



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:50 PM UTC

PDB ID : 2YVZ / pdb\_00002yvv  
Title : Crystal structure of magnesium transporter MgtE cytosolic domain, Mg<sup>2+</sup>-free form  
Authors : Hattori, M.; Tanaka, Y.; Fukai, S.; Ishitani, R.; Nureki, O.  
Deposited on : 2007-04-18  
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

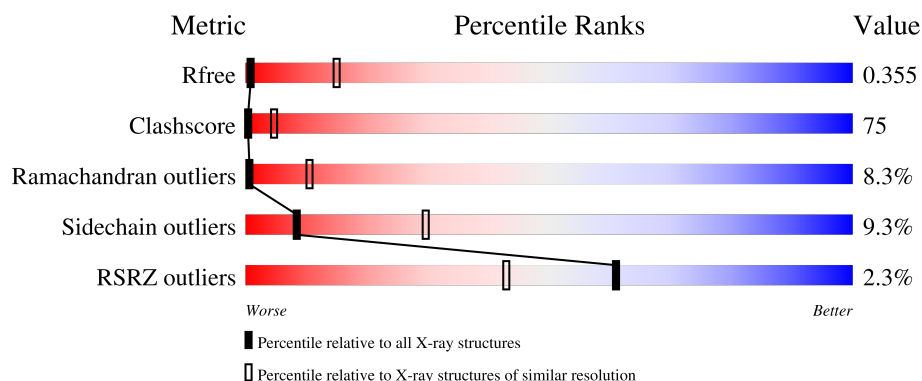
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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                      | 1270 (4.10-3.70)                                      |
| Clashscore            | 190562                      | 1034 (4.08-3.72)                                      |
| Ramachandran outliers | 187476                      | 1251 (4.10-3.70)                                      |
| Sidechain outliers    | 187428                      | 1243 (4.10-3.70)                                      |
| RSRZ outliers         | 180081                      | 1269 (4.10-3.70)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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     | 278    |                  |
| 1   | B     | 278    |                  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3982 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 Mg<sup>2+</sup> transporter MgtE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 248      | Total | C    | N   | O   | Se | 0       | 0       | 0     |
|     |       |          | 1991  | 1262 | 336 | 389 | 4  |         |         |       |
| 1   | B     | 248      | Total | C    | N   | O   | Se | 0       | 0       | 0     |
|     |       |          | 1991  | 1262 | 336 | 389 | 4  |         |         |       |

There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | -2      | GLY      | -      | expression tag   | UNP Q5SMG8 |
| A     | -1      | SER      | -      | expression tag   | UNP Q5SMG8 |
| A     | 0       | HIS      | -      | expression tag   | UNP Q5SMG8 |
| A     | 1       | MSE      | MET    | modified residue | UNP Q5SMG8 |
| A     | 138     | MSE      | MET    | modified residue | UNP Q5SMG8 |
| A     | 149     | MSE      | MET    | modified residue | UNP Q5SMG8 |
| A     | 202     | MSE      | MET    | modified residue | UNP Q5SMG8 |
| A     | 222     | MSE      | MET    | modified residue | UNP Q5SMG8 |
| B     | -2      | GLY      | -      | expression tag   | UNP Q5SMG8 |
| B     | -1      | SER      | -      | expression tag   | UNP Q5SMG8 |
| B     | 0       | HIS      | -      | expression tag   | UNP Q5SMG8 |
| B     | 1       | MSE      | MET    | modified residue | UNP Q5SMG8 |
| B     | 138     | MSE      | MET    | modified residue | UNP Q5SMG8 |
| B     | 149     | MSE      | MET    | modified residue | UNP Q5SMG8 |
| B     | 202     | MSE      | MET    | modified residue | UNP Q5SMG8 |
| B     | 222     | MSE      | MET    | modified residue | UNP Q5SMG8 |



THR  
GLU  
ASP  
ILE  
HIS  
LYS  
LEU  
GLY  
ALA  
VAL  
ASP  
VAL  
PRO  
ASP  
LEU  
VAL  
TYR  
SER  
GLU

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 77.11Å 100.18Å 100.16Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 44.80 – 3.90<br>44.80 – 3.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.4 (44.80-3.90)<br>99.4 (44.80-3.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.38 (at 3.88Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.2                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.346 , 0.370<br>0.350 , 0.355                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 402 reflections (5.41%)                                     | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 177.9                                                       | Xtriage          |
| Anisotropy                                                              | 0.326                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 755.0                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$ | Xtriage          |
| Estimated twinning fraction                                             | 0.419 for -h,l,k                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 3982                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 227.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$    |
| 1   | A     | 0.88         | 1/2018 (0.0%) | 1.35        | 28/2738 (1.0%) |
| 1   | B     | 0.84         | 2/2018 (0.1%) | 1.31        | 28/2738 (1.0%) |
| All | All   | 0.86         | 3/4036 (0.1%) | 1.33        | 56/5476 (1.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |
| 1   | B     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | A     | 133 | GLU  | CA-C  | -10.73 | 1.38        | 1.52     |
| 1   | B     | 132 | ASP  | CA-C  | -5.26  | 1.45        | 1.52     |
| 1   | B     | 138 | MSE  | CG-SE | 5.15   | 2.10        | 1.95     |

All (56) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 133 | GLU  | N-CA-C | 17.28  | 136.05      | 110.48   |
| 1   | B     | 162 | ALA  | CA-C-N | 10.96  | 131.27      | 119.87   |
| 1   | B     | 162 | ALA  | C-N-CA | 10.96  | 131.27      | 119.87   |
| 1   | A     | 162 | ALA  | CA-C-N | 10.19  | 130.47      | 119.87   |
| 1   | A     | 162 | ALA  | C-N-CA | 10.19  | 130.47      | 119.87   |
| 1   | A     | 127 | ALA  | N-CA-C | 10.16  | 132.44      | 110.80   |
| 1   | B     | 168 | ILE  | N-CA-C | -10.04 | 102.97      | 111.91   |
| 1   | B     | 127 | ALA  | N-CA-C | 9.12   | 130.24      | 110.80   |
| 1   | B     | 230 | LEU  | CA-C-N | 8.55   | 128.56      | 119.76   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | B     | 230 | LEU  | C-N-CA   | 8.55  | 128.56      | 119.76   |
| 1   | B     | 126 | LEU  | N-CA-C   | -8.52 | 102.70      | 113.43   |
| 1   | A     | 89  | SER  | N-CA-C   | -8.23 | 98.31       | 110.48   |
| 1   | B     | 93  | LEU  | N-CA-C   | -8.12 | 103.50      | 113.41   |
| 1   | A     | 230 | LEU  | CA-C-N   | 7.71  | 127.70      | 119.76   |
| 1   | A     | 230 | LEU  | C-N-CA   | 7.71  | 127.70      | 119.76   |
| 1   | A     | 249 | LEU  | N-CA-C   | -7.64 | 103.42      | 112.89   |
| 1   | B     | 89  | SER  | N-CA-C   | -7.57 | 99.28       | 110.48   |
| 1   | B     | 249 | LEU  | N-CA-C   | -7.28 | 103.86      | 112.89   |
| 1   | A     | 133 | GLU  | O-C-N    | 6.84  | 130.69      | 122.96   |
| 1   | A     | 126 | LEU  | N-CA-C   | 6.80  | 125.28      | 110.80   |
| 1   | A     | 129 | TYR  | CA-CB-CG | -6.70 | 101.84      | 113.90   |
| 1   | B     | 128 | ARG  | CA-C-N   | -6.17 | 113.34      | 122.41   |
| 1   | B     | 128 | ARG  | C-N-CA   | -6.17 | 113.34      | 122.41   |
| 1   | A     | 93  | LEU  | N-CA-C   | -6.15 | 103.91      | 112.45   |
| 1   | A     | 54  | LYS  | N-CA-C   | 5.81  | 123.18      | 110.80   |
| 1   | B     | 109 | GLN  | N-CA-C   | 5.69  | 117.56      | 111.36   |
| 1   | B     | 54  | LYS  | N-CA-C   | 5.62  | 122.76      | 110.80   |
| 1   | A     | 132 | ASP  | N-CA-C   | -5.60 | 98.87       | 110.80   |
| 1   | B     | 133 | GLU  | CA-C-N   | 5.60  | 128.04      | 120.65   |
| 1   | B     | 133 | GLU  | C-N-CA   | 5.60  | 128.04      | 120.65   |
| 1   | A     | 107 | TYR  | N-CA-C   | -5.59 | 106.29      | 113.23   |
| 1   | A     | 177 | LYS  | N-CA-C   | 5.57  | 119.59      | 112.34   |
| 1   | B     | 162 | ALA  | N-CA-C   | -5.57 | 105.25      | 113.16   |
| 1   | B     | 19  | ARG  | N-CA-C   | 5.57  | 119.48      | 111.02   |
| 1   | A     | 129 | TYR  | N-CA-C   | 5.53  | 117.72      | 107.99   |
| 1   | B     | 225 | TYR  | N-CA-C   | 5.52  | 120.02      | 113.28   |
| 1   | A     | 216 | GLU  | N-CA-C   | -5.41 | 106.52      | 113.23   |
| 1   | B     | 60  | VAL  | CB-CA-C  | -5.40 | 104.81      | 111.94   |
| 1   | A     | 192 | ALA  | N-CA-C   | 5.39  | 118.04      | 110.23   |
| 1   | B     | 216 | GLU  | N-CA-C   | -5.38 | 106.56      | 113.23   |
| 1   | B     | 15  | GLU  | N-CA-C   | 5.35  | 120.67      | 113.72   |
| 1   | B     | 177 | LYS  | N-CA-C   | 5.35  | 119.29      | 112.34   |
| 1   | B     | 107 | TYR  | N-CA-C   | -5.30 | 106.65      | 113.23   |
| 1   | A     | 219 | ALA  | N-CA-C   | -5.28 | 104.44      | 112.04   |
| 1   | A     | 207 | VAL  | N-CA-C   | 5.27  | 115.95      | 107.73   |
| 1   | A     | 129 | TYR  | CA-C-N   | -5.27 | 113.60      | 123.03   |
| 1   | A     | 129 | TYR  | C-N-CA   | -5.27 | 113.60      | 123.03   |
| 1   | A     | 134 | ALA  | N-CA-C   | -5.17 | 99.79       | 110.80   |
| 1   | A     | 162 | ALA  | N-CA-C   | -5.14 | 105.86      | 113.16   |
| 1   | B     | 11  | GLU  | N-CA-C   | -5.13 | 105.86      | 112.68   |
| 1   | B     | 219 | ALA  | N-CA-C   | -5.11 | 104.68      | 112.04   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 11  | GLU  | N-CA-C | -5.11 | 105.88      | 112.68   |
| 1   | A     | 109 | GLN  | N-CA-C | 5.10  | 117.97      | 111.69   |
| 1   | B     | 76  | LEU  | CA-C-N | 5.09  | 125.62      | 120.38   |
| 1   | B     | 76  | LEU  | C-N-CA | 5.09  | 125.62      | 120.38   |
| 1   | A     | 15  | GLU  | N-CA-C | 5.03  | 120.25      | 113.72   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 129 | TYR  | Sidechain |
| 1   | A     | 172 | TYR  | Sidechain |
| 1   | B     | 170 | TYR  | Sidechain |

## 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     | 1991  | 0        | 2006     | 340     | 0            |
| 1   | B     | 1991  | 0        | 2006     | 290     | 0            |
| All | All   | 3982  | 0        | 4012     | 601     | 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 75.

All (601) 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:A:130:GLU:HB3 | 1:A:133:GLU:HB2  | 1.27                     | 1.17              |
| 1:A:133:GLU:O   | 1:A:135:GLY:N    | 1.78                     | 1.16              |
| 1:B:13:LEU:HD11 | 1:B:21:LEU:HD13  | 1.29                     | 1.14              |
| 1:B:113:ASP:HA  | 1:B:120:ARG:NH1  | 1.66                     | 1.10              |
| 1:B:146:ARG:NH2 | 1:B:176:GLU:HA   | 1.67                     | 1.10              |
| 1:B:113:ASP:HA  | 1:B:120:ARG:HH12 | 1.14                     | 1.03              |
| 1:B:9:LEU:HD11  | 1:B:21:LEU:HA    | 1.38                     | 1.02              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:113:ASP:HA   | 1:A:120:ARG:HH12 | 1.26                     | 1.01              |
| 1:A:203:ASN:OD1  | 1:A:205:LYS:HE3  | 1.65                     | 0.97              |
| 1:A:71:GLU:HA    | 1:A:74:LYS:HE2   | 1.45                     | 0.95              |
| 1:B:24:VAL:O     | 1:B:28:ILE:HB    | 1.67                     | 0.95              |
| 1:B:76:LEU:HD23  | 1:B:77:PRO:HD2   | 1.50                     | 0.94              |
| 1:A:36:LEU:HD23  | 1:A:36:LEU:H     | 1.33                     | 0.93              |
| 1:A:24:VAL:O     | 1:A:28:ILE:HB    | 1.69                     | 0.91              |
| 1:A:187:ARG:HG3  | 1:B:168:ILE:HD11 | 1.52                     | 0.91              |
| 1:A:120:ARG:O    | 1:A:124:GLU:HG3  | 1.70                     | 0.91              |
| 1:A:131:GLU:C    | 1:A:133:GLU:OE1  | 2.15                     | 0.89              |
| 1:B:77:PRO:HG2   | 1:B:80:ARG:CB    | 2.04                     | 0.88              |
| 1:A:113:ASP:HA   | 1:A:120:ARG:NH1  | 1.87                     | 0.88              |
| 1:A:130:GLU:CB   | 1:A:133:GLU:HB2  | 2.04                     | 0.88              |
| 1:B:36:LEU:HD23  | 1:B:36:LEU:H     | 1.38                     | 0.88              |
| 1:B:5:LEU:HD22   | 1:B:24:VAL:HG13  | 1.56                     | 0.87              |
| 1:B:146:ARG:HH22 | 1:B:176:GLU:HA   | 1.39                     | 0.86              |
| 1:B:120:ARG:O    | 1:B:124:GLU:HG3  | 1.76                     | 0.86              |
| 1:B:135:GLY:HA2  | 1:B:138:MSE:HE3  | 1.57                     | 0.85              |
| 1:A:70:ALA:O     | 1:A:74:LYS:HG3   | 1.76                     | 0.85              |
| 1:B:124:GLU:O    | 1:B:128:ARG:NH1  | 2.10                     | 0.85              |
| 1:A:184:LEU:HD21 | 1:A:189:LEU:HD21 | 1.57                     | 0.84              |
| 1:A:250:ASP:O    | 1:A:252:LEU:HD13 | 1.77                     | 0.84              |
| 1:A:119:THR:O    | 1:A:123:VAL:HG23 | 1.78                     | 0.84              |
| 1:B:77:PRO:HG2   | 1:B:80:ARG:HB3   | 1.60                     | 0.83              |
| 1:A:5:LEU:HD22   | 1:A:24:VAL:HG13  | 1.60                     | 0.83              |
| 1:A:134:ALA:HB3  | 1:A:211:THR:O    | 1.79                     | 0.83              |
| 1:B:162:ALA:HB3  | 1:B:163:PRO:HD3  | 1.61                     | 0.83              |
| 1:A:77:PRO:HG2   | 1:A:80:ARG:CB    | 2.09                     | 0.83              |
| 1:B:19:ARG:HG3   | 1:B:20:ALA:H     | 1.43                     | 0.82              |
| 1:A:162:ALA:HB3  | 1:A:163:PRO:HD3  | 1.60                     | 0.82              |
| 1:A:61:LEU:HD12  | 1:A:64:LEU:HD12  | 1.62                     | 0.81              |
| 1:A:9:LEU:HD11   | 1:A:21:LEU:HD12  | 1.62                     | 0.81              |
| 1:A:52:LEU:HD23  | 1:A:57:ALA:HA    | 1.63                     | 0.80              |
| 1:A:187:ARG:NH2  | 1:B:166:GLU:O    | 2.15                     | 0.79              |
| 1:B:76:LEU:CD2   | 1:B:77:PRO:HD2   | 2.13                     | 0.79              |
| 1:A:193:ASP:OD2  | 1:A:195:ARG:HB2  | 1.82                     | 0.79              |
| 1:B:52:LEU:HD23  | 1:B:57:ALA:HA    | 1.65                     | 0.79              |
| 1:A:128:ARG:HH21 | 1:A:136:GLY:HA2  | 1.47                     | 0.79              |
| 1:B:162:ALA:N    | 1:B:163:PRO:CD   | 2.44                     | 0.79              |
| 1:A:162:ALA:N    | 1:A:163:PRO:CD   | 2.47                     | 0.78              |
| 1:A:179:ARG:HA   | 1:A:238:ARG:HA   | 1.64                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:112:LYS:O    | 1:B:120:ARG:HG3  | 1.84                     | 0.78              |
| 1:A:190:ILE:HD12 | 1:A:190:ILE:H    | 1.49                     | 0.78              |
| 1:B:13:LEU:HD23  | 1:B:44:HIS:ND1   | 1.99                     | 0.77              |
| 1:A:132:ASP:HB3  | 1:A:215:GLN:NE2  | 2.00                     | 0.77              |
| 1:A:112:LYS:HE3  | 1:A:124:GLU:HG2  | 1.65                     | 0.77              |
| 1:B:179:ARG:HA   | 1:B:238:ARG:HA   | 1.67                     | 0.77              |
| 1:B:136:GLY:O    | 1:B:137:LEU:HD23 | 1.84                     | 0.76              |
| 1:A:207:VAL:HG11 | 1:A:225:TYR:CE2  | 2.21                     | 0.76              |
| 1:B:193:ASP:OD2  | 1:B:195:ARG:HG3  | 1.86                     | 0.76              |
| 1:B:29:HIS:CE1   | 1:B:31:GLN:HB2   | 2.20                     | 0.76              |
| 1:B:66:PRO:HG2   | 1:B:67:GLU:OE2   | 1.85                     | 0.76              |
| 1:B:207:VAL:HG21 | 1:B:227:PHE:HE1  | 1.49                     | 0.75              |
| 1:A:37:TRP:O     | 1:A:39:GLU:N     | 2.20                     | 0.75              |
| 1:B:172:TYR:CE2  | 1:B:231:PRO:HB3  | 2.22                     | 0.75              |
| 1:A:128:ARG:HE   | 1:A:135:GLY:C    | 1.95                     | 0.75              |
| 1:A:132:ASP:N    | 1:A:133:GLU:OE1  | 2.20                     | 0.74              |
| 1:A:36:LEU:HD23  | 1:A:36:LEU:N     | 2.02                     | 0.74              |
| 1:A:77:PRO:HG2   | 1:A:80:ARG:HB2   | 1.68                     | 0.74              |
| 1:A:133:GLU:C    | 1:A:135:GLY:N    | 2.45                     | 0.74              |
| 1:B:115:LEU:HD23 | 1:B:120:ARG:HA   | 1.69                     | 0.74              |
| 1:A:7:VAL:HG22   | 1:A:10:GLN:NE2   | 2.02                     | 0.74              |
| 1:B:107:TYR:CE2  | 1:B:111:LEU:HD11 | 2.22                     | 0.74              |
| 1:B:37:TRP:O     | 1:B:39:GLU:N     | 2.21                     | 0.73              |
| 1:A:37:TRP:HE1   | 1:A:45:ARG:NH1   | 1.85                     | 0.73              |
| 1:A:180:LEU:HD23 | 1:A:181:LYS:N    | 2.02                     | 0.73              |
| 1:B:150:THR:O    | 1:B:154:VAL:HG23 | 1.89                     | 0.73              |
| 1:A:130:GLU:CD   | 1:A:212:ASP:HA   | 2.12                     | 0.73              |
| 1:B:208:TYR:CD2  | 1:B:209:VAL:N    | 2.56                     | 0.73              |
| 1:A:162:ALA:CB   | 1:B:191:VAL:HG11 | 2.19                     | 0.72              |
| 1:A:48:VAL:HG23  | 1:A:49:LEU:H     | 1.52                     | 0.72              |
| 1:A:105:PRO:O    | 1:A:108:PHE:HB3  | 1.89                     | 0.72              |
| 1:A:128:ARG:HH21 | 1:A:135:GLY:C    | 1.98                     | 0.72              |
| 1:A:128:ARG:NH2  | 1:A:136:GLY:HA2  | 2.04                     | 0.72              |
| 1:A:88:LEU:HD23  | 1:A:93:LEU:HA    | 1.69                     | 0.72              |
| 1:A:162:ALA:HB1  | 1:B:191:VAL:HG11 | 1.72                     | 0.72              |
| 1:B:94:ALA:HB2   | 1:B:126:LEU:HD23 | 1.72                     | 0.71              |
| 1:B:110:ARG:O    | 1:B:114:LEU:HG   | 1.90                     | 0.71              |
| 1:A:151:VAL:HB   | 1:A:194:PRO:HA   | 1.73                     | 0.71              |
| 1:B:153:GLU:HG2  | 1:B:156:ARG:HH22 | 1.55                     | 0.71              |
| 1:A:138:MSE:HE1  | 1:A:211:THR:HG22 | 1.73                     | 0.71              |
| 1:A:135:GLY:HA2  | 1:A:138:MSE:HE2  | 1.72                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:77:PRO:HG2   | 1:B:80:ARG:HB2   | 1.71                     | 0.71              |
| 1:B:142:TYR:HB3  | 1:B:242:ILE:HG21 | 1.71                     | 0.71              |
| 1:B:151:VAL:HB   | 1:B:194:PRO:HA   | 1.72                     | 0.70              |
| 1:A:168:ILE:O    | 1:A:186:LEU:HD13 | 1.91                     | 0.70              |
| 1:A:131:GLU:CA   | 1:A:133:GLU:OE1  | 2.39                     | 0.70              |
| 1:A:130:GLU:HB3  | 1:A:133:GLU:CB   | 2.16                     | 0.70              |
| 1:A:142:TYR:HB3  | 1:A:242:ILE:HG21 | 1.71                     | 0.70              |
| 1:B:9:LEU:CD1    | 1:B:21:LEU:HA    | 2.18                     | 0.70              |
| 1:B:13:LEU:CD1   | 1:B:21:LEU:HD13  | 2.15                     | 0.70              |
| 1:A:166:GLU:O    | 1:B:187:ARG:NH2  | 2.21                     | 0.70              |
| 1:B:105:PRO:O    | 1:B:108:PHE:HB3  | 1.92                     | 0.69              |
| 1:A:77:PRO:HG2   | 1:A:80:ARG:HB3   | 1.73                     | 0.69              |
| 1:A:167:THR:OG1  | 1:A:169:TYR:HB2  | 1.93                     | 0.69              |
| 1:A:52:LEU:HD23  | 1:A:57:ALA:CA    | 2.23                     | 0.69              |
| 1:B:52:LEU:HD23  | 1:B:57:ALA:CA    | 2.23                     | 0.69              |
| 1:B:167:THR:OG1  | 1:B:169:TYR:HB2  | 1.92                     | 0.69              |
| 1:B:171:ILE:N    | 1:B:171:ILE:HD12 | 2.08                     | 0.68              |
| 1:A:188:ASP:O    | 1:A:191:VAL:HG22 | 1.93                     | 0.68              |
| 1:A:101:ARG:NH2  | 1:A:129:TYR:O    | 2.27                     | 0.68              |
| 1:A:69:GLN:O     | 1:A:73:LEU:HG    | 1.93                     | 0.68              |
| 1:B:5:LEU:CD2    | 1:B:24:VAL:HG13  | 2.24                     | 0.68              |
| 1:A:36:LEU:H     | 1:A:36:LEU:CD2   | 2.04                     | 0.68              |
| 1:B:101:ARG:HH21 | 1:B:130:GLU:HB2  | 1.59                     | 0.68              |
| 1:B:139:THR:O    | 1:B:141:GLU:N    | 2.26                     | 0.68              |
| 1:A:76:LEU:HD23  | 1:A:77:PRO:HD2   | 1.74                     | 0.68              |
| 1:A:187:ARG:NH2  | 1:B:167:THR:HA   | 2.09                     | 0.68              |
| 1:B:180:LEU:HD23 | 1:B:181:LYS:N    | 2.09                     | 0.68              |
| 1:A:112:LYS:O    | 1:A:120:ARG:HG3  | 1.94                     | 0.67              |
| 1:B:13:LEU:HD23  | 1:B:44:HIS:CE1   | 2.30                     | 0.67              |
| 1:A:133:GLU:OE1  | 1:A:133:GLU:N    | 2.27                     | 0.67              |
| 1:A:135:GLY:HA2  | 1:A:138:MSE:CE   | 2.24                     | 0.67              |
| 1:A:202:MSE:O    | 1:A:202:MSE:HG3  | 1.94                     | 0.67              |
| 1:A:13:LEU:HD23  | 1:A:44:HIS:ND1   | 2.10                     | 0.67              |
| 1:A:111:LEU:O    | 1:A:115:LEU:HD13 | 1.95                     | 0.67              |
| 1:A:218:VAL:O    | 1:A:222:MSE:HE2  | 1.95                     | 0.67              |
| 1:B:250:ASP:C    | 1:B:252:LEU:H    | 2.03                     | 0.66              |
| 1:A:5:LEU:CD2    | 1:A:24:VAL:HG13  | 2.25                     | 0.66              |
| 1:B:65:SER:OG    | 1:B:68:GLU:OE1   | 2.13                     | 0.66              |
| 1:A:136:GLY:O    | 1:A:137:LEU:HD23 | 1.94                     | 0.66              |
| 1:A:139:THR:O    | 1:A:141:GLU:N    | 2.28                     | 0.66              |
| 1:B:135:GLY:HA2  | 1:B:138:MSE:CE   | 2.25                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:112:LYS:O    | 1:A:115:LEU:HB2  | 1.96                     | 0.66              |
| 1:B:67:GLU:H     | 1:B:67:GLU:CD    | 2.03                     | 0.65              |
| 1:A:5:LEU:HD13   | 1:A:27:GLU:O     | 1.97                     | 0.65              |
| 1:B:5:LEU:HA     | 1:B:8:SER:HB3    | 1.78                     | 0.65              |
| 1:B:70:ALA:HB1   | 1:B:100:VAL:HG13 | 1.78                     | 0.65              |
| 1:A:67:GLU:CD    | 1:A:67:GLU:H     | 2.05                     | 0.65              |
| 1:A:190:ILE:HG23 | 1:B:155:LEU:HD22 | 1.78                     | 0.65              |
| 1:A:107:TYR:CE2  | 1:A:111:LEU:HD11 | 2.31                     | 0.65              |
| 1:B:175:ASP:O    | 1:B:176:GLU:C    | 2.37                     | 0.65              |
| 1:A:66:PRO:HG2   | 1:A:67:GLU:OE2   | 1.97                     | 0.65              |
| 1:A:175:ASP:O    | 1:A:176:GLU:C    | 2.38                     | 0.65              |
| 1:A:76:LEU:CD2   | 1:A:77:PRO:HD2   | 2.27                     | 0.65              |
| 1:B:210:ARG:HH11 | 1:B:235:GLU:HA   | 1.61                     | 0.65              |
| 1:B:203:ASN:OD1  | 1:B:205:LYS:HE3  | 1.96                     | 0.64              |
| 1:A:172:TYR:CE2  | 1:A:231:PRO:HB3  | 2.32                     | 0.64              |
| 1:A:142:TYR:HB3  | 1:A:242:ILE:HD13 | 1.78                     | 0.64              |
| 1:A:180:LEU:HD23 | 1:A:182:GLY:H    | 1.63                     | 0.64              |
| 1:A:190:ILE:HG21 | 1:B:158:LEU:HD23 | 1.80                     | 0.64              |
| 1:A:203:ASN:OD1  | 1:A:205:LYS:HB2  | 1.98                     | 0.64              |
| 1:B:7:VAL:HG13   | 1:B:10:GLN:NE2   | 2.12                     | 0.63              |
| 1:B:61:LEU:HD12  | 1:B:64:LEU:HD12  | 1.80                     | 0.63              |
| 1:B:81:LEU:O     | 1:B:85:LEU:HG    | 1.97                     | 0.63              |
| 1:B:19:ARG:HG3   | 1:B:20:ALA:N     | 2.13                     | 0.63              |
| 1:A:249:LEU:O    | 1:A:249:LEU:HD23 | 1.98                     | 0.63              |
| 1:A:61:LEU:CD1   | 1:A:64:LEU:HD12  | 2.28                     | 0.63              |
| 1:B:77:PRO:O     | 1:B:81:LEU:HG    | 1.98                     | 0.63              |
| 1:B:242:ILE:HG13 | 1:B:242:ILE:O    | 1.97                     | 0.63              |
| 1:A:169:TYR:CE2  | 1:B:187:ARG:HB2  | 2.34                     | 0.63              |
| 1:A:146:ARG:NH2  | 1:A:176:GLU:HA   | 2.13                     | 0.63              |
| 1:B:5:LEU:HB3    | 1:B:24:VAL:HG13  | 1.80                     | 0.63              |
| 1:B:125:ALA:HA   | 1:B:128:ARG:NH1  | 2.14                     | 0.62              |
| 1:B:48:VAL:HG23  | 1:B:49:LEU:H     | 1.63                     | 0.62              |
| 1:B:107:TYR:CD2  | 1:B:111:LEU:HD11 | 2.34                     | 0.62              |
| 1:A:128:ARG:HH21 | 1:A:136:GLY:CA   | 2.13                     | 0.62              |
| 1:B:36:LEU:H     | 1:B:36:LEU:CD2   | 2.10                     | 0.62              |
| 1:A:133:GLU:O    | 1:A:135:GLY:CA   | 2.48                     | 0.62              |
| 1:B:53:PRO:O     | 1:B:55:ALA:N     | 2.32                     | 0.62              |
| 1:B:139:THR:C    | 1:B:141:GLU:H    | 2.08                     | 0.62              |
| 1:A:132:ASP:OD2  | 1:A:215:GLN:NE2  | 2.24                     | 0.62              |
| 1:A:190:ILE:HD12 | 1:A:190:ILE:N    | 2.13                     | 0.62              |
| 1:A:250:ASP:C    | 1:A:252:LEU:H    | 2.07                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:13:LEU:C     | 1:A:15:GLU:H     | 2.06                     | 0.62              |
| 1:A:128:ARG:HE   | 1:A:135:GLY:CA   | 2.13                     | 0.62              |
| 1:A:29:HIS:ND1   | 1:A:30:PRO:HD2   | 2.15                     | 0.61              |
| 1:B:180:LEU:HD23 | 1:B:182:GLY:H    | 1.64                     | 0.61              |
| 1:A:9:LEU:HD13   | 1:A:24:VAL:HB    | 1.82                     | 0.61              |
| 1:A:133:GLU:OE2  | 1:A:215:GLN:HB3  | 2.00                     | 0.61              |
| 1:A:128:ARG:NH2  | 1:A:135:GLY:O    | 2.32                     | 0.61              |
| 1:A:53:PRO:O     | 1:A:55:ALA:N     | 2.34                     | 0.61              |
| 1:A:167:THR:HA   | 1:B:187:ARG:CZ   | 2.30                     | 0.61              |
| 1:B:172:TYR:OH   | 1:B:231:PRO:HD3  | 2.00                     | 0.61              |
| 1:A:248:VAL:HA   | 1:A:251:VAL:HG22 | 1.83                     | 0.61              |
| 1:A:208:TYR:CD2  | 1:A:209:VAL:N    | 2.69                     | 0.61              |
| 1:A:210:ARG:HB3  | 1:A:212:ASP:OD1  | 1.99                     | 0.61              |
| 1:A:25:LEU:HA    | 1:A:28:ILE:CG2   | 2.31                     | 0.61              |
| 1:B:147:GLU:OE1  | 1:B:181:LYS:HG3  | 2.01                     | 0.61              |
| 1:A:222:MSE:HE1  | 1:A:248:VAL:HG21 | 1.82                     | 0.60              |
| 1:B:41:LYS:O     | 1:B:42:GLY:C     | 2.44                     | 0.60              |
| 1:A:115:LEU:HD23 | 1:A:120:ARG:HA   | 1.83                     | 0.60              |
| 1:B:203:ASN:CG   | 1:B:205:LYS:HE3  | 2.26                     | 0.60              |
| 1:A:41:LYS:O     | 1:A:42:GLY:C     | 2.42                     | 0.60              |
| 1:B:90:LEU:O     | 1:B:93:LEU:HB3   | 2.00                     | 0.60              |
| 1:A:147:GLU:OE1  | 1:A:181:LYS:HG3  | 2.02                     | 0.60              |
| 1:B:36:LEU:HD23  | 1:B:36:LEU:N     | 2.11                     | 0.60              |
| 1:B:80:ARG:O     | 1:B:84:ILE:HG12  | 2.02                     | 0.60              |
| 1:B:13:LEU:C     | 1:B:15:GLU:H     | 2.09                     | 0.60              |
| 1:B:207:VAL:HG23 | 1:B:230:LEU:HD11 | 1.83                     | 0.60              |
| 1:A:190:ILE:HD11 | 1:B:190:ILE:HD11 | 1.84                     | 0.60              |
| 1:A:180:LEU:HD23 | 1:A:182:GLY:N    | 2.17                     | 0.60              |
| 1:B:89:SER:O     | 1:B:93:LEU:HB2   | 2.02                     | 0.59              |
| 1:B:173:VAL:HG21 | 1:B:202:MSE:SE   | 2.52                     | 0.59              |
| 1:A:13:LEU:HD23  | 1:A:44:HIS:CE1   | 2.37                     | 0.59              |
| 1:A:7:VAL:HG12   | 1:A:7:VAL:O      | 2.01                     | 0.59              |
| 1:A:105:PRO:O    | 1:A:108:PHE:N    | 2.35                     | 0.59              |
| 1:A:186:LEU:HD11 | 1:B:190:ILE:HD12 | 1.82                     | 0.59              |
| 1:B:193:ASP:CG   | 1:B:194:PRO:HD2  | 2.28                     | 0.59              |
| 1:B:203:ASN:ND2  | 1:B:205:LYS:HE3  | 2.17                     | 0.59              |
| 1:B:5:LEU:HD13   | 1:B:27:GLU:HG3   | 1.84                     | 0.59              |
| 1:B:5:LEU:HB3    | 1:B:24:VAL:CG1   | 2.32                     | 0.58              |
| 1:A:7:VAL:HA     | 1:A:10:GLN:HE21  | 1.67                     | 0.58              |
| 1:A:94:ALA:O     | 1:A:98:GLN:HG3   | 2.04                     | 0.58              |
| 1:A:107:TYR:CD2  | 1:A:111:LEU:HD11 | 2.38                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:105:PRO:O    | 1:B:108:PHE:N    | 2.36                     | 0.58              |
| 1:A:110:ARG:O    | 1:A:114:LEU:HG   | 2.03                     | 0.58              |
| 1:A:19:ARG:CD    | 1:A:20:ALA:N     | 2.67                     | 0.58              |
| 1:A:203:ASN:ND2  | 1:A:205:LYS:O    | 2.36                     | 0.58              |
| 1:A:217:GLU:OE1  | 1:A:217:GLU:HA   | 2.04                     | 0.58              |
| 1:A:13:LEU:O     | 1:A:15:GLU:N     | 2.36                     | 0.58              |
| 1:A:139:THR:C    | 1:A:141:GLU:H    | 2.11                     | 0.58              |
| 1:A:191:VAL:HG23 | 1:A:192:ALA:N    | 2.18                     | 0.58              |
| 1:B:168:ILE:O    | 1:B:186:LEU:HD13 | 2.04                     | 0.58              |
| 1:B:169:TYR:C    | 1:B:170:TYR:CD1  | 2.82                     | 0.58              |
| 1:A:130:GLU:C    | 1:A:132:ASP:H    | 2.12                     | 0.57              |
| 1:B:119:THR:O    | 1:B:123:VAL:HG23 | 2.04                     | 0.57              |
| 1:A:207:VAL:HG23 | 1:A:207:VAL:O    | 2.02                     | 0.57              |
| 1:B:13:LEU:O     | 1:B:15:GLU:N     | 2.37                     | 0.57              |
| 1:B:168:ILE:O    | 1:B:171:ILE:HD11 | 2.04                     | 0.57              |
| 1:B:203:ASN:OD1  | 1:B:205:LYS:CE   | 2.53                     | 0.57              |
| 1:B:54:LYS:O     | 1:B:87:GLU:HG3   | 2.05                     | 0.57              |
| 1:A:5:LEU:HB3    | 1:A:24:VAL:HG13  | 1.86                     | 0.57              |
| 1:A:132:ASP:HB3  | 1:A:215:GLN:CD   | 2.30                     | 0.57              |
| 1:B:9:LEU:HD12   | 1:B:12:ALA:HB3   | 1.85                     | 0.57              |
| 1:A:128:ARG:NE   | 1:A:135:GLY:O    | 2.37                     | 0.57              |
| 1:B:225:TYR:N    | 1:B:225:TYR:CD1  | 2.69                     | 0.57              |
| 1:A:6:ALA:C      | 1:A:8:SER:H      | 2.13                     | 0.57              |
| 1:A:105:PRO:O    | 1:A:108:PHE:CB   | 2.53                     | 0.57              |
| 1:A:53:PRO:HG2   | 1:A:56:LYS:HD2   | 1.86                     | 0.57              |
| 1:A:133:GLU:O    | 1:A:134:ALA:C    | 2.40                     | 0.56              |
| 1:A:13:LEU:CD1   | 1:A:21:LEU:HD13  | 2.35                     | 0.56              |
| 1:A:107:TYR:CZ   | 1:A:111:LEU:HD21 | 2.40                     | 0.56              |
| 1:A:131:GLU:N    | 1:A:133:GLU:OE1  | 2.39                     | 0.56              |
| 1:B:217:GLU:HA   | 1:B:217:GLU:OE1  | 2.05                     | 0.56              |
| 1:A:168:ILE:HD11 | 1:B:187:ARG:HG3  | 1.87                     | 0.56              |
| 1:B:5:LEU:CD1    | 1:B:27:GLU:HG3   | 2.36                     | 0.56              |
| 1:B:218:VAL:HG12 | 1:B:218:VAL:O    | 2.04                     | 0.56              |
| 1:A:132:ASP:OD2  | 1:A:251:VAL:HG12 | 2.05                     | 0.56              |
| 1:B:160:ARG:NH1  | 1:B:160:ARG:HG3  | 2.21                     | 0.56              |
| 1:B:247:ASP:O    | 1:B:251:VAL:HG13 | 2.05                     | 0.56              |
| 1:A:90:LEU:O     | 1:A:93:LEU:CB    | 2.54                     | 0.56              |
| 1:B:31:GLN:C     | 1:B:33:LEU:N     | 2.60                     | 0.56              |
| 1:B:210:ARG:NH1  | 1:B:235:GLU:HA   | 2.21                     | 0.56              |
| 1:A:202:MSE:HE3  | 1:A:204:PRO:HA   | 1.87                     | 0.55              |
| 1:B:53:PRO:CG    | 1:B:56:LYS:HD2   | 2.35                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:12:ALA:C     | 1:B:13:LEU:HD12  | 2.30                     | 0.55              |
| 1:B:33:LEU:C     | 1:B:35:ALA:H     | 2.14                     | 0.55              |
| 1:A:91:ASP:O     | 1:A:94:ALA:HB3   | 2.06                     | 0.55              |
| 1:A:31:GLN:C     | 1:A:33:LEU:N     | 2.62                     | 0.55              |
| 1:B:107:TYR:CZ   | 1:B:111:LEU:HD21 | 2.41                     | 0.55              |
| 1:B:207:VAL:HG21 | 1:B:227:PHE:CE1  | 2.37                     | 0.55              |
| 1:A:62:SER:HA    | 1:A:69:GLN:HE22  | 1.70                     | 0.55              |
| 1:A:9:LEU:HD11   | 1:A:21:LEU:CD1   | 2.35                     | 0.55              |
| 1:A:53:PRO:CG    | 1:A:56:LYS:HD2   | 2.37                     | 0.55              |
| 1:A:202:MSE:HE3  | 1:A:204:PRO:CA   | 2.37                     | 0.54              |
| 1:A:94:ALA:HB2   | 1:A:126:LEU:HD23 | 1.90                     | 0.54              |
| 1:A:105:PRO:HA   | 1:A:108:PHE:HB2  | 1.89                     | 0.54              |
| 1:A:133:GLU:OE2  | 1:A:215:GLN:CB   | 2.55                     | 0.54              |
| 1:B:53:PRO:HG2   | 1:B:56:LYS:HG3   | 1.89                     | 0.54              |
| 1:B:88:LEU:HD23  | 1:B:93:LEU:HA    | 1.87                     | 0.54              |
| 1:A:48:VAL:O     | 1:A:52:LEU:HB2   | 2.08                     | 0.54              |
| 1:A:89:SER:O     | 1:A:93:LEU:HB2   | 2.07                     | 0.54              |
| 1:A:186:LEU:O    | 1:A:190:ILE:CD1  | 2.55                     | 0.54              |
| 1:B:13:LEU:HD12  | 1:B:13:LEU:N     | 2.22                     | 0.54              |
| 1:B:168:ILE:HD13 | 1:B:168:ILE:H    | 1.73                     | 0.54              |
| 1:B:203:ASN:OD1  | 1:B:205:LYS:HB2  | 2.08                     | 0.54              |
| 1:A:25:LEU:O     | 1:A:28:ILE:HG22  | 2.07                     | 0.54              |
| 1:A:162:ALA:HB2  | 1:B:191:VAL:CG1  | 2.38                     | 0.54              |
| 1:A:95:ASP:OD1   | 1:A:95:ASP:N     | 2.41                     | 0.54              |
| 1:B:207:VAL:HG23 | 1:B:207:VAL:O    | 2.06                     | 0.54              |
| 1:A:17:ASP:OD1   | 1:A:19:ARG:HG3   | 2.08                     | 0.54              |
| 1:A:146:ARG:HH11 | 1:A:146:ARG:HB3  | 1.72                     | 0.54              |
| 1:A:147:GLU:HB3  | 1:A:173:VAL:CG1  | 2.38                     | 0.54              |
| 1:A:5:LEU:HA     | 1:A:8:SER:HB3    | 1.89                     | 0.54              |
| 1:A:162:ALA:CB   | 1:B:191:VAL:CG1  | 2.84                     | 0.54              |
| 1:A:180:LEU:HD21 | 1:A:206:VAL:HG11 | 1.89                     | 0.54              |
| 1:A:133:GLU:N    | 1:A:133:GLU:CD   | 2.66                     | 0.53              |
| 1:A:142:TYR:HB3  | 1:A:242:ILE:CG2  | 2.36                     | 0.53              |
| 1:A:62:SER:HA    | 1:A:69:GLN:NE2   | 2.23                     | 0.53              |
| 1:A:19:ARG:HD3   | 1:A:20:ALA:N     | 2.24                     | 0.53              |
| 1:A:131:GLU:O    | 1:A:132:ASP:HB2  | 2.08                     | 0.53              |
| 1:A:187:ARG:NH1  | 1:B:167:THR:OG1  | 2.42                     | 0.53              |
| 1:B:53:PRO:HG2   | 1:B:56:LYS:CG    | 2.39                     | 0.53              |
| 1:B:71:GLU:HA    | 1:B:74:LYS:HE2   | 1.90                     | 0.53              |
| 1:A:130:GLU:OE1  | 1:A:212:ASP:O    | 2.27                     | 0.53              |
| 1:A:33:LEU:C     | 1:A:35:ALA:H     | 2.17                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:89:SER:HB3   | 1:A:91:ASP:OD1   | 2.09                     | 0.52              |
| 1:B:31:GLN:O     | 1:B:33:LEU:N     | 2.43                     | 0.52              |
| 1:B:48:VAL:O     | 1:B:52:LEU:HB2   | 2.10                     | 0.52              |
| 1:A:129:TYR:C    | 1:A:129:TYR:CD2  | 2.85                     | 0.52              |
| 1:A:9:LEU:C      | 1:A:11:GLU:H     | 2.17                     | 0.52              |
| 1:A:207:VAL:HG11 | 1:A:225:TYR:CZ   | 2.43                     | 0.52              |
| 1:A:232:VAL:CG2  | 1:A:243:VAL:HG23 | 2.39                     | 0.52              |
| 1:B:9:LEU:C      | 1:B:11:GLU:H     | 2.16                     | 0.52              |
| 1:B:139:THR:O    | 1:B:139:THR:HG23 | 2.09                     | 0.52              |
| 1:A:13:LEU:C     | 1:A:15:GLU:N     | 2.67                     | 0.52              |
| 1:A:130:GLU:CB   | 1:A:133:GLU:CB   | 2.84                     | 0.52              |
| 1:B:250:ASP:C    | 1:B:252:LEU:N    | 2.64                     | 0.52              |
| 1:B:6:ALA:C      | 1:B:8:SER:H      | 2.18                     | 0.52              |
| 1:B:162:ALA:N    | 1:B:163:PRO:HD3  | 2.22                     | 0.52              |
| 1:B:142:TYR:HB3  | 1:B:242:ILE:CG2  | 2.39                     | 0.52              |
| 1:B:134:ALA:HB3  | 1:B:211:THR:O    | 2.10                     | 0.52              |
| 1:B:138:MSE:HA   | 1:B:242:ILE:O    | 2.10                     | 0.52              |
| 1:A:37:TRP:NE1   | 1:A:45:ARG:NH1   | 2.57                     | 0.51              |
| 1:A:162:ALA:HB2  | 1:B:191:VAL:HG12 | 1.91                     | 0.51              |
| 1:A:41:LYS:HB2   | 1:A:44:HIS:HD2   | 1.75                     | 0.51              |
| 1:A:128:ARG:NH2  | 1:A:135:GLY:C    | 2.68                     | 0.51              |
| 1:A:250:ASP:C    | 1:A:252:LEU:N    | 2.66                     | 0.51              |
| 1:B:232:VAL:CG2  | 1:B:243:VAL:HG23 | 2.39                     | 0.51              |
| 1:B:24:VAL:HG12  | 1:B:28:ILE:HD13  | 1.92                     | 0.51              |
| 1:B:91:ASP:O     | 1:B:94:ALA:HB3   | 2.10                     | 0.51              |
| 1:A:162:ALA:CB   | 1:A:163:PRO:HD3  | 2.30                     | 0.51              |
| 1:B:147:GLU:HB3  | 1:B:173:VAL:CG1  | 2.40                     | 0.51              |
| 1:A:37:TRP:C     | 1:A:39:GLU:H     | 2.18                     | 0.51              |
| 1:A:162:ALA:N    | 1:A:163:PRO:HD3  | 2.23                     | 0.51              |
| 1:B:13:LEU:CD1   | 1:B:13:LEU:N     | 2.74                     | 0.51              |
| 1:B:101:ARG:O    | 1:B:103:GLU:N    | 2.43                     | 0.51              |
| 1:A:177:LYS:NZ   | 1:A:179:ARG:HH22 | 2.09                     | 0.51              |
| 1:B:150:THR:C    | 1:B:152:GLU:N    | 2.68                     | 0.50              |
| 1:B:162:ALA:N    | 1:B:163:PRO:HD2  | 2.25                     | 0.50              |
| 1:A:65:SER:OG    | 1:A:68:GLU:OE1   | 2.29                     | 0.50              |
| 1:A:184:LEU:CD2  | 1:A:189:LEU:HD21 | 2.36                     | 0.50              |
| 1:B:31:GLN:C     | 1:B:33:LEU:H     | 2.18                     | 0.50              |
| 1:B:49:LEU:HD23  | 1:B:57:ALA:HA    | 1.93                     | 0.50              |
| 1:A:177:LYS:HZ2  | 1:A:179:ARG:NH2  | 2.09                     | 0.50              |
| 1:B:180:LEU:CD2  | 1:B:182:GLY:H    | 2.24                     | 0.50              |
| 1:A:138:MSE:HA   | 1:A:242:ILE:O    | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:187:ARG:CZ   | 1:B:167:THR:HA   | 2.41                     | 0.50              |
| 1:A:214:ASP:OD2  | 1:A:216:GLU:HB2  | 2.12                     | 0.50              |
| 1:B:9:LEU:HD11   | 1:B:21:LEU:HD12  | 1.94                     | 0.50              |
| 1:B:13:LEU:C     | 1:B:15:GLU:N     | 2.68                     | 0.50              |
| 1:B:115:LEU:HB3  | 1:B:120:ARG:HB2  | 1.94                     | 0.50              |
| 1:A:180:LEU:HD23 | 1:A:180:LEU:C    | 2.37                     | 0.50              |
| 1:A:31:GLN:O     | 1:A:33:LEU:N     | 2.45                     | 0.50              |
| 1:B:62:SER:HA    | 1:B:69:GLN:NE2   | 2.26                     | 0.50              |
| 1:A:19:ARG:HG3   | 1:A:20:ALA:H     | 1.77                     | 0.50              |
| 1:A:19:ARG:CG    | 1:A:20:ALA:H     | 2.24                     | 0.50              |
| 1:A:177:LYS:HZ2  | 1:A:179:ARG:HH22 | 1.60                     | 0.49              |
| 1:A:187:ARG:HG3  | 1:B:168:ILE:CD1  | 2.32                     | 0.49              |
| 1:A:203:ASN:HD21 | 1:A:205:LYS:HB2  | 1.77                     | 0.49              |
| 1:B:70:ALA:O     | 1:B:74:LYS:HG3   | 2.12                     | 0.49              |
| 1:A:158:LEU:O    | 1:A:162:ALA:HB2  | 2.12                     | 0.49              |
| 1:B:101:ARG:NH2  | 1:B:130:GLU:HB2  | 2.27                     | 0.49              |
| 1:B:105:PRO:O    | 1:B:108:PHE:CB   | 2.59                     | 0.49              |
| 1:B:180:LEU:CD2  | 1:B:182:GLY:N    | 2.75                     | 0.49              |
| 1:B:196:THR:HG22 | 1:B:200:GLU:HB2  | 1.94                     | 0.49              |
| 1:B:199:ALA:O    | 1:B:201:ILE:N    | 2.45                     | 0.49              |
| 1:A:130:GLU:CG   | 1:A:212:ASP:HA   | 2.42                     | 0.49              |
| 1:A:184:LEU:HD21 | 1:A:189:LEU:CD2  | 2.35                     | 0.49              |
| 1:B:10:GLN:O     | 1:B:14:GLN:CD    | 2.55                     | 0.49              |
| 1:B:139:THR:C    | 1:B:141:GLU:N    | 2.70                     | 0.49              |
| 1:A:41:LYS:HB2   | 1:A:44:HIS:CD2   | 2.48                     | 0.49              |
| 1:A:88:LEU:HD23  | 1:A:92:ASP:O     | 2.13                     | 0.49              |
| 1:A:218:VAL:O    | 1:A:218:VAL:HG12 | 2.13                     | 0.49              |
| 1:B:37:TRP:C     | 1:B:39:GLU:H     | 2.20                     | 0.49              |
| 1:B:208:TYR:HD2  | 1:B:209:VAL:H    | 1.59                     | 0.49              |
| 1:B:179:ARG:CB   | 1:B:237:GLY:O    | 2.61                     | 0.49              |
| 1:B:180:LEU:HD21 | 1:B:206:VAL:HG11 | 1.95                     | 0.49              |
| 1:A:132:ASP:CB   | 1:A:215:GLN:NE2  | 2.73                     | 0.49              |
| 1:A:101:ARG:O    | 1:A:103:GLU:N    | 2.45                     | 0.49              |
| 1:A:138:MSE:HE1  | 1:A:211:THR:CG2  | 2.42                     | 0.49              |
| 1:B:33:LEU:O     | 1:B:35:ALA:N     | 2.45                     | 0.49              |
| 1:B:132:ASP:O    | 1:B:133:GLU:CB   | 2.61                     | 0.49              |
| 1:A:168:ILE:C    | 1:A:168:ILE:HD12 | 2.38                     | 0.48              |
| 1:B:115:LEU:HD23 | 1:B:120:ARG:CA   | 2.42                     | 0.48              |
| 1:B:222:MSE:HE1  | 1:B:248:VAL:HG21 | 1.94                     | 0.48              |
| 1:A:31:GLN:C     | 1:A:33:LEU:H     | 2.21                     | 0.48              |
| 1:A:107:TYR:CE2  | 1:A:111:LEU:HD21 | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:214:ASP:OD2  | 1:B:216:GLU:HB2  | 2.13                     | 0.48              |
| 1:A:199:ALA:O    | 1:A:201:ILE:N    | 2.46                     | 0.48              |
| 1:B:7:VAL:HA     | 1:B:10:GLN:HE21  | 1.77                     | 0.48              |
| 1:B:158:LEU:O    | 1:B:162:ALA:HB2  | 2.13                     | 0.48              |
| 1:B:162:ALA:CB   | 1:B:163:PRO:HD3  | 2.30                     | 0.48              |
| 1:A:5:LEU:CD1    | 1:A:27:GLU:O     | 2.61                     | 0.48              |
| 1:A:25:LEU:HA    | 1:A:28:ILE:HG21  | 1.95                     | 0.48              |
| 1:A:36:LEU:O     | 1:A:37:TRP:C     | 2.57                     | 0.48              |
| 1:B:35:ALA:C     | 1:B:37:TRP:H     | 2.21                     | 0.48              |
| 1:B:132:ASP:C    | 1:B:133:GLU:CG   | 2.86                     | 0.48              |
| 1:B:234:ASP:OD2  | 1:B:238:ARG:HB2  | 2.14                     | 0.48              |
| 1:B:210:ARG:HB2  | 1:B:213:THR:OG1  | 2.13                     | 0.48              |
| 1:A:135:GLY:CA   | 1:A:138:MSE:HE2  | 2.41                     | 0.48              |
| 1:A:226:ASP:N    | 1:A:226:ASP:OD1  | 2.47                     | 0.48              |
| 1:A:35:ALA:C     | 1:A:37:TRP:N     | 2.72                     | 0.48              |
| 1:A:150:THR:C    | 1:A:152:GLU:N    | 2.69                     | 0.48              |
| 1:A:191:VAL:HA   | 1:B:159:ARG:HG2  | 1.95                     | 0.48              |
| 1:B:94:ALA:CB    | 1:B:126:LEU:HD23 | 2.42                     | 0.48              |
| 1:B:203:ASN:HD21 | 1:B:205:LYS:HE3  | 1.77                     | 0.48              |
| 1:A:207:VAL:CG2  | 1:A:227:PHE:HE1  | 2.27                     | 0.48              |
| 1:B:207:VAL:CG2  | 1:B:227:PHE:HE1  | 2.24                     | 0.48              |
| 1:A:18:THR:HG22  | 1:A:22:ARG:HE    | 1.79                     | 0.48              |
| 1:A:19:ARG:CG    | 1:A:20:ALA:N     | 2.77                     | 0.48              |
| 1:A:101:ARG:HH22 | 1:A:129:TYR:N    | 2.12                     | 0.48              |
| 1:A:180:LEU:CD2  | 1:A:182:GLY:N    | 2.77                     | 0.48              |
| 1:B:52:LEU:HD12  | 1:B:53:PRO:HD2   | 1.96                     | 0.48              |
| 1:B:160:ARG:HG3  | 1:B:160:ARG:HH11 | 1.77                     | 0.48              |
| 1:B:33:LEU:C     | 1:B:35:ALA:N     | 2.72                     | 0.47              |
| 1:B:128:ARG:HG3  | 1:B:129:TYR:CE2  | 2.49                     | 0.47              |
| 1:A:67:GLU:CD    | 1:A:67:GLU:N     | 2.71                     | 0.47              |
| 1:A:138:MSE:SE   | 1:A:241:GLY:HA3  | 2.64                     | 0.47              |
| 1:A:193:ASP:OD1  | 1:A:194:PRO:HD2  | 2.14                     | 0.47              |
| 1:A:128:ARG:NE   | 1:A:135:GLY:C    | 2.68                     | 0.47              |
| 1:B:138:MSE:HE1  | 1:B:211:THR:HG22 | 1.96                     | 0.47              |
| 1:B:234:ASP:OD1  | 1:B:235:GLU:N    | 2.48                     | 0.47              |
| 1:A:29:HIS:CE1   | 1:A:31:GLN:HB2   | 2.50                     | 0.47              |
| 1:A:133:GLU:OE2  | 1:A:215:GLN:HG2  | 2.15                     | 0.47              |
| 1:A:146:ARG:HH11 | 1:A:146:ARG:CG   | 2.27                     | 0.47              |
| 1:B:36:LEU:O     | 1:B:37:TRP:C     | 2.56                     | 0.47              |
| 1:A:130:GLU:HG3  | 1:A:212:ASP:HA   | 1.95                     | 0.47              |
| 1:A:187:ARG:CG   | 1:B:168:ILE:HD11 | 2.36                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:19:ARG:CG    | 1:B:20:ALA:N     | 2.78                     | 0.47              |
| 1:B:105:PRO:C    | 1:B:108:PHE:H    | 2.23                     | 0.47              |
| 1:A:153:GLU:HA   | 1:A:156:ARG:NH2  | 2.29                     | 0.47              |
| 1:A:66:PRO:O     | 1:A:67:GLU:C     | 2.58                     | 0.47              |
| 1:A:105:PRO:C    | 1:A:108:PHE:H    | 2.23                     | 0.47              |
| 1:A:154:VAL:O    | 1:A:155:LEU:C    | 2.58                     | 0.47              |
| 1:B:153:GLU:HA   | 1:B:156:ARG:NH2  | 2.30                     | 0.47              |
| 1:A:172:TYR:N    | 1:A:172:TYR:CD1  | 2.83                     | 0.47              |
| 1:A:227:PHE:HD1  | 1:A:230:LEU:CD1  | 2.27                     | 0.47              |
| 1:B:202:MSE:O    | 1:B:202:MSE:HG3  | 2.15                     | 0.47              |
| 1:A:33:LEU:C     | 1:A:35:ALA:N     | 2.73                     | 0.46              |
| 1:A:80:ARG:O     | 1:A:84:ILE:HG12  | 2.14                     | 0.46              |
| 1:A:139:THR:C    | 1:A:141:GLU:N    | 2.73                     | 0.46              |
| 1:A:33:LEU:O     | 1:A:35:ALA:N     | 2.48                     | 0.46              |
| 1:A:97:LEU:HD12  | 1:A:123:VAL:HG11 | 1.97                     | 0.46              |
| 1:A:232:VAL:HG21 | 1:A:243:VAL:HG23 | 1.97                     | 0.46              |
| 1:B:173:VAL:HG11 | 1:B:202:MSE:SE   | 2.65                     | 0.46              |
| 1:A:168:ILE:HD11 | 1:B:187:ARG:HA   | 1.96                     | 0.46              |
| 1:A:169:TYR:C    | 1:A:170:TYR:CD1  | 2.93                     | 0.46              |
| 1:B:35:ALA:C     | 1:B:37:TRP:N     | 2.70                     | 0.46              |
| 1:A:6:ALA:C      | 1:A:8:SER:N      | 2.71                     | 0.46              |
| 1:A:37:TRP:NE1   | 1:A:45:ARG:CZ    | 2.79                     | 0.46              |
| 1:A:29:HIS:HB3   | 1:A:32:ASP:OD2   | 2.16                     | 0.46              |
| 1:A:35:ALA:C     | 1:A:37:TRP:H     | 2.23                     | 0.46              |
| 1:A:48:VAL:HG23  | 1:A:49:LEU:N     | 2.27                     | 0.46              |
| 1:A:146:ARG:HH22 | 1:A:176:GLU:HA   | 1.79                     | 0.46              |
| 1:A:207:VAL:HG11 | 1:A:225:TYR:OH   | 2.16                     | 0.46              |
| 1:A:133:GLU:OE2  | 1:A:215:GLN:CG   | 2.64                     | 0.46              |
| 1:B:154:VAL:O    | 1:B:155:LEU:C    | 2.59                     | 0.46              |
| 1:A:179:ARG:HB2  | 1:A:237:GLY:O    | 2.16                     | 0.46              |
| 1:A:208:TYR:OH   | 1:A:210:ARG:NH2  | 2.49                     | 0.46              |
| 1:B:132:ASP:C    | 1:B:133:GLU:HG2  | 2.41                     | 0.46              |
| 1:A:150:THR:OG1  | 1:A:152:GLU:HB3  | 2.16                     | 0.46              |
| 1:B:171:ILE:N    | 1:B:171:ILE:CD1  | 2.77                     | 0.46              |
| 1:B:172:TYR:HE2  | 1:B:231:PRO:HG3  | 1.81                     | 0.46              |
| 1:A:91:ASP:C     | 1:A:93:LEU:H     | 2.24                     | 0.45              |
| 1:B:105:PRO:HA   | 1:B:108:PHE:HB2  | 1.98                     | 0.45              |
| 1:A:37:TRP:C     | 1:A:39:GLU:N     | 2.74                     | 0.45              |
| 1:B:37:TRP:C     | 1:B:39:GLU:N     | 2.74                     | 0.45              |
| 1:B:138:MSE:SE   | 1:B:241:GLY:HA3  | 2.66                     | 0.45              |
| 1:B:66:PRO:O     | 1:B:67:GLU:C     | 2.59                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:206:VAL:HG13 | 1:B:206:VAL:O    | 2.16                     | 0.45              |
| 1:A:193:ASP:OD2  | 1:A:195:ARG:CB   | 2.60                     | 0.45              |
| 1:B:29:HIS:ND1   | 1:B:31:GLN:HB2   | 2.29                     | 0.45              |
| 1:B:229:VAL:HG12 | 1:B:230:LEU:N    | 2.31                     | 0.45              |
| 1:A:11:GLU:C     | 1:A:13:LEU:N     | 2.75                     | 0.45              |
| 1:A:167:THR:HA   | 1:B:187:ARG:NH2  | 2.31                     | 0.45              |
| 1:B:10:GLN:O     | 1:B:14:GLN:OE1   | 2.34                     | 0.45              |
| 1:B:37:TRP:NE1   | 1:B:45:ARG:NH1   | 2.64                     | 0.45              |
| 1:B:25:LEU:HA    | 1:B:28:ILE:CG2   | 2.46                     | 0.45              |
| 1:B:130:GLU:HG3  | 1:B:131:GLU:N    | 2.32                     | 0.45              |
| 1:B:180:LEU:CD2  | 1:B:180:LEU:C    | 2.89                     | 0.45              |
| 1:B:167:THR:HG1  | 1:B:169:TYR:HB2  | 1.81                     | 0.45              |
| 1:A:71:GLU:O     | 1:A:71:GLU:HG2   | 2.16                     | 0.45              |
| 1:B:70:ALA:HB2   | 1:B:100:VAL:HG22 | 1.99                     | 0.45              |
| 1:A:90:LEU:HA    | 1:A:93:LEU:HB2   | 1.98                     | 0.45              |
| 1:A:203:ASN:ND2  | 1:A:205:LYS:HB2  | 2.31                     | 0.45              |
| 1:A:88:LEU:HD23  | 1:A:93:LEU:CA    | 2.44                     | 0.44              |
| 1:A:5:LEU:CD1    | 1:A:27:GLU:HG3   | 2.48                     | 0.44              |
| 1:A:101:ARG:HH21 | 1:A:129:TYR:HB3  | 1.82                     | 0.44              |
| 1:A:66:PRO:C     | 1:A:68:GLU:N     | 2.74                     | 0.44              |
| 1:A:158:LEU:HD23 | 1:B:190:ILE:HG21 | 1.97                     | 0.44              |
| 1:A:215:GLN:NE2  | 1:A:251:VAL:CG1  | 2.80                     | 0.44              |
| 1:B:70:ALA:HB2   | 1:B:100:VAL:HA   | 1.99                     | 0.44              |
| 1:B:101:ARG:HH21 | 1:B:130:GLU:CB   | 2.26                     | 0.44              |
| 1:A:190:ILE:H    | 1:A:190:ILE:CD1  | 2.24                     | 0.44              |
| 1:B:73:LEU:O     | 1:B:107:TYR:OH   | 2.26                     | 0.44              |
| 1:B:177:LYS:HZ2  | 1:B:179:ARG:NH2  | 2.16                     | 0.44              |
| 1:B:218:VAL:O    | 1:B:222:MSE:HE2  | 2.17                     | 0.44              |
| 1:A:155:LEU:HD22 | 1:B:190:ILE:HG23 | 1.99                     | 0.44              |
| 1:B:6:ALA:C      | 1:B:8:SER:N      | 2.75                     | 0.44              |
| 1:B:11:GLU:C     | 1:B:13:LEU:N     | 2.73                     | 0.44              |
| 1:A:130:GLU:O    | 1:A:132:ASP:N    | 2.47                     | 0.44              |
| 1:A:177:LYS:NZ   | 1:A:179:ARG:NH2  | 2.64                     | 0.44              |
| 1:A:56:LYS:O     | 1:A:57:ALA:C     | 2.60                     | 0.44              |
| 1:A:203:ASN:CG   | 1:A:205:LYS:HB2  | 2.43                     | 0.44              |
| 1:A:12:ALA:HB1   | 1:A:21:LEU:HB2   | 1.98                     | 0.44              |
| 1:A:19:ARG:C     | 1:A:21:LEU:H     | 2.26                     | 0.44              |
| 1:B:225:TYR:N    | 1:B:225:TYR:HD1  | 2.13                     | 0.44              |
| 1:A:227:PHE:CD1  | 1:A:230:LEU:CD1  | 3.00                     | 0.44              |
| 1:A:130:GLU:CD   | 1:A:212:ASP:CA   | 2.86                     | 0.43              |
| 1:B:151:VAL:HG13 | 1:B:189:LEU:HD22 | 2.00                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:98:GLN:HE21 | 1:A:127:ALA:CB   | 2.30                     | 0.43              |
| 1:A:138:MSE:CE  | 1:A:211:THR:HG22 | 2.46                     | 0.43              |
| 1:B:62:SER:HA   | 1:B:69:GLN:HE22  | 1.83                     | 0.43              |
| 1:A:28:ILE:O    | 1:A:28:ILE:HG23  | 2.17                     | 0.43              |
| 1:A:146:ARG:HA  | 1:A:146:ARG:HD2  | 1.82                     | 0.43              |
| 1:B:37:TRP:HE1  | 1:B:45:ARG:NH1   | 2.16                     | 0.43              |
| 1:B:91:ASP:C    | 1:B:93:LEU:H     | 2.25                     | 0.43              |
| 1:A:193:ASP:CG  | 1:A:194:PRO:HD2  | 2.44                     | 0.43              |
| 1:B:177:LYS:NZ  | 1:B:179:ARG:NH2  | 2.66                     | 0.43              |
| 1:A:169:TYR:HB3 | 1:A:170:TYR:CD1  | 2.53                     | 0.43              |
| 1:A:215:GLN:NE2 | 1:A:251:VAL:HG11 | 2.33                     | 0.43              |
| 1:B:5:LEU:HD13  | 1:B:27:GLU:O     | 2.19                     | 0.43              |
| 1:B:69:GLN:O    | 1:B:73:LEU:HG    | 2.18                     | 0.43              |
| 1:B:58:ALA:C    | 1:B:60:VAL:N     | 2.77                     | 0.43              |
| 1:B:80:ARG:HD2  | 1:B:80:ARG:HA    | 1.81                     | 0.43              |
| 1:B:208:TYR:CG  | 1:B:209:VAL:N    | 2.80                     | 0.43              |
| 1:A:37:TRP:O    | 1:A:40:LEU:N     | 2.51                     | 0.43              |
| 1:A:180:LEU:CD2 | 1:A:182:GLY:H    | 2.31                     | 0.43              |
| 1:A:227:PHE:CD1 | 1:A:230:LEU:HD13 | 2.53                     | 0.43              |
| 1:B:53:PRO:HG2  | 1:B:56:LYS:HD2   | 1.99                     | 0.43              |
| 1:B:61:LEU:CD1  | 1:B:64:LEU:HD12  | 2.48                     | 0.43              |
| 1:A:37:TRP:CE2  | 1:A:45:ARG:HG2   | 2.53                     | 0.43              |
| 1:B:169:TYR:HB3 | 1:B:170:TYR:CD1  | 2.54                     | 0.43              |
| 1:A:9:LEU:C     | 1:A:11:GLU:N     | 2.77                     | 0.43              |
| 1:B:169:TYR:HB3 | 1:B:170:TYR:CE1  | 2.53                     | 0.43              |
| 1:A:5:LEU:HB3   | 1:A:24:VAL:CG1   | 2.49                     | 0.43              |
| 1:A:162:ALA:N   | 1:A:163:PRO:HD2  | 2.31                     | 0.43              |
| 1:B:5:LEU:CB    | 1:B:24:VAL:HG13  | 2.48                     | 0.43              |
| 1:B:9:LEU:C     | 1:B:11:GLU:N     | 2.76                     | 0.43              |
| 1:B:11:GLU:C    | 1:B:13:LEU:H     | 2.27                     | 0.43              |
| 1:A:19:ARG:HD2  | 1:A:20:ALA:HB2   | 2.01                     | 0.42              |
| 1:A:123:VAL:O   | 1:A:126:LEU:HB2  | 2.19                     | 0.42              |
| 1:A:45:ARG:HB2  | 1:A:72:TYR:OH    | 2.19                     | 0.42              |
| 1:A:187:ARG:NH2 | 1:B:167:THR:CA   | 2.79                     | 0.42              |
| 1:A:7:VAL:HG22  | 1:A:10:GLN:HE22  | 1.78                     | 0.42              |
| 1:B:19:ARG:C    | 1:B:21:LEU:H     | 2.27                     | 0.42              |
| 1:A:19:ARG:CD   | 1:A:20:ALA:H     | 2.31                     | 0.42              |
| 1:B:199:ALA:C   | 1:B:201:ILE:H    | 2.27                     | 0.42              |
| 1:A:90:LEU:O    | 1:A:93:LEU:HB2   | 2.20                     | 0.42              |
| 1:A:176:GLU:H   | 1:A:176:GLU:HG3  | 1.65                     | 0.42              |
| 1:A:180:LEU:C   | 1:A:180:LEU:CD2  | 2.93                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:5:LEU:HD11   | 1:A:27:GLU:OE1   | 2.19                     | 0.42              |
| 1:A:29:HIS:ND1   | 1:A:30:PRO:CD    | 2.81                     | 0.42              |
| 1:A:207:VAL:HG11 | 1:A:225:TYR:HE2  | 1.75                     | 0.42              |
| 1:B:56:LYS:O     | 1:B:57:ALA:C     | 2.61                     | 0.42              |
| 1:B:132:ASP:O    | 1:B:133:GLU:HB3  | 2.19                     | 0.42              |
| 1:A:58:ALA:C     | 1:A:60:VAL:N     | 2.75                     | 0.42              |
| 1:A:70:ALA:HB2   | 1:A:100:VAL:HA   | 2.02                     | 0.42              |
| 1:A:158:LEU:HA   | 1:A:158:LEU:HD12 | 1.84                     | 0.42              |
| 1:A:190:ILE:HG23 | 1:B:155:LEU:CD2  | 2.47                     | 0.42              |
| 1:B:21:LEU:O     | 1:B:25:LEU:HG    | 2.20                     | 0.42              |
| 1:B:130:GLU:HB3  | 1:B:133:GLU:OE1  | 2.20                     | 0.42              |
| 1:A:175:ASP:OD1  | 1:A:179:ARG:HG2  | 2.20                     | 0.42              |
| 1:B:169:TYR:HD2  | 1:B:169:TYR:HA   | 1.79                     | 0.42              |
| 1:B:222:MSE:CE   | 1:B:248:VAL:HG21 | 2.50                     | 0.42              |
| 1:A:147:GLU:HB3  | 1:A:173:VAL:HG11 | 2.02                     | 0.41              |
| 1:A:186:LEU:CD1  | 1:B:190:ILE:HD12 | 2.50                     | 0.41              |
| 1:B:7:VAL:HG22   | 1:B:10:GLN:NE2   | 2.35                     | 0.41              |
| 1:B:53:PRO:HG2   | 1:B:56:LYS:CD    | 2.50                     | 0.41              |
| 1:B:66:PRO:C     | 1:B:68:GLU:N     | 2.75                     | 0.41              |
| 1:A:101:ARG:HH22 | 1:A:129:TYR:H    | 1.67                     | 0.41              |
| 1:A:11:GLU:C     | 1:A:13:LEU:H     | 2.29                     | 0.41              |
| 1:A:199:ALA:C    | 1:A:201:ILE:H    | 2.28                     | 0.41              |
| 1:B:219:ALA:HA   | 1:B:248:VAL:HG11 | 2.02                     | 0.41              |
| 1:A:21:LEU:O     | 1:A:25:LEU:HG    | 2.19                     | 0.41              |
| 1:A:128:ARG:CZ   | 1:A:135:GLY:O    | 2.67                     | 0.41              |
| 1:B:10:GLN:O     | 1:B:14:GLN:NE2   | 2.53                     | 0.41              |
| 1:A:205:LYS:HE3  | 1:A:205:LYS:HB2  | 1.87                     | 0.41              |
| 1:B:37:TRP:O     | 1:B:40:LEU:N     | 2.50                     | 0.41              |
| 1:B:142:TYR:CB   | 1:B:242:ILE:HG21 | 2.48                     | 0.41              |
| 1:A:5:LEU:CA     | 1:A:8:SER:HB3    | 2.50                     | 0.41              |
| 1:A:90:LEU:O     | 1:A:93:LEU:HB3   | 2.21                     | 0.41              |
| 1:A:91:ASP:C     | 1:A:93:LEU:N     | 2.79                     | 0.41              |
| 1:A:142:TYR:CB   | 1:A:242:ILE:HG21 | 2.44                     | 0.41              |
| 1:A:208:TYR:HD2  | 1:A:209:VAL:H    | 1.68                     | 0.41              |
| 1:A:113:ASP:C    | 1:A:115:LEU:N    | 2.76                     | 0.41              |
| 1:B:28:ILE:HD12  | 1:B:28:ILE:HA    | 1.93                     | 0.41              |
| 1:B:47:VAL:O     | 1:B:47:VAL:HG12  | 2.21                     | 0.41              |
| 1:A:88:LEU:CD2   | 1:A:93:LEU:HA    | 2.47                     | 0.41              |
| 1:A:168:ILE:CD1  | 1:A:186:LEU:HD22 | 2.51                     | 0.41              |
| 1:A:207:VAL:HG23 | 1:A:230:LEU:HD11 | 2.03                     | 0.41              |
| 1:B:5:LEU:HB3    | 1:B:28:ILE:HD13  | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:179:ARG:HB2  | 1:B:237:GLY:O    | 2.21                     | 0.41              |
| 1:B:129:TYR:N    | 1:B:129:TYR:CD2  | 2.89                     | 0.41              |
| 1:A:80:ARG:HD2   | 1:A:80:ARG:HA    | 1.83                     | 0.40              |
| 1:B:218:VAL:O    | 1:B:218:VAL:CG1  | 2.69                     | 0.40              |
| 1:B:218:VAL:O    | 1:B:222:MSE:CB   | 2.69                     | 0.40              |
| 1:A:66:PRO:HG2   | 1:A:67:GLU:H     | 1.87                     | 0.40              |
| 1:B:90:LEU:O     | 1:B:94:ALA:N     | 2.54                     | 0.40              |
| 1:B:94:ALA:O     | 1:B:98:GLN:HG3   | 2.21                     | 0.40              |
| 1:B:203:ASN:OD1  | 1:B:205:LYS:N    | 2.40                     | 0.40              |
| 1:A:159:ARG:HG2  | 1:B:191:VAL:HA   | 2.03                     | 0.40              |
| 1:B:94:ALA:HB2   | 1:B:126:LEU:CD2  | 2.47                     | 0.40              |
| 1:B:218:VAL:O    | 1:B:222:MSE:HB3  | 2.21                     | 0.40              |
| 1:A:132:ASP:CG   | 1:A:215:GLN:HE22 | 2.23                     | 0.40              |
| 1:B:113:ASP:C    | 1:B:115:LEU:N    | 2.78                     | 0.40              |
| 1:B:208:TYR:O    | 1:B:209:VAL:HB   | 2.21                     | 0.40              |
| 1:B:90:LEU:O     | 1:B:93:LEU:CB    | 2.68                     | 0.40              |
| 1:B:101:ARG:NH1  | 1:B:128:ARG:HA   | 2.37                     | 0.40              |
| 1:B:172:TYR:CE2  | 1:B:231:PRO:CB   | 2.99                     | 0.40              |
| 1:B:207:VAL:CG2  | 1:B:227:PHE:CE1  | 3.00                     | 0.40              |
| 1:B:218:VAL:HG12 | 1:B:222:MSE:HE2  | 2.02                     | 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     | 246/278 (88%) | 182 (74%) | 43 (18%) | 21 (8%)  | 0           | 10 |
| 1   | B     | 246/278 (88%) | 185 (75%) | 41 (17%) | 20 (8%)  | 1           | 11 |
| All | All   | 492/556 (88%) | 367 (75%) | 84 (17%) | 41 (8%)  | 0           | 10 |

All (41) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 37  | TRP  |
| 1   | A     | 38  | ASP  |
| 1   | A     | 54  | LYS  |
| 1   | A     | 102 | LYS  |
| 1   | A     | 127 | ALA  |
| 1   | A     | 131 | GLU  |
| 1   | A     | 132 | ASP  |
| 1   | A     | 134 | ALA  |
| 1   | A     | 200 | GLU  |
| 1   | B     | 37  | TRP  |
| 1   | B     | 38  | ASP  |
| 1   | B     | 54  | LYS  |
| 1   | B     | 127 | ALA  |
| 1   | B     | 133 | GLU  |
| 1   | B     | 200 | GLU  |
| 1   | A     | 6   | ALA  |
| 1   | A     | 14  | GLN  |
| 1   | A     | 69  | GLN  |
| 1   | A     | 140 | PRO  |
| 1   | A     | 209 | VAL  |
| 1   | B     | 6   | ALA  |
| 1   | B     | 14  | GLN  |
| 1   | B     | 69  | GLN  |
| 1   | B     | 102 | LYS  |
| 1   | B     | 128 | ARG  |
| 1   | B     | 140 | PRO  |
| 1   | A     | 32  | ASP  |
| 1   | A     | 34  | LEU  |
| 1   | A     | 40  | LEU  |
| 1   | A     | 128 | ARG  |
| 1   | B     | 32  | ASP  |
| 1   | B     | 34  | LEU  |
| 1   | B     | 40  | LEU  |
| 1   | B     | 209 | VAL  |
| 1   | A     | 10  | GLN  |
| 1   | B     | 10  | GLN  |
| 1   | B     | 96  | ALA  |
| 1   | A     | 66  | PRO  |
| 1   | A     | 96  | ALA  |
| 1   | B     | 66  | PRO  |
| 1   | B     | 131 | GLU  |

### 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     | 215/235 (92%) | 196 (91%) | 19 (9%)  | 9           | 32 |
| 1   | B     | 215/235 (92%) | 194 (90%) | 21 (10%) | 7           | 28 |
| All | All   | 430/470 (92%) | 390 (91%) | 40 (9%)  | 8           | 30 |

All (40) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 19  | ARG  |
| 1   | A     | 31  | GLN  |
| 1   | A     | 33  | LEU  |
| 1   | A     | 36  | LEU  |
| 1   | A     | 45  | ARG  |
| 1   | A     | 67  | GLU  |
| 1   | A     | 89  | SER  |
| 1   | A     | 93  | LEU  |
| 1   | A     | 95  | ASP  |
| 1   | A     | 103 | GLU  |
| 1   | A     | 117 | PRO  |
| 1   | A     | 128 | ARG  |
| 1   | A     | 139 | THR  |
| 1   | A     | 146 | ARG  |
| 1   | A     | 158 | LEU  |
| 1   | A     | 196 | THR  |
| 1   | A     | 226 | ASP  |
| 1   | A     | 250 | ASP  |
| 1   | A     | 252 | LEU  |
| 1   | B     | 19  | ARG  |
| 1   | B     | 30  | PRO  |
| 1   | B     | 31  | GLN  |
| 1   | B     | 33  | LEU  |
| 1   | B     | 36  | LEU  |
| 1   | B     | 48  | VAL  |
| 1   | B     | 93  | LEU  |
| 1   | B     | 115 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 128 | ARG  |
| 1   | B     | 133 | GLU  |
| 1   | B     | 146 | ARG  |
| 1   | B     | 168 | ILE  |
| 1   | B     | 169 | TYR  |
| 1   | B     | 171 | ILE  |
| 1   | B     | 180 | LEU  |
| 1   | B     | 196 | THR  |
| 1   | B     | 198 | VAL  |
| 1   | B     | 202 | MSE  |
| 1   | B     | 216 | GLU  |
| 1   | B     | 226 | ASP  |
| 1   | B     | 252 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | GLN  |
| 1   | A     | 215 | GLN  |
| 1   | B     | 10  | GLN  |
| 1   | B     | 215 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 1   | A     | 244/278 (87%) | -0.37  | 5 (2%) 65 45  | 161, 228, 266, 287    | 0     |
| 1   | B     | 244/278 (87%) | -0.50  | 6 (2%) 58 41  | 162, 225, 261, 277    | 0     |
| All | All   | 488/556 (87%) | -0.44  | 11 (2%) 61 43 | 161, 226, 265, 287    | 0     |

All (11) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 50  | THR  | 4.5  |
| 1   | A     | 47  | VAL  | 3.5  |
| 1   | B     | 40  | LEU  | 3.3  |
| 1   | B     | 197 | ARG  | 2.5  |
| 1   | A     | 144 | ALA  | 2.2  |
| 1   | A     | 173 | VAL  | 2.2  |
| 1   | B     | 43  | GLU  | 2.2  |
| 1   | B     | 148 | GLY  | 2.2  |
| 1   | A     | 198 | VAL  | 2.1  |
| 1   | B     | 72  | TYR  | 2.1  |
| 1   | B     | 131 | GLU  | 2.1  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.