



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:56 PM UTC

PDB ID : 2IBM / pdb\_00002ibm  
Title : A novel dimer interface and conformational changes revealed by an X-ray structure of B. subtilis SecA  
Authors : Zimmer, J.; Li, W.; Rapoport, T.A.  
Deposited on : 2006-09-11  
Resolution : 3.20 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  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

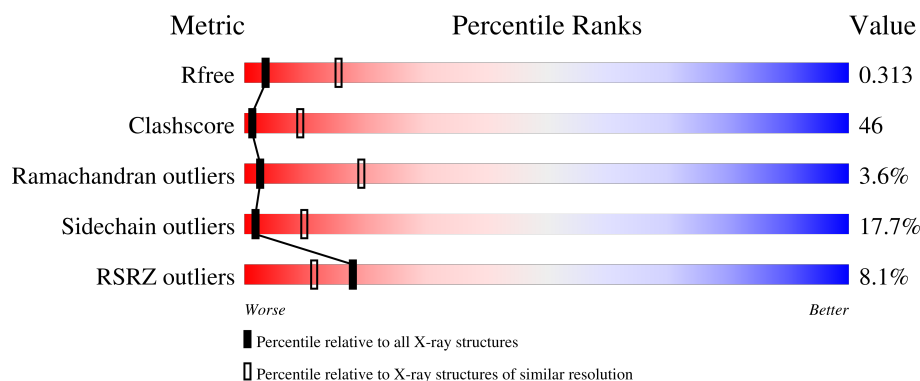
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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                      | 1466 (3.20-3.20)                                      |
| Clashscore            | 190562                      | 1573 (3.20-3.20)                                      |
| Ramachandran outliers | 187476                      | 1548 (3.20-3.20)                                      |
| Sidechain outliers    | 187428                      | 1547 (3.20-3.20)                                      |
| RSRZ outliers         | 180081                      | 1466 (3.20-3.20)                                      |

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     | 780    | <div> <div>9%</div> <div>41%</div> <div>45%</div> <div>13%</div> <div>.</div> </div>  |
| 1   | B     | 780    | <div> <div>7%</div> <div>41%</div> <div>43%</div> <div>12%</div> <div>..</div> </div> |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 12403 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 Preprotein translocase secA subunit.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 780      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6228  | 3899 | 1084 | 1210 | 35 |         |         |       |
| 1   | B     | 770      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6148  | 3846 | 1072 | 1197 | 33 |         |         |       |

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

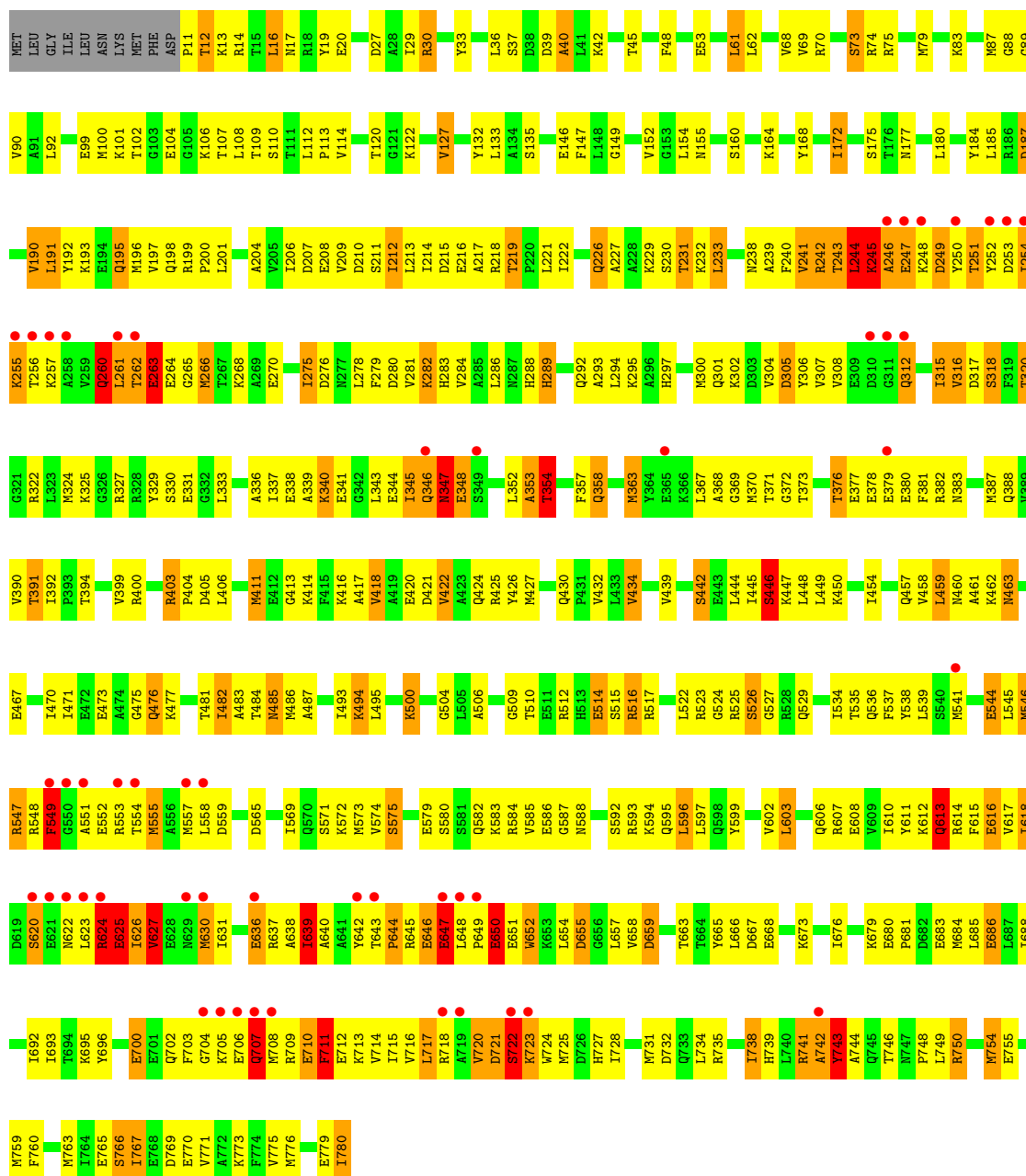


| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |





● Molecule 1: Preprotein translocase secA subunit



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | I 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 125.83Å 166.83Å 211.99Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 40.53 – 3.20<br>40.53 – 3.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 92.7 (40.53-3.20)<br>92.6 (40.53-3.20)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.07                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.18 (at 3.12Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.321 , 0.323<br>0.304 , 0.313                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3431 reflections (8.64%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 69.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.095                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 36.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.85                                                        | EDS              |
| Total number of atoms                                                   | 12403                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 47.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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 [i](#)

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

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

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     | 0.82         | 8/6316 (0.1%)   | 1.26        | 54/8492 (0.6%)   |
| 1   | B     | 0.88         | 9/6235 (0.1%)   | 1.29        | 72/8384 (0.9%)   |
| All | All   | 0.85         | 17/12551 (0.1%) | 1.28        | 126/16876 (0.7%) |

All (17) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | B     | 354 | THR  | CB-OG1 | -16.79 | 1.16        | 1.43     |
| 1   | A     | 279 | PHE  | C-N    | 11.55  | 1.49        | 1.33     |
| 1   | B     | 352 | LEU  | C-N    | 9.59   | 1.45        | 1.33     |
| 1   | A     | 701 | GLU  | N-CA   | 7.96   | 1.56        | 1.46     |
| 1   | B     | 243 | THR  | C-N    | 7.52   | 1.42        | 1.33     |
| 1   | A     | 280 | ASP  | N-CA   | 7.24   | 1.55        | 1.46     |
| 1   | B     | 247 | GLU  | CA-C   | -7.19  | 1.45        | 1.53     |
| 1   | B     | 244 | LEU  | N-CA   | 6.53   | 1.54        | 1.46     |
| 1   | B     | 639 | ILE  | CA-CB  | 6.12   | 1.60        | 1.54     |
| 1   | B     | 354 | THR  | C-N    | 6.09   | 1.42        | 1.33     |
| 1   | A     | 624 | ARG  | CA-C   | -6.08  | 1.45        | 1.53     |
| 1   | B     | 622 | ASN  | CA-C   | 6.02   | 1.60        | 1.52     |
| 1   | A     | 277 | ASN  | CA-C   | 5.55   | 1.60        | 1.52     |
| 1   | A     | 700 | GLU  | CA-C   | 5.27   | 1.59        | 1.52     |
| 1   | B     | 244 | LEU  | CA-C   | 5.24   | 1.58        | 1.52     |
| 1   | A     | 11  | PRO  | C-N    | 5.12   | 1.39        | 1.33     |
| 1   | A     | 303 | ASP  | N-CA   | -5.07  | 1.39        | 1.46     |

All (126) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 14  | ARG  | N-CA-C | -18.24 | 93.82       | 114.62   |
| 1   | B     | 244 | LEU  | CA-C-N | 13.49  | 147.31      | 121.54   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | B     | 244 | LEU  | C-N-CA     | 13.49  | 147.31      | 121.54   |
| 1   | A     | 10  | ASP  | CA-C-N     | 12.82  | 135.87      | 119.84   |
| 1   | A     | 10  | ASP  | C-N-CA     | 12.82  | 135.87      | 119.84   |
| 1   | B     | 244 | LEU  | N-CA-C     | 11.93  | 127.04      | 108.79   |
| 1   | B     | 702 | GLN  | OE1-CD-NE2 | -10.65 | 111.95      | 122.60   |
| 1   | A     | 702 | GLN  | OE1-CD-NE2 | -10.64 | 111.95      | 122.60   |
| 1   | A     | 620 | SER  | N-CA-C     | 10.49  | 124.69      | 112.72   |
| 1   | A     | 707 | GLN  | OE1-CD-NE2 | -10.48 | 112.11      | 122.60   |
| 1   | B     | 707 | GLN  | OE1-CD-NE2 | -10.26 | 112.34      | 122.60   |
| 1   | B     | 260 | GLN  | OE1-CD-NE2 | -10.20 | 112.40      | 122.60   |
| 1   | A     | 312 | GLN  | OE1-CD-NE2 | -10.17 | 112.43      | 122.60   |
| 1   | B     | 346 | GLN  | OE1-CD-NE2 | -10.14 | 112.46      | 122.60   |
| 1   | A     | 260 | GLN  | OE1-CD-NE2 | -9.88  | 112.72      | 122.60   |
| 1   | B     | 312 | GLN  | OE1-CD-NE2 | -9.80  | 112.80      | 122.60   |
| 1   | A     | 745 | GLN  | OE1-CD-NE2 | -9.80  | 112.80      | 122.60   |
| 1   | A     | 301 | GLN  | OE1-CD-NE2 | -9.79  | 112.81      | 122.60   |
| 1   | B     | 613 | GLN  | OE1-CD-NE2 | -9.64  | 112.96      | 122.60   |
| 1   | B     | 529 | GLN  | OE1-CD-NE2 | -9.28  | 113.32      | 122.60   |
| 1   | A     | 346 | GLN  | OE1-CD-NE2 | -9.15  | 113.45      | 122.60   |
| 1   | A     | 226 | GLN  | OE1-CD-NE2 | -9.12  | 113.48      | 122.60   |
| 1   | B     | 354 | THR  | CA-CB-OG1  | 9.11   | 123.26      | 109.60   |
| 1   | A     | 11  | PRO  | N-CA-C     | 8.99   | 130.99      | 112.47   |
| 1   | B     | 346 | GLN  | N-CA-C     | 8.74   | 123.21      | 112.54   |
| 1   | A     | 301 | GLN  | N-CA-C     | 8.74   | 123.77      | 109.96   |
| 1   | B     | 618 | ILE  | N-CA-C     | 8.35   | 119.13      | 110.62   |
| 1   | B     | 249 | ASP  | CA-CB-CG   | 8.27   | 120.87      | 112.60   |
| 1   | B     | 40  | ALA  | N-CA-C     | -8.21  | 102.98      | 113.16   |
| 1   | B     | 247 | GLU  | O-C-N      | 8.18   | 132.64      | 122.91   |
| 1   | B     | 717 | LEU  | CA-C-N     | -8.16  | 109.08      | 122.54   |
| 1   | B     | 717 | LEU  | C-N-CA     | -8.16  | 109.08      | 122.54   |
| 1   | A     | 279 | PHE  | CA-CB-CG   | 8.13   | 121.93      | 113.80   |
| 1   | B     | 244 | LEU  | O-C-N      | 7.93   | 131.90      | 123.42   |
| 1   | B     | 741 | ARG  | N-CA-C     | 7.65   | 122.11      | 109.95   |
| 1   | B     | 247 | GLU  | N-CA-C     | -7.63  | 100.98      | 111.28   |
| 1   | A     | 543 | ASP  | N-CA-C     | 7.59   | 120.28      | 108.96   |
| 1   | A     | 280 | ASP  | CA-C-N     | 7.54   | 135.54      | 121.97   |
| 1   | A     | 280 | ASP  | C-N-CA     | 7.54   | 135.54      | 121.97   |
| 1   | B     | 705 | LYS  | N-CA-C     | -7.38  | 103.41      | 113.30   |
| 1   | B     | 403 | ARG  | CA-C-N     | 7.31   | 127.74      | 119.92   |
| 1   | B     | 403 | ARG  | C-N-CA     | 7.31   | 127.74      | 119.92   |
| 1   | B     | 652 | TRP  | N-CA-C     | 7.25   | 121.31      | 109.72   |
| 1   | A     | 252 | TYR  | N-CA-C     | 7.24   | 117.57      | 108.45   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 301 | GLN  | CG-CD-NE2  | 7.21  | 127.22      | 116.40   |
| 1   | B     | 346 | GLN  | CG-CD-NE2  | 7.18  | 127.17      | 116.40   |
| 1   | B     | 247 | GLU  | CA-C-O     | 7.13  | 130.95      | 122.03   |
| 1   | B     | 613 | GLN  | CG-CD-NE2  | 7.13  | 127.10      | 116.40   |
| 1   | B     | 244 | LEU  | CA-C-O     | 7.08  | 128.80      | 121.23   |
| 1   | B     | 702 | GLN  | CG-CD-NE2  | 7.02  | 126.93      | 116.40   |
| 1   | A     | 702 | GLN  | CG-CD-NE2  | 7.01  | 126.92      | 116.40   |
| 1   | B     | 353 | ALA  | N-CA-CB    | 7.01  | 122.42      | 111.56   |
| 1   | A     | 707 | GLN  | CG-CD-NE2  | 6.99  | 126.89      | 116.40   |
| 1   | A     | 230 | SER  | N-CA-C     | 6.98  | 125.67      | 110.80   |
| 1   | A     | 705 | LYS  | N-CA-C     | -6.97 | 103.96      | 113.30   |
| 1   | B     | 650 | GLU  | N-CA-C     | 6.92  | 121.34      | 112.34   |
| 1   | B     | 529 | GLN  | CG-CD-NE2  | 6.91  | 126.77      | 116.40   |
| 1   | A     | 260 | GLN  | CG-CD-NE2  | 6.81  | 126.62      | 116.40   |
| 1   | B     | 260 | GLN  | CG-CD-NE2  | 6.70  | 126.44      | 116.40   |
| 1   | A     | 745 | GLN  | CG-CD-NE2  | 6.68  | 126.42      | 116.40   |
| 1   | A     | 279 | PHE  | CB-CA-C    | 6.67  | 119.67      | 109.34   |
| 1   | B     | 246 | ALA  | N-CA-C     | -6.62 | 105.27      | 113.15   |
| 1   | B     | 710 | GLU  | CA-C-N     | 6.62  | 129.15      | 120.28   |
| 1   | B     | 710 | GLU  | C-N-CA     | 6.62  | 129.15      | 120.28   |
| 1   | A     | 7   | LYS  | CA-C-N     | -6.61 | 110.16      | 121.85   |
| 1   | A     | 7   | LYS  | C-N-CA     | -6.61 | 110.16      | 121.85   |
| 1   | A     | 704 | GLY  | N-CA-C     | 6.50  | 127.12      | 115.80   |
| 1   | B     | 711 | PHE  | CB-CA-C    | -6.48 | 100.04      | 110.79   |
| 1   | B     | 707 | GLN  | CG-CD-NE2  | 6.37  | 125.96      | 116.40   |
| 1   | A     | 312 | GLN  | CG-CD-NE2  | 6.32  | 125.88      | 116.40   |
| 1   | B     | 704 | GLY  | N-CA-C     | 6.29  | 128.08      | 113.18   |
| 1   | B     | 702 | GLN  | CA-C-N     | -6.21 | 113.43      | 122.44   |
| 1   | B     | 702 | GLN  | C-N-CA     | -6.21 | 113.43      | 122.44   |
| 1   | A     | 346 | GLN  | CG-CD-NE2  | 6.19  | 125.69      | 116.40   |
| 1   | B     | 722 | SER  | CB-CA-C    | -6.16 | 100.70      | 110.86   |
| 1   | B     | 624 | ARG  | CB-CA-C    | 6.15  | 122.10      | 110.35   |
| 1   | B     | 624 | ARG  | CA-CB-CG   | 6.14  | 126.39      | 114.10   |
| 1   | A     | 280 | ASP  | CA-CB-CG   | -6.12 | 106.48      | 112.60   |
| 1   | A     | 226 | GLN  | CG-CD-NE2  | 6.01  | 125.42      | 116.40   |
| 1   | B     | 650 | GLU  | N-CA-CB    | -6.01 | 99.36       | 110.18   |
| 1   | B     | 208 | GLU  | N-CA-C     | -5.97 | 103.91      | 111.92   |
| 1   | B     | 312 | GLN  | CG-CD-NE2  | 5.94  | 125.31      | 116.40   |
| 1   | B     | 623 | LEU  | CA-C-O     | 5.89  | 126.09      | 119.78   |
| 1   | B     | 418 | VAL  | N-CA-C     | -5.89 | 105.38      | 110.74   |
| 1   | A     | 652 | TRP  | N-CA-C     | 5.87  | 118.62      | 109.52   |
| 1   | B     | 354 | THR  | OG1-CB-CG2 | 5.86  | 121.01      | 109.30   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 758 | ALA  | N-CA-C   | -5.85 | 104.59      | 110.97   |
| 1   | B     | 245 | LYS  | N-CA-C   | -5.77 | 98.51       | 110.80   |
| 1   | B     | 346 | GLN  | CA-C-N   | -5.73 | 113.69      | 122.62   |
| 1   | B     | 346 | GLN  | C-N-CA   | -5.73 | 113.69      | 122.62   |
| 1   | A     | 747 | ASN  | CA-C-N   | 5.67  | 126.92      | 119.84   |
| 1   | A     | 747 | ASN  | C-N-CA   | 5.67  | 126.92      | 119.84   |
| 1   | A     | 212 | ILE  | N-CA-C   | 5.62  | 115.75      | 110.30   |
| 1   | B     | 647 | GLU  | CB-CG-CD | 5.61  | 122.14      | 112.60   |
| 1   | A     | 280 | ASP  | N-CA-CB  | 5.60  | 119.96      | 110.49   |
| 1   | B     | 347 | ASN  | N-CA-C   | 5.60  | 118.35      | 109.50   |
| 1   | A     | 277 | ASN  | N-CA-C   | -5.60 | 101.62      | 109.96   |
| 1   | B     | 427 | MET  | N-CA-C   | -5.58 | 105.30      | 111.71   |
| 1   | A     | 10  | ASP  | O-C-N    | 5.50  | 127.65      | 121.32   |
| 1   | A     | 483 | ALA  | N-CA-C   | 5.50  | 118.44      | 107.62   |
| 1   | B     | 623 | LEU  | O-C-N    | 5.49  | 129.73      | 122.04   |
| 1   | B     | 343 | LEU  | N-CA-C   | -5.49 | 102.08      | 110.14   |
| 1   | A     | 563 | MET  | N-CA-C   | 5.38  | 122.25      | 110.80   |
| 1   | A     | 11  | PRO  | CB-CA-C  | -5.36 | 102.72      | 111.56   |
| 1   | B     | 245 | LYS  | N-CA-CB  | 5.34  | 119.52      | 110.49   |
| 1   | A     | 277 | ASN  | CB-CA-C  | 5.34  | 117.84      | 110.16   |
| 1   | B     | 767 | ILE  | CB-CA-C  | -5.33 | 105.15      | 111.97   |
| 1   | B     | 743 | TYR  | N-CA-C   | 5.32  | 122.13      | 110.80   |
| 1   | B     | 214 | ILE  | N-CA-C   | 5.30  | 115.50      | 110.42   |
| 1   | B     | 549 | PHE  | N-CA-C   | 5.29  | 116.92      | 110.41   |
| 1   | B     | 742 | ALA  | CA-C-N   | 5.24  | 131.54      | 121.54   |
| 1   | B     | 742 | ALA  | C-N-CA   | 5.24  | 131.54      | 121.54   |
| 1   | B     | 353 | ALA  | CB-CA-C  | -5.23 | 100.89      | 110.62   |
| 1   | A     | 687 | LEU  | N-CA-C   | 5.22  | 116.97      | 111.28   |
| 1   | A     | 303 | ASP  | N-CA-C   | 5.20  | 118.76      | 111.74   |
| 1   | B     | 622 | ASN  | N-CA-C   | 5.18  | 117.73      | 109.96   |
| 1   | B     | 721 | ASP  | N-CA-C   | 5.15  | 119.60      | 112.45   |
| 1   | A     | 311 | GLY  | N-CA-C   | -5.11 | 101.07      | 113.18   |
| 1   | B     | 620 | SER  | CB-CA-C  | 5.09  | 118.54      | 109.38   |
| 1   | A     | 549 | PHE  | O-C-N    | -5.08 | 116.24      | 122.34   |
| 1   | B     | 625 | GLU  | N-CA-C   | 5.04  | 121.54      | 110.80   |
| 1   | A     | 213 | LEU  | CA-C-N   | -5.04 | 116.40      | 122.35   |
| 1   | A     | 213 | LEU  | C-N-CA   | -5.04 | 116.40      | 122.35   |
| 1   | A     | 276 | ASP  | CA-C-N   | -5.03 | 113.57      | 121.02   |
| 1   | A     | 276 | ASP  | C-N-CA   | -5.03 | 113.57      | 121.02   |
| 1   | B     | 596 | LEU  | N-CA-C   | -5.00 | 105.52      | 110.97   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 6228  | 0        | 6227     | 576     | 0            |
| 1   | B     | 6148  | 0        | 6139     | 605     | 0            |
| 2   | A     | 27    | 0        | 12       | 3       | 0            |
| All | All   | 12403 | 0        | 12378    | 1148    | 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 46.

All (1148) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:620:SER:HB3  | 1:B:625:GLU:CG   | 1.49                     | 1.39              |
| 1:A:723:LYS:HD3  | 1:A:763:MET:SD   | 1.67                     | 1.35              |
| 1:A:747:ASN:H    | 1:A:748:PRO:CD   | 1.39                     | 1.31              |
| 1:A:10:ASP:HB3   | 1:A:11:PRO:CD    | 1.61                     | 1.29              |
| 1:A:303:ASP:O    | 1:A:304:VAL:HG23 | 1.10                     | 1.28              |
| 1:A:747:ASN:N    | 1:A:748:PRO:HD2  | 1.34                     | 1.27              |
| 1:B:650:GLU:C    | 1:B:650:GLU:OE1  | 1.78                     | 1.26              |
| 1:B:723:LYS:CE   | 1:B:767:ILE:HD11 | 1.66                     | 1.25              |
| 1:A:10:ASP:CB    | 1:A:11:PRO:HD2   | 1.57                     | 1.25              |
| 1:B:620:SER:HB3  | 1:B:625:GLU:CB   | 1.67                     | 1.25              |
| 1:B:723:LYS:HE3  | 1:B:767:ILE:CD1  | 1.65                     | 1.25              |
| 1:A:723:LYS:CD   | 1:A:763:MET:SD   | 2.31                     | 1.18              |
| 1:A:303:ASP:O    | 1:A:304:VAL:CG2  | 1.93                     | 1.16              |
| 1:B:245:LYS:HE3  | 1:B:247:GLU:OE1  | 1.40                     | 1.16              |
| 1:B:624:ARG:HH21 | 1:B:707:GLN:CB   | 1.57                     | 1.16              |
| 1:B:248:LYS:HB2  | 1:B:265:GLY:CA   | 1.76                     | 1.15              |
| 1:B:650:GLU:OE1  | 1:B:650:GLU:O    | 1.63                     | 1.14              |
| 1:B:248:LYS:HB2  | 1:B:265:GLY:HA3  | 1.15                     | 1.14              |
| 1:B:718:ARG:HG3  | 1:B:770:GLU:OE2  | 1.48                     | 1.13              |
| 1:B:624:ARG:HH21 | 1:B:707:GLN:HB3  | 0.96                     | 1.13              |
| 1:A:278:LEU:HB3  | 1:A:283:HIS:CG   | 1.83                     | 1.11              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:281:VAL:HB   | 1:A:283:HIS:CD2  | 1.86                     | 1.11              |
| 1:A:661:ILE:HG22 | 1:A:666:LEU:HD21 | 1.23                     | 1.10              |
| 1:B:750:ARG:HG2  | 1:B:750:ARG:HH11 | 1.07                     | 1.09              |
| 1:B:620:SER:HB3  | 1:B:625:GLU:HG2  | 1.13                     | 1.08              |
| 1:B:647:GLU:C    | 1:B:652:TRP:HH2  | 1.61                     | 1.08              |
| 1:B:630:MET:SD   | 1:B:775:VAL:HG21 | 1.93                     | 1.07              |
| 1:B:620:SER:CB   | 1:B:625:GLU:HG2  | 1.85                     | 1.06              |
| 1:A:661:ILE:HG22 | 1:A:666:LEU:CD2  | 1.85                     | 1.06              |
| 1:A:349:SER:HB3  | 1:B:557:MET:HG3  | 1.37                     | 1.05              |
| 1:B:620:SER:CB   | 1:B:625:GLU:CG   | 2.33                     | 1.05              |
| 1:A:349:SER:CB   | 1:B:557:MET:HG3  | 1.86                     | 1.05              |
| 1:A:558:LEU:HG   | 1:A:563:MET:CE   | 1.87                     | 1.04              |
| 1:B:516:ARG:CZ   | 1:B:582:GLN:HG2  | 1.86                     | 1.04              |
| 1:B:723:LYS:HB2  | 1:B:763:MET:CG   | 1.87                     | 1.04              |
| 1:B:647:GLU:CB   | 1:B:652:TRP:CZ3  | 2.42                     | 1.03              |
| 1:A:254:ILE:HG22 | 1:A:255:LYS:H    | 0.86                     | 1.03              |
| 1:B:718:ARG:HG3  | 1:B:770:GLU:CD   | 1.82                     | 1.03              |
| 1:A:284:VAL:HG21 | 1:A:717:LEU:HD21 | 1.35                     | 1.01              |
| 1:A:279:PHE:HA   | 1:A:778:ALA:HB1  | 1.42                     | 1.01              |
| 1:B:243:THR:C    | 1:B:244:LEU:HD23 | 1.85                     | 1.01              |
| 1:B:637:ARG:HH21 | 1:B:769:ASP:HB3  | 1.21                     | 1.01              |
| 1:B:620:SER:CB   | 1:B:625:GLU:HB3  | 1.89                     | 1.01              |
| 1:A:254:ILE:HG22 | 1:A:255:LYS:N    | 1.66                     | 1.00              |
| 1:A:708:MET:SD   | 1:A:711:PHE:HE1  | 1.84                     | 1.00              |
| 1:A:254:ILE:CG2  | 1:A:255:LYS:H    | 1.72                     | 0.99              |
| 1:A:563:MET:O    | 1:A:564:ASP:OD1  | 1.80                     | 0.99              |
| 1:A:723:LYS:HD3  | 1:A:763:MET:CE   | 1.92                     | 0.99              |
| 1:B:275:ILE:HD11 | 1:B:283:HIS:CD2  | 1.98                     | 0.99              |
| 1:A:553:ARG:HH21 | 1:A:560:ARG:HH21 | 1.02                     | 0.99              |
| 1:A:661:ILE:CG2  | 1:A:666:LEU:HD21 | 1.93                     | 0.99              |
| 1:B:295:LYS:HE2  | 1:B:333:LEU:HD22 | 1.39                     | 0.99              |
| 1:A:226:GLN:HE21 | 1:A:228:ALA:H    | 1.11                     | 0.98              |
| 1:B:248:LYS:CB   | 1:B:265:GLY:CA   | 2.41                     | 0.98              |
| 1:B:218:ARG:HD3  | 1:B:592:SER:HB3  | 1.44                     | 0.98              |
| 1:A:485:ASN:O    | 1:A:486:MET:HG2  | 1.63                     | 0.98              |
| 1:B:620:SER:HB3  | 1:B:625:GLU:HB3  | 1.39                     | 0.97              |
| 1:A:457:GLN:HE21 | 1:A:470:ILE:HD12 | 1.27                     | 0.97              |
| 1:A:558:LEU:HG   | 1:A:563:MET:HE1  | 1.45                     | 0.97              |
| 1:B:624:ARG:NH2  | 1:B:707:GLN:HB3  | 1.79                     | 0.97              |
| 1:B:647:GLU:HB3  | 1:B:652:TRP:CZ3  | 1.98                     | 0.97              |
| 1:B:245:LYS:HE3  | 1:B:247:GLU:CD   | 1.90                     | 0.96              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:637:ARG:HE   | 1:B:769:ASP:CB   | 1.77                     | 0.96              |
| 1:B:647:GLU:C    | 1:B:652:TRP:CH2  | 2.43                     | 0.96              |
| 1:B:12:THR:O     | 1:B:16:LEU:HD22  | 1.63                     | 0.96              |
| 1:B:647:GLU:CA   | 1:B:652:TRP:CH2  | 2.48                     | 0.96              |
| 1:A:278:LEU:HB3  | 1:A:283:HIS:CB   | 1.95                     | 0.96              |
| 1:A:746:THR:HG22 | 1:A:746:THR:O    | 1.64                     | 0.96              |
| 1:B:637:ARG:NH2  | 1:B:769:ASP:HB3  | 1.80                     | 0.96              |
| 1:A:337:ILE:HD12 | 1:A:346:GLN:NE2  | 1.79                     | 0.96              |
| 1:A:275:ILE:CG2  | 1:A:276:ASP:H    | 1.78                     | 0.96              |
| 1:A:221:LEU:HD11 | 1:A:357:PHE:CZ   | 2.01                     | 0.96              |
| 1:B:418:VAL:O    | 1:B:422:VAL:HG23 | 1.66                     | 0.95              |
| 1:B:625:GLU:O    | 1:B:625:GLU:HG3  | 1.65                     | 0.95              |
| 1:B:603:LEU:HD11 | 1:B:731:MET:HG2  | 1.47                     | 0.95              |
| 1:A:666:LEU:CD1  | 1:A:691:ARG:HB3  | 1.96                     | 0.95              |
| 1:A:708:MET:SD   | 1:A:711:PHE:CE1  | 2.59                     | 0.95              |
| 1:B:647:GLU:HB3  | 1:B:652:TRP:HZ3  | 1.31                     | 0.94              |
| 1:A:275:ILE:HG23 | 1:A:276:ASP:H    | 1.31                     | 0.94              |
| 1:A:610:ILE:HG13 | 1:A:723:LYS:HE3  | 1.47                     | 0.94              |
| 1:B:626:ILE:HD12 | 1:B:715:ILE:HD12 | 1.49                     | 0.94              |
| 1:A:627:VAL:O    | 1:A:631:ILE:HG12 | 1.66                     | 0.94              |
| 1:A:278:LEU:HB3  | 1:A:283:HIS:HB3  | 1.48                     | 0.93              |
| 1:A:5:LEU:HB3    | 1:A:383:ASN:OD1  | 1.69                     | 0.93              |
| 1:B:647:GLU:N    | 1:B:652:TRP:CH2  | 2.37                     | 0.92              |
| 1:B:331:GLU:OE2  | 1:B:722:SER:HB2  | 1.69                     | 0.92              |
| 1:B:620:SER:CB   | 1:B:625:GLU:CB   | 2.48                     | 0.92              |
| 1:A:278:LEU:CB   | 1:A:283:HIS:HB3  | 2.00                     | 0.91              |
| 1:B:647:GLU:O    | 1:B:652:TRP:CH2  | 2.23                     | 0.91              |
| 1:B:614:ARG:HH12 | 1:B:720:VAL:CG2  | 1.84                     | 0.90              |
| 1:A:182:PHE:HB3  | 1:A:186:ARG:HH21 | 1.36                     | 0.90              |
| 1:A:275:ILE:CG2  | 1:A:276:ASP:N    | 2.34                     | 0.90              |
| 1:B:336:ALA:O    | 1:B:340:LYS:HD3  | 1.72                     | 0.90              |
| 1:A:660:LEU:HD23 | 1:A:661:ILE:HG13 | 1.52                     | 0.90              |
| 1:B:248:LYS:CD   | 1:B:265:GLY:HA2  | 2.02                     | 0.90              |
| 1:B:636:GLU:HA   | 1:B:636:GLU:OE1  | 1.69                     | 0.89              |
| 1:B:647:GLU:O    | 1:B:652:TRP:HH2  | 1.52                     | 0.89              |
| 1:A:232:LYS:H    | 1:A:232:LYS:HD2  | 1.37                     | 0.89              |
| 1:B:324:MET:HA   | 1:B:741:ARG:HD2  | 1.53                     | 0.89              |
| 1:A:244:LEU:O    | 1:A:248:LYS:HB2  | 1.72                     | 0.89              |
| 1:A:749:LEU:O    | 1:A:753:GLN:HG2  | 1.73                     | 0.89              |
| 1:B:750:ARG:HG2  | 1:B:750:ARG:NH1  | 1.82                     | 0.89              |
| 1:B:750:ARG:HH11 | 1:B:750:ARG:CG   | 1.86                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:228:ALA:HB3  | 1:A:230:SER:OG   | 1.74                     | 0.88              |
| 1:A:317:ASP:HB3  | 1:A:320:THR:HG22 | 1.55                     | 0.88              |
| 1:A:576:ARG:HH22 | 1:B:346:GLN:CD   | 1.80                     | 0.88              |
| 1:A:313:VAL:HG22 | 1:A:337:ILE:HD13 | 1.56                     | 0.88              |
| 1:A:338:GLU:HG2  | 1:A:345:ILE:HG13 | 1.55                     | 0.87              |
| 1:A:666:LEU:HD12 | 1:A:691:ARG:HB3  | 1.55                     | 0.87              |
| 1:B:713:LYS:O    | 1:B:717:LEU:HB2  | 1.72                     | 0.87              |
| 1:A:485:ASN:O    | 1:A:486:MET:CG   | 2.23                     | 0.87              |
| 1:A:640:ALA:O    | 1:A:644:PRO:HD3  | 1.74                     | 0.87              |
| 1:A:647:GLU:HG3  | 1:A:649:PRO:CD   | 2.05                     | 0.87              |
| 1:A:226:GLN:HB2  | 1:A:350:MET:HB2  | 1.54                     | 0.87              |
| 1:A:673:LYS:HB2  | 1:A:677:PHE:HB3  | 1.54                     | 0.86              |
| 1:A:722:SER:O    | 1:A:726:ASP:HB2  | 1.74                     | 0.86              |
| 1:A:561:PHE:O    | 1:A:569:ILE:HG13 | 1.76                     | 0.85              |
| 1:B:248:LYS:CB   | 1:B:265:GLY:HA2  | 2.05                     | 0.85              |
| 1:B:368:ALA:HA   | 1:B:387:MET:HE1  | 1.59                     | 0.85              |
| 1:A:630:MET:HE3  | 1:A:775:VAL:HG11 | 1.59                     | 0.85              |
| 1:A:281:VAL:HG12 | 1:A:281:VAL:O    | 1.74                     | 0.85              |
| 1:B:522:LEU:O    | 1:B:525:ARG:HG3  | 1.76                     | 0.85              |
| 1:A:647:GLU:HG3  | 1:A:649:PRO:HD3  | 1.59                     | 0.85              |
| 1:A:755:GLU:O    | 1:A:759:MET:HG3  | 1.75                     | 0.84              |
| 1:B:229:LYS:HB3  | 1:B:289:HIS:NE2  | 1.92                     | 0.84              |
| 1:B:718:ARG:CG   | 1:B:770:GLU:OE2  | 2.24                     | 0.84              |
| 1:B:152:VAL:HG13 | 1:B:172:ILE:HG22 | 1.58                     | 0.84              |
| 1:B:614:ARG:HH12 | 1:B:720:VAL:HG23 | 1.43                     | 0.84              |
| 1:A:723:LYS:HD2  | 1:A:763:MET:SD   | 2.16                     | 0.83              |
| 1:A:657:LEU:HD12 | 1:A:660:LEU:HD22 | 1.59                     | 0.83              |
| 1:A:700:GLU:O    | 1:A:704:GLY:HA3  | 1.78                     | 0.83              |
| 1:B:12:THR:O     | 1:B:16:LEU:CD2   | 2.26                     | 0.83              |
| 1:B:703:PHE:CE1  | 1:B:707:GLN:NE2  | 2.45                     | 0.83              |
| 1:A:249:ASP:OD2  | 1:A:294:LEU:HD21 | 1.78                     | 0.83              |
| 1:A:741:ARG:HH22 | 1:B:376:THR:HG22 | 1.43                     | 0.83              |
| 1:B:723:LYS:HB2  | 1:B:763:MET:HG3  | 1.61                     | 0.83              |
| 1:A:673:LYS:HB2  | 1:A:677:PHE:CB   | 2.08                     | 0.82              |
| 1:B:459:LEU:HD22 | 1:B:487:ALA:HB1  | 1.61                     | 0.82              |
| 1:B:610:ILE:CD1  | 1:B:723:LYS:HZ3  | 1.92                     | 0.82              |
| 1:B:626:ILE:CG2  | 1:B:715:ILE:HD11 | 2.09                     | 0.82              |
| 1:B:706:GLU:O    | 1:B:709:ARG:HB2  | 1.79                     | 0.82              |
| 1:A:338:GLU:HG2  | 1:A:345:ILE:HA   | 1.61                     | 0.82              |
| 1:B:514:GLU:HA   | 1:B:514:GLU:OE1  | 1.79                     | 0.82              |
| 1:B:637:ARG:HE   | 1:B:769:ASP:HB3  | 1.45                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:650:GLU:C    | 1:B:650:GLU:CD   | 2.46                     | 0.82              |
| 1:B:295:LYS:HE2  | 1:B:333:LEU:CD2  | 2.10                     | 0.82              |
| 1:B:248:LYS:HZ3  | 1:B:268:LYS:HB2  | 1.43                     | 0.81              |
| 1:A:599:TYR:HD2  | 1:A:735:ARG:HG3  | 1.45                     | 0.81              |
| 1:B:637:ARG:HE   | 1:B:769:ASP:CA   | 1.92                     | 0.81              |
| 1:A:351:THR:HG22 | 1:A:728:ILE:HG22 | 1.62                     | 0.81              |
| 1:A:255:LYS:CD   | 1:A:762:HIS:HE1  | 1.93                     | 0.81              |
| 1:B:217:ALA:HB1  | 1:B:358:GLN:HE22 | 1.45                     | 0.81              |
| 1:B:650:GLU:O    | 1:B:650:GLU:CD   | 2.24                     | 0.81              |
| 1:A:348:GLU:OE2  | 1:B:573:MET:CB   | 2.29                     | 0.81              |
| 1:B:624:ARG:NH2  | 1:B:707:GLN:CB   | 2.41                     | 0.81              |
| 1:A:322:ARG:NE   | 1:A:324:MET:HE1  | 1.96                     | 0.81              |
| 1:B:348:GLU:OE1  | 1:B:348:GLU:HA   | 1.81                     | 0.81              |
| 1:B:647:GLU:CB   | 1:B:652:TRP:HZ3  | 1.88                     | 0.81              |
| 1:A:253:ASP:OD2  | 1:A:645:ARG:HG2  | 1.81                     | 0.80              |
| 1:A:611:TYR:O    | 1:A:615:PHE:HD1  | 1.65                     | 0.80              |
| 1:A:5:LEU:H      | 1:A:5:LEU:CD2    | 1.94                     | 0.80              |
| 1:B:248:LYS:CB   | 1:B:265:GLY:HA3  | 2.01                     | 0.80              |
| 1:A:221:LEU:HD11 | 1:A:357:PHE:CE2  | 2.17                     | 0.80              |
| 1:B:248:LYS:HD2  | 1:B:265:GLY:HA2  | 1.62                     | 0.80              |
| 1:B:256:THR:HG21 | 1:B:295:LYS:HD2  | 1.63                     | 0.79              |
| 1:B:720:VAL:O    | 1:B:725:MET:HG3  | 1.82                     | 0.79              |
| 1:A:557:MET:HG2  | 1:B:226:GLN:NE2  | 1.97                     | 0.79              |
| 1:A:255:LYS:HD3  | 1:A:762:HIS:CE1  | 2.18                     | 0.79              |
| 1:A:610:ILE:HG13 | 1:A:723:LYS:CE   | 2.12                     | 0.79              |
| 1:B:695:LYS:HD3  | 1:B:776:MET:HE3  | 1.64                     | 0.79              |
| 1:A:218:ARG:O    | 1:B:549:PHE:HB3  | 1.83                     | 0.79              |
| 1:A:744:ALA:O    | 1:A:748:PRO:HD3  | 1.83                     | 0.79              |
| 1:B:368:ALA:HA   | 1:B:387:MET:CE   | 2.12                     | 0.79              |
| 1:B:637:ARG:HB3  | 1:B:665:TYR:OH   | 1.82                     | 0.79              |
| 1:B:275:ILE:HD11 | 1:B:283:HIS:NE2  | 1.98                     | 0.79              |
| 1:A:626:ILE:HG23 | 1:A:711:PHE:CD1  | 2.18                     | 0.79              |
| 1:A:110:SER:O    | 1:A:114:VAL:HG23 | 1.82                     | 0.78              |
| 1:A:243:THR:HG22 | 1:A:243:THR:O    | 1.84                     | 0.78              |
| 1:A:400:ARG:HD2  | 1:A:526:SER:HB3  | 1.65                     | 0.78              |
| 1:B:626:ILE:HG21 | 1:B:715:ILE:HD11 | 1.64                     | 0.78              |
| 1:B:626:ILE:HD12 | 1:B:715:ILE:CD1  | 2.13                     | 0.78              |
| 1:A:275:ILE:HG22 | 1:A:276:ASP:N    | 1.99                     | 0.78              |
| 1:A:553:ARG:HH21 | 1:A:560:ARG:NH2  | 1.81                     | 0.78              |
| 1:B:695:LYS:HD3  | 1:B:776:MET:CE   | 2.12                     | 0.78              |
| 1:B:703:PHE:O    | 1:B:703:PHE:CD1  | 2.37                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:278:LEU:N    | 1:A:278:LEU:HD23 | 1.99                     | 0.78              |
| 1:B:582:GLN:HE21 | 1:B:586:GLU:HG3  | 1.48                     | 0.78              |
| 1:A:226:GLN:HE21 | 1:A:228:ALA:N    | 1.81                     | 0.77              |
| 1:A:740:LEU:H    | 1:A:740:LEU:HD23 | 1.49                     | 0.77              |
| 1:B:301:GLN:HB3  | 1:B:304:VAL:HB   | 1.66                     | 0.77              |
| 1:B:448:LEU:HD12 | 1:B:449:LEU:N    | 1.98                     | 0.77              |
| 1:B:637:ARG:NE   | 1:B:769:ASP:HB3  | 1.99                     | 0.77              |
| 1:A:558:LEU:HG   | 1:A:563:MET:HE3  | 1.66                     | 0.77              |
| 1:A:207:ASP:HB2  | 1:A:370:MET:HE3  | 1.65                     | 0.77              |
| 1:A:284:VAL:HG21 | 1:A:717:LEU:CD2  | 2.14                     | 0.77              |
| 1:A:279:PHE:CA   | 1:A:778:ALA:HB1  | 2.14                     | 0.77              |
| 1:A:279:PHE:CD1  | 1:A:778:ALA:O    | 2.37                     | 0.77              |
| 1:A:278:LEU:HD11 | 1:A:286:LEU:HB2  | 1.67                     | 0.76              |
| 1:A:10:ASP:CB    | 1:A:11:PRO:CD    | 2.36                     | 0.76              |
| 1:B:245:LYS:CE   | 1:B:247:GLU:OE1  | 2.28                     | 0.76              |
| 1:B:241:VAL:O    | 1:B:244:LEU:HG   | 1.86                     | 0.76              |
| 1:B:463:ASN:O    | 1:B:467:GLU:HG3  | 1.85                     | 0.76              |
| 1:A:210:ASP:OD2  | 1:A:371:THR:HG21 | 1.84                     | 0.76              |
| 1:B:425:ARG:HD2  | 1:B:430:GLN:OE1  | 1.85                     | 0.76              |
| 1:B:711:PHE:O    | 1:B:715:ILE:HG13 | 1.86                     | 0.76              |
| 1:A:9:PHE:CD2    | 1:A:10:ASP:N     | 2.53                     | 0.75              |
| 1:A:217:ALA:HB1  | 1:A:358:GLN:NE2  | 2.01                     | 0.75              |
| 1:B:250:TYR:HE2  | 1:B:659:ASP:HB3  | 1.49                     | 0.75              |
| 1:B:516:ARG:NE   | 1:B:582:GLN:HG2  | 2.00                     | 0.75              |
| 1:B:647:GLU:HB2  | 1:B:652:TRP:CZ3  | 2.20                     | 0.75              |
| 1:B:552:GLU:HA   | 1:B:555:MET:HG3  | 1.67                     | 0.75              |
| 1:A:654:LEU:HD12 | 1:A:657:LEU:HB3  | 1.68                     | 0.75              |
| 1:B:307:VAL:HG12 | 1:B:308:VAL:N    | 2.01                     | 0.75              |
| 1:B:248:LYS:HZ3  | 1:B:268:LYS:CB   | 2.00                     | 0.74              |
| 1:B:246:ALA:HB1  | 1:B:268:LYS:HZ1  | 1.51                     | 0.74              |
| 1:B:637:ARG:HE   | 1:B:769:ASP:HA   | 1.51                     | 0.74              |
| 1:A:276:ASP:O    | 1:A:278:LEU:HD23 | 1.88                     | 0.74              |
| 1:B:206:ILE:HG21 | 1:B:209:VAL:HG23 | 1.70                     | 0.74              |
| 1:B:476:GLN:HE22 | 1:B:494:LYS:HZ3  | 1.35                     | 0.74              |
| 1:A:626:ILE:CG2  | 1:A:711:PHE:HD1  | 2.00                     | 0.74              |
| 1:B:354:THR:CG2  | 1:B:735:ARG:HH22 | 2.00                     | 0.74              |
| 1:B:723:LYS:HB2  | 1:B:763:MET:HG2  | 1.70                     | 0.74              |
| 1:B:637:ARG:CZ   | 1:B:769:ASP:HB3  | 2.17                     | 0.74              |
| 1:A:194:GLU:HG3  | 1:A:195:GLN:N    | 2.02                     | 0.73              |
| 1:A:654:LEU:HB3  | 1:A:675:ASP:HB2  | 1.69                     | 0.73              |
| 1:B:655:ASP:O    | 1:B:659:ASP:HB2  | 1.86                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:414:LYS:O    | 1:B:418:VAL:HG23 | 1.88                     | 0.73              |
| 1:A:654:LEU:HD22 | 1:A:677:PHE:HE2  | 1.53                     | 0.73              |
| 1:A:182:PHE:HB3  | 1:A:186:ARG:NH2  | 2.03                     | 0.73              |
| 1:A:747:ASN:N    | 1:A:748:PRO:CD   | 2.10                     | 0.73              |
| 1:B:199:ARG:HB3  | 1:B:200:PRO:CD   | 2.18                     | 0.73              |
| 1:B:514:GLU:OE1  | 1:B:585:VAL:HG11 | 1.88                     | 0.73              |
| 1:A:351:THR:HG22 | 1:A:728:ILE:CG2  | 2.17                     | 0.73              |
| 1:A:666:LEU:HD11 | 1:A:691:ARG:HB3  | 1.70                     | 0.73              |
| 1:A:207:ASP:HB2  | 1:A:370:MET:CE   | 2.18                     | 0.73              |
| 1:A:291:ASN:O    | 1:A:295:LYS:HG3  | 1.89                     | 0.73              |
| 1:A:382:ARG:CZ   | 1:A:388:GLN:HG2  | 2.18                     | 0.72              |
| 1:A:654:LEU:HD23 | 1:A:675:ASP:HA   | 1.71                     | 0.72              |
| 1:A:255:LYS:HD3  | 1:A:762:HIS:HE1  | 1.49                     | 0.72              |
| 1:A:349:SER:HB2  | 1:B:557:MET:HG3  | 1.69                     | 0.72              |
| 1:A:315:ILE:HD12 | 1:A:327:ARG:HB3  | 1.71                     | 0.72              |
| 1:A:142:GLY:HA2  | 1:A:152:VAL:HG21 | 1.72                     | 0.72              |
| 1:B:295:LYS:CE   | 1:B:333:LEU:HD22 | 2.18                     | 0.72              |
| 1:A:303:ASP:C    | 1:A:304:VAL:HG23 | 2.10                     | 0.72              |
| 1:A:562:GLY:CA   | 1:A:569:ILE:HG13 | 2.19                     | 0.72              |
| 1:B:722:SER:OG   | 1:B:723:LYS:N    | 2.12                     | 0.72              |
| 1:A:348:GLU:OE2  | 1:B:573:MET:HB2  | 1.89                     | 0.71              |
| 1:B:288:HIS:CD2  | 1:B:718:ARG:HH12 | 2.06                     | 0.71              |
| 1:B:190:VAL:HG22 | 1:B:195:GLN:HG3  | 1.72                     | 0.71              |
| 1:B:198:GLN:O    | 1:B:199:ARG:HD2  | 1.91                     | 0.71              |
| 1:B:243:THR:O    | 1:B:243:THR:HG22 | 1.90                     | 0.71              |
| 1:B:636:GLU:OE1  | 1:B:636:GLU:CA   | 2.38                     | 0.71              |
| 1:A:348:GLU:OE2  | 1:B:573:MET:HB3  | 1.90                     | 0.71              |
| 1:A:610:ILE:HD12 | 1:A:723:LYS:HZ1  | 1.56                     | 0.71              |
| 1:A:246:ALA:HB1  | 1:A:264:GLU:HB3  | 1.73                     | 0.71              |
| 1:B:39:ASP:HA    | 1:B:42:LYS:HB3   | 1.73                     | 0.71              |
| 1:A:213:LEU:HD22 | 1:A:385:TYR:CZ   | 2.27                     | 0.70              |
| 1:B:459:LEU:HD21 | 1:B:467:GLU:HB3  | 1.72                     | 0.70              |
| 1:B:654:LEU:O    | 1:B:657:LEU:N    | 2.23                     | 0.70              |
| 1:B:354:THR:HG21 | 1:B:735:ARG:HH22 | 1.54                     | 0.70              |
| 1:A:279:PHE:HD1  | 1:A:779:GLU:CA   | 2.03                     | 0.70              |
| 1:A:485:ASN:OD1  | 1:A:485:ASN:C    | 2.34                     | 0.70              |
| 1:A:706:GLU:O    | 1:A:709:ARG:HB3  | 1.92                     | 0.70              |
| 1:B:642:TYR:HE1  | 1:B:685:LEU:HA   | 1.56                     | 0.70              |
| 1:A:66:PHE:CE2   | 1:A:112:LEU:HB3  | 2.26                     | 0.70              |
| 1:A:426:TYR:HE1  | 1:A:455:PRO:HG2  | 1.56                     | 0.70              |
| 1:A:662:ASN:HA   | 1:A:666:LEU:O    | 1.90                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:662:ASN:HB3  | 1:A:670:ALA:HB3  | 1.72                     | 0.70              |
| 1:A:279:PHE:HA   | 1:A:778:ALA:CB   | 2.20                     | 0.70              |
| 1:A:627:VAL:O    | 1:A:631:ILE:CG1  | 2.38                     | 0.69              |
| 1:B:626:ILE:CG2  | 1:B:715:ILE:CD1  | 2.70                     | 0.69              |
| 1:A:258:ALA:HB3  | 1:A:295:LYS:HG2  | 1.74                     | 0.69              |
| 1:A:647:GLU:HG3  | 1:A:649:PRO:HD2  | 1.74                     | 0.69              |
| 1:B:626:ILE:HG21 | 1:B:715:ILE:CD1  | 2.22                     | 0.69              |
| 1:A:744:ALA:O    | 1:A:748:PRO:CD   | 2.40                     | 0.69              |
| 1:A:562:GLY:HA2  | 1:A:569:ILE:HG13 | 1.75                     | 0.69              |
| 1:B:233:LEU:HB3  | 1:B:289:HIS:HD1  | 1.58                     | 0.69              |
| 1:B:246:ALA:HB3  | 1:B:248:LYS:HG2  | 1.73                     | 0.69              |
| 1:A:426:TYR:CD1  | 1:A:454:ILE:HG23 | 2.27                     | 0.68              |
| 1:A:746:THR:O    | 1:A:746:THR:CG2  | 2.37                     | 0.68              |
| 1:B:325:LYS:H    | 1:B:741:ARG:HD3  | 1.57                     | 0.68              |
| 1:A:627:VAL:HG11 | 1:A:696:TYR:OH   | 1.93                     | 0.68              |
| 1:B:36:LEU:H     | 1:B:75:ARG:HH22  | 1.42                     | 0.68              |
| 1:A:328:ARG:HG2  | 1:A:328:ARG:HH11 | 1.59                     | 0.68              |
| 1:B:380:GLU:CD   | 1:B:593:ARG:HH12 | 2.02                     | 0.68              |
| 1:A:279:PHE:O    | 1:A:778:ALA:HB1  | 1.94                     | 0.68              |
| 1:A:254:ILE:CG2  | 1:A:255:LYS:N    | 2.42                     | 0.68              |
| 1:B:626:ILE:HB   | 1:B:711:PHE:CD1  | 2.29                     | 0.68              |
| 1:A:278:LEU:HD23 | 1:A:278:LEU:H    | 1.58                     | 0.68              |
| 1:A:528:ARG:HH11 | 1:A:528:ARG:HG3  | 1.59                     | 0.68              |
| 1:A:553:ARG:NH2  | 1:A:560:ARG:HH21 | 1.85                     | 0.68              |
| 1:B:723:LYS:HE2  | 1:B:763:MET:HE3  | 1.76                     | 0.68              |
| 1:A:300:MET:SD   | 1:A:306:TYR:CE2  | 2.87                     | 0.67              |
| 1:B:380:GLU:OE2  | 1:B:593:ARG:NH1  | 2.27                     | 0.67              |
| 1:B:246:ALA:HB1  | 1:B:268:LYS:NZ   | 2.08                     | 0.67              |
| 1:A:255:LYS:CD   | 1:A:762:HIS:CE1  | 2.75                     | 0.67              |
| 1:A:406:LEU:CD2  | 1:A:570:GLN:HE21 | 2.07                     | 0.67              |
| 1:B:206:ILE:O    | 1:B:369:GLY:HA2  | 1.94                     | 0.67              |
| 1:A:337:ILE:HD12 | 1:A:346:GLN:HE22 | 1.55                     | 0.67              |
| 1:B:647:GLU:CB   | 1:B:652:TRP:CH2  | 2.78                     | 0.67              |
| 1:A:249:ASP:OD2  | 1:A:294:LEU:CD2  | 2.42                     | 0.67              |
| 1:B:261:LEU:C    | 1:B:261:LEU:CD1  | 2.67                     | 0.67              |
| 1:A:182:PHE:CB   | 1:A:186:ARG:HH21 | 2.06                     | 0.67              |
| 1:A:717:LEU:HG   | 1:A:718:ARG:N    | 2.09                     | 0.67              |
| 1:B:218:ARG:CD   | 1:B:592:SER:HB3  | 2.23                     | 0.67              |
| 1:B:610:ILE:CD1  | 1:B:723:LYS:NZ   | 2.57                     | 0.67              |
| 1:B:627:VAL:HG22 | 1:B:711:PHE:CZ   | 2.30                     | 0.67              |
| 1:B:201:LEU:HD12 | 1:B:363:MET:HE2  | 1.77                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:769:ASP:OD1  | 1:B:770:GLU:N    | 2.28                     | 0.67              |
| 1:A:544:GLU:O    | 1:A:545:LEU:HB2  | 1.95                     | 0.66              |
| 1:B:307:VAL:CG1  | 1:B:308:VAL:N    | 2.57                     | 0.66              |
| 1:B:248:LYS:NZ   | 1:B:268:LYS:HB2  | 2.08                     | 0.66              |
| 1:A:599:TYR:CD2  | 1:A:735:ARG:HG3  | 2.28                     | 0.66              |
| 1:B:206:ILE:HG23 | 1:B:212:ILE:HD12 | 1.77                     | 0.66              |
| 1:B:261:LEU:HD12 | 1:B:262:THR:HB   | 1.75                     | 0.66              |
| 1:B:301:GLN:HA   | 1:B:301:GLN:OE1  | 1.94                     | 0.66              |
| 1:A:458:VAL:HA   | 1:A:482:ILE:HG23 | 1.77                     | 0.66              |
| 1:B:400:ARG:HD2  | 1:B:535:THR:HG23 | 1.76                     | 0.66              |
| 1:A:246:ALA:O    | 1:A:262:THR:HB   | 1.96                     | 0.66              |
| 1:A:611:TYR:O    | 1:A:615:PHE:CD1  | 2.49                     | 0.66              |
| 1:B:248:LYS:HA   | 1:B:261:LEU:HB3  | 1.78                     | 0.66              |
| 1:B:302:LYS:O    | 1:B:302:LYS:CG   | 2.43                     | 0.66              |
| 1:A:561:PHE:O    | 1:A:561:PHE:HD1  | 1.78                     | 0.66              |
| 1:A:421:ASP:O    | 1:A:425:ARG:HG2  | 1.95                     | 0.66              |
| 1:B:16:LEU:CD2   | 1:B:16:LEU:H     | 2.07                     | 0.66              |
| 1:B:344:GLU:O    | 1:B:346:GLN:N    | 2.29                     | 0.66              |
| 1:A:313:VAL:HG22 | 1:A:337:ILE:CD1  | 2.25                     | 0.66              |
| 1:A:361:PHE:HB3  | 1:A:367:LEU:HD21 | 1.78                     | 0.66              |
| 1:B:206:ILE:CG2  | 1:B:209:VAL:HG23 | 2.25                     | 0.66              |
| 1:A:426:TYR:C    | 1:A:426:TYR:CD2  | 2.73                     | 0.65              |
| 1:A:576:ARG:HH12 | 1:B:346:GLN:HE22 | 1.44                     | 0.65              |
| 1:B:720:VAL:HG12 | 1:B:721:ASP:N    | 2.09                     | 0.65              |
| 1:B:582:GLN:NE2  | 1:B:586:GLU:HG3  | 2.11                     | 0.65              |
| 1:A:677:PHE:CE1  | 1:A:684:MET:HE1  | 2.31                     | 0.65              |
| 1:A:206:ILE:HG23 | 1:A:212:ILE:HD12 | 1.78                     | 0.65              |
| 1:A:724:TRP:HA   | 1:A:724:TRP:CE3  | 2.31                     | 0.65              |
| 1:A:761:GLU:O    | 1:A:765:GLU:HG3  | 1.97                     | 0.65              |
| 1:B:516:ARG:N    | 1:B:516:ARG:HH11 | 1.94                     | 0.65              |
| 1:A:433:LEU:HD21 | 1:A:525:ARG:HD3  | 1.78                     | 0.65              |
| 1:A:274:GLY:O    | 1:A:275:ILE:HG13 | 1.96                     | 0.65              |
| 1:A:317:ASP:HB3  | 1:A:320:THR:CG2  | 2.26                     | 0.65              |
| 1:A:654:LEU:HD22 | 1:A:677:PHE:CE2  | 2.33                     | 0.64              |
| 1:B:554:THR:O    | 1:B:558:LEU:HG   | 1.98                     | 0.64              |
| 1:A:278:LEU:HB2  | 1:A:283:HIS:HB3  | 1.79                     | 0.64              |
| 1:A:279:PHE:HD1  | 1:A:779:GLU:HA   | 1.61                     | 0.64              |
| 1:A:637:ARG:NE   | 1:A:769:ASP:HB2  | 2.13                     | 0.64              |
| 1:A:680:GLU:HB2  | 1:A:683:GLU:HB2  | 1.80                     | 0.64              |
| 1:A:684:MET:HA   | 1:A:684:MET:HE3  | 1.78                     | 0.64              |
| 1:B:439:VAL:HA   | 1:B:442:SER:HB2  | 1.79                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:463:ASN:C    | 1:B:463:ASN:HD22 | 2.05                     | 0.64              |
| 1:B:620:SER:HB2  | 1:B:625:GLU:HB3  | 1.75                     | 0.64              |
| 1:B:248:LYS:HB3  | 1:B:265:GLY:CA   | 2.28                     | 0.64              |
| 1:B:637:ARG:HH21 | 1:B:769:ASP:CB   | 2.05                     | 0.64              |
| 1:A:426:TYR:CE1  | 1:A:455:PRO:HG2  | 2.32                     | 0.64              |
| 1:B:630:MET:SD   | 1:B:775:VAL:CG2  | 2.79                     | 0.64              |
| 1:B:649:PRO:O    | 1:B:652:TRP:CH2  | 2.50                     | 0.64              |
| 1:A:667:ASP:OD1  | 1:A:777:LYS:HE2  | 1.97                     | 0.64              |
| 1:B:135:SER:OG   | 1:B:154:LEU:HD21 | 1.98                     | 0.64              |
| 1:B:254:ILE:HG23 | 1:B:255:LYS:H    | 1.61                     | 0.64              |
| 1:B:110:SER:O    | 1:B:114:VAL:HG23 | 1.97                     | 0.64              |
| 1:B:270:GLU:HA   | 1:B:275:ILE:HG22 | 1.79                     | 0.64              |
| 1:B:233:LEU:HB2  | 1:B:289:HIS:CE1  | 2.34                     | 0.63              |
| 1:B:379:GLU:HG2  | 1:B:383:ASN:HD22 | 1.63                     | 0.63              |
| 1:A:471:ILE:HG21 | 1:A:491:THR:HB   | 1.81                     | 0.63              |
| 1:B:248:LYS:HZ3  | 1:B:268:LYS:HD2  | 1.63                     | 0.63              |
| 1:A:637:ARG:HE   | 1:A:769:ASP:HB2  | 1.63                     | 0.63              |
| 1:A:654:LEU:CD1  | 1:A:657:LEU:HB3  | 2.28                     | 0.63              |
| 1:B:325:LYS:N    | 1:B:741:ARG:HD3  | 2.13                     | 0.63              |
| 1:B:377:GLU:HG2  | 1:B:517:ARG:HD3  | 1.81                     | 0.63              |
| 1:A:249:ASP:HB2  | 1:A:260:GLN:HG2  | 1.78                     | 0.63              |
| 1:A:645:ARG:O    | 1:A:646:GLU:HG3  | 1.98                     | 0.63              |
| 1:B:238:ASN:HD21 | 1:B:340:LYS:HA   | 1.63                     | 0.63              |
| 1:A:410:THR:HG21 | 1:B:462:LYS:HE3  | 1.81                     | 0.63              |
| 1:A:5:LEU:H      | 1:A:5:LEU:HD22   | 1.63                     | 0.63              |
| 1:A:206:ILE:H    | 1:A:206:ILE:HD12 | 1.61                     | 0.63              |
| 1:A:627:VAL:HA   | 1:A:630:MET:SD   | 2.39                     | 0.63              |
| 1:B:546:MET:HB3  | 1:B:555:MET:HE1  | 1.81                     | 0.63              |
| 1:B:723:LYS:HE2  | 1:B:763:MET:HG2  | 1.80                     | 0.63              |
| 1:A:626:ILE:HG23 | 1:A:711:PHE:HD1  | 1.59                     | 0.63              |
| 1:A:645:ARG:HG3  | 1:A:657:LEU:HD13 | 1.80                     | 0.63              |
| 1:B:238:ASN:OD1  | 1:B:297:HIS:HE1  | 1.81                     | 0.63              |
| 1:B:245:LYS:CE   | 1:B:247:GLU:CD   | 2.69                     | 0.63              |
| 1:B:307:VAL:HG21 | 1:B:316:VAL:HG21 | 1.81                     | 0.63              |
| 1:A:106:LYS:HD3  | 1:A:370:MET:HB3  | 1.81                     | 0.62              |
| 1:A:640:ALA:O    | 1:A:644:PRO:CD   | 2.47                     | 0.62              |
| 1:B:254:ILE:HG23 | 1:B:255:LYS:N    | 2.14                     | 0.62              |
| 1:A:547:ARG:O    | 1:B:219:THR:HG22 | 1.99                     | 0.62              |
| 1:A:261:LEU:HD23 | 1:A:266:MET:HG2  | 1.82                     | 0.62              |
| 1:B:421:ASP:OD1  | 1:B:425:ARG:NH1  | 2.32                     | 0.62              |
| 1:B:627:VAL:O    | 1:B:631:ILE:N    | 2.28                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:255:LYS:NZ   | 1:A:762:HIS:HE1  | 1.98                     | 0.62              |
| 1:A:279:PHE:HD1  | 1:A:778:ALA:C    | 2.07                     | 0.62              |
| 1:A:420:GLU:O    | 1:A:424:GLN:HG3  | 2.00                     | 0.62              |
| 1:B:354:THR:HG21 | 1:B:735:ARG:HH12 | 1.65                     | 0.62              |
| 1:A:561:PHE:CD1  | 1:A:561:PHE:C    | 2.77                     | 0.62              |
| 1:B:185:LEU:HD22 | 1:B:353:ALA:HB1  | 1.80                     | 0.62              |
| 1:B:190:VAL:HG22 | 1:B:195:GLN:CG   | 2.29                     | 0.62              |
| 1:B:512:ARG:HG2  | 1:B:539:LEU:HD21 | 1.80                     | 0.62              |
| 1:B:676:ILE:HG12 | 1:B:684:MET:HG2  | 1.80                     | 0.62              |
| 1:A:426:TYR:C    | 1:A:426:TYR:HD2  | 2.08                     | 0.62              |
| 1:B:354:THR:HG21 | 1:B:735:ARG:NH2  | 2.13                     | 0.62              |
| 1:A:324:MET:HA   | 1:A:740:LEU:HD13 | 1.82                     | 0.62              |
| 1:B:723:LYS:CB   | 1:B:763:MET:HG3  | 2.30                     | 0.62              |
| 1:B:250:TYR:O    | 1:B:251:THR:HB   | 1.99                     | 0.61              |
| 1:B:213:LEU:O    | 1:B:217:ALA:HB2  | 2.00                     | 0.61              |
| 1:B:74:ARG:HG3   | 1:B:74:ARG:HH11  | 1.64                     | 0.61              |
| 1:B:624:ARG:CZ   | 1:B:700:GLU:HG2  | 2.30                     | 0.61              |
| 1:A:281:VAL:O    | 1:A:281:VAL:CG1  | 2.49                     | 0.61              |
| 1:B:640:ALA:O    | 1:B:644:PRO:HD3  | 2.01                     | 0.61              |
| 1:A:686:GLU:HG2  | 1:A:687:LEU:N    | 2.14                     | 0.61              |
| 1:B:732:ASP:O    | 1:B:735:ARG:HB3  | 2.01                     | 0.61              |
| 1:B:191:LEU:HD21 | 1:B:716:VAL:HG11 | 1.82                     | 0.61              |
| 1:B:723:LYS:HG2  | 1:B:767:ILE:HG12 | 1.83                     | 0.61              |
| 1:A:668:GLU:C    | 1:A:670:ALA:H    | 2.09                     | 0.61              |
| 1:A:406:LEU:HG   | 1:A:536:GLN:NE2  | 2.15                     | 0.61              |
| 1:B:711:PHE:O    | 1:B:715:ILE:CG1  | 2.49                     | 0.61              |
| 1:A:254:ILE:HG22 | 1:A:255:LYS:HG3  | 1.81                     | 0.61              |
| 1:A:255:LYS:O    | 1:A:256:THR:HB   | 2.00                     | 0.61              |
| 1:B:317:ASP:HB3  | 1:B:320:THR:HG23 | 1.83                     | 0.61              |
| 1:B:238:ASN:ND2  | 1:B:340:LYS:HD2  | 2.15                     | 0.60              |
| 1:A:288:HIS:O    | 1:A:292:GLN:HG2  | 2.00                     | 0.60              |
| 1:A:322:ARG:HE   | 1:A:324:MET:HE1  | 1.65                     | 0.60              |
| 1:A:404:PRO:O    | 1:A:536:GLN:NE2  | 2.34                     | 0.60              |
| 1:A:541:MET:SD   | 1:A:561:PHE:HZ   | 2.25                     | 0.60              |
| 1:B:626:ILE:O    | 1:B:627:VAL:C    | 2.44                     | 0.60              |
| 1:A:217:ALA:HB1  | 1:A:358:GLN:HE21 | 1.66                     | 0.60              |
| 1:A:259:VAL:HG21 | 1:A:769:ASP:OD2  | 1.99                     | 0.60              |
| 1:A:312:GLN:NE2  | 1:B:572:LYS:HD3  | 2.17                     | 0.60              |
| 1:A:610:ILE:HD12 | 1:A:723:LYS:NZ   | 2.17                     | 0.60              |
| 1:B:718:ARG:HG3  | 1:B:770:GLU:OE1  | 2.01                     | 0.60              |
| 1:A:270:GLU:O    | 1:A:274:GLY:N    | 2.33                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:418:VAL:O    | 1:A:422:VAL:HG23 | 2.02                     | 0.60              |
| 1:A:700:GLU:O    | 1:A:704:GLY:CA   | 2.48                     | 0.60              |
| 1:A:724:TRP:HA   | 1:A:724:TRP:HE3  | 1.66                     | 0.60              |
| 1:B:645:ARG:HG3  | 1:B:657:LEU:HB2  | 1.84                     | 0.60              |
| 1:A:279:PHE:CD1  | 1:A:778:ALA:C    | 2.80                     | 0.60              |
| 1:B:102:THR:HB   | 1:B:524:GLY:O    | 2.02                     | 0.60              |
| 1:B:243:THR:O    | 1:B:244:LEU:HD23 | 2.01                     | 0.60              |
| 1:A:100:MET:HE3  | 1:A:106:LYS:HG2  | 1.84                     | 0.60              |
| 1:B:218:ARG:HD3  | 1:B:592:SER:CB   | 2.26                     | 0.60              |
| 1:B:494:LYS:H    | 1:B:494:LYS:HD3  | 1.65                     | 0.60              |
| 1:B:713:LYS:O    | 1:B:717:LEU:CB   | 2.49                     | 0.60              |
| 1:B:288:HIS:O    | 1:B:292:GLN:HG2  | 2.01                     | 0.60              |
| 1:A:661:ILE:CG2  | 1:A:666:LEU:CD2  | 2.65                     | 0.60              |
| 1:A:723:LYS:HG2  | 1:A:767:ILE:HD11 | 1.84                     | 0.60              |
| 1:A:142:GLY:O    | 1:A:146:GLU:HG3  | 2.02                     | 0.60              |
| 1:A:646:GLU:HA   | 1:A:651:GLU:HA   | 1.84                     | 0.60              |
| 1:A:747:ASN:H    | 1:A:748:PRO:HD2  | 0.51                     | 0.60              |
| 1:B:627:VAL:HG22 | 1:B:711:PHE:HZ   | 1.66                     | 0.60              |
| 1:B:627:VAL:HG12 | 1:B:631:ILE:HG13 | 1.84                     | 0.60              |
| 1:A:325:LYS:HB2  | 1:A:740:LEU:HB3  | 1.82                     | 0.59              |
| 1:A:337:ILE:HD12 | 1:A:346:GLN:CD   | 2.27                     | 0.59              |
| 1:A:401:ASP:OD2  | 1:A:403:ARG:HD3  | 2.02                     | 0.59              |
| 1:A:672:GLU:O    | 1:A:673:LYS:C    | 2.45                     | 0.59              |
| 1:B:541:MET:HE1  | 1:B:559:ASP:OD2  | 2.02                     | 0.59              |
| 1:A:255:LYS:NZ   | 1:A:762:HIS:CE1  | 2.69                     | 0.59              |
| 1:A:284:VAL:HG13 | 1:A:718:ARG:HH21 | 1.67                     | 0.59              |
| 1:A:560:ARG:O    | 1:A:561:PHE:CG   | 2.55                     | 0.59              |
| 1:A:677:PHE:HE1  | 1:A:684:MET:HE1  | 1.67                     | 0.59              |
| 1:A:736:GLN:O    | 1:A:737:GLY:C    | 2.43                     | 0.59              |
| 1:B:19:TYR:HE1   | 1:B:390:VAL:HG11 | 1.68                     | 0.59              |
| 1:B:297:HIS:CE1  | 1:B:340:LYS:HB3  | 2.37                     | 0.59              |
| 1:B:248:LYS:NZ   | 1:B:268:LYS:HD2  | 2.17                     | 0.59              |
| 1:B:617:VAL:O    | 1:B:617:VAL:HG12 | 2.02                     | 0.59              |
| 1:B:624:ARG:HH21 | 1:B:707:GLN:HB2  | 1.59                     | 0.59              |
| 1:A:249:ASP:HB3  | 1:A:260:GLN:O    | 2.02                     | 0.59              |
| 1:A:529:GLN:OE1  | 1:A:529:GLN:HA   | 2.00                     | 0.59              |
| 1:B:102:THR:HA   | 1:B:106:LYS:HZ3  | 1.67                     | 0.59              |
| 1:B:230:SER:C    | 1:B:232:LYS:H    | 2.10                     | 0.59              |
| 1:B:723:LYS:CE   | 1:B:763:MET:HE3  | 2.32                     | 0.59              |
| 1:A:358:GLN:HG3  | 1:A:385:TYR:OH   | 2.02                     | 0.59              |
| 1:A:406:LEU:HD23 | 1:A:570:GLN:HE21 | 1.66                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:554:THR:HG21 | 1:A:557:MET:O    | 2.02                     | 0.59              |
| 1:A:160:SER:C    | 1:A:162:ASP:H    | 2.09                     | 0.59              |
| 1:A:374:ALA:O    | 1:A:389:VAL:HG21 | 2.02                     | 0.59              |
| 1:B:187:ASP:OD1  | 1:B:196:MET:HA   | 2.02                     | 0.59              |
| 1:B:300:MET:HG3  | 1:B:337:ILE:HD11 | 1.84                     | 0.59              |
| 1:B:417:ALA:HA   | 1:B:420:GLU:HB3  | 1.84                     | 0.59              |
| 1:B:442:SER:O    | 1:B:446:SER:HB3  | 2.03                     | 0.59              |
| 1:A:278:LEU:CD1  | 1:A:286:LEU:HB2  | 2.32                     | 0.59              |
| 1:A:592:SER:O    | 1:A:595:GLN:HG2  | 2.03                     | 0.59              |
| 1:A:684:MET:SD   | 1:A:684:MET:N    | 2.75                     | 0.59              |
| 1:A:83:LYS:HA    | 1:A:86:LEU:HD12  | 1.85                     | 0.59              |
| 1:B:614:ARG:NH1  | 1:B:720:VAL:HG23 | 2.14                     | 0.59              |
| 1:B:686:GLU:HA   | 1:B:686:GLU:OE1  | 2.02                     | 0.59              |
| 1:A:328:ARG:HG2  | 1:A:328:ARG:NH1  | 2.14                     | 0.58              |
| 1:B:244:LEU:HD22 | 1:B:248:LYS:HE3  | 1.84                     | 0.58              |
| 1:A:626:ILE:O    | 1:A:630:MET:HB3  | 2.04                     | 0.58              |
| 1:A:647:GLU:HG3  | 1:A:648:LEU:N    | 2.18                     | 0.58              |
| 1:B:206:ILE:CG2  | 1:B:209:VAL:HA   | 2.34                     | 0.58              |
| 1:B:483:ALA:HB1  | 1:B:487:ALA:HB3  | 1.84                     | 0.58              |
| 1:A:279:PHE:HD1  | 1:A:778:ALA:O    | 1.83                     | 0.58              |
| 1:B:88:GLY:HA3   | 1:B:109:THR:HG21 | 1.86                     | 0.58              |
| 1:A:764:ILE:O    | 1:A:768:GLU:HG3  | 2.03                     | 0.58              |
| 1:A:226:GLN:OE1  | 1:A:350:MET:HE2  | 2.04                     | 0.58              |
| 1:B:703:PHE:CZ   | 1:B:707:GLN:NE2  | 2.71                     | 0.58              |
| 1:B:87:MET:HA    | 1:B:90:VAL:HG12  | 1.86                     | 0.58              |
| 1:B:100:MET:O    | 1:B:372:GLY:HA2  | 2.04                     | 0.58              |
| 1:B:676:ILE:CG1  | 1:B:684:MET:HG2  | 2.34                     | 0.58              |
| 1:A:257:LYS:NZ   | 1:A:660:LEU:HD12 | 2.18                     | 0.58              |
| 1:A:626:ILE:CG2  | 1:A:711:PHE:CD1  | 2.81                     | 0.58              |
| 1:B:476:GLN:HE22 | 1:B:494:LYS:NZ   | 2.00                     | 0.58              |
| 1:B:703:PHE:O    | 1:B:703:PHE:CG   | 2.57                     | 0.58              |
| 1:B:741:ARG:HG3  | 1:B:742:ALA:N    | 2.17                     | 0.58              |
| 1:B:302:LYS:O    | 1:B:302:LYS:HG3  | 2.04                     | 0.57              |
| 1:B:460:ASN:ND2  | 1:B:462:LYS:HB2  | 2.19                     | 0.57              |
| 1:A:610:ILE:HG21 | 1:A:723:LYS:HE2  | 1.85                     | 0.57              |
| 1:A:5:LEU:CB     | 1:A:383:ASN:OD1  | 2.49                     | 0.57              |
| 1:A:324:MET:HB3  | 1:A:327:ARG:HD2  | 1.86                     | 0.57              |
| 1:A:510:THR:O    | 1:A:511:GLU:HB3  | 2.04                     | 0.57              |
| 1:B:718:ARG:HD2  | 1:B:722:SER:HB3  | 1.87                     | 0.57              |
| 1:B:647:GLU:HB3  | 1:B:652:TRP:CH2  | 2.39                     | 0.57              |
| 1:A:561:PHE:O    | 1:A:561:PHE:CD1  | 2.57                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:766:SER:O    | 1:B:769:ASP:OD1  | 2.21                     | 0.57              |
| 1:A:649:PRO:O    | 1:A:650:GLU:HG3  | 2.04                     | 0.57              |
| 1:A:723:LYS:HG3  | 1:A:724:TRP:N    | 2.20                     | 0.57              |
| 1:B:307:VAL:CG2  | 1:B:316:VAL:HG21 | 2.35                     | 0.57              |
| 1:A:301:GLN:O    | 1:A:306:TYR:HB2  | 2.05                     | 0.56              |
| 1:A:329:TYR:HB3  | 1:A:333:LEU:HB2  | 1.86                     | 0.56              |
| 1:B:152:VAL:HG13 | 1:B:172:ILE:CG2  | 2.34                     | 0.56              |
| 1:B:168:TYR:CD1  | 1:B:197:VAL:HG12 | 2.39                     | 0.56              |
| 1:A:300:MET:SD   | 1:A:306:TYR:HE2  | 2.28                     | 0.56              |
| 1:A:637:ARG:NH2  | 1:A:769:ASP:HB2  | 2.20                     | 0.56              |
| 1:B:403:ARG:HB3  | 1:B:536:GLN:OE1  | 2.05                     | 0.56              |
| 1:B:430:GLN:HG2  | 1:B:504:GLY:O    | 2.06                     | 0.56              |
| 1:B:637:ARG:HB3  | 1:B:665:TYR:HH   | 1.71                     | 0.56              |
| 1:B:696:TYR:OH   | 1:B:711:PHE:CE2  | 2.58                     | 0.56              |
| 1:A:190:VAL:CG1  | 1:A:192:TYR:O    | 2.53                     | 0.56              |
| 1:B:612:LYS:O    | 1:B:613:GLN:C    | 2.48                     | 0.56              |
| 1:A:283:HIS:O    | 1:A:284:VAL:C    | 2.48                     | 0.56              |
| 1:A:358:GLN:CG   | 1:A:385:TYR:OH   | 2.54                     | 0.56              |
| 1:A:747:ASN:O    | 1:A:750:ARG:HB2  | 2.05                     | 0.56              |
| 1:B:27:ASP:O     | 1:B:30:ARG:HB3   | 2.04                     | 0.56              |
| 1:B:249:ASP:H    | 1:B:261:LEU:HB2  | 1.70                     | 0.56              |
| 1:A:647:GLU:HG3  | 1:A:648:LEU:H    | 1.70                     | 0.56              |
| 1:B:221:LEU:HD11 | 1:B:357:PHE:CE2  | 2.40                     | 0.56              |
| 1:A:438:ALA:HB1  | 1:A:440:GLU:OE1  | 2.06                     | 0.56              |
| 1:B:184:TYR:CE1  | 1:B:363:MET:HE1  | 2.40                     | 0.56              |
| 1:B:250:TYR:CE2  | 1:B:659:ASP:HB3  | 2.37                     | 0.56              |
| 1:A:348:GLU:OE1  | 1:B:573:MET:SD   | 2.63                     | 0.56              |
| 1:A:512:ARG:HD2  | 1:A:519:ASP:OD1  | 2.05                     | 0.56              |
| 1:B:233:LEU:HB3  | 1:B:289:HIS:ND1  | 2.19                     | 0.56              |
| 1:B:723:LYS:HB2  | 1:B:763:MET:SD   | 2.46                     | 0.56              |
| 1:A:426:TYR:HD1  | 1:A:454:ILE:HG23 | 1.68                     | 0.56              |
| 1:B:642:TYR:O    | 1:B:646:GLU:HG3  | 2.06                     | 0.56              |
| 1:B:17:ASN:O     | 1:B:20:GLU:HB2   | 2.06                     | 0.55              |
| 1:B:380:GLU:CD   | 1:B:593:ARG:NH1  | 2.64                     | 0.55              |
| 1:B:637:ARG:NE   | 1:B:769:ASP:HA   | 2.19                     | 0.55              |
| 1:A:373:THR:O    | 1:A:517:ARG:HD2  | 2.06                     | 0.55              |
| 1:B:344:GLU:O    | 1:B:345:ILE:C    | 2.48                     | 0.55              |
| 1:A:644:PRO:C    | 1:A:646:GLU:H    | 2.13                     | 0.55              |
| 1:A:734:LEU:O    | 1:A:738:ILE:HB   | 2.06                     | 0.55              |
| 1:A:270:GLU:OE2  | 1:A:278:LEU:HD21 | 2.07                     | 0.55              |
| 1:B:252:TYR:HE2  | 1:B:254:ILE:HG22 | 1.71                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:626:ILE:HG23 | 1:B:715:ILE:CD1  | 2.36                     | 0.55              |
| 1:A:300:MET:SD   | 1:A:306:TYR:CD2  | 2.99                     | 0.55              |
| 1:A:641:ALA:HB1  | 1:A:660:LEU:HD11 | 1.87                     | 0.55              |
| 1:B:16:LEU:HD22  | 1:B:16:LEU:H     | 1.72                     | 0.55              |
| 1:A:43:HIS:HA    | 1:A:46:ILE:HD12  | 1.89                     | 0.55              |
| 1:A:541:MET:SD   | 1:A:561:PHE:CZ   | 3.00                     | 0.55              |
| 1:A:626:ILE:HG21 | 1:A:711:PHE:HD1  | 1.71                     | 0.55              |
| 1:A:552:GLU:H    | 1:A:560:ARG:HH12 | 1.54                     | 0.55              |
| 1:B:315:ILE:HG13 | 1:B:327:ARG:HB2  | 1.88                     | 0.55              |
| 1:B:720:VAL:CG1  | 1:B:721:ASP:N    | 2.69                     | 0.55              |
| 1:A:561:PHE:O    | 1:A:569:ILE:CG1  | 2.53                     | 0.55              |
| 1:B:354:THR:HG21 | 1:B:735:ARG:NH1  | 2.21                     | 0.55              |
| 1:A:356:THR:HB   | 1:A:358:GLN:OE1  | 2.07                     | 0.55              |
| 1:A:606:GLN:NE2  | 1:A:760:PHE:HB2  | 2.21                     | 0.55              |
| 1:A:301:GLN:O    | 1:A:306:TYR:CB   | 2.55                     | 0.54              |
| 1:B:624:ARG:NH1  | 1:B:700:GLU:HG2  | 2.22                     | 0.54              |
| 1:B:711:PHE:O    | 1:B:715:ILE:CD1  | 2.55                     | 0.54              |
| 1:A:337:ILE:HG22 | 1:A:344:GLU:O    | 2.07                     | 0.54              |
| 1:A:650:GLU:HB3  | 1:A:652:TRP:HB2  | 1.89                     | 0.54              |
| 1:B:647:GLU:O    | 1:B:652:TRP:CZ2  | 2.59                     | 0.54              |
| 1:A:769:ASP:O    | 1:A:770:GLU:C    | 2.50                     | 0.54              |
| 1:B:646:GLU:OE1  | 1:B:681:PRO:HG3  | 2.08                     | 0.54              |
| 1:B:706:GLU:O    | 1:B:709:ARG:CB   | 2.55                     | 0.54              |
| 1:B:92:LEU:HB2   | 1:B:113:PRO:HG3  | 1.89                     | 0.54              |
| 1:B:344:GLU:O    | 1:B:344:GLU:CG   | 2.56                     | 0.54              |
| 1:B:614:ARG:HH12 | 1:B:720:VAL:HG22 | 1.69                     | 0.54              |
| 1:A:257:LYS:HZ1  | 1:A:660:LEU:HD12 | 1.73                     | 0.54              |
| 1:A:279:PHE:CD1  | 1:A:779:GLU:HA   | 2.40                     | 0.54              |
| 1:A:606:GLN:HG2  | 1:A:760:PHE:CE1  | 2.43                     | 0.54              |
| 1:A:625:GLU:O    | 1:A:629:ASN:ND2  | 2.40                     | 0.54              |
| 1:B:595:GLN:HE22 | 1:B:739:HIS:CE1  | 2.25                     | 0.54              |
| 1:B:610:ILE:HG13 | 1:B:724:TRP:CZ3  | 2.42                     | 0.54              |
| 1:A:50:GLU:O     | 1:A:54:LYS:HG3   | 2.07                     | 0.54              |
| 1:B:325:LYS:H    | 1:B:741:ARG:CD   | 2.20                     | 0.54              |
| 1:B:217:ALA:HB1  | 1:B:358:GLN:NE2  | 2.20                     | 0.54              |
| 1:B:723:LYS:O    | 1:B:727:HIS:HB2  | 2.07                     | 0.54              |
| 1:A:606:GLN:HE21 | 1:A:760:PHE:HB2  | 1.72                     | 0.54              |
| 1:A:676:ILE:O    | 1:A:676:ILE:HG22 | 2.08                     | 0.54              |
| 1:A:723:LYS:CG   | 1:A:767:ILE:HD11 | 2.38                     | 0.54              |
| 1:B:177:ASN:HD22 | 1:B:212:ILE:HG23 | 1.73                     | 0.54              |
| 1:B:184:TYR:HE1  | 1:B:363:MET:HE1  | 1.73                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:231:THR:HB   | 1:B:348:GLU:HG3  | 1.88                     | 0.54              |
| 1:B:476:GLN:NE2  | 1:B:494:LYS:NZ   | 2.56                     | 0.54              |
| 1:B:595:GLN:HE22 | 1:B:739:HIS:HE1  | 1.56                     | 0.54              |
| 1:B:642:TYR:N    | 1:B:642:TYR:CD2  | 2.73                     | 0.54              |
| 1:B:718:ARG:NH1  | 1:B:770:GLU:OE1  | 2.35                     | 0.54              |
| 1:A:604:ARG:O    | 1:A:608:GLU:HG2  | 2.08                     | 0.54              |
| 1:B:238:ASN:HD21 | 1:B:340:LYS:CA   | 2.21                     | 0.54              |
| 1:B:347:ASN:O    | 1:B:348:GLU:CD   | 2.51                     | 0.54              |
| 1:B:447:LYS:HD3  | 1:B:450:LYS:HE3  | 1.90                     | 0.54              |
| 1:B:718:ARG:HD2  | 1:B:722:SER:CB   | 2.38                     | 0.54              |
| 1:A:322:ARG:NH1  | 1:A:743:TYR:HE1  | 2.06                     | 0.54              |
| 1:B:209:VAL:HG13 | 1:B:210:ASP:N    | 2.22                     | 0.54              |
| 1:A:671:LEU:HD11 | 1:A:674:SER:HA   | 1.90                     | 0.53              |
| 1:A:695:LYS:O    | 1:A:698:GLU:HG2  | 2.08                     | 0.53              |
| 1:B:523:ARG:HB3  | 1:B:535:THR:HG21 | 1.90                     | 0.53              |
| 1:B:652:TRP:HB2  | 1:B:654:LEU:HG   | 1.89                     | 0.53              |
| 1:A:279:PHE:C    | 1:A:778:ALA:HB1  | 2.33                     | 0.53              |
| 1:A:459:LEU:HD22 | 1:A:467:GLU:HB3  | 1.89                     | 0.53              |
| 1:A:548:ARG:HH12 | 1:B:735:ARG:HD3  | 1.73                     | 0.53              |
| 1:B:486:MET:HE2  | 1:B:486:MET:HA   | 1.91                     | 0.53              |
| 1:B:494:LYS:HD3  | 1:B:494:LYS:N    | 2.21                     | 0.53              |
| 1:A:105:GLY:HA2  | 2:A:781:ADP:PA   | 2.48                     | 0.53              |
| 1:A:284:VAL:CG1  | 1:A:718:ARG:HH21 | 2.21                     | 0.53              |
| 1:B:610:ILE:HG13 | 1:B:724:TRP:CE3  | 2.44                     | 0.53              |
| 1:A:252:TYR:CD2  | 1:A:257:LYS:O    | 2.62                     | 0.53              |
| 1:A:259:VAL:HA   | 1:A:291:ASN:OD1  | 2.08                     | 0.53              |
| 1:A:302:LYS:HG2  | 1:A:303:ASP:N    | 2.23                     | 0.53              |
| 1:B:261:LEU:C    | 1:B:261:LEU:HD13 | 2.34                     | 0.53              |
| 1:A:610:ILE:CD1  | 1:A:723:LYS:NZ   | 2.71                     | 0.53              |
| 1:B:244:LEU:HD22 | 1:B:248:LYS:CE   | 2.39                     | 0.53              |
| 1:B:248:LYS:NZ   | 1:B:268:LYS:CB   | 2.70                     | 0.53              |
| 1:B:336:ALA:O    | 1:B:340:LYS:CD   | 2.53                     | 0.53              |
| 1:A:127:VAL:HB   | 1:A:206:ILE:HA   | 1.91                     | 0.53              |
| 1:B:647:GLU:OE1  | 1:B:647:GLU:HA   | 2.09                     | 0.53              |
| 1:A:270:GLU:CD   | 1:A:278:LEU:HD21 | 2.33                     | 0.53              |
| 1:B:199:ARG:HB3  | 1:B:200:PRO:HD3  | 1.90                     | 0.53              |
| 1:B:206:ILE:HG22 | 1:B:209:VAL:HA   | 1.91                     | 0.53              |
| 1:B:210:ASP:OD1  | 1:B:371:THR:HG21 | 2.09                     | 0.53              |
| 1:A:206:ILE:CG2  | 1:A:212:ILE:HD12 | 2.39                     | 0.52              |
| 1:A:630:MET:O    | 1:A:634:SER:OG   | 2.25                     | 0.52              |
| 1:A:672:GLU:C    | 1:A:673:LYS:HG2  | 2.35                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:447:LYS:HB3  | 1:B:450:LYS:HG3  | 1.90                     | 0.52              |
| 1:B:718:ARG:CG   | 1:B:770:GLU:CD   | 2.71                     | 0.52              |
| 1:A:93:HIS:CD2   | 1:A:116:LEU:HD23 | 2.45                     | 0.52              |
| 1:A:279:PHE:CD1  | 1:A:779:GLU:CA   | 2.89                     | 0.52              |
| 1:B:201:LEU:CD1  | 1:B:363:MET:HE2  | 2.40                     | 0.52              |
| 1:B:221:LEU:O    | 1:B:354:THR:HA   | 2.09                     | 0.52              |
| 1:A:210:ASP:OD2  | 1:A:371:THR:CG2  | 2.57                     | 0.52              |
| 1:B:245:LYS:C    | 1:B:247:GLU:H    | 2.17                     | 0.52              |
| 1:A:576:ARG:HE   | 1:B:312:GLN:HE21 | 1.56                     | 0.52              |
| 1:B:302:LYS:HD3  | 1:B:341:GLU:CD   | 2.35                     | 0.52              |
| 1:B:434:VAL:HB   | 1:B:482:ILE:HG13 | 1.92                     | 0.52              |
| 1:A:27:ASP:O     | 1:A:30:ARG:HB3   | 2.10                     | 0.52              |
| 1:A:317:ASP:CB   | 1:A:320:THR:HG22 | 2.34                     | 0.52              |
| 1:A:637:ARG:HH21 | 1:A:769:ASP:HB2  | 1.75                     | 0.52              |
| 1:A:686:GLU:OE2  | 1:A:687:LEU:HG   | 2.10                     | 0.52              |
| 1:B:522:LEU:O    | 1:B:525:ARG:CG   | 2.55                     | 0.52              |
| 1:A:5:LEU:H      | 1:A:5:LEU:HD23   | 1.75                     | 0.52              |
| 1:B:650:GLU:OE1  | 1:B:651:GLU:N    | 2.37                     | 0.52              |
| 1:A:91:ALA:O     | 1:A:96:ASN:HB2   | 2.10                     | 0.52              |
| 1:A:407:ILE:HB   | 1:A:569:ILE:HG22 | 1.92                     | 0.52              |
| 1:A:637:ARG:CZ   | 1:A:769:ASP:HB2  | 2.40                     | 0.52              |
| 1:B:322:ARG:HG3  | 1:B:742:ALA:HB3  | 1.92                     | 0.52              |
| 1:B:637:ARG:O    | 1:B:638:ALA:C    | 2.52                     | 0.52              |
| 1:B:770:GLU:O    | 1:B:771:VAL:C    | 2.52                     | 0.52              |
| 1:A:457:GLN:NE2  | 1:A:470:ILE:HD12 | 2.10                     | 0.51              |
| 1:A:643:THR:N    | 1:A:644:PRO:CD   | 2.74                     | 0.51              |
| 1:B:322:ARG:HD3  | 1:B:324:MET:HE2  | 1.91                     | 0.51              |
| 1:B:262:THR:OG1  | 1:B:668:GLU:CD   | 2.53                     | 0.51              |
| 1:B:418:VAL:O    | 1:B:422:VAL:CG2  | 2.51                     | 0.51              |
| 1:B:625:GLU:CG   | 1:B:625:GLU:O    | 2.42                     | 0.51              |
| 1:A:206:ILE:HD12 | 1:A:206:ILE:N    | 2.24                     | 0.51              |
| 1:A:221:LEU:O    | 1:A:354:THR:HA   | 2.10                     | 0.51              |
| 1:A:436:THR:HG22 | 1:A:438:ALA:H    | 1.75                     | 0.51              |
| 1:B:13:LYS:HA    | 1:B:16:LEU:HD21  | 1.93                     | 0.51              |
| 1:B:39:ASP:HA    | 1:B:42:LYS:CB    | 2.39                     | 0.51              |
| 1:A:654:LEU:CD2  | 1:A:677:PHE:CE2  | 2.94                     | 0.51              |
| 1:B:233:LEU:HB2  | 1:B:289:HIS:HE1  | 1.73                     | 0.51              |
| 1:B:325:LYS:O    | 1:B:741:ARG:NH1  | 2.43                     | 0.51              |
| 1:B:371:THR:HG22 | 1:B:372:GLY:N    | 2.26                     | 0.51              |
| 1:B:642:TYR:CE1  | 1:B:685:LEU:HA   | 2.42                     | 0.51              |
| 1:B:718:ARG:HG3  | 1:B:718:ARG:HH11 | 1.76                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:411:MET:HG2  | 1:A:542:GLU:OE2  | 2.10                     | 0.51              |
| 1:A:741:ARG:NH2  | 1:B:376:THR:HG22 | 2.21                     | 0.51              |
| 1:B:199:ARG:CB   | 1:B:200:PRO:CD   | 2.88                     | 0.51              |
| 1:B:239:ALA:HA   | 1:B:242:ARG:NH1  | 2.25                     | 0.51              |
| 1:B:512:ARG:HG2  | 1:B:539:LEU:CD2  | 2.41                     | 0.51              |
| 1:B:710:GLU:O    | 1:B:714:VAL:HG23 | 2.11                     | 0.51              |
| 1:A:327:ARG:HH21 | 1:A:755:GLU:HG2  | 1.76                     | 0.51              |
| 1:A:522:LEU:O    | 1:A:525:ARG:HG3  | 2.11                     | 0.51              |
| 1:B:718:ARG:CD   | 1:B:722:SER:HB3  | 2.39                     | 0.51              |
| 1:A:255:LYS:HZ2  | 1:A:762:HIS:CE1  | 2.29                     | 0.51              |
| 1:A:278:LEU:HB3  | 1:A:283:HIS:CD2  | 2.41                     | 0.51              |
| 1:A:279:PHE:HD1  | 1:A:779:GLU:N    | 2.09                     | 0.51              |
| 1:A:680:GLU:O    | 1:A:684:MET:SD   | 2.69                     | 0.51              |
| 1:B:400:ARG:HD3  | 1:B:526:SER:O    | 2.10                     | 0.51              |
| 1:B:639:ILE:HG22 | 1:B:640:ALA:N    | 2.26                     | 0.51              |
| 1:B:42:LYS:HE3   | 1:B:149:GLY:HA3  | 1.92                     | 0.50              |
| 1:B:250:TYR:CE1  | 1:B:261:LEU:HA   | 2.45                     | 0.50              |
| 1:B:344:GLU:O    | 1:B:344:GLU:HG2  | 2.11                     | 0.50              |
| 1:B:376:THR:C    | 1:B:378:GLU:H    | 2.19                     | 0.50              |
| 1:A:247:GLU:O    | 1:A:249:ASP:N    | 2.44                     | 0.50              |
| 1:A:562:GLY:HA2  | 1:A:569:ILE:CG1  | 2.39                     | 0.50              |
| 1:B:647:GLU:N    | 1:B:652:TRP:CZ2  | 2.78                     | 0.50              |
| 1:A:251:THR:OG1  | 1:A:252:TYR:N    | 2.45                     | 0.50              |
| 1:B:69:VAL:O     | 1:B:73:SER:HB2   | 2.12                     | 0.50              |
| 1:B:101:LYS:O    | 1:B:104:GLU:HB2  | 2.10                     | 0.50              |
| 1:B:193:LYS:O    | 1:B:196:MET:HG3  | 2.11                     | 0.50              |
| 1:B:610:ILE:HD12 | 1:B:723:LYS:NZ   | 2.26                     | 0.50              |
| 1:B:549:PHE:N    | 1:B:549:PHE:CD2  | 2.79                     | 0.50              |
| 1:B:666:LEU:HD21 | 1:B:692:ILE:HG13 | 1.94                     | 0.50              |
| 1:A:100:MET:HG2  | 1:A:392:ILE:HB   | 1.92                     | 0.50              |
| 1:A:207:ASP:CB   | 1:A:370:MET:HE3  | 2.39                     | 0.50              |
| 1:A:548:ARG:NH1  | 1:B:735:ARG:HD3  | 2.26                     | 0.50              |
| 1:A:689:MET:O    | 1:A:693:ILE:HG22 | 2.12                     | 0.50              |
| 1:B:48:PHE:HE1   | 1:B:68:VAL:HG21  | 1.75                     | 0.50              |
| 1:B:190:VAL:CG2  | 1:B:195:GLN:HG3  | 2.38                     | 0.50              |
| 1:B:215:ASP:OD1  | 1:B:517:ARG:NH2  | 2.45                     | 0.50              |
| 1:B:249:ASP:N    | 1:B:261:LEU:HB2  | 2.27                     | 0.50              |
| 1:A:160:SER:C    | 1:A:162:ASP:N    | 2.69                     | 0.50              |
| 1:A:475:GLY:O    | 1:A:495:LEU:HA   | 2.11                     | 0.50              |
| 1:A:559:ASP:O    | 1:A:563:MET:HE2  | 2.12                     | 0.50              |
| 1:A:588:ASN:OD1  | 1:B:588:ASN:HB3  | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:240:PHE:O    | 1:B:244:LEU:HD21 | 2.12                     | 0.50              |
| 1:A:330:SER:C    | 1:A:331:GLU:HG3  | 2.36                     | 0.50              |
| 1:A:442:SER:HA   | 1:A:482:ILE:HD11 | 1.93                     | 0.50              |
| 1:A:659:ASP:O    | 1:A:660:LEU:C    | 2.55                     | 0.50              |
| 1:B:642:TYR:HE1  | 1:B:685:LEU:CA   | 2.23                     | 0.50              |
| 1:A:3:GLY:O      | 1:A:4:ILE:HG13   | 2.12                     | 0.49              |
| 1:A:107:THR:HG22 | 1:A:141:MET:SD   | 2.52                     | 0.49              |
| 1:A:210:ASP:OD2  | 1:A:210:ASP:N    | 2.40                     | 0.49              |
| 1:B:371:THR:HG22 | 1:B:373:THR:H    | 1.77                     | 0.49              |
| 1:A:486:MET:O    | 1:A:486:MET:HG3  | 2.12                     | 0.49              |
| 1:B:432:VAL:HG13 | 1:B:506:ALA:HB3  | 1.93                     | 0.49              |
| 1:B:261:LEU:HD13 | 1:B:261:LEU:O    | 2.13                     | 0.49              |
| 1:B:484:THR:O    | 1:B:486:MET:N    | 2.45                     | 0.49              |
| 1:A:66:PHE:HE2   | 1:A:112:LEU:C    | 2.20                     | 0.49              |
| 1:A:232:LYS:H    | 1:A:232:LYS:CD   | 2.19                     | 0.49              |
| 1:A:190:VAL:HG13 | 1:A:195:GLN:HB2  | 1.94                     | 0.49              |
| 1:B:647:GLU:N    | 1:B:652:TRP:CZ3  | 2.76                     | 0.49              |
| 1:A:243:THR:O    | 1:A:243:THR:CG2  | 2.55                     | 0.49              |
| 1:B:248:LYS:HG3  | 1:B:248:LYS:O    | 2.13                     | 0.49              |
| 1:A:737:GLY:C    | 1:A:739:HIS:H    | 2.21                     | 0.49              |
| 1:B:233:LEU:CB   | 1:B:289:HIS:CE1  | 2.95                     | 0.49              |
| 1:A:645:ARG:C    | 1:A:646:GLU:HG3  | 2.37                     | 0.49              |
| 1:A:708:MET:N    | 1:A:708:MET:HE2  | 2.28                     | 0.49              |
| 1:B:275:ILE:CD1  | 1:B:283:HIS:CD2  | 2.83                     | 0.49              |
| 1:B:637:ARG:NE   | 1:B:769:ASP:CB   | 2.55                     | 0.49              |
| 1:A:301:GLN:HB2  | 1:A:306:TYR:CE1  | 2.48                     | 0.49              |
| 1:B:238:ASN:CG   | 1:B:340:LYS:HD2  | 2.37                     | 0.49              |
| 1:B:368:ALA:HA   | 1:B:387:MET:HE3  | 1.93                     | 0.49              |
| 1:B:637:ARG:NE   | 1:B:769:ASP:CA   | 2.70                     | 0.49              |
| 1:A:7:LYS:O      | 1:B:743:TYR:CD2  | 2.66                     | 0.49              |
| 1:A:324:MET:CB   | 1:A:327:ARG:HD2  | 2.43                     | 0.49              |
| 1:A:647:GLU:CG   | 1:A:649:PRO:HD2  | 2.42                     | 0.49              |
| 1:B:199:ARG:CB   | 1:B:200:PRO:HD3  | 2.42                     | 0.49              |
| 1:B:445:ILE:O    | 1:B:447:LYS:N    | 2.45                     | 0.48              |
| 1:B:620:SER:OG   | 1:B:625:GLU:HG2  | 2.14                     | 0.48              |
| 1:B:48:PHE:CE1   | 1:B:68:VAL:HG21  | 2.49                     | 0.48              |
| 1:B:284:VAL:HG12 | 1:B:718:ARG:NH2  | 2.28                     | 0.48              |
| 1:B:400:ARG:HD2  | 1:B:535:THR:CG2  | 2.42                     | 0.48              |
| 1:B:673:LYS:HA   | 1:B:676:ILE:HG22 | 1.94                     | 0.48              |
| 1:A:89:GLY:HA2   | 1:A:92:LEU:HD12  | 1.95                     | 0.48              |
| 1:A:177:ASN:OD1  | 1:A:177:ASN:N    | 2.46                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:379:GLU:O    | 1:A:383:ASN:HB3  | 2.13                     | 0.48              |
| 1:B:246:ALA:CB   | 1:B:268:LYS:NZ   | 2.75                     | 0.48              |
| 1:B:248:LYS:HZ3  | 1:B:268:LYS:CD   | 2.26                     | 0.48              |
| 1:B:185:LEU:HD22 | 1:B:353:ALA:CB   | 2.44                     | 0.48              |
| 1:B:262:THR:O    | 1:B:263:GLU:C    | 2.55                     | 0.48              |
| 1:B:727:HIS:NE2  | 1:B:731:MET:HE2  | 2.28                     | 0.48              |
| 1:A:624:ARG:HG2  | 1:A:627:VAL:HB   | 1.95                     | 0.48              |
| 1:B:539:LEU:HD13 | 1:B:546:MET:CE   | 2.42                     | 0.48              |
| 1:B:708:MET:HA   | 1:B:711:PHE:HB2  | 1.96                     | 0.48              |
| 1:A:637:ARG:HG2  | 1:A:769:ASP:HA   | 1.94                     | 0.48              |
| 1:A:2:LEU:O      | 1:A:3:GLY:C      | 2.55                     | 0.48              |
| 1:A:82:PHE:CE1   | 2:A:781:ADP:N6   | 2.82                     | 0.48              |
| 1:A:513:HIS:CE1  | 1:A:518:ILE:HG22 | 2.49                     | 0.48              |
| 1:A:688:ILE:HG12 | 1:A:692:ILE:HD12 | 1.96                     | 0.48              |
| 1:A:249:ASP:CB   | 1:A:260:GLN:O    | 2.62                     | 0.48              |
| 1:A:645:ARG:O    | 1:A:646:GLU:CG   | 2.62                     | 0.48              |
| 1:B:616:GLU:OE1  | 1:B:616:GLU:HA   | 2.14                     | 0.48              |
| 1:B:624:ARG:NH2  | 1:B:707:GLN:HB2  | 2.23                     | 0.48              |
| 1:B:340:LYS:CD   | 1:B:340:LYS:N    | 2.77                     | 0.48              |
| 1:B:649:PRO:O    | 1:B:652:TRP:CZ3  | 2.67                     | 0.48              |
| 1:A:284:VAL:HG11 | 1:A:717:LEU:HD11 | 1.95                     | 0.48              |
| 1:A:414:LYS:HD3  | 1:A:540:SER:N    | 2.28                     | 0.48              |
| 1:A:576:ARG:HH22 | 1:B:346:GLN:NE2  | 2.11                     | 0.48              |
| 1:B:626:ILE:HG23 | 1:B:715:ILE:HD11 | 1.93                     | 0.48              |
| 1:B:741:ARG:O    | 1:B:742:ALA:C    | 2.56                     | 0.48              |
| 1:A:322:ARG:NH1  | 1:A:743:TYR:CE1  | 2.81                     | 0.47              |
| 1:A:662:ASN:HB3  | 1:A:670:ALA:CB   | 2.42                     | 0.47              |
| 1:B:500:LYS:HE2  | 1:B:500:LYS:H    | 1.78                     | 0.47              |
| 1:B:572:LYS:O    | 1:B:575:SER:HB3  | 2.13                     | 0.47              |
| 1:A:279:PHE:HB2  | 1:A:779:GLU:N    | 2.30                     | 0.47              |
| 1:A:380:GLU:OE1  | 1:A:593:ARG:NH1  | 2.46                     | 0.47              |
| 1:B:617:VAL:HG11 | 1:B:716:VAL:CG2  | 2.45                     | 0.47              |
| 1:B:624:ARG:NH2  | 1:B:700:GLU:HG2  | 2.29                     | 0.47              |
| 1:A:10:ASP:HB3   | 1:A:11:PRO:HD2   | 0.68                     | 0.47              |
| 1:A:203:PHE:CD2  | 1:A:204:ALA:N    | 2.82                     | 0.47              |
| 1:A:209:VAL:HG12 | 1:A:371:THR:HG22 | 1.95                     | 0.47              |
| 1:A:324:MET:HG3  | 1:A:327:ARG:NH1  | 2.29                     | 0.47              |
| 1:A:549:PHE:CD2  | 1:A:561:PHE:HE2  | 2.32                     | 0.47              |
| 1:B:261:LEU:C    | 1:B:261:LEU:HD12 | 2.39                     | 0.47              |
| 1:A:382:ARG:O    | 1:A:382:ARG:HG3  | 2.14                     | 0.47              |
| 1:B:248:LYS:HD2  | 1:B:265:GLY:CA   | 2.39                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:484:THR:HG22 | 1:B:485:ASN:OD1  | 2.14                     | 0.47              |
| 1:B:627:VAL:HG13 | 1:B:696:TYR:CZ   | 2.49                     | 0.47              |
| 1:B:750:ARG:NH1  | 1:B:750:ARG:CG   | 2.56                     | 0.47              |
| 1:B:260:GLN:HB3  | 1:B:266:MET:HE3  | 1.96                     | 0.47              |
| 1:B:445:ILE:C    | 1:B:447:LYS:H    | 2.22                     | 0.47              |
| 1:A:228:ALA:C    | 1:A:230:SER:N    | 2.69                     | 0.47              |
| 1:B:61:LEU:O     | 1:B:62:LEU:C     | 2.58                     | 0.47              |
| 1:B:262:THR:O    | 1:B:264:GLU:N    | 2.48                     | 0.47              |
| 1:B:548:ARG:HG3  | 1:B:549:PHE:H    | 1.80                     | 0.47              |
| 1:B:679:LYS:HB3  | 1:B:683:GLU:HG3  | 1.97                     | 0.47              |
| 1:A:194:GLU:HG3  | 1:A:195:GLN:H    | 1.77                     | 0.47              |
| 1:A:738:ILE:HD11 | 1:A:743:TYR:HE2  | 1.80                     | 0.47              |
| 1:A:293:ALA:O    | 1:A:297:HIS:HD2  | 1.97                     | 0.47              |
| 1:A:360:TYR:O    | 1:A:363:MET:HG3  | 2.14                     | 0.47              |
| 1:B:248:LYS:HA   | 1:B:261:LEU:CB   | 2.45                     | 0.47              |
| 1:B:363:MET:HE3  | 1:B:363:MET:HB3  | 1.77                     | 0.47              |
| 1:A:226:GLN:NE2  | 1:A:228:ALA:HB2  | 2.30                     | 0.47              |
| 1:A:647:GLU:CG   | 1:A:648:LEU:H    | 2.28                     | 0.47              |
| 1:B:485:ASN:OD1  | 1:B:486:MET:HG2  | 2.14                     | 0.47              |
| 1:A:558:LEU:CG   | 1:A:563:MET:HE3  | 2.40                     | 0.46              |
| 1:A:662:ASN:O    | 1:A:777:LYS:NZ   | 2.47                     | 0.46              |
| 1:B:74:ARG:HG3   | 1:B:74:ARG:NH1   | 2.29                     | 0.46              |
| 1:B:88:GLY:HA3   | 1:B:109:THR:CG2  | 2.45                     | 0.46              |
| 1:B:708:MET:HA   | 1:B:711:PHE:CD1  | 2.50                     | 0.46              |
| 1:A:302:LYS:HG2  | 1:A:303:ASP:HB2  | 1.98                     | 0.46              |
| 1:A:338:GLU:CG   | 1:A:345:ILE:HG13 | 2.35                     | 0.46              |
| 1:B:229:LYS:HD3  | 1:B:289:HIS:CD2  | 2.50                     | 0.46              |
| 1:B:307:VAL:CG1  | 1:B:308:VAL:H    | 2.28                     | 0.46              |
| 1:B:554:THR:HG21 | 1:B:574:VAL:HA   | 1.97                     | 0.46              |
| 1:A:706:GLU:O    | 1:A:709:ARG:N    | 2.49                     | 0.46              |
| 1:B:39:ASP:CG    | 1:B:42:LYS:HB3   | 2.40                     | 0.46              |
| 1:B:256:THR:CG2  | 1:B:295:LYS:HD2  | 2.42                     | 0.46              |
| 1:A:754:MET:HE2  | 1:A:754:MET:HB3  | 1.71                     | 0.46              |
| 1:B:39:ASP:OD2   | 1:B:42:LYS:HB3   | 2.15                     | 0.46              |
| 1:A:328:ARG:HH11 | 1:A:328:ARG:CG   | 2.25                     | 0.46              |
| 1:A:600:ASP:O    | 1:A:604:ARG:N    | 2.36                     | 0.46              |
| 1:B:611:TYR:O    | 1:B:614:ARG:HG2  | 2.16                     | 0.46              |
| 1:A:9:PHE:HD2    | 1:A:10:ASP:N     | 2.09                     | 0.46              |
| 1:A:84:VAL:HG21  | 1:A:395:ASN:HB2  | 1.97                     | 0.46              |
| 1:A:123:GLY:HA2  | 1:A:171:ASP:O    | 2.16                     | 0.46              |
| 1:B:238:ASN:HD21 | 1:B:340:LYS:HD2  | 1.79                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:279:PHE:HZ   | 1:B:773:LYS:HE2  | 1.80                     | 0.46              |
| 1:B:403:ARG:HG2  | 1:B:404:PRO:HD2  | 1.96                     | 0.46              |
| 1:A:164:LYS:NZ   | 1:A:183:ASP:OD1  | 2.48                     | 0.46              |
| 1:A:439:VAL:HG23 | 1:B:411:MET:CE   | 2.46                     | 0.46              |
| 1:A:463:ASN:O    | 1:A:467:GLU:HG3  | 2.15                     | 0.46              |
| 1:A:513:HIS:ND1  | 1:A:519:ASP:OD2  | 2.49                     | 0.46              |
| 1:A:739:HIS:HB3  | 1:B:583:LYS:HD2  | 1.98                     | 0.46              |
| 1:A:745:GLN:NE2  | 1:B:584:ARG:HA   | 2.31                     | 0.46              |
| 1:B:324:MET:HA   | 1:B:741:ARG:CD   | 2.37                     | 0.46              |
| 1:B:406:LEU:HD12 | 1:B:538:TYR:CE1  | 2.51                     | 0.46              |
| 1:B:414:LYS:NZ   | 1:B:510:THR:O    | 2.29                     | 0.46              |
| 1:B:484:THR:O    | 1:B:485:ASN:C    | 2.58                     | 0.46              |
| 1:A:112:LEU:HB2  | 1:A:113:PRO:HD3  | 1.98                     | 0.46              |
| 1:A:226:GLN:NE2  | 1:A:228:ALA:CB   | 2.79                     | 0.46              |
| 1:A:244:LEU:HD22 | 1:A:248:LYS:HG3  | 1.98                     | 0.46              |
| 1:A:484:THR:O    | 1:A:485:ASN:C    | 2.57                     | 0.46              |
| 1:A:512:ARG:HH11 | 1:A:582:GLN:NE2  | 2.14                     | 0.46              |
| 1:A:552:GLU:O    | 1:A:560:ARG:NH1  | 2.48                     | 0.46              |
| 1:B:551:ALA:C    | 1:B:553:ARG:H    | 2.23                     | 0.46              |
| 1:B:686:GLU:OE1  | 1:B:686:GLU:CA   | 2.63                     | 0.46              |
| 1:B:711:PHE:O    | 1:B:715:ILE:HD12 | 2.15                     | 0.46              |
| 1:A:207:ASP:HB2  | 1:A:370:MET:HE1  | 1.96                     | 0.46              |
| 1:A:255:LYS:CE   | 1:A:762:HIS:HE1  | 2.29                     | 0.46              |
| 1:A:609:VAL:HG12 | 1:A:610:ILE:HD13 | 1.97                     | 0.46              |
| 1:B:147:PHE:C    | 1:B:149:GLY:N    | 2.73                     | 0.46              |
| 1:B:155:ASN:HB3  | 1:B:175:SER:HB2  | 1.98                     | 0.46              |
| 1:B:708:MET:C    | 1:B:711:PHE:HB2  | 2.41                     | 0.46              |
| 1:A:176:THR:O    | 1:A:177:ASN:C    | 2.59                     | 0.45              |
| 1:A:226:GLN:HE22 | 1:A:228:ALA:HB2  | 1.80                     | 0.45              |
| 1:A:410:THR:HA   | 1:A:542:GLU:HB2  | 1.98                     | 0.45              |
| 1:B:425:ARG:CD   | 1:B:430:GLN:OE1  | 2.61                     | 0.45              |
| 1:B:539:LEU:HB3  | 1:B:546:MET:HE2  | 1.98                     | 0.45              |
| 1:A:740:LEU:H    | 1:A:740:LEU:CD2  | 2.24                     | 0.45              |
| 1:B:602:VAL:O    | 1:B:606:GLN:HG3  | 2.16                     | 0.45              |
| 1:B:611:TYR:O    | 1:B:615:PHE:HD1  | 2.00                     | 0.45              |
| 1:B:630:MET:HE3  | 1:B:630:MET:O    | 2.17                     | 0.45              |
| 1:B:37:SER:N     | 1:B:40:ALA:HB3   | 2.30                     | 0.45              |
| 1:B:231:THR:HB   | 1:B:348:GLU:CG   | 2.46                     | 0.45              |
| 1:B:248:LYS:HD3  | 1:B:265:GLY:HA2  | 1.94                     | 0.45              |
| 1:B:426:TYR:CD2  | 1:B:454:ILE:HG23 | 2.50                     | 0.45              |
| 1:B:617:VAL:O    | 1:B:617:VAL:CG1  | 2.65                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:442:SER:O    | 1:A:482:ILE:HD11 | 2.15                     | 0.45              |
| 1:A:528:ARG:HG3  | 1:A:528:ARG:NH1  | 2.27                     | 0.45              |
| 1:B:424:GLN:C    | 1:B:426:TYR:H    | 2.24                     | 0.45              |
| 1:B:607:ARG:O    | 1:B:608:GLU:C    | 2.58                     | 0.45              |
| 1:A:5:LEU:HG     | 1:A:590:PHE:HZ   | 1.82                     | 0.45              |
| 1:A:45:THR:O     | 1:A:49:LYS:HG3   | 2.16                     | 0.45              |
| 1:A:88:GLY:HA2   | 1:A:392:ILE:CD1  | 2.46                     | 0.45              |
| 1:A:283:HIS:O    | 1:A:285:ALA:N    | 2.50                     | 0.45              |
| 1:A:682:ASP:HA   | 1:A:685:LEU:HG   | 1.99                     | 0.45              |
| 1:A:741:ARG:NH2  | 1:B:376:THR:O    | 2.50                     | 0.45              |
| 1:B:191:LEU:HD13 | 1:B:191:LEU:O    | 2.16                     | 0.45              |
| 1:B:252:TYR:CE2  | 1:B:254:ILE:HG22 | 2.50                     | 0.45              |
| 1:B:376:THR:HB   | 1:B:377:GLU:OE2  | 2.16                     | 0.45              |
| 1:B:515:SER:C    | 1:B:516:ARG:HH11 | 2.25                     | 0.45              |
| 1:B:593:ARG:O    | 1:B:594:LYS:C    | 2.59                     | 0.45              |
| 1:B:738:ILE:HD12 | 1:B:748:PRO:HB2  | 1.98                     | 0.45              |
| 1:A:203:PHE:HD2  | 1:A:204:ALA:N    | 2.14                     | 0.45              |
| 1:A:258:ALA:CB   | 1:A:295:LYS:HG2  | 2.45                     | 0.45              |
| 1:A:642:TYR:CE1  | 1:A:684:MET:HB3  | 2.52                     | 0.45              |
| 1:B:89:GLY:HA2   | 1:B:113:PRO:HD3  | 1.98                     | 0.45              |
| 1:B:639:ILE:HG13 | 1:B:685:LEU:HD22 | 1.98                     | 0.45              |
| 1:A:279:PHE:O    | 1:A:778:ALA:CB   | 2.65                     | 0.45              |
| 1:A:747:ASN:C    | 1:A:749:LEU:N    | 2.74                     | 0.45              |
| 1:B:248:LYS:HB3  | 1:B:265:GLY:HA2  | 1.89                     | 0.45              |
| 1:B:506:ALA:HA   | 1:B:534:ILE:HG23 | 1.99                     | 0.45              |
| 1:A:5:LEU:O      | 1:A:6:ASN:HB2    | 2.16                     | 0.45              |
| 1:A:206:ILE:O    | 1:A:369:GLY:HA2  | 2.17                     | 0.45              |
| 1:A:368:ALA:HA   | 1:A:387:MET:HE3  | 1.99                     | 0.45              |
| 1:A:653:LYS:HE3  | 1:A:653:LYS:O    | 2.17                     | 0.45              |
| 1:B:112:LEU:HB2  | 1:B:113:PRO:HD3  | 1.98                     | 0.45              |
| 1:B:218:ARG:O    | 1:B:218:ARG:HG2  | 2.16                     | 0.45              |
| 1:B:230:SER:C    | 1:B:232:LYS:N    | 2.75                     | 0.45              |
| 1:A:436:THR:HG22 | 1:A:437:VAL:N    | 2.31                     | 0.45              |
| 1:A:643:THR:N    | 1:A:644:PRO:HD2  | 2.32                     | 0.45              |
| 1:B:723:LYS:HG2  | 1:B:767:ILE:CG1  | 2.46                     | 0.45              |
| 1:B:512:ARG:HD2  | 1:B:537:PHE:CD2  | 2.53                     | 0.44              |
| 1:A:439:VAL:HG23 | 1:B:411:MET:HE1  | 1.99                     | 0.44              |
| 1:A:571:SER:O    | 1:A:572:LYS:C    | 2.59                     | 0.44              |
| 1:A:642:TYR:C    | 1:A:644:PRO:HD2  | 2.43                     | 0.44              |
| 1:B:256:THR:O    | 1:B:257:LYS:HD3  | 2.16                     | 0.44              |
| 1:B:283:HIS:HB3  | 1:B:286:LEU:HB3  | 1.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:596:LEU:HD12 | 1:B:596:LEU:HA   | 1.79                     | 0.44              |
| 1:A:210:ASP:OD2  | 1:A:371:THR:CB   | 2.64                     | 0.44              |
| 1:A:718:ARG:NH1  | 1:A:722:SER:HB3  | 2.32                     | 0.44              |
| 1:B:13:LYS:O     | 1:B:16:LEU:HD23  | 2.18                     | 0.44              |
| 1:B:222:ILE:HG12 | 1:B:354:THR:HG23 | 1.98                     | 0.44              |
| 1:B:731:MET:O    | 1:B:735:ARG:HB2  | 2.17                     | 0.44              |
| 1:A:238:ASN:O    | 1:A:241:VAL:HG23 | 2.17                     | 0.44              |
| 1:A:362:ARG:HH21 | 1:A:597:LEU:HD11 | 1.82                     | 0.44              |
| 1:A:718:ARG:HD3  | 1:A:770:GLU:HG2  | 1.98                     | 0.44              |
| 1:B:354:THR:HG21 | 1:B:735:ARG:CZ   | 2.48                     | 0.44              |
| 1:B:413:GLY:O    | 1:B:416:LYS:HB3  | 2.17                     | 0.44              |
| 1:B:493:ILE:HD13 | 1:B:525:ARG:HB3  | 1.98                     | 0.44              |
| 1:A:215:ASP:OD2  | 1:A:517:ARG:NH2  | 2.43                     | 0.44              |
| 1:A:753:GLN:HG3  | 1:A:754:MET:H    | 1.83                     | 0.44              |
| 1:B:322:ARG:NH2  | 1:B:742:ALA:O    | 2.51                     | 0.44              |
| 1:B:516:ARG:N    | 1:B:516:ARG:HD2  | 2.33                     | 0.44              |
| 1:B:243:THR:O    | 1:B:243:THR:CG2  | 2.62                     | 0.44              |
| 1:B:554:THR:CG2  | 1:B:574:VAL:HG22 | 2.48                     | 0.44              |
| 1:B:610:ILE:HD12 | 1:B:723:LYS:HZ3  | 1.78                     | 0.44              |
| 1:B:755:GLU:O    | 1:B:759:MET:HG3  | 2.18                     | 0.44              |
| 1:A:554:THR:CG2  | 1:A:555:MET:N    | 2.78                     | 0.44              |
| 1:A:558:LEU:HD12 | 1:A:558:LEU:HA   | 1.76                     | 0.44              |
| 1:A:637:ARG:HE   | 1:A:769:ASP:CA   | 2.31                     | 0.44              |
| 1:A:709:ARG:HD3  | 1:A:709:ARG:C    | 2.42                     | 0.44              |
| 1:A:718:ARG:HD3  | 1:A:770:GLU:CG   | 2.48                     | 0.44              |
| 1:A:731:MET:HE1  | 1:A:756:GLY:HA3  | 1.99                     | 0.44              |
| 1:B:102:THR:HA   | 1:B:106:LYS:NZ   | 2.32                     | 0.44              |
| 1:B:379:GLU:HG2  | 1:B:383:ASN:ND2  | 2.29                     | 0.44              |
| 1:B:461:ALA:HA   | 1:B:467:GLU:OE2  | 2.18                     | 0.44              |
| 1:A:641:ALA:HB1  | 1:A:660:LEU:CD1  | 2.48                     | 0.44              |
| 1:A:62:LEU:O     | 1:A:63:VAL:C     | 2.60                     | 0.44              |
| 1:A:513:HIS:C    | 1:A:515:SER:H    | 2.26                     | 0.44              |
| 1:B:99:GLU:OE2   | 1:B:391:THR:HG23 | 2.18                     | 0.44              |
| 1:B:337:ILE:HA   | 1:B:340:LYS:HG2  | 1.98                     | 0.44              |
| 1:B:614:ARG:NH1  | 1:B:720:VAL:CG2  | 2.67                     | 0.44              |
| 1:A:266:MET:HB3  | 1:A:277:ASN:OD1  | 2.18                     | 0.43              |
| 1:A:457:GLN:HE21 | 1:A:470:ILE:CD1  | 2.15                     | 0.43              |
| 1:A:667:ASP:O    | 1:A:669:GLY:N    | 2.51                     | 0.43              |
| 1:B:16:LEU:CD2   | 1:B:16:LEU:N     | 2.77                     | 0.43              |
| 1:B:108:LEU:O    | 1:B:109:THR:C    | 2.60                     | 0.43              |
| 1:B:262:THR:HG1  | 1:B:668:GLU:CD   | 2.26                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:346:GLN:CD   | 1:B:346:GLN:O    | 2.61                     | 0.43              |
| 1:B:457:GLN:HE21 | 1:B:470:ILE:HG23 | 1.82                     | 0.43              |
| 1:A:105:GLY:N    | 2:A:781:ADP:O3A  | 2.49                     | 0.43              |
| 1:A:723:LYS:HB2  | 1:A:763:MET:HG2  | 2.00                     | 0.43              |
| 1:B:238:ASN:HD21 | 1:B:340:LYS:N    | 2.15                     | 0.43              |
| 1:B:368:ALA:CA   | 1:B:387:MET:HE1  | 2.40                     | 0.43              |
| 1:B:630:MET:HB3  | 1:B:630:MET:HE2  | 1.65                     | 0.43              |
| 1:A:279:PHE:HB2  | 1:A:778:ALA:C    | 2.43                     | 0.43              |
| 1:A:723:LYS:CD   | 1:A:763:MET:CE   | 2.82                     | 0.43              |
| 1:B:250:TYR:CD1  | 1:B:261:LEU:HA   | 2.52                     | 0.43              |
| 1:B:270:GLU:HB3  | 1:B:275:ILE:O    | 2.18                     | 0.43              |
| 1:B:716:VAL:O    | 1:B:720:VAL:HB   | 2.18                     | 0.43              |
| 1:B:760:PHE:O    | 1:B:763:MET:HB3  | 2.19                     | 0.43              |
| 1:A:166:GLU:O    | 1:A:169:ALA:HB3  | 2.19                     | 0.43              |
| 1:A:737:GLY:C    | 1:A:739:HIS:N    | 2.76                     | 0.43              |
| 1:B:16:LEU:H     | 1:B:16:LEU:HD23  | 1.80                     | 0.43              |
| 1:A:278:LEU:H    | 1:A:278:LEU:CD2  | 2.20                     | 0.43              |
| 1:A:459:LEU:HB2  | 1:A:483:ALA:HA   | 1.99                     | 0.43              |
| 1:A:647:GLU:CG   | 1:A:648:LEU:N    | 2.81                     | 0.43              |
| 1:A:657:LEU:O    | 1:A:660:LEU:HD23 | 2.18                     | 0.43              |
| 1:A:745:GLN:NE2  | 1:B:587:GLY:HA3  | 2.34                     | 0.43              |
| 1:B:336:ALA:O    | 1:B:337:ILE:C    | 2.61                     | 0.43              |
| 1:B:422:VAL:HG13 | 1:B:432:VAL:HG11 | 2.00                     | 0.43              |
| 1:B:539:LEU:HD13 | 1:B:546:MET:HE1  | 2.00                     | 0.43              |
| 1:A:425:ARG:HB2  | 1:A:432:VAL:HG21 | 2.00                     | 0.43              |
| 1:A:610:ILE:CG2  | 1:A:723:LYS:HE2  | 2.47                     | 0.43              |
| 1:A:776:MET:HE2  | 1:A:776:MET:HA   | 2.00                     | 0.43              |
| 1:B:19:TYR:C     | 1:B:87:MET:HE3   | 2.43                     | 0.43              |
| 1:B:204:ALA:HB3  | 1:B:367:LEU:HD12 | 2.01                     | 0.43              |
| 1:B:509:GLY:O    | 1:B:538:TYR:N    | 2.45                     | 0.43              |
| 1:B:238:ASN:O    | 1:B:239:ALA:C    | 2.62                     | 0.43              |
| 1:B:639:ILE:CG2  | 1:B:640:ALA:N    | 2.82                     | 0.43              |
| 1:B:643:THR:HA   | 1:B:646:GLU:OE2  | 2.18                     | 0.43              |
| 1:A:134:ALA:O    | 1:A:135:SER:C    | 2.61                     | 0.43              |
| 1:A:218:ARG:HB3  | 1:B:549:PHE:CD2  | 2.54                     | 0.43              |
| 1:A:244:LEU:O    | 1:A:244:LEU:HD13 | 2.18                     | 0.43              |
| 1:B:160:SER:O    | 1:B:164:LYS:HG3  | 2.19                     | 0.43              |
| 1:B:227:ALA:HB3  | 1:B:348:GLU:OE1  | 2.19                     | 0.43              |
| 1:B:354:THR:HG22 | 1:B:735:ARG:HH22 | 1.80                     | 0.43              |
| 1:B:603:LEU:HD12 | 1:B:603:LEU:HA   | 1.82                     | 0.43              |
| 1:A:108:LEU:HD12 | 1:A:108:LEU:HA   | 1.76                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:313:VAL:CG2  | 1:A:337:ILE:CD1  | 2.96                     | 0.43              |
| 1:A:666:LEU:HD23 | 1:A:670:ALA:HB2  | 2.00                     | 0.43              |
| 1:B:11:PRO:O     | 1:B:13:LYS:N     | 2.51                     | 0.43              |
| 1:B:262:THR:HG23 | 1:B:263:GLU:N    | 2.34                     | 0.43              |
| 1:B:627:VAL:HG22 | 1:B:711:PHE:CE1  | 2.53                     | 0.43              |
| 1:B:716:VAL:O    | 1:B:716:VAL:HG12 | 2.18                     | 0.43              |
| 1:A:604:ARG:HA   | 1:A:607:ARG:CZ   | 2.49                     | 0.43              |
| 1:B:36:LEU:HD13  | 1:B:40:ALA:O     | 2.19                     | 0.43              |
| 1:B:127:VAL:HG13 | 1:B:180:LEU:HD12 | 2.01                     | 0.43              |
| 1:B:199:ARG:HB3  | 1:B:200:PRO:HD2  | 1.97                     | 0.43              |
| 1:B:209:VAL:CG1  | 1:B:210:ASP:N    | 2.81                     | 0.43              |
| 1:B:642:TYR:O    | 1:B:645:ARG:N    | 2.52                     | 0.43              |
| 1:A:160:SER:O    | 1:A:162:ASP:N    | 2.52                     | 0.42              |
| 1:A:226:GLN:HA   | 1:A:350:MET:HE3  | 2.00                     | 0.42              |
| 1:A:576:ARG:HH12 | 1:B:346:GLN:NE2  | 2.14                     | 0.42              |
| 1:A:182:PHE:CB   | 1:A:186:ARG:NH2  | 2.75                     | 0.42              |
| 1:A:207:ASP:HA   | 1:A:370:MET:HE3  | 2.02                     | 0.42              |
| 1:B:475:GLY:HA3  | 1:B:494:LYS:O    | 2.19                     | 0.42              |
| 1:B:306:TYR:CD1  | 1:B:306:TYR:C    | 2.96                     | 0.42              |
| 1:B:724:TRP:CZ2  | 1:B:728:ILE:HD11 | 2.54                     | 0.42              |
| 1:A:334:HIS:HA   | 1:A:337:ILE:HG13 | 2.00                     | 0.42              |
| 1:A:685:LEU:O    | 1:A:689:MET:HB2  | 2.19                     | 0.42              |
| 1:B:29:ILE:HD12  | 1:B:33:TYR:HE1   | 1.83                     | 0.42              |
| 1:B:70:ARG:O     | 1:B:70:ARG:HG2   | 2.19                     | 0.42              |
| 1:B:256:THR:OG1  | 1:B:295:LYS:HE3  | 2.19                     | 0.42              |
| 1:B:317:ASP:O    | 1:B:318:SER:C    | 2.62                     | 0.42              |
| 1:A:115:TYR:O    | 1:A:116:LEU:C    | 2.61                     | 0.42              |
| 1:A:426:TYR:CD2  | 1:A:426:TYR:O    | 2.71                     | 0.42              |
| 1:A:564:ASP:OD2  | 1:A:566:SER:HB2  | 2.20                     | 0.42              |
| 1:A:637:ARG:HE   | 1:A:769:ASP:CB   | 2.28                     | 0.42              |
| 1:A:708:MET:CE   | 1:A:711:PHE:CE1  | 3.03                     | 0.42              |
| 1:B:107:THR:O    | 1:B:110:SER:OG   | 2.29                     | 0.42              |
| 1:A:338:GLU:O    | 1:A:343:LEU:HA   | 2.19                     | 0.42              |
| 1:B:241:VAL:HG21 | 1:B:293:ALA:HB3  | 2.01                     | 0.42              |
| 1:B:582:GLN:C    | 1:B:584:ARG:N    | 2.76                     | 0.42              |
| 1:A:252:TYR:HB2  | 1:A:253:ASP:H    | 1.51                     | 0.42              |
| 1:A:642:TYR:CD1  | 1:A:684:MET:HB3  | 2.55                     | 0.42              |
| 1:A:103:GLY:HA3  | 1:A:528:ARG:HB2  | 2.02                     | 0.42              |
| 1:A:224:SER:HA   | 1:A:350:MET:O    | 2.19                     | 0.42              |
| 1:B:617:VAL:HG11 | 1:B:716:VAL:HG23 | 2.02                     | 0.42              |
| 1:A:66:PHE:CE2   | 1:A:112:LEU:C    | 2.97                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:648:LEU:N    | 1:A:649:PRO:CD   | 2.82                     | 0.42              |
| 1:A:679:LYS:C    | 1:A:680:GLU:HG2  | 2.45                     | 0.42              |
| 1:A:699:LYS:HD2  | 1:A:707:GLN:HE22 | 1.85                     | 0.42              |
| 1:B:322:ARG:HG3  | 1:B:742:ALA:CB   | 2.50                     | 0.42              |
| 1:B:486:MET:O    | 1:B:487:ALA:C    | 2.63                     | 0.42              |
| 1:A:93:HIS:HD2   | 1:A:117:ASN:HD21 | 1.68                     | 0.42              |
| 1:A:331:GLU:OE2  | 1:A:766:SER:OG   | 2.31                     | 0.42              |
| 1:A:425:ARG:NH1  | 1:A:534:ILE:HD11 | 2.34                     | 0.42              |
| 1:A:553:ARG:HE   | 1:A:560:ARG:NH2  | 2.18                     | 0.42              |
| 1:B:302:LYS:HD3  | 1:B:341:GLU:OE2  | 2.19                     | 0.42              |
| 1:B:315:ILE:HD13 | 1:B:329:TYR:CZ   | 2.55                     | 0.42              |
| 1:A:252:TYR:CE1  | 1:A:256:THR:HA   | 2.55                     | 0.41              |
| 1:A:339:ALA:O    | 1:A:340:LYS:C    | 2.64                     | 0.41              |
| 1:A:689:MET:SD   | 1:A:693:ILE:HB   | 2.60                     | 0.41              |
| 1:A:544:GLU:C    | 1:A:546:MET:H    | 2.27                     | 0.41              |
| 1:A:699:LYS:HE3  | 1:A:779:GLU:OE1  | 2.20                     | 0.41              |
| 1:B:207:ASP:CG   | 1:B:370:MET:HE3  | 2.45                     | 0.41              |
| 1:B:211:SER:O    | 1:B:216:GLU:HG3  | 2.20                     | 0.41              |
| 1:B:254:ILE:CG2  | 1:B:255:LYS:N    | 2.83                     | 0.41              |
| 1:B:460:ASN:O    | 1:B:461:ALA:HB3  | 2.19                     | 0.41              |
| 1:A:109:THR:O    | 1:A:113:PRO:HD2  | 2.20                     | 0.41              |
| 1:A:405:ASP:HB3  | 1:A:539:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:625:GLU:HA   | 1:A:628:GLU:HB3  | 2.02                     | 0.41              |
| 1:A:636:GLU:HG2  | 1:A:768:GLU:CD   | 2.46                     | 0.41              |
| 1:B:301:GLN:H    | 1:B:305:ASP:HB2  | 1.84                     | 0.41              |
| 1:B:331:GLU:OE2  | 1:B:722:SER:CB   | 2.55                     | 0.41              |
| 1:B:780:ILE:OXT  | 1:B:780:ILE:HG22 | 2.20                     | 0.41              |
| 1:A:258:ALA:H    | 1:A:295:LYS:HE2  | 1.85                     | 0.41              |
| 1:A:677:PHE:CZ   | 1:A:684:MET:HE1  | 2.55                     | 0.41              |
| 1:B:190:VAL:HG13 | 1:B:192:TYR:H    | 1.85                     | 0.41              |
| 1:B:642:TYR:O    | 1:B:643:THR:C    | 2.63                     | 0.41              |
| 1:B:708:MET:CA   | 1:B:711:PHE:HB2  | 2.50                     | 0.41              |
| 1:B:723:LYS:C    | 1:B:763:MET:SD   | 3.04                     | 0.41              |
| 1:A:728:ILE:HD13 | 1:A:728:ILE:HA   | 1.82                     | 0.41              |
| 1:B:20:GLU:N     | 1:B:87:MET:HE3   | 2.35                     | 0.41              |
| 1:B:42:LYS:O     | 1:B:45:THR:HB    | 2.20                     | 0.41              |
| 1:B:282:LYS:NZ   | 1:B:283:HIS:NE2  | 2.69                     | 0.41              |
| 1:B:461:ALA:HB2  | 1:B:487:ALA:HA   | 2.02                     | 0.41              |
| 1:B:582:GLN:O    | 1:B:583:LYS:C    | 2.64                     | 0.41              |
| 1:A:141:MET:O    | 1:A:142:GLY:C    | 2.64                     | 0.41              |
| 1:A:261:LEU:HD13 | 1:A:294:LEU:HD22 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:741:ARG:HH22 | 1:B:376:THR:CG2  | 2.22                     | 0.41              |
| 1:B:112:LEU:HB2  | 1:B:113:PRO:CD   | 2.51                     | 0.41              |
| 1:B:448:LEU:HD12 | 1:B:448:LEU:C    | 2.45                     | 0.41              |
| 1:B:458:VAL:O    | 1:B:458:VAL:HG12 | 2.20                     | 0.41              |
| 1:A:374:ALA:HB1  | 1:A:381:PHE:CE1  | 2.56                     | 0.41              |
| 1:A:686:GLU:CG   | 1:A:687:LEU:N    | 2.83                     | 0.41              |
| 1:B:168:TYR:HD1  | 1:B:197:VAL:HG12 | 1.86                     | 0.41              |
| 1:B:217:ALA:HB3  | 1:B:593:ARG:CD   | 2.51                     | 0.41              |
| 1:B:302:LYS:O    | 1:B:302:LYS:HG2  | 2.20                     | 0.41              |
| 1:B:516:ARG:HD2  | 1:B:516:ARG:H    | 1.86                     | 0.41              |
| 1:B:744:ALA:HB1  | 1:B:748:PRO:HG3  | 2.03                     | 0.41              |
| 1:A:637:ARG:HA   | 1:A:637:ARG:HD3  | 1.58                     | 0.41              |
| 1:A:668:GLU:C    | 1:A:670:ALA:N    | 2.77                     | 0.41              |
| 1:A:72:ALA:HB2   | 1:A:148:LEU:HD21 | 2.03                     | 0.41              |
| 1:A:247:GLU:HB2  | 1:A:261:LEU:HG   | 2.03                     | 0.41              |
| 1:A:563:MET:C    | 1:A:564:ASP:OD1  | 2.59                     | 0.41              |
| 1:A:572:LYS:NZ   | 1:B:344:GLU:OE2  | 2.52                     | 0.41              |
| 1:A:576:ARG:O    | 1:A:579:GLU:HB2  | 2.20                     | 0.41              |
| 1:A:652:TRP:O    | 1:A:653:LYS:HG3  | 2.21                     | 0.41              |
| 1:A:659:ASP:HA   | 1:A:662:ASN:OD1  | 2.21                     | 0.41              |
| 1:B:218:ARG:HH11 | 1:B:592:SER:CB   | 2.33                     | 0.41              |
| 1:B:263:GLU:N    | 1:B:263:GLU:OE2  | 2.50                     | 0.41              |
| 1:B:339:ALA:HB2  | 1:B:345:ILE:HG12 | 2.03                     | 0.41              |
| 1:B:549:PHE:C    | 1:B:551:ALA:H    | 2.29                     | 0.41              |
| 1:B:599:TYR:HD1  | 1:B:599:TYR:N    | 2.18                     | 0.41              |
| 1:A:332:GLY:HA2  | 1:A:334:HIS:NE2  | 2.36                     | 0.41              |
| 1:A:624:ARG:HG2  | 1:A:624:ARG:O    | 2.21                     | 0.41              |
| 1:A:748:PRO:O    | 1:A:749:LEU:C    | 2.64                     | 0.41              |
| 1:A:685:LEU:O    | 1:A:689:MET:CB   | 2.69                     | 0.40              |
| 1:B:637:ARG:NH2  | 1:B:765:GLU:O    | 2.54                     | 0.40              |
| 1:B:754:MET:HE2  | 1:B:754:MET:HB2  | 1.63                     | 0.40              |
| 1:A:206:ILE:H    | 1:A:206:ILE:CD1  | 2.33                     | 0.40              |
| 1:A:279:PHE:CZ   | 1:A:780:ILE:HG23 | 2.56                     | 0.40              |
| 1:A:280:ASP:C    | 1:A:280:ASP:OD1  | 2.63                     | 0.40              |
| 1:A:348:GLU:CD   | 1:B:573:MET:SD   | 3.04                     | 0.40              |
| 1:A:613:GLN:O    | 1:A:617:VAL:HG23 | 2.20                     | 0.40              |
| 1:B:358:GLN:HB3  | 1:B:597:LEU:HD13 | 2.03                     | 0.40              |
| 1:B:642:TYR:OH   | 1:B:688:ILE:HD12 | 2.22                     | 0.40              |
| 1:A:442:SER:O    | 1:A:482:ILE:CD1  | 2.69                     | 0.40              |
| 1:A:540:SER:C    | 1:A:542:GLU:H    | 2.29                     | 0.40              |
| 1:A:747:ASN:HD22 | 1:A:747:ASN:HA   | 1.57                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:79:MET:HE3  | 1:B:108:LEU:HD13 | 2.03                     | 0.40              |
| 1:B:377:GLU:HB2 | 1:B:381:PHE:HE1  | 1.86                     | 0.40              |
| 1:A:100:MET:O   | 1:A:372:GLY:HA2  | 2.22                     | 0.40              |
| 1:A:317:ASP:O   | 1:A:319:PHE:N    | 2.55                     | 0.40              |
| 1:A:374:ALA:HB1 | 1:A:381:PHE:HE1  | 1.87                     | 0.40              |
| 1:A:442:SER:CA  | 1:A:482:ILE:HD11 | 2.51                     | 0.40              |
| 1:A:665:TYR:O   | 1:A:776:MET:HB3  | 2.21                     | 0.40              |
| 1:A:671:LEU:CD1 | 1:A:674:SER:HA   | 2.52                     | 0.40              |
| 1:B:400:ARG:HB2 | 1:B:527:GLY:HA3  | 2.04                     | 0.40              |
| 1:B:512:ARG:CG  | 1:B:539:LEU:HD21 | 2.51                     | 0.40              |
| 1:B:599:TYR:N   | 1:B:599:TYR:CD1  | 2.89                     | 0.40              |
| 1:B:657:LEU:O   | 1:B:658:VAL:C    | 2.65                     | 0.40              |
| 1:A:168:TYR:OH  | 1:A:180:LEU:HD23 | 2.21                     | 0.40              |
| 1:A:203:PHE:HD2 | 1:A:204:ALA:H    | 1.69                     | 0.40              |
| 1:A:230:SER:O   | 1:A:231:THR:C    | 2.64                     | 0.40              |
| 1:A:458:VAL:CG1 | 1:A:459:LEU:N    | 2.84                     | 0.40              |
| 1:A:541:MET:HA  | 1:A:546:MET:HG2  | 2.04                     | 0.40              |
| 1:A:641:ALA:CB  | 1:A:660:LEU:HD11 | 2.52                     | 0.40              |
| 1:A:679:LYS:O   | 1:A:680:GLU:HG2  | 2.21                     | 0.40              |
| 1:B:302:LYS:HA  | 1:B:306:TYR:CZ   | 2.56                     | 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     | 778/780 (100%)  | 647 (83%)  | 99 (13%)  | 32 (4%)  | 2           | 17 |
| 1   | B     | 768/780 (98%)   | 626 (82%)  | 118 (15%) | 24 (3%)  | 3           | 22 |
| All | All   | 1546/1560 (99%) | 1273 (82%) | 217 (14%) | 56 (4%)  | 2           | 19 |

All (56) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 230 | SER  |
| 1   | A     | 259 | VAL  |
| 1   | A     | 275 | ILE  |
| 1   | A     | 280 | ASP  |
| 1   | A     | 304 | VAL  |
| 1   | A     | 544 | GLU  |
| 1   | A     | 563 | MET  |
| 1   | A     | 668 | GLU  |
| 1   | B     | 12  | THR  |
| 1   | B     | 120 | THR  |
| 1   | B     | 122 | LYS  |
| 1   | B     | 245 | LYS  |
| 1   | B     | 345 | ILE  |
| 1   | B     | 485 | ASN  |
| 1   | A     | 161 | LYS  |
| 1   | A     | 284 | VAL  |
| 1   | A     | 299 | ALA  |
| 1   | A     | 342 | GLY  |
| 1   | A     | 548 | ARG  |
| 1   | A     | 690 | ASP  |
| 1   | A     | 737 | GLY  |
| 1   | B     | 133 | LEU  |
| 1   | B     | 446 | SER  |
| 1   | B     | 655 | ASP  |
| 1   | A     | 248 | LYS  |
| 1   | A     | 254 | ILE  |
| 1   | A     | 257 | LYS  |
| 1   | A     | 311 | GLY  |
| 1   | A     | 318 | SER  |
| 1   | B     | 253 | ASP  |
| 1   | B     | 318 | SER  |
| 1   | B     | 625 | GLU  |
| 1   | B     | 743 | TYR  |
| 1   | A     | 310 | ASP  |
| 1   | A     | 679 | LYS  |
| 1   | B     | 263 | GLU  |
| 1   | B     | 544 | GLU  |
| 1   | A     | 3   | GLY  |
| 1   | A     | 376 | THR  |
| 1   | A     | 461 | ALA  |
| 1   | A     | 485 | ASN  |
| 1   | A     | 674 | SER  |
| 1   | B     | 251 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 575 | SER  |
| 1   | B     | 627 | VAL  |
| 1   | A     | 562 | GLY  |
| 1   | A     | 660 | LEU  |
| 1   | A     | 681 | PRO  |
| 1   | B     | 132 | TYR  |
| 1   | B     | 547 | ARG  |
| 1   | B     | 565 | ASP  |
| 1   | A     | 738 | ILE  |
| 1   | B     | 254 | ILE  |
| 1   | A     | 274 | GLY  |
| 1   | B     | 212 | ILE  |
| 1   | B     | 644 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 670/670 (100%)  | 557 (83%)  | 113 (17%) | 2           | 11 |
| 1   | B     | 661/670 (99%)   | 539 (82%)  | 122 (18%) | 1           | 9  |
| All | All   | 1331/1340 (99%) | 1096 (82%) | 235 (18%) | 2           | 10 |

All (235) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | LEU  |
| 1   | A     | 13  | LYS  |
| 1   | A     | 16  | LEU  |
| 1   | A     | 21  | LYS  |
| 1   | A     | 30  | ARG  |
| 1   | A     | 35  | ASN  |
| 1   | A     | 61  | LEU  |
| 1   | A     | 62  | LEU  |
| 1   | A     | 79  | MET  |
| 1   | A     | 120 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 127 | VAL  |
| 1   | A     | 158 | SER  |
| 1   | A     | 194 | GLU  |
| 1   | A     | 200 | PRO  |
| 1   | A     | 206 | ILE  |
| 1   | A     | 207 | ASP  |
| 1   | A     | 210 | ASP  |
| 1   | A     | 218 | ARG  |
| 1   | A     | 221 | LEU  |
| 1   | A     | 224 | SER  |
| 1   | A     | 238 | ASN  |
| 1   | A     | 244 | LEU  |
| 1   | A     | 250 | TYR  |
| 1   | A     | 251 | THR  |
| 1   | A     | 259 | VAL  |
| 1   | A     | 260 | GLN  |
| 1   | A     | 275 | ILE  |
| 1   | A     | 278 | LEU  |
| 1   | A     | 279 | PHE  |
| 1   | A     | 284 | VAL  |
| 1   | A     | 287 | ASN  |
| 1   | A     | 298 | VAL  |
| 1   | A     | 301 | GLN  |
| 1   | A     | 308 | VAL  |
| 1   | A     | 309 | GLU  |
| 1   | A     | 313 | VAL  |
| 1   | A     | 316 | VAL  |
| 1   | A     | 323 | LEU  |
| 1   | A     | 328 | ARG  |
| 1   | A     | 331 | GLU  |
| 1   | A     | 337 | ILE  |
| 1   | A     | 343 | LEU  |
| 1   | A     | 344 | GLU  |
| 1   | A     | 345 | ILE  |
| 1   | A     | 348 | GLU  |
| 1   | A     | 350 | MET  |
| 1   | A     | 354 | THR  |
| 1   | A     | 363 | MET  |
| 1   | A     | 371 | THR  |
| 1   | A     | 376 | THR  |
| 1   | A     | 377 | GLU  |
| 1   | A     | 378 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 382 | ARG  |
| 1   | A     | 426 | TYR  |
| 1   | A     | 428 | THR  |
| 1   | A     | 432 | VAL  |
| 1   | A     | 437 | VAL  |
| 1   | A     | 439 | VAL  |
| 1   | A     | 442 | SER  |
| 1   | A     | 443 | GLU  |
| 1   | A     | 448 | LEU  |
| 1   | A     | 471 | ILE  |
| 1   | A     | 481 | THR  |
| 1   | A     | 482 | ILE  |
| 1   | A     | 485 | ASN  |
| 1   | A     | 491 | THR  |
| 1   | A     | 500 | LYS  |
| 1   | A     | 501 | GLU  |
| 1   | A     | 512 | ARG  |
| 1   | A     | 534 | ILE  |
| 1   | A     | 535 | THR  |
| 1   | A     | 554 | THR  |
| 1   | A     | 558 | LEU  |
| 1   | A     | 559 | ASP  |
| 1   | A     | 569 | ILE  |
| 1   | A     | 583 | LYS  |
| 1   | A     | 601 | ASP  |
| 1   | A     | 630 | MET  |
| 1   | A     | 631 | ILE  |
| 1   | A     | 632 | LYS  |
| 1   | A     | 634 | SER  |
| 1   | A     | 636 | GLU  |
| 1   | A     | 637 | ARG  |
| 1   | A     | 648 | LEU  |
| 1   | A     | 655 | ASP  |
| 1   | A     | 660 | LEU  |
| 1   | A     | 663 | THR  |
| 1   | A     | 666 | LEU  |
| 1   | A     | 673 | LYS  |
| 1   | A     | 684 | MET  |
| 1   | A     | 686 | GLU  |
| 1   | A     | 687 | LEU  |
| 1   | A     | 688 | ILE  |
| 1   | A     | 691 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 695 | LYS  |
| 1   | A     | 696 | TYR  |
| 1   | A     | 699 | LYS  |
| 1   | A     | 700 | GLU  |
| 1   | A     | 707 | GLN  |
| 1   | A     | 708 | MET  |
| 1   | A     | 710 | GLU  |
| 1   | A     | 715 | ILE  |
| 1   | A     | 717 | LEU  |
| 1   | A     | 718 | ARG  |
| 1   | A     | 722 | SER  |
| 1   | A     | 723 | LYS  |
| 1   | A     | 724 | TRP  |
| 1   | A     | 740 | LEU  |
| 1   | A     | 747 | ASN  |
| 1   | A     | 749 | LEU  |
| 1   | A     | 751 | GLU  |
| 1   | A     | 763 | MET  |
| 1   | A     | 771 | VAL  |
| 1   | B     | 14  | ARG  |
| 1   | B     | 16  | LEU  |
| 1   | B     | 30  | ARG  |
| 1   | B     | 53  | GLU  |
| 1   | B     | 61  | LEU  |
| 1   | B     | 73  | SER  |
| 1   | B     | 83  | LYS  |
| 1   | B     | 127 | VAL  |
| 1   | B     | 146 | GLU  |
| 1   | B     | 172 | ILE  |
| 1   | B     | 187 | ASP  |
| 1   | B     | 190 | VAL  |
| 1   | B     | 191 | LEU  |
| 1   | B     | 195 | GLN  |
| 1   | B     | 219 | THR  |
| 1   | B     | 226 | GLN  |
| 1   | B     | 231 | THR  |
| 1   | B     | 233 | LEU  |
| 1   | B     | 241 | VAL  |
| 1   | B     | 242 | ARG  |
| 1   | B     | 244 | LEU  |
| 1   | B     | 255 | LYS  |
| 1   | B     | 260 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 261 | LEU  |
| 1   | B     | 262 | THR  |
| 1   | B     | 263 | GLU  |
| 1   | B     | 266 | MET  |
| 1   | B     | 275 | ILE  |
| 1   | B     | 276 | ASP  |
| 1   | B     | 278 | LEU  |
| 1   | B     | 280 | ASP  |
| 1   | B     | 281 | VAL  |
| 1   | B     | 282 | LYS  |
| 1   | B     | 289 | HIS  |
| 1   | B     | 294 | LEU  |
| 1   | B     | 305 | ASP  |
| 1   | B     | 315 | ILE  |
| 1   | B     | 316 | VAL  |
| 1   | B     | 320 | THR  |
| 1   | B     | 330 | SER  |
| 1   | B     | 338 | GLU  |
| 1   | B     | 340 | LYS  |
| 1   | B     | 347 | ASN  |
| 1   | B     | 348 | GLU  |
| 1   | B     | 354 | THR  |
| 1   | B     | 358 | GLN  |
| 1   | B     | 363 | MET  |
| 1   | B     | 376 | THR  |
| 1   | B     | 382 | ARG  |
| 1   | B     | 388 | GLN  |
| 1   | B     | 391 | THR  |
| 1   | B     | 392 | ILE  |
| 1   | B     | 394 | THR  |
| 1   | B     | 399 | VAL  |
| 1   | B     | 405 | ASP  |
| 1   | B     | 411 | MET  |
| 1   | B     | 422 | VAL  |
| 1   | B     | 434 | VAL  |
| 1   | B     | 442 | SER  |
| 1   | B     | 444 | LEU  |
| 1   | B     | 446 | SER  |
| 1   | B     | 459 | LEU  |
| 1   | B     | 463 | ASN  |
| 1   | B     | 471 | ILE  |
| 1   | B     | 473 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 476 | GLN  |
| 1   | B     | 477 | LYS  |
| 1   | B     | 481 | THR  |
| 1   | B     | 482 | ILE  |
| 1   | B     | 494 | LYS  |
| 1   | B     | 495 | LEU  |
| 1   | B     | 500 | LYS  |
| 1   | B     | 514 | GLU  |
| 1   | B     | 516 | ARG  |
| 1   | B     | 526 | SER  |
| 1   | B     | 544 | GLU  |
| 1   | B     | 545 | LEU  |
| 1   | B     | 546 | MET  |
| 1   | B     | 547 | ARG  |
| 1   | B     | 549 | PHE  |
| 1   | B     | 555 | MET  |
| 1   | B     | 569 | ILE  |
| 1   | B     | 571 | SER  |
| 1   | B     | 579 | GLU  |
| 1   | B     | 580 | SER  |
| 1   | B     | 603 | LEU  |
| 1   | B     | 613 | GLN  |
| 1   | B     | 616 | GLU  |
| 1   | B     | 618 | ILE  |
| 1   | B     | 624 | ARG  |
| 1   | B     | 626 | ILE  |
| 1   | B     | 627 | VAL  |
| 1   | B     | 630 | MET  |
| 1   | B     | 636 | GLU  |
| 1   | B     | 639 | ILE  |
| 1   | B     | 646 | GLU  |
| 1   | B     | 647 | GLU  |
| 1   | B     | 648 | LEU  |
| 1   | B     | 650 | GLU  |
| 1   | B     | 659 | ASP  |
| 1   | B     | 663 | THR  |
| 1   | B     | 667 | ASP  |
| 1   | B     | 680 | GLU  |
| 1   | B     | 686 | GLU  |
| 1   | B     | 693 | ILE  |
| 1   | B     | 700 | GLU  |
| 1   | B     | 707 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 711 | PHE  |
| 1   | B     | 712 | GLU  |
| 1   | B     | 720 | VAL  |
| 1   | B     | 722 | SER  |
| 1   | B     | 723 | LYS  |
| 1   | B     | 734 | LEU  |
| 1   | B     | 738 | ILE  |
| 1   | B     | 743 | TYR  |
| 1   | B     | 746 | THR  |
| 1   | B     | 749 | LEU  |
| 1   | B     | 750 | ARG  |
| 1   | B     | 754 | MET  |
| 1   | B     | 766 | SER  |
| 1   | B     | 779 | GLU  |
| 1   | B     | 780 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 24  | ASN  |
| 1   | A     | 35  | ASN  |
| 1   | A     | 93  | HIS  |
| 1   | A     | 125 | HIS  |
| 1   | A     | 188 | ASN  |
| 1   | A     | 226 | GLN  |
| 1   | A     | 238 | ASN  |
| 1   | A     | 260 | GLN  |
| 1   | A     | 287 | ASN  |
| 1   | A     | 297 | HIS  |
| 1   | A     | 312 | GLN  |
| 1   | A     | 335 | GLN  |
| 1   | A     | 457 | GLN  |
| 1   | A     | 460 | ASN  |
| 1   | A     | 570 | GLN  |
| 1   | A     | 582 | GLN  |
| 1   | A     | 697 | ASN  |
| 1   | A     | 727 | HIS  |
| 1   | A     | 733 | GLN  |
| 1   | A     | 745 | GLN  |
| 1   | A     | 747 | ASN  |
| 1   | A     | 762 | HIS  |
| 1   | B     | 17  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 157 | ASN  |
| 1   | B     | 202 | HIS  |
| 1   | B     | 226 | GLN  |
| 1   | B     | 260 | GLN  |
| 1   | B     | 288 | HIS  |
| 1   | B     | 292 | GLN  |
| 1   | B     | 297 | HIS  |
| 1   | B     | 312 | GLN  |
| 1   | B     | 358 | GLN  |
| 1   | B     | 383 | ASN  |
| 1   | B     | 395 | ASN  |
| 1   | B     | 424 | GLN  |
| 1   | B     | 457 | GLN  |
| 1   | B     | 463 | ASN  |
| 1   | B     | 464 | HIS  |
| 1   | B     | 476 | GLN  |
| 1   | B     | 521 | GLN  |
| 1   | B     | 582 | GLN  |
| 1   | B     | 739 | HIS  |

### 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 ⓘ

1 ligand is 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   | ADP  | A     | 781 | -    | 28,29,29     | 1.73 | 5 (17%)     | 43,45,45    | 1.96 | 11 (25%)    |

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   | ADP  | A     | 781 | -    | -       | 3/16/32/32 | 0/3/3/3 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | A     | 781 | ADP  | C5-C4   | 5.47 | 1.48        | 1.39     |
| 2   | A     | 781 | ADP  | C5-C6   | 3.37 | 1.50        | 1.41     |
| 2   | A     | 781 | ADP  | O3'-C3' | 2.94 | 1.50        | 1.43     |
| 2   | A     | 781 | ADP  | C8-N7   | 2.62 | 1.36        | 1.31     |
| 2   | A     | 781 | ADP  | PA-O3A  | 2.62 | 1.62        | 1.59     |

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 781 | ADP  | C5-C4-N3    | -5.96 | 118.51      | 126.72   |
| 2   | A     | 781 | ADP  | N3-C4-N9    | 4.78  | 135.30      | 127.17   |
| 2   | A     | 781 | ADP  | C2-N3-C4    | 4.01  | 121.62      | 111.83   |
| 2   | A     | 781 | ADP  | C4-C5-N7    | -3.76 | 106.28      | 110.58   |
| 2   | A     | 781 | ADP  | N3-C2-N1    | -3.71 | 122.97      | 128.58   |
| 2   | A     | 781 | ADP  | C3'-C2'-C1' | 3.09  | 107.31      | 101.46   |
| 2   | A     | 781 | ADP  | C5-N7-C8    | 2.90  | 108.01      | 103.45   |
| 2   | A     | 781 | ADP  | C4-N9-C8    | 2.52  | 108.38      | 105.74   |
| 2   | A     | 781 | ADP  | C6-C5-N7    | 2.47  | 136.85      | 132.09   |
| 2   | A     | 781 | ADP  | O4'-C4'-C3' | 2.32  | 109.76      | 105.15   |
| 2   | A     | 781 | ADP  | C2-N1-C6    | 2.12  | 122.21      | 118.73   |

There are no chirality outliers.

All (3) torsion outliers are listed below:

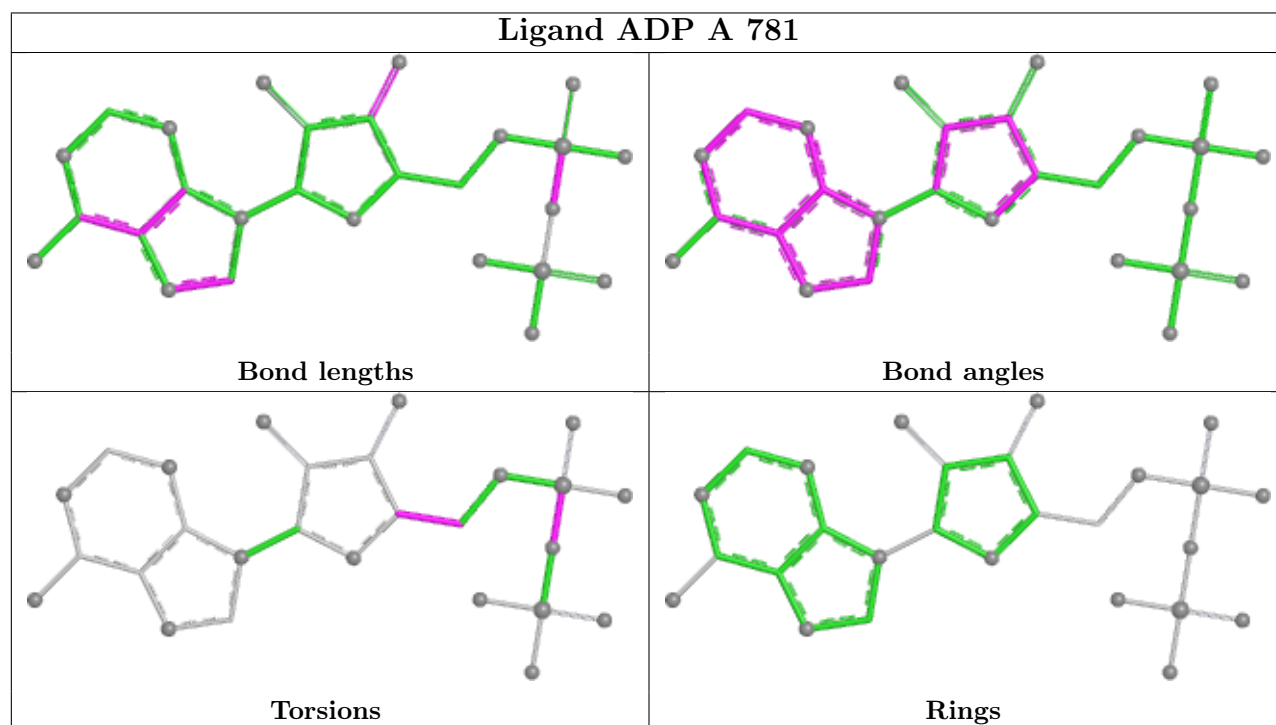
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 781 | ADP  | O4'-C4'-C5'-O5' |
| 2   | A     | 781 | ADP  | C3'-C4'-C5'-O5' |
| 2   | A     | 781 | ADP  | PB-O3A-PA-O2A   |

There are no ring outliers.

1 monomer is involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 781 | ADP  | 3       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------|-------|-----------------------|-------|
| 1   | A     | 780/780 (100%)  | 0.58   | 74 (9%)  | 14 9  | 20, 45, 80, 187       | 0     |
| 1   | B     | 770/780 (98%)   | 0.53   | 51 (6%)  | 24 15 | 18, 46, 61, 187       | 0     |
| All | All   | 1550/1560 (99%) | 0.56   | 125 (8%) | 18 11 | 18, 46, 73, 187       | 0     |

All (125) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 261 | LEU  | 9.2  |
| 1   | B     | 248 | LYS  | 7.3  |
| 1   | B     | 723 | LYS  | 6.0  |
| 1   | B     | 262 | THR  | 5.4  |
| 1   | B     | 622 | ASN  | 5.1  |
| 1   | B     | 250 | TYR  | 5.1  |
| 1   | A     | 646 | GLU  | 5.0  |
| 1   | A     | 338 | GLU  | 4.8  |
| 1   | A     | 642 | TYR  | 4.7  |
| 1   | B     | 643 | THR  | 4.6  |
| 1   | A     | 723 | LYS  | 4.5  |
| 1   | B     | 742 | ALA  | 4.5  |
| 1   | A     | 280 | ASP  | 4.5  |
| 1   | A     | 270 | GLU  | 4.3  |
| 1   | B     | 253 | ASP  | 4.1  |
| 1   | B     | 246 | ALA  | 4.0  |
| 1   | B     | 647 | GLU  | 3.9  |
| 1   | B     | 256 | THR  | 3.8  |
| 1   | A     | 675 | ASP  | 3.7  |
| 1   | B     | 623 | LEU  | 3.7  |
| 1   | A     | 256 | THR  | 3.6  |
| 1   | A     | 705 | LYS  | 3.6  |
| 1   | B     | 621 | GLU  | 3.6  |
| 1   | B     | 705 | LYS  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 708 | MET  | 3.5  |
| 1   | A     | 344 | GLU  | 3.5  |
| 1   | B     | 554 | THR  | 3.4  |
| 1   | A     | 743 | TYR  | 3.4  |
| 1   | A     | 281 | VAL  | 3.4  |
| 1   | B     | 311 | GLY  | 3.4  |
| 1   | A     | 247 | GLU  | 3.4  |
| 1   | B     | 642 | TYR  | 3.3  |
| 1   | B     | 312 | GLN  | 3.3  |
| 1   | B     | 549 | PHE  | 3.3  |
| 1   | B     | 550 | GLY  | 3.3  |
| 1   | A     | 706 | GLU  | 3.2  |
| 1   | A     | 676 | ILE  | 3.2  |
| 1   | A     | 239 | ALA  | 3.1  |
| 1   | A     | 7   | LYS  | 3.1  |
| 1   | A     | 313 | VAL  | 3.1  |
| 1   | A     | 688 | ILE  | 3.0  |
| 1   | B     | 346 | GLN  | 3.0  |
| 1   | A     | 6   | ASN  | 3.0  |
| 1   | A     | 701 | GLU  | 3.0  |
| 1   | A     | 277 | ASN  | 2.9  |
| 1   | A     | 562 | GLY  | 2.9  |
| 1   | A     | 622 | ASN  | 2.9  |
| 1   | A     | 630 | MET  | 2.9  |
| 1   | A     | 253 | ASP  | 2.9  |
| 1   | A     | 626 | ILE  | 2.9  |
| 1   | A     | 563 | MET  | 2.8  |
| 1   | A     | 486 | MET  | 2.8  |
| 1   | A     | 303 | ASP  | 2.8  |
| 1   | B     | 706 | GLU  | 2.8  |
| 1   | A     | 702 | GLN  | 2.7  |
| 1   | B     | 629 | ASN  | 2.7  |
| 1   | B     | 719 | ALA  | 2.7  |
| 1   | A     | 337 | ILE  | 2.7  |
| 1   | B     | 254 | ILE  | 2.7  |
| 1   | B     | 636 | GLU  | 2.7  |
| 1   | A     | 674 | SER  | 2.7  |
| 1   | B     | 553 | ARG  | 2.7  |
| 1   | A     | 244 | LEU  | 2.7  |
| 1   | B     | 649 | PRO  | 2.7  |
| 1   | A     | 651 | GLU  | 2.7  |
| 1   | A     | 225 | GLY  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 309 | GLU  | 2.7  |
| 1   | A     | 690 | ASP  | 2.7  |
| 1   | A     | 264 | GLU  | 2.6  |
| 1   | A     | 650 | GLU  | 2.6  |
| 1   | B     | 624 | ARG  | 2.6  |
| 1   | A     | 266 | MET  | 2.6  |
| 1   | A     | 623 | LEU  | 2.6  |
| 1   | A     | 287 | ASN  | 2.6  |
| 1   | B     | 558 | LEU  | 2.5  |
| 1   | A     | 746 | THR  | 2.5  |
| 1   | A     | 248 | LYS  | 2.5  |
| 1   | A     | 249 | ASP  | 2.5  |
| 1   | A     | 8   | MET  | 2.5  |
| 1   | B     | 707 | GLN  | 2.5  |
| 1   | A     | 227 | ALA  | 2.5  |
| 1   | B     | 551 | ALA  | 2.5  |
| 1   | A     | 259 | VAL  | 2.4  |
| 1   | B     | 258 | ALA  | 2.4  |
| 1   | B     | 257 | LYS  | 2.4  |
| 1   | B     | 722 | SER  | 2.4  |
| 1   | A     | 3   | GLY  | 2.4  |
| 1   | A     | 311 | GLY  | 2.4  |
| 1   | A     | 780 | ILE  | 2.4  |
| 1   | A     | 257 | LYS  | 2.4  |
| 1   | A     | 561 | PHE  | 2.4  |
| 1   | B     | 252 | TYR  | 2.3  |
| 1   | A     | 335 | GLN  | 2.3  |
| 1   | B     | 648 | LEU  | 2.3  |
| 1   | A     | 461 | ALA  | 2.3  |
| 1   | B     | 379 | GLU  | 2.3  |
| 1   | A     | 775 | VAL  | 2.3  |
| 1   | A     | 1   | MET  | 2.3  |
| 1   | B     | 630 | MET  | 2.3  |
| 1   | A     | 620 | SER  | 2.3  |
| 1   | A     | 336 | ALA  | 2.3  |
| 1   | A     | 278 | LEU  | 2.3  |
| 1   | A     | 228 | ALA  | 2.2  |
| 1   | A     | 246 | ALA  | 2.2  |
| 1   | B     | 620 | SER  | 2.2  |
| 1   | A     | 4   | ILE  | 2.2  |
| 1   | B     | 718 | ARG  | 2.2  |
| 1   | A     | 2   | LEU  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 655 | ASP  | 2.2  |
| 1   | B     | 704 | GLY  | 2.2  |
| 1   | A     | 721 | ASP  | 2.2  |
| 1   | B     | 541 | MET  | 2.1  |
| 1   | A     | 341 | GLU  | 2.1  |
| 1   | B     | 365 | GLU  | 2.1  |
| 1   | A     | 699 | LYS  | 2.1  |
| 1   | A     | 559 | ASP  | 2.1  |
| 1   | B     | 310 | ASP  | 2.1  |
| 1   | B     | 557 | MET  | 2.1  |
| 1   | B     | 247 | GLU  | 2.1  |
| 1   | B     | 255 | LYS  | 2.1  |
| 1   | A     | 250 | TYR  | 2.1  |
| 1   | A     | 251 | THR  | 2.1  |
| 1   | A     | 770 | GLU  | 2.1  |
| 1   | A     | 304 | VAL  | 2.0  |
| 1   | B     | 349 | SER  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

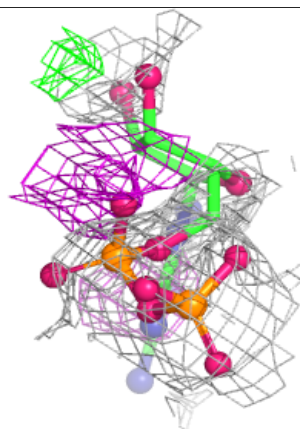
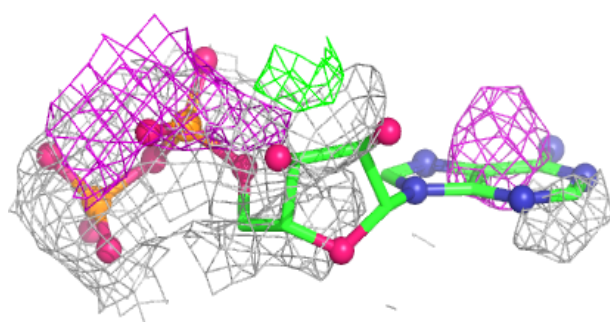
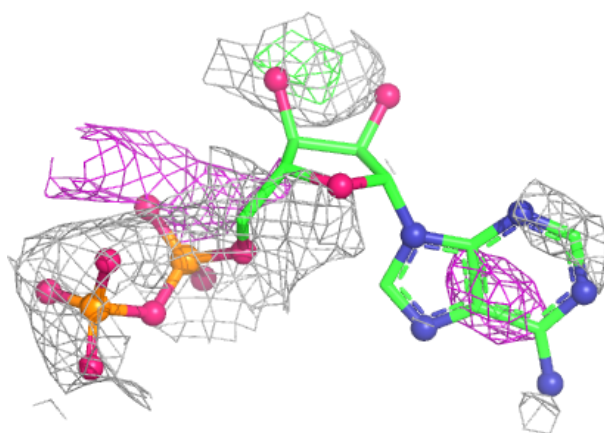
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | ADP  | A     | 781 | 27/27 | 0.60 | 0.18 | 47,108,108,108             | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around ADP A 781:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.