



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:10 AM UTC

PDB ID : 2R4L / pdb\_00002r4l  
Title : Crystal structure of the long-chain fatty acid transporter FadL mutant P34A  
Authors : Hearn, E.M.; Patel, D.R.; Lepore, B.W.; Indic, M.; van den Berg, B.  
Deposited on : 2007-08-31  
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

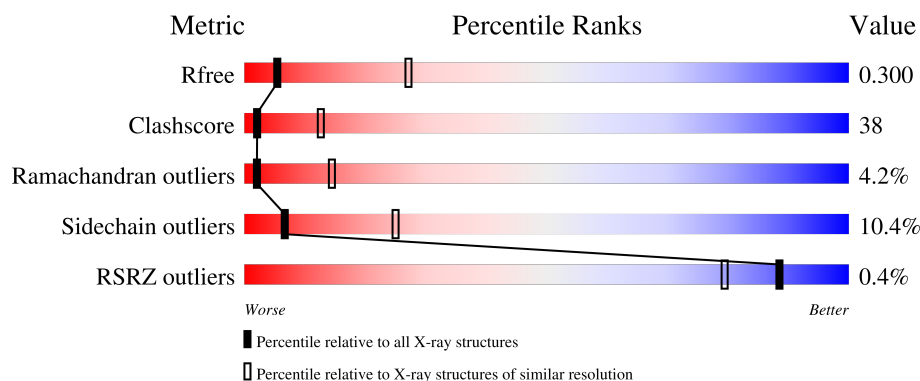
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1169 (3.32-3.28)                                      |
| Clashscore            | 190562                      | 1209 (3.32-3.28)                                      |
| Ramachandran outliers | 187476                      | 1188 (3.32-3.28)                                      |
| Sidechain outliers    | 187428                      | 1187 (3.32-3.28)                                      |
| RSRZ outliers         | 180081                      | 1169 (3.32-3.28)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 427    | <div> <div>46%</div> <div>42%</div> <div>8%</div> <div>.</div> </div>                |
| 1   | B     | 427    | <div> <div>41%</div> <div>45%</div> <div>11%</div> <div>..</div> </div>              |
| 1   | C     | 427    | <div> <div>%</div> <div>40%</div> <div>46%</div> <div>10%</div> <div>..</div> </div> |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | LDA  | A     | 506 | -         | -        | X       | -                |
| 2   | LDA  | B     | 503 | -         | -        | X       | -                |
| 2   | LDA  | C     | 501 | -         | -        | X       | -                |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9740 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 Long-chain fatty acid transport protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 412      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3184  | 2016 | 539 | 623 | 6 |         |         |       |
| 1   | B     | 421      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3249  | 2053 | 552 | 638 | 6 |         |         |       |
| 1   | C     | 416      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3211  | 2032 | 544 | 629 | 6 |         |         |       |

There are 24 discrepancies between the modelled and reference sequences:

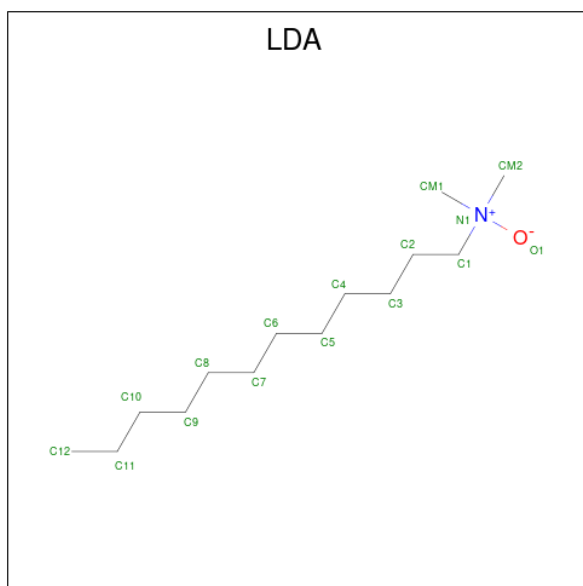
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 34      | ALA      | PRO    | engineered mutation | UNP P10384 |
| A     | 197     | THR      | ILE    | conflict            | UNP P10384 |
| A     | 422     | HIS      | -      | expression tag      | UNP P10384 |
| A     | 423     | HIS      | -      | expression tag      | UNP P10384 |
| A     | 424     | HIS      | -      | expression tag      | UNP P10384 |
| A     | 425     | HIS      | -      | expression tag      | UNP P10384 |
| A     | 426     | HIS      | -      | expression tag      | UNP P10384 |
| A     | 427     | HIS      | -      | expression tag      | UNP P10384 |
| B     | 34      | ALA      | PRO    | engineered mutation | UNP P10384 |
| B     | 197     | THR      | ILE    | conflict            | UNP P10384 |
| B     | 422     | HIS      | -      | expression tag      | UNP P10384 |
| B     | 423     | HIS      | -      | expression tag      | UNP P10384 |
| B     | 424     | HIS      | -      | expression tag      | UNP P10384 |
| B     | 425     | HIS      | -      | expression tag      | UNP P10384 |
| B     | 426     | HIS      | -      | expression tag      | UNP P10384 |
| B     | 427     | HIS      | -      | expression tag      | UNP P10384 |
| C     | 34      | ALA      | PRO    | engineered mutation | UNP P10384 |
| C     | 197     | THR      | ILE    | conflict            | UNP P10384 |
| C     | 422     | HIS      | -      | expression tag      | UNP P10384 |
| C     | 423     | HIS      | -      | expression tag      | UNP P10384 |
| C     | 424     | HIS      | -      | expression tag      | UNP P10384 |
| C     | 425     | HIS      | -      | expression tag      | UNP P10384 |
| C     | 426     | HIS      | -      | expression tag      | UNP P10384 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 427     | HIS      | -      | expression tag | UNP P10384 |

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula:  $C_{14}H_{31}NO$ ).

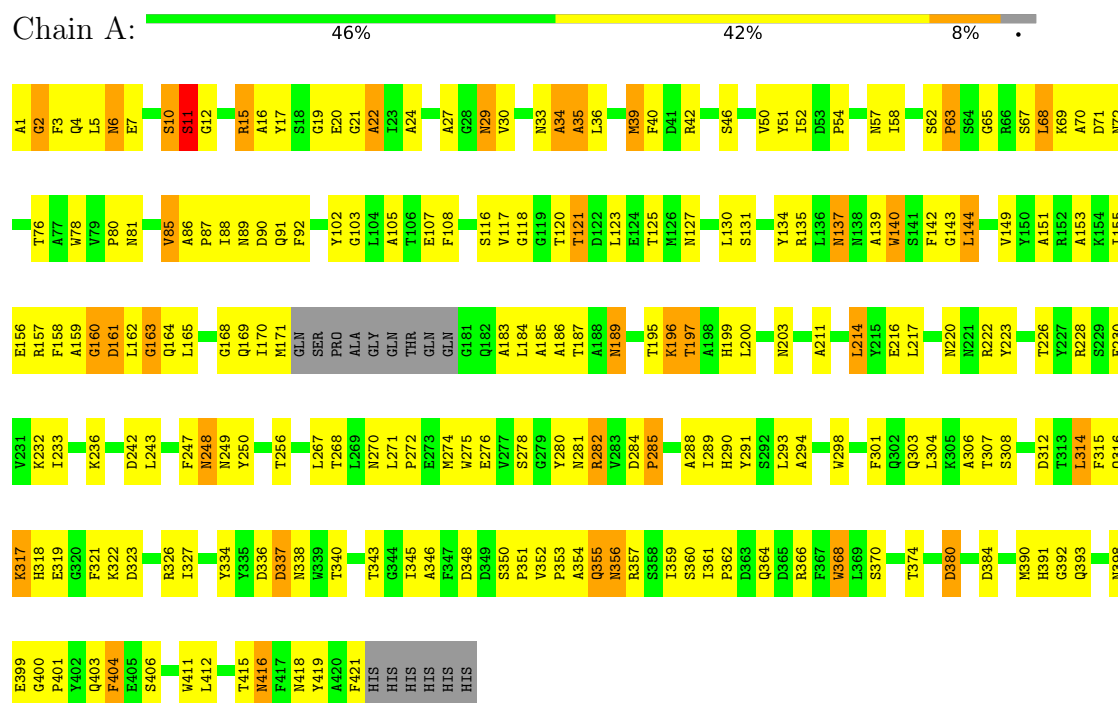


| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 2   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 2   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 2   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 2   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 2   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |

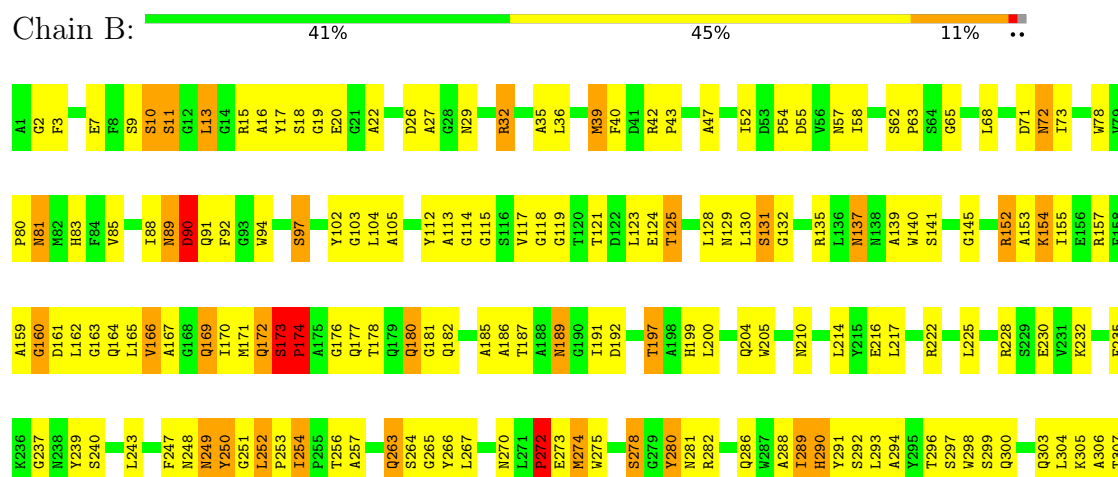
### 3 Residue-property plots

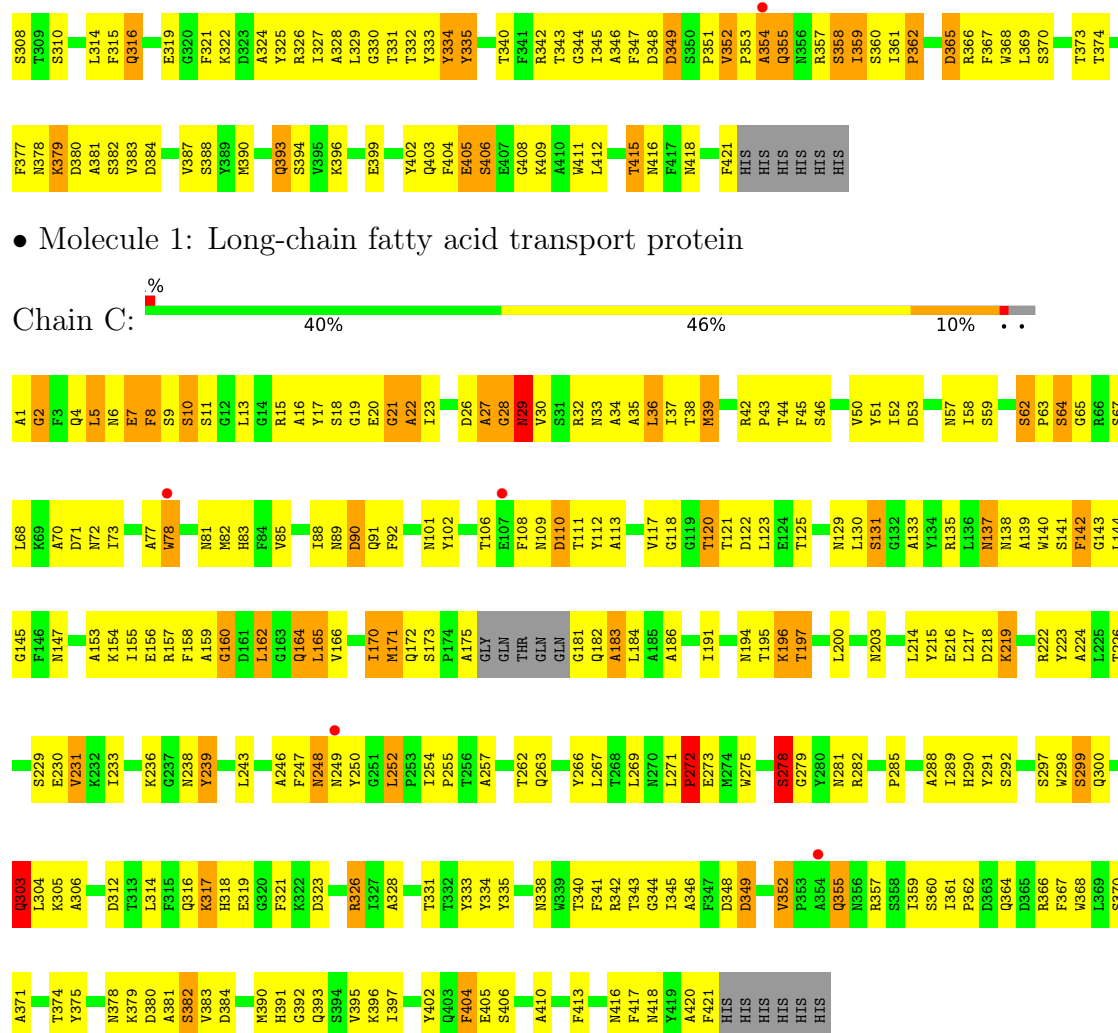
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Long-chain fatty acid transport protein



#### • Molecule 1: Long-chain fatty acid transport protein





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 112.80Å 167.04Å 197.40Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 10.00 – 3.30<br>10.00 – 3.30                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.2 (10.00-3.30)<br>91.4 (10.00-3.30)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.16                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.92 (at 3.33Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.234 , 0.302<br>0.240 , 0.300                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2721 reflections (9.54%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 49.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.683                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.38 , 46.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.88                                                        | EDS              |
| Total number of atoms                                                   | 9740                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 24.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.59         | 0/3270      | 1.08        | 19/4450 (0.4%)  |
| 1   | B     | 0.56         | 0/3337      | 1.09        | 19/4543 (0.4%)  |
| 1   | C     | 0.55         | 0/3298      | 1.12        | 30/4489 (0.7%)  |
| All | All   | 0.57         | 0/9905      | 1.10        | 68/13482 (0.5%) |

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

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

There are no bond length outliers.

All (68) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | B     | 173 | SER  | CA-C-N | 14.19  | 137.58      | 119.84   |
| 1   | B     | 173 | SER  | C-N-CA | 14.19  | 137.58      | 119.84   |
| 1   | C     | 88  | ILE  | N-CA-C | -12.79 | 100.56      | 111.56   |
| 1   | C     | 352 | VAL  | N-CA-C | 10.38  | 117.01      | 107.56   |
| 1   | C     | 170 | ILE  | N-CA-C | -9.60  | 103.99      | 113.20   |
| 1   | B     | 299 | SER  | N-CA-C | -9.54  | 100.96      | 111.36   |
| 1   | C     | 172 | GLN  | N-CA-C | -9.45  | 101.88      | 113.97   |
| 1   | C     | 395 | VAL  | N-CA-C | 8.88   | 121.59      | 108.45   |
| 1   | A     | 161 | ASP  | N-CA-C | -8.65  | 99.52       | 113.19   |
| 1   | B     | 29  | ASN  | N-CA-C | 8.54   | 123.93      | 113.17   |
| 1   | B     | 11  | SER  | N-CA-C | -8.45  | 102.03      | 111.07   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 248 | ASN  | N-CA-C | 8.43  | 120.64      | 110.19   |
| 1   | B     | 186 | ALA  | N-CA-C | -8.31 | 103.59      | 114.31   |
| 1   | C     | 8   | PHE  | N-CA-C | -8.14 | 103.37      | 113.38   |
| 1   | A     | 189 | ASN  | N-CA-C | -7.96 | 103.37      | 113.72   |
| 1   | A     | 230 | GLU  | N-CA-C | -7.79 | 100.48      | 110.53   |
| 1   | A     | 35  | ALA  | N-CA-C | -7.75 | 103.96      | 113.41   |
| 1   | A     | 271 | LEU  | CA-C-N | 7.68  | 129.44      | 119.84   |
| 1   | A     | 271 | LEU  | C-N-CA | 7.68  | 129.44      | 119.84   |
| 1   | C     | 299 | SER  | N-CA-C | -7.61 | 102.12      | 111.33   |
| 1   | B     | 349 | ASP  | N-CA-C | 7.51  | 120.00      | 110.24   |
| 1   | C     | 183 | ALA  | N-CA-C | -7.36 | 103.26      | 112.90   |
| 1   | C     | 10  | SER  | N-CA-C | -7.04 | 103.03      | 111.69   |
| 1   | A     | 356 | ASN  | N-CA-C | -6.95 | 105.99      | 114.75   |
| 1   | A     | 10  | SER  | N-CA-C | -6.58 | 104.51      | 112.54   |
| 1   | A     | 29  | ASN  | N-CA-C | 6.55  | 121.36      | 113.23   |
| 1   | C     | 22  | ALA  | N-CA-C | -6.33 | 105.86      | 113.97   |
| 1   | A     | 107 | GLU  | N-CA-C | 6.11  | 119.97      | 107.69   |
| 1   | B     | 230 | GLU  | N-CA-C | -6.09 | 102.06      | 110.35   |
| 1   | C     | 252 | LEU  | CA-C-N | 6.05  | 127.40      | 119.84   |
| 1   | C     | 252 | LEU  | C-N-CA | 6.05  | 127.40      | 119.84   |
| 1   | B     | 131 | SER  | N-CA-C | 6.04  | 117.96      | 108.96   |
| 1   | A     | 183 | ALA  | N-CA-C | -6.00 | 105.22      | 112.54   |
| 1   | C     | 248 | ASN  | N-CA-C | 5.97  | 119.36      | 110.52   |
| 1   | C     | 379 | LYS  | N-CA-C | -5.90 | 106.70      | 114.31   |
| 1   | B     | 394 | SER  | N-CA-C | -5.90 | 101.55      | 110.28   |
| 1   | B     | 174 | PRO  | N-CA-C | 5.83  | 124.49      | 112.47   |
| 1   | C     | 397 | ILE  | N-CA-C | 5.81  | 115.96      | 106.72   |
| 1   | A     | 368 | TRP  | N-CA-C | 5.79  | 117.95      | 108.52   |
| 1   | C     | 21  | GLY  | N-CA-C | -5.78 | 107.41      | 114.92   |
| 1   | B     | 35  | ALA  | N-CA-C | -5.70 | 105.43      | 112.90   |
| 1   | C     | 131 | SER  | N-CA-C | 5.70  | 117.93      | 108.99   |
| 1   | C     | 53  | ASP  | CA-C-N | 5.65  | 126.12      | 120.14   |
| 1   | C     | 53  | ASP  | C-N-CA | 5.65  | 126.12      | 120.14   |
| 1   | B     | 352 | VAL  | CA-C-N | 5.51  | 125.27      | 119.76   |
| 1   | B     | 352 | VAL  | C-N-CA | 5.51  | 125.27      | 119.76   |
| 1   | C     | 29  | ASN  | N-CA-C | 5.49  | 122.50      | 110.80   |
| 1   | C     | 186 | ALA  | N-CA-C | -5.49 | 106.58      | 113.28   |
| 1   | A     | 184 | LEU  | N-CA-C | -5.42 | 105.93      | 112.54   |
| 1   | C     | 67  | SER  | N-CA-C | 5.39  | 118.72      | 110.20   |
| 1   | B     | 180 | GLN  | N-CA-C | -5.38 | 106.65      | 113.43   |
| 1   | C     | 249 | ASN  | N-CA-C | 5.38  | 119.01      | 111.90   |
| 1   | A     | 11  | SER  | N-CA-C | -5.37 | 105.32      | 111.07   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 13  | LEU  | N-CA-C | -5.32 | 105.59      | 111.71   |
| 1   | B     | 316 | GLN  | N-CA-C | 5.30  | 116.98      | 107.80   |
| 1   | A     | 22  | ALA  | N-CA-C | -5.30 | 107.48      | 114.31   |
| 1   | C     | 303 | GLN  | N-CA-C | 5.27  | 116.15      | 108.14   |
| 1   | C     | 184 | LEU  | N-CA-C | -5.25 | 106.94      | 113.19   |
| 1   | C     | 64  | SER  | N-CA-C | -5.22 | 106.17      | 112.54   |
| 1   | B     | 119 | GLY  | N-CA-C | -5.18 | 100.89      | 113.18   |
| 1   | A     | 68  | LEU  | N-CA-C | -5.16 | 104.60      | 111.87   |
| 1   | B     | 278 | SER  | N-CA-C | 5.14  | 116.66      | 108.79   |
| 1   | C     | 278 | SER  | N-CA-C | 5.14  | 116.33      | 108.52   |
| 1   | A     | 88  | ILE  | N-CA-C | -5.14 | 107.39      | 111.81   |
| 1   | C     | 36  | LEU  | N-CA-C | -5.14 | 107.08      | 113.19   |
| 1   | C     | 62  | SER  | N-CA-C | 5.06  | 117.28      | 110.29   |
| 1   | A     | 228 | ARG  | N-CA-C | -5.05 | 100.18      | 108.41   |
| 1   | C     | 162 | LEU  | N-CA-C | -5.01 | 106.01      | 111.82   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 291 | TYR  | Sidechain |
| 1   | C     | 239 | TYR  | Sidechain |

## 5.2 Too-close contacts [i](#)

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     | 3184  | 0        | 2967     | 208     | 0            |
| 1   | B     | 3249  | 0        | 3027     | 233     | 0            |
| 1   | C     | 3211  | 0        | 2992     | 272     | 0            |
| 2   | A     | 32    | 0        | 62       | 19      | 0            |
| 2   | B     | 32    | 0        | 62       | 11      | 0            |
| 2   | C     | 32    | 0        | 62       | 19      | 0            |
| All | All   | 9740  | 0        | 9172     | 711     | 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 38.

All (711) 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:34:ALA:O     | 1:C:143:GLY:HA3  | 1.46                     | 1.15              |
| 1:C:361:ILE:HD11 | 2:C:501:LDA:H22  | 1.22                     | 1.10              |
| 1:C:58:ILE:HB    | 1:C:70:ALA:HB3   | 1.39                     | 1.05              |
| 1:B:346:ALA:HB3  | 1:B:368:TRP:HB2  | 1.40                     | 1.03              |
| 1:B:252:LEU:HB3  | 1:B:254:ILE:HG12 | 1.41                     | 1.00              |
| 1:B:382:SER:HB3  | 1:B:418:ASN:HB2  | 1.45                     | 0.96              |
| 1:C:64:SER:HB3   | 1:C:165:LEU:HD21 | 1.49                     | 0.94              |
| 1:C:10:SER:H     | 1:C:416:ASN:HD22 | 1.18                     | 0.92              |
| 1:A:293:LEU:HD13 | 1:A:327:ILE:HG12 | 1.49                     | 0.92              |
| 1:A:10:SER:OG    | 1:A:416:ASN:HB2  | 1.70                     | 0.91              |
| 1:C:21:GLY:HA2   | 1:C:36:LEU:HD11  | 1.50                     | 0.90              |
| 1:C:10:SER:H     | 1:C:416:ASN:ND2  | 1.68                     | 0.90              |
| 1:A:21:GLY:H     | 1:A:29:ASN:HD22  | 1.17                     | 0.89              |
| 1:A:117:VAL:HG23 | 1:A:359:ILE:HD11 | 1.55                     | 0.88              |
| 1:B:293:LEU:HD13 | 1:B:327:ILE:CD1  | 2.04                     | 0.87              |
| 1:C:368:TRP:HZ2  | 2:C:502:LDA:HM23 | 1.39                     | 0.87              |
| 1:C:303:GLN:HE22 | 1:C:316:GLN:HE21 | 1.22                     | 0.87              |
| 1:B:63:PRO:HA    | 1:C:138:ASN:OD1  | 1.74                     | 0.87              |
| 1:B:293:LEU:HD13 | 1:B:327:ILE:HD11 | 1.58                     | 0.86              |
| 1:C:278:SER:HB3  | 1:C:292:SER:HB3  | 1.56                     | 0.85              |
| 1:A:319:GLU:OE2  | 2:A:506:LDA:HM22 | 1.76                     | 0.85              |
| 1:C:346:ALA:HB3  | 1:C:368:TRP:HB2  | 1.58                     | 0.84              |
| 1:A:102:TYR:O    | 1:A:125:THR:HB   | 1.78                     | 0.83              |
| 1:A:354:ALA:O    | 1:A:355:GLN:HB2  | 1.78                     | 0.82              |
| 1:A:343:THR:HG23 | 1:A:370:SER:O    | 1.80                     | 0.82              |
| 1:A:267:LEU:HD23 | 1:A:268:THR:N    | 1.95                     | 0.81              |
| 1:C:390:MET:HG3  | 1:C:410:ALA:HB3  | 1.60                     | 0.81              |
| 1:A:4:GLN:C      | 1:A:5:LEU:HD12   | 2.06                     | 0.80              |
| 1:B:319:GLU:OE1  | 2:B:503:LDA:HM21 | 1.82                     | 0.80              |
| 1:C:361:ILE:HD11 | 2:C:501:LDA:C2   | 2.10                     | 0.80              |
| 1:C:38:THR:HG21  | 1:C:141:SER:OG   | 1.81                     | 0.79              |
| 1:C:110:ASP:O    | 1:C:194:ASN:HB3  | 1.82                     | 0.79              |
| 1:C:390:MET:HE1  | 2:C:502:LDA:HM22 | 1.62                     | 0.79              |
| 1:C:21:GLY:H     | 1:C:29:ASN:HD22  | 1.27                     | 0.79              |
| 1:C:131:SER:HB3  | 1:C:145:GLY:HA3  | 1.63                     | 0.79              |
| 1:C:27:ALA:HB2   | 1:C:44:THR:HG22  | 1.63                     | 0.79              |
| 1:A:89:ASN:ND2   | 1:A:90:ASP:H     | 1.81                     | 0.79              |
| 1:B:199:HIS:C    | 1:B:200:LEU:HD12 | 2.08                     | 0.78              |
| 1:B:306:ALA:HB3  | 1:B:315:PHE:HB3  | 1.63                     | 0.78              |
| 1:A:196:LYS:HB2  | 1:A:242:ASP:OD2  | 1.84                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:164:GLN:HG3  | 1:A:189:ASN:ND2  | 1.99                     | 0.78              |
| 1:A:39:MET:HE1   | 1:A:216:GLU:OE2  | 1.84                     | 0.78              |
| 1:B:102:TYR:O    | 1:B:125:THR:HB   | 1.85                     | 0.77              |
| 1:C:137:ASN:HD22 | 1:C:137:ASN:C    | 1.92                     | 0.77              |
| 1:C:281:ASN:HB2  | 1:C:289:ILE:HG23 | 1.66                     | 0.76              |
| 1:A:153:ALA:CB   | 2:A:506:LDA:H91  | 2.16                     | 0.76              |
| 1:B:65:GLY:C     | 1:C:91:GLN:HE21  | 1.94                     | 0.75              |
| 1:C:157:ARG:HH12 | 2:C:501:LDA:HM22 | 1.51                     | 0.75              |
| 1:B:62:SER:HB2   | 1:B:68:LEU:HD21  | 1.67                     | 0.75              |
| 1:B:131:SER:HB3  | 1:B:145:GLY:HA2  | 1.69                     | 0.75              |
| 1:A:200:LEU:HB3  | 2:A:506:LDA:H123 | 1.67                     | 0.74              |
| 1:A:303:GLN:HE22 | 1:A:316:GLN:HE21 | 1.33                     | 0.74              |
| 1:A:168:GLY:O    | 1:A:171:MET:HG2  | 1.88                     | 0.74              |
| 1:C:137:ASN:HD21 | 1:C:140:TRP:H    | 1.34                     | 0.73              |
| 1:A:276:GLU:HG3  | 1:A:294:ALA:HB2  | 1.70                     | 0.73              |
| 1:C:137:ASN:HD21 | 1:C:140:TRP:N    | 1.86                     | 0.73              |
| 1:C:164:GLN:O    | 1:C:166:VAL:N    | 2.20                     | 0.73              |
| 1:C:131:SER:HB3  | 1:C:145:GLY:CA   | 2.18                     | 0.73              |
| 1:C:278:SER:HB3  | 1:C:292:SER:CB   | 2.19                     | 0.72              |
| 1:B:154:LYS:HA   | 1:B:200:LEU:O    | 1.88                     | 0.72              |
| 1:C:281:ASN:ND2  | 1:C:291:TYR:HE2  | 1.88                     | 0.72              |
| 1:B:19:GLY:H     | 1:B:292:SER:HB3  | 1.55                     | 0.72              |
| 1:C:338:ASN:HB3  | 1:C:375:TYR:HE1  | 1.55                     | 0.72              |
| 1:B:273:GLU:H    | 1:B:300:GLN:NE2  | 1.88                     | 0.72              |
| 1:B:42:ARG:HD2   | 1:B:421:PHE:O    | 1.91                     | 0.71              |
| 1:C:102:TYR:O    | 1:C:125:THR:HB   | 1.89                     | 0.71              |
| 1:C:254:ILE:HG13 | 1:C:255:PRO:HD2  | 1.72                     | 0.71              |
| 1:B:396:LYS:H    | 1:B:396:LYS:HD2  | 1.56                     | 0.70              |
| 1:B:396:LYS:HD2  | 1:B:396:LYS:N    | 2.06                     | 0.70              |
| 1:B:393:GLN:HA   | 1:B:393:GLN:HE21 | 1.55                     | 0.70              |
| 1:A:17:TYR:HA    | 1:A:20:GLU:OE1   | 1.90                     | 0.70              |
| 1:A:39:MET:HE1   | 1:A:216:GLU:CD   | 2.16                     | 0.70              |
| 1:A:5:LEU:HA     | 2:A:505:LDA:HM13 | 1.72                     | 0.70              |
| 1:C:5:LEU:HD22   | 1:C:6:ASN:H      | 1.57                     | 0.70              |
| 1:A:364:GLN:HG3  | 1:A:393:GLN:O    | 1.91                     | 0.69              |
| 1:B:346:ALA:HB3  | 1:B:368:TRP:CB   | 2.20                     | 0.69              |
| 1:C:20:GLU:OE2   | 1:C:20:GLU:HA    | 1.92                     | 0.69              |
| 1:A:232:LYS:HE2  | 1:A:270:ASN:ND2  | 2.07                     | 0.69              |
| 1:B:303:GLN:HE22 | 1:B:316:GLN:NE2  | 1.90                     | 0.69              |
| 1:C:21:GLY:CA    | 1:C:36:LEU:HD11  | 2.20                     | 0.69              |
| 1:A:67:SER:C     | 1:A:68:LEU:HD23  | 2.18                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:352:VAL:HG11 | 1:A:357:ARG:HA   | 1.75                     | 0.69              |
| 1:A:415:THR:HG22 | 1:A:416:ASN:H    | 1.57                     | 0.68              |
| 1:B:178:THR:HG22 | 1:B:180:GLN:H    | 1.56                     | 0.68              |
| 1:C:374:THR:HG23 | 1:C:384:ASP:OD2  | 1.94                     | 0.68              |
| 1:B:378:ASN:O    | 1:B:379:LYS:HB2  | 1.94                     | 0.68              |
| 1:C:52:ILE:HG21  | 2:C:502:LDA:H52  | 1.76                     | 0.68              |
| 1:C:393:GLN:HE21 | 1:C:393:GLN:HA   | 1.58                     | 0.68              |
| 1:C:27:ALA:O     | 1:C:30:VAL:HG22  | 1.94                     | 0.67              |
| 1:C:7:GLU:HG2    | 1:C:50:VAL:HG11  | 1.76                     | 0.67              |
| 1:B:131:SER:HB3  | 1:B:145:GLY:CA   | 2.24                     | 0.67              |
| 1:C:137:ASN:C    | 1:C:137:ASN:ND2  | 2.52                     | 0.67              |
| 1:C:303:GLN:HE22 | 1:C:316:GLN:NE2  | 1.92                     | 0.66              |
| 1:B:135:ARG:HG3  | 1:B:137:ASN:O    | 1.95                     | 0.66              |
| 1:A:360:SER:C    | 1:A:362:PRO:HD3  | 2.20                     | 0.66              |
| 1:C:338:ASN:HB3  | 1:C:375:TYR:CE1  | 2.31                     | 0.66              |
| 1:C:281:ASN:HB2  | 1:C:289:ILE:CG2  | 2.26                     | 0.66              |
| 1:A:33:ASN:HB2   | 1:A:226:THR:HG21 | 1.78                     | 0.66              |
| 1:C:39:MET:HE1   | 1:C:216:GLU:OE1  | 1.96                     | 0.66              |
| 1:C:159:ALA:O    | 1:C:160:GLY:C    | 2.38                     | 0.65              |
| 1:B:17:TYR:HA    | 1:B:20:GLU:OE1   | 1.96                     | 0.65              |
| 1:B:272:PRO:HA   | 1:B:300:GLN:HE21 | 1.59                     | 0.65              |
| 1:A:89:ASN:HD22  | 1:A:90:ASP:H     | 1.44                     | 0.65              |
| 1:B:199:HIS:O    | 1:B:200:LEU:HD12 | 1.96                     | 0.65              |
| 1:B:306:ALA:O    | 1:B:314:LEU:HB2  | 1.97                     | 0.65              |
| 1:C:7:GLU:HA     | 1:C:17:TYR:OH    | 1.96                     | 0.65              |
| 1:A:326:ARG:HG3  | 1:A:348:ASP:HB3  | 1.76                     | 0.65              |
| 1:B:10:SER:HB3   | 1:B:416:ASN:ND2  | 2.12                     | 0.65              |
| 1:B:68:LEU:HD13  | 1:B:404:PHE:CE2  | 2.32                     | 0.65              |
| 1:C:305:LYS:HD2  | 1:C:316:GLN:NE2  | 2.12                     | 0.65              |
| 1:B:137:ASN:HD21 | 1:B:140:TRP:H    | 1.44                     | 0.65              |
| 1:B:170:ILE:HG21 | 1:B:185:ALA:HB2  | 1.79                     | 0.65              |
| 1:C:346:ALA:HB3  | 1:C:368:TRP:CB   | 2.28                     | 0.64              |
| 1:B:358:SER:HB2  | 1:B:399:GLU:CD   | 2.22                     | 0.64              |
| 1:C:173:SER:O    | 1:C:175:ALA:N    | 2.31                     | 0.64              |
| 1:C:110:ASP:O    | 1:C:194:ASN:CB   | 2.45                     | 0.64              |
| 1:B:237:GLY:O    | 1:B:265:GLY:N    | 2.30                     | 0.63              |
| 1:C:157:ARG:HB2  | 1:C:197:THR:HG22 | 1.80                     | 0.63              |
| 1:C:380:ASP:HA   | 1:C:420:ALA:HB3  | 1.81                     | 0.63              |
| 1:A:7:GLU:OE1    | 1:A:7:GLU:N      | 2.32                     | 0.63              |
| 1:A:284:ASP:OD1  | 1:A:285:PRO:HD2  | 1.98                     | 0.63              |
| 1:A:355:GLN:C    | 1:A:356:ASN:HD22 | 2.06                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:6:ASN:O      | 1:C:7:GLU:HB2    | 1.98                     | 0.63              |
| 1:B:52:ILE:O     | 1:B:54:PRO:HD3   | 1.99                     | 0.62              |
| 1:B:293:LEU:HD13 | 1:B:327:ILE:HD13 | 1.80                     | 0.62              |
| 1:C:238:ASN:HD22 | 1:C:262:THR:HG21 | 1.63                     | 0.62              |
| 1:C:396:LYS:H    | 1:C:396:LYS:HD2  | 1.65                     | 0.62              |
| 1:C:321:PHE:CE2  | 1:C:352:VAL:HG22 | 2.34                     | 0.62              |
| 1:A:33:ASN:C     | 1:A:35:ALA:H     | 2.08                     | 0.62              |
| 1:A:303:GLN:HE22 | 1:A:316:GLN:NE2  | 1.95                     | 0.62              |
| 1:C:35:ALA:C     | 1:C:37:ILE:H     | 2.07                     | 0.62              |
| 1:B:137:ASN:ND2  | 1:B:139:ALA:H    | 1.96                     | 0.62              |
| 1:A:42:ARG:HD2   | 1:A:421:PHE:O    | 1.99                     | 0.62              |
| 1:A:415:THR:HG22 | 1:A:416:ASN:N    | 2.13                     | 0.62              |
| 1:B:32:ARG:HG2   | 1:B:32:ARG:HH11  | 1.65                     | 0.62              |
| 1:C:10:SER:N     | 1:C:416:ASN:HD22 | 1.94                     | 0.61              |
| 1:C:106:THR:HG21 | 1:C:360:SER:HA   | 1.81                     | 0.61              |
| 1:A:411:TRP:C    | 1:A:412:LEU:HD12 | 2.26                     | 0.61              |
| 1:C:272:PRO:HA   | 1:C:300:GLN:HE21 | 1.66                     | 0.61              |
| 1:C:303:GLN:NE2  | 1:C:316:GLN:HE21 | 1.94                     | 0.61              |
| 1:A:92:PHE:CE2   | 1:A:134:TYR:HB2  | 2.36                     | 0.60              |
| 1:A:398:ASN:OD1  | 1:A:403:GLN:HG3  | 2.00                     | 0.60              |
| 1:C:250:TYR:C    | 1:C:252:LEU:H    | 2.09                     | 0.60              |
| 1:A:360:SER:O    | 1:A:362:PRO:HD3  | 2.02                     | 0.60              |
| 1:C:171:MET:HE2  | 1:C:171:MET:HA   | 1.83                     | 0.60              |
| 1:B:228:ARG:HB3  | 1:B:274:MET:HB3  | 1.84                     | 0.60              |
| 1:C:352:VAL:HG11 | 1:C:357:ARG:HA   | 1.84                     | 0.60              |
| 1:B:57:ASN:HD22  | 1:B:71:ASP:HA    | 1.67                     | 0.60              |
| 1:B:159:ALA:O    | 1:B:160:GLY:C    | 2.44                     | 0.60              |
| 1:B:280:TYR:C    | 1:B:280:TYR:CD2  | 2.79                     | 0.60              |
| 1:C:26:ASP:HB2   | 1:C:418:ASN:ND2  | 2.17                     | 0.59              |
| 1:A:308:SER:HB3  | 1:A:314:LEU:HD11 | 1.83                     | 0.59              |
| 1:C:19:GLY:H     | 1:C:292:SER:CB   | 2.15                     | 0.59              |
| 1:C:51:TYR:N     | 1:C:413:PHE:O    | 2.21                     | 0.59              |
| 1:A:304:LEU:HD11 | 2:A:506:LDA:H32  | 1.85                     | 0.59              |
| 1:A:345:ILE:HA   | 1:A:368:TRP:O    | 2.02                     | 0.59              |
| 1:A:243:LEU:HD22 | 1:A:247:PHE:CE1  | 2.38                     | 0.59              |
| 1:B:10:SER:CB    | 1:B:416:ASN:HD22 | 2.16                     | 0.59              |
| 1:C:18:SER:OG    | 1:C:290:HIS:HD2  | 1.85                     | 0.59              |
| 1:A:12:GLY:HA2   | 1:A:15:ARG:CZ    | 2.33                     | 0.59              |
| 1:B:89:ASN:O     | 1:B:91:GLN:N     | 2.35                     | 0.59              |
| 1:C:38:THR:HG21  | 1:C:141:SER:HG   | 1.68                     | 0.59              |
| 1:B:281:ASN:HB2  | 1:B:289:ILE:HG23 | 1.84                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:319:GLU:HB3  | 1:A:321:PHE:CE2  | 2.37                     | 0.58              |
| 1:B:396:LYS:HG3  | 1:B:405:GLU:OE2  | 2.04                     | 0.58              |
| 1:C:155:ILE:HD11 | 2:C:501:LDA:H62  | 1.86                     | 0.58              |
| 1:B:347:PHE:HE1  | 1:B:365:ASP:HB3  | 1.69                     | 0.58              |
| 1:C:120:THR:HG23 | 1:C:122:ASP:OD1  | 2.03                     | 0.58              |
| 1:C:236:LYS:HE3  | 1:C:266:TYR:OH   | 2.04                     | 0.58              |
| 1:C:378:ASN:OD1  | 1:C:380:ASP:N    | 2.35                     | 0.58              |
| 1:A:293:LEU:CD1  | 1:A:327:ILE:HG12 | 2.29                     | 0.58              |
| 1:B:273:GLU:N    | 1:B:300:GLN:NE2  | 2.51                     | 0.58              |
| 1:A:39:MET:HE1   | 1:A:216:GLU:OE1  | 2.03                     | 0.58              |
| 1:B:55:ASP:HB3   | 1:B:409:LYS:HG2  | 1.85                     | 0.58              |
| 1:A:62:SER:O     | 1:A:65:GLY:N     | 2.33                     | 0.58              |
| 1:B:65:GLY:C     | 1:C:91:GLN:NE2   | 2.62                     | 0.58              |
| 1:C:29:ASN:HB3   | 1:C:36:LEU:CD1   | 2.34                     | 0.58              |
| 1:B:157:ARG:HB2  | 1:B:197:THR:HG22 | 1.85                     | 0.58              |
| 1:B:170:ILE:HD12 | 1:B:185:ALA:HB2  | 1.84                     | 0.58              |
| 1:C:191:ILE:HD11 | 1:C:247:PHE:CZ   | 2.38                     | 0.58              |
| 1:A:58:ILE:HB    | 1:A:70:ALA:HB3   | 1.86                     | 0.58              |
| 1:B:27:ALA:HA    | 1:B:40:PHE:CZ    | 2.39                     | 0.58              |
| 1:C:239:TYR:CD2  | 1:C:314:LEU:HD23 | 2.39                     | 0.58              |
| 1:A:199:HIS:C    | 1:A:200:LEU:HD12 | 2.29                     | 0.57              |
| 1:C:223:TYR:HA   | 1:C:279:GLY:HA2  | 1.85                     | 0.57              |
| 1:A:135:ARG:NH2  | 1:A:216:GLU:OE2  | 2.37                     | 0.57              |
| 1:A:195:THR:O    | 1:A:197:THR:N    | 2.36                     | 0.57              |
| 1:C:368:TRP:HZ2  | 2:C:502:LDA:CM2  | 2.16                     | 0.57              |
| 1:B:81:ASN:HD21  | 1:B:416:ASN:HD21 | 1.52                     | 0.57              |
| 1:B:402:TYR:HB2  | 1:B:404:PHE:CE1  | 2.39                     | 0.57              |
| 1:C:39:MET:HE1   | 1:C:216:GLU:CD   | 2.28                     | 0.57              |
| 1:C:267:LEU:HD12 | 1:C:306:ALA:HB2  | 1.86                     | 0.57              |
| 1:A:304:LEU:HD12 | 2:A:506:LDA:HM21 | 1.86                     | 0.57              |
| 1:A:155:ILE:HD11 | 2:A:506:LDA:H81  | 1.86                     | 0.57              |
| 1:B:26:ASP:O     | 1:B:40:PHE:HZ    | 1.88                     | 0.57              |
| 1:A:354:ALA:HA   | 1:A:357:ARG:CG   | 2.35                     | 0.57              |
| 1:A:7:GLU:HG2    | 1:A:50:VAL:HG11  | 1.87                     | 0.57              |
| 1:A:19:GLY:O     | 1:A:22:ALA:HB3   | 2.05                     | 0.57              |
| 1:B:360:SER:C    | 1:B:362:PRO:HD3  | 2.30                     | 0.57              |
| 1:A:27:ALA:HB1   | 1:A:85:VAL:HG23  | 1.87                     | 0.57              |
| 1:B:324:ALA:HB2  | 1:B:351:PRO:HG3  | 1.87                     | 0.57              |
| 1:C:281:ASN:ND2  | 1:C:291:TYR:CE2  | 2.70                     | 0.57              |
| 1:B:27:ALA:HB1   | 1:B:85:VAL:HG23  | 1.86                     | 0.56              |
| 1:A:153:ALA:HB1  | 2:A:506:LDA:H91  | 1.85                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:153:ALA:HB3  | 2:A:506:LDA:H91  | 1.86                     | 0.56              |
| 1:A:391:HIS:ND1  | 1:A:392:GLY:N    | 2.53                     | 0.56              |
| 1:B:57:ASN:ND2   | 1:B:71:ASP:HA    | 2.20                     | 0.56              |
| 1:B:88:ILE:HB    | 1:B:92:PHE:O     | 2.05                     | 0.56              |
| 1:C:137:ASN:ND2  | 1:C:139:ALA:N    | 2.53                     | 0.56              |
| 1:C:273:GLU:H    | 1:C:300:GLN:NE2  | 2.03                     | 0.56              |
| 1:B:104:LEU:HG   | 1:B:105:ALA:N    | 2.20                     | 0.56              |
| 1:A:21:GLY:H     | 1:A:29:ASN:ND2   | 1.96                     | 0.56              |
| 1:A:267:LEU:HD23 | 1:A:267:LEU:C    | 2.31                     | 0.56              |
| 1:B:272:PRO:HG2  | 1:B:298:TRP:CE3  | 2.41                     | 0.56              |
| 1:B:346:ALA:CB   | 1:B:368:TRP:HB2  | 2.27                     | 0.56              |
| 1:A:355:GLN:C    | 1:A:356:ASN:ND2  | 2.63                     | 0.56              |
| 1:C:36:LEU:HD23  | 1:C:214:LEU:HD13 | 1.88                     | 0.56              |
| 1:C:266:TYR:O    | 1:C:306:ALA:HA   | 2.05                     | 0.56              |
| 1:B:304:LEU:HD13 | 2:B:503:LDA:H12  | 1.88                     | 0.56              |
| 1:B:390:MET:SD   | 2:B:504:LDA:CM2  | 2.94                     | 0.56              |
| 1:C:254:ILE:HG23 | 1:C:255:PRO:O    | 2.06                     | 0.56              |
| 1:C:1:ALA:O      | 1:C:2:GLY:C      | 2.47                     | 0.55              |
| 1:B:367:PHE:O    | 1:B:390:MET:HA   | 2.05                     | 0.55              |
| 1:C:191:ILE:HD11 | 1:C:247:PHE:HZ   | 1.72                     | 0.55              |
| 1:A:11:SER:HB2   | 1:A:384:ASP:OD1  | 2.06                     | 0.55              |
| 1:B:170:ILE:CD1  | 1:B:185:ALA:HB2  | 2.37                     | 0.55              |
| 1:C:166:VAL:O    | 1:C:170:ILE:HG13 | 2.07                     | 0.55              |
| 1:C:281:ASN:HD22 | 1:C:291:TYR:HE2  | 1.54                     | 0.55              |
| 1:C:21:GLY:O     | 1:C:36:LEU:HD21  | 2.06                     | 0.55              |
| 1:C:360:SER:OG   | 2:C:501:LDA:HM21 | 2.07                     | 0.55              |
| 1:C:367:PHE:O    | 1:C:390:MET:HA   | 2.06                     | 0.55              |
| 1:A:12:GLY:HA2   | 1:A:15:ARG:NH1   | 2.21                     | 0.55              |
| 1:C:368:TRP:CZ2  | 2:C:502:LDA:HM23 | 2.31                     | 0.55              |
| 1:A:89:ASN:ND2   | 1:A:90:ASP:N     | 2.52                     | 0.55              |
| 1:C:223:TYR:CD2  | 1:C:279:GLY:HA3  | 2.41                     | 0.55              |
| 1:C:304:LEU:HD11 | 2:C:501:LDA:H32  | 1.89                     | 0.55              |
| 1:A:5:LEU:HD13   | 1:A:103:GLY:N    | 2.21                     | 0.55              |
| 1:A:57:ASN:ND2   | 1:A:71:ASP:HA    | 2.22                     | 0.55              |
| 1:A:336:ASP:O    | 1:A:338:ASN:N    | 2.40                     | 0.55              |
| 1:C:10:SER:CB    | 1:C:416:ASN:HD22 | 2.20                     | 0.55              |
| 1:C:142:PHE:N    | 1:C:142:PHE:CD1  | 2.74                     | 0.55              |
| 1:B:13:LEU:HA    | 1:B:17:TYR:CE1   | 2.41                     | 0.55              |
| 1:B:374:THR:HG23 | 1:B:384:ASP:OD2  | 2.07                     | 0.55              |
| 1:B:216:GLU:HA   | 1:B:222:ARG:HA   | 1.88                     | 0.55              |
| 1:C:343:THR:HG23 | 1:C:370:SER:O    | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:312:ASP:O    | 1:A:314:LEU:HD13 | 2.08                     | 0.54              |
| 1:B:83:HIS:HA    | 1:B:97:SER:HB3   | 1.90                     | 0.54              |
| 1:B:358:SER:HB2  | 1:B:399:GLU:OE1  | 2.07                     | 0.54              |
| 1:B:304:LEU:CD1  | 2:B:503:LDA:H11  | 2.38                     | 0.54              |
| 1:B:384:ASP:O    | 1:B:415:THR:HA   | 2.08                     | 0.54              |
| 1:A:90:ASP:O     | 1:A:91:GLN:HG2   | 2.07                     | 0.54              |
| 1:B:374:THR:HG23 | 1:B:383:VAL:O    | 2.08                     | 0.54              |
| 1:B:153:ALA:HB3  | 2:B:503:LDA:H102 | 1.89                     | 0.54              |
| 1:B:58:ILE:CD1   | 1:B:406:SER:HB2  | 2.38                     | 0.54              |
| 1:A:364:GLN:N    | 1:A:364:GLN:OE1  | 2.39                     | 0.54              |
| 1:A:67:SER:O     | 1:A:68:LEU:HD23  | 2.08                     | 0.54              |
| 1:A:361:ILE:HG13 | 2:A:506:LDA:H22  | 1.90                     | 0.54              |
| 1:B:329:LEU:HD12 | 1:B:330:GLY:H    | 1.72                     | 0.54              |
| 1:B:16:ALA:O     | 1:B:326:ARG:NH2  | 2.41                     | 0.54              |
| 1:B:303:GLN:HE22 | 1:B:316:GLN:HE21 | 1.51                     | 0.54              |
| 1:C:326:ARG:HG3  | 1:C:326:ARG:HH11 | 1.73                     | 0.54              |
| 1:A:419:TYR:HE2  | 1:A:421:PHE:CE1  | 2.26                     | 0.53              |
| 1:C:273:GLU:HG2  | 1:C:300:GLN:OE1  | 2.09                     | 0.53              |
| 1:C:10:SER:N     | 1:C:416:ASN:ND2  | 2.49                     | 0.53              |
| 1:C:254:ILE:HG13 | 1:C:255:PRO:CD   | 2.36                     | 0.53              |
| 1:A:155:ILE:CD1  | 2:A:506:LDA:H81  | 2.38                     | 0.53              |
| 1:B:352:VAL:HG11 | 1:B:357:ARG:HA   | 1.91                     | 0.53              |
| 1:A:151:ALA:CB   | 1:A:233:ILE:HD13 | 2.39                     | 0.53              |
| 1:C:238:ASN:HB3  | 1:C:262:THR:HG23 | 1.90                     | 0.53              |
| 1:C:319:GLU:OE1  | 2:C:501:LDA:HM13 | 2.08                     | 0.53              |
| 1:C:342:ARG:NH1  | 1:C:374:THR:OG1  | 2.38                     | 0.53              |
| 1:B:137:ASN:C    | 1:B:137:ASN:HD22 | 2.17                     | 0.53              |
| 1:A:140:TRP:HA   | 1:A:214:LEU:O    | 2.09                     | 0.53              |
| 1:C:252:LEU:C    | 1:C:254:ILE:H    | 2.17                     | 0.53              |
| 1:A:33:ASN:O     | 1:A:35:ALA:N     | 2.38                     | 0.52              |
| 1:A:137:ASN:HD21 | 1:A:140:TRP:HD1  | 1.56                     | 0.52              |
| 1:B:9:SER:C      | 1:B:11:SER:H     | 2.16                     | 0.52              |
| 1:B:294:ALA:HB3  | 1:B:326:ARG:HB3  | 1.91                     | 0.52              |
| 1:C:238:ASN:HB3  | 1:C:262:THR:CG2  | 2.39                     | 0.52              |
| 1:C:272:PRO:HA   | 1:C:300:GLN:NE2  | 2.24                     | 0.52              |
| 1:C:390:MET:O    | 1:C:410:ALA:N    | 2.43                     | 0.52              |
| 1:A:108:PHE:HB2  | 1:A:118:GLY:O    | 2.08                     | 0.52              |
| 1:B:243:LEU:HD22 | 1:B:247:PHE:CD1  | 2.45                     | 0.52              |
| 1:C:18:SER:HA    | 1:C:292:SER:OG   | 2.09                     | 0.52              |
| 1:A:276:GLU:HG3  | 1:A:294:ALA:CB   | 2.38                     | 0.52              |
| 1:A:281:ASN:O    | 1:A:288:ALA:HA   | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:359:ILE:O    | 1:A:362:PRO:HG3  | 2.08                     | 0.52              |
| 1:B:176:GLY:O    | 1:B:182:GLN:HG3  | 2.08                     | 0.52              |
| 1:B:303:GLN:NE2  | 1:B:316:GLN:HE21 | 2.07                     | 0.52              |
| 1:A:170:ILE:HG22 | 1:A:170:ILE:O    | 2.09                     | 0.52              |
| 1:A:361:ILE:HD11 | 2:A:506:LDA:H31  | 1.92                     | 0.52              |
| 1:B:308:SER:HB3  | 1:B:314:LEU:HD11 | 1.92                     | 0.52              |
| 1:A:2:GLY:H      | 1:A:351:PRO:CG   | 2.23                     | 0.52              |
| 1:B:94:TRP:HA    | 1:B:132:GLY:HA2  | 1.92                     | 0.52              |
| 1:C:297:SER:HA   | 1:C:323:ASP:OD2  | 2.09                     | 0.52              |
| 1:A:284:ASP:CG   | 1:A:285:PRO:HD2  | 2.35                     | 0.52              |
| 1:B:47:ALA:HA    | 1:B:81:ASN:O     | 2.09                     | 0.52              |
| 1:A:5:LEU:CD1    | 1:A:103:GLY:N    | 2.73                     | 0.52              |
| 1:B:19:GLY:HA2   | 1:B:278:SER:HB2  | 1.92                     | 0.52              |
| 1:C:15:ARG:NH1   | 1:C:20:GLU:OE1   | 2.43                     | 0.52              |
| 1:B:165:LEU:C    | 1:B:167:ALA:H    | 2.18                     | 0.52              |
| 1:B:326:ARG:HB2  | 1:B:348:ASP:HB2  | 1.92                     | 0.52              |
| 1:A:69:LYS:HE2   | 1:A:71:ASP:OD2   | 2.10                     | 0.51              |
| 1:B:112:TYR:HH   | 1:B:404:PHE:HE2  | 1.58                     | 0.51              |
| 1:B:319:GLU:HB3  | 1:B:321:PHE:CE2  | 2.44                     | 0.51              |
| 1:A:58:ILE:HD13  | 1:A:406:SER:HB2  | 1.92                     | 0.51              |
| 1:B:334:TYR:O    | 1:B:335:TYR:C    | 2.52                     | 0.51              |
| 1:A:19:GLY:HA3   | 1:A:290:HIS:HB2  | 1.93                     | 0.51              |
| 1:B:173:SER:CB   | 1:B:174:PRO:HD2  | 2.38                     | 0.51              |
| 1:A:5:LEU:HA     | 2:A:505:LDA:CM1  | 2.38                     | 0.51              |
| 1:C:229:SER:C    | 1:C:230:GLU:O    | 2.51                     | 0.51              |
| 1:B:173:SER:HB2  | 1:B:174:PRO:HD2  | 1.91                     | 0.51              |
| 1:C:9:SER:OG     | 1:C:11:SER:HB3   | 2.11                     | 0.51              |
| 1:A:89:ASN:C     | 1:A:91:GLN:H     | 2.19                     | 0.51              |
| 1:C:16:ALA:HB1   | 1:C:346:ALA:HB2  | 1.92                     | 0.51              |
| 1:C:20:GLU:HB2   | 1:C:32:ARG:HD3   | 1.93                     | 0.51              |
| 1:C:89:ASN:OD1   | 1:C:92:PHE:HB2   | 2.10                     | 0.51              |
| 1:B:166:VAL:HG12 | 1:B:166:VAL:O    | 2.10                     | 0.51              |
| 1:B:204:GLN:OE1  | 1:B:205:TRP:N    | 2.34                     | 0.51              |
| 1:A:140:TRP:CD1  | 1:A:140:TRP:N    | 2.78                     | 0.51              |
| 1:B:172:GLN:O    | 1:B:173:SER:HB3  | 2.11                     | 0.51              |
| 1:B:248:ASN:OD1  | 1:B:257:ALA:HB3  | 2.11                     | 0.51              |
| 1:B:326:ARG:HD2  | 1:B:348:ASP:HB3  | 1.92                     | 0.51              |
| 1:B:39:MET:HE1   | 1:B:135:ARG:HH22 | 1.76                     | 0.51              |
| 1:C:29:ASN:HB3   | 1:C:36:LEU:HD13  | 1.93                     | 0.51              |
| 1:C:390:MET:CE   | 2:C:502:LDA:HM22 | 2.39                     | 0.51              |
| 1:A:2:GLY:H      | 1:A:351:PRO:HG2  | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:16:ALA:HB1   | 1:C:346:ALA:CB   | 2.40                     | 0.50              |
| 1:B:329:LEU:HD12 | 1:B:330:GLY:N    | 2.26                     | 0.50              |
| 1:B:252:LEU:HB3  | 1:B:254:ILE:CG1  | 2.29                     | 0.50              |
| 1:C:396:LYS:H    | 1:C:396:LYS:CD   | 2.24                     | 0.50              |
| 1:C:68:LEU:HD22  | 1:C:404:PHE:CE2  | 2.47                     | 0.50              |
| 1:C:81:ASN:HD22  | 1:C:83:HIS:CE1   | 2.30                     | 0.50              |
| 1:C:272:PRO:HG2  | 1:C:298:TRP:CD2  | 2.46                     | 0.50              |
| 1:A:137:ASN:HD22 | 1:A:137:ASN:H    | 1.59                     | 0.50              |
| 1:A:351:PRO:O    | 1:A:353:PRO:HD3  | 2.12                     | 0.50              |
| 1:B:18:SER:HB3   | 1:B:328:ALA:HB1  | 1.92                     | 0.50              |
| 1:C:224:ALA:N    | 1:C:278:SER:O    | 2.42                     | 0.50              |
| 1:A:137:ASN:HD21 | 1:A:139:ALA:HB3  | 1.75                     | 0.50              |
| 1:C:42:ARG:HD2   | 1:C:421:PHE:O    | 2.12                     | 0.50              |
| 1:C:51:TYR:HD1   | 1:C:78:TRP:HD1   | 1.60                     | 0.50              |
| 1:B:239:TYR:CG   | 1:B:240:SER:N    | 2.80                     | 0.50              |
| 1:C:273:GLU:N    | 1:C:300:GLN:HE22 | 2.09                     | 0.50              |
| 1:C:248:ASN:HD21 | 1:C:257:ALA:H    | 1.58                     | 0.50              |
| 1:C:123:LEU:CD1  | 1:C:153:ALA:HB2  | 2.42                     | 0.49              |
| 1:C:108:PHE:HB2  | 1:C:118:GLY:O    | 2.11                     | 0.49              |
| 1:A:355:GLN:O    | 1:A:356:ASN:ND2  | 2.41                     | 0.49              |
| 1:C:304:LEU:CD1  | 2:C:501:LDA:H11  | 2.43                     | 0.49              |
| 1:A:220:ASN:HB3  | 1:A:282:ARG:CB   | 2.42                     | 0.49              |
| 1:A:301:PHE:CE2  | 1:A:319:GLU:HG3  | 2.47                     | 0.49              |
| 1:A:354:ALA:HA   | 1:A:357:ARG:HG2  | 1.93                     | 0.49              |
| 1:C:35:ALA:C     | 1:C:37:ILE:N     | 2.67                     | 0.49              |
| 1:C:62:SER:O     | 1:C:65:GLY:N     | 2.29                     | 0.49              |
| 1:C:137:ASN:ND2  | 1:C:139:ALA:H    | 2.09                     | 0.49              |
| 1:C:164:GLN:CG   | 1:C:165:LEU:H    | 2.26                     | 0.49              |
| 1:C:291:TYR:N    | 1:C:291:TYR:CD2  | 2.79                     | 0.49              |
| 1:B:129:ASN:CG   | 1:B:130:LEU:N    | 2.70                     | 0.49              |
| 1:B:137:ASN:ND2  | 1:B:140:TRP:H    | 2.07                     | 0.49              |
| 1:B:239:TYR:OH   | 1:B:256:THR:O    | 2.18                     | 0.49              |
| 1:B:354:ALA:O    | 1:B:355:GLN:HB3  | 2.13                     | 0.49              |
| 1:C:1:ALA:CB     | 1:C:4:GLN:HB3    | 2.43                     | 0.49              |
| 1:C:20:GLU:CB    | 1:C:32:ARG:HD3   | 2.42                     | 0.49              |
| 1:C:312:ASP:O    | 1:C:314:LEU:HD13 | 2.12                     | 0.49              |
| 1:C:28:GLY:HA2   | 1:C:83:HIS:CD2   | 2.48                     | 0.49              |
| 1:C:51:TYR:CD1   | 1:C:78:TRP:HD1   | 2.30                     | 0.49              |
| 1:C:70:ALA:HB1   | 1:C:73:ILE:CG2   | 2.42                     | 0.49              |
| 1:B:359:ILE:O    | 1:B:362:PRO:HG3  | 2.13                     | 0.49              |
| 1:A:103:GLY:HA2  | 1:A:123:LEU:O    | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:158:PHE:HA   | 1:A:197:THR:HB   | 1.95                     | 0.48              |
| 1:C:27:ALA:O     | 1:C:28:GLY:C     | 2.56                     | 0.48              |
| 1:C:156:GLU:OE2  | 1:C:196:LYS:HE2  | 2.13                     | 0.48              |
| 1:C:333:TYR:N    | 1:C:341:PHE:O    | 2.39                     | 0.48              |
| 1:A:121:THR:OG1  | 1:A:157:ARG:NH2  | 2.45                     | 0.48              |
| 1:A:280:TYR:CD2  | 1:A:280:TYR:C    | 2.91                     | 0.48              |
| 1:A:306:ALA:HB3  | 1:A:315:PHE:HB3  | 1.94                     | 0.48              |
| 1:B:177:GLN:HE21 | 1:B:177:GLN:HA   | 1.79                     | 0.48              |
| 1:B:332:THR:HG22 | 1:B:334:TYR:CE1  | 2.48                     | 0.48              |
| 1:C:19:GLY:HA2   | 1:C:278:SER:HB2  | 1.95                     | 0.48              |
| 1:C:326:ARG:HG3  | 1:C:348:ASP:HB3  | 1.94                     | 0.48              |
| 1:A:321:PHE:CE2  | 1:A:352:VAL:HG22 | 2.49                     | 0.48              |
| 1:C:6:ASN:O      | 1:C:7:GLU:CB     | 2.60                     | 0.48              |
| 1:C:157:ARG:CB   | 1:C:197:THR:HG22 | 2.43                     | 0.48              |
| 1:A:352:VAL:CG1  | 1:A:357:ARG:HA   | 2.42                     | 0.48              |
| 1:B:170:ILE:CG2  | 1:B:185:ALA:HB2  | 2.43                     | 0.48              |
| 1:B:307:THR:O    | 1:B:314:LEU:HD22 | 2.13                     | 0.48              |
| 1:C:33:ASN:HB2   | 1:C:226:THR:HG21 | 1.94                     | 0.48              |
| 1:C:181:GLY:C    | 1:C:183:ALA:H    | 2.21                     | 0.48              |
| 1:B:9:SER:O      | 1:B:11:SER:N     | 2.40                     | 0.48              |
| 1:A:366:ARG:HD3  | 1:A:390:MET:HE3  | 1.94                     | 0.48              |
| 1:C:1:ALA:HB1    | 1:C:4:GLN:HB3    | 1.96                     | 0.48              |
| 1:C:20:GLU:HB2   | 1:C:32:ARG:CD    | 2.44                     | 0.48              |
| 1:B:281:ASN:HB2  | 1:B:289:ILE:CG2  | 2.43                     | 0.48              |
| 1:B:322:LYS:HG3  | 1:B:351:PRO:O    | 2.13                     | 0.48              |
| 1:C:20:GLU:CB    | 1:C:32:ARG:CD    | 2.92                     | 0.48              |
| 1:C:23:ILE:HG23  | 1:C:29:ASN:ND2   | 2.28                     | 0.48              |
| 1:C:250:TYR:O    | 1:C:252:LEU:N    | 2.47                     | 0.48              |
| 1:A:354:ALA:HA   | 1:A:357:ARG:HG3  | 1.95                     | 0.47              |
| 1:B:13:LEU:HD11  | 1:B:388:SER:CB   | 2.43                     | 0.47              |
| 1:B:308:SER:CB   | 1:B:314:LEU:HD11 | 2.44                     | 0.47              |
| 1:C:81:ASN:HD22  | 1:C:83:HIS:HE1   | 1.61                     | 0.47              |
| 1:C:108:PHE:CG   | 1:C:118:GLY:O    | 2.67                     | 0.47              |
| 1:A:151:ALA:HB3  | 1:A:233:ILE:HD13 | 1.95                     | 0.47              |
| 1:A:304:LEU:HD12 | 2:A:506:LDA:H11  | 1.94                     | 0.47              |
| 1:C:46:SER:HA    | 1:C:417:PHE:O    | 2.14                     | 0.47              |
| 1:C:62:SER:C     | 1:C:64:SER:N     | 2.71                     | 0.47              |
| 1:C:139:ALA:HB1  | 1:C:215:TYR:CE2  | 2.49                     | 0.47              |
| 1:A:158:PHE:HA   | 1:A:197:THR:H    | 1.79                     | 0.47              |
| 1:B:9:SER:O      | 1:B:416:ASN:ND2  | 2.46                     | 0.47              |
| 1:B:10:SER:HB3   | 1:B:416:ASN:HD22 | 1.75                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:124:GLU:HB2  | 1:B:152:ARG:HB2  | 1.95                     | 0.47              |
| 1:B:250:TYR:O    | 1:B:251:GLY:C    | 2.57                     | 0.47              |
| 1:C:381:ALA:HA   | 1:C:418:ASN:O    | 2.13                     | 0.47              |
| 1:C:396:LYS:HD2  | 1:C:396:LYS:N    | 2.28                     | 0.47              |
| 1:B:169:GLN:HA   | 1:B:169:GLN:OE1  | 2.13                     | 0.47              |
| 1:C:51:TYR:HD1   | 1:C:78:TRP:CD1   | 2.31                     | 0.47              |
| 1:C:20:GLU:OE2   | 1:C:20:GLU:CA    | 2.60                     | 0.47              |
| 1:C:233:ILE:HD12 | 1:C:269:LEU:HD23 | 1.97                     | 0.47              |
| 1:C:269:LEU:CD2  | 1:C:271:LEU:HD21 | 2.45                     | 0.47              |
| 1:A:6:ASN:N      | 1:A:6:ASN:ND2    | 2.62                     | 0.47              |
| 1:B:52:ILE:C     | 1:B:54:PRO:HD3   | 2.39                     | 0.47              |
| 1:C:18:SER:OG    | 1:C:290:HIS:CD2  | 2.65                     | 0.47              |
| 1:C:21:GLY:HA2   | 1:C:36:LEU:CD1   | 2.35                     | 0.47              |
| 1:A:116:SER:HA   | 1:A:158:PHE:O    | 2.14                     | 0.47              |
| 1:A:195:THR:O    | 1:A:196:LYS:C    | 2.57                     | 0.47              |
| 1:A:380:ASP:OD2  | 1:A:380:ASP:N    | 2.47                     | 0.47              |
| 1:B:90:ASP:OD2   | 1:B:90:ASP:N     | 2.35                     | 0.47              |
| 1:B:280:TYR:C    | 1:B:280:TYR:HD2  | 2.22                     | 0.47              |
| 1:B:334:TYR:N    | 1:B:334:TYR:CD1  | 2.83                     | 0.47              |
| 1:C:8:PHE:CD2    | 1:C:8:PHE:C      | 2.92                     | 0.47              |
| 1:A:52:ILE:HG22  | 1:A:54:PRO:HD3   | 1.96                     | 0.47              |
| 1:A:80:PRO:O     | 1:A:81:ASN:HB3   | 2.15                     | 0.47              |
| 1:A:158:PHE:C    | 1:A:197:THR:HB   | 2.39                     | 0.47              |
| 1:A:304:LEU:CD1  | 2:A:506:LDA:H11  | 2.45                     | 0.47              |
| 1:B:159:ALA:O    | 1:B:160:GLY:O    | 2.31                     | 0.47              |
| 1:B:297:SER:O    | 1:B:300:GLN:HG3  | 2.14                     | 0.47              |
| 1:C:317:LYS:HD3  | 1:C:318:HIS:N    | 2.30                     | 0.47              |
| 1:A:168:GLY:O    | 1:A:169:GLN:C    | 2.58                     | 0.47              |
| 1:C:58:ILE:O     | 1:C:70:ALA:N     | 2.45                     | 0.47              |
| 1:C:64:SER:CB    | 1:C:165:LEU:HD21 | 2.34                     | 0.47              |
| 1:A:33:ASN:C     | 1:A:35:ALA:N     | 2.72                     | 0.47              |
| 1:B:216:GLU:HB3  | 1:B:222:ARG:HB3  | 1.96                     | 0.47              |
| 1:B:235:PHE:HB2  | 1:B:267:LEU:O    | 2.15                     | 0.47              |
| 1:A:256:THR:OG1  | 1:A:314:LEU:HA   | 2.15                     | 0.46              |
| 1:A:304:LEU:O    | 1:A:316:GLN:HA   | 2.14                     | 0.46              |
| 1:C:18:SER:HB3   | 1:C:328:ALA:HB1  | 1.97                     | 0.46              |
| 1:C:101:ASN:C    | 1:C:102:TYR:CD1  | 2.94                     | 0.46              |
| 1:A:24:ALA:HB2   | 1:A:36:LEU:HD22  | 1.96                     | 0.46              |
| 1:C:6:ASN:C      | 1:C:7:GLU:CD     | 2.83                     | 0.46              |
| 1:C:343:THR:CG2  | 1:C:344:GLY:N    | 2.78                     | 0.46              |
| 1:A:162:LEU:HD21 | 1:A:401:PRO:HG3  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:374:THR:HG23 | 1:A:384:ASP:OD2  | 2.16                     | 0.46              |
| 1:B:393:GLN:HE21 | 1:B:393:GLN:CA   | 2.25                     | 0.46              |
| 1:C:273:GLU:H    | 1:C:300:GLN:HE22 | 1.63                     | 0.46              |
| 1:A:1:ALA:HB1    | 1:A:298:TRP:HE1  | 1.81                     | 0.46              |
| 1:B:191:ILE:HD11 | 1:B:247:PHE:CZ   | 2.50                     | 0.46              |
| 1:B:354:ALA:HB2  | 1:B:357:ARG:NH2  | 2.30                     | 0.46              |
| 1:A:46:SER:HB2   | 1:A:418:ASN:ND2  | 2.31                     | 0.46              |
| 1:A:62:SER:HB3   | 1:A:68:LEU:HD21  | 1.96                     | 0.46              |
| 1:C:26:ASP:O     | 1:C:28:GLY:N     | 2.49                     | 0.46              |
| 1:A:7:GLU:OE2    | 1:A:52:ILE:HD11  | 2.16                     | 0.46              |
| 1:B:137:ASN:HD22 | 1:B:137:ASN:N    | 2.13                     | 0.46              |
| 1:B:286:GLN:O    | 1:B:333:TYR:HD1  | 1.99                     | 0.46              |
| 1:B:354:ALA:HB2  | 1:B:357:ARG:CZ   | 2.45                     | 0.46              |
| 1:C:155:ILE:HD11 | 2:C:501:LDA:C6   | 2.45                     | 0.46              |
| 1:B:19:GLY:N     | 1:B:292:SER:HB3  | 2.26                     | 0.46              |
| 1:B:191:ILE:HD11 | 1:B:247:PHE:CE2  | 2.51                     | 0.46              |
| 1:C:158:PHE:HA   | 1:C:197:THR:H    | 1.80                     | 0.46              |
| 1:C:218:ASP:C    | 1:C:218:ASP:OD1  | 2.59                     | 0.46              |
| 1:C:317:LYS:HD3  | 1:C:318:HIS:H    | 1.80                     | 0.46              |
| 1:A:62:SER:CB    | 1:A:68:LEU:HD21  | 2.46                     | 0.46              |
| 1:B:304:LEU:CD1  | 2:B:503:LDA:C1   | 2.94                     | 0.46              |
| 1:A:220:ASN:HB3  | 1:A:282:ARG:HB2  | 1.99                     | 0.45              |
| 1:B:164:GLN:HG3  | 1:B:189:ASN:ND2  | 2.31                     | 0.45              |
| 1:B:228:ARG:HB3  | 1:B:274:MET:CB   | 2.46                     | 0.45              |
| 1:C:11:SER:HB2   | 1:C:384:ASP:OD1  | 2.16                     | 0.45              |
| 1:A:19:GLY:O     | 1:A:20:GLU:C     | 2.60                     | 0.45              |
| 1:B:135:ARG:NH2  | 1:B:216:GLU:OE2  | 2.50                     | 0.45              |
| 1:B:155:ILE:HG13 | 2:B:503:LDA:H92  | 1.98                     | 0.45              |
| 1:C:7:GLU:HB3    | 1:C:50:VAL:HG21  | 1.99                     | 0.45              |
| 1:C:45:PHE:CG    | 1:C:46:SER:N     | 2.84                     | 0.45              |
| 1:C:58:ILE:CD1   | 1:C:406:SER:HB2  | 2.47                     | 0.45              |
| 1:C:109:ASN:O    | 1:C:111:THR:N    | 2.47                     | 0.45              |
| 1:A:356:ASN:O    | 1:A:357:ARG:C    | 2.60                     | 0.45              |
| 1:B:162:LEU:O    | 1:B:166:VAL:HG23 | 2.16                     | 0.45              |
| 1:B:343:THR:HA   | 1:B:370:SER:O    | 2.16                     | 0.45              |
| 1:C:33:ASN:OD1   | 1:C:33:ASN:C     | 2.60                     | 0.45              |
| 1:C:137:ASN:ND2  | 1:C:140:TRP:N    | 2.60                     | 0.45              |
| 1:A:10:SER:CB    | 1:A:416:ASN:HD22 | 2.29                     | 0.45              |
| 1:C:51:TYR:CD1   | 1:C:78:TRP:CD1   | 3.05                     | 0.45              |
| 1:B:114:GLY:HA2  | 1:B:402:TYR:CZ   | 2.52                     | 0.45              |
| 1:C:123:LEU:HD12 | 1:C:153:ALA:HB2  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:158:PHE:CA   | 1:A:197:THR:HB   | 2.47                     | 0.45              |
| 1:A:199:HIS:HE1  | 1:B:192:ASP:OD1  | 1.99                     | 0.45              |
| 1:A:303:GLN:NE2  | 1:A:316:GLN:HG3  | 2.32                     | 0.45              |
| 1:B:9:SER:C      | 1:B:11:SER:N     | 2.75                     | 0.45              |
| 1:B:216:GLU:CB   | 1:B:222:ARG:HB3  | 2.47                     | 0.45              |
| 1:B:324:ALA:CB   | 1:B:351:PRO:HG3  | 2.46                     | 0.45              |
| 1:C:42:ARG:NH1   | 1:C:420:ALA:HB1  | 2.31                     | 0.45              |
| 1:C:281:ASN:O    | 1:C:288:ALA:HA   | 2.16                     | 0.45              |
| 1:C:361:ILE:CD1  | 2:C:501:LDA:H22  | 2.16                     | 0.45              |
| 1:A:248:ASN:O    | 1:A:250:TYR:CD2  | 2.70                     | 0.45              |
| 2:B:503:LDA:H51  | 2:B:503:LDA:H21  | 1.29                     | 0.45              |
| 1:C:334:TYR:CD2  | 1:C:340:THR:HG23 | 2.52                     | 0.45              |
| 1:C:393:GLN:HA   | 1:C:393:GLN:NE2  | 2.28                     | 0.45              |
| 1:A:3:PHE:O      | 1:A:3:PHE:CD2    | 2.70                     | 0.45              |
| 1:B:121:THR:OG1  | 1:B:157:ARG:NH2  | 2.49                     | 0.45              |
| 1:B:378:ASN:O    | 1:B:379:LYS:CB   | 2.60                     | 0.45              |
| 1:A:159:ALA:O    | 1:A:160:GLY:O    | 2.35                     | 0.44              |
| 1:A:185:ALA:O    | 1:A:187:THR:N    | 2.50                     | 0.44              |
| 1:B:103:GLY:HA2  | 1:B:123:LEU:O    | 2.17                     | 0.44              |
| 1:C:154:LYS:HA   | 1:C:200:LEU:O    | 2.17                     | 0.44              |
| 1:C:216:GLU:HA   | 1:C:222:ARG:HB3  | 1.99                     | 0.44              |
| 1:A:5:LEU:HD13   | 1:A:102:TYR:HA   | 1.99                     | 0.44              |
| 1:A:15:ARG:NH1   | 1:A:20:GLU:OE1   | 2.50                     | 0.44              |
| 1:B:272:PRO:HG2  | 1:B:298:TRP:CD2  | 2.51                     | 0.44              |
| 1:C:348:ASP:O    | 1:C:348:ASP:OD2  | 2.36                     | 0.44              |
| 1:A:51:TYR:OH    | 1:A:76:THR:HG21  | 2.18                     | 0.44              |
| 1:B:165:LEU:C    | 1:B:167:ALA:N    | 2.72                     | 0.44              |
| 1:B:305:LYS:HD3  | 1:B:316:GLN:NE2  | 2.33                     | 0.44              |
| 1:A:162:LEU:O    | 1:A:163:GLY:C    | 2.61                     | 0.44              |
| 1:A:319:GLU:CD   | 2:A:506:LDA:HM22 | 2.41                     | 0.44              |
| 1:B:91:GLN:NE2   | 1:B:135:ARG:O    | 2.51                     | 0.44              |
| 1:B:326:ARG:HB2  | 1:B:348:ASP:CB   | 2.48                     | 0.44              |
| 1:C:89:ASN:O     | 1:C:90:ASP:C     | 2.59                     | 0.44              |
| 1:C:238:ASN:HD22 | 1:C:262:THR:CG2  | 2.30                     | 0.44              |
| 1:A:40:PHE:CD1   | 1:A:40:PHE:N     | 2.85                     | 0.44              |
| 1:A:361:ILE:HG22 | 1:A:361:ILE:O    | 2.17                     | 0.44              |
| 1:B:248:ASN:HD21 | 1:B:256:THR:HA   | 1.82                     | 0.44              |
| 1:B:321:PHE:CE2  | 1:B:352:VAL:HG22 | 2.53                     | 0.44              |
| 1:B:377:PHE:HB2  | 1:B:381:ALA:HB3  | 1.99                     | 0.44              |
| 1:B:378:ASN:OD1  | 1:B:380:ASP:N    | 2.38                     | 0.44              |
| 1:C:13:LEU:HD13  | 1:C:17:TYR:OH    | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:11:SER:OG    | 1:A:15:ARG:NH2   | 2.51                     | 0.44              |
| 1:A:366:ARG:NH1  | 2:A:505:LDA:H12  | 2.32                     | 0.44              |
| 1:B:254:ILE:HD13 | 1:B:254:ILE:H    | 1.83                     | 0.44              |
| 1:B:343:THR:CG2  | 1:B:344:GLY:N    | 2.80                     | 0.44              |
| 1:C:82:MET:HE3   | 1:C:82:MET:HB2   | 1.70                     | 0.44              |
| 1:A:15:ARG:NH1   | 1:A:20:GLU:OE2   | 2.49                     | 0.44              |
| 1:A:216:GLU:HB2  | 1:A:222:ARG:HB3  | 2.00                     | 0.44              |
| 1:B:171:MET:HE1  | 1:B:182:GLN:HG2  | 2.00                     | 0.44              |
| 1:B:280:TYR:CD2  | 1:B:281:ASN:N    | 2.86                     | 0.44              |
| 1:C:57:ASN:ND2   | 1:C:71:ASP:HA    | 2.33                     | 0.44              |
| 1:C:343:THR:HG22 | 1:C:344:GLY:N    | 2.32                     | 0.44              |
| 1:A:6:ASN:O      | 1:A:17:TYR:CE1   | 2.70                     | 0.44              |
| 1:A:214:LEU:O    | 1:A:214:LEU:HD23 | 2.18                     | 0.44              |
| 1:B:304:LEU:HD13 | 2:B:503:LDA:C1   | 2.48                     | 0.44              |
| 1:B:352:VAL:HA   | 1:B:353:PRO:HD3  | 1.82                     | 0.44              |
| 1:C:1:ALA:HB1    | 1:C:4:GLN:CB     | 2.48                     | 0.44              |
| 1:C:15:ARG:HG2   | 1:C:342:ARG:HD3  | 2.00                     | 0.44              |
| 1:B:7:GLU:OE2    | 2:B:504:LDA:HM12 | 2.18                     | 0.43              |
| 1:B:178:THR:CG2  | 1:B:181:GLY:H    | 2.31                     | 0.43              |
| 1:B:361:ILE:N    | 1:B:362:PRO:HD3  | 2.32                     | 0.43              |
| 1:C:298:TRP:O    | 1:C:299:SER:C    | 2.59                     | 0.43              |
| 1:B:137:ASN:HD21 | 1:B:139:ALA:HB3  | 1.82                     | 0.43              |
| 1:B:155:ILE:HD11 | 2:B:503:LDA:H71  | 2.00                     | 0.43              |
| 1:B:256:THR:OG1  | 1:B:314:LEU:HA   | 2.17                     | 0.43              |
| 1:B:36:LEU:HD23  | 1:B:214:LEU:HD13 | 2.00                     | 0.43              |
| 1:B:78:TRP:O     | 1:B:80:PRO:HD3   | 2.17                     | 0.43              |
| 1:B:113:ALA:HB1  | 1:B:161:ASP:OD2  | 2.18                     | 0.43              |
| 1:B:117:VAL:HB   | 1:B:399:GLU:CD   | 2.42                     | 0.43              |
| 2:C:502:LDA:H12  | 2:C:502:LDA:H41  | 1.89                     | 0.43              |
| 1:A:36:LEU:O     | 1:A:39:MET:HB2   | 2.19                     | 0.43              |
| 1:A:326:ARG:HG3  | 1:A:326:ARG:HH11 | 1.83                     | 0.43              |
| 1:A:350:SER:HA   | 1:A:351:PRO:HD3  | 1.83                     | 0.43              |
| 1:B:13:LEU:HA    | 1:B:17:TYR:CZ    | 2.54                     | 0.43              |
| 1:B:89:ASN:O     | 1:B:90:ASP:C     | 2.61                     | 0.43              |
| 1:C:195:THR:O    | 1:C:197:THR:N    | 2.51                     | 0.43              |
| 1:A:3:PHE:O      | 1:A:3:PHE:HD2    | 2.01                     | 0.43              |
| 1:A:15:ARG:O     | 1:A:16:ALA:HB3   | 2.19                     | 0.43              |
| 1:A:34:ALA:HB1   | 1:A:131:SER:OG   | 2.18                     | 0.43              |
| 1:B:303:GLN:NE2  | 1:B:316:GLN:NE2  | 2.63                     | 0.43              |
| 1:C:43:PRO:HA    | 1:C:85:VAL:O     | 2.18                     | 0.43              |
| 1:C:246:ALA:C    | 1:C:248:ASN:H    | 2.25                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:273:GLU:N    | 1:C:300:GLN:NE2  | 2.65                     | 0.43              |
| 1:C:334:TYR:CD2  | 1:C:340:THR:CG2  | 3.02                     | 0.43              |
| 1:C:345:ILE:CG2  | 1:C:346:ALA:N    | 2.82                     | 0.43              |
| 1:A:21:GLY:HA2   | 1:A:36:LEU:HD11  | 2.00                     | 0.43              |
| 1:B:13:LEU:HD11  | 1:B:388:SER:HB2  | 2.01                     | 0.43              |
| 1:B:378:ASN:OD1  | 1:B:379:LYS:N    | 2.52                     | 0.43              |
| 1:C:19:GLY:H     | 1:C:292:SER:HB3  | 1.82                     | 0.43              |
| 1:C:170:ILE:HA   | 1:C:173:SER:HB3  | 2.00                     | 0.43              |
| 1:A:223:TYR:N    | 1:A:223:TYR:CD1  | 2.86                     | 0.43              |
| 1:B:13:LEU:CD1   | 1:B:388:SER:HB2  | 2.48                     | 0.43              |
| 1:C:57:ASN:ND2   | 1:C:71:ASP:OD2   | 2.52                     | 0.43              |
| 1:C:112:TYR:HE2  | 1:C:404:PHE:HE2  | 1.65                     | 0.43              |
| 1:C:165:LEU:H    | 1:C:165:LEU:HD23 | 1.83                     | 0.43              |
| 1:A:5:LEU:CD1    | 1:A:103:GLY:H    | 2.32                     | 0.43              |
| 1:A:86:ALA:HA    | 1:A:87:PRO:HD3   | 1.69                     | 0.43              |
| 1:A:419:TYR:HE2  | 1:A:421:PHE:CD1  | 2.37                     | 0.43              |
| 1:B:58:ILE:HD13  | 1:B:406:SER:HB2  | 1.99                     | 0.43              |
| 1:B:252:LEU:HD23 | 1:B:254:ILE:HG13 | 2.01                     | 0.43              |
| 1:C:250:TYR:C    | 1:C:252:LEU:N    | 2.76                     | 0.43              |
| 1:C:321:PHE:CD2  | 1:C:352:VAL:HG22 | 2.52                     | 0.43              |
| 1:C:345:ILE:HG22 | 1:C:346:ALA:N    | 2.34                     | 0.43              |
| 1:C:391:HIS:ND1  | 1:C:392:GLY:N    | 2.67                     | 0.43              |
| 1:C:404:PHE:CD1  | 1:C:404:PHE:N    | 2.86                     | 0.43              |
| 1:C:20:GLU:HB3   | 1:C:32:ARG:HD2   | 2.01                     | 0.43              |
| 1:C:326:ARG:HG3  | 1:C:326:ARG:NH1  | 2.34                     | 0.43              |
| 1:B:10:SER:O     | 1:B:13:LEU:HB3   | 2.18                     | 0.42              |
| 1:B:43:PRO:HA    | 1:B:85:VAL:O     | 2.19                     | 0.42              |
| 1:B:55:ASP:O     | 1:B:408:GLY:HA2  | 2.19                     | 0.42              |
| 1:B:117:VAL:HG23 | 1:B:359:ILE:HD11 | 2.01                     | 0.42              |
| 1:B:266:TYR:HB2  | 1:B:307:THR:OG1  | 2.19                     | 0.42              |
| 1:C:33:ASN:ND2   | 1:C:226:THR:HG22 | 2.34                     | 0.42              |
| 1:C:243:LEU:HD23 | 1:C:243:LEU:HA   | 1.84                     | 0.42              |
| 1:B:290:HIS:HE1  | 1:B:332:THR:OG1  | 2.01                     | 0.42              |
| 1:B:326:ARG:HA   | 1:B:348:ASP:CB   | 2.49                     | 0.42              |
| 1:B:411:TRP:C    | 1:B:412:LEU:HD12 | 2.44                     | 0.42              |
| 1:C:33:ASN:ND2   | 1:C:226:THR:CG2  | 2.82                     | 0.42              |
| 1:A:161:ASP:O    | 1:A:162:LEU:C    | 2.62                     | 0.42              |
| 1:B:165:LEU:O    | 1:B:167:ALA:N    | 2.52                     | 0.42              |
| 1:C:20:GLU:HA    | 1:C:29:ASN:ND2   | 2.34                     | 0.42              |
| 1:C:68:LEU:HD23  | 1:C:113:ALA:HB3  | 2.01                     | 0.42              |
| 1:C:383:VAL:HG22 | 1:C:384:ASP:N    | 2.34                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:157:ARG:C    | 1:A:197:THR:HG22 | 2.44                     | 0.42              |
| 1:A:220:ASN:HB3  | 1:A:282:ARG:HB3  | 2.01                     | 0.42              |
| 1:A:322:LYS:O    | 1:A:323:ASP:C    | 2.62                     | 0.42              |
| 1:B:58:ILE:HG12  | 1:B:73:ILE:HD13  | 2.00                     | 0.42              |
| 1:B:249:ASN:O    | 1:B:250:TYR:CG   | 2.73                     | 0.42              |
| 1:C:20:GLU:HB3   | 1:C:32:ARG:CD    | 2.50                     | 0.42              |
| 1:C:129:ASN:HB2  | 1:C:147:ASN:OD1  | 2.19                     | 0.42              |
| 1:C:135:ARG:HG3  | 1:C:137:ASN:O    | 2.19                     | 0.42              |
| 1:C:171:MET:HE1  | 1:C:182:GLN:CB   | 2.50                     | 0.42              |
| 1:C:236:LYS:HD3  | 1:C:266:TYR:CE2  | 2.55                     | 0.42              |
| 1:C:343:THR:HA   | 1:C:371:ALA:HA   | 2.01                     | 0.42              |
| 1:C:392:GLY:O    | 1:C:393:GLN:C    | 2.61                     | 0.42              |
| 1:A:127:ASN:ND2  | 1:A:149:VAL:HG22 | 2.34                     | 0.42              |
| 1:B:172:GLN:O    | 1:B:173:SER:CB   | 2.68                     | 0.42              |
| 1:B:232:LYS:HE2  | 1:B:270:ASN:ND2  | 2.34                     | 0.42              |
| 1:C:164:GLN:HG2  | 1:C:165:LEU:H    | 1.83                     | 0.42              |
| 1:A:10:SER:HB3   | 1:A:416:ASN:HD22 | 1.85                     | 0.42              |
| 1:A:336:ASP:O    | 1:A:337:ASP:C    | 2.63                     | 0.42              |
| 1:C:157:ARG:C    | 1:C:197:THR:HG22 | 2.45                     | 0.42              |
| 1:C:164:GLN:O    | 1:C:165:LEU:C    | 2.60                     | 0.42              |
| 1:A:120:THR:HB   | 1:A:156:GLU:HB2  | 2.02                     | 0.42              |
| 1:B:243:LEU:HD22 | 1:B:247:PHE:CE1  | 2.55                     | 0.42              |
| 1:B:347:PHE:CE1  | 1:B:365:ASP:HB3  | 2.53                     | 0.42              |
| 1:C:156:GLU:CD   | 1:C:196:LYS:HE2  | 2.45                     | 0.42              |
| 1:A:153:ALA:HB1  | 2:A:506:LDA:H82  | 2.01                     | 0.42              |
| 1:B:325:TYR:O    | 1:B:348:ASP:HB2  | 2.19                     | 0.42              |
| 1:C:360:SER:C    | 1:C:362:PRO:HD3  | 2.45                     | 0.42              |
| 1:A:89:ASN:HD22  | 1:A:90:ASP:N     | 2.11                     | 0.41              |
| 1:A:121:THR:HG21 | 2:A:506:LDA:H21  | 2.02                     | 0.41              |
| 1:B:308:SER:C    | 1:B:310:SER:N    | 2.75                     | 0.41              |
| 1:C:37:ILE:C     | 1:C:39:MET:H     | 2.27                     | 0.41              |
| 1:C:59:SER:OG    | 1:C:405:GLU:HB3  | 2.19                     | 0.41              |
| 1:C:109:ASN:C    | 1:C:111:THR:H    | 2.28                     | 0.41              |
| 1:C:129:ASN:CG   | 1:C:130:LEU:N    | 2.78                     | 0.41              |
| 1:A:20:GLU:C     | 1:A:22:ALA:H     | 2.28                     | 0.41              |
| 1:B:32:ARG:HH11  | 1:B:32:ARG:CG    | 2.29                     | 0.41              |
| 1:B:137:ASN:ND2  | 1:B:137:ASN:C    | 2.77                     | 0.41              |
| 1:B:167:ALA:HB1  | 1:B:185:ALA:O    | 2.20                     | 0.41              |
| 1:B:402:TYR:CB   | 1:B:404:PHE:CE1  | 3.03                     | 0.41              |
| 1:B:161:ASP:C    | 1:B:163:GLY:N    | 2.78                     | 0.41              |
| 1:B:263:GLN:OE1  | 1:B:314:LEU:HD21 | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:42:ARG:NH1   | 1:C:420:ALA:O    | 2.53                     | 0.41              |
| 1:A:156:GLU:C    | 1:A:157:ARG:HG2  | 2.45                     | 0.41              |
| 1:A:404:PHE:CD1  | 1:A:404:PHE:N    | 2.89                     | 0.41              |
| 1:B:137:ASN:ND2  | 1:B:137:ASN:N    | 2.67                     | 0.41              |
| 1:A:4:GLN:O      | 1:A:5:LEU:HD12   | 2.21                     | 0.41              |
| 1:A:15:ARG:HH11  | 1:A:15:ARG:HG3   | 1.84                     | 0.41              |
| 1:A:399:GLU:O    | 1:A:400:GLY:C    | 2.63                     | 0.41              |
| 1:C:112:TYR:O    | 1:C:113:ALA:C    | 2.62                     | 0.41              |
| 1:C:361:ILE:O    | 1:C:361:ILE:HG22 | 2.19                     | 0.41              |
| 1:A:30:VAL:HG21  | 1:A:85:VAL:HG22  | 2.03                     | 0.41              |
| 1:A:185:ALA:C    | 1:A:187:THR:N    | 2.79                     | 0.41              |
| 1:B:71:ASP:O     | 1:B:72:ASN:C     | 2.64                     | 0.41              |
| 1:C:117:VAL:HG23 | 1:C:359:ILE:HD11 | 2.02                     | 0.41              |
| 1:C:231:VAL:O    | 1:C:231:VAL:HG12 | 2.20                     | 0.41              |
| 1:A:6:ASN:HD22   | 1:A:6:ASN:H      | 1.69                     | 0.41              |
| 1:A:326:ARG:CG   | 1:A:348:ASP:HB3  | 2.47                     | 0.41              |
| 1:A:334:TYR:HA   | 1:A:340:THR:HG23 | 2.02                     | 0.41              |
| 1:B:342:ARG:NH2  | 1:B:374:THR:OG1  | 2.48                     | 0.41              |
| 1:C:170:ILE:O    | 1:C:170:ILE:HG22 | 2.20                     | 0.41              |
| 1:C:195:THR:O    | 1:C:196:LYS:C    | 2.63                     | 0.41              |
| 1:A:69:LYS:HE2   | 1:A:71:ASP:CG    | 2.46                     | 0.41              |
| 1:A:162:LEU:HD23 | 1:A:162:LEU:HA   | 1.90                     | 0.41              |
| 1:A:317:LYS:HD3  | 1:A:318:HIS:N    | 2.35                     | 0.41              |
| 1:A:346:ALA:HB3  | 1:A:368:TRP:HB2  | 2.03                     | 0.41              |
| 1:B:288:ALA:O    | 1:B:331:THR:HB   | 2.21                     | 0.41              |
| 1:C:19:GLY:O     | 1:C:22:ALA:HB3   | 2.21                     | 0.41              |
| 1:C:133:ALA:HA   | 1:C:143:GLY:HA2  | 2.02                     | 0.41              |
| 1:A:217:LEU:C    | 1:A:217:LEU:HD23 | 2.46                     | 0.41              |
| 1:B:131:SER:HB3  | 1:B:145:GLY:HA3  | 2.00                     | 0.41              |
| 1:B:253:PRO:O    | 1:B:254:ILE:C    | 2.64                     | 0.41              |
| 1:B:291:TYR:O    | 1:B:291:TYR:CD1  | 2.74                     | 0.41              |
| 1:C:252:LEU:C    | 1:C:254:ILE:N    | 2.78                     | 0.41              |
| 1:C:381:ALA:O    | 1:C:382:SER:HB3  | 2.21                     | 0.41              |
| 1:B:321:PHE:N    | 1:B:321:PHE:CD2  | 2.89                     | 0.40              |
| 1:C:402:TYR:HB2  | 1:C:404:PHE:CE1  | 2.55                     | 0.40              |
| 1:A:142:PHE:CD1  | 1:A:142:PHE:N    | 2.89                     | 0.40              |
| 1:A:307:THR:C    | 1:A:314:LEU:HD22 | 2.46                     | 0.40              |
| 1:B:112:TYR:OH   | 1:B:404:PHE:HE2  | 2.03                     | 0.40              |
| 1:B:128:LEU:HD12 | 1:B:205:TRP:CZ3  | 2.56                     | 0.40              |
| 1:B:164:GLN:H    | 1:B:164:GLN:CD   | 2.29                     | 0.40              |
| 1:B:274:MET:HG2  | 1:B:296:THR:OG1  | 2.21                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:347:PHE:HA   | 1:B:366:ARG:O   | 2.21                     | 0.40              |
| 1:C:157:ARG:HB2  | 1:C:197:THR:CG2 | 2.49                     | 0.40              |
| 1:C:366:ARG:NH1  | 2:C:502:LDA:H21 | 2.36                     | 0.40              |
| 1:A:131:SER:HB2  | 1:A:144:LEU:O   | 2.21                     | 0.40              |
| 1:A:143:GLY:O    | 1:A:211:ALA:HA  | 2.21                     | 0.40              |
| 1:A:159:ALA:O    | 1:A:160:GLY:C   | 2.64                     | 0.40              |
| 1:A:162:LEU:O    | 1:A:165:LEU:HB2 | 2.22                     | 0.40              |
| 1:B:177:GLN:HA   | 1:B:177:GLN:NE2 | 2.35                     | 0.40              |
| 1:C:157:ARG:HH12 | 2:C:501:LDA:CM2 | 2.26                     | 0.40              |
| 1:A:158:PHE:CD1  | 1:A:158:PHE:N   | 2.89                     | 0.40              |
| 1:B:253:PRO:O    | 1:B:254:ILE:O   | 2.40                     | 0.40              |
| 1:B:387:VAL:HA   | 1:B:412:LEU:O   | 2.21                     | 0.40              |
| 1:C:52:ILE:HB    | 1:C:77:ALA:HB3  | 2.04                     | 0.40              |
| 1:C:140:TRP:O    | 1:C:141:SER:HB2 | 2.21                     | 0.40              |
| 1:C:359:ILE:O    | 1:C:362:PRO:HG3 | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 408/427 (96%)   | 352 (86%)  | 43 (10%)  | 13 (3%)  | 3           | 19 |
| 1   | B     | 419/427 (98%)   | 355 (85%)  | 42 (10%)  | 22 (5%)  | 1           | 10 |
| 1   | C     | 412/427 (96%)   | 340 (82%)  | 55 (13%)  | 17 (4%)  | 2           | 15 |
| All | All   | 1239/1281 (97%) | 1047 (84%) | 140 (11%) | 52 (4%)  | 2           | 14 |

All (52) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 196 | LYS  |
| 1   | A     | 337 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 355 | GLN  |
| 1   | B     | 90  | ASP  |
| 1   | B     | 174 | PRO  |
| 1   | B     | 254 | ILE  |
| 1   | B     | 355 | GLN  |
| 1   | B     | 379 | LYS  |
| 1   | C     | 2   | GLY  |
| 1   | C     | 27  | ALA  |
| 1   | C     | 164 | GLN  |
| 1   | C     | 165 | LEU  |
| 1   | C     | 355 | GLN  |
| 1   | A     | 2   | GLY  |
| 1   | A     | 34  | ALA  |
| 1   | A     | 160 | GLY  |
| 1   | A     | 186 | ALA  |
| 1   | B     | 72  | ASN  |
| 1   | B     | 160 | GLY  |
| 1   | B     | 217 | LEU  |
| 1   | B     | 250 | TYR  |
| 1   | B     | 272 | PRO  |
| 1   | B     | 354 | ALA  |
| 1   | B     | 359 | ILE  |
| 1   | C     | 29  | ASN  |
| 1   | C     | 90  | ASP  |
| 1   | C     | 110 | ASP  |
| 1   | C     | 160 | GLY  |
| 1   | C     | 272 | PRO  |
| 1   | A     | 105 | ALA  |
| 1   | A     | 249 | ASN  |
| 1   | A     | 272 | PRO  |
| 1   | B     | 154 | LYS  |
| 1   | B     | 362 | PRO  |
| 1   | C     | 7   | GLU  |
| 1   | C     | 28  | GLY  |
| 1   | C     | 196 | LYS  |
| 1   | C     | 219 | LYS  |
| 1   | C     | 349 | ASP  |
| 1   | B     | 365 | ASP  |
| 1   | C     | 382 | SER  |
| 1   | A     | 72  | ASN  |
| 1   | B     | 22  | ALA  |
| 1   | C     | 335 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 2   | GLY  |
| 1   | B     | 115 | GLY  |
| 1   | B     | 335 | TYR  |
| 1   | B     | 166 | VAL  |
| 1   | B     | 173 | SER  |
| 1   | B     | 118 | GLY  |
| 1   | A     | 63  | PRO  |
| 1   | A     | 163 | 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     | 323/336 (96%)  | 296 (92%) | 27 (8%)   | 10          | 34 |
| 1   | B     | 330/336 (98%)  | 286 (87%) | 44 (13%)  | 4           | 17 |
| 1   | C     | 326/336 (97%)  | 295 (90%) | 31 (10%)  | 8           | 29 |
| All | All   | 979/1008 (97%) | 877 (90%) | 102 (10%) | 7           | 25 |

All (102) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | ASN  |
| 1   | A     | 11  | SER  |
| 1   | A     | 15  | ARG  |
| 1   | A     | 39  | MET  |
| 1   | A     | 63  | PRO  |
| 1   | A     | 78  | TRP  |
| 1   | A     | 85  | VAL  |
| 1   | A     | 121 | THR  |
| 1   | A     | 130 | LEU  |
| 1   | A     | 137 | ASN  |
| 1   | A     | 140 | TRP  |
| 1   | A     | 144 | LEU  |
| 1   | A     | 197 | THR  |
| 1   | A     | 203 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 214 | LEU  |
| 1   | A     | 236 | LYS  |
| 1   | A     | 274 | MET  |
| 1   | A     | 275 | TRP  |
| 1   | A     | 278 | SER  |
| 1   | A     | 282 | ARG  |
| 1   | A     | 285 | PRO  |
| 1   | A     | 289 | ILE  |
| 1   | A     | 314 | LEU  |
| 1   | A     | 317 | LYS  |
| 1   | A     | 380 | ASP  |
| 1   | A     | 404 | PHE  |
| 1   | A     | 416 | ASN  |
| 1   | B     | 3   | PHE  |
| 1   | B     | 10  | SER  |
| 1   | B     | 15  | ARG  |
| 1   | B     | 32  | ARG  |
| 1   | B     | 39  | MET  |
| 1   | B     | 81  | ASN  |
| 1   | B     | 89  | ASN  |
| 1   | B     | 90  | ASP  |
| 1   | B     | 97  | SER  |
| 1   | B     | 125 | THR  |
| 1   | B     | 137 | ASN  |
| 1   | B     | 141 | SER  |
| 1   | B     | 152 | ARG  |
| 1   | B     | 169 | GLN  |
| 1   | B     | 172 | GLN  |
| 1   | B     | 174 | PRO  |
| 1   | B     | 187 | THR  |
| 1   | B     | 189 | ASN  |
| 1   | B     | 197 | THR  |
| 1   | B     | 210 | ASN  |
| 1   | B     | 225 | LEU  |
| 1   | B     | 249 | ASN  |
| 1   | B     | 252 | LEU  |
| 1   | B     | 263 | GLN  |
| 1   | B     | 264 | SER  |
| 1   | B     | 272 | PRO  |
| 1   | B     | 274 | MET  |
| 1   | B     | 275 | TRP  |
| 1   | B     | 280 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 282 | ARG  |
| 1   | B     | 289 | ILE  |
| 1   | B     | 290 | HIS  |
| 1   | B     | 334 | TYR  |
| 1   | B     | 340 | THR  |
| 1   | B     | 345 | ILE  |
| 1   | B     | 349 | ASP  |
| 1   | B     | 358 | SER  |
| 1   | B     | 369 | LEU  |
| 1   | B     | 373 | THR  |
| 1   | B     | 393 | GLN  |
| 1   | B     | 403 | GLN  |
| 1   | B     | 405 | GLU  |
| 1   | B     | 406 | SER  |
| 1   | B     | 415 | THR  |
| 1   | C     | 5   | LEU  |
| 1   | C     | 39  | MET  |
| 1   | C     | 63  | PRO  |
| 1   | C     | 72  | ASN  |
| 1   | C     | 78  | TRP  |
| 1   | C     | 120 | THR  |
| 1   | C     | 121 | THR  |
| 1   | C     | 137 | ASN  |
| 1   | C     | 142 | PHE  |
| 1   | C     | 144 | LEU  |
| 1   | C     | 162 | LEU  |
| 1   | C     | 171 | MET  |
| 1   | C     | 197 | THR  |
| 1   | C     | 203 | ASN  |
| 1   | C     | 217 | LEU  |
| 1   | C     | 219 | LYS  |
| 1   | C     | 231 | VAL  |
| 1   | C     | 263 | GLN  |
| 1   | C     | 272 | PRO  |
| 1   | C     | 275 | TRP  |
| 1   | C     | 278 | SER  |
| 1   | C     | 282 | ARG  |
| 1   | C     | 285 | PRO  |
| 1   | C     | 303 | GLN  |
| 1   | C     | 317 | LYS  |
| 1   | C     | 326 | ARG  |
| 1   | C     | 331 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 349 | ASP  |
| 1   | C     | 355 | GLN  |
| 1   | C     | 364 | GLN  |
| 1   | C     | 404 | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | ASN  |
| 1   | A     | 29  | ASN  |
| 1   | A     | 57  | ASN  |
| 1   | A     | 72  | ASN  |
| 1   | A     | 89  | ASN  |
| 1   | A     | 109 | ASN  |
| 1   | A     | 127 | ASN  |
| 1   | A     | 137 | ASN  |
| 1   | A     | 147 | ASN  |
| 1   | A     | 189 | ASN  |
| 1   | A     | 199 | HIS  |
| 1   | A     | 210 | ASN  |
| 1   | A     | 248 | ASN  |
| 1   | A     | 300 | GLN  |
| 1   | A     | 303 | GLN  |
| 1   | A     | 316 | GLN  |
| 1   | A     | 355 | GLN  |
| 1   | A     | 356 | ASN  |
| 1   | A     | 393 | GLN  |
| 1   | A     | 416 | ASN  |
| 1   | A     | 418 | ASN  |
| 1   | B     | 6   | ASN  |
| 1   | B     | 29  | ASN  |
| 1   | B     | 57  | ASN  |
| 1   | B     | 72  | ASN  |
| 1   | B     | 83  | HIS  |
| 1   | B     | 89  | ASN  |
| 1   | B     | 91  | GLN  |
| 1   | B     | 109 | ASN  |
| 1   | B     | 129 | ASN  |
| 1   | B     | 137 | ASN  |
| 1   | B     | 147 | ASN  |
| 1   | B     | 164 | GLN  |
| 1   | B     | 177 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 182 | GLN  |
| 1   | B     | 189 | ASN  |
| 1   | B     | 203 | ASN  |
| 1   | B     | 210 | ASN  |
| 1   | B     | 270 | ASN  |
| 1   | B     | 281 | ASN  |
| 1   | B     | 290 | HIS  |
| 1   | B     | 300 | GLN  |
| 1   | B     | 302 | GLN  |
| 1   | B     | 303 | GLN  |
| 1   | B     | 316 | GLN  |
| 1   | B     | 338 | ASN  |
| 1   | B     | 356 | ASN  |
| 1   | B     | 393 | GLN  |
| 1   | B     | 416 | ASN  |
| 1   | B     | 418 | ASN  |
| 1   | C     | 6   | ASN  |
| 1   | C     | 29  | ASN  |
| 1   | C     | 57  | ASN  |
| 1   | C     | 72  | ASN  |
| 1   | C     | 81  | ASN  |
| 1   | C     | 91  | GLN  |
| 1   | C     | 129 | ASN  |
| 1   | C     | 137 | ASN  |
| 1   | C     | 189 | ASN  |
| 1   | C     | 210 | ASN  |
| 1   | C     | 220 | ASN  |
| 1   | C     | 238 | ASN  |
| 1   | C     | 244 | ASN  |
| 1   | C     | 248 | ASN  |
| 1   | C     | 270 | ASN  |
| 1   | C     | 281 | ASN  |
| 1   | C     | 290 | HIS  |
| 1   | C     | 300 | GLN  |
| 1   | C     | 316 | GLN  |
| 1   | C     | 338 | ASN  |
| 1   | C     | 355 | GLN  |
| 1   | C     | 356 | ASN  |
| 1   | C     | 393 | GLN  |
| 1   | C     | 416 | ASN  |
| 1   | C     | 418 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | LDA  | C     | 502 | -    | 13,15,15     | 2.08 | 2 (15%)  | 14,17,17    | 1.57 | 3 (21%)  |
| 2   | LDA  | B     | 504 | -    | 13,15,15     | 2.03 | 2 (15%)  | 14,17,17    | 1.88 | 3 (21%)  |
| 2   | LDA  | C     | 501 | -    | 13,15,15     | 2.07 | 1 (7%)   | 14,17,17    | 1.32 | 2 (14%)  |
| 2   | LDA  | A     | 505 | -    | 13,15,15     | 1.92 | 1 (7%)   | 14,17,17    | 1.70 | 3 (21%)  |
| 2   | LDA  | A     | 506 | -    | 13,15,15     | 1.89 | 1 (7%)   | 14,17,17    | 1.81 | 5 (35%)  |
| 2   | LDA  | B     | 503 | -    | 13,15,15     | 2.06 | 1 (7%)   | 14,17,17    | 1.41 | 1 (7%)   |

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 |
|-----|------|-------|-----|------|---------|------------|-------|
| 2   | LDA  | C     | 502 | -    | -       | 6/13/13/13 | -     |
| 2   | LDA  | B     | 504 | -    | -       | 7/13/13/13 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 2   | LDA  | C     | 501 | -    | -       | 8/13/13/13 | -     |
| 2   | LDA  | A     | 505 | -    | -       | 8/13/13/13 | -     |
| 2   | LDA  | A     | 506 | -    | -       | 6/13/13/13 | -     |
| 2   | LDA  | B     | 503 | -    | -       | 7/13/13/13 | -     |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | B     | 503 | LDA  | O1-N1 | -6.91 | 1.25        | 1.42     |
| 2   | C     | 501 | LDA  | O1-N1 | -6.83 | 1.25        | 1.42     |
| 2   | A     | 506 | LDA  | O1-N1 | -6.37 | 1.26        | 1.42     |
| 2   | C     | 502 | LDA  | O1-N1 | -6.32 | 1.26        | 1.42     |
| 2   | A     | 505 | LDA  | O1-N1 | -5.96 | 1.27        | 1.42     |
| 2   | B     | 504 | LDA  | O1-N1 | -5.91 | 1.27        | 1.42     |
| 2   | B     | 504 | LDA  | C1-N1 | 3.26  | 1.54        | 1.51     |
| 2   | C     | 502 | LDA  | C1-N1 | 2.77  | 1.54        | 1.51     |

All (17) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | B     | 504 | LDA  | CM1-N1-C1 | -4.81 | 100.13      | 110.23   |
| 2   | A     | 505 | LDA  | CM1-N1-C1 | -4.01 | 101.82      | 110.23   |
| 2   | A     | 506 | LDA  | CM1-N1-C1 | -3.93 | 101.98      | 110.23   |
| 2   | C     | 502 | LDA  | O1-N1-C1  | 3.00  | 116.62      | 109.27   |
| 2   | B     | 504 | LDA  | CM2-N1-C1 | 2.89  | 116.30      | 110.23   |
| 2   | C     | 502 | LDA  | CM1-N1-C1 | -2.86 | 104.23      | 110.23   |
| 2   | B     | 503 | LDA  | CM1-N1-C1 | -2.83 | 104.30      | 110.23   |
| 2   | B     | 504 | LDA  | O1-N1-C1  | 2.74  | 116.00      | 109.27   |
| 2   | A     | 505 | LDA  | O1-N1-C1  | 2.70  | 115.89      | 109.27   |
| 2   | A     | 506 | LDA  | C6-C5-C4  | -2.32 | 102.64      | 114.37   |
| 2   | C     | 502 | LDA  | C9-C8-C7  | -2.30 | 102.72      | 114.37   |
| 2   | A     | 506 | LDA  | O1-N1-C1  | 2.26  | 114.82      | 109.27   |
| 2   | A     | 505 | LDA  | C9-C8-C7  | -2.24 | 103.02      | 114.37   |
| 2   | A     | 506 | LDA  | C9-C8-C7  | -2.24 | 103.05      | 114.37   |
| 2   | A     | 506 | LDA  | CM2-N1-C1 | 2.16  | 114.78      | 110.23   |
| 2   | C     | 501 | LDA  | CM2-N1-C1 | 2.13  | 114.71      | 110.23   |
| 2   | C     | 501 | LDA  | CM1-N1-C1 | -2.11 | 105.81      | 110.23   |

There are no chirality outliers.

All (42) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 2   | A     | 505 | LDA  | C2-C1-N1-O1   |
| 2   | A     | 505 | LDA  | C2-C1-N1-CM1  |
| 2   | A     | 505 | LDA  | C2-C1-N1-CM2  |
| 2   | A     | 506 | LDA  | N1-C1-C2-C3   |
| 2   | B     | 504 | LDA  | C2-C1-N1-O1   |
| 2   | B     | 504 | LDA  | C2-C1-N1-CM2  |
| 2   | C     | 501 | LDA  | C2-C1-N1-O1   |
| 2   | C     | 501 | LDA  | C2-C1-N1-CM1  |
| 2   | C     | 501 | LDA  | C2-C1-N1-CM2  |
| 2   | C     | 502 | LDA  | C2-C1-N1-O1   |
| 2   | C     | 502 | LDA  | C2-C1-N1-CM1  |
| 2   | C     | 502 | LDA  | C2-C1-N1-CM2  |
| 2   | C     | 502 | LDA  | C1-C2-C3-C4   |
| 2   | B     | 503 | LDA  | C2-C3-C4-C5   |
| 2   | A     | 506 | LDA  | C11-C10-C9-C8 |
| 2   | B     | 503 | LDA  | C11-C10-C9-C8 |
| 2   | C     | 502 | LDA  | C11-C10-C9-C8 |
| 2   | B     | 503 | LDA  | C3-C4-C5-C6   |
| 2   | B     | 503 | LDA  | C1-C2-C3-C4   |
| 2   | A     | 506 | LDA  | C1-C2-C3-C4   |
| 2   | C     | 501 | LDA  | C6-C7-C8-C9   |
| 2   | A     | 506 | LDA  | C3-C4-C5-C6   |
| 2   | A     | 505 | LDA  | C3-C4-C5-C6   |
| 2   | B     | 503 | LDA  | C7-C8-C9-C10  |
| 2   | A     | 505 | LDA  | C6-C7-C8-C9   |
| 2   | A     | 506 | LDA  | C7-C8-C9-C10  |
| 2   | B     | 504 | LDA  | C11-C10-C9-C8 |
| 2   | B     | 504 | LDA  | C2-C3-C4-C5   |
| 2   | A     | 505 | LDA  | C1-C2-C3-C4   |
| 2   | C     | 502 | LDA  | C2-C3-C4-C5   |
| 2   | B     | 504 | LDA  | C7-C8-C9-C10  |
| 2   | A     | 506 | LDA  | C2-C3-C4-C5   |
| 2   | B     | 503 | LDA  | C2-C1-N1-CM2  |
| 2   | B     | 504 | LDA  | C2-C1-N1-CM1  |
| 2   | B     | 503 | LDA  | C6-C7-C8-C9   |
| 2   | B     | 504 | LDA  | C3-C4-C5-C6   |
| 2   | C     | 501 | LDA  | C1-C2-C3-C4   |
| 2   | C     | 501 | LDA  | N1-C1-C2-C3   |
| 2   | C     | 501 | LDA  | C2-C3-C4-C5   |
| 2   | A     | 505 | LDA  | C11-C10-C9-C8 |
| 2   | A     | 505 | LDA  | C2-C3-C4-C5   |
| 2   | C     | 501 | LDA  | C11-C10-C9-C8 |

There are no ring outliers.

6 monomers are involved in 49 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | C     | 502 | LDA  | 8       | 0            |
| 2   | B     | 504 | LDA  | 2       | 0            |
| 2   | C     | 501 | LDA  | 11      | 0            |
| 2   | A     | 505 | LDA  | 3       | 0            |
| 2   | A     | 506 | LDA  | 16      | 0            |
| 2   | B     | 503 | LDA  | 9       | 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|--------------|-----------------------|-------|
| 1   | A     | 412/427 (96%)   | -0.30  | 0 100 100    | 4, 20, 35, 50         | 0     |
| 1   | B     | 421/427 (98%)   | -0.24  | 1 (0%) 91 86 | 10, 24, 35, 46        | 0     |
| 1   | C     | 416/427 (97%)   | -0.20  | 4 (0%) 79 63 | 7, 25, 38, 45         | 0     |
| All | All   | 1249/1281 (97%) | -0.25  | 5 (0%) 88 79 | 4, 23, 36, 50         | 0     |

All (5) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 78  | TRP  | 2.4  |
| 1   | C     | 107 | GLU  | 2.4  |
| 1   | C     | 249 | ASN  | 2.3  |
| 1   | C     | 354 | ALA  | 2.2  |
| 1   | B     | 354 | ALA  | 2.1  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.



| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | LDA  | C     | 502 | 16/16 | 0.66 | 0.14 | 30,37,47,47                 | 0     |
| 2   | LDA  | B     | 504 | 16/16 | 0.78 | 0.12 | 22,32,37,37                 | 0     |
| 2   | LDA  | C     | 501 | 16/16 | 0.84 | 0.12 | 18,21,31,31                 | 0     |
| 2   | LDA  | A     | 505 | 16/16 | 0.86 | 0.11 | 25,29,30,30                 | 0     |
| 2   | LDA  | B     | 503 | 16/16 | 0.87 | 0.11 | 23,26,39,40                 | 0     |
| 2   | LDA  | A     | 506 | 16/16 | 0.90 | 0.11 | 21,30,46,46                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.