0.56              |
| 1:B:17:THR:O     | 1:B:18:ALA:HB2   | 2.06                     | 0.56              |
| 1:B:279:LYS:O    | 1:B:280:THR:O    | 2.24                     | 0.55              |
| 1:A:296:GLN:HG2  | 1:A:298:GLN:O    | 2.06                     | 0.55              |
| 1:B:151:LEU:HD23 | 1:B:180:GLN:C    | 2.30                     | 0.55              |
| 1:A:319:LEU:HD13 | 1:A:321:ASN:HB2  | 1.88                     | 0.55              |
| 1:B:273:THR:HG23 | 1:B:284:HIS:CD2  | 2.42                     | 0.55              |
| 1:B:111:GLY:HA2  | 1:B:148:GLN:HB3  | 1.88                     | 0.55              |
| 1:B:315:LEU:HA   | 1:B:346:LEU:O    | 2.06                     | 0.55              |
| 1:A:305:VAL:HG12 | 1:A:309:THR:HG21 | 1.89                     | 0.55              |
| 1:B:204:VAL:O    | 1:B:205:GLU:CB   | 2.54                     | 0.55              |
| 1:B:86:VAL:HG12  | 1:B:87:GLU:N     | 2.22                     | 0.55              |
| 1:A:279:LYS:O    | 1:A:280:THR:O    | 2.24                     | 0.55              |
| 1:B:62:TRP:HA    | 1:B:66:ASN:O     | 2.07                     | 0.55              |
| 1:A:244:ASP:CB   | 1:A:245:PRO:CD   | 2.84                     | 0.55              |
| 1:B:37:LEU:HB2   | 1:B:45:THR:O     | 2.06                     | 0.55              |
| 1:A:251:LYS:HB2  | 1:A:251:LYS:NZ   | 2.21                     | 0.54              |
| 1:B:294:ALA:HA   | 1:B:303:CYS:SG   | 2.47                     | 0.54              |
| 1:A:157:TRP:CD1  | 1:A:174:ILE:HD12 | 2.43                     | 0.54              |
| 1:B:177:LEU:HD23 | 1:B:178:ALA:N    | 2.21                     | 0.54              |
| 1:B:29:LYS:HA    | 1:B:34:ILE:O     | 2.06                     | 0.54              |
| 1:A:178:ALA:CB   | 1:A:283:LEU:HD22 | 2.38                     | 0.54              |
| 1:B:212:GLU:HB3  | 1:B:228:THR:HG23 | 1.88                     | 0.54              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:110:GLN:NE2 | 1:B:178:ALA:CB   | 2.71                     | 0.54              |
| 1:B:98:PHE:HZ   | 1:B:163:GLN:HE21 | 1.54                     | 0.54              |
| 1:B:305:VAL:CG1 | 1:B:309:THR:HG21 | 2.37                     | 0.54              |
| 1:A:164:ASN:C   | 1:A:166:LYS:H    | 2.16                     | 0.54              |
| 1:B:28:TRP:CE2  | 1:B:69:LEU:HB2   | 2.43                     | 0.54              |
| 1:A:299:LYS:H   | 1:A:299:LYS:HD3  | 1.72                     | 0.54              |
| 1:A:124:SER:CB  | 1:A:163:GLN:HE22 | 2.19                     | 0.54              |
| 1:A:298:GLN:OE1 | 1:A:299:LYS:HG2  | 2.08                     | 0.54              |
| 1:A:259:LEU:O   | 1:A:260:PRO:O    | 2.26                     | 0.53              |
| 1:B:233:ASN:O   | 1:B:253:LEU:HD21 | 2.07                     | 0.53              |
| 1:A:121:PRO:HG2 | 1:A:124:SER:OG   | 2.09                     | 0.53              |
| 1:A:326:VAL:O   | 1:A:326:VAL:HG13 | 2.09                     | 0.53              |
| 1:A:320:GLU:OE1 | 1:B:358:ASN:HB2  | 2.09                     | 0.53              |
| 1:B:292:MET:HE2 | 1:B:345:CYS:SG   | 2.49                     | 0.53              |
| 1:A:5:LEU:HD11  | 1:A:166:LYS:HB3  | 1.91                     | 0.53              |
| 1:B:274:LEU:O   | 1:B:283:LEU:N    | 2.41                     | 0.53              |
| 1:A:178:ALA:HA  | 1:A:283:LEU:HD11 | 1.91                     | 0.52              |
| 1:B:19:SER:C    | 1:B:21:LYS:H     | 2.16                     | 0.52              |
| 1:B:177:LEU:CD1 | 1:B:283:LEU:HD13 | 2.32                     | 0.52              |
| 1:A:19:SER:C    | 1:A:21:LYS:H     | 2.16                     | 0.52              |
| 1:B:185:ILE:CG1 | 1:B:288:ASN:HB2  | 2.38                     | 0.52              |
| 1:A:52:ASN:OD1  | 1:A:53:ASP:N     | 2.43                     | 0.52              |
| 1:A:16:CYS:SG   | 1:A:84:CYS:SG    | 3.02                     | 0.52              |
| 1:A:212:GLU:HB3 | 1:A:228:THR:HG23 | 1.92                     | 0.52              |
| 1:A:33:GLN:OE1  | 1:A:33:GLN:HA    | 2.09                     | 0.52              |
| 1:A:194:VAL:HB  | 1:A:259:LEU:CB   | 2.39                     | 0.52              |
| 1:B:110:GLN:NE2 | 1:B:178:ALA:HB1  | 2.25                     | 0.52              |
| 1:B:157:TRP:CD1 | 1:B:174:ILE:HD12 | 2.45                     | 0.52              |
| 1:B:244:ASP:CB  | 1:B:245:PRO:CD   | 2.88                     | 0.52              |
| 1:A:220:ALA:C   | 1:A:222:SER:H    | 2.17                     | 0.52              |
| 1:A:356:GLU:HG2 | 1:B:320:GLU:CG   | 2.39                     | 0.52              |
| 1:B:2:LYS:HB2   | 1:B:93:VAL:HG13  | 1.91                     | 0.52              |
| 1:B:177:LEU:O   | 1:B:178:ALA:HB2  | 2.09                     | 0.52              |
| 1:A:87:GLU:O    | 1:A:88:ASP:CG    | 2.53                     | 0.52              |
| 1:A:107:HIS:CE1 | 1:A:205:GLU:OE1  | 2.62                     | 0.52              |
| 1:A:246:LYS:HB3 | 1:A:260:PRO:HG2  | 1.91                     | 0.52              |
| 1:B:151:LEU:O   | 1:B:154:SER:HB2  | 2.10                     | 0.52              |
| 1:A:141:GLY:C   | 1:A:143:THR:H    | 2.15                     | 0.52              |
| 1:B:310:SER:C   | 1:B:312:LYS:H    | 2.18                     | 0.52              |
| 1:B:100:LEU:HA  | 1:B:118:LEU:HD12 | 1.91                     | 0.52              |
| 1:A:80:ASP:O    | 1:A:94:GLN:HA    | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:28:TRP:CE2   | 1:B:84:CYS:SG    | 3.02                     | 0.51              |
| 1:B:161:VAL:HB   | 1:B:168:VAL:HG13 | 1.92                     | 0.51              |
| 1:B:13:GLU:OE1   | 1:B:58:ARG:NH2   | 2.43                     | 0.51              |
| 1:A:19:SER:O     | 1:A:21:LYS:N     | 2.38                     | 0.51              |
| 1:A:35:LYS:O     | 1:A:47:GLY:HA3   | 2.11                     | 0.51              |
| 1:A:100:LEU:HD12 | 1:A:118:LEU:HD12 | 1.92                     | 0.51              |
| 1:A:161:VAL:HB   | 1:A:168:VAL:HG13 | 1.92                     | 0.51              |
| 1:B:220:ALA:C    | 1:B:222:SER:N    | 2.68                     | 0.51              |
| 1:A:266:TYR:O    | 1:A:289:LEU:HD23 | 2.11                     | 0.51              |
| 1:A:326:VAL:HG11 | 1:A:335:VAL:HG22 | 1.93                     | 0.51              |
| 1:B:114:LEU:O    | 1:B:145:SER:HB3  | 2.10                     | 0.51              |
| 1:B:129:GLN:HA   | 1:B:139:GLN:HB3  | 1.93                     | 0.51              |
| 1:A:204:VAL:O    | 1:A:205:GLU:CB   | 2.59                     | 0.51              |
| 1:A:290:VAL:HG13 | 1:A:306:TRP:O    | 2.10                     | 0.51              |
| 1:B:206:LYS:HB3  | 1:B:207:LEU:HG   | 1.93                     | 0.51              |
| 1:A:233:ASN:O    | 1:A:253:LEU:HD21 | 2.10                     | 0.51              |
| 1:A:29:LYS:HA    | 1:A:34:ILE:O     | 2.11                     | 0.51              |
| 1:B:19:SER:O     | 1:B:21:LYS:N     | 2.43                     | 0.51              |
| 1:A:27:HIS:HD2   | 1:A:85:GLU:HB2   | 1.72                     | 0.51              |
| 1:A:310:SER:O    | 1:A:313:LEU:HG   | 2.11                     | 0.51              |
| 1:B:319:LEU:HB3  | 1:B:343:TRP:CE2  | 2.46                     | 0.51              |
| 1:B:205:GLU:HG3  | 1:B:208:THR:HG21 | 1.92                     | 0.51              |
| 1:A:206:LYS:O    | 1:A:208:THR:N    | 2.44                     | 0.50              |
| 1:A:342:MET:SD   | 1:A:360:LYS:HD2  | 2.50                     | 0.50              |
| 1:A:86:VAL:HG12  | 1:A:87:GLU:N     | 2.26                     | 0.50              |
| 1:A:26:PHE:CD2   | 1:A:67:PHE:HB3   | 2.46                     | 0.50              |
| 1:A:204:VAL:O    | 1:A:205:GLU:HB3  | 2.11                     | 0.50              |
| 1:A:276:LEU:N    | 1:A:276:LEU:HD22 | 2.21                     | 0.50              |
| 1:A:291:VAL:O    | 1:A:305:VAL:HA   | 2.10                     | 0.50              |
| 1:B:59:ARG:HH11  | 1:B:59:ARG:HB2   | 1.75                     | 0.50              |
| 1:B:182:ALA:O    | 1:B:286:GLU:HB3  | 2.12                     | 0.50              |
| 1:A:24:ILE:HD12  | 1:A:87:GLU:HB2   | 1.93                     | 0.50              |
| 1:B:27:HIS:CD2   | 1:B:85:GLU:HB2   | 2.46                     | 0.50              |
| 1:B:151:LEU:HD23 | 1:B:181:LYS:N    | 2.26                     | 0.50              |
| 1:A:221:SER:O    | 1:A:223:SER:N    | 2.45                     | 0.50              |
| 1:A:59:ARG:HA    | 1:A:62:TRP:CD2   | 2.45                     | 0.50              |
| 1:B:229:PHE:CE2  | 1:B:255:LEU:HD21 | 2.46                     | 0.50              |
| 1:B:345:CYS:C    | 1:B:346:LEU:HD12 | 2.35                     | 0.50              |
| 1:A:219:ARG:NH1  | 1:A:306:TRP:HZ3  | 2.10                     | 0.49              |
| 1:B:89:GLN:HG2   | 1:B:90:LYS:H     | 1.76                     | 0.49              |
| 1:B:294:ALA:CA   | 1:B:303:CYS:SG   | 3.00                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:221:SER:O    | 1:B:223:SER:N    | 2.45                     | 0.49              |
| 1:A:44:LEU:HD13  | 1:A:62:TRP:HZ2   | 1.77                     | 0.49              |
| 1:B:314:MET:SD   | 1:B:329:ARG:CD   | 3.00                     | 0.49              |
| 1:A:315:LEU:HD13 | 1:A:333:VAL:HB   | 1.93                     | 0.49              |
| 1:A:46:LYS:HD2   | 1:A:55:ALA:HB3   | 1.94                     | 0.49              |
| 1:B:80:ASP:O     | 1:B:94:GLN:HA    | 2.13                     | 0.49              |
| 1:A:189:LYS:O    | 1:A:190:GLU:C    | 2.56                     | 0.49              |
| 1:A:208:THR:HG22 | 1:A:277:GLU:H    | 1.77                     | 0.49              |
| 1:B:190:GLU:HA   | 1:B:262:ALA:O    | 2.13                     | 0.49              |
| 1:A:12:VAL:HG21  | 1:A:95:LEU:HD11  | 1.94                     | 0.49              |
| 1:A:345:CYS:C    | 1:A:346:LEU:HD12 | 2.36                     | 0.49              |
| 1:B:14:LEU:HB2   | 1:B:69:LEU:HB3   | 1.95                     | 0.49              |
| 1:B:183:SER:OG   | 1:B:286:GLU:HG2  | 2.13                     | 0.49              |
| 1:A:46:LYS:HD2   | 1:A:52:ASN:O     | 2.13                     | 0.48              |
| 1:A:336:LEU:O    | 1:A:336:LEU:HD23 | 2.13                     | 0.48              |
| 1:B:130:CYS:CB   | 1:B:159:CYS:HG   | 2.26                     | 0.48              |
| 1:A:212:GLU:HG3  | 1:A:214:TRP:HE1  | 1.76                     | 0.48              |
| 1:A:310:SER:C    | 1:A:312:LYS:H    | 2.19                     | 0.48              |
| 1:B:128:VAL:HA   | 1:B:160:THR:O    | 2.13                     | 0.48              |
| 1:A:26:PHE:CG    | 1:A:67:PHE:HB3   | 2.49                     | 0.48              |
| 1:A:100:LEU:HD21 | 1:A:159:CYS:SG   | 2.52                     | 0.48              |
| 1:B:37:LEU:HD12  | 1:B:37:LEU:C     | 2.39                     | 0.48              |
| 1:B:114:LEU:HD21 | 1:B:174:ILE:HD13 | 1.94                     | 0.48              |
| 1:A:54:ARG:HG2   | 1:A:72:LYS:HB2   | 1.94                     | 0.48              |
| 1:A:132:SER:OG   | 1:A:135:GLY:O    | 2.28                     | 0.48              |
| 1:B:132:SER:OG   | 1:B:136:LYS:HB3  | 2.13                     | 0.48              |
| 1:A:13:GLU:CD    | 1:A:58:ARG:HH21  | 2.21                     | 0.48              |
| 1:A:275:ALA:HB2  | 1:A:282:LYS:HB3  | 1.96                     | 0.48              |
| 1:A:178:ALA:HB1  | 1:A:283:LEU:HD22 | 1.96                     | 0.48              |
| 1:B:162:LEU:CD2  | 1:B:162:LEU:C    | 2.87                     | 0.48              |
| 1:A:130:CYS:N    | 1:A:138:ILE:O    | 2.45                     | 0.48              |
| 1:A:220:ALA:C    | 1:A:222:SER:N    | 2.72                     | 0.48              |
| 1:A:314:MET:SD   | 1:A:329:ARG:CD   | 3.01                     | 0.48              |
| 1:B:44:LEU:HD13  | 1:B:62:TRP:HZ2   | 1.78                     | 0.48              |
| 1:B:130:CYS:N    | 1:B:138:ILE:O    | 2.47                     | 0.48              |
| 1:B:288:ASN:HB3  | 1:B:308:PRO:HG3  | 1.94                     | 0.48              |
| 1:A:161:VAL:O    | 1:A:161:VAL:HG12 | 2.14                     | 0.48              |
| 1:B:208:THR:O    | 1:B:276:LEU:HB3  | 2.14                     | 0.48              |
| 1:B:342:MET:SD   | 1:B:360:LYS:HD2  | 2.53                     | 0.48              |
| 1:B:72:LYS:O     | 1:B:73:ASN:C     | 2.56                     | 0.48              |
| 1:B:25:GLN:HG3   | 1:B:26:PHE:N     | 2.28                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:177:LEU:HD11 | 1:B:200:LEU:HD11 | 1.87                     | 0.47              |
| 1:A:72:LYS:O     | 1:A:73:ASN:C     | 2.56                     | 0.47              |
| 1:A:344:GLN:OE1  | 1:B:344:GLN:NE2  | 2.46                     | 0.47              |
| 1:B:141:GLY:C    | 1:B:143:THR:H    | 2.22                     | 0.47              |
| 1:A:102:ALA:HA   | 1:A:115:THR:O    | 2.14                     | 0.47              |
| 1:A:109:LEU:HD12 | 1:A:109:LEU:H    | 1.78                     | 0.47              |
| 1:B:100:LEU:HD12 | 1:B:118:LEU:CD1  | 2.44                     | 0.47              |
| 1:B:198:PHE:HB3  | 1:B:285:GLN:OE1  | 2.14                     | 0.47              |
| 1:B:333:VAL:HG13 | 1:B:334:TRP:N    | 2.29                     | 0.47              |
| 1:A:107:HIS:CE1  | 1:A:278:ALA:HB1  | 2.48                     | 0.47              |
| 1:A:293:ARG:O    | 1:A:303:CYS:HA   | 2.15                     | 0.47              |
| 1:A:362:LEU:HB2  | 1:A:363:PRO:HD3  | 1.96                     | 0.47              |
| 1:B:59:ARG:HG2   | 1:B:62:TRP:CZ3   | 2.49                     | 0.47              |
| 1:B:338:PRO:HB2  | 1:B:361:VAL:HG21 | 1.97                     | 0.47              |
| 1:B:114:LEU:CD2  | 1:B:174:ILE:HD13 | 2.45                     | 0.47              |
| 1:A:28:TRP:CE2   | 1:A:84:CYS:SG    | 2.98                     | 0.47              |
| 1:A:29:LYS:HB3   | 1:A:29:LYS:HE3   | 1.77                     | 0.47              |
| 1:A:89:GLN:HE21  | 1:A:89:GLN:HB3   | 1.55                     | 0.47              |
| 1:A:109:LEU:HD22 | 1:A:281:GLY:N    | 2.29                     | 0.47              |
| 1:A:183:SER:OG   | 1:A:286:GLU:HG2  | 2.15                     | 0.47              |
| 1:B:215:TRP:CD1  | 1:B:216:GLN:N    | 2.83                     | 0.47              |
| 1:A:198:PHE:HB3  | 1:A:285:GLN:OE1  | 2.15                     | 0.47              |
| 1:B:117:THR:HA   | 1:B:143:THR:OG1  | 2.15                     | 0.47              |
| 1:B:275:ALA:HB2  | 1:B:282:LYS:HB3  | 1.96                     | 0.47              |
| 1:A:51:LEU:HD12  | 1:A:51:LEU:HA    | 1.73                     | 0.47              |
| 1:A:111:GLY:HA2  | 1:A:148:GLN:HB3  | 1.97                     | 0.47              |
| 1:A:212:GLU:HG3  | 1:A:214:TRP:NE1  | 2.30                     | 0.47              |
| 1:A:141:GLY:C    | 1:A:143:THR:N    | 2.73                     | 0.47              |
| 1:B:189:LYS:HA   | 1:B:292:MET:H    | 1.79                     | 0.47              |
| 1:A:195:GLU:HG2  | 1:A:258:THR:HG22 | 1.97                     | 0.46              |
| 1:A:342:MET:CG   | 1:A:360:LYS:HG2  | 2.44                     | 0.46              |
| 1:B:82:TYR:N     | 1:B:82:TYR:CD1   | 2.83                     | 0.46              |
| 1:B:110:GLN:HE21 | 1:B:110:GLN:HB3  | 1.58                     | 0.46              |
| 1:B:194:VAL:HG23 | 1:B:262:ALA:HB2  | 1.97                     | 0.46              |
| 1:A:202:PHE:O    | 1:A:203:THR:O    | 2.33                     | 0.46              |
| 1:B:206:LYS:HB3  | 1:B:207:LEU:H    | 1.49                     | 0.46              |
| 1:B:276:LEU:N    | 1:B:276:LEU:HD22 | 2.21                     | 0.46              |
| 1:A:13:GLU:OE1   | 1:A:58:ARG:NH2   | 2.48                     | 0.46              |
| 1:A:303:CYS:HG   | 1:A:345:CYS:HG   | 1.55                     | 0.46              |
| 1:A:305:VAL:HG21 | 1:A:347:LEU:HG   | 1.96                     | 0.46              |
| 1:B:115:THR:HA   | 1:B:145:SER:CB   | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:205:GLU:HG2  | 1:A:208:THR:HG21 | 1.98                     | 0.46              |
| 1:B:87:GLU:O     | 1:B:88:ASP:CG    | 2.59                     | 0.46              |
| 1:B:194:VAL:CG2  | 1:B:262:ALA:HB2  | 2.46                     | 0.46              |
| 1:B:305:VAL:O    | 1:B:331:LYS:HB2  | 2.15                     | 0.46              |
| 1:A:59:ARG:HH11  | 1:A:59:ARG:HB2   | 1.80                     | 0.46              |
| 1:A:130:CYS:HG   | 1:A:159:CYS:CB   | 2.23                     | 0.46              |
| 1:B:213:LEU:O    | 1:B:226:TRP:HB3  | 2.16                     | 0.46              |
| 1:A:59:ARG:HA    | 1:A:62:TRP:CG    | 2.50                     | 0.46              |
| 1:A:117:THR:HA   | 1:A:143:THR:OG1  | 2.16                     | 0.46              |
| 1:A:129:GLN:HA   | 1:A:139:GLN:HB3  | 1.98                     | 0.46              |
| 1:A:302:THR:HG23 | 1:A:303:CYS:N    | 2.29                     | 0.46              |
| 1:B:98:PHE:CG    | 1:B:161:VAL:HG11 | 2.51                     | 0.46              |
| 1:B:251:LYS:HB2  | 1:B:251:LYS:NZ   | 2.31                     | 0.46              |
| 1:A:106:THR:O    | 1:A:279:LYS:HB2  | 2.15                     | 0.46              |
| 1:B:299:LYS:HD3  | 1:B:299:LYS:N    | 2.29                     | 0.46              |
| 1:A:213:LEU:O    | 1:A:226:TRP:HB3  | 2.16                     | 0.45              |
| 1:B:36:ILE:O     | 1:B:47:GLY:N     | 2.49                     | 0.45              |
| 1:B:294:ALA:HB2  | 1:B:303:CYS:SG   | 2.56                     | 0.45              |
| 1:A:115:THR:HA   | 1:A:145:SER:CB   | 2.46                     | 0.45              |
| 1:A:151:LEU:O    | 1:A:154:SER:HB2  | 2.17                     | 0.45              |
| 1:A:190:GLU:HA   | 1:A:262:ALA:O    | 2.15                     | 0.45              |
| 1:A:202:PHE:HE2  | 1:A:234:LYS:NZ   | 2.14                     | 0.45              |
| 1:B:187:TYR:HB3  | 1:B:355:LEU:HG   | 1.98                     | 0.45              |
| 1:B:189:LYS:O    | 1:B:190:GLU:C    | 2.58                     | 0.45              |
| 1:A:20:GLN:O     | 1:A:22:LYS:N     | 2.49                     | 0.45              |
| 1:A:342:MET:HG2  | 1:A:360:LYS:HG2  | 1.98                     | 0.45              |
| 1:B:309:THR:HB   | 1:B:313:LEU:CD1  | 2.40                     | 0.45              |
| 1:A:111:GLY:O    | 1:A:112:GLN:C    | 2.60                     | 0.45              |
| 1:A:161:VAL:HB   | 1:A:168:VAL:CG1  | 2.46                     | 0.45              |
| 1:A:290:VAL:HG22 | 1:A:308:PRO:HG2  | 1.97                     | 0.45              |
| 1:A:333:VAL:HG13 | 1:A:334:TRP:N    | 2.30                     | 0.45              |
| 1:B:52:ASN:OD1   | 1:B:53:ASP:N     | 2.50                     | 0.45              |
| 1:B:130:CYS:HB2  | 1:B:138:ILE:HG23 | 1.98                     | 0.45              |
| 1:A:109:LEU:HD12 | 1:A:109:LEU:N    | 2.31                     | 0.45              |
| 1:A:231:LEU:C    | 1:A:232:LYS:HG3  | 2.42                     | 0.45              |
| 1:A:267:ALA:HB1  | 1:A:307:GLY:CA   | 2.46                     | 0.45              |
| 1:A:356:GLU:CG   | 1:B:320:GLU:CG   | 2.95                     | 0.45              |
| 1:B:219:ARG:O    | 1:B:221:SER:N    | 2.49                     | 0.45              |
| 1:B:27:HIS:HD2   | 1:B:85:GLU:HB2   | 1.81                     | 0.45              |
| 1:B:196:PHE:HE2  | 1:B:259:LEU:HD12 | 1.81                     | 0.45              |
| 1:B:315:LEU:HD22 | 1:B:316:SER:H    | 1.82                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:14:LEU:HD22  | 1:A:69:LEU:HD23  | 1.99                     | 0.45              |
| 1:B:27:HIS:HB2   | 1:B:35:LYS:HZ3   | 1.81                     | 0.45              |
| 1:B:290:VAL:CG1  | 1:B:306:TRP:O    | 2.62                     | 0.45              |
| 1:A:118:LEU:HD23 | 1:A:120:SER:OG   | 2.16                     | 0.45              |
| 1:A:178:ALA:O    | 1:A:200:LEU:CD2  | 2.52                     | 0.45              |
| 1:A:294:ALA:HB2  | 1:A:303:CYS:SG   | 2.56                     | 0.45              |
| 1:A:296:GLN:HA   | 1:A:301:LEU:HA   | 1.98                     | 0.45              |
| 1:B:29:LYS:HD3   | 1:B:33:GLN:OE1   | 2.16                     | 0.45              |
| 1:A:162:LEU:C    | 1:A:162:LEU:CD2  | 2.89                     | 0.45              |
| 1:B:263:LEU:O    | 1:B:266:TYR:HD1  | 2.00                     | 0.44              |
| 1:B:30:ASN:O     | 1:B:32:ASN:N     | 2.50                     | 0.44              |
| 1:B:72:LYS:O     | 1:B:74:LEU:N     | 2.51                     | 0.44              |
| 1:B:86:VAL:O     | 1:B:88:ASP:N     | 2.42                     | 0.44              |
| 1:A:214:TRP:CE3  | 1:A:226:TRP:HZ3  | 2.34                     | 0.44              |
| 1:B:8:LYS:C      | 1:B:10:ASP:H     | 2.26                     | 0.44              |
| 1:B:44:LEU:HD13  | 1:B:62:TRP:CZ2   | 2.52                     | 0.44              |
| 1:A:30:ASN:HA    | 1:A:82:TYR:HA    | 2.00                     | 0.44              |
| 1:A:37:LEU:C     | 1:A:37:LEU:HD12  | 2.43                     | 0.44              |
| 1:A:198:PHE:CD2  | 1:A:272:LEU:HD22 | 2.52                     | 0.44              |
| 1:B:261:GLN:NE2  | 1:B:263:LEU:HD11 | 2.30                     | 0.44              |
| 1:A:110:GLN:NE2  | 1:A:178:ALA:HB2  | 2.33                     | 0.44              |
| 1:B:13:GLU:CD    | 1:B:58:ARG:HH21  | 2.25                     | 0.44              |
| 1:B:130:CYS:O    | 1:B:138:ILE:HG22 | 2.18                     | 0.44              |
| 1:B:195:GLU:HG2  | 1:B:258:THR:HG22 | 1.99                     | 0.44              |
| 1:B:219:ARG:NH1  | 1:B:306:TRP:HZ3  | 2.16                     | 0.44              |
| 1:B:231:LEU:C    | 1:B:232:LYS:HG3  | 2.43                     | 0.44              |
| 1:B:121:PRO:HA   | 1:B:122:PRO:HD3  | 1.84                     | 0.44              |
| 1:B:303:CYS:HG   | 1:B:345:CYS:CB   | 2.31                     | 0.44              |
| 1:B:30:ASN:C     | 1:B:32:ASN:N     | 2.74                     | 0.43              |
| 1:A:59:ARG:HG2   | 1:A:62:TRP:CE3   | 2.54                     | 0.43              |
| 1:B:116:LEU:O    | 1:B:143:THR:HA   | 2.18                     | 0.43              |
| 1:A:259:LEU:HD13 | 1:A:289:LEU:HD22 | 1.99                     | 0.43              |
| 1:B:296:GLN:HA   | 1:B:301:LEU:HA   | 2.01                     | 0.43              |
| 1:B:298:GLN:HB2  | 1:B:299:LYS:H    | 1.61                     | 0.43              |
| 1:B:298:GLN:HB2  | 1:B:299:LYS:HD3  | 2.00                     | 0.43              |
| 1:B:315:LEU:HD23 | 1:B:346:LEU:O    | 2.18                     | 0.43              |
| 1:A:26:PHE:CD1   | 1:A:67:PHE:CD1   | 3.06                     | 0.43              |
| 1:A:44:LEU:HD13  | 1:A:62:TRP:CZ2   | 2.53                     | 0.43              |
| 1:A:128:VAL:HB   | 1:A:144:LEU:HD23 | 2.00                     | 0.43              |
| 1:A:130:CYS:SG   | 1:A:159:CYS:CB   | 3.06                     | 0.43              |
| 1:A:178:ALA:HA   | 1:A:283:LEU:HD22 | 1.80                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:193:GLN:HE21 | 1:A:193:GLN:HB3  | 1.62                     | 0.43              |
| 1:A:298:GLN:HB2  | 1:A:299:LYS:H    | 1.65                     | 0.43              |
| 1:B:17:THR:HG23  | 1:B:65:GLY:C     | 2.44                     | 0.43              |
| 1:A:76:ILE:H     | 1:A:76:ILE:CD1   | 2.18                     | 0.43              |
| 1:A:82:TYR:N     | 1:A:82:TYR:CD1   | 2.86                     | 0.43              |
| 1:A:124:SER:HB2  | 1:A:163:GLN:NE2  | 2.28                     | 0.43              |
| 1:B:36:ILE:HD12  | 1:B:51:LEU:HD23  | 2.01                     | 0.43              |
| 1:B:234:LYS:HA   | 1:B:253:LEU:CG   | 2.29                     | 0.43              |
| 1:A:215:TRP:CD1  | 1:A:216:GLN:N    | 2.87                     | 0.43              |
| 1:A:114:LEU:HD21 | 1:A:174:ILE:HD13 | 1.99                     | 0.43              |
| 1:B:26:PHE:CD2   | 1:B:67:PHE:HB3   | 2.53                     | 0.43              |
| 1:B:112:GLN:O    | 1:B:149:LEU:HD12 | 2.19                     | 0.43              |
| 1:B:198:PHE:CD2  | 1:B:272:LEU:HD22 | 2.54                     | 0.43              |
| 1:B:319:LEU:HA   | 1:B:343:TRP:HA   | 2.00                     | 0.43              |
| 1:A:293:ARG:C    | 1:A:303:CYS:SG   | 3.01                     | 0.43              |
| 1:B:164:ASN:C    | 1:B:166:LYS:H    | 2.25                     | 0.43              |
| 1:A:52:ASN:CG    | 1:A:53:ASP:N     | 2.77                     | 0.43              |
| 1:A:98:PHE:CG    | 1:A:161:VAL:HG11 | 2.54                     | 0.43              |
| 1:A:206:LYS:O    | 1:A:207:LEU:C    | 2.61                     | 0.43              |
| 1:A:206:LYS:HB3  | 1:A:207:LEU:HG   | 2.01                     | 0.43              |
| 1:B:133:PRO:HG3  | 1:B:156:THR:O    | 2.19                     | 0.43              |
| 1:B:205:GLU:CG   | 1:B:208:THR:CG2  | 2.93                     | 0.43              |
| 1:A:107:HIS:CE1  | 1:A:278:ALA:CB   | 2.99                     | 0.43              |
| 1:A:187:TYR:HB3  | 1:A:355:LEU:HG   | 2.00                     | 0.43              |
| 1:B:214:TRP:CE3  | 1:B:226:TRP:HZ3  | 2.34                     | 0.43              |
| 1:B:297:LEU:N    | 1:B:300:ASN:O    | 2.52                     | 0.43              |
| 1:A:128:VAL:HA   | 1:A:160:THR:O    | 2.18                     | 0.42              |
| 1:A:208:THR:O    | 1:A:276:LEU:HB2  | 2.19                     | 0.42              |
| 1:A:212:GLU:HB2  | 1:A:227:ILE:O    | 2.19                     | 0.42              |
| 1:A:226:TRP:HD1  | 1:A:241:VAL:HG11 | 1.84                     | 0.42              |
| 1:B:189:LYS:O    | 1:B:191:GLY:N    | 2.52                     | 0.42              |
| 1:A:100:LEU:HD12 | 1:A:118:LEU:CD1  | 2.48                     | 0.42              |
| 1:A:214:TRP:CD1  | 1:A:214:TRP:N    | 2.87                     | 0.42              |
| 1:A:267:ALA:HB1  | 1:A:307:GLY:HA3  | 2.01                     | 0.42              |
| 1:B:161:VAL:HB   | 1:B:168:VAL:CG1  | 2.49                     | 0.42              |
| 1:B:212:GLU:HG3  | 1:B:214:TRP:NE1  | 2.34                     | 0.42              |
| 1:A:109:LEU:HD22 | 1:A:281:GLY:C    | 2.44                     | 0.42              |
| 1:B:89:GLN:HE21  | 1:B:89:GLN:HB3   | 1.65                     | 0.42              |
| 1:B:130:CYS:SG   | 1:B:144:LEU:HD21 | 2.59                     | 0.42              |
| 1:B:326:VAL:HG11 | 1:B:335:VAL:HG22 | 2.00                     | 0.42              |
| 1:A:248:GLN:O    | 1:A:258:THR:OG1  | 2.38                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:288:ASN:HB3  | 1:A:308:PRO:HG3  | 2.01                     | 0.42              |
| 1:B:30:ASN:C     | 1:B:32:ASN:H     | 2.27                     | 0.42              |
| 1:B:109:LEU:HD12 | 1:B:109:LEU:H    | 1.85                     | 0.42              |
| 1:A:121:PRO:HA   | 1:A:122:PRO:HD3  | 1.93                     | 0.42              |
| 1:A:356:GLU:CG   | 1:B:320:GLU:HG2  | 2.50                     | 0.42              |
| 1:B:111:GLY:HA2  | 1:B:148:GLN:CB   | 2.49                     | 0.42              |
| 1:B:333:VAL:CG1  | 1:B:334:TRP:N    | 2.81                     | 0.42              |
| 1:A:186:VAL:HG12 | 1:A:188:LYS:HG2  | 2.02                     | 0.42              |
| 1:B:196:PHE:HD2  | 1:B:257:LEU:O    | 2.03                     | 0.42              |
| 1:A:114:LEU:HB2  | 1:A:149:LEU:HD11 | 2.01                     | 0.42              |
| 1:A:166:LYS:HZ3  | 1:A:166:LYS:HG3  | 1.56                     | 0.42              |
| 1:A:315:LEU:HD23 | 1:A:346:LEU:O    | 2.20                     | 0.42              |
| 1:A:342:MET:SD   | 1:A:360:LYS:CG   | 3.08                     | 0.42              |
| 1:B:362:LEU:CB   | 1:B:363:PRO:HD3  | 2.49                     | 0.42              |
| 1:B:293:ARG:O    | 1:B:303:CYS:HA   | 2.20                     | 0.41              |
| 1:A:20:GLN:HG3   | 1:A:24:ILE:HD13  | 2.02                     | 0.41              |
| 1:A:194:VAL:HG23 | 1:A:262:ALA:HB2  | 2.02                     | 0.41              |
| 1:A:263:LEU:HB2  | 1:A:266:TYR:CE1  | 2.56                     | 0.41              |
| 1:B:17:THR:HG22  | 1:B:18:ALA:N     | 2.33                     | 0.41              |
| 1:A:61:LEU:HD23  | 1:A:61:LEU:HA    | 1.90                     | 0.41              |
| 1:A:296:GLN:HA   | 1:A:301:LEU:CB   | 2.51                     | 0.41              |
| 1:A:347:LEU:O    | 1:A:354:LEU:HB2  | 2.20                     | 0.41              |
| 1:B:30:ASN:C     | 1:B:30:ASN:OD1   | 2.62                     | 0.41              |
| 1:B:46:LYS:HB2   | 1:B:46:LYS:HE2   | 1.72                     | 0.41              |
| 1:B:162:LEU:HD23 | 1:B:162:LEU:C    | 2.45                     | 0.41              |
| 1:B:180:GLN:O    | 1:B:180:GLN:HG3  | 2.20                     | 0.41              |
| 1:B:303:CYS:CB   | 1:B:345:CYS:HG   | 2.32                     | 0.41              |
| 1:A:14:LEU:CD2   | 1:A:69:LEU:HD23  | 2.50                     | 0.41              |
| 1:A:128:VAL:HB   | 1:A:144:LEU:CD2  | 2.50                     | 0.41              |
| 1:B:54:ARG:HG2   | 1:B:72:LYS:HB2   | 2.01                     | 0.41              |
| 1:B:100:LEU:HD12 | 1:B:118:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:331:LYS:HE3  | 1:A:331:LYS:HB2  | 1.85                     | 0.41              |
| 1:A:130:CYS:SG   | 1:A:144:LEU:HD11 | 2.60                     | 0.41              |
| 1:A:194:VAL:CG2  | 1:A:262:ALA:HB2  | 2.51                     | 0.41              |
| 1:B:349:ASP:O    | 1:B:351:GLY:N    | 2.51                     | 0.41              |
| 1:A:86:VAL:O     | 1:A:88:ASP:N     | 2.43                     | 0.41              |
| 1:A:148:GLN:H    | 1:A:148:GLN:HG3  | 1.69                     | 0.41              |
| 1:A:213:LEU:HD12 | 1:A:271:ASN:O    | 2.21                     | 0.41              |
| 1:A:245:PRO:CB   | 1:A:266:TYR:CE2  | 2.81                     | 0.41              |
| 1:A:300:ASN:HA   | 1:A:338:PRO:HD3  | 2.03                     | 0.41              |
| 1:B:87:GLU:O     | 1:B:88:ASP:CB    | 2.69                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:294:ALA:N    | 1:A:303:CYS:SG   | 2.93                     | 0.41              |
| 1:B:128:VAL:HB   | 1:B:144:LEU:CD2  | 2.51                     | 0.41              |
| 1:B:300:ASN:OD1  | 1:B:337:ASN:N    | 2.54                     | 0.41              |
| 1:B:319:LEU:HB3  | 1:B:343:TRP:NE1  | 2.36                     | 0.41              |
| 1:B:362:LEU:HB2  | 1:B:363:PRO:CD   | 2.50                     | 0.41              |
| 1:A:206:LYS:HB3  | 1:A:207:LEU:H    | 1.68                     | 0.41              |
| 1:A:302:THR:CG2  | 1:A:303:CYS:N    | 2.84                     | 0.41              |
| 1:A:317:LEU:HB2  | 1:A:326:VAL:HG12 | 2.02                     | 0.41              |
| 1:A:326:VAL:O    | 1:A:326:VAL:CG1  | 2.69                     | 0.41              |
| 1:B:16:CYS:SG    | 1:B:67:PHE:HB2   | 2.60                     | 0.41              |
| 1:B:20:GLN:O     | 1:B:22:LYS:N     | 2.54                     | 0.41              |
| 1:B:136:LYS:HD2  | 1:B:138:ILE:HB   | 2.02                     | 0.41              |
| 1:B:265:GLN:H    | 1:B:265:GLN:CD   | 2.28                     | 0.41              |
| 1:B:111:GLY:O    | 1:B:112:GLN:C    | 2.64                     | 0.41              |
| 1:B:296:GLN:HG3  | 1:B:301:LEU:HB3  | 2.02                     | 0.41              |
| 1:A:178:ALA:C    | 1:A:283:LEU:CD1  | 2.92                     | 0.40              |
| 1:B:343:TRP:N    | 1:B:359:ILE:O    | 2.53                     | 0.40              |
| 1:A:42:SER:HG    | 1:A:43:PHE:HD1   | 1.68                     | 0.40              |
| 1:A:58:ARG:NE    | 1:A:61:LEU:HD12  | 2.36                     | 0.40              |
| 1:A:100:LEU:HD22 | 1:A:159:CYS:HB2  | 2.03                     | 0.40              |
| 1:A:177:LEU:HD21 | 1:A:276:LEU:CD1  | 2.47                     | 0.40              |
| 1:B:7:LYS:HB2    | 1:B:10:ASP:CB    | 2.50                     | 0.40              |
| 1:B:59:ARG:HA    | 1:B:62:TRP:CD2   | 2.57                     | 0.40              |
| 1:A:175:VAL:O    | 1:A:175:VAL:HG12 | 2.20                     | 0.40              |
| 1:A:319:LEU:HB3  | 1:A:343:TRP:NE1  | 2.36                     | 0.40              |
| 1:B:17:THR:O     | 1:B:18:ALA:CB    | 2.69                     | 0.40              |
| 1:B:51:LEU:HD12  | 1:B:51:LEU:HA    | 1.77                     | 0.40              |
| 1:B:247:LEU:HD23 | 1:B:247:LEU:H    | 1.85                     | 0.40              |
| 1:A:51:LEU:O     | 1:A:52:ASN:C     | 2.64                     | 0.40              |
| 1:A:296:GLN:HG3  | 1:A:301:LEU:HB3  | 2.04                     | 0.40              |
| 1:A:349:ASP:O    | 1:A:351:GLY:N    | 2.53                     | 0.40              |
| 1:B:59:ARG:HA    | 1:B:62:TRP:CG    | 2.57                     | 0.40              |

All (32) 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:A:124:SER:CA | 1:B:362:LEU:CD1[3_664] | 0.99                     | 1.21              |
| 1:A:124:SER:N  | 1:B:362:LEU:CD1[3_664] | 1.08                     | 1.12              |
| 1:A:142:LYS:CB | 1:B:297:LEU:O[3_664]   | 1.13                     | 1.07              |

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| Atom-1         | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:A:123:GLY:CA | 1:B:362:LEU:CD2[3_664] | 1.24                     | 0.96              |
| 1:A:123:GLY:O  | 1:B:362:LEU:CB[3_664]  | 1.24                     | 0.96              |
| 1:A:142:LYS:NZ | 1:B:295:THR:O[3_664]   | 1.40                     | 0.80              |
| 1:A:123:GLY:C  | 1:B:362:LEU:CD2[3_664] | 1.47                     | 0.73              |
| 1:A:127:SER:N  | 1:B:299:LYS:NZ[3_664]  | 1.49                     | 0.71              |
| 1:B:48:PRO:CA  | 1:B:241:VAL:CG2[4_647] | 1.50                     | 0.70              |
| 1:A:124:SER:C  | 1:B:362:LEU:CD1[3_664] | 1.55                     | 0.65              |
| 1:A:123:GLY:C  | 1:B:362:LEU:CG[3_664]  | 1.56                     | 0.64              |
| 1:A:127:SER:CB | 1:B:299:LYS:NZ[3_664]  | 1.65                     | 0.55              |
| 1:A:127:SER:CA | 1:B:299:LYS:NZ[3_664]  | 1.69                     | 0.51              |
| 1:A:142:LYS:CB | 1:B:297:LEU:C[3_664]   | 1.72                     | 0.48              |
| 1:A:127:SER:OG | 1:B:299:LYS:CE[3_664]  | 1.73                     | 0.47              |
| 1:A:124:SER:N  | 1:B:362:LEU:CG[3_664]  | 1.77                     | 0.43              |
| 1:A:126:PRO:C  | 1:B:299:LYS:NZ[3_664]  | 1.78                     | 0.42              |
| 1:A:126:PRO:O  | 1:B:298:GLN:CB[3_664]  | 1.81                     | 0.39              |
| 1:A:142:LYS:CG | 1:B:297:LEU:CA[3_664]  | 1.81                     | 0.39              |
| 1:A:123:GLY:O  | 1:B:362:LEU:CG[3_664]  | 1.87                     | 0.33              |
| 1:A:125:SER:CB | 1:B:299:LYS:CA[3_664]  | 1.91                     | 0.29              |
| 1:A:127:SER:OG | 1:B:299:LYS:NZ[3_664]  | 1.92                     | 0.28              |
| 1:A:123:GLY:C  | 1:B:362:LEU:CD1[3_664] | 1.98                     | 0.22              |
| 1:A:123:GLY:C  | 1:B:362:LEU:CB[3_664]  | 1.99                     | 0.21              |
| 1:A:124:SER:O  | 1:B:362:LEU:CD1[3_664] | 2.03                     | 0.17              |
| 1:B:52:ASN:ND2 | 1:B:240:ARG:CB[4_647]  | 2.08                     | 0.12              |
| 1:A:124:SER:N  | 1:B:362:LEU:CD2[3_664] | 2.09                     | 0.11              |
| 1:A:125:SER:OG | 1:B:299:LYS:CA[3_664]  | 2.09                     | 0.11              |
| 1:A:126:PRO:O  | 1:B:299:LYS:NZ[3_664]  | 2.09                     | 0.11              |
| 1:A:142:LYS:CA | 1:B:297:LEU:O[3_664]   | 2.09                     | 0.11              |
| 1:A:125:SER:OG | 1:B:298:GLN:O[3_664]   | 2.12                     | 0.08              |
| 1:B:48:PRO:CB  | 1:B:241:VAL:CG1[4_647] | 2.17                     | 0.03              |

## 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     | 359/363 (99%) | 259 (72%) | 58 (16%)  | 42 (12%) | 0           | 5 |
| 1   | B     | 359/363 (99%) | 259 (72%) | 59 (16%)  | 41 (11%) | 0           | 5 |
| All | All   | 718/726 (99%) | 518 (72%) | 117 (16%) | 83 (12%) | 0           | 5 |

All (83) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 21  | LYS  |
| 1   | A     | 52  | ASN  |
| 1   | A     | 73  | ASN  |
| 1   | A     | 87  | GLU  |
| 1   | A     | 88  | ASP  |
| 1   | A     | 105 | ASP  |
| 1   | A     | 136 | LYS  |
| 1   | A     | 147 | SER  |
| 1   | A     | 151 | LEU  |
| 1   | A     | 190 | GLU  |
| 1   | A     | 202 | PHE  |
| 1   | A     | 203 | THR  |
| 1   | A     | 205 | GLU  |
| 1   | A     | 222 | SER  |
| 1   | A     | 241 | VAL  |
| 1   | A     | 242 | THR  |
| 1   | A     | 244 | ASP  |
| 1   | A     | 255 | LEU  |
| 1   | A     | 260 | PRO  |
| 1   | A     | 280 | THR  |
| 1   | A     | 349 | ASP  |
| 1   | B     | 18  | ALA  |
| 1   | B     | 21  | LYS  |
| 1   | B     | 52  | ASN  |
| 1   | B     | 73  | ASN  |
| 1   | B     | 87  | GLU  |
| 1   | B     | 88  | ASP  |
| 1   | B     | 105 | ASP  |
| 1   | B     | 136 | LYS  |
| 1   | B     | 147 | SER  |
| 1   | B     | 151 | LEU  |
| 1   | B     | 190 | GLU  |
| 1   | B     | 202 | PHE  |
| 1   | B     | 205 | GLU  |
| 1   | B     | 222 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 241 | VAL  |
| 1   | B     | 242 | THR  |
| 1   | B     | 244 | ASP  |
| 1   | B     | 255 | LEU  |
| 1   | B     | 261 | GLN  |
| 1   | B     | 280 | THR  |
| 1   | B     | 349 | ASP  |
| 1   | A     | 53  | ASP  |
| 1   | A     | 106 | THR  |
| 1   | A     | 112 | GLN  |
| 1   | A     | 207 | LEU  |
| 1   | A     | 278 | ALA  |
| 1   | B     | 10  | ASP  |
| 1   | B     | 106 | THR  |
| 1   | B     | 206 | LYS  |
| 1   | B     | 207 | LEU  |
| 1   | B     | 243 | GLN  |
| 1   | B     | 278 | ALA  |
| 1   | A     | 10  | ASP  |
| 1   | A     | 19  | SER  |
| 1   | A     | 20  | GLN  |
| 1   | A     | 233 | ASN  |
| 1   | A     | 253 | LEU  |
| 1   | A     | 297 | LEU  |
| 1   | A     | 324 | ALA  |
| 1   | B     | 20  | GLN  |
| 1   | B     | 53  | ASP  |
| 1   | B     | 112 | GLN  |
| 1   | B     | 220 | ALA  |
| 1   | B     | 240 | ARG  |
| 1   | B     | 253 | LEU  |
| 1   | B     | 324 | ALA  |
| 1   | B     | 351 | GLY  |
| 1   | A     | 16  | CYS  |
| 1   | A     | 201 | ALA  |
| 1   | A     | 206 | LYS  |
| 1   | A     | 240 | ARG  |
| 1   | A     | 351 | GLY  |
| 1   | B     | 16  | CYS  |
| 1   | B     | 23  | SER  |
| 1   | B     | 201 | ALA  |
| 1   | B     | 326 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 113 | SER  |
| 1   | A     | 220 | ALA  |
| 1   | A     | 326 | VAL  |
| 1   | B     | 126 | PRO  |
| 1   | A     | 362 | LEU  |
| 1   | B     | 122 | 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     | 318/324 (98%) | 216 (68%) | 102 (32%) | 0           | 2 |
| 1   | B     | 318/324 (98%) | 223 (70%) | 95 (30%)  | 0           | 2 |
| All | All   | 636/648 (98%) | 439 (69%) | 197 (31%) | 0           | 2 |

All (197) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | LYS  |
| 1   | A     | 3   | VAL  |
| 1   | A     | 11  | THR  |
| 1   | A     | 14  | LEU  |
| 1   | A     | 15  | THR  |
| 1   | A     | 16  | CYS  |
| 1   | A     | 19  | SER  |
| 1   | A     | 23  | SER  |
| 1   | A     | 25  | GLN  |
| 1   | A     | 29  | LYS  |
| 1   | A     | 35  | LYS  |
| 1   | A     | 36  | ILE  |
| 1   | A     | 43  | PHE  |
| 1   | A     | 46  | LYS  |
| 1   | A     | 59  | ARG  |
| 1   | A     | 63  | ASP  |
| 1   | A     | 68  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 70  | ILE  |
| 1   | A     | 76  | ILE  |
| 1   | A     | 84  | CYS  |
| 1   | A     | 89  | GLN  |
| 1   | A     | 97  | VAL  |
| 1   | A     | 101 | THR  |
| 1   | A     | 103 | ASN  |
| 1   | A     | 104 | SER  |
| 1   | A     | 115 | THR  |
| 1   | A     | 118 | LEU  |
| 1   | A     | 124 | SER  |
| 1   | A     | 125 | SER  |
| 1   | A     | 132 | SER  |
| 1   | A     | 134 | ARG  |
| 1   | A     | 136 | LYS  |
| 1   | A     | 139 | GLN  |
| 1   | A     | 143 | THR  |
| 1   | A     | 144 | LEU  |
| 1   | A     | 148 | GLN  |
| 1   | A     | 151 | LEU  |
| 1   | A     | 152 | GLN  |
| 1   | A     | 154 | SER  |
| 1   | A     | 156 | THR  |
| 1   | A     | 158 | THR  |
| 1   | A     | 163 | GLN  |
| 1   | A     | 164 | ASN  |
| 1   | A     | 166 | LYS  |
| 1   | A     | 171 | LYS  |
| 1   | A     | 175 | VAL  |
| 1   | A     | 185 | ILE  |
| 1   | A     | 193 | GLN  |
| 1   | A     | 195 | GLU  |
| 1   | A     | 197 | SER  |
| 1   | A     | 198 | PHE  |
| 1   | A     | 207 | LEU  |
| 1   | A     | 208 | THR  |
| 1   | A     | 216 | GLN  |
| 1   | A     | 221 | SER  |
| 1   | A     | 223 | SER  |
| 1   | A     | 225 | SER  |
| 1   | A     | 226 | TRP  |
| 1   | A     | 228 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 229 | PHE  |
| 1   | A     | 230 | ASP  |
| 1   | A     | 234 | LYS  |
| 1   | A     | 235 | GLU  |
| 1   | A     | 237 | SER  |
| 1   | A     | 238 | VAL  |
| 1   | A     | 243 | GLN  |
| 1   | A     | 247 | LEU  |
| 1   | A     | 251 | LYS  |
| 1   | A     | 253 | LEU  |
| 1   | A     | 257 | LEU  |
| 1   | A     | 259 | LEU  |
| 1   | A     | 260 | PRO  |
| 1   | A     | 266 | TYR  |
| 1   | A     | 272 | LEU  |
| 1   | A     | 273 | THR  |
| 1   | A     | 274 | LEU  |
| 1   | A     | 276 | LEU  |
| 1   | A     | 279 | LYS  |
| 1   | A     | 282 | LYS  |
| 1   | A     | 285 | GLN  |
| 1   | A     | 286 | GLU  |
| 1   | A     | 295 | THR  |
| 1   | A     | 298 | GLN  |
| 1   | A     | 299 | LYS  |
| 1   | A     | 302 | THR  |
| 1   | A     | 304 | GLU  |
| 1   | A     | 305 | VAL  |
| 1   | A     | 310 | SER  |
| 1   | A     | 312 | LYS  |
| 1   | A     | 313 | LEU  |
| 1   | A     | 315 | LEU  |
| 1   | A     | 316 | SER  |
| 1   | A     | 320 | GLU  |
| 1   | A     | 329 | ARG  |
| 1   | A     | 330 | GLU  |
| 1   | A     | 333 | VAL  |
| 1   | A     | 336 | LEU  |
| 1   | A     | 339 | GLU  |
| 1   | A     | 342 | MET  |
| 1   | A     | 350 | SER  |
| 1   | A     | 353 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 362 | LEU  |
| 1   | B     | 3   | VAL  |
| 1   | B     | 11  | THR  |
| 1   | B     | 12  | VAL  |
| 1   | B     | 14  | LEU  |
| 1   | B     | 15  | THR  |
| 1   | B     | 19  | SER  |
| 1   | B     | 23  | SER  |
| 1   | B     | 25  | GLN  |
| 1   | B     | 29  | LYS  |
| 1   | B     | 35  | LYS  |
| 1   | B     | 43  | PHE  |
| 1   | B     | 58  | ARG  |
| 1   | B     | 59  | ARG  |
| 1   | B     | 63  | ASP  |
| 1   | B     | 68  | PRO  |
| 1   | B     | 70  | ILE  |
| 1   | B     | 76  | ILE  |
| 1   | B     | 82  | TYR  |
| 1   | B     | 89  | GLN  |
| 1   | B     | 97  | VAL  |
| 1   | B     | 101 | THR  |
| 1   | B     | 103 | ASN  |
| 1   | B     | 115 | THR  |
| 1   | B     | 118 | LEU  |
| 1   | B     | 125 | SER  |
| 1   | B     | 127 | SER  |
| 1   | B     | 132 | SER  |
| 1   | B     | 134 | ARG  |
| 1   | B     | 139 | GLN  |
| 1   | B     | 143 | THR  |
| 1   | B     | 144 | LEU  |
| 1   | B     | 148 | GLN  |
| 1   | B     | 151 | LEU  |
| 1   | B     | 152 | GLN  |
| 1   | B     | 154 | SER  |
| 1   | B     | 156 | THR  |
| 1   | B     | 158 | THR  |
| 1   | B     | 162 | LEU  |
| 1   | B     | 163 | GLN  |
| 1   | B     | 164 | ASN  |
| 1   | B     | 166 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 175 | VAL  |
| 1   | B     | 185 | ILE  |
| 1   | B     | 193 | GLN  |
| 1   | B     | 195 | GLU  |
| 1   | B     | 197 | SER  |
| 1   | B     | 198 | PHE  |
| 1   | B     | 203 | THR  |
| 1   | B     | 207 | LEU  |
| 1   | B     | 208 | THR  |
| 1   | B     | 216 | GLN  |
| 1   | B     | 221 | SER  |
| 1   | B     | 223 | SER  |
| 1   | B     | 225 | SER  |
| 1   | B     | 226 | TRP  |
| 1   | B     | 228 | THR  |
| 1   | B     | 229 | PHE  |
| 1   | B     | 230 | ASP  |
| 1   | B     | 235 | GLU  |
| 1   | B     | 236 | VAL  |
| 1   | B     | 237 | SER  |
| 1   | B     | 238 | VAL  |
| 1   | B     | 243 | GLN  |
| 1   | B     | 247 | LEU  |
| 1   | B     | 251 | LYS  |
| 1   | B     | 253 | LEU  |
| 1   | B     | 257 | LEU  |
| 1   | B     | 259 | LEU  |
| 1   | B     | 273 | THR  |
| 1   | B     | 274 | LEU  |
| 1   | B     | 276 | LEU  |
| 1   | B     | 279 | LYS  |
| 1   | B     | 282 | LYS  |
| 1   | B     | 285 | GLN  |
| 1   | B     | 286 | GLU  |
| 1   | B     | 298 | GLN  |
| 1   | B     | 299 | LYS  |
| 1   | B     | 302 | THR  |
| 1   | B     | 304 | GLU  |
| 1   | B     | 305 | VAL  |
| 1   | B     | 310 | SER  |
| 1   | B     | 312 | LYS  |
| 1   | B     | 313 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 315 | LEU  |
| 1   | B     | 316 | SER  |
| 1   | B     | 320 | GLU  |
| 1   | B     | 329 | ARG  |
| 1   | B     | 330 | GLU  |
| 1   | B     | 333 | VAL  |
| 1   | B     | 336 | LEU  |
| 1   | B     | 339 | GLU  |
| 1   | B     | 342 | MET  |
| 1   | B     | 350 | SER  |
| 1   | B     | 353 | VAL  |
| 1   | B     | 362 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 20  | GLN  |
| 1   | A     | 66  | ASN  |
| 1   | A     | 89  | GLN  |
| 1   | A     | 103 | ASN  |
| 1   | A     | 110 | GLN  |
| 1   | A     | 163 | GLN  |
| 1   | A     | 180 | GLN  |
| 1   | A     | 193 | GLN  |
| 1   | A     | 261 | GLN  |
| 1   | A     | 284 | HIS  |
| 1   | A     | 288 | ASN  |
| 1   | A     | 321 | ASN  |
| 1   | B     | 20  | GLN  |
| 1   | B     | 66  | ASN  |
| 1   | B     | 89  | GLN  |
| 1   | B     | 103 | ASN  |
| 1   | B     | 110 | GLN  |
| 1   | B     | 163 | GLN  |
| 1   | B     | 180 | GLN  |
| 1   | B     | 261 | GLN  |
| 1   | B     | 284 | HIS  |
| 1   | B     | 288 | ASN  |

### 5.3.3 RNA [i](#)

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](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | A     | 1                |
| 1   | B     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 178:ALA   | C      | 179:PHE   | N      | 2.89         |
| 1     | B     | 178:ALA   | C      | 179:PHE   | N      | 2.73         |

## 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.