



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:12 PM UTC

PDB ID : 1OFR / pdb\_00001ofr  
Title : CRYSTAL STRUCTURE OF THE TYROSINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE FROM SACCCHAROMYCES CEREVISIAE COMPLEXED WITH PHENYLALANINE AND MANGANESE  
Authors : Koenig, V.; Pfeil, A.; Heinrich, G.; Braus, G.; Schneider, T.R.  
Deposited on : 2003-04-18  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

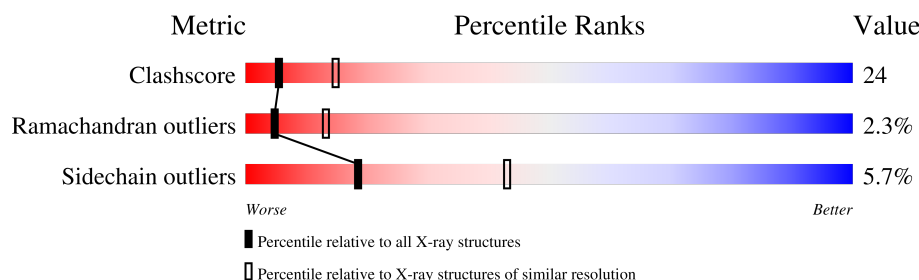
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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                      | 3843 (2.70-2.70)                                      |
| Ramachandran outliers | 187476                      | 3778 (2.70-2.70)                                      |
| Sidechain outliers    | 187428                      | 3778 (2.70-2.70)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 370    |                  |
| 1   | B     | 370    |                  |
| 1   | C     | 370    |                  |
| 1   | D     | 370    |                  |
| 1   | E     | 370    |                  |
| 1   | F     | 370    |                  |
| 1   | G     | 370    |                  |
| 1   | H     | 370    |                  |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 20930 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 PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 350      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 2631  | 1636 | 474 | 511 | 10 |         |         |       |
| 1   | B     | 348      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 2618  | 1629 | 469 | 510 | 10 |         |         |       |
| 1   | C     | 349      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 2626  | 1634 | 471 | 511 | 10 |         |         |       |
| 1   | D     | 351      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 2623  | 1630 | 470 | 513 | 10 |         |         |       |
| 1   | E     | 339      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 2560  | 1591 | 460 | 499 | 10 |         |         |       |
| 1   | F     | 347      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 2604  | 1620 | 467 | 507 | 10 |         |         |       |
| 1   | G     | 344      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 2581  | 1605 | 462 | 504 | 10 |         |         |       |
| 1   | H     | 347      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 2599  | 1614 | 466 | 509 | 10 |         |         |       |

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

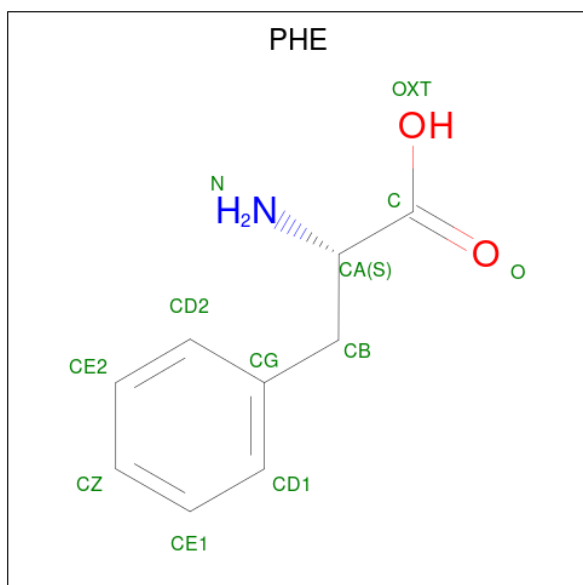
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 1        | Total | Mn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | B     | 1        | Total | Mn | 0       | 0       |
|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

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | G     | 1        | Total | Mn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | H     | 1        | Total | Mn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is PHENYLALANINE (CCD ID: PHE) (formula:  $C_9H_{11}NO_2$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 9 | 1 | 2 |         |         |
| 3   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 9 | 1 | 2 |         |         |
| 3   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 9 | 1 | 2 |         |         |
| 3   | H     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 9 | 1 | 2 |         |         |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 4   | A     | 6        | Total | O | 0       | 0       |
|     |       |          | 6     | 6 |         |         |
| 4   | B     | 4        | Total | O | 0       | 0       |
|     |       |          | 4     | 4 |         |         |
| 4   | C     | 5        | Total | O | 0       | 0       |
|     |       |          | 5     | 5 |         |         |

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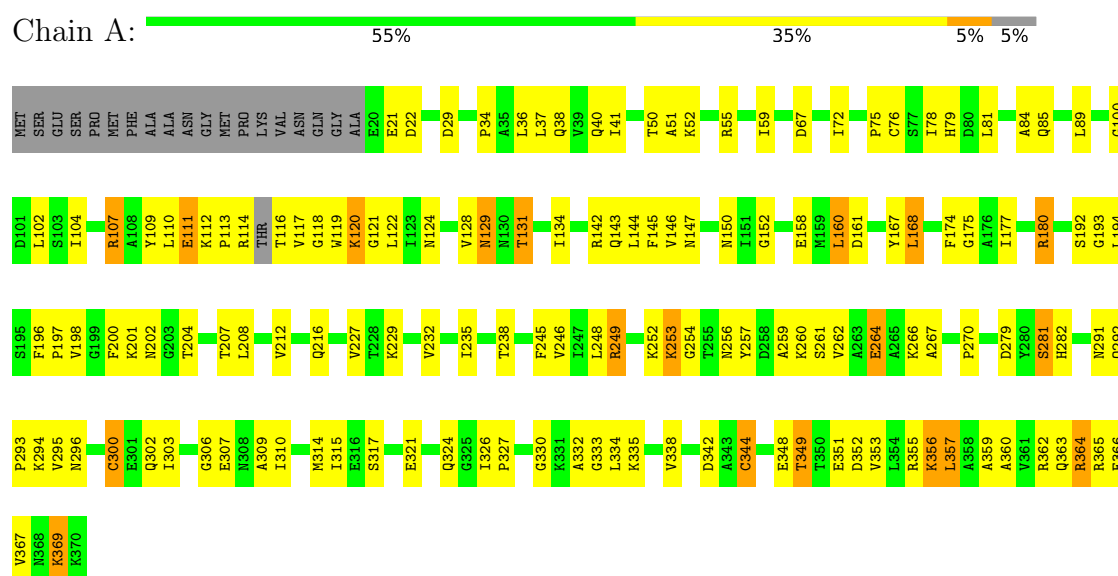
| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 4   | D     | 5        | Total<br>5 | O<br>5 | 0       | 0       |
| 4   | E     | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 4   | F     | 4        | Total<br>4 | O<br>4 | 0       | 0       |
| 4   | G     | 3        | Total<br>3 | O<br>3 | 0       | 0       |
| 4   | H     | 3        | Total<br>3 | O<br>3 | 0       | 0       |

### 3 Residue-property plots

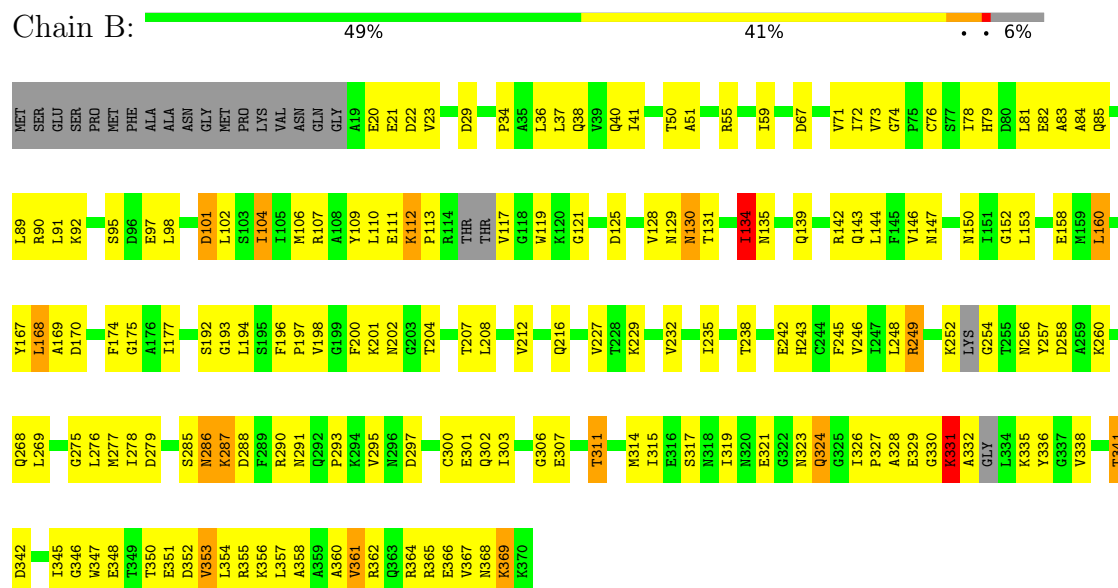
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

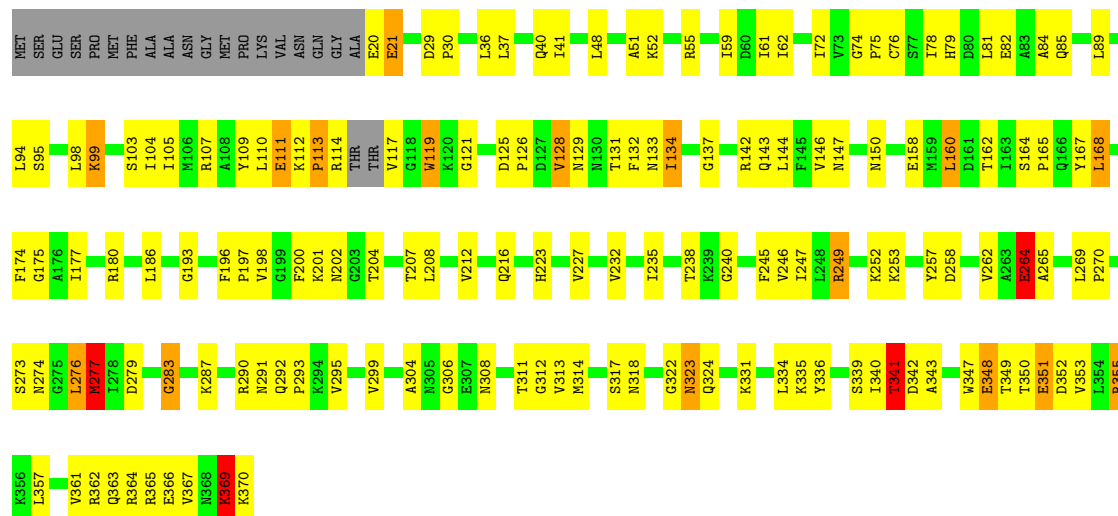


#### • Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE



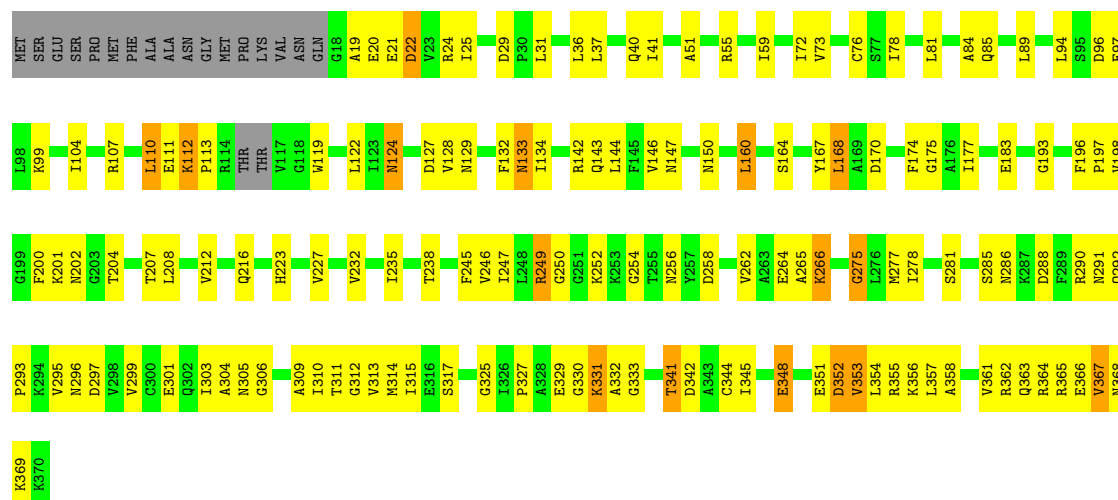
• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain C: 



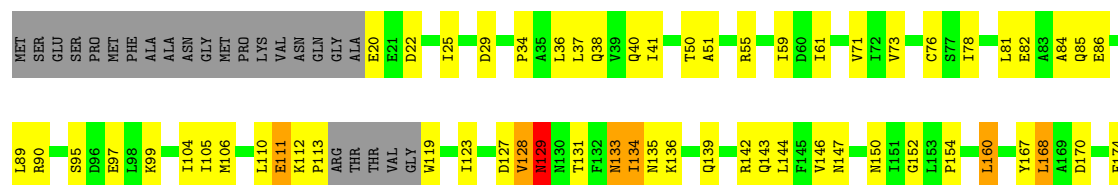
• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

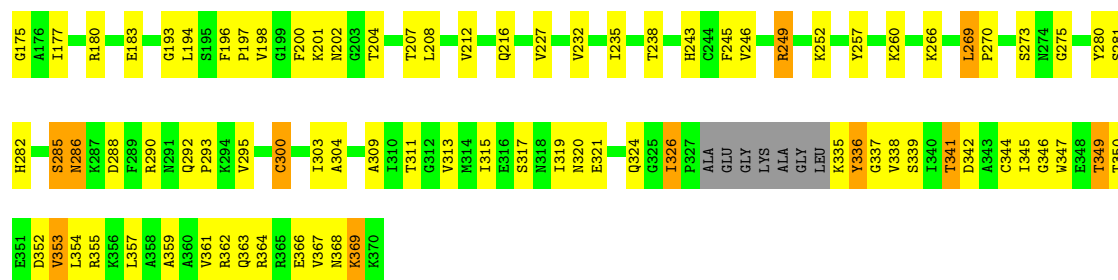
Chain D: 



• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

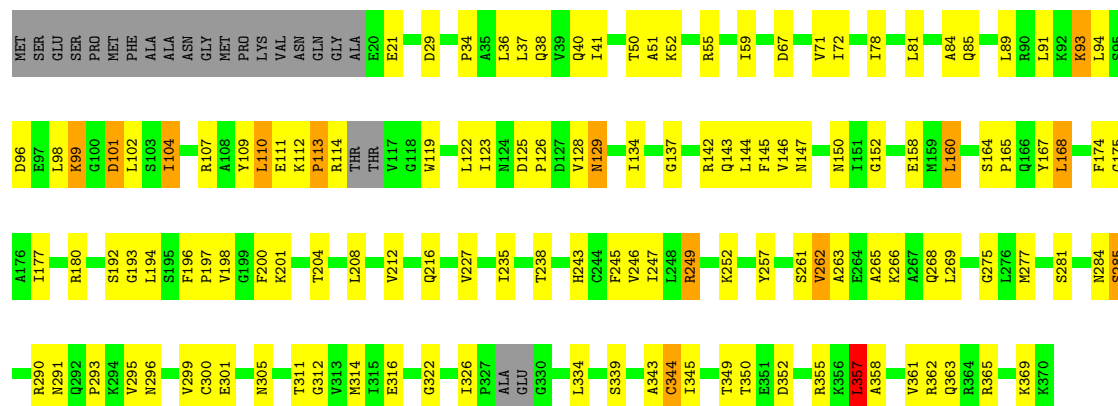
Chain E: 





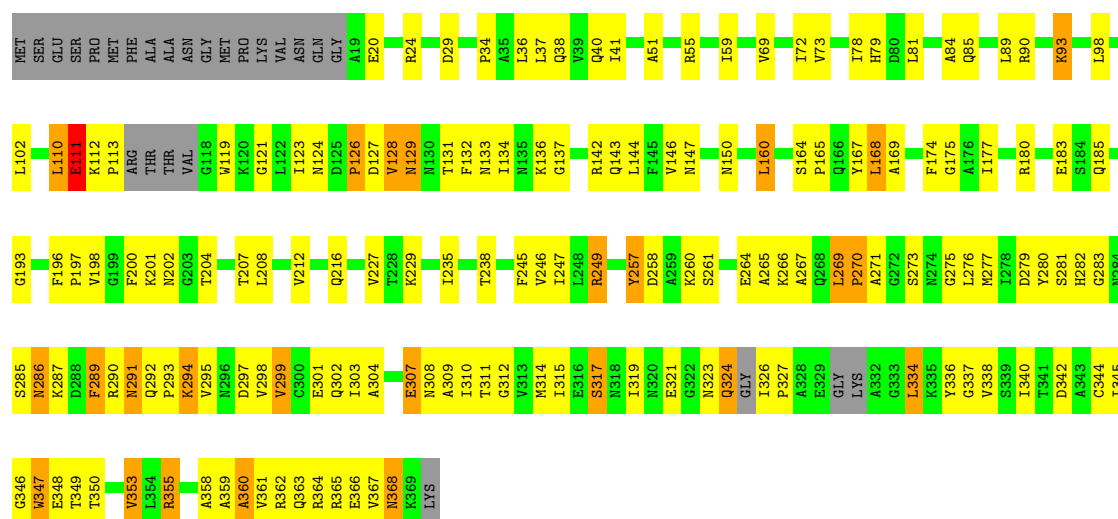
• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain F: 59% 31% 6%



• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain G: 50% 36% 7% 7%



• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain H: 50% 39% 6%

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|------|------|------|------|------|------|------|------|------|------|
| W347 | E348 | T349 | T350 | D352 | V353 | L354 | K355 | L357 | V361 | R362 | Q363 | R364 | R365 | E366 | V367 | N368 | K369 | LYS | G275 | L276 | M277 | I278 | D279 | S285 | D288 | F289 | R290 | N291 | Q292 | P293 | K294 | V295 | N296 | V299 | C300 | E301 | Q302 | I303 | A304 | N305 | G306 | E307 | N308 | V313 | M314 | I315 | E316 | S317 | N318 | I319 | N320 | E321 | G322 | N323 | Q324 | G325 | I326 | P327 | A328 | GLU  | GLY  | LYS | A332 | Y336 | G337 | V338 | S339 | D342 | A343 | C344 | I345 | G346 |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     | A176 | I177 | R180 | E183 | G193 | L194 | S195 | F196 | P197 | V198 | G199 | F200 | K201 | T204 | L208 | V212 | Q216 | V227 | T228 | K229 | V232 | I235 | T238 | K239 | G240 | F245 | V246 | I247 | L248 | R249 | K252 | K253 | G254 | D258 | S261 | V262 | A263 | E264 | A265 | K266 | P270 | S273 | N274 |     |      |      |      |      |      |      |      |      |      |      |
| MET  | SER  | GLU  | SER  | PRO  | MET  | PHE  | ALA  | ALA  | ASN  | GLY  | MET  | PRO  | PRO  | LYS  | VAL  | ASN  | GLN  | GLY | ALA  | E20  | D29  | P30  | L31  | P34  | A35  | L36  | L37  | Q38  | V39  | Q40  | I41  | A51  | R55  | I59  | D60  | I61  | I62  | L70  | V71  | I72  | V73  | G74  | P75  | C76  | S77  | I78  | H79  | D80  | L81  | E82  | A83  | A84  | Q85  | E86  |      |      |      |      |      |      |      |     |      |      |      |      |      |      |      |      |      |      |

## 4 Data and refinement statistics

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

| Property                                                 | Value                                         | Source    |
|----------------------------------------------------------|-----------------------------------------------|-----------|
| Space group                                              | P 1                                           | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 82.29Å 94.03Å 105.12Å<br>65.14° 85.68° 75.73° | Depositor |
| Resolution (Å)                                           | 37.20 – 2.70                                  | Depositor |
| % Data completeness<br>(in resolution range)             | 85.9 (37.20-2.70)                             | Depositor |
| $R_{merge}$                                              | 0.07                                          | Depositor |
| $R_{sym}$                                                | (Not available)                               | Depositor |
| Refinement program                                       | CNS 1.1                                       | Depositor |
| R, $R_{free}$                                            | 0.232 , 0.274                                 | Depositor |
| Estimated twinning fraction                              | No twinning to report.                        | Xtriage   |
| Total number of atoms                                    | 20930                                         | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 46.0                                          | wwPDB-VP  |

## 5 Model quality [i](#)

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

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

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.54         | 1/2669 (0.0%)  | 0.93        | 5/3613 (0.1%)   |
| 1   | B     | 0.55         | 1/2654 (0.0%)  | 0.95        | 6/3590 (0.2%)   |
| 1   | C     | 0.53         | 1/2664 (0.0%)  | 0.98        | 12/3605 (0.3%)  |
| 1   | D     | 0.54         | 1/2661 (0.0%)  | 0.97        | 4/3605 (0.1%)   |
| 1   | E     | 0.49         | 1/2596 (0.0%)  | 0.95        | 7/3513 (0.2%)   |
| 1   | F     | 0.51         | 1/2641 (0.0%)  | 0.97        | 3/3575 (0.1%)   |
| 1   | G     | 0.51         | 1/2617 (0.0%)  | 0.94        | 8/3544 (0.2%)   |
| 1   | H     | 0.50         | 1/2637 (0.0%)  | 0.93        | 4/3577 (0.1%)   |
| All | All   | 0.52         | 8/21139 (0.0%) | 0.95        | 49/28622 (0.2%) |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | B     | 369 | LYS  | C-N   | -5.68 | 1.25        | 1.33     |
| 1   | E     | 369 | LYS  | C-N   | -5.52 | 1.25        | 1.33     |
| 1   | F     | 369 | LYS  | C-N   | -5.52 | 1.25        | 1.33     |
| 1   | A     | 369 | LYS  | C-N   | -5.50 | 1.25        | 1.33     |
| 1   | H     | 368 | ASN  | C-N   | -5.39 | 1.25        | 1.33     |
| 1   | D     | 369 | LYS  | C-N   | -5.34 | 1.25        | 1.33     |
| 1   | C     | 369 | LYS  | C-N   | -5.33 | 1.25        | 1.33     |
| 1   | G     | 368 | ASN  | C-N   | -5.31 | 1.25        | 1.33     |

All (49) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | G     | 309 | ALA  | N-CA-C | -8.09 | 103.61      | 113.97   |
| 1   | G     | 303 | ILE  | N-CA-C | -7.48 | 103.57      | 110.82   |
| 1   | C     | 125 | ASP  | CA-C-N | 7.47  | 126.74      | 118.97   |
| 1   | C     | 125 | ASP  | C-N-CA | 7.47  | 126.74      | 118.97   |
| 1   | D     | 104 | ILE  | N-CA-C | 7.44  | 119.33      | 109.21   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | E     | 269 | LEU  | CA-C-N | 7.27  | 127.22      | 120.03   |
| 1   | E     | 269 | LEU  | C-N-CA | 7.27  | 127.22      | 120.03   |
| 1   | B     | 104 | ILE  | N-CA-C | 6.90  | 117.99      | 108.89   |
| 1   | F     | 104 | ILE  | N-CA-C | 6.85  | 117.30      | 108.12   |
| 1   | C     | 111 | GLU  | N-CA-C | 6.70  | 116.71      | 107.73   |
| 1   | E     | 353 | VAL  | N-CA-C | -6.65 | 104.00      | 110.72   |
| 1   | F     | 285 | SER  | N-CA-C | -6.53 | 105.23      | 113.72   |
| 1   | C     | 264 | GLU  | N-CA-C | -6.48 | 104.30      | 111.36   |
| 1   | G     | 111 | GLU  | N-CA-C | 6.27  | 116.72      | 107.88   |
| 1   | H     | 319 | ILE  | N-CA-C | -6.19 | 104.71      | 110.53   |
| 1   | A     | 315 | ILE  | N-CA-C | 6.10  | 116.65      | 108.11   |
| 1   | D     | 325 | GLY  | N-CA-C | -6.04 | 103.36      | 112.60   |
| 1   | B     | 328 | ALA  | N-CA-C | -5.91 | 105.17      | 112.38   |
| 1   | B     | 321 | GLU  | N-CA-C | 5.89  | 118.15      | 110.43   |
| 1   | E     | 321 | GLU  | N-CA-C | 5.86  | 117.05      | 108.14   |
| 1   | E     | 104 | ILE  | N-CA-C | 5.81  | 116.67      | 108.36   |
| 1   | G     | 269 | LEU  | CA-C-N | 5.77  | 126.23      | 120.52   |
| 1   | G     | 269 | LEU  | C-N-CA | 5.77  | 126.23      | 120.52   |
| 1   | A     | 264 | GLU  | N-CA-C | -5.75 | 105.02      | 111.28   |
| 1   | G     | 297 | ASP  | N-CA-C | 5.65  | 117.89      | 111.11   |
| 1   | C     | 277 | MET  | N-CA-C | -5.61 | 101.45      | 110.14   |
| 1   | D     | 124 | ASN  | N-CA-C | 5.61  | 118.32      | 111.82   |
| 1   | A     | 309 | ALA  | N-CA-C | -5.60 | 106.28      | 113.23   |
| 1   | G     | 270 | PRO  | N-CA-C | 5.53  | 119.38      | 111.13   |
| 1   | B     | 287 | LYS  | N-CA-C | 5.50  | 119.02      | 111.54   |
| 1   | B     | 134 | ILE  | N-CA-C | 5.48  | 116.87      | 110.62   |
| 1   | E     | 111 | GLU  | N-CA-C | 5.47  | 116.45      | 108.14   |
| 1   | C     | 347 | TRP  | N-CA-C | 5.46  | 116.92      | 110.97   |
| 1   | C     | 306 | GLY  | N-CA-C | 5.41  | 123.89      | 115.72   |
| 1   | C     | 351 | GLU  | N-CA-C | -5.39 | 105.40      | 111.28   |
| 1   | D     | 358 | ALA  | N-CA-C | -5.35 | 105.11      | 111.69   |
| 1   | A     | 356 | LYS  | N-CA-C | -5.33 | 105.51      | 112.23   |
| 1   | C     | 105 | ILE  | N-CA-C | -5.33 | 100.80      | 108.53   |
| 1   | C     | 355 | ARG  | N-CA-C | -5.29 | 105.59      | 111.36   |
| 1   | H     | 326 | ILE  | CA-C-N | 5.28  | 126.44      | 119.84   |
| 1   | H     | 326 | ILE  | C-N-CA | 5.28  | 126.44      | 119.84   |
| 1   | E     | 275 | GLY  | N-CA-C | 5.21  | 120.01      | 110.95   |
| 1   | C     | 104 | ILE  | N-CA-C | 5.21  | 115.59      | 107.99   |
| 1   | A     | 104 | ILE  | N-CA-C | 5.19  | 116.06      | 108.58   |
| 1   | B     | 268 | GLN  | N-CA-C | 5.18  | 119.08      | 112.34   |
| 1   | G     | 299 | VAL  | N-CA-C | -5.12 | 106.69      | 111.45   |
| 1   | C     | 311 | THR  | N-CA-C | 5.05  | 119.50      | 113.23   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | F     | 357 | LEU  | N-CA-C | -5.02 | 105.99      | 111.82   |
| 1   | H     | 351 | GLU  | N-CA-C | -5.02 | 105.81      | 111.28   |

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     | 2631  | 0        | 2634     | 130     | 0            |
| 1   | B     | 2618  | 0        | 2618     | 136     | 0            |
| 1   | C     | 2626  | 0        | 2631     | 130     | 0            |
| 1   | D     | 2623  | 0        | 2605     | 124     | 0            |
| 1   | E     | 2560  | 0        | 2562     | 127     | 0            |
| 1   | F     | 2604  | 0        | 2596     | 104     | 0            |
| 1   | G     | 2581  | 0        | 2564     | 154     | 0            |
| 1   | H     | 2599  | 0        | 2576     | 139     | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 2   | E     | 1     | 0        | 0        | 0       | 0            |
| 2   | F     | 1     | 0        | 0        | 0       | 0            |
| 2   | G     | 1     | 0        | 0        | 0       | 0            |
| 2   | H     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 12    | 0        | 8        | 0       | 0            |
| 3   | D     | 12    | 0        | 8        | 0       | 0            |
| 3   | G     | 12    | 0        | 8        | 1       | 0            |
| 3   | H     | 12    | 0        | 8        | 1       | 0            |
| 4   | A     | 6     | 0        | 0        | 2       | 0            |
| 4   | B     | 4     | 0        | 0        | 0       | 0            |
| 4   | C     | 5     | 0        | 0        | 1       | 0            |
| 4   | D     | 5     | 0        | 0        | 1       | 0            |
| 4   | E     | 2     | 0        | 0        | 0       | 0            |
| 4   | F     | 4     | 0        | 0        | 1       | 0            |
| 4   | G     | 3     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | H     | 3     | 0        | 0        | 0       | 0            |
| All | All   | 20930 | 0        | 20818    | 994     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (994) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:134:ILE:HD12 | 1:C:134:ILE:H    | 1.19                     | 1.05              |
| 1:B:134:ILE:H    | 1:B:134:ILE:HD12 | 1.19                     | 1.05              |
| 1:E:324:GLN:HE21 | 1:E:338:VAL:HB   | 1.18                     | 1.01              |
| 1:D:247:ILE:HD13 | 1:D:314:MET:HE1  | 1.45                     | 0.96              |
| 1:C:247:ILE:HD13 | 1:C:314:MET:HE1  | 1.48                     | 0.94              |
| 1:G:355:ARG:HH11 | 1:G:355:ARG:HG3  | 1.28                     | 0.94              |
| 1:C:208:LEU:HD11 | 1:C:246:VAL:HG11 | 1.50                     | 0.94              |
| 1:H:208:LEU:HD11 | 1:H:246:VAL:HG11 | 1.49                     | 0.94              |
| 1:G:208:LEU:HD11 | 1:G:246:VAL:HG11 | 1.51                     | 0.92              |
| 1:A:208:LEU:HD11 | 1:A:246:VAL:HG11 | 1.52                     | 0.92              |
| 1:B:208:LEU:HD11 | 1:B:246:VAL:HG11 | 1.51                     | 0.92              |
| 1:D:208:LEU:HD11 | 1:D:246:VAL:HG11 | 1.49                     | 0.92              |
| 1:E:208:LEU:HD11 | 1:E:246:VAL:HG11 | 1.52                     | 0.91              |
| 1:G:257:TYR:CD2  | 1:G:295:VAL:HG13 | 2.06                     | 0.91              |
| 1:F:208:LEU:HD11 | 1:F:246:VAL:HG11 | 1.51                     | 0.89              |
| 1:D:348:GLU:H    | 1:D:348:GLU:CD   | 1.77                     | 0.89              |
| 1:H:319:ILE:HD12 | 1:H:319:ILE:H    | 1.37                     | 0.88              |
| 1:B:95:SER:HA    | 1:B:104:ILE:HD12 | 1.54                     | 0.88              |
| 1:H:308:ASN:HA   | 1:H:364:ARG:HH11 | 1.36                     | 0.87              |
| 1:E:134:ILE:HD12 | 1:E:134:ILE:H    | 1.40                     | 0.86              |
| 1:G:289:PHE:CE1  | 1:G:321:GLU:HB2  | 2.12                     | 0.85              |
| 1:G:289:PHE:HE1  | 1:G:321:GLU:HB2  | 1.41                     | 0.84              |
| 1:H:357:LEU:O    | 1:H:361:VAL:HG23 | 1.77                     | 0.84              |
| 1:G:359:ALA:HA   | 1:G:362:ARG:HD2  | 1.59                     | 0.83              |
| 1:A:359:ALA:HA   | 1:A:362:ARG:NH1  | 1.91                     | 0.83              |
| 1:B:355:ARG:HG2  | 1:B:355:ARG:HH11 | 1.44                     | 0.83              |
| 1:H:290:ARG:O    | 1:H:293:PRO:HD2  | 1.79                     | 0.82              |
| 1:C:72:ILE:HG12  | 1:C:277:MET:HE1  | 1.60                     | 0.82              |
| 1:C:349:THR:O    | 1:C:353:VAL:HG23 | 1.80                     | 0.82              |
| 1:B:134:ILE:HD12 | 1:B:134:ILE:N    | 1.96                     | 0.81              |
| 1:C:95:SER:O     | 1:C:99:LYS:HB3   | 1.81                     | 0.81              |
| 1:B:134:ILE:H    | 1:B:134:ILE:CD1  | 1.92                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:317:SER:HA   | 1:E:344:CYS:HB3  | 1.63                     | 0.80              |
| 1:H:308:ASN:HA   | 1:H:364:ARG:NH1  | 1.95                     | 0.80              |
| 1:A:112:LYS:HZ3  | 1:A:114:ARG:HA   | 1.45                     | 0.80              |
| 1:F:112:LYS:HD2  | 1:F:113:PRO:HD2  | 1.62                     | 0.80              |
| 1:B:72:ILE:HG12  | 1:B:277:MET:HE1  | 1.64                     | 0.79              |
| 1:C:114:ARG:O    | 1:C:117:VAL:HG12 | 1.82                     | 0.79              |
| 1:H:303:ILE:O    | 1:H:364:ARG:HB2  | 1.83                     | 0.79              |
| 1:H:348:GLU:CD   | 1:H:348:GLU:H    | 1.91                     | 0.79              |
| 1:A:161:ASP:HB2  | 4:A:2001:HOH:O   | 1.82                     | 0.78              |
| 1:G:257:TYR:CE2  | 1:G:295:VAL:HA   | 2.20                     | 0.77              |
| 1:C:134:ILE:H    | 1:C:134:ILE:CD1  | 1.93                     | 0.77              |
| 1:C:355:ARG:HG3  | 1:C:355:ARG:HH11 | 1.50                     | 0.76              |
| 1:D:317:SER:HA   | 1:D:344:CYS:HB3  | 1.68                     | 0.76              |
| 1:C:291:ASN:O    | 1:C:295:VAL:HG23 | 1.86                     | 0.76              |
| 1:G:111:GLU:HB3  | 1:G:121:GLY:CA   | 2.15                     | 0.75              |
| 1:H:112:LYS:HG2  | 1:H:113:PRO:HD2  | 1.68                     | 0.75              |
| 1:H:304:ALA:C    | 1:H:305:ASN:HD22 | 1.95                     | 0.74              |
| 1:A:160:LEU:HD22 | 1:A:160:LEU:H    | 1.51                     | 0.74              |
| 1:E:324:GLN:NE2  | 1:E:338:VAL:HB   | 1.99                     | 0.74              |
| 1:G:269:LEU:HD11 | 1:G:276:LEU:HD21 | 1.70                     | 0.74              |
| 1:B:160:LEU:H    | 1:B:160:LEU:HD22 | 1.52                     | 0.73              |
| 1:F:247:ILE:HD13 | 1:F:314:MET:HE1  | 1.70                     | 0.73              |
| 1:A:359:ALA:HA   | 1:A:362:ARG:HH12 | 1.51                     | 0.73              |
| 1:C:160:LEU:HD22 | 1:C:160:LEU:H    | 1.54                     | 0.73              |
| 1:C:318:ASN:ND2  | 1:C:339:SER:HB2  | 2.03                     | 0.73              |
| 1:F:160:LEU:HD22 | 1:F:160:LEU:H    | 1.54                     | 0.73              |
| 1:H:160:LEU:HD22 | 1:H:160:LEU:H    | 1.53                     | 0.72              |
| 1:H:319:ILE:HD12 | 1:H:319:ILE:N    | 2.04                     | 0.72              |
| 1:D:110:LEU:H    | 1:D:110:LEU:HD22 | 1.54                     | 0.72              |
| 1:E:134:ILE:HD13 | 1:F:235:ILE:HG21 | 1.71                     | 0.72              |
| 1:A:110:LEU:HD21 | 1:A:145:PHE:CZ   | 2.25                     | 0.72              |
| 1:G:324:GLN:HE22 | 1:G:334:LEU:HB3  | 1.54                     | 0.72              |
| 1:G:160:LEU:H    | 1:G:160:LEU:HD22 | 1.53                     | 0.71              |
| 1:G:291:ASN:N    | 1:G:291:ASN:HD22 | 1.86                     | 0.71              |
| 1:C:331:LYS:O    | 1:C:331:LYS:HD3  | 1.89                     | 0.71              |
| 1:E:160:LEU:H    | 1:E:160:LEU:HD22 | 1.55                     | 0.71              |
| 1:H:124:ASN:HA   | 1:H:134:ILE:HD13 | 1.71                     | 0.71              |
| 1:A:21:GLU:OE1   | 1:B:169:ALA:HB3  | 1.91                     | 0.71              |
| 1:F:96:ASP:HA    | 1:F:99:LYS:HD2   | 1.72                     | 0.71              |
| 1:F:262:VAL:HG12 | 1:F:263:ALA:N    | 2.06                     | 0.71              |
| 1:B:297:ASP:OD1  | 1:B:356:LYS:HE2  | 1.90                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:292:GLN:HB2  | 1:E:293:PRO:HD3  | 1.73                     | 0.71              |
| 1:C:348:GLU:CD   | 1:C:348:GLU:H    | 1.99                     | 0.70              |
| 1:D:160:LEU:H    | 1:D:160:LEU:HD22 | 1.54                     | 0.70              |
| 1:G:111:GLU:HB3  | 1:G:121:GLY:HA2  | 1.72                     | 0.70              |
| 1:F:93:LYS:HB2   | 1:F:93:LYS:NZ    | 2.07                     | 0.70              |
| 1:A:114:ARG:H    | 1:A:114:ARG:HD3  | 1.57                     | 0.70              |
| 1:G:308:ASN:OD1  | 1:G:364:ARG:HD2  | 1.93                     | 0.69              |
| 1:E:183:GLU:HB3  | 1:F:180:ARG:HB3  | 1.74                     | 0.69              |
| 1:E:300:CYS:SG   | 1:E:357:LEU:HA   | 2.33                     | 0.69              |
| 1:G:110:LEU:H    | 1:G:110:LEU:HD22 | 1.56                     | 0.69              |
| 1:H:295:VAL:O    | 1:H:299:VAL:HG23 | 1.93                     | 0.69              |
| 1:A:349:THR:HA   | 1:A:352:ASP:OD2  | 1.93                     | 0.69              |
| 1:G:355:ARG:HG3  | 1:G:355:ARG:NH1  | 2.05                     | 0.68              |
| 1:G:185:GLN:OE1  | 1:H:114:ARG:HB3  | 1.93                     | 0.68              |
| 1:E:20:GLU:HG2   | 1:F:52:LYS:HD3   | 1.74                     | 0.68              |
| 1:B:355:ARG:HG2  | 1:B:355:ARG:NH1  | 2.08                     | 0.68              |
| 1:D:291:ASN:O    | 1:D:295:VAL:HG23 | 1.93                     | 0.68              |
| 1:E:134:ILE:HD12 | 1:E:134:ILE:N    | 2.09                     | 0.68              |
| 1:H:319:ILE:H    | 1:H:319:ILE:CD1  | 2.07                     | 0.68              |
| 1:G:302:GLN:O    | 1:G:307:GLU:HB3  | 1.94                     | 0.67              |
| 1:H:98:LEU:HD13  | 1:H:102:LEU:HD22 | 1.76                     | 0.67              |
| 1:E:304:ALA:O    | 1:E:363:GLN:HG3  | 1.94                     | 0.67              |
| 1:G:90:ARG:HD3   | 1:G:347:TRP:NE1  | 2.09                     | 0.67              |
| 1:E:134:ILE:H    | 1:E:134:ILE:CD1  | 2.08                     | 0.67              |
| 1:A:307:GLU:HG2  | 1:A:310:ILE:HD12 | 1.77                     | 0.67              |
| 1:G:290:ARG:O    | 1:G:293:PRO:HD2  | 1.95                     | 0.67              |
| 1:G:291:ASN:O    | 1:G:295:VAL:HG23 | 1.93                     | 0.67              |
| 1:A:300:CYS:SG   | 1:A:357:LEU:HA   | 2.35                     | 0.67              |
| 1:E:119:TRP:NE1  | 1:E:128:VAL:HG22 | 2.09                     | 0.67              |
| 1:G:294:LYS:HB2  | 1:G:294:LYS:NZ   | 2.10                     | 0.67              |
| 1:H:261:SER:HA   | 1:H:264:GLU:OE1  | 1.94                     | 0.67              |
| 1:B:76:CYS:SG    | 1:B:342:ASP:HB2  | 2.35                     | 0.67              |
| 1:F:71:VAL:HG21  | 1:F:102:LEU:HD22 | 1.77                     | 0.67              |
| 1:C:258:ASP:O    | 1:C:262:VAL:HG23 | 1.95                     | 0.66              |
| 1:D:97:GLU:CD    | 1:D:355:ARG:HH12 | 2.03                     | 0.66              |
| 1:E:76:CYS:SG    | 1:E:342:ASP:HB2  | 2.35                     | 0.66              |
| 1:C:264:GLU:HG3  | 1:C:265:ALA:N    | 2.10                     | 0.66              |
| 1:C:349:THR:O    | 1:C:352:ASP:HB2  | 1.95                     | 0.66              |
| 1:A:260:LYS:O    | 1:A:264:GLU:HG3  | 1.95                     | 0.66              |
| 1:G:257:TYR:HD2  | 1:G:295:VAL:HG13 | 1.56                     | 0.66              |
| 1:F:357:LEU:O    | 1:F:361:VAL:HG23 | 1.95                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:247:ILE:HD13 | 1:D:314:MET:CE   | 2.24                     | 0.66              |
| 1:A:253:LYS:O    | 1:A:253:LYS:HG2  | 1.93                     | 0.66              |
| 1:C:292:GLN:HB2  | 1:C:293:PRO:HD3  | 1.78                     | 0.66              |
| 1:A:114:ARG:O    | 1:A:116:THR:HA   | 1.96                     | 0.66              |
| 1:A:207:THR:HG21 | 1:B:252:LYS:NZ   | 2.11                     | 0.66              |
| 1:C:134:ILE:HD12 | 1:C:134:ILE:N    | 2.04                     | 0.66              |
| 1:B:129:ASN:O    | 1:B:131:THR:HG23 | 1.96                     | 0.65              |
| 1:A:117:VAL:HG12 | 1:A:118:GLY:N    | 2.09                     | 0.65              |
| 1:E:22:ASP:HB3   | 1:E:25:ILE:HB    | 1.78                     | 0.65              |
| 1:C:308:ASN:OD1  | 1:C:364:ARG:HD2  | 1.96                     | 0.65              |
| 1:G:319:ILE:HB   | 1:G:337:GLY:HA3  | 1.78                     | 0.65              |
| 1:H:318:ASN:HD21 | 1:H:339:SER:HB3  | 1.61                     | 0.65              |
| 1:G:129:ASN:H    | 1:G:129:ASN:HD22 | 1.45                     | 0.65              |
| 1:G:321:GLU:HA   | 1:G:344:CYS:O    | 1.95                     | 0.65              |
| 1:E:129:ASN:HD22 | 1:E:129:ASN:N    | 1.92                     | 0.65              |
| 1:H:293:PRO:O    | 1:H:296:ASN:HB3  | 1.96                     | 0.65              |
| 1:C:323:ASN:HB3  | 1:C:343:ALA:HA   | 1.77                     | 0.65              |
| 1:F:129:ASN:HD22 | 1:F:129:ASN:H    | 1.43                     | 0.65              |
| 1:G:257:TYR:HE2  | 1:G:295:VAL:HA   | 1.60                     | 0.64              |
| 1:C:269:LEU:HD11 | 1:C:276:LEU:CD1  | 2.28                     | 0.64              |
| 1:G:51:ALA:O     | 1:G:55:ARG:HG3   | 1.97                     | 0.64              |
| 1:D:55:ARG:O     | 1:D:59:ILE:HG13  | 1.98                     | 0.64              |
| 1:F:275:GLY:HA3  | 1:F:311:THR:CG2  | 2.28                     | 0.64              |
| 1:E:303:ILE:O    | 1:E:364:ARG:HB2  | 1.97                     | 0.64              |
| 1:H:291:ASN:O    | 1:H:295:VAL:HG23 | 1.98                     | 0.64              |
| 1:D:51:ALA:O     | 1:D:55:ARG:HG3   | 1.98                     | 0.64              |
| 1:E:51:ALA:O     | 1:E:55:ARG:HG3   | 1.98                     | 0.64              |
| 1:F:277:MET:HA   | 1:F:312:GLY:O    | 1.97                     | 0.64              |
| 1:G:123:ILE:O    | 1:G:137:GLY:HA3  | 1.98                     | 0.64              |
| 1:H:55:ARG:O     | 1:H:59:ILE:HG13  | 1.98                     | 0.64              |
| 1:G:20:GLU:O     | 1:G:20:GLU:HG3   | 1.97                     | 0.63              |
| 1:G:349:THR:O    | 1:G:353:VAL:HG22 | 1.98                     | 0.63              |
| 1:B:366:GLU:O    | 1:B:369:LYS:N    | 2.30                     | 0.63              |
| 1:E:112:LYS:HB3  | 1:E:341:THR:HG21 | 1.80                     | 0.63              |
| 1:F:51:ALA:O     | 1:F:55:ARG:HG3   | 1.98                     | 0.63              |
| 1:C:277:MET:HE2  | 1:C:313:VAL:C    | 2.23                     | 0.63              |
| 1:C:362:ARG:O    | 1:C:365:ARG:HB2  | 1.98                     | 0.63              |
| 1:B:72:ILE:HG12  | 1:B:277:MET:CE   | 2.29                     | 0.63              |
| 1:E:324:GLN:NE2  | 1:E:335:LYS:HB2  | 2.14                     | 0.63              |
| 1:A:294:LYS:HD2  | 1:A:294:LYS:N    | 2.14                     | 0.63              |
| 1:C:363:GLN:O    | 1:C:367:VAL:HG23 | 1.98                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:281:SER:HA   | 1:D:285:SER:HB3  | 1.81                     | 0.63              |
| 1:H:289:PHE:CD1  | 1:H:343:ALA:HB1  | 2.33                     | 0.63              |
| 1:B:71:VAL:HG21  | 1:B:102:LEU:HD22 | 1.81                     | 0.62              |
| 1:A:216:GLN:NE2  | 1:A:270:PRO:HG3  | 2.14                     | 0.62              |
| 1:C:277:MET:HE3  | 1:C:313:VAL:N    | 2.14                     | 0.62              |
| 1:D:313:VAL:HG21 | 1:D:357:LEU:HD11 | 1.82                     | 0.62              |
| 1:D:327:PRO:HG2  | 1:D:333:GLY:O    | 1.99                     | 0.62              |
| 1:H:294:LYS:HD2  | 1:H:294:LYS:N    | 2.14                     | 0.62              |
| 1:E:170:ASP:HB3  | 1:F:21:GLU:CD    | 2.23                     | 0.62              |
| 1:F:263:ALA:HA   | 1:F:266:LYS:HD3  | 1.80                     | 0.62              |
| 1:G:111:GLU:HB3  | 1:G:121:GLY:HA3  | 1.80                     | 0.62              |
| 1:A:327:PRO:HG3  | 1:A:333:GLY:O    | 1.99                     | 0.62              |
| 1:D:128:VAL:HB   | 1:D:331:LYS:HB2  | 1.81                     | 0.62              |
| 1:E:90:ARG:NH1   | 1:E:319:ILE:HG23 | 2.12                     | 0.62              |
| 1:C:52:LYS:HD3   | 1:D:20:GLU:HG3   | 1.81                     | 0.61              |
| 1:F:110:LEU:N    | 1:F:110:LEU:HD22 | 2.15                     | 0.61              |
| 1:G:216:GLN:NE2  | 1:G:270:PRO:HG3  | 2.15                     | 0.61              |
| 1:E:326:ILE:N    | 1:E:326:ILE:HD12 | 2.15                     | 0.61              |
| 1:G:112:LYS:HG3  | 1:G:113:PRO:HD2  | 1.81                     | 0.61              |
| 1:B:101:ASP:HB3  | 1:B:361:VAL:HG11 | 1.81                     | 0.61              |
| 1:H:116:THR:HG23 | 1:H:117:VAL:HG23 | 1.82                     | 0.61              |
| 1:F:322:GLY:O    | 1:F:343:ALA:HA   | 1.99                     | 0.61              |
| 1:A:279:ASP:HA   | 1:A:314:MET:HB3  | 1.83                     | 0.61              |
| 1:B:51:ALA:O     | 1:B:55:ARG:HG3   | 2.00                     | 0.61              |
| 1:B:82:GLU:N     | 1:B:82:GLU:OE2   | 2.34                     | 0.61              |
| 1:F:110:LEU:HD21 | 1:F:145:PHE:HZ   | 1.66                     | 0.61              |
| 1:D:212:VAL:O    | 1:D:216:GLN:HG2  | 2.01                     | 0.61              |
| 1:D:262:VAL:O    | 1:D:266:LYS:HG3  | 2.01                     | 0.61              |
| 1:H:124:ASN:HA   | 1:H:134:ILE:CD1  | 2.31                     | 0.61              |
| 1:A:110:LEU:HD21 | 1:A:145:PHE:HZ   | 1.63                     | 0.60              |
| 1:A:110:LEU:O    | 1:A:111:GLU:HB3  | 2.00                     | 0.60              |
| 1:G:281:SER:HA   | 1:G:285:SER:HB2  | 1.82                     | 0.60              |
| 1:G:126:PRO:HB3  | 1:G:137:GLY:HA2  | 1.83                     | 0.60              |
| 1:G:249:ARG:O    | 1:G:283:GLY:HA3  | 2.01                     | 0.60              |
| 1:C:82:GLU:HA    | 1:C:82:GLU:OE1   | 2.01                     | 0.60              |
| 1:C:357:LEU:O    | 1:C:361:VAL:HG23 | 2.01                     | 0.60              |
| 1:B:212:VAL:O    | 1:B:216:GLN:HG2  | 2.02                     | 0.60              |
| 1:G:291:ASN:N    | 1:G:291:ASN:ND2  | 2.49                     | 0.60              |
| 1:A:21:GLU:OE2   | 1:B:170:ASP:HB3  | 2.02                     | 0.60              |
| 1:A:76:CYS:SG    | 1:A:342:ASP:HB2  | 2.42                     | 0.60              |
| 1:B:326:ILE:N    | 1:B:326:ILE:HD12 | 2.16                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:280:TYR:O    | 1:E:292:GLN:HG2  | 2.00                     | 0.60              |
| 1:H:51:ALA:O     | 1:H:55:ARG:HG3   | 2.01                     | 0.60              |
| 1:G:308:ASN:HA   | 1:G:364:ARG:NH1  | 2.16                     | 0.60              |
| 1:H:82:GLU:N     | 1:H:82:GLU:CD    | 2.59                     | 0.60              |
| 1:A:281:SER:OG   | 1:A:282:HIS:N    | 2.34                     | 0.60              |
| 1:G:275:GLY:HA3  | 1:G:311:THR:CG2  | 2.32                     | 0.60              |
| 1:A:112:LYS:HZ2  | 1:A:114:ARG:HB3  | 1.67                     | 0.60              |
| 1:B:73:VAL:HG23  | 1:B:315:ILE:HB   | 1.83                     | 0.60              |
| 1:C:111:GLU:HB3  | 1:C:121:GLY:CA   | 2.31                     | 0.60              |
| 1:C:269:LEU:HD11 | 1:C:276:LEU:HD11 | 1.83                     | 0.60              |
| 1:B:257:TYR:CD1  | 1:B:295:VAL:HG13 | 2.38                     | 0.59              |
| 1:D:295:VAL:O    | 1:D:299:VAL:HG23 | 2.02                     | 0.59              |
| 1:D:330:GLY:C    | 1:D:332:ALA:H    | 2.09                     | 0.59              |
| 1:G:260:LYS:O    | 1:G:264:GLU:HG3  | 2.02                     | 0.59              |
| 1:C:143:GLN:HG3  | 1:C:147:ASN:HD21 | 1.68                     | 0.59              |
| 1:H:299:VAL:O    | 1:H:303:ILE:HG13 | 2.03                     | 0.59              |
| 1:B:72:ILE:CG1   | 1:B:277:MET:HE1  | 2.32                     | 0.59              |
| 1:H:317:SER:HA   | 1:H:344:CYS:HB3  | 1.84                     | 0.59              |
| 1:C:48:LEU:HD13  | 1:D:19:ALA:HB2   | 1.83                     | 0.59              |
| 1:E:349:THR:O    | 1:E:353:VAL:HG23 | 2.02                     | 0.59              |
| 1:A:232:VAL:HG21 | 1:D:232:VAL:HG21 | 1.85                     | 0.59              |
| 1:G:364:ARG:O    | 1:G:368:ASN:ND2  | 2.36                     | 0.59              |
| 1:C:51:ALA:O     | 1:C:55:ARG:HG3   | 2.02                     | 0.59              |
| 1:C:111:GLU:HB3  | 1:C:121:GLY:HA2  | 1.84                     | 0.59              |
| 1:B:232:VAL:HG21 | 1:C:232:VAL:HG21 | 1.85                     | 0.59              |
| 1:H:201:LYS:HD3  | 1:H:249:ARG:HG2  | 1.84                     | 0.59              |
| 1:G:129:ASN:HD22 | 1:G:129:ASN:N    | 2.00                     | 0.58              |
| 1:H:319:ILE:HD13 | 1:H:337:GLY:HA2  | 1.84                     | 0.58              |
| 1:G:299:VAL:HG13 | 1:G:310:ILE:HD13 | 1.85                     | 0.58              |
| 1:E:143:GLN:HG3  | 1:E:147:ASN:HD21 | 1.68                     | 0.58              |
| 1:G:98:LEU:HD13  | 1:G:358:ALA:HB2  | 1.85                     | 0.58              |
| 1:E:110:LEU:HD13 | 1:E:123:ILE:HD11 | 1.84                     | 0.58              |
| 1:H:36:LEU:O     | 1:H:40:GLN:HG3   | 2.03                     | 0.58              |
| 1:E:90:ARG:HH12  | 1:E:319:ILE:HG23 | 1.68                     | 0.58              |
| 1:F:291:ASN:O    | 1:F:295:VAL:HG23 | 2.03                     | 0.58              |
| 1:D:330:GLY:O    | 1:D:332:ALA:N    | 2.37                     | 0.58              |
| 1:E:55:ARG:O     | 1:E:59:ILE:HG13  | 2.03                     | 0.58              |
| 1:G:323:ASN:HA   | 1:G:338:VAL:HG12 | 1.86                     | 0.58              |
| 1:A:117:VAL:HG12 | 1:A:118:GLY:H    | 1.69                     | 0.58              |
| 1:A:252:LYS:C    | 1:A:254:GLY:H    | 2.11                     | 0.58              |
| 1:C:76:CYS:SG    | 1:C:342:ASP:HB2  | 2.43                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:51:ALA:O     | 1:A:55:ARG:HG3   | 2.03                     | 0.58              |
| 1:C:112:LYS:HD2  | 1:C:113:PRO:HD2  | 1.85                     | 0.58              |
| 1:F:212:VAL:O    | 1:F:216:GLN:HG2  | 2.04                     | 0.58              |
| 1:G:201:LYS:HD3  | 1:G:249:ARG:HG2  | 1.86                     | 0.58              |
| 1:B:106:MET:HB2  | 1:B:153:LEU:HD21 | 1.85                     | 0.57              |
| 1:G:212:VAL:O    | 1:G:216:GLN:HG2  | 2.05                     | 0.57              |
| 1:G:264:GLU:O    | 1:G:267:ALA:HB3  | 2.04                     | 0.57              |
| 1:H:212:VAL:O    | 1:H:216:GLN:HG2  | 2.04                     | 0.57              |
| 1:F:110:LEU:HD21 | 1:F:145:PHE:CZ   | 2.39                     | 0.57              |
| 1:A:212:VAL:O    | 1:A:216:GLN:HG2  | 2.04                     | 0.57              |
| 1:E:281:SER:HA   | 1:E:285:SER:HB2  | 1.85                     | 0.57              |
| 1:F:129:ASN:H    | 1:F:129:ASN:ND2  | 2.02                     | 0.57              |
| 1:C:30:PRO:HA    | 4:C:2001:HOH:O   | 2.04                     | 0.57              |
| 1:E:20:GLU:HG3   | 1:E:20:GLU:O     | 2.05                     | 0.57              |
| 1:H:175:GLY:O    | 1:H:198:VAL:HA   | 2.05                     | 0.57              |
| 1:C:55:ARG:O     | 1:C:59:ILE:HG13  | 2.04                     | 0.57              |
| 1:C:110:LEU:N    | 1:C:110:LEU:HD22 | 2.20                     | 0.57              |
| 1:D:247:ILE:HG12 | 1:D:277:MET:HB3  | 1.86                     | 0.57              |
| 1:D:266:LYS:HE2  | 1:D:309:ALA:HB2  | 1.86                     | 0.57              |
| 1:C:72:ILE:HG22  | 1:C:107:ARG:HG3  | 1.87                     | 0.57              |
| 1:E:335:LYS:O    | 1:E:336:TYR:HB2  | 2.04                     | 0.57              |
| 1:G:143:GLN:HG3  | 1:G:147:ASN:HD21 | 1.70                     | 0.57              |
| 1:G:350:THR:HA   | 1:G:353:VAL:CG2  | 2.35                     | 0.57              |
| 1:A:67:ASP:OD1   | 1:A:365:ARG:NE   | 2.37                     | 0.57              |
| 1:D:297:ASP:OD1  | 1:D:356:LYS:HE3  | 2.05                     | 0.57              |
| 1:A:143:GLN:HG3  | 1:A:147:ASN:HD21 | 1.69                     | 0.57              |
| 1:D:73:VAL:HG23  | 1:D:315:ILE:HB   | 1.86                     | 0.57              |
| 1:H:325:GLY:O    | 1:H:327:PRO:HD3  | 2.04                     | 0.57              |
| 1:A:55:ARG:O     | 1:A:59:ILE:HG13  | 2.05                     | 0.56              |
| 1:A:120:LYS:HE3  | 1:A:120:LYS:HA   | 1.86                     | 0.56              |
| 1:D:20:GLU:O     | 1:D:21:GLU:HG2   | 2.05                     | 0.56              |
| 1:D:22:ASP:HB3   | 1:D:25:ILE:HB    | 1.85                     | 0.56              |
| 1:E:257:TYR:CD1  | 1:E:295:VAL:HG13 | 2.40                     | 0.56              |
| 1:C:257:TYR:CD2  | 1:C:295:VAL:HG13 | 2.40                     | 0.56              |
| 1:A:201:LYS:HD3  | 1:A:249:ARG:HG2  | 1.86                     | 0.56              |
| 1:E:212:VAL:O    | 1:E:216:GLN:HG2  | 2.05                     | 0.56              |
| 1:F:55:ARG:O     | 1:F:59:ILE:HG13  | 2.06                     | 0.56              |
| 1:F:101:ASP:HB3  | 1:F:361:VAL:HB   | 1.87                     | 0.56              |
| 1:G:55:ARG:O     | 1:G:59:ILE:HG13  | 2.06                     | 0.56              |
| 1:G:167:TYR:C    | 1:G:168:LEU:HG   | 2.30                     | 0.56              |
| 1:H:91:LEU:HA    | 1:H:347:TRP:HH2  | 1.70                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:212:VAL:O    | 1:C:216:GLN:HG2  | 2.05                     | 0.56              |
| 1:C:324:GLN:HE22 | 1:C:335:LYS:H    | 1.54                     | 0.56              |
| 1:B:143:GLN:HG3  | 1:B:147:ASN:HD21 | 1.71                     | 0.56              |
| 1:E:204:THR:HA   | 1:E:249:ARG:HH12 | 1.71                     | 0.56              |
| 1:E:317:SER:CA   | 1:E:344:CYS:HB3  | 2.34                     | 0.56              |
| 1:A:102:LEU:HD21 | 1:A:357:LEU:HD13 | 1.87                     | 0.56              |
| 1:D:143:GLN:HG3  | 1:D:147:ASN:HD21 | 1.70                     | 0.56              |
| 1:D:306:GLY:HA2  | 1:D:364:ARG:HG3  | 1.88                     | 0.56              |
| 1:B:257:TYR:CZ   | 1:B:295:VAL:HG22 | 2.41                     | 0.56              |
| 1:C:167:TYR:C    | 1:C:168:LEU:HG   | 2.30                     | 0.56              |
| 1:B:79:HIS:HB3   | 1:B:119:TRP:CH2  | 2.41                     | 0.56              |
| 1:F:36:LEU:O     | 1:F:40:GLN:HG3   | 2.05                     | 0.56              |
| 1:A:36:LEU:O     | 1:A:40:GLN:HG3   | 2.06                     | 0.56              |
| 1:A:204:THR:HA   | 1:A:249:ARG:HH12 | 1.71                     | 0.56              |
| 1:A:72:ILE:HG22  | 1:A:107:ARG:HG2  | 1.87                     | 0.56              |
| 1:D:167:TYR:C    | 1:D:168:LEU:HG   | 2.30                     | 0.56              |
| 1:D:367:VAL:HG12 | 1:D:367:VAL:O    | 2.06                     | 0.56              |
| 1:B:55:ARG:O     | 1:B:59:ILE:HG13  | 2.06                     | 0.55              |
| 1:E:129:ASN:ND2  | 1:E:131:THR:HB   | 2.21                     | 0.55              |
| 1:E:201:LYS:HD3  | 1:E:249:ARG:HG2  | 1.88                     | 0.55              |
| 1:E:232:VAL:HG21 | 1:H:232:VAL:CG2  | 2.36                     | 0.55              |
| 1:H:127:ASP:OD1  | 1:H:131:THR:HB   | 2.07                     | 0.55              |
| 1:B:74:GLY:HA3   | 1:B:107:ARG:HB2  | 1.89                     | 0.55              |
| 1:B:125:ASP:OD2  | 1:B:128:VAL:HA   | 2.06                     | 0.55              |
| 1:B:101:ASP:HB3  | 1:B:361:VAL:CG1  | 2.36                     | 0.55              |
| 1:C:36:LEU:O     | 1:C:40:GLN:HG3   | 2.06                     | 0.55              |
| 1:F:290:ARG:O    | 1:F:293:PRO:HD2  | 2.06                     | 0.55              |
| 1:D:76:CYS:SG    | 1:D:342:ASP:HB2  | 2.46                     | 0.55              |
| 1:G:307:GLU:OE2  | 1:G:307:GLU:HA   | 2.05                     | 0.55              |
| 1:C:348:GLU:CD   | 1:C:348:GLU:N    | 2.64                     | 0.55              |
| 1:H:294:LYS:CD   | 1:H:294:LYS:H    | 2.20                     | 0.55              |
| 1:D:175:GLY:O    | 1:D:198:VAL:HA   | 2.06                     | 0.55              |
| 1:D:201:LYS:HD3  | 1:D:249:ARG:HG2  | 1.89                     | 0.55              |
| 1:G:257:TYR:CD2  | 1:G:295:VAL:HA   | 2.41                     | 0.55              |
| 1:G:275:GLY:HA3  | 1:G:311:THR:HG21 | 1.88                     | 0.55              |
| 1:H:208:LEU:CD2  | 1:H:265:ALA:HA   | 2.37                     | 0.55              |
| 1:A:112:LYS:NZ   | 1:A:114:ARG:HA   | 2.18                     | 0.55              |
| 1:E:232:VAL:HG21 | 1:H:232:VAL:HG21 | 1.87                     | 0.55              |
| 1:B:167:TYR:C    | 1:B:168:LEU:HG   | 2.32                     | 0.55              |
| 1:B:36:LEU:O     | 1:B:40:GLN:HG3   | 2.07                     | 0.55              |
| 1:B:204:THR:HA   | 1:B:249:ARG:HH12 | 1.72                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:143:GLN:HG3  | 1:H:147:ASN:HD21 | 1.72                     | 0.55              |
| 1:B:232:VAL:CG2  | 1:C:232:VAL:HG21 | 2.37                     | 0.55              |
| 1:G:363:GLN:O    | 1:G:367:VAL:HG23 | 2.07                     | 0.55              |
| 1:H:252:LYS:C    | 1:H:254:GLY:H    | 2.15                     | 0.55              |
| 1:F:201:LYS:HD3  | 1:F:249:ARG:HG2  | 1.90                     | 0.54              |
| 1:F:345:ILE:HG13 | 1:F:345:ILE:O    | 2.07                     | 0.54              |
| 1:G:169:ALA:HB1  | 3:H:1002:PHE:OXT | 2.07                     | 0.54              |
| 1:G:235:ILE:HD13 | 1:H:134:ILE:HB   | 1.89                     | 0.54              |
| 1:E:357:LEU:O    | 1:E:361:VAL:HG23 | 2.06                     | 0.54              |
| 1:G:204:THR:HA   | 1:G:249:ARG:HH12 | 1.72                     | 0.54              |
| 1:A:324:GLN:HE21 | 1:A:338:VAL:HB   | 1.73                     | 0.54              |
| 1:E:366:GLU:CD   | 1:E:366:GLU:H    | 2.15                     | 0.54              |
| 1:F:247:ILE:HD13 | 1:F:314:MET:CE   | 2.38                     | 0.54              |
| 1:F:263:ALA:HB2  | 4:F:2004:HOH:O   | 2.07                     | 0.54              |
| 1:A:262:VAL:O    | 1:A:266:LYS:HG3  | 2.07                     | 0.54              |
| 1:G:281:SER:HA   | 1:G:285:SER:CB   | 2.37                     | 0.54              |
| 1:F:143:GLN:HG3  | 1:F:147:ASN:HD21 | 1.71                     | 0.54              |
| 1:E:324:GLN:HB3  | 1:E:335:LYS:HD3  | 1.90                     | 0.54              |
| 1:B:324:GLN:HE21 | 1:B:338:VAL:HB   | 1.73                     | 0.54              |
| 1:H:302:GLN:O    | 1:H:307:GLU:HB3  | 2.07                     | 0.54              |
| 1:H:352:ASP:OD1  | 1:H:356:LYS:NZ   | 2.39                     | 0.54              |
| 1:A:129:ASN:C    | 1:A:129:ASN:HD22 | 2.16                     | 0.54              |
| 1:A:366:GLU:OE2  | 1:A:369:LYS:HE2  | 2.08                     | 0.54              |
| 1:B:128:VAL:CG2  | 1:B:331:LYS:HE3  | 2.37                     | 0.54              |
| 1:G:317:SER:HA   | 1:G:344:CYS:HB3  | 1.89                     | 0.54              |
| 1:C:201:LYS:HD3  | 1:C:249:ARG:HG2  | 1.89                     | 0.54              |
| 1:E:207:THR:HG21 | 1:F:252:LYS:NZ   | 2.23                     | 0.54              |
| 1:G:90:ARG:HD3   | 1:G:347:TRP:CD1  | 2.43                     | 0.54              |
| 1:C:175:GLY:O    | 1:C:198:VAL:HA   | 2.08                     | 0.53              |
| 1:E:167:TYR:C    | 1:E:168:LEU:HG   | 2.33                     | 0.53              |
| 1:H:120:LYS:HE3  | 1:H:132:PHE:CZ   | 2.43                     | 0.53              |
| 1:E:282:HIS:N    | 1:E:285:SER:HB2  | 2.23                     | 0.53              |
| 1:G:257:TYR:CG   | 1:G:257:TYR:O    | 2.61                     | 0.53              |
| 1:H:263:ALA:HA   | 1:H:266:LYS:HD3  | 1.90                     | 0.53              |
| 1:B:248:LEU:HB2  | 1:B:278:ILE:HD13 | 1.90                     | 0.53              |
| 1:H:111:GLU:HB3  | 1:H:121:GLY:HA3  | 1.91                     | 0.53              |
| 1:H:294:LYS:N    | 1:H:294:LYS:CD   | 2.71                     | 0.53              |
| 1:E:324:GLN:CD   | 1:E:335:LYS:HB2  | 2.32                     | 0.53              |
| 1:G:110:LEU:HD22 | 1:G:110:LEU:N    | 2.22                     | 0.53              |
| 1:G:175:GLY:O    | 1:G:198:VAL:HA   | 2.08                     | 0.53              |
| 1:H:362:ARG:HG3  | 1:H:362:ARG:HH11 | 1.74                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:204:THR:HA   | 1:A:249:ARG:NH1  | 2.23                     | 0.53              |
| 1:E:36:LEU:O     | 1:E:40:GLN:HG3   | 2.09                     | 0.53              |
| 1:E:113:PRO:HG3  | 1:E:180:ARG:NH1  | 2.23                     | 0.53              |
| 1:G:261:SER:O    | 1:G:264:GLU:HB2  | 2.08                     | 0.53              |
| 1:G:350:THR:HA   | 1:G:353:VAL:HG22 | 1.90                     | 0.53              |
| 1:B:362:ARG:O    | 1:B:365:ARG:HB3  | 2.08                     | 0.53              |
| 1:E:320:ASN:ND2  | 1:E:337:GLY:HA3  | 2.24                     | 0.53              |
| 1:G:36:LEU:O     | 1:G:40:GLN:HG3   | 2.09                     | 0.53              |
| 1:G:93:LYS:HB2   | 1:G:93:LYS:NZ    | 2.23                     | 0.53              |
| 1:A:324:GLN:NE2  | 1:A:335:LYS:HB2  | 2.23                     | 0.53              |
| 1:H:300:CYS:SG   | 1:H:357:LEU:HA   | 2.49                     | 0.53              |
| 1:B:269:LEU:HD11 | 1:B:276:LEU:CD2  | 2.39                     | 0.52              |
| 1:D:366:GLU:C    | 1:D:368:ASN:H    | 2.16                     | 0.52              |
| 1:H:204:THR:HA   | 1:H:249:ARG:HH12 | 1.74                     | 0.52              |
| 1:G:355:ARG:HH11 | 1:G:355:ARG:CG   | 2.09                     | 0.52              |
| 1:G:355:ARG:NH1  | 1:G:355:ARG:CG   | 2.71                     | 0.52              |
| 1:A:75:PRO:HA    | 1:A:317:SER:O    | 2.09                     | 0.52              |
| 1:B:348:GLU:CD   | 1:B:348:GLU:H    | 2.18                     | 0.52              |
| 1:C:366:GLU:HA   | 1:C:369:LYS:HG2  | 1.90                     | 0.52              |
| 1:D:112:LYS:HD3  | 1:D:112:LYS:C    | 2.34                     | 0.52              |
| 1:E:204:THR:HA   | 1:E:249:ARG:NH1  | 2.23                     | 0.52              |
| 1:G:324:GLN:O    | 1:G:326:ILE:N    | 2.42                     | 0.52              |
| 1:B:201:LYS:HD3  | 1:B:249:ARG:HG2  | 1.91                     | 0.52              |
| 1:D:304:ALA:C    | 1:D:306:GLY:H    | 2.17                     | 0.52              |
| 1:B:269:LEU:HD11 | 1:B:276:LEU:HD21 | 1.92                     | 0.52              |
| 1:E:336:TYR:CD1  | 1:E:337:GLY:N    | 2.78                     | 0.52              |
| 1:A:207:THR:HG21 | 1:B:252:LYS:HZ3  | 1.71                     | 0.52              |
| 1:D:36:LEU:O     | 1:D:40:GLN:HG3   | 2.09                     | 0.52              |
| 1:F:167:TYR:C    | 1:F:168:LEU:HG   | 2.33                     | 0.52              |
| 1:A:232:VAL:HG21 | 1:D:232:VAL:CG2  | 2.39                     | 0.52              |
| 1:A:307:GLU:HG2  | 1:A:310:ILE:CD1  | 2.40                     | 0.52              |
| 1:B:335:LYS:CE   | 1:B:338:VAL:HG21 | 2.40                     | 0.52              |
| 1:E:134:ILE:HD13 | 1:F:235:ILE:CG2  | 2.38                     | 0.52              |
| 1:E:175:GLY:O    | 1:E:198:VAL:HA   | 2.10                     | 0.52              |
| 1:E:266:LYS:HE2  | 1:E:309:ALA:HB2  | 1.91                     | 0.52              |
| 1:G:247:ILE:HD13 | 1:G:314:MET:HE1  | 1.92                     | 0.52              |
| 1:A:175:GLY:O    | 1:A:198:VAL:HA   | 2.09                     | 0.52              |
| 1:G:204:THR:HA   | 1:G:249:ARG:NH1  | 2.25                     | 0.52              |
| 1:G:308:ASN:HA   | 1:G:364:ARG:HH11 | 1.74                     | 0.52              |
| 1:A:167:TYR:C    | 1:A:168:LEU:HG   | 2.34                     | 0.52              |
| 1:B:248:LEU:HD12 | 1:B:278:ILE:HD11 | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:204:THR:HA   | 1:C:249:ARG:HH12 | 1.75                     | 0.52              |
| 1:H:110:LEU:N    | 1:H:110:LEU:HD22 | 2.25                     | 0.52              |
| 1:A:303:ILE:HG22 | 1:A:360:ALA:O    | 2.10                     | 0.52              |
| 1:G:180:ARG:HB3  | 1:H:183:GLU:HB3  | 1.92                     | 0.52              |
| 1:B:324:GLN:HE22 | 1:B:335:LYS:H    | 1.58                     | 0.51              |
| 1:C:109:TYR:CD2  | 1:C:158:GLU:HB2  | 2.45                     | 0.51              |
| 1:F:111:GLU:HB2  | 1:F:160:LEU:HD11 | 1.92                     | 0.51              |
| 1:F:144:LEU:HA   | 1:F:147:ASN:HD22 | 1.75                     | 0.51              |
| 1:H:81:LEU:HG    | 1:H:144:LEU:HD13 | 1.91                     | 0.51              |
| 1:B:358:ALA:O    | 1:B:361:VAL:HB   | 2.11                     | 0.51              |
| 1:C:340:ILE:O    | 1:C:341:THR:HG23 | 2.10                     | 0.51              |
| 1:F:94:LEU:HD11  | 1:F:98:LEU:HD11  | 1.92                     | 0.51              |
| 1:C:340:ILE:O    | 1:C:340:ILE:HG13 | 2.11                     | 0.51              |
| 1:D:266:LYS:NZ   | 1:D:266:LYS:HB3  | 2.26                     | 0.51              |
| 1:F:355:ARG:HG2  | 1:F:355:ARG:HH11 | 1.74                     | 0.51              |
| 1:H:349:THR:O    | 1:H:353:VAL:HG23 | 2.10                     | 0.51              |
| 1:A:257:TYR:CD1  | 1:A:295:VAL:HG13 | 2.46                     | 0.51              |
| 1:D:247:ILE:CD1  | 1:D:314:MET:HE1  | 2.29                     | 0.51              |
| 1:A:134:ILE:HD12 | 1:A:134:ILE:H    | 1.75                     | 0.51              |
| 1:A:248:LEU:HB3  | 1:A:256:ASN:OD1  | 2.10                     | 0.51              |
| 1:C:177:ILE:HG13 | 1:C:200:PHE:CE1  | 2.46                     | 0.51              |
| 1:D:292:GLN:N    | 1:D:293:PRO:CD   | 2.74                     | 0.51              |
| 1:D:330:GLY:C    | 1:D:332:ALA:N    | 2.68                     | 0.51              |
| 1:E:105:ILE:HG12 | 1:E:154:PRO:HB2  | 1.92                     | 0.51              |
| 1:E:110:LEU:HD13 | 1:E:123:ILE:CD1  | 2.40                     | 0.51              |
| 1:H:71:VAL:HG11  | 1:H:354:LEU:HD21 | 1.91                     | 0.51              |
| 1:F:72:ILE:HG22  | 1:F:107:ARG:HG3  | 1.92                     | 0.51              |
| 1:F:110:LEU:HD22 | 1:F:110:LEU:H    | 1.74                     | 0.51              |
| 1:D:81:LEU:HG    | 1:D:144:LEU:HD13 | 1.92                     | 0.51              |
| 1:E:235:ILE:HB   | 1:F:29:ASP:HB2   | 1.93                     | 0.51              |
| 1:A:72:ILE:HG22  | 1:A:107:ARG:CG   | 2.40                     | 0.51              |
| 1:B:67:ASP:OD1   | 1:B:365:ARG:NH2  | 2.44                     | 0.51              |
| 1:C:355:ARG:HG3  | 1:C:355:ARG:NH1  | 2.21                     | 0.51              |
| 1:D:177:ILE:HG13 | 1:D:200:PHE:CE1  | 2.46                     | 0.51              |
| 1:F:355:ARG:O    | 1:F:358:ALA:HB3  | 2.11                     | 0.51              |
| 1:A:100:GLY:O    | 1:A:365:ARG:NH2  | 2.44                     | 0.51              |
| 1:A:359:ALA:CA   | 1:A:362:ARG:HH12 | 2.22                     | 0.51              |
| 1:B:175:GLY:O    | 1:B:198:VAL:HA   | 2.10                     | 0.51              |
| 1:B:204:THR:HA   | 1:B:249:ARG:NH1  | 2.25                     | 0.51              |
| 1:G:304:ALA:O    | 1:G:367:VAL:HG21 | 2.11                     | 0.51              |
| 1:H:292:GLN:HB2  | 1:H:293:PRO:HD3  | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:252:LYS:C    | 1:D:254:GLY:H    | 2.18                     | 0.51              |
| 1:G:90:ARG:HH11  | 1:G:347:TRP:CD1  | 2.29                     | 0.51              |
| 1:B:252:LYS:O    | 1:B:254:GLY:N    | 2.44                     | 0.50              |
| 1:B:258:ASP:OD2  | 1:B:260:LYS:HB3  | 2.11                     | 0.50              |
| 1:F:204:THR:HA   | 1:F:249:ARG:HH12 | 1.76                     | 0.50              |
| 1:D:204:THR:HA   | 1:D:249:ARG:HH12 | 1.77                     | 0.50              |
| 1:C:204:THR:HA   | 1:C:249:ARG:NH1  | 2.26                     | 0.50              |
| 1:D:72:ILE:HG22  | 1:D:107:ARG:HG3  | 1.94                     | 0.50              |
| 1:D:250:GLY:N    | 1:D:256:ASN:OD1  | 2.41                     | 0.50              |
| 1:F:175:GLY:O    | 1:F:198:VAL:HA   | 2.11                     | 0.50              |
| 1:G:146:VAL:O    | 1:G:150:ASN:HB2  | 2.11                     | 0.50              |
| 1:A:122:LEU:O    | 1:A:122:LEU:HG   | 2.10                     | 0.50              |
| 1:B:117:VAL:O    | 1:B:117:VAL:HG23 | 2.10                     | 0.50              |
| 1:E:85:GLN:O     | 1:E:89:LEU:HD23  | 2.12                     | 0.50              |
| 1:E:113:PRO:HG3  | 1:E:180:ARG:HH11 | 1.76                     | 0.50              |
| 1:F:277:MET:HG3  | 1:F:312:GLY:C    | 2.37                     | 0.50              |
| 1:F:128:VAL:O    | 1:F:128:VAL:HG12 | 2.11                     | 0.50              |
| 1:H:216:GLN:NE2  | 1:H:270:PRO:HG3  | 2.27                     | 0.50              |
| 1:A:177:ILE:HG13 | 1:A:200:PHE:CE1  | 2.47                     | 0.50              |
| 1:G:177:ILE:HG13 | 1:G:200:PHE:CE1  | 2.47                     | 0.50              |
| 1:A:144:LEU:HA   | 1:A:147:ASN:HD22 | 1.76                     | 0.50              |
| 1:B:345:ILE:HD11 | 1:B:350:THR:OG1  | 2.11                     | 0.50              |
| 1:D:356:LYS:O    | 1:D:356:LYS:HG3  | 2.11                     | 0.50              |
| 1:F:262:VAL:O    | 1:F:265:ALA:HB3  | 2.12                     | 0.50              |
| 1:E:281:SER:CA   | 1:E:285:SER:HB2  | 2.42                     | 0.50              |
| 1:G:280:TYR:CD2  | 1:G:315:ILE:HG12 | 2.47                     | 0.50              |
| 1:F:293:PRO:O    | 1:F:296:ASN:HB3  | 2.12                     | 0.49              |
| 1:H:204:THR:HA   | 1:H:249:ARG:NH1  | 2.27                     | 0.49              |
| 1:H:144:LEU:HA   | 1:H:147:ASN:HD22 | 1.76                     | 0.49              |
| 1:H:177:ILE:HG13 | 1:H:200:PHE:CE1  | 2.47                     | 0.49              |
| 1:C:174:PHE:HE1  | 1:C:245:PHE:CZ   | 2.31                     | 0.49              |
| 1:D:266:LYS:HB3  | 1:D:266:LYS:HZ3  | 1.76                     | 0.49              |
| 1:G:90:ARG:HB3   | 1:G:347:TRP:CZ2  | 2.47                     | 0.49              |
| 1:E:112:LYS:HG2  | 1:E:113:PRO:HD2  | 1.94                     | 0.49              |
| 1:H:321:GLU:HB3  | 1:H:346:GLY:N    | 2.27                     | 0.49              |
| 1:A:229:LYS:NZ   | 1:B:21:GLU:OE2   | 2.33                     | 0.49              |
| 1:B:81:LEU:HG    | 1:B:144:LEU:HD13 | 1.94                     | 0.49              |
| 1:B:112:LYS:HG2  | 1:B:341:THR:CG2  | 2.43                     | 0.49              |
| 1:F:265:ALA:O    | 1:F:268:GLN:HB2  | 2.12                     | 0.49              |
| 1:A:327:PRO:HD2  | 1:A:334:LEU:HD21 | 1.94                     | 0.49              |
| 1:B:303:ILE:O    | 1:B:364:ARG:HB2  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:348:GLU:CD   | 1:D:348:GLU:N    | 2.55                     | 0.49              |
| 1:E:95:SER:O     | 1:E:99:LYS:HB2   | 2.11                     | 0.49              |
| 1:G:129:ASN:N    | 1:G:129:ASN:ND2  | 2.61                     | 0.49              |
| 1:G:289:PHE:N    | 1:G:289:PHE:CD2  | 2.80                     | 0.49              |
| 1:B:302:GLN:O    | 1:B:307:GLU:HB3  | 2.12                     | 0.49              |
| 1:B:347:TRP:O    | 1:B:350:THR:HB   | 2.13                     | 0.49              |
| 1:D:96:ASP:O     | 1:D:99:LYS:HG2   | 2.11                     | 0.49              |
| 1:F:93:LYS:HB2   | 1:F:93:LYS:HZ3   | 1.78                     | 0.49              |
| 1:F:134:ILE:HD12 | 1:F:134:ILE:H    | 1.78                     | 0.49              |
| 1:E:129:ASN:HD21 | 1:E:131:THR:HB   | 1.76                     | 0.49              |
| 1:E:177:ILE:HG13 | 1:E:200:PHE:CE1  | 2.48                     | 0.49              |
| 1:G:247:ILE:HD13 | 1:G:314:MET:CE   | 2.42                     | 0.49              |
| 1:B:85:GLN:O     | 1:B:89:LEU:HD23  | 2.13                     | 0.49              |
| 1:B:177:ILE:HG13 | 1:B:200:PHE:CE1  | 2.47                     | 0.49              |
| 1:C:81:LEU:HG    | 1:C:144:LEU:HD13 | 1.95                     | 0.49              |
| 1:D:94:LEU:HD11  | 1:D:351:GLU:HG3  | 1.95                     | 0.49              |
| 1:D:164:SER:HB2  | 4:D:2003:HOH:O   | 2.12                     | 0.49              |
| 1:E:82:GLU:OE1   | 1:E:82:GLU:N     | 2.38                     | 0.49              |
| 1:B:112:LYS:HD3  | 1:B:342:ASP:OD2  | 2.13                     | 0.49              |
| 1:B:335:LYS:HE3  | 1:B:338:VAL:HG21 | 1.95                     | 0.49              |
| 1:F:257:TYR:CD1  | 1:F:295:VAL:HG13 | 2.48                     | 0.49              |
| 1:C:249:ARG:O    | 1:C:283:GLY:HA3  | 2.13                     | 0.48              |
| 1:E:78:ILE:HG23  | 1:E:84:ALA:HB2   | 1.95                     | 0.48              |
| 1:E:324:GLN:CB   | 1:E:335:LYS:HD3  | 2.43                     | 0.48              |
| 1:G:129:ASN:ND2  | 1:G:131:THR:OG1  | 2.47                     | 0.48              |
| 1:G:144:LEU:HA   | 1:G:147:ASN:HD22 | 1.78                     | 0.48              |
| 1:H:167:TYR:C    | 1:H:168:LEU:HG   | 2.35                     | 0.48              |
| 1:A:78:ILE:HG23  | 1:A:84:ALA:HB2   | 1.95                     | 0.48              |
| 1:A:134:ILE:HD13 | 1:B:235:ILE:HG21 | 1.94                     | 0.48              |
| 1:E:304:ALA:O    | 1:E:367:VAL:HG21 | 2.13                     | 0.48              |
| 1:E:345:ILE:HG13 | 1:E:350:THR:OG1  | 2.13                     | 0.48              |
| 1:H:304:ALA:HB1  | 1:H:363:GLN:HG2  | 1.95                     | 0.48              |
| 1:A:79:HIS:HB3   | 1:A:119:TRP:CH2  | 2.48                     | 0.48              |
| 1:A:110:LEU:N    | 1:A:110:LEU:HD22 | 2.28                     | 0.48              |
| 1:A:146:VAL:O    | 1:A:150:ASN:HB2  | 2.13                     | 0.48              |
| 1:C:78:ILE:HG23  | 1:C:84:ALA:HB2   | 1.95                     | 0.48              |
| 1:D:204:THR:HA   | 1:D:249:ARG:NH1  | 2.29                     | 0.48              |
| 1:F:67:ASP:OD1   | 1:F:365:ARG:NE   | 2.47                     | 0.48              |
| 1:F:349:THR:O    | 1:F:352:ASP:HB3  | 2.12                     | 0.48              |
| 1:A:134:ILE:HB   | 1:B:235:ILE:HD13 | 1.95                     | 0.48              |
| 1:B:144:LEU:HA   | 1:B:147:ASN:HD22 | 1.78                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:304:ALA:O    | 1:C:367:VAL:HG21 | 2.14                     | 0.48              |
| 1:G:85:GLN:O     | 1:G:89:LEU:HD23  | 2.13                     | 0.48              |
| 1:G:174:PHE:HE1  | 1:G:245:PHE:CZ   | 2.32                     | 0.48              |
| 1:F:122:LEU:HD12 | 1:F:126:PRO:HA   | 1.95                     | 0.48              |
| 1:F:275:GLY:HA3  | 1:F:311:THR:HG21 | 1.94                     | 0.48              |
| 1:F:300:CYS:O    | 1:F:301:GLU:C    | 2.54                     | 0.48              |
| 1:H:361:VAL:HG12 | 1:H:365:ARG:HH12 | 1.79                     | 0.48              |
| 1:G:280:TYR:O    | 1:G:285:SER:HB2  | 2.14                     | 0.48              |
| 1:H:78:ILE:HG23  | 1:H:84:ALA:HB2   | 1.95                     | 0.48              |
| 1:A:113:PRO:HB2  | 1:A:180:ARG:CZ   | 2.44                     | 0.48              |
| 1:B:291:ASN:O    | 1:B:295:VAL:HG23 | 2.14                     | 0.48              |
| 1:B:330:GLY:C    | 1:B:332:ALA:H    | 2.21                     | 0.48              |
| 1:D:76:CYS:HA    | 1:D:107:ARG:HH21 | 1.78                     | 0.48              |
| 1:D:110:LEU:HD22 | 1:D:110:LEU:N    | 2.26                     | 0.48              |
| 1:F:204:THR:HA   | 1:F:249:ARG:NH1  | 2.28                     | 0.48              |
| 1:G:362:ARG:O    | 1:G:365:ARG:HB2  | 2.13                     | 0.48              |
| 1:H:74:GLY:CA    | 1:H:107:ARG:HB2  | 2.43                     | 0.48              |
| 1:B:146:VAL:O    | 1:B:150:ASN:HB2  | 2.14                     | 0.48              |
| 1:E:112:LYS:HB3  | 1:E:341:THR:CG2  | 2.42                     | 0.48              |
| 1:E:144:LEU:HA   | 1:E:147:ASN:HD22 | 1.79                     | 0.48              |
| 1:E:146:VAL:O    | 1:E:150:ASN:HB2  | 2.14                     | 0.48              |
| 1:E:359:ALA:HA   | 1:E:362:ARG:CZ   | 2.44                     | 0.48              |
| 1:F:112:LYS:HD2  | 1:F:113:PRO:CD   | 2.37                     | 0.48              |
| 1:H:363:GLN:HE21 | 1:H:367:VAL:HG23 | 1.78                     | 0.48              |
| 1:A:363:GLN:O    | 1:A:365:ARG:N    | 2.47                     | 0.48              |
| 1:C:369:LYS:HG3  | 1:C:370:LYS:N    | 2.28                     | 0.48              |
| 1:D:290:ARG:O    | 1:D:293:PRO:HD2  | 2.14                     | 0.48              |
| 1:F:71:VAL:CG2   | 1:F:102:LEU:HD22 | 2.43                     | 0.48              |
| 1:F:93:LYS:HB2   | 1:F:93:LYS:HZ2   | 1.77                     | 0.48              |
| 1:G:29:ASP:HB2   | 1:H:235:ILE:HB   | 1.96                     | 0.48              |
| 1:G:78:ILE:HG23  | 1:G:84:ALA:HB2   | 1.95                     | 0.48              |
| 1:A:292:GLN:HB2  | 1:A:293:PRO:HD3  | 1.94                     | 0.47              |
| 1:B:128:VAL:HG23 | 1:B:331:LYS:HE3  | 1.96                     | 0.47              |
| 1:D:94:LEU:CD1   | 1:D:351:GLU:HG3  | 2.44                     | 0.47              |
| 1:F:112:LYS:O    | 1:F:114:ARG:N    | 2.47                     | 0.47              |
| 1:F:119:TRP:HB2  | 1:F:326:ILE:CD1  | 2.44                     | 0.47              |
| 1:H:74:GLY:HA3   | 1:H:107:ARG:HB2  | 1.95                     | 0.47              |
| 1:C:128:VAL:HG13 | 1:C:128:VAL:O    | 2.14                     | 0.47              |
| 1:C:287:LYS:HD2  | 1:C:287:LYS:N    | 2.29                     | 0.47              |
| 1:C:295:VAL:O    | 1:C:299:VAL:HG23 | 2.13                     | 0.47              |
| 1:C:324:GLN:NE2  | 1:C:335:LYS:H    | 2.12                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:281:SER:C    | 1:E:285:SER:HB2  | 2.39                     | 0.47              |
| 1:E:320:ASN:O    | 1:E:346:GLY:HA2  | 2.14                     | 0.47              |
| 1:E:336:TYR:CD1  | 1:E:336:TYR:C    | 2.93                     | 0.47              |
| 1:G:289:PHE:N    | 1:G:289:PHE:HD2  | 2.11                     | 0.47              |
| 1:H:94:LEU:O     | 1:H:94:LEU:HD23  | 2.14                     | 0.47              |
| 1:H:322:GLY:O    | 1:H:323:ASN:HB3  | 2.13                     | 0.47              |
| 1:A:235:ILE:HG21 | 1:B:134:ILE:HD13 | 1.97                     | 0.47              |
| 1:B:78:ILE:HG23  | 1:B:84:ALA:HB2   | 1.95                     | 0.47              |
| 1:B:111:GLU:HB3  | 1:B:121:GLY:HA3  | 1.95                     | 0.47              |
| 1:F:295:VAL:O    | 1:F:299:VAL:HG23 | 2.15                     | 0.47              |
| 1:G:185:GLN:OE1  | 1:H:114:ARG:CB   | 2.62                     | 0.47              |
| 3:G:1002:PHE:OXT | 1:H:169:ALA:HB1  | 2.14                     | 0.47              |
| 1:H:111:GLU:O    | 1:H:111:GLU:HG3  | 2.15                     | 0.47              |
| 1:H:349:THR:O    | 1:H:352:ASP:HB3  | 2.14                     | 0.47              |
| 1:D:78:ILE:HG23  | 1:D:84:ALA:HB2   | 1.97                     | 0.47              |
| 1:F:257:TYR:CG   | 1:F:295:VAL:HG13 | 2.50                     | 0.47              |
| 1:D:362:ARG:O    | 1:D:365:ARG:HB3  | 2.14                     | 0.47              |
| 1:E:286:ASN:HD22 | 1:E:286:ASN:HA   | 1.56                     | 0.47              |
| 1:A:85:GLN:O     | 1:A:89:LEU:HD23  | 2.15                     | 0.47              |
| 1:A:235:ILE:HB   | 1:B:29:ASP:HB2   | 1.97                     | 0.47              |
| 1:B:290:ARG:O    | 1:B:293:PRO:HD2  | 2.15                     | 0.47              |
| 1:C:146:VAL:O    | 1:C:150:ASN:HB2  | 2.15                     | 0.47              |
| 1:C:257:TYR:CD1  | 1:C:257:TYR:C    | 2.93                     | 0.47              |
| 1:E:73:VAL:O     | 1:E:106:MET:HA   | 2.15                     | 0.47              |
| 1:F:81:LEU:HG    | 1:F:144:LEU:HD13 | 1.95                     | 0.47              |
| 1:B:317:SER:HB2  | 1:B:345:ILE:HG12 | 1.96                     | 0.47              |
| 1:E:281:SER:HA   | 1:E:285:SER:CB   | 2.45                     | 0.47              |
| 1:E:304:ALA:HA   | 1:E:363:GLN:HB3  | 1.97                     | 0.47              |
| 1:E:355:ARG:HG2  | 1:E:355:ARG:HH11 | 1.78                     | 0.47              |
| 1:G:324:GLN:OE1  | 1:G:334:LEU:HD22 | 2.14                     | 0.47              |
| 1:H:258:ASP:O    | 1:H:262:VAL:HG23 | 2.15                     | 0.47              |
| 1:A:327:PRO:HD2  | 1:A:334:LEU:CD2  | 2.45                     | 0.47              |
| 1:B:351:GLU:O    | 1:B:355:ARG:HG3  | 2.15                     | 0.47              |
| 1:C:74:GLY:CA    | 1:C:107:ARG:HB2  | 2.45                     | 0.47              |
| 1:D:144:LEU:HA   | 1:D:147:ASN:HD22 | 1.79                     | 0.47              |
| 1:H:196:PHE:HB2  | 1:H:197:PRO:CD   | 2.45                     | 0.47              |
| 1:A:232:VAL:CG2  | 1:D:232:VAL:HG21 | 2.45                     | 0.47              |
| 1:C:85:GLN:O     | 1:C:89:LEU:HD23  | 2.15                     | 0.47              |
| 1:C:144:LEU:HA   | 1:C:147:ASN:HD22 | 1.80                     | 0.47              |
| 1:D:277:MET:HA   | 1:D:312:GLY:O    | 2.15                     | 0.47              |
| 1:D:317:SER:HB3  | 1:D:345:ILE:HG13 | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:196:PHE:HB2  | 1:F:197:PRO:CD   | 2.45                     | 0.47              |
| 1:B:34:PRO:O     | 1:B:38:GLN:HG3   | 2.15                     | 0.46              |
| 1:C:94:LEU:HD11  | 1:C:98:LEU:HD11  | 1.97                     | 0.46              |
| 1:C:247:ILE:CD1  | 1:C:314:MET:HE1  | 2.33                     | 0.46              |
| 1:E:71:VAL:HG22  | 1:E:313:VAL:HG22 | 1.97                     | 0.46              |
| 1:F:129:ASN:HD22 | 1:F:129:ASN:N    | 2.04                     | 0.46              |
| 1:H:247:ILE:HD13 | 1:H:314:MET:HE1  | 1.97                     | 0.46              |
| 1:A:352:ASP:HB3  | 1:A:356:LYS:NZ   | 2.30                     | 0.46              |
| 1:C:314:MET:HE3  | 1:C:314:MET:HB2  | 1.76                     | 0.46              |
| 1:F:174:PHE:HE1  | 1:F:245:PHE:CZ   | 2.33                     | 0.46              |
| 1:F:316:GLU:O    | 1:F:344:CYS:HB2  | 2.14                     | 0.46              |
| 1:G:24:ARG:HD3   | 1:H:240:GLY:O    | 2.15                     | 0.46              |
| 1:H:131:THR:HG22 | 1:H:132:PHE:N    | 2.30                     | 0.46              |
| 1:C:235:ILE:HG13 | 1:D:31:LEU:HB2   | 1.98                     | 0.46              |
| 1:E:61:ILE:HG22  | 1:E:311:THR:HB   | 1.97                     | 0.46              |
| 1:G:289:PHE:HD2  | 1:G:289:PHE:H    | 1.64                     | 0.46              |
| 1:G:321:GLU:HB3  | 1:G:346:GLY:H    | 1.79                     | 0.46              |
| 1:B:97:GLU:HG2   | 1:B:98:LEU:HD23  | 1.97                     | 0.46              |
| 1:E:266:LYS:NZ   | 1:E:266:LYS:HB3  | 2.31                     | 0.46              |
| 1:H:85:GLN:O     | 1:H:89:LEU:HD23  | 2.14                     | 0.46              |
| 1:A:34:PRO:O     | 1:A:38:GLN:HG3   | 2.16                     | 0.46              |
| 1:D:85:GLN:O     | 1:D:89:LEU:HD23  | 2.15                     | 0.46              |
| 1:G:317:SER:CA   | 1:G:344:CYS:HB3  | 2.45                     | 0.46              |
| 1:G:324:GLN:HE22 | 1:G:334:LEU:CB   | 2.24                     | 0.46              |
| 1:A:117:VAL:CG1  | 1:A:118:GLY:H    | 2.29                     | 0.46              |
| 1:B:90:ARG:NH1   | 1:B:319:ILE:HG23 | 2.29                     | 0.46              |
| 1:C:20:GLU:OE1   | 1:D:55:ARG:HD2   | 2.15                     | 0.46              |
| 1:D:208:LEU:CD2  | 1:D:265:ALA:HA   | 2.46                     | 0.46              |
| 1:E:193:GLY:HA3  | 1:E:238:THR:CG2  | 2.46                     | 0.46              |
| 1:F:134:ILE:HD12 | 1:F:134:ILE:N    | 2.31                     | 0.46              |
| 1:G:294:LYS:HB2  | 1:G:294:LYS:HZ3  | 1.79                     | 0.46              |
| 1:A:109:TYR:CD2  | 1:A:158:GLU:HB2  | 2.51                     | 0.46              |
| 1:B:21:GLU:O     | 1:B:23:VAL:N     | 2.48                     | 0.46              |
| 1:B:74:GLY:CA    | 1:B:107:ARG:HB2  | 2.44                     | 0.46              |
| 1:B:248:LEU:HB2  | 1:B:278:ILE:CD1  | 2.45                     | 0.46              |
| 1:C:180:ARG:NH1  | 1:D:183:GLU:O    | 2.49                     | 0.46              |
| 1:D:110:LEU:N    | 1:D:110:LEU:HD13 | 2.31                     | 0.46              |
| 1:E:128:VAL:O    | 1:E:129:ASN:HB3  | 2.15                     | 0.46              |
| 1:G:348:GLU:CD   | 1:G:348:GLU:N    | 2.74                     | 0.46              |
| 1:A:117:VAL:CG1  | 1:A:118:GLY:N    | 2.75                     | 0.46              |
| 1:A:201:LYS:NZ   | 4:A:2004:HOH:O   | 2.42                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:72:ILE:HB    | 1:D:314:MET:HG3  | 1.98                     | 0.46              |
| 1:E:315:ILE:CD1  | 1:E:354:LEU:HD21 | 2.46                     | 0.46              |
| 1:H:34:PRO:O     | 1:H:38:GLN:HG3   | 2.16                     | 0.46              |
| 1:B:303:ILE:HG22 | 1:B:360:ALA:O    | 2.15                     | 0.46              |
| 1:C:341:THR:O    | 1:C:342:ASP:C    | 2.57                     | 0.46              |
| 1:E:368:ASN:O    | 1:E:369:LYS:HG3  | 2.15                     | 0.46              |
| 1:H:174:PHE:HE1  | 1:H:245:PHE:CZ   | 2.33                     | 0.46              |
| 1:H:308:ASN:ND2  | 1:H:364:ARG:HD2  | 2.30                     | 0.46              |
| 1:A:129:ASN:HD22 | 1:A:131:THR:H    | 1.64                     | 0.46              |
| 1:A:349:THR:O    | 1:A:353:VAL:HG23 | 2.16                     | 0.46              |
| 1:B:196:PHE:HB2  | 1:B:197:PRO:CD   | 2.46                     | 0.46              |
| 1:C:62:ILE:HD12  | 1:C:274:ASN:ND2  | 2.31                     | 0.46              |
| 1:C:196:PHE:HB2  | 1:C:197:PRO:CD   | 2.46                     | 0.46              |
| 1:H:146:VAL:O    | 1:H:150:ASN:HB2  | 2.16                     | 0.46              |
| 1:A:266:LYS:NZ   | 1:A:307:GLU:OE2  | 2.42                     | 0.45              |
| 1:C:174:PHE:CE1  | 1:C:245:PHE:HZ   | 2.34                     | 0.45              |
| 1:D:266:LYS:HE2  | 1:D:309:ALA:CB   | 2.46                     | 0.45              |
| 1:D:352:ASP:O    | 1:D:353:VAL:C    | 2.57                     | 0.45              |
| 1:H:98:LEU:HD13  | 1:H:102:LEU:CD2  | 2.44                     | 0.45              |
| 1:H:110:LEU:HD22 | 1:H:110:LEU:H    | 1.80                     | 0.45              |
| 1:A:174:PHE:HE1  | 1:A:245:PHE:CZ   | 2.34                     | 0.45              |
| 1:C:111:GLU:HB3  | 1:C:121:GLY:HA3  | 1.97                     | 0.45              |
| 1:C:257:TYR:CG   | 1:C:295:VAL:HG13 | 2.51                     | 0.45              |
| 1:C:323:ASN:CG   | 1:C:323:ASN:O    | 2.59                     | 0.45              |
| 1:D:174:PHE:HE1  | 1:D:245:PHE:CZ   | 2.35                     | 0.45              |
| 1:B:323:ASN:O    | 1:B:324:GLN:HB3  | 2.16                     | 0.45              |
| 1:C:369:LYS:NZ   | 1:C:369:LYS:HB3  | 2.32                     | 0.45              |
| 1:G:257:TYR:HD1  | 1:G:257:TYR:H    | 1.64                     | 0.45              |
| 1:H:102:LEU:HD23 | 1:H:354:LEU:HD22 | 1.99                     | 0.45              |
| 1:A:112:LYS:HG2  | 1:A:113:PRO:HD2  | 1.97                     | 0.45              |
| 1:C:247:ILE:HG12 | 1:C:277:MET:HB3  | 1.99                     | 0.45              |
| 1:G:142:ARG:O    | 1:G:146:VAL:HG23 | 2.17                     | 0.45              |
| 1:B:362:ARG:HG3  | 1:B:362:ARG:HH11 | 1.82                     | 0.45              |
| 1:E:97:GLU:C     | 1:E:99:LYS:H     | 2.24                     | 0.45              |
| 1:F:78:ILE:HG23  | 1:F:84:ALA:HB2   | 1.98                     | 0.45              |
| 1:H:323:ASN:HA   | 1:H:339:SER:O    | 2.17                     | 0.45              |
| 1:B:279:ASP:HA   | 1:B:314:MET:HB2  | 1.99                     | 0.45              |
| 1:C:270:PRO:O    | 1:C:273:SER:HB2  | 2.16                     | 0.45              |
| 1:F:91:LEU:HD11  | 1:F:104:ILE:HG21 | 1.97                     | 0.45              |
| 1:G:93:LYS:HB2   | 1:G:93:LYS:HZ2   | 1.82                     | 0.45              |
| 1:H:76:CYS:SG    | 1:H:112:LYS:HG3  | 2.57                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:196:PHE:HB2  | 1:A:197:PRO:CD   | 2.47                     | 0.45              |
| 1:C:235:ILE:HB   | 1:D:29:ASP:HB2   | 1.99                     | 0.45              |
| 1:D:352:ASP:O    | 1:D:354:LEU:N    | 2.49                     | 0.45              |
| 1:D:366:GLU:C    | 1:D:368:ASN:N    | 2.73                     | 0.45              |
| 1:E:29:ASP:HB2   | 1:F:235:ILE:HB   | 1.98                     | 0.45              |
| 1:H:362:ARG:HG3  | 1:H:362:ARG:NH1  | 2.31                     | 0.45              |
| 1:D:196:PHE:HB2  | 1:D:197:PRO:CD   | 2.47                     | 0.45              |
| 1:E:207:THR:HG21 | 1:F:252:LYS:HZ2  | 1.81                     | 0.45              |
| 1:F:177:ILE:HG13 | 1:F:200:PHE:CE1  | 2.52                     | 0.45              |
| 1:H:70:LEU:HD11  | 1:H:105:ILE:CD1  | 2.47                     | 0.45              |
| 1:H:94:LEU:CD2   | 1:H:98:LEU:HD11  | 2.47                     | 0.45              |
| 1:A:193:GLY:HA3  | 1:A:238:THR:CG2  | 2.46                     | 0.45              |
| 1:C:324:GLN:HE22 | 1:C:335:LYS:N    | 2.15                     | 0.45              |
| 1:D:278:ILE:HD12 | 1:D:310:ILE:HD13 | 1.97                     | 0.45              |
| 1:E:81:LEU:HG    | 1:E:144:LEU:HD13 | 1.99                     | 0.45              |
| 1:H:91:LEU:HA    | 1:H:347:TRP:CH2  | 2.50                     | 0.45              |
| 1:B:352:ASP:O    | 1:B:353:VAL:C    | 2.60                     | 0.44              |
| 1:C:61:ILE:HD11  | 1:C:103:SER:HB2  | 1.98                     | 0.44              |
| 1:F:101:ASP:OD2  | 1:F:362:ARG:NH1  | 2.49                     | 0.44              |
| 1:G:196:PHE:HB2  | 1:G:197:PRO:CD   | 2.47                     | 0.44              |
| 1:H:216:GLN:HE22 | 1:H:270:PRO:HG3  | 1.82                     | 0.44              |
| 1:A:252:LYS:C    | 1:A:254:GLY:N    | 2.75                     | 0.44              |
| 1:A:291:ASN:O    | 1:A:294:LYS:HB2  | 2.17                     | 0.44              |
| 1:C:129:ASN:OD1  | 1:C:131:THR:HB   | 2.16                     | 0.44              |
| 1:D:296:ASN:CG   | 1:D:353:VAL:HG13 | 2.42                     | 0.44              |
| 1:D:303:ILE:O    | 1:D:364:ARG:HB2  | 2.17                     | 0.44              |
| 1:F:193:GLY:HA3  | 1:F:238:THR:CG2  | 2.47                     | 0.44              |
| 1:A:81:LEU:HG    | 1:A:144:LEU:HD13 | 2.00                     | 0.44              |
| 1:C:110:LEU:HD22 | 1:C:110:LEU:H    | 1.81                     | 0.44              |
| 1:D:146:VAL:O    | 1:D:150:ASN:HB2  | 2.17                     | 0.44              |
| 1:E:270:PRO:HD2  | 1:E:273:SER:OG   | 2.18                     | 0.44              |
| 1:G:307:GLU:OE2  | 1:G:307:GLU:CA   | 2.65                     | 0.44              |
| 1:H:82:GLU:N     | 1:H:82:GLU:OE2   | 2.48                     | 0.44              |
| 1:H:86:GLU:CD    | 1:H:336:TYR:OH   | 2.60                     | 0.44              |
| 1:H:193:GLY:HA3  | 1:H:238:THR:CG2  | 2.47                     | 0.44              |
| 1:B:193:GLY:HA3  | 1:B:238:THR:CG2  | 2.48                     | 0.44              |
| 1:B:302:GLN:O    | 1:B:307:GLU:CB   | 2.66                     | 0.44              |
| 1:C:75:PRO:HA    | 1:C:317:SER:O    | 2.16                     | 0.44              |
| 1:D:111:GLU:O    | 1:D:112:LYS:HB2  | 2.17                     | 0.44              |
| 1:F:301:GLU:HG3  | 1:F:305:ASN:ND2  | 2.33                     | 0.44              |
| 1:G:294:LYS:HB2  | 1:G:294:LYS:HZ2  | 1.82                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:247:ILE:HG12 | 1:H:277:MET:HB3  | 1.99                     | 0.44              |
| 1:D:127:ASP:HB2  | 1:D:129:ASN:ND2  | 2.33                     | 0.44              |
| 1:G:81:LEU:HG    | 1:G:144:LEU:HD13 | 1.99                     | 0.44              |
| 1:D:262:VAL:HG12 | 1:D:266:LYS:HD2  | 1.99                     | 0.44              |
| 1:F:146:VAL:O    | 1:F:150:ASN:HB2  | 2.17                     | 0.44              |
| 1:H:106:MET:CG   | 1:H:107:ARG:N    | 2.80                     | 0.44              |
| 1:B:83:ALA:HB2   | 1:B:336:TYR:CE1  | 2.53                     | 0.44              |
| 1:E:34:PRO:O     | 1:E:38:GLN:HG3   | 2.16                     | 0.44              |
| 1:B:91:LEU:HD11  | 1:B:104:ILE:HG21 | 2.00                     | 0.44              |
| 1:B:300:CYS:SG   | 1:B:357:LEU:HA   | 2.58                     | 0.44              |
| 1:B:345:ILE:HG13 | 1:B:346:GLY:O    | 2.18                     | 0.44              |
| 1:D:341:THR:HB   | 1:D:342:ASP:H    | 1.57                     | 0.44              |
| 1:E:355:ARG:HG2  | 1:E:355:ARG:NH1  | 2.33                     | 0.44              |
| 1:H:285:SER:HB2  | 1:H:288:ASP:O    | 2.18                     | 0.44              |
| 1:C:129:ASN:C    | 1:C:131:THR:H    | 2.26                     | 0.44              |
| 1:H:104:ILE:CG2  | 1:H:105:ILE:N    | 2.81                     | 0.44              |
| 1:A:29:ASP:HB2   | 1:B:235:ILE:HB   | 1.99                     | 0.43              |
| 1:A:192:SER:O    | 1:A:238:THR:HB   | 2.18                     | 0.43              |
| 1:A:259:ALA:HA   | 1:A:302:GLN:OE1  | 2.18                     | 0.43              |
| 1:B:174:PHE:HE1  | 1:B:245:PHE:CZ   | 2.36                     | 0.43              |
| 1:C:126:PRO:HB3  | 1:C:137:GLY:HA2  | 2.00                     | 0.43              |
| 1:G:79:HIS:HB3   | 1:G:340:ILE:HD11 | 2.00                     | 0.43              |
| 1:G:127:ASP:OD2  | 1:G:136:LYS:NZ   | 2.35                     | 0.43              |
| 1:G:359:ALA:O    | 1:G:361:VAL:N    | 2.51                     | 0.43              |
| 1:A:264:GLU:O    | 1:A:267:ALA:HB3  | 2.18                     | 0.43              |
| 1:A:321:GLU:HA   | 1:A:344:CYS:O    | 2.18                     | 0.43              |
| 1:E:193:GLY:HA3  | 1:E:238:THR:HG22 | 1.99                     | 0.43              |
| 1:H:322:GLY:O    | 1:H:343:ALA:HA   | 2.18                     | 0.43              |
| 1:A:306:GLY:HA3  | 1:A:367:VAL:HG11 | 1.99                     | 0.43              |
| 1:E:134:ILE:HB   | 1:F:235:ILE:HD13 | 2.00                     | 0.43              |
| 1:E:324:GLN:HE22 | 1:E:335:LYS:HB2  | 1.82                     | 0.43              |
| 1:G:174:PHE:CE1  | 1:G:245:PHE:HZ   | 2.37                     | 0.43              |
| 1:H:76:CYS:SG    | 1:H:342:ASP:HB2  | 2.57                     | 0.43              |
| 1:H:110:LEU:HD21 | 1:H:145:PHE:CZ   | 2.54                     | 0.43              |
| 1:H:279:ASP:HA   | 1:H:314:MET:HB3  | 2.01                     | 0.43              |
| 1:H:318:ASN:ND2  | 1:H:339:SER:HB3  | 2.31                     | 0.43              |
| 1:B:34:PRO:HD2   | 1:B:229:LYS:O    | 2.18                     | 0.43              |
| 1:C:174:PHE:HE1  | 1:C:245:PHE:HZ   | 1.66                     | 0.43              |
| 1:C:313:VAL:HG21 | 1:C:357:LEU:HD21 | 2.01                     | 0.43              |
| 1:H:62:ILE:O     | 1:H:274:ASN:HB3  | 2.18                     | 0.43              |
| 1:A:110:LEU:O    | 1:A:111:GLU:CB   | 2.66                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:326:ILE:HA   | 1:A:327:PRO:HD2  | 1.84                     | 0.43              |
| 1:B:364:ARG:O    | 1:B:368:ASN:ND2  | 2.52                     | 0.43              |
| 1:C:208:LEU:HD11 | 1:C:246:VAL:CG1  | 2.37                     | 0.43              |
| 1:E:123:ILE:O    | 1:E:134:ILE:HA   | 2.18                     | 0.43              |
| 1:F:275:GLY:HA3  | 1:F:311:THR:HG23 | 1.98                     | 0.43              |
| 1:G:202:ASN:HB2  | 1:G:207:THR:O    | 2.19                     | 0.43              |
| 1:H:277:MET:SD   | 1:H:314:MET:HE3  | 2.59                     | 0.43              |
| 1:C:74:GLY:HA3   | 1:C:107:ARG:HB2  | 2.01                     | 0.43              |
| 1:C:322:GLY:O    | 1:C:323:ASN:HB3  | 2.18                     | 0.43              |
| 1:G:112:LYS:HE2  | 1:G:342:ASP:OD1  | 2.19                     | 0.43              |
| 1:A:261:SER:HA   | 1:A:264:GLU:OE2  | 2.18                     | 0.43              |
| 1:B:275:GLY:C    | 1:B:311:THR:OG1  | 2.62                     | 0.43              |
| 1:E:73:VAL:HG23  | 1:E:315:ILE:HB   | 2.00                     | 0.43              |
| 1:E:196:PHE:HB2  | 1:E:197:PRO:CD   | 2.48                     | 0.43              |
| 1:E:202:ASN:HB2  | 1:E:207:THR:O    | 2.19                     | 0.43              |
| 1:E:335:LYS:O    | 1:E:336:TYR:CB   | 2.66                     | 0.43              |
| 1:G:124:ASN:O    | 1:G:132:PHE:HA   | 2.18                     | 0.43              |
| 1:G:285:SER:O    | 1:G:286:ASN:C    | 2.61                     | 0.43              |
| 1:G:345:ILE:O    | 1:G:345:ILE:HG13 | 2.17                     | 0.43              |
| 1:A:118:GLY:O    | 1:A:120:LYS:NZ   | 2.51                     | 0.43              |
| 1:A:193:GLY:HA3  | 1:A:238:THR:HG22 | 2.01                     | 0.43              |
| 1:B:306:GLY:HA2  | 1:B:364:ARG:HG3  | 2.01                     | 0.43              |
| 1:E:90:ARG:HD3   | 1:E:347:TRP:CD1  | 2.53                     | 0.43              |
| 1:H:174:PHE:CE1  | 1:H:245:PHE:HZ   | 2.37                     | 0.43              |
| 1:A:129:ASN:ND2  | 1:A:131:THR:OG1  | 2.52                     | 0.43              |
| 1:C:62:ILE:O     | 1:C:274:ASN:HB3  | 2.19                     | 0.43              |
| 1:D:258:ASP:OD1  | 1:D:258:ASP:C    | 2.61                     | 0.43              |
| 1:D:275:GLY:HA3  | 1:D:311:THR:OG1  | 2.18                     | 0.43              |
| 1:G:93:LYS:NZ    | 1:G:93:LYS:CB    | 2.82                     | 0.43              |
| 1:H:78:ILE:O     | 1:H:119:TRP:HH2  | 2.02                     | 0.43              |
| 1:E:290:ARG:O    | 1:E:293:PRO:HD2  | 2.19                     | 0.43              |
| 1:G:258:ASP:OD2  | 1:G:260:LYS:HB3  | 2.19                     | 0.43              |
| 1:G:265:ALA:O    | 1:G:267:ALA:N    | 2.52                     | 0.43              |
| 1:H:366:GLU:C    | 1:H:368:ASN:N    | 2.75                     | 0.43              |
| 1:B:109:TYR:CE2  | 1:B:158:GLU:HB2  | 2.54                     | 0.42              |
| 1:B:142:ARG:O    | 1:B:146:VAL:HG23 | 2.19                     | 0.42              |
| 1:B:192:SER:O    | 1:B:238:THR:HB   | 2.19                     | 0.42              |
| 1:C:257:TYR:HD1  | 1:C:258:ASP:N    | 2.16                     | 0.42              |
| 1:D:262:VAL:O    | 1:D:262:VAL:HG12 | 2.19                     | 0.42              |
| 1:F:123:ILE:O    | 1:F:137:GLY:HA3  | 2.19                     | 0.42              |
| 1:G:235:ILE:HB   | 1:H:29:ASP:HB2   | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:102:LEU:CD2  | 1:A:357:LEU:HD13 | 2.48                     | 0.42              |
| 1:A:355:ARG:HG2  | 1:A:355:ARG:HH11 | 1.84                     | 0.42              |
| 1:A:366:GLU:O    | 1:A:367:VAL:C    | 2.61                     | 0.42              |
| 1:B:92:LYS:O     | 1:B:95:SER:HB3   | 2.19                     | 0.42              |
| 1:G:193:GLY:HA3  | 1:G:238:THR:CG2  | 2.49                     | 0.42              |
| 1:C:355:ARG:NH1  | 1:C:355:ARG:CG   | 2.80                     | 0.42              |
| 1:D:193:GLY:HA3  | 1:D:238:THR:CG2  | 2.48                     | 0.42              |
| 1:D:304:ALA:C    | 1:D:306:GLY:N    | 2.77                     | 0.42              |
| 1:E:363:GLN:O    | 1:E:367:VAL:HG23 | 2.19                     | 0.42              |
| 1:F:85:GLN:O     | 1:F:89:LEU:HD23  | 2.18                     | 0.42              |
| 1:G:265:ALA:C    | 1:G:267:ALA:N    | 2.77                     | 0.42              |
| 1:G:365:ARG:O    | 1:G:366:GLU:C    | 2.61                     | 0.42              |
| 1:B:335:LYS:HE2  | 1:B:338:VAL:HG21 | 2.01                     | 0.42              |
| 1:C:21:GLU:CD    | 1:D:170:ASP:HB3  | 2.44                     | 0.42              |
| 1:C:119:TRP:CD1  | 1:C:128:VAL:HG23 | 2.54                     | 0.42              |
| 1:C:240:GLY:O    | 1:D:24:ARG:HD3   | 2.19                     | 0.42              |
| 1:C:279:ASP:HA   | 1:C:314:MET:HB3  | 2.00                     | 0.42              |
| 1:D:133:ASN:O    | 1:D:134:ILE:C    | 2.62                     | 0.42              |
| 1:F:355:ARG:HG2  | 1:F:355:ARG:NH1  | 2.33                     | 0.42              |
| 1:G:41:ILE:HB    | 1:G:142:ARG:HD3  | 2.00                     | 0.42              |
| 1:H:112:LYS:O    | 1:H:113:PRO:C    | 2.63                     | 0.42              |
| 1:A:351:GLU:O    | 1:A:355:ARG:HG3  | 2.19                     | 0.42              |
| 1:A:363:GLN:O    | 1:A:364:ARG:C    | 2.63                     | 0.42              |
| 1:B:362:ARG:HG3  | 1:B:362:ARG:NH1  | 2.35                     | 0.42              |
| 1:D:288:ASP:OD1  | 1:D:290:ARG:HG3  | 2.19                     | 0.42              |
| 1:E:194:LEU:HD13 | 1:E:196:PHE:CE1  | 2.54                     | 0.42              |
| 1:G:327:PRO:HD3  | 1:G:334:LEU:CD2  | 2.50                     | 0.42              |
| 1:G:359:ALA:O    | 1:G:360:ALA:C    | 2.63                     | 0.42              |
| 1:H:79:HIS:HB3   | 1:H:119:TRP:CH2  | 2.54                     | 0.42              |
| 1:A:52:LYS:HD3   | 1:B:20:GLU:HB2   | 2.02                     | 0.42              |
| 1:A:194:LEU:HD13 | 1:A:196:PHE:CE1  | 2.55                     | 0.42              |
| 1:B:72:ILE:HG22  | 1:B:107:ARG:HG3  | 2.01                     | 0.42              |
| 1:C:257:TYR:C    | 1:C:257:TYR:HD1  | 2.28                     | 0.42              |
| 1:D:110:LEU:HB3  | 1:D:122:LEU:HB3  | 2.01                     | 0.42              |
| 1:D:266:LYS:NZ   | 1:D:266:LYS:CB   | 2.82                     | 0.42              |
| 1:F:193:GLY:HA3  | 1:F:238:THR:HG22 | 2.02                     | 0.42              |
| 1:G:289:PHE:CD2  | 1:G:290:ARG:N    | 2.88                     | 0.42              |
| 1:A:111:GLU:HB3  | 1:A:121:GLY:HA3  | 2.01                     | 0.42              |
| 1:B:50:THR:OG1   | 1:B:152:GLY:HA2  | 2.20                     | 0.42              |
| 1:C:162:THR:HG21 | 1:C:186:LEU:HD11 | 2.01                     | 0.42              |
| 1:E:59:ILE:HD13  | 1:E:243:HIS:CE1  | 2.55                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:104:ILE:HG22 | 1:H:105:ILE:N    | 2.35                     | 0.42              |
| 1:C:351:GLU:HG2  | 1:C:355:ARG:NH1  | 2.35                     | 0.42              |
| 1:G:348:GLU:CD   | 1:G:348:GLU:H    | 2.28                     | 0.42              |
| 1:A:129:ASN:ND2  | 1:A:131:THR:H    | 2.17                     | 0.42              |
| 1:D:310:ILE:O    | 1:D:310:ILE:HG22 | 2.20                     | 0.42              |
| 1:D:357:LEU:O    | 1:D:361:VAL:HG23 | 2.20                     | 0.42              |
| 1:F:50:THR:OG1   | 1:F:152:GLY:HA2  | 2.19                     | 0.42              |
| 1:F:194:LEU:HD13 | 1:F:196:PHE:CE1  | 2.55                     | 0.42              |
| 1:H:41:ILE:HB    | 1:H:142:ARG:HD3  | 2.01                     | 0.42              |
| 1:A:114:ARG:HB2  | 1:A:116:THR:O    | 2.20                     | 0.42              |
| 1:B:285:SER:O    | 1:B:286:ASN:C    | 2.62                     | 0.42              |
| 1:C:323:ASN:HA   | 1:C:339:SER:O    | 2.20                     | 0.42              |
| 1:D:363:GLN:NE2  | 1:D:367:VAL:HG23 | 2.34                     | 0.42              |
| 1:E:41:ILE:HB    | 1:E:142:ARG:HD3  | 2.01                     | 0.42              |
| 1:E:142:ARG:O    | 1:E:146:VAL:HG23 | 2.20                     | 0.42              |
| 1:E:288:ASP:C    | 1:E:290:ARG:H    | 2.28                     | 0.42              |
| 1:F:34:PRO:O     | 1:F:38:GLN:HG3   | 2.19                     | 0.42              |
| 1:B:366:GLU:O    | 1:B:368:ASN:N    | 2.53                     | 0.41              |
| 1:C:366:GLU:OE2  | 1:C:369:LYS:HD2  | 2.20                     | 0.41              |
| 1:D:208:LEU:HD11 | 1:D:246:VAL:CG1  | 2.35                     | 0.41              |
| 1:D:317:SER:HB3  | 1:D:345:ILE:CG1  | 2.50                     | 0.41              |
| 1:E:133:ASN:ND2  | 1:E:136:LYS:CB   | 2.82                     | 0.41              |
| 1:A:41:ILE:HB    | 1:A:142:ARG:HD3  | 2.02                     | 0.41              |
| 1:B:59:ILE:HD13  | 1:B:243:HIS:CE1  | 2.55                     | 0.41              |
| 1:C:41:ILE:HB    | 1:C:142:ARG:HD3  | 2.02                     | 0.41              |
| 1:C:132:PHE:CD2  | 1:D:223:HIS:HB2  | 2.54                     | 0.41              |
| 1:E:174:PHE:HE1  | 1:E:245:PHE:CZ   | 2.39                     | 0.41              |
| 1:E:235:ILE:HD13 | 1:F:134:ILE:HB   | 2.02                     | 0.41              |
| 1:G:298:VAL:O    | 1:G:298:VAL:HG12 | 2.20                     | 0.41              |
| 1:C:29:ASP:HB2   | 1:D:235:ILE:HB   | 2.02                     | 0.41              |
| 1:C:223:HIS:HB2  | 1:D:132:PHE:CD1  | 2.55                     | 0.41              |
| 1:D:119:TRP:CZ2  | 1:D:122:LEU:N    | 2.88                     | 0.41              |
| 1:E:269:LEU:HA   | 1:E:270:PRO:HD3  | 1.79                     | 0.41              |
| 1:F:109:TYR:CE2  | 1:F:158:GLU:HB2  | 2.55                     | 0.41              |
| 1:G:164:SER:HB2  | 1:G:165:PRO:HD3  | 2.01                     | 0.41              |
| 1:H:122:LEU:O    | 1:H:126:PRO:HB3  | 2.21                     | 0.41              |
| 1:A:202:ASN:HB2  | 1:A:207:THR:O    | 2.20                     | 0.41              |
| 1:B:327:PRO:C    | 1:B:329:GLU:N    | 2.73                     | 0.41              |
| 1:B:369:LYS:HB2  | 1:B:369:LYS:HE3  | 1.81                     | 0.41              |
| 1:C:290:ARG:HH11 | 1:C:290:ARG:HG2  | 1.85                     | 0.41              |
| 1:D:41:ILE:HB    | 1:D:142:ARG:HD3  | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:132:PHE:N    | 1:D:132:PHE:CD2  | 2.88                     | 0.41              |
| 1:E:339:SER:C    | 1:E:341:THR:H    | 2.28                     | 0.41              |
| 1:E:347:TRP:CE3  | 1:E:347:TRP:HA   | 2.56                     | 0.41              |
| 1:G:281:SER:O    | 1:G:282:HIS:HB2  | 2.20                     | 0.41              |
| 1:H:120:LYS:HE3  | 1:H:132:PHE:CE2  | 2.56                     | 0.41              |
| 1:H:194:LEU:HD13 | 1:H:196:PHE:CE1  | 2.55                     | 0.41              |
| 1:H:366:GLU:O    | 1:H:368:ASN:O    | 2.38                     | 0.41              |
| 1:B:303:ILE:HG23 | 1:B:364:ARG:HD3  | 2.03                     | 0.41              |
| 1:B:330:GLY:O    | 1:B:332:ALA:N    | 2.49                     | 0.41              |
| 1:C:111:GLU:CB   | 1:C:121:GLY:HA2  | 2.48                     | 0.41              |
| 1:D:193:GLY:HA3  | 1:D:238:THR:HG22 | 2.03                     | 0.41              |
| 1:D:329:GLU:H    | 1:D:329:GLU:CD   | 2.29                     | 0.41              |
| 1:E:86:GLU:OE2   | 1:E:319:ILE:HD13 | 2.21                     | 0.41              |
| 1:F:41:ILE:HB    | 1:F:142:ARG:HD3  | 2.01                     | 0.41              |
| 1:F:59:ILE:HD13  | 1:F:243:HIS:CE1  | 2.56                     | 0.41              |
| 1:F:212:VAL:HG22 | 1:F:269:LEU:HD23 | 2.01                     | 0.41              |
| 1:G:164:SER:N    | 1:G:165:PRO:CD   | 2.84                     | 0.41              |
| 1:G:235:ILE:HG13 | 1:H:31:LEU:HB2   | 2.03                     | 0.41              |
| 1:B:41:ILE:HB    | 1:B:142:ARG:HD3  | 2.03                     | 0.41              |
| 1:B:135:ASN:O    | 1:B:139:GLN:HG3  | 2.20                     | 0.41              |
| 1:E:89:LEU:HD13  | 1:E:89:LEU:HA    | 1.92                     | 0.41              |
| 1:F:142:ARG:O    | 1:F:146:VAL:HG23 | 2.20                     | 0.41              |
| 1:G:193:GLY:HA3  | 1:G:238:THR:HG22 | 2.03                     | 0.41              |
| 1:G:299:VAL:O    | 1:G:302:GLN:N    | 2.49                     | 0.41              |
| 1:H:94:LEU:HD11  | 1:H:351:GLU:HG3  | 2.03                     | 0.41              |
| 1:B:242:GLU:HG2  | 1:B:243:HIS:CD2  | 2.56                     | 0.41              |
| 1:D:174:PHE:CE1  | 1:D:245:PHE:HZ   | 2.38                     | 0.41              |
| 1:E:366:GLU:CD   | 1:E:366:GLU:N    | 2.77                     | 0.41              |
| 1:F:281:SER:HA   | 1:F:285:SER:OG   | 2.20                     | 0.41              |
| 1:G:269:LEU:HD22 | 1:G:273:SER:OG   | 2.21                     | 0.41              |
| 1:G:280:TYR:CD1  | 1:G:295:VAL:CG1  | 3.03                     | 0.41              |
| 1:G:292:GLN:HB2  | 1:G:293:PRO:HD3  | 2.02                     | 0.41              |
| 1:D:124:ASN:O    | 1:D:132:PHE:HA   | 2.20                     | 0.41              |
| 1:G:34:PRO:O     | 1:G:38:GLN:HG3   | 2.20                     | 0.41              |
| 1:G:69:VAL:HG13  | 1:G:312:GLY:HA2  | 2.02                     | 0.41              |
| 1:H:73:VAL:HG23  | 1:H:315:ILE:HB   | 2.02                     | 0.41              |
| 1:H:193:GLY:HA3  | 1:H:238:THR:HG22 | 2.02                     | 0.41              |
| 1:H:348:GLU:CD   | 1:H:348:GLU:N    | 2.67                     | 0.41              |
| 1:A:112:LYS:HE3  | 1:A:112:LYS:HB3  | 1.91                     | 0.41              |
| 1:A:174:PHE:CE1  | 1:A:245:PHE:HZ   | 2.39                     | 0.41              |
| 1:A:303:ILE:HG23 | 1:A:364:ARG:HD3  | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:248:LEU:HD12 | 1:B:278:ILE:CD1  | 2.51                     | 0.41              |
| 1:C:109:TYR:CE2  | 1:C:158:GLU:HB2  | 2.56                     | 0.41              |
| 1:C:252:LYS:O    | 1:C:253:LYS:C    | 2.64                     | 0.41              |
| 1:D:202:ASN:HB2  | 1:D:207:THR:O    | 2.21                     | 0.41              |
| 1:E:135:ASN:O    | 1:E:139:GLN:HG3  | 2.21                     | 0.41              |
| 1:F:164:SER:N    | 1:F:165:PRO:CD   | 2.84                     | 0.41              |
| 1:F:174:PHE:CE1  | 1:F:245:PHE:HZ   | 2.38                     | 0.41              |
| 1:G:112:LYS:HG3  | 1:G:113:PRO:CD   | 2.47                     | 0.41              |
| 1:G:127:ASP:O    | 1:G:128:VAL:HB   | 2.21                     | 0.41              |
| 1:G:183:GLU:HB3  | 1:H:180:ARG:HB3  | 2.03                     | 0.41              |
| 1:G:279:ASP:HA   | 1:G:314:MET:HB3  | 2.03                     | 0.41              |
| 1:H:61:ILE:HD11  | 1:H:103:SER:HB2  | 2.03                     | 0.41              |
| 1:H:273:SER:C    | 1:H:274:ASN:O    | 2.64                     | 0.41              |
| 1:A:142:ARG:O    | 1:A:146:VAL:HG23 | 2.21                     | 0.41              |
| 1:C:193:GLY:HA3  | 1:C:238:THR:CG2  | 2.50                     | 0.41              |
| 1:D:134:ILE:H    | 1:D:134:ILE:HD12 | 1.86                     | 0.41              |
| 1:E:50:THR:OG1   | 1:E:152:GLY:HA2  | 2.21                     | 0.41              |
| 1:F:249:ARG:HA   | 1:F:284:ASN:ND2  | 2.35                     | 0.41              |
| 1:H:128:VAL:O    | 1:H:129:ASN:HB3  | 2.21                     | 0.41              |
| 1:A:111:GLU:HG3  | 1:A:112:LYS:N    | 2.36                     | 0.40              |
| 1:B:193:GLY:HA3  | 1:B:238:THR:HG22 | 2.02                     | 0.40              |
| 1:B:194:LEU:HD13 | 1:B:196:PHE:CE1  | 2.56                     | 0.40              |
| 1:B:202:ASN:HB2  | 1:B:207:THR:O    | 2.21                     | 0.40              |
| 1:B:275:GLY:HA3  | 1:B:311:THR:OG1  | 2.21                     | 0.40              |
| 1:F:192:SER:O    | 1:F:238:THR:HB   | 2.20                     | 0.40              |
| 1:G:174:PHE:HE1  | 1:G:245:PHE:HZ   | 1.68                     | 0.40              |
| 1:G:319:ILE:CD1  | 1:G:336:TYR:HE1  | 2.34                     | 0.40              |
| 1:H:262:VAL:O    | 1:H:265:ALA:HB3  | 2.21                     | 0.40              |
| 1:A:257:TYR:CG   | 1:A:295:VAL:HG13 | 2.56                     | 0.40              |
| 1:B:107:ARG:HH11 | 1:B:314:MET:HE2  | 1.86                     | 0.40              |
| 1:C:79:HIS:NE2   | 1:C:334:LEU:HD23 | 2.36                     | 0.40              |
| 1:C:202:ASN:HB2  | 1:C:207:THR:O    | 2.21                     | 0.40              |
| 1:C:277:MET:HA   | 1:C:312:GLY:O    | 2.20                     | 0.40              |
| 1:G:72:ILE:HG12  | 1:G:277:MET:HE1  | 2.03                     | 0.40              |
| 1:H:94:LEU:HD11  | 1:H:351:GLU:HA   | 2.03                     | 0.40              |
| 1:A:50:THR:OG1   | 1:A:152:GLY:HA2  | 2.21                     | 0.40              |
| 1:A:353:VAL:O    | 1:A:357:LEU:HB2  | 2.21                     | 0.40              |
| 1:B:287:LYS:O    | 1:B:288:ASP:HB2  | 2.20                     | 0.40              |
| 1:B:352:ASP:O    | 1:B:354:LEU:N    | 2.54                     | 0.40              |
| 1:D:134:ILE:H    | 1:D:134:ILE:CD1  | 2.34                     | 0.40              |
| 1:D:292:GLN:HB2  | 1:D:293:PRO:HD3  | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:216:GLN:NE2  | 1:E:270:PRO:HG2  | 2.36                     | 0.40              |
| 1:E:366:GLU:O    | 1:E:367:VAL:C    | 2.65                     | 0.40              |
| 1:G:34:PRO:HD2   | 1:G:229:LYS:O    | 2.22                     | 0.40              |
| 1:A:114:ARG:NE   | 1:A:120:LYS:HE3  | 2.36                     | 0.40              |
| 1:B:232:VAL:HG21 | 1:C:232:VAL:CG2  | 2.50                     | 0.40              |
| 1:C:164:SER:N    | 1:C:165:PRO:CD   | 2.85                     | 0.40              |
| 1:C:249:ARG:O    | 1:C:283:GLY:CA   | 2.69                     | 0.40              |
| 1:D:262:VAL:HG21 | 1:D:310:ILE:HD11 | 2.03                     | 0.40              |
| 1:F:266:LYS:C    | 1:F:268:GLN:H    | 2.29                     | 0.40              |
| 1:G:73:VAL:HA    | 1:G:315:ILE:O    | 2.21                     | 0.40              |
| 1:H:34:PRO:HD2   | 1:H:229:LYS:O    | 2.21                     | 0.40              |
| 1:A:296:ASN:CG   | 1:A:353:VAL:HG13 | 2.46                     | 0.40              |
| 1:B:160:LEU:H    | 1:B:160:LEU:CD2  | 2.29                     | 0.40              |
| 1:D:89:LEU:HD13  | 1:D:89:LEU:HA    | 1.93                     | 0.40              |
| 1:D:97:GLU:OE1   | 1:D:355:ARG:NH1  | 2.41                     | 0.40              |
| 1:D:142:ARG:O    | 1:D:146:VAL:HG23 | 2.22                     | 0.40              |
| 1:G:301:GLU:O    | 1:G:301:GLU:HG2  | 2.21                     | 0.40              |
| 1:H:314:MET:HE3  | 1:H:314:MET:HB2  | 1.99                     | 0.40              |
| 1:H:323:ASN:HB3  | 1:H:343:ALA:HA   | 2.02                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | A     | 346/370 (94%) | 298 (86%) | 41 (12%) | 7 (2%)   | 6           | 16 |
| 1   | B     | 340/370 (92%) | 296 (87%) | 35 (10%) | 9 (3%)   | 4           | 11 |
| 1   | C     | 345/370 (93%) | 302 (88%) | 35 (10%) | 8 (2%)   | 5           | 13 |
| 1   | D     | 347/370 (94%) | 299 (86%) | 38 (11%) | 10 (3%)  | 3           | 9  |
| 1   | E     | 333/370 (90%) | 294 (88%) | 35 (10%) | 4 (1%)   | 10          | 27 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | F     | 341/370 (92%)   | 307 (90%)  | 32 (9%)   | 2 (1%)   | 21          | 44 |
| 1   | G     | 336/370 (91%)   | 287 (85%)  | 38 (11%)  | 11 (3%)  | 3           | 7  |
| 1   | H     | 343/370 (93%)   | 298 (87%)  | 34 (10%)  | 11 (3%)  | 3           | 7  |
| All | All   | 2731/2960 (92%) | 2381 (87%) | 288 (10%) | 62 (2%)  | 5           | 13 |

All (62) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 111 | GLU  |
| 1   | B     | 22  | ASP  |
| 1   | B     | 286 | ASN  |
| 1   | B     | 324 | GLN  |
| 1   | C     | 323 | ASN  |
| 1   | E     | 129 | ASN  |
| 1   | G     | 334 | LEU  |
| 1   | H     | 129 | ASN  |
| 1   | H     | 327 | PRO  |
| 1   | A     | 253 | LYS  |
| 1   | A     | 330 | GLY  |
| 1   | A     | 364 | ARG  |
| 1   | B     | 130 | ASN  |
| 1   | B     | 331 | LYS  |
| 1   | C     | 283 | GLY  |
| 1   | C     | 336 | TYR  |
| 1   | D     | 331 | LYS  |
| 1   | E     | 336 | TYR  |
| 1   | F     | 334 | LEU  |
| 1   | G     | 271 | ALA  |
| 1   | G     | 286 | ASN  |
| 1   | H     | 253 | LYS  |
| 1   | H     | 274 | ASN  |
| 1   | H     | 323 | ASN  |
| 1   | A     | 332 | ALA  |
| 1   | B     | 353 | VAL  |
| 1   | C     | 133 | ASN  |
| 1   | D     | 286 | ASN  |
| 1   | D     | 305 | ASN  |
| 1   | D     | 353 | VAL  |
| 1   | E     | 133 | ASN  |
| 1   | F     | 113 | PRO  |
| 1   | G     | 119 | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 133 | ASN  |
| 1   | G     | 266 | LYS  |
| 1   | G     | 360 | ALA  |
| 1   | H     | 113 | PRO  |
| 1   | B     | 256 | ASN  |
| 1   | C     | 113 | PRO  |
| 1   | C     | 119 | TRP  |
| 1   | C     | 128 | VAL  |
| 1   | C     | 341 | THR  |
| 1   | D     | 133 | ASN  |
| 1   | H     | 101 | ASP  |
| 1   | H     | 117 | VAL  |
| 1   | A     | 22  | ASP  |
| 1   | A     | 281 | SER  |
| 1   | D     | 352 | ASP  |
| 1   | D     | 367 | VAL  |
| 1   | G     | 287 | LYS  |
| 1   | B     | 367 | VAL  |
| 1   | E     | 128 | VAL  |
| 1   | G     | 126 | PRO  |
| 1   | G     | 128 | VAL  |
| 1   | G     | 134 | ILE  |
| 1   | D     | 112 | LYS  |
| 1   | H     | 118 | GLY  |
| 1   | B     | 113 | PRO  |
| 1   | D     | 113 | PRO  |
| 1   | H     | 128 | VAL  |
| 1   | H     | 275 | GLY  |
| 1   | D     | 275 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 280/298 (94%) | 263 (94%) | 17 (6%)  | 17          | 40 |
| 1   | B     | 279/298 (94%) | 264 (95%) | 15 (5%)  | 20          | 45 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | C     | 280/298 (94%)   | 265 (95%)  | 15 (5%)  | 20          | 45 |
| 1   | D     | 277/298 (93%)   | 265 (96%)  | 12 (4%)  | 26          | 54 |
| 1   | E     | 275/298 (92%)   | 257 (94%)  | 18 (6%)  | 15          | 37 |
| 1   | F     | 277/298 (93%)   | 259 (94%)  | 18 (6%)  | 15          | 37 |
| 1   | G     | 274/298 (92%)   | 254 (93%)  | 20 (7%)  | 13          | 32 |
| 1   | H     | 276/298 (93%)   | 264 (96%)  | 12 (4%)  | 26          | 54 |
| All | All   | 2218/2384 (93%) | 2091 (94%) | 127 (6%) | 18          | 43 |

All (127) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 37  | LEU  |
| 1   | A     | 107 | ARG  |
| 1   | A     | 120 | LYS  |
| 1   | A     | 124 | ASN  |
| 1   | A     | 128 | VAL  |
| 1   | A     | 129 | ASN  |
| 1   | A     | 131 | THR  |
| 1   | A     | 160 | LEU  |
| 1   | A     | 168 | LEU  |
| 1   | A     | 180 | ARG  |
| 1   | A     | 227 | VAL  |
| 1   | A     | 249 | ARG  |
| 1   | A     | 300 | CYS  |
| 1   | A     | 344 | CYS  |
| 1   | A     | 348 | GLU  |
| 1   | A     | 349 | THR  |
| 1   | A     | 357 | LEU  |
| 1   | B     | 37  | LEU  |
| 1   | B     | 101 | ASP  |
| 1   | B     | 110 | LEU  |
| 1   | B     | 112 | LYS  |
| 1   | B     | 130 | ASN  |
| 1   | B     | 134 | ILE  |
| 1   | B     | 160 | LEU  |
| 1   | B     | 168 | LEU  |
| 1   | B     | 227 | VAL  |
| 1   | B     | 249 | ARG  |
| 1   | B     | 301 | GLU  |
| 1   | B     | 311 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 331 | LYS  |
| 1   | B     | 341 | THR  |
| 1   | B     | 361 | VAL  |
| 1   | C     | 21  | GLU  |
| 1   | C     | 37  | LEU  |
| 1   | C     | 99  | LYS  |
| 1   | C     | 134 | ILE  |
| 1   | C     | 160 | LEU  |
| 1   | C     | 168 | LEU  |
| 1   | C     | 227 | VAL  |
| 1   | C     | 249 | ARG  |
| 1   | C     | 264 | GLU  |
| 1   | C     | 276 | LEU  |
| 1   | C     | 277 | MET  |
| 1   | C     | 341 | THR  |
| 1   | C     | 348 | GLU  |
| 1   | C     | 350 | THR  |
| 1   | C     | 369 | LYS  |
| 1   | D     | 22  | ASP  |
| 1   | D     | 37  | LEU  |
| 1   | D     | 110 | LEU  |
| 1   | D     | 160 | LEU  |
| 1   | D     | 168 | LEU  |
| 1   | D     | 227 | VAL  |
| 1   | D     | 249 | ARG  |
| 1   | D     | 264 | GLU  |
| 1   | D     | 266 | LYS  |
| 1   | D     | 301 | GLU  |
| 1   | D     | 341 | THR  |
| 1   | D     | 348 | GLU  |
| 1   | E     | 37  | LEU  |
| 1   | E     | 111 | GLU  |
| 1   | E     | 127 | ASP  |
| 1   | E     | 129 | ASN  |
| 1   | E     | 134 | ILE  |
| 1   | E     | 160 | LEU  |
| 1   | E     | 168 | LEU  |
| 1   | E     | 227 | VAL  |
| 1   | E     | 249 | ARG  |
| 1   | E     | 252 | LYS  |
| 1   | E     | 260 | LYS  |
| 1   | E     | 285 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 286 | ASN  |
| 1   | E     | 300 | CYS  |
| 1   | E     | 326 | ILE  |
| 1   | E     | 341 | THR  |
| 1   | E     | 349 | THR  |
| 1   | E     | 352 | ASP  |
| 1   | F     | 37  | LEU  |
| 1   | F     | 93  | LYS  |
| 1   | F     | 99  | LYS  |
| 1   | F     | 101 | ASP  |
| 1   | F     | 110 | LEU  |
| 1   | F     | 125 | ASP  |
| 1   | F     | 129 | ASN  |
| 1   | F     | 160 | LEU  |
| 1   | F     | 168 | LEU  |
| 1   | F     | 227 | VAL  |
| 1   | F     | 249 | ARG  |
| 1   | F     | 261 | SER  |
| 1   | F     | 262 | VAL  |
| 1   | F     | 339 | SER  |
| 1   | F     | 344 | CYS  |
| 1   | F     | 350 | THR  |
| 1   | F     | 357 | LEU  |
| 1   | F     | 363 | GLN  |
| 1   | G     | 37  | LEU  |
| 1   | G     | 93  | LYS  |
| 1   | G     | 102 | LEU  |
| 1   | G     | 110 | LEU  |
| 1   | G     | 111 | GLU  |
| 1   | G     | 129 | ASN  |
| 1   | G     | 160 | LEU  |
| 1   | G     | 168 | LEU  |
| 1   | G     | 227 | VAL  |
| 1   | G     | 249 | ARG  |
| 1   | G     | 257 | TYR  |
| 1   | G     | 289 | PHE  |
| 1   | G     | 291 | ASN  |
| 1   | G     | 294 | LYS  |
| 1   | G     | 307 | GLU  |
| 1   | G     | 317 | SER  |
| 1   | G     | 324 | GLN  |
| 1   | G     | 347 | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 353 | VAL  |
| 1   | G     | 355 | ARG  |
| 1   | H     | 37  | LEU  |
| 1   | H     | 113 | PRO  |
| 1   | H     | 114 | ARG  |
| 1   | H     | 116 | THR  |
| 1   | H     | 127 | ASP  |
| 1   | H     | 160 | LEU  |
| 1   | H     | 168 | LEU  |
| 1   | H     | 227 | VAL  |
| 1   | H     | 249 | ARG  |
| 1   | H     | 294 | LYS  |
| 1   | H     | 313 | VAL  |
| 1   | H     | 319 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 40  | GLN  |
| 1   | A     | 129 | ASN  |
| 1   | A     | 143 | GLN  |
| 1   | A     | 147 | ASN  |
| 1   | A     | 216 | GLN  |
| 1   | A     | 282 | HIS  |
| 1   | A     | 324 | GLN  |
| 1   | B     | 40  | GLN  |
| 1   | B     | 133 | ASN  |
| 1   | B     | 139 | GLN  |
| 1   | B     | 143 | GLN  |
| 1   | B     | 147 | ASN  |
| 1   | B     | 150 | ASN  |
| 1   | B     | 243 | HIS  |
| 1   | B     | 268 | GLN  |
| 1   | B     | 324 | GLN  |
| 1   | B     | 363 | GLN  |
| 1   | B     | 368 | ASN  |
| 1   | C     | 40  | GLN  |
| 1   | C     | 124 | ASN  |
| 1   | C     | 143 | GLN  |
| 1   | C     | 147 | ASN  |
| 1   | C     | 216 | GLN  |
| 1   | C     | 286 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 296 | ASN  |
| 1   | C     | 318 | ASN  |
| 1   | D     | 40  | GLN  |
| 1   | D     | 124 | ASN  |
| 1   | D     | 129 | ASN  |
| 1   | D     | 139 | GLN  |
| 1   | D     | 143 | GLN  |
| 1   | D     | 147 | ASN  |
| 1   | D     | 216 | GLN  |
| 1   | D     | 268 | GLN  |
| 1   | D     | 320 | ASN  |
| 1   | D     | 363 | GLN  |
| 1   | D     | 368 | ASN  |
| 1   | E     | 40  | GLN  |
| 1   | E     | 129 | ASN  |
| 1   | E     | 133 | ASN  |
| 1   | E     | 143 | GLN  |
| 1   | E     | 147 | ASN  |
| 1   | E     | 216 | GLN  |
| 1   | E     | 286 | ASN  |
| 1   | E     | 291 | ASN  |
| 1   | E     | 296 | ASN  |
| 1   | E     | 320 | ASN  |
| 1   | E     | 324 | GLN  |
| 1   | F     | 40  | GLN  |
| 1   | F     | 129 | ASN  |
| 1   | F     | 139 | GLN  |
| 1   | F     | 143 | GLN  |
| 1   | F     | 147 | ASN  |
| 1   | F     | 216 | GLN  |
| 1   | F     | 296 | ASN  |
| 1   | F     | 302 | GLN  |
| 1   | F     | 305 | ASN  |
| 1   | F     | 320 | ASN  |
| 1   | G     | 40  | GLN  |
| 1   | G     | 124 | ASN  |
| 1   | G     | 129 | ASN  |
| 1   | G     | 143 | GLN  |
| 1   | G     | 147 | ASN  |
| 1   | G     | 216 | GLN  |
| 1   | G     | 268 | GLN  |
| 1   | G     | 286 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 291 | ASN  |
| 1   | G     | 292 | GLN  |
| 1   | G     | 296 | ASN  |
| 1   | H     | 40  | GLN  |
| 1   | H     | 143 | GLN  |
| 1   | H     | 147 | ASN  |
| 1   | H     | 216 | GLN  |
| 1   | H     | 230 | HIS  |
| 1   | H     | 291 | ASN  |
| 1   | H     | 292 | GLN  |
| 1   | H     | 305 | ASN  |
| 1   | H     | 308 | ASN  |
| 1   | H     | 318 | ASN  |
| 1   | H     | 363 | GLN  |

### 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](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | PHE  | G     | 1002 | -    | 11,12,12     | 0.74 | 0        | 11,15,15    | 0.31 | 0        |
| 3   | PHE  | H     | 1002 | -    | 11,12,12     | 0.68 | 0        | 11,15,15    | 0.32 | 0        |
| 3   | PHE  | C     | 1002 | -    | 11,12,12     | 0.75 | 0        | 11,15,15    | 0.34 | 0        |
| 3   | PHE  | D     | 1002 | -    | 11,12,12     | 0.84 | 0        | 11,15,15    | 0.28 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 3   | PHE  | G     | 1002 | -    | -       | 4/8/8/8  | 0/1/1/1 |
| 3   | PHE  | H     | 1002 | -    | -       | 2/8/8/8  | 0/1/1/1 |
| 3   | PHE  | C     | 1002 | -    | -       | 3/8/8/8  | 0/1/1/1 |
| 3   | PHE  | D     | 1002 | -    | -       | 2/8/8/8  | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 3   | G     | 1002 | PHE  | OXT-C-CA-N   |
| 3   | D     | 1002 | PHE  | OXT-C-CA-N   |
| 3   | G     | 1002 | PHE  | O-C-CA-CB    |
| 3   | H     | 1002 | PHE  | OXT-C-CA-N   |
| 3   | G     | 1002 | PHE  | OXT-C-CA-CB  |
| 3   | D     | 1002 | PHE  | O-C-CA-N     |
| 3   | C     | 1002 | PHE  | CA-CB-CG-CD2 |
| 3   | C     | 1002 | PHE  | CA-CB-CG-CD1 |
| 3   | C     | 1002 | PHE  | C-CA-CB-CG   |
| 3   | G     | 1002 | PHE  | O-C-CA-N     |
| 3   | H     | 1002 | PHE  | O-C-CA-N     |

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | G     | 1002 | PHE  | 1       | 0            |
| 3   | H     | 1002 | PHE  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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.