



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:47 PM UTC

PDB ID : 1QC9 / pdb\_00001qc9  
Title : THE CRYSTALLOGRAPHIC STRUCTURE OF RESTRICTION ENDONUCLEASE ECO RI AT 3.3 Å IN THE ABSENCE OF DNA  
Authors : Chandrasekhar, K.; Horvath, M.M.; Samudzi, C.; Choi, J.; Rosenberg, J.M.  
Deposited on : 1999-05-18  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

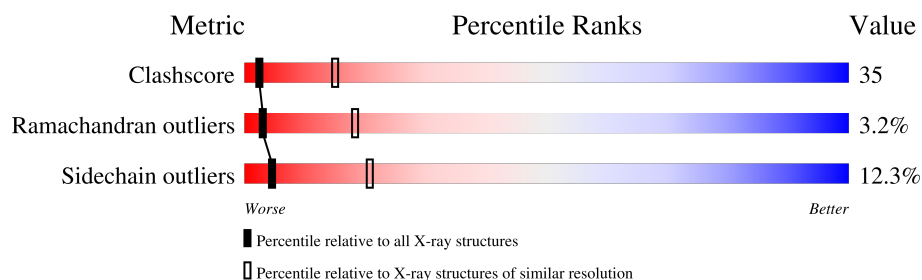
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 2977 (3.00-3.00)                                      |
| Ramachandran outliers | 187476                      | 2877 (3.00-3.00)                                      |
| Sidechain outliers    | 187428                      | 2880 (3.00-3.00)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 276    |                  |
| 1   | B     | 276    |                  |
| 1   | C     | 276    |                  |

## 2 Entry composition

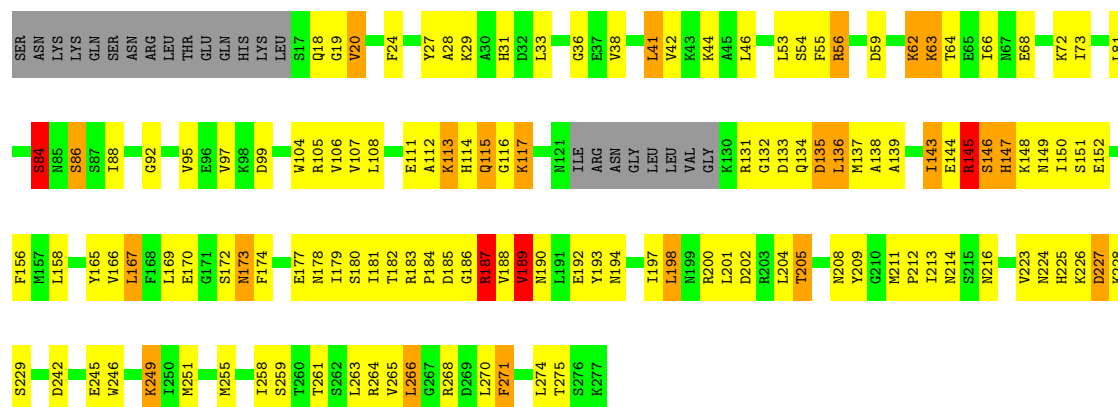
There is only 1 type of molecule in this entry. The entry contains 5979 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (ECO RI ENDONUCLEASE).

| Mol | Chain | Residues | Atoms         |           |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| 1   | A     | 253      | Total<br>1993 | C<br>1257 | N<br>344 | O<br>385 | S<br>7 | 0       | 0       | 0     |
| 1   | B     | 253      | Total<br>1993 | C<br>1257 | N<br>344 | O<br>385 | S<br>7 | 0       | 0       | 0     |
| 1   | C     | 253      | Total<br>1993 | C<br>1257 | N<br>344 | O<br>385 | S<br>7 | 0       | 0       | 0     |





## 4 Data and refinement statistics

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

| Property                                                 | Value                                          | Source    |
|----------------------------------------------------------|------------------------------------------------|-----------|
| Space group                                              | C 1 2 1                                        | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 208.68Å 127.35Å 49.87Å<br>90.00° 98.57° 90.00° | Depositor |
| Resolution (Å)                                           | 8.00 – 3.00                                    | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (8.00-3.00)                    | Depositor |
| $R_{merge}$                                              | (Not available)                                | Depositor |
| $R_{sym}$                                                | (Not available)                                | Depositor |
| Refinement program                                       | X-PLOR 3.1                                     | Depositor |
| R, $R_{free}$                                            | 0.251 , 0.295                                  | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtrriage  |
| Total number of atoms                                    | 5979                                           | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 30.0                                           | wwPDB-VP  |

## 5 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 1   | A     | 0.78         | 5/2025 (0.2%)  | 1.11        | 11/2724 (0.4%) |
| 1   | B     | 0.77         | 5/2025 (0.2%)  | 1.11        | 11/2724 (0.4%) |
| 1   | C     | 0.78         | 5/2025 (0.2%)  | 1.11        | 11/2724 (0.4%) |
| All | All   | 0.78         | 15/6075 (0.2%) | 1.11        | 33/8172 (0.4%) |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 145 | ARG  | C-N   | -8.88 | 1.21        | 1.33     |
| 1   | B     | 145 | ARG  | C-N   | -8.88 | 1.21        | 1.33     |
| 1   | C     | 145 | ARG  | C-N   | -8.87 | 1.21        | 1.33     |
| 1   | A     | 19  | GLY  | N-CA  | 7.67  | 1.50        | 1.45     |
| 1   | C     | 19  | GLY  | N-CA  | 7.63  | 1.50        | 1.45     |
| 1   | B     | 19  | GLY  | N-CA  | 7.62  | 1.50        | 1.45     |
| 1   | A     | 145 | ARG  | CA-C  | -7.43 | 1.42        | 1.52     |
| 1   | B     | 145 | ARG  | CA-C  | -7.41 | 1.42        | 1.52     |
| 1   | C     | 145 | ARG  | CA-C  | -7.40 | 1.42        | 1.52     |
| 1   | C     | 146 | SER  | N-CA  | -6.48 | 1.37        | 1.46     |
| 1   | A     | 19  | GLY  | CA-C  | 6.45  | 1.55        | 1.51     |
| 1   | C     | 19  | GLY  | CA-C  | 6.43  | 1.55        | 1.51     |
| 1   | B     | 146 | SER  | N-CA  | -6.41 | 1.38        | 1.46     |
| 1   | A     | 146 | SER  | N-CA  | -6.40 | 1.38        | 1.46     |
| 1   | B     | 19  | GLY  | CA-C  | 6.34  | 1.55        | 1.51     |

All (33) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | C     | 19  | GLY  | N-CA-C | 6.76 | 116.36      | 110.21   |
| 1   | A     | 19  | GLY  | N-CA-C | 6.76 | 116.36      | 110.21   |
| 1   | B     | 19  | GLY  | N-CA-C | 6.69 | 116.30      | 110.21   |
| 1   | A     | 246 | TRP  | N-CA-C | 6.33 | 119.39      | 109.96   |
| 1   | C     | 246 | TRP  | N-CA-C | 6.26 | 119.43      | 110.10   |
| 1   | B     | 246 | TRP  | N-CA-C | 6.23 | 119.38      | 110.10   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 145 | ARG  | N-CA-C    | 6.15  | 120.39      | 113.01   |
| 1   | B     | 145 | ARG  | N-CA-C    | 6.12  | 120.35      | 113.01   |
| 1   | C     | 145 | ARG  | N-CA-C    | 6.11  | 120.34      | 113.01   |
| 1   | B     | 59  | ASP  | N-CA-C    | 5.86  | 120.27      | 112.30   |
| 1   | A     | 59  | ASP  | N-CA-C    | 5.86  | 120.27      | 112.30   |
| 1   | C     | 242 | ASP  | N-CA-C    | -5.86 | 106.10      | 113.72   |
| 1   | B     | 242 | ASP  | N-CA-C    | -5.84 | 106.12      | 113.72   |
| 1   | A     | 242 | ASP  | N-CA-C    | -5.83 | 106.14      | 113.72   |
| 1   | C     | 59  | ASP  | N-CA-C    | 5.83  | 120.22      | 112.30   |
| 1   | C     | 205 | THR  | N-CA-C    | 5.69  | 118.22      | 111.33   |
| 1   | B     | 205 | THR  | N-CA-C    | 5.64  | 118.16      | 111.33   |
| 1   | A     | 205 | THR  | N-CA-C    | 5.63  | 118.14      | 111.33   |
| 1   | A     | 173 | ASN  | N-CA-C    | -5.47 | 107.86      | 114.75   |
| 1   | C     | 173 | ASN  | N-CA-C    | -5.45 | 107.88      | 114.75   |
| 1   | B     | 173 | ASN  | N-CA-C    | -5.45 | 107.89      | 114.75   |
| 1   | C     | 145 | ARG  | NE-CZ-NH2 | 5.40  | 124.06      | 119.20   |
| 1   | A     | 145 | ARG  | NE-CZ-NH2 | 5.39  | 124.05      | 119.20   |
| 1   | B     | 187 | ARG  | NE-CZ-NH2 | 5.39  | 124.05      | 119.20   |
| 1   | B     | 145 | ARG  | NE-CZ-NH2 | 5.34  | 124.01      | 119.20   |
| 1   | C     | 187 | ARG  | NE-CZ-NH2 | 5.33  | 123.99      | 119.20   |
| 1   | A     | 187 | ARG  | NE-CZ-NH2 | 5.30  | 123.97      | 119.20   |
| 1   | B     | 198 | LEU  | N-CA-C    | 5.28  | 121.53      | 113.61   |
| 1   | A     | 198 | LEU  | N-CA-C    | 5.27  | 121.51      | 113.61   |
| 1   | C     | 198 | LEU  | N-CA-C    | 5.26  | 121.50      | 113.61   |
| 1   | C     | 84  | SER  | N-CA-C    | 5.08  | 121.61      | 110.80   |
| 1   | B     | 84  | SER  | N-CA-C    | 5.07  | 121.60      | 110.80   |
| 1   | A     | 84  | SER  | N-CA-C    | 5.05  | 121.56      | 110.80   |

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     | 1993  | 0        | 1989     | 139     | 1            |
| 1   | B     | 1993  | 0        | 1989     | 140     | 5            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | C     | 1993  | 0        | 1989     | 138     | 5            |
| All | All   | 5979  | 0        | 5967     | 417     | 6            |

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 35.

All (417) 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:183:ARG:CD   | 1:A:187:ARG:HB2  | 1.92                     | 1.00              |
| 1:C:183:ARG:CD   | 1:C:187:ARG:HB2  | 1.92                     | 0.99              |
| 1:B:183:ARG:CD   | 1:B:187:ARG:HB2  | 1.92                     | 0.98              |
| 1:C:224:ASN:HD22 | 1:C:229:SER:HB3  | 1.30                     | 0.95              |
| 1:B:136:LEU:HD11 | 1:B:138:ALA:HB3  | 1.50                     | 0.94              |
| 1:C:185:ASP:HB3  | 1:C:187:ARG:NH2  | 1.84                     | 0.93              |
| 1:A:185:ASP:HB3  | 1:A:187:ARG:NH2  | 1.84                     | 0.93              |
| 1:A:224:ASN:HD22 | 1:A:229:SER:HB3  | 1.30                     | 0.93              |
| 1:B:224:ASN:HD22 | 1:B:229:SER:HB3  | 1.30                     | 0.92              |
| 1:A:136:LEU:HD11 | 1:A:138:ALA:HB3  | 1.50                     | 0.92              |
| 1:B:185:ASP:HB3  | 1:B:187:ARG:NH2  | 1.84                     | 0.92              |
| 1:C:136:LEU:HD11 | 1:C:138:ALA:HB3  | 1.50                     | 0.92              |
| 1:C:28:ALA:HA    | 1:C:33:LEU:HD12  | 1.54                     | 0.90              |
| 1:B:28:ALA:HA    | 1:B:33:LEU:HD12  | 1.53                     | 0.90              |
| 1:C:224:ASN:HA   | 1:C:228:LYS:O    | 1.72                     | 0.89              |
| 1:A:28:ALA:HA    | 1:A:33:LEU:HD12  | 1.54                     | 0.89              |
| 1:B:224:ASN:HA   | 1:B:228:LYS:O    | 1.72                     | 0.89              |
| 1:A:224:ASN:HA   | 1:A:228:LYS:O    | 1.72                     | 0.89              |
| 1:B:224:ASN:ND2  | 1:B:229:SER:HB3  | 1.87                     | 0.88              |
| 1:C:224:ASN:ND2  | 1:C:229:SER:HB3  | 1.87                     | 0.88              |
| 1:A:224:ASN:ND2  | 1:A:229:SER:HB3  | 1.87                     | 0.88              |
| 1:B:136:LEU:HD13 | 1:B:136:LEU:O    | 1.75                     | 0.87              |
| 1:C:97:VAL:HG11  | 1:C:263:LEU:HD21 | 1.56                     | 0.87              |
| 1:B:136:LEU:HD22 | 1:B:137:MET:N    | 1.91                     | 0.86              |
| 1:C:136:LEU:HD13 | 1:C:136:LEU:O    | 1.74                     | 0.86              |
| 1:C:136:LEU:HD22 | 1:C:137:MET:N    | 1.91                     | 0.85              |
| 1:A:97:VAL:HG11  | 1:A:263:LEU:HD21 | 1.56                     | 0.85              |
| 1:A:136:LEU:HD13 | 1:A:136:LEU:O    | 1.74                     | 0.85              |
| 1:B:136:LEU:HD21 | 1:B:138:ALA:HB2  | 1.58                     | 0.85              |
| 1:A:136:LEU:HD22 | 1:A:137:MET:N    | 1.91                     | 0.85              |
| 1:B:183:ARG:HD2  | 1:B:187:ARG:HB2  | 1.57                     | 0.85              |
| 1:B:97:VAL:HG11  | 1:B:263:LEU:HD21 | 1.56                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:183:ARG:HD2  | 1:C:187:ARG:HB2  | 1.57                     | 0.84              |
| 1:A:136:LEU:HD21 | 1:A:138:ALA:HB2  | 1.58                     | 0.84              |
| 1:A:183:ARG:HD2  | 1:A:187:ARG:HB2  | 1.57                     | 0.84              |
| 1:C:136:LEU:HD21 | 1:C:138:ALA:HB2  | 1.58                     | 0.84              |
| 1:C:145:ARG:C    | 1:C:147:HIS:H    | 1.89                     | 0.81              |
| 1:C:185:ASP:HB3  | 1:C:187:ARG:HH21 | 1.45                     | 0.81              |
| 1:B:145:ARG:C    | 1:B:147:HIS:H    | 1.89                     | 0.80              |
| 1:A:185:ASP:HB3  | 1:A:187:ARG:HH21 | 1.45                     | 0.79              |
| 1:A:145:ARG:C    | 1:A:147:HIS:H    | 1.89                     | 0.79              |
| 1:B:185:ASP:HB3  | 1:B:187:ARG:HH21 | 1.45                     | 0.79              |
| 1:A:139:ALA:HB1  | 1:A:200:ARG:NH2  | 1.98                     | 0.79              |
| 1:B:178:ASN:HD22 | 1:B:192:GLU:HA   | 1.47                     | 0.78              |
| 1:B:139:ALA:HB1  | 1:B:200:ARG:NH2  | 1.98                     | 0.78              |
| 1:A:178:ASN:HD22 | 1:A:192:GLU:HA   | 1.47                     | 0.78              |
| 1:C:178:ASN:HD22 | 1:C:192:GLU:HA   | 1.47                     | 0.77              |
| 1:C:139:ALA:HB1  | 1:C:200:ARG:NH2  | 1.99                     | 0.76              |
| 1:C:166:VAL:HG21 | 1:C:258:ILE:HG13 | 1.68                     | 0.76              |
| 1:A:166:VAL:HG21 | 1:A:258:ILE:HG13 | 1.68                     | 0.76              |
| 1:B:183:ARG:HB2  | 1:B:184:PRO:HD2  | 1.68                     | 0.75              |
| 1:A:183:ARG:HB2  | 1:A:184:PRO:HD2  | 1.68                     | 0.75              |
| 1:B:166:VAL:HG21 | 1:B:258:ILE:HG13 | 1.68                     | 0.74              |
| 1:C:178:ASN:ND2  | 1:C:192:GLU:HA   | 2.02                     | 0.74              |
| 1:A:178:ASN:ND2  | 1:A:192:GLU:HA   | 2.03                     | 0.74              |
| 1:A:224:ASN:CA   | 1:A:228:LYS:O    | 2.37                     | 0.73              |
| 1:B:178:ASN:ND2  | 1:B:192:GLU:HA   | 2.02                     | 0.73              |
| 1:C:183:ARG:HB2  | 1:C:184:PRO:HD2  | 1.68                     | 0.73              |
| 1:B:224:ASN:CA   | 1:B:228:LYS:O    | 2.37                     | 0.73              |
| 1:A:145:ARG:C    | 1:A:147:HIS:N    | 2.46                     | 0.72              |
| 1:C:145:ARG:C    | 1:C:147:HIS:N    | 2.46                     | 0.72              |
| 1:C:224:ASN:CA   | 1:C:228:LYS:O    | 2.37                     | 0.71              |
| 1:A:139:ALA:HB2  | 1:A:197:ILE:O    | 1.91                     | 0.71              |
| 1:C:131:ARG:HG3  | 1:C:135:ASP:HA   | 1.73                     | 0.70              |
| 1:B:148:LYS:HE3  | 1:B:149:ASN:OD1  | 1.92                     | 0.70              |
| 1:C:139:ALA:HB2  | 1:C:197:ILE:O    | 1.91                     | 0.70              |
| 1:C:148:LYS:HE3  | 1:C:149:ASN:OD1  | 1.92                     | 0.70              |
| 1:B:139:ALA:HB2  | 1:B:197:ILE:O    | 1.91                     | 0.70              |
| 1:A:131:ARG:HG3  | 1:A:135:ASP:HA   | 1.74                     | 0.70              |
| 1:B:131:ARG:HG3  | 1:B:135:ASP:HA   | 1.74                     | 0.70              |
| 1:A:148:LYS:HE3  | 1:A:149:ASN:OD1  | 1.92                     | 0.69              |
| 1:B:138:ALA:O    | 1:B:198:LEU:HD12 | 1.93                     | 0.69              |
| 1:C:138:ALA:O    | 1:C:198:LEU:HD12 | 1.93                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:138:ALA:O    | 1:A:198:LEU:HD12 | 1.93                     | 0.68              |
| 1:B:145:ARG:C    | 1:B:147:HIS:N    | 2.45                     | 0.68              |
| 1:A:182:THR:HA   | 1:A:188:VAL:HA   | 1.74                     | 0.68              |
| 1:C:182:THR:HA   | 1:C:188:VAL:HA   | 1.74                     | 0.68              |
| 1:B:182:THR:HA   | 1:B:188:VAL:HA   | 1.74                     | 0.68              |
| 1:A:183:ARG:HD2  | 1:A:187:ARG:CB   | 2.24                     | 0.67              |
| 1:B:183:ARG:NH1  | 1:B:185:ASP:H    | 1.92                     | 0.67              |
| 1:C:183:ARG:NH1  | 1:C:185:ASP:H    | 1.92                     | 0.67              |
| 1:A:183:ARG:HD3  | 1:A:187:ARG:HB2  | 1.76                     | 0.67              |
| 1:A:183:ARG:NH1  | 1:A:185:ASP:H    | 1.92                     | 0.67              |
| 1:C:183:ARG:HD2  | 1:C:187:ARG:CB   | 2.24                     | 0.67              |
| 1:B:183:ARG:HD2  | 1:B:187:ARG:CB   | 2.24                     | 0.67              |
| 1:B:183:ARG:HD3  | 1:B:187:ARG:HB2  | 1.76                     | 0.67              |
| 1:B:136:LEU:HD11 | 1:B:138:ALA:CB   | 2.24                     | 0.66              |
| 1:B:145:ARG:O    | 1:B:147:HIS:N    | 2.29                     | 0.66              |
| 1:C:145:ARG:O    | 1:C:147:HIS:N    | 2.29                     | 0.66              |
| 1:C:105:ARG:HG3  | 1:C:105:ARG:HH11 | 1.60                     | 0.66              |
| 1:A:105:ARG:HH11 | 1:A:105:ARG:HG3  | 1.60                     | 0.66              |
| 1:A:145:ARG:O    | 1:A:147:HIS:N    | 2.29                     | 0.65              |
| 1:C:227:ASP:O    | 1:C:227:ASP:OD2  | 2.14                     | 0.65              |
| 1:A:136:LEU:HD22 | 1:A:136:LEU:C    | 2.22                     | 0.65              |
| 1:C:136:LEU:HD11 | 1:C:138:ALA:CB   | 2.24                     | 0.65              |
| 1:B:105:ARG:HG3  | 1:B:105:ARG:HH11 | 1.60                     | 0.65              |
| 1:B:136:LEU:HD13 | 1:B:136:LEU:C    | 2.22                     | 0.65              |
| 1:A:136:LEU:HD13 | 1:A:136:LEU:C    | 2.22                     | 0.64              |
| 1:B:136:LEU:HD22 | 1:B:136:LEU:C    | 2.22                     | 0.64              |
| 1:C:183:ARG:HD3  | 1:C:187:ARG:HB2  | 1.76                     | 0.64              |
| 1:B:227:ASP:O    | 1:B:227:ASP:OD2  | 2.14                     | 0.64              |
| 1:C:136:LEU:HD13 | 1:C:136:LEU:C    | 2.22                     | 0.64              |
| 1:A:227:ASP:O    | 1:A:227:ASP:OD2  | 2.15                     | 0.64              |
| 1:C:136:LEU:HD22 | 1:C:136:LEU:C    | 2.22                     | 0.63              |
| 1:B:224:ASN:ND2  | 1:B:229:SER:CB   | 2.61                     | 0.63              |
| 1:C:36:GLY:HA2   | 1:C:92:GLY:HA2   | 1.80                     | 0.63              |
| 1:A:136:LEU:HD11 | 1:A:138:ALA:CB   | 2.24                     | 0.63              |
| 1:A:36:GLY:HA2   | 1:A:92:GLY:HA2   | 1.80                     | 0.63              |
| 1:A:224:ASN:ND2  | 1:A:229:SER:CB   | 2.61                     | 0.63              |
| 1:B:36:GLY:HA2   | 1:B:92:GLY:HA2   | 1.80                     | 0.63              |
| 1:B:224:ASN:CG   | 1:B:228:LYS:O    | 2.42                     | 0.62              |
| 1:A:224:ASN:HD22 | 1:A:229:SER:CB   | 2.08                     | 0.62              |
| 1:C:224:ASN:HD22 | 1:C:229:SER:CB   | 2.08                     | 0.62              |
| 1:C:224:ASN:CG   | 1:C:228:LYS:O    | 2.42                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:224:ASN:ND2  | 1:C:229:SER:CB   | 2.61                     | 0.61              |
| 1:C:173:ASN:HA   | 1:C:198:LEU:O    | 2.00                     | 0.61              |
| 1:A:224:ASN:CG   | 1:A:228:LYS:O    | 2.42                     | 0.61              |
| 1:C:143:ILE:HG21 | 1:C:174:PHE:HZ   | 1.65                     | 0.61              |
| 1:C:183:ARG:NH2  | 1:C:184:PRO:HG2  | 2.16                     | 0.61              |
| 1:A:173:ASN:HA   | 1:A:198:LEU:O    | 2.00                     | 0.61              |
| 1:A:183:ARG:NH2  | 1:A:184:PRO:HG2  | 2.16                     | 0.61              |
| 1:B:173:ASN:HA   | 1:B:198:LEU:O    | 2.00                     | 0.61              |
| 1:B:143:ILE:HG21 | 1:B:174:PHE:HZ   | 1.65                     | 0.61              |
| 1:B:211:MET:HB3  | 1:B:212:PRO:HD2  | 1.83                     | 0.61              |
| 1:C:211:MET:HB3  | 1:C:212:PRO:HD2  | 1.83                     | 0.61              |
| 1:C:224:ASN:CG   | 1:C:228:LYS:C    | 2.69                     | 0.61              |
| 1:A:211:MET:HB3  | 1:A:212:PRO:HD2  | 1.83                     | 0.60              |
| 1:B:224:ASN:CG   | 1:B:228:LYS:C    | 2.69                     | 0.60              |
| 1:A:224:ASN:CG   | 1:A:228:LYS:C    | 2.69                     | 0.60              |
| 1:A:46:LEU:HD21  | 1:A:259:SER:HB3  | 1.84                     | 0.60              |
| 1:A:97:VAL:HG13  | 1:A:107:VAL:HG21 | 1.84                     | 0.60              |
| 1:B:97:VAL:HG13  | 1:B:107:VAL:HG21 | 1.84                     | 0.60              |
| 1:B:108:LEU:HD21 | 1:B:255:MET:HB3  | 1.84                     | 0.60              |
| 1:B:261:THR:O    | 1:B:265:VAL:HG23 | 2.02                     | 0.60              |
| 1:B:183:ARG:NH2  | 1:B:184:PRO:HG2  | 2.16                     | 0.60              |
| 1:C:46:LEU:HD21  | 1:C:259:SER:HB3  | 1.84                     | 0.60              |
| 1:C:108:LEU:HD21 | 1:C:255:MET:HB3  | 1.84                     | 0.60              |
| 1:C:261:THR:O    | 1:C:265:VAL:HG23 | 2.02                     | 0.60              |
| 1:C:97:VAL:HG13  | 1:C:107:VAL:HG21 | 1.84                     | 0.60              |
| 1:A:131:ARG:CG   | 1:A:135:ASP:HA   | 2.32                     | 0.60              |
| 1:A:143:ILE:HG21 | 1:A:174:PHE:HZ   | 1.65                     | 0.59              |
| 1:B:131:ARG:CG   | 1:B:135:ASP:HA   | 2.32                     | 0.59              |
| 1:B:188:VAL:O    | 1:B:188:VAL:HG13 | 2.01                     | 0.59              |
| 1:C:188:VAL:HG13 | 1:C:188:VAL:O    | 2.01                     | 0.59              |
| 1:A:108:LEU:HD21 | 1:A:255:MET:HB3  | 1.84                     | 0.59              |
| 1:C:131:ARG:CG   | 1:C:135:ASP:HA   | 2.32                     | 0.59              |
| 1:A:105:ARG:HG3  | 1:A:105:ARG:NH1  | 2.17                     | 0.59              |
| 1:A:188:VAL:HG13 | 1:A:188:VAL:O    | 2.01                     | 0.59              |
| 1:B:46:LEU:HD21  | 1:B:259:SER:HB3  | 1.84                     | 0.59              |
| 1:B:105:ARG:HG3  | 1:B:105:ARG:NH1  | 2.17                     | 0.59              |
| 1:A:251:MET:HG2  | 1:A:255:MET:HE3  | 1.84                     | 0.59              |
| 1:C:188:VAL:O    | 1:C:188:VAL:HG22 | 2.02                     | 0.59              |
| 1:A:261:THR:O    | 1:A:265:VAL:HG23 | 2.02                     | 0.59              |
| 1:B:224:ASN:HD22 | 1:B:229:SER:CB   | 2.09                     | 0.59              |
| 1:B:188:VAL:O    | 1:B:188:VAL:HG22 | 2.02                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:251:MET:HG2  | 1:C:255:MET:HE3  | 1.85                     | 0.58              |
| 1:B:131:ARG:HG3  | 1:B:134:GLN:O    | 2.04                     | 0.58              |
| 1:A:188:VAL:O    | 1:A:188:VAL:HG22 | 2.02                     | 0.58              |
| 1:C:105:ARG:HG3  | 1:C:105:ARG:NH1  | 2.16                     | 0.58              |
| 1:C:138:ALA:HB1  | 1:C:197:ILE:HD11 | 1.85                     | 0.57              |
| 1:C:131:ARG:HG3  | 1:C:134:GLN:O    | 2.04                     | 0.57              |
| 1:C:114:HIS:HA   | 1:C:170:GLU:O    | 2.04                     | 0.57              |
| 1:B:138:ALA:HB1  | 1:B:197:ILE:HD11 | 1.85                     | 0.57              |
| 1:B:251:MET:HG2  | 1:B:255:MET:HE3  | 1.84                     | 0.57              |
| 1:A:131:ARG:HG3  | 1:A:134:GLN:O    | 2.04                     | 0.57              |
| 1:A:138:ALA:HB1  | 1:A:197:ILE:HD11 | 1.85                     | 0.57              |
| 1:A:27:TYR:O     | 1:A:31:HIS:HD2   | 1.88                     | 0.56              |
| 1:B:27:TYR:O     | 1:B:31:HIS:HD2   | 1.88                     | 0.56              |
| 1:A:114:HIS:HA   | 1:A:170:GLU:O    | 2.04                     | 0.56              |
| 1:B:117:LYS:O    | 1:B:117:LYS:HG2  | 2.05                     | 0.56              |
| 1:C:27:TYR:O     | 1:C:31:HIS:HD2   | 1.88                     | 0.56              |
| 1:A:117:LYS:O    | 1:A:117:LYS:HG2  | 2.05                     | 0.56              |
| 1:B:114:HIS:HA   | 1:B:170:GLU:O    | 2.04                     | 0.56              |
| 1:C:117:LYS:O    | 1:C:117:LYS:HG2  | 2.05                     | 0.56              |
| 1:C:115:GLN:OE1  | 1:C:143:ILE:HG13 | 2.06                     | 0.56              |
| 1:A:115:GLN:OE1  | 1:A:143:ILE:HG13 | 2.06                     | 0.56              |
| 1:B:201:LEU:HD21 | 1:B:213:ILE:CD1  | 2.36                     | 0.55              |
| 1:B:169:LEU:N    | 1:B:169:LEU:HD22 | 2.22                     | 0.55              |
| 1:C:201:LEU:HD21 | 1:C:213:ILE:CD1  | 2.36                     | 0.55              |
| 1:C:66:ILE:CD1   | 1:C:156:PHE:HB2  | 2.37                     | 0.55              |
| 1:A:66:ILE:CD1   | 1:A:156:PHE:HB2  | 2.37                     | 0.55              |
| 1:A:169:LEU:N    | 1:A:169:LEU:HD22 | 2.22                     | 0.55              |
| 1:A:201:LEU:HD21 | 1:A:213:ILE:CD1  | 2.36                     | 0.55              |
| 1:B:66:ILE:CD1   | 1:B:156:PHE:HB2  | 2.37                     | 0.55              |
| 1:C:73:ILE:CD1   | 1:C:158:LEU:HB3  | 2.37                     | 0.55              |
| 1:C:226:LYS:O    | 1:C:227:ASP:OD1  | 2.25                     | 0.55              |
| 1:C:169:LEU:N    | 1:C:169:LEU:HD22 | 2.22                     | 0.55              |
| 1:B:73:ILE:CD1   | 1:B:158:LEU:HB3  | 2.37                     | 0.54              |
| 1:B:115:GLN:OE1  | 1:B:143:ILE:HG13 | 2.06                     | 0.54              |
| 1:B:226:LYS:O    | 1:B:227:ASP:OD1  | 2.25                     | 0.54              |
| 1:C:20:VAL:HG12  | 1:C:24:PHE:CE1   | 2.43                     | 0.54              |
| 1:A:73:ILE:CD1   | 1:A:158:LEU:HB3  | 2.37                     | 0.54              |
| 1:B:223:VAL:HG12 | 1:B:224:ASN:N    | 2.22                     | 0.54              |
| 1:C:223:VAL:HG12 | 1:C:224:ASN:N    | 2.22                     | 0.54              |
| 1:A:20:VAL:HG12  | 1:A:24:PHE:CE1   | 2.43                     | 0.54              |
| 1:A:226:LYS:O    | 1:A:227:ASP:OD1  | 2.25                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:224:ASN:ND2  | 1:A:229:SER:CA   | 2.71                     | 0.53              |
| 1:C:224:ASN:ND2  | 1:C:229:SER:CA   | 2.71                     | 0.53              |
| 1:B:20:VAL:HG12  | 1:B:24:PHE:CE1   | 2.43                     | 0.53              |
| 1:B:185:ASP:CB   | 1:B:187:ARG:HH21 | 2.20                     | 0.53              |
| 1:C:185:ASP:CB   | 1:C:187:ARG:HH21 | 2.20                     | 0.53              |
| 1:B:183:ARG:N    | 1:B:187:ARG:O    | 2.42                     | 0.53              |
| 1:A:183:ARG:N    | 1:A:187:ARG:O    | 2.42                     | 0.53              |
| 1:C:166:VAL:CG2  | 1:C:258:ILE:HG13 | 2.38                     | 0.53              |
| 1:A:223:VAL:HG12 | 1:A:224:ASN:N    | 2.22                     | 0.53              |
| 1:C:183:ARG:N    | 1:C:187:ARG:O    | 2.42                     | 0.53              |
| 1:A:264:ARG:HB2  | 1:A:264:ARG:CZ   | 2.39                     | 0.53              |
| 1:B:225:HIS:N    | 1:B:228:LYS:O    | 2.42                     | 0.53              |
| 1:B:224:ASN:ND2  | 1:B:229:SER:CA   | 2.71                     | 0.53              |
| 1:C:225:HIS:N    | 1:C:228:LYS:O    | 2.42                     | 0.53              |
| 1:B:264:ARG:HB2  | 1:B:264:ARG:CZ   | 2.39                     | 0.52              |
| 1:A:225:HIS:N    | 1:A:228:LYS:O    | 2.42                     | 0.52              |
| 1:B:166:VAL:CG2  | 1:B:258:ILE:HG13 | 2.38                     | 0.52              |
| 1:A:266:LEU:O    | 1:A:270:LEU:HG   | 2.10                     | 0.51              |
| 1:B:266:LEU:O    | 1:B:270:LEU:HG   | 2.10                     | 0.51              |
| 1:C:266:LEU:O    | 1:C:270:LEU:HG   | 2.10                     | 0.51              |
| 1:A:183:ARG:HG2  | 1:A:187:ARG:N    | 2.26                     | 0.51              |
| 1:B:183:ARG:CB   | 1:B:184:PRO:HD2  | 2.40                     | 0.51              |
| 1:C:264:ARG:HB2  | 1:C:264:ARG:CZ   | 2.39                     | 0.51              |
| 1:C:183:ARG:HG2  | 1:C:187:ARG:N    | 2.26                     | 0.51              |
| 1:A:143:ILE:HG21 | 1:A:174:PHE:CZ   | 2.46                     | 0.51              |
| 1:B:183:ARG:HG2  | 1:B:187:ARG:N    | 2.26                     | 0.51              |
| 1:A:177:GLU:O    | 1:A:193:TYR:HB3  | 2.11                     | 0.51              |
| 1:B:138:ALA:O    | 1:B:198:LEU:CD1  | 2.59                     | 0.51              |
| 1:A:18:GLN:HG3   | 1:A:18:GLN:O     | 2.11                     | 0.50              |
| 1:C:41:LEU:O     | 1:C:44:LYS:HB2   | 2.12                     | 0.50              |
| 1:A:166:VAL:CG2  | 1:A:258:ILE:HG13 | 2.38                     | 0.50              |
| 1:A:41:LEU:O     | 1:A:44:LYS:HB2   | 2.12                     | 0.50              |
| 1:A:72:LYS:N     | 1:A:72:LYS:HD3   | 2.26                     | 0.50              |
| 1:A:183:ARG:CB   | 1:A:184:PRO:HD2  | 2.40                     | 0.50              |
| 1:B:41:LEU:O     | 1:B:44:LYS:HB2   | 2.12                     | 0.50              |
| 1:B:177:GLU:O    | 1:B:193:TYR:HB3  | 2.11                     | 0.50              |
| 1:A:185:ASP:CB   | 1:A:187:ARG:HH21 | 2.20                     | 0.50              |
| 1:A:131:ARG:HG3  | 1:A:135:ASP:CA   | 2.41                     | 0.50              |
| 1:B:143:ILE:HG21 | 1:B:174:PHE:CZ   | 2.46                     | 0.50              |
| 1:A:138:ALA:O    | 1:A:198:LEU:CD1  | 2.59                     | 0.50              |
| 1:C:72:LYS:HD3   | 1:C:72:LYS:N     | 2.26                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:38:VAL:O     | 1:B:42:VAL:HG23  | 2.12                     | 0.50              |
| 1:C:177:GLU:O    | 1:C:193:TYR:HB3  | 2.11                     | 0.50              |
| 1:B:18:GLN:O     | 1:B:18:GLN:HG3   | 2.11                     | 0.49              |
| 1:C:18:GLN:O     | 1:C:18:GLN:HG3   | 2.11                     | 0.49              |
| 1:C:38:VAL:O     | 1:C:42:VAL:HG23  | 2.12                     | 0.49              |
| 1:B:20:VAL:O     | 1:B:24:PHE:CD1   | 2.65                     | 0.49              |
| 1:C:20:VAL:O     | 1:C:24:PHE:CD1   | 2.65                     | 0.49              |
| 1:C:131:ARG:HG3  | 1:C:135:ASP:CA   | 2.41                     | 0.49              |
| 1:B:72:LYS:HD3   | 1:B:72:LYS:N     | 2.26                     | 0.49              |
| 1:A:20:VAL:O     | 1:A:24:PHE:CD1   | 2.65                     | 0.49              |
| 1:C:143:ILE:HG21 | 1:C:174:PHE:CZ   | 2.46                     | 0.49              |
| 1:A:20:VAL:HG12  | 1:A:24:PHE:CZ    | 2.48                     | 0.49              |
| 1:B:131:ARG:HG3  | 1:B:135:ASP:CA   | 2.41                     | 0.49              |
| 1:B:227:ASP:OD2  | 1:B:228:LYS:NZ   | 2.38                     | 0.49              |
| 1:B:55:PHE:HZ    | 1:B:263:LEU:HD11 | 1.78                     | 0.49              |
| 1:A:55:PHE:HZ    | 1:A:263:LEU:HD11 | 1.78                     | 0.48              |
| 1:A:131:ARG:CD   | 1:A:135:ASP:HA   | 2.43                     | 0.48              |
| 1:A:224:ASN:ND2  | 1:A:229:SER:N    | 2.62                     | 0.48              |
| 1:C:55:PHE:HZ    | 1:C:263:LEU:HD11 | 1.78                     | 0.48              |
| 1:A:38:VAL:O     | 1:A:42:VAL:HG23  | 2.12                     | 0.48              |
| 1:B:131:ARG:CD   | 1:B:135:ASP:HA   | 2.43                     | 0.48              |
| 1:C:224:ASN:ND2  | 1:C:229:SER:N    | 2.62                     | 0.48              |
| 1:A:188:VAL:O    | 1:A:189:VAL:C    | 2.57                     | 0.48              |
| 1:B:81:LEU:CD2   | 1:B:84:SER:HA    | 2.43                     | 0.48              |
| 1:C:81:LEU:CD2   | 1:C:84:SER:HA    | 2.43                     | 0.48              |
| 1:A:169:LEU:HD12 | 1:A:174:PHE:CZ   | 2.49                     | 0.48              |
| 1:B:169:LEU:HD12 | 1:B:174:PHE:CZ   | 2.49                     | 0.48              |
| 1:C:138:ALA:O    | 1:C:198:LEU:CD1  | 2.59                     | 0.48              |
| 1:C:20:VAL:HG12  | 1:C:24:PHE:CZ    | 2.48                     | 0.48              |
| 1:B:20:VAL:HG12  | 1:B:24:PHE:CZ    | 2.48                     | 0.48              |
| 1:B:188:VAL:O    | 1:B:189:VAL:C    | 2.57                     | 0.48              |
| 1:C:131:ARG:CD   | 1:C:135:ASP:HA   | 2.43                     | 0.48              |
| 1:A:81:LEU:CD2   | 1:A:84:SER:HA    | 2.44                     | 0.47              |
| 1:B:224:ASN:ND2  | 1:B:229:SER:N    | 2.62                     | 0.47              |
| 1:C:169:LEU:HD12 | 1:C:174:PHE:CZ   | 2.49                     | 0.47              |
| 1:B:208:ASN:O    | 1:B:211:MET:HG3  | 2.14                     | 0.47              |
| 1:C:188:VAL:O    | 1:C:189:VAL:C    | 2.57                     | 0.47              |
| 1:C:208:ASN:O    | 1:C:211:MET:HG3  | 2.14                     | 0.47              |
| 1:C:116:GLY:HA3  | 1:C:172:SER:H    | 1.79                     | 0.47              |
| 1:A:116:GLY:HA3  | 1:A:172:SER:H    | 1.79                     | 0.47              |
| 1:A:208:ASN:O    | 1:A:211:MET:HG3  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:66:ILE:HD12  | 1:B:156:PHE:HB2 | 1.97                     | 0.46              |
| 1:B:116:GLY:HA3  | 1:B:172:SER:H   | 1.79                     | 0.46              |
| 1:A:193:TYR:CE1  | 1:A:194:ASN:HB3 | 2.51                     | 0.46              |
| 1:A:268:ARG:NH1  | 1:A:268:ARG:HB3 | 2.31                     | 0.46              |
| 1:B:268:ARG:HB3  | 1:B:268:ARG:NH1 | 2.31                     | 0.46              |
| 1:A:139:ALA:CB   | 1:A:200:ARG:NH2 | 2.76                     | 0.46              |
| 1:C:193:TYR:CE1  | 1:C:194:ASN:HB3 | 2.51                     | 0.46              |
| 1:C:150:ILE:HG12 | 1:C:165:TYR:CE1 | 2.51                     | 0.46              |
| 1:B:150:ILE:HG12 | 1:B:165:TYR:CE1 | 2.51                     | 0.46              |
| 1:A:227:ASP:OD2  | 1:A:228:LYS:NZ  | 2.38                     | 0.45              |
| 1:A:263:LEU:HD23 | 1:A:263:LEU:HA  | 1.82                     | 0.45              |
| 1:B:193:TYR:CE1  | 1:B:194:ASN:HB3 | 2.51                     | 0.45              |
| 1:A:150:ILE:HG12 | 1:A:165:TYR:CE1 | 2.51                     | 0.45              |
| 1:C:268:ARG:HB3  | 1:C:268:ARG:NH1 | 2.31                     | 0.45              |
| 1:A:66:ILE:HD12  | 1:A:156:PHE:HB2 | 1.98                     | 0.45              |
| 1:C:112:ALA:C    | 1:C:113:LYS:HD2 | 2.41                     | 0.45              |
| 1:C:183:ARG:CB   | 1:C:184:PRO:HD2 | 2.40                     | 0.45              |
| 1:A:181:ILE:HD12 | 1:A:182:THR:H   | 1.81                     | 0.45              |
| 1:B:112:ALA:C    | 1:B:113:LYS:HD2 | 2.41                     | 0.45              |
| 1:A:88:ILE:HD12  | 1:A:152:GLU:HG3 | 1.98                     | 0.45              |
| 1:C:66:ILE:HD12  | 1:C:156:PHE:HB2 | 1.97                     | 0.45              |
| 1:C:181:ILE:HD12 | 1:C:182:THR:H   | 1.82                     | 0.45              |
| 1:A:112:ALA:C    | 1:A:113:LYS:HD2 | 2.41                     | 0.45              |
| 1:A:200:ARG:HA   | 1:A:200:ARG:HD3 | 1.84                     | 0.45              |
| 1:B:116:GLY:O    | 1:B:117:LYS:HB3 | 2.17                     | 0.45              |
| 1:B:46:LEU:CD1   | 1:B:95:VAL:HG11 | 2.48                     | 0.44              |
| 1:B:88:ILE:HD12  | 1:B:152:GLU:HG3 | 1.99                     | 0.44              |
| 1:C:116:GLY:O    | 1:C:117:LYS:HB3 | 2.17                     | 0.44              |
| 1:A:111:GLU:O    | 1:A:167:LEU:HA  | 2.17                     | 0.44              |
| 1:A:183:ARG:CG   | 1:A:187:ARG:HB2 | 2.47                     | 0.44              |
| 1:C:223:VAL:CG1  | 1:C:224:ASN:N   | 2.80                     | 0.44              |
| 1:A:223:VAL:CG1  | 1:A:224:ASN:N   | 2.80                     | 0.44              |
| 1:A:116:GLY:O    | 1:A:117:LYS:HB3 | 2.17                     | 0.44              |
| 1:B:139:ALA:CB   | 1:B:200:ARG:NH2 | 2.76                     | 0.44              |
| 1:C:46:LEU:CD1   | 1:C:95:VAL:HG11 | 2.47                     | 0.44              |
| 1:B:181:ILE:HD12 | 1:B:182:THR:H   | 1.81                     | 0.44              |
| 1:A:46:LEU:CD1   | 1:A:95:VAL:HG11 | 2.48                     | 0.44              |
| 1:B:111:GLU:O    | 1:B:167:LEU:HA  | 2.17                     | 0.44              |
| 1:B:223:VAL:CG1  | 1:B:224:ASN:N   | 2.80                     | 0.44              |
| 1:B:116:GLY:HA2  | 1:B:173:ASN:OD1 | 2.17                     | 0.44              |
| 1:C:28:ALA:HA    | 1:C:33:LEU:CD1  | 2.37                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:88:ILE:HD12  | 1:C:152:GLU:HG3  | 1.99                     | 0.44              |
| 1:A:131:ARG:NH2  | 1:A:134:GLN:HA   | 2.33                     | 0.44              |
| 1:A:227:ASP:O    | 1:A:227:ASP:CG   | 2.61                     | 0.44              |
| 1:B:131:ARG:NH2  | 1:B:134:GLN:HA   | 2.33                     | 0.44              |
| 1:C:116:GLY:HA2  | 1:C:173:ASN:OD1  | 2.17                     | 0.44              |
| 1:B:99:ASP:HB3   | 1:B:105:ARG:HH11 | 1.83                     | 0.43              |
| 1:C:111:GLU:O    | 1:C:167:LEU:HA   | 2.17                     | 0.43              |
| 1:C:169:LEU:HD12 | 1:C:174:PHE:CE1  | 2.53                     | 0.43              |
| 1:C:224:ASN:OD1  | 1:C:228:LYS:O    | 2.37                     | 0.43              |
| 1:A:271:PHE:O    | 1:A:274:LEU:HB2  | 2.18                     | 0.43              |
| 1:B:81:LEU:HD22  | 1:B:84:SER:HA    | 2.00                     | 0.43              |
| 1:C:131:ARG:NH2  | 1:C:134:GLN:HA   | 2.33                     | 0.43              |
| 1:B:169:LEU:HD12 | 1:B:174:PHE:CE1  | 2.53                     | 0.43              |
| 1:B:181:ILE:HG13 | 1:B:182:THR:O    | 2.18                     | 0.43              |
| 1:B:224:ASN:OD1  | 1:B:228:LYS:O    | 2.37                     | 0.43              |
| 1:A:99:ASP:HB3   | 1:A:105:ARG:HH11 | 1.83                     | 0.43              |
| 1:C:227:ASP:O    | 1:C:227:ASP:CG   | 2.61                     | 0.43              |
| 1:A:116:GLY:HA2  | 1:A:173:ASN:OD1  | 2.17                     | 0.43              |
| 1:B:263:LEU:HD23 | 1:B:263:LEU:HA   | 1.82                     | 0.43              |
| 1:B:132:GLY:C    | 1:B:134:GLN:N    | 2.76                     | 0.43              |
| 1:B:271:PHE:O    | 1:B:274:LEU:HB2  | 2.18                     | 0.43              |
| 1:C:56:ARG:HB3   | 1:C:104:TRP:CZ3  | 2.54                     | 0.43              |
| 1:C:200:ARG:HD3  | 1:C:200:ARG:HA   | 1.84                     | 0.43              |
| 1:C:81:LEU:HD22  | 1:C:84:SER:HA    | 2.00                     | 0.42              |
| 1:A:169:LEU:HD12 | 1:A:174:PHE:CE1  | 2.53                     | 0.42              |
| 1:B:68:GLU:O     | 1:B:72:LYS:HD3   | 2.19                     | 0.42              |
| 1:C:181:ILE:HG13 | 1:C:182:THR:O    | 2.18                     | 0.42              |
| 1:A:180:SER:OG   | 1:A:190:ASN:HA   | 2.20                     | 0.42              |
| 1:A:181:ILE:HG13 | 1:A:182:THR:O    | 2.18                     | 0.42              |
| 1:C:131:ARG:NH1  | 1:C:132:GLY:O    | 2.53                     | 0.42              |
| 1:C:193:TYR:CD1  | 1:C:193:TYR:C    | 2.97                     | 0.42              |
| 1:C:271:PHE:O    | 1:C:274:LEU:HB2  | 2.18                     | 0.42              |
| 1:A:68:GLU:O     | 1:A:72:LYS:HD3   | 2.19                     | 0.42              |
| 1:C:68:GLU:O     | 1:C:72:LYS:HD3   | 2.19                     | 0.42              |
| 1:C:216:ASN:OD1  | 1:C:258:ILE:HD13 | 2.20                     | 0.42              |
| 1:A:62:LYS:C     | 1:A:64:THR:N     | 2.77                     | 0.42              |
| 1:B:29:LYS:HB2   | 1:B:249:LYS:HB2  | 2.02                     | 0.42              |
| 1:B:105:ARG:HH11 | 1:B:105:ARG:CG   | 2.31                     | 0.42              |
| 1:B:131:ARG:NH1  | 1:B:132:GLY:O    | 2.53                     | 0.42              |
| 1:B:200:ARG:HD3  | 1:B:200:ARG:HA   | 1.84                     | 0.42              |
| 1:C:99:ASP:HB3   | 1:C:105:ARG:HH11 | 1.83                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:33:LEU:HA    | 1:A:33:LEU:HD23  | 1.87                     | 0.42              |
| 1:A:216:ASN:OD1  | 1:A:258:ILE:HD13 | 2.20                     | 0.42              |
| 1:B:180:SER:OG   | 1:B:190:ASN:HA   | 2.20                     | 0.42              |
| 1:A:81:LEU:HD22  | 1:A:84:SER:HA    | 2.00                     | 0.42              |
| 1:A:131:ARG:NH1  | 1:A:132:GLY:O    | 2.53                     | 0.42              |
| 1:B:63:LYS:HB2   | 1:B:86:SER:O     | 2.20                     | 0.42              |
| 1:A:56:ARG:HB3   | 1:A:104:TRP:CZ3  | 2.54                     | 0.42              |
| 1:A:136:LEU:C    | 1:A:136:LEU:CD2  | 2.89                     | 0.42              |
| 1:B:56:ARG:HB3   | 1:B:104:TRP:CZ3  | 2.54                     | 0.42              |
| 1:B:113:LYS:HD2  | 1:B:113:LYS:N    | 2.35                     | 0.42              |
| 1:B:193:TYR:CD1  | 1:B:193:TYR:C    | 2.97                     | 0.42              |
| 1:C:63:LYS:HB2   | 1:C:86:SER:O     | 2.20                     | 0.42              |
| 1:A:132:GLY:C    | 1:A:134:GLN:N    | 2.76                     | 0.42              |
| 1:C:136:LEU:HD22 | 1:C:137:MET:C    | 2.45                     | 0.42              |
| 1:C:136:LEU:C    | 1:C:136:LEU:CD1  | 2.89                     | 0.42              |
| 1:A:224:ASN:OD1  | 1:A:228:LYS:O    | 2.37                     | 0.41              |
| 1:B:227:ASP:O    | 1:B:227:ASP:CG   | 2.61                     | 0.41              |
| 1:C:180:SER:OG   | 1:C:190:ASN:HA   | 2.20                     | 0.41              |
| 1:A:136:LEU:HD22 | 1:A:137:MET:C    | 2.45                     | 0.41              |
| 1:A:193:TYR:CD1  | 1:A:193:TYR:C    | 2.97                     | 0.41              |
| 1:C:139:ALA:CB   | 1:C:200:ARG:NH2  | 2.76                     | 0.41              |
| 1:A:224:ASN:OD1  | 1:A:228:LYS:C    | 2.64                     | 0.41              |
| 1:C:113:LYS:HD2  | 1:C:113:LYS:N    | 2.35                     | 0.41              |
| 1:C:224:ASN:OD1  | 1:C:228:LYS:C    | 2.64                     | 0.41              |
| 1:A:29:LYS:HB2   | 1:A:249:LYS:HB2  | 2.02                     | 0.41              |
| 1:A:63:LYS:HB2   | 1:A:86:SER:O     | 2.20                     | 0.41              |
| 1:A:136:LEU:C    | 1:A:136:LEU:CD1  | 2.89                     | 0.41              |
| 1:C:66:ILE:HD13  | 1:C:156:PHE:HB2  | 2.03                     | 0.41              |
| 1:C:263:LEU:HA   | 1:C:263:LEU:HD23 | 1.82                     | 0.41              |
| 1:A:223:VAL:O    | 1:A:229:SER:HA   | 2.21                     | 0.41              |
| 1:C:223:VAL:O    | 1:C:229:SER:HA   | 2.21                     | 0.41              |
| 1:B:223:VAL:O    | 1:B:229:SER:HA   | 2.21                     | 0.41              |
| 1:B:46:LEU:HD22  | 1:B:55:PHE:CE1   | 2.56                     | 0.41              |
| 1:C:172:SER:O    | 1:C:198:LEU:HG   | 2.21                     | 0.41              |
| 1:C:183:ARG:CG   | 1:C:187:ARG:HB2  | 2.47                     | 0.41              |
| 1:B:136:LEU:HD22 | 1:B:137:MET:C    | 2.45                     | 0.41              |
| 1:B:150:ILE:O    | 1:B:151:SER:C    | 2.64                     | 0.41              |
| 1:C:150:ILE:O    | 1:C:151:SER:C    | 2.64                     | 0.41              |
| 1:A:113:LYS:HD2  | 1:A:113:LYS:N    | 2.35                     | 0.41              |
| 1:B:183:ARG:CG   | 1:B:187:ARG:HB2  | 2.47                     | 0.41              |
| 1:B:224:ASN:OD1  | 1:B:228:LYS:C    | 2.64                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:29:LYS:HB2   | 1:C:249:LYS:HB2  | 2.02                     | 0.41              |
| 1:A:28:ALA:HA    | 1:A:33:LEU:CD1   | 2.37                     | 0.41              |
| 1:B:66:ILE:HD13  | 1:B:156:PHE:HB2  | 2.03                     | 0.41              |
| 1:A:46:LEU:HD22  | 1:A:55:PHE:CE1   | 2.56                     | 0.40              |
| 1:B:62:LYS:C     | 1:B:64:THR:N     | 2.77                     | 0.40              |
| 1:B:172:SER:O    | 1:B:198:LEU:HG   | 2.21                     | 0.40              |
| 1:B:216:ASN:OD1  | 1:B:258:ILE:HD13 | 2.20                     | 0.40              |
| 1:C:62:LYS:C     | 1:C:64:THR:N     | 2.77                     | 0.40              |
| 1:C:213:ILE:HG22 | 1:C:214:ASN:ND2  | 2.36                     | 0.40              |
| 1:A:208:ASN:O    | 1:A:209:TYR:HB2  | 2.22                     | 0.40              |
| 1:B:136:LEU:C    | 1:B:136:LEU:CD1  | 2.89                     | 0.40              |
| 1:C:208:ASN:O    | 1:C:209:TYR:HB2  | 2.22                     | 0.40              |
| 1:A:213:ILE:HG22 | 1:A:214:ASN:ND2  | 2.36                     | 0.40              |
| 1:B:73:ILE:HD13  | 1:B:158:LEU:HB3  | 2.04                     | 0.40              |
| 1:B:213:ILE:HG22 | 1:B:214:ASN:ND2  | 2.36                     | 0.40              |
| 1:C:46:LEU:HD22  | 1:C:55:PHE:CE1   | 2.56                     | 0.40              |

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:B:147:HIS:CB | 1:C:144:GLU:O[2_555]   | 1.96                     | 0.24              |
| 1:A:144:GLU:O  | 1:A:147:HIS:CB[2_555]  | 2.02                     | 0.18              |
| 1:B:27:TYR:CD2 | 1:C:271:PHE:CE1[3_444] | 2.02                     | 0.18              |
| 1:B:27:TYR:CG  | 1:C:271:PHE:CE1[3_444] | 2.12                     | 0.08              |
| 1:B:27:TYR:CD2 | 1:C:271:PHE:CD1[3_444] | 2.13                     | 0.07              |
| 1:B:144:GLU:O  | 1:C:147:HIS:CB[2_555]  | 2.16                     | 0.04              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | A     | 249/276 (90%) | 209 (84%) | 32 (13%) | 8 (3%)   | 3           | 18 |
| 1   | B     | 249/276 (90%) | 209 (84%) | 32 (13%) | 8 (3%)   | 3           | 18 |
| 1   | C     | 249/276 (90%) | 209 (84%) | 32 (13%) | 8 (3%)   | 3           | 18 |
| All | All   | 747/828 (90%) | 627 (84%) | 96 (13%) | 24 (3%)  | 3           | 18 |

All (24) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 84  | SER  |
| 1   | B     | 84  | SER  |
| 1   | C     | 84  | SER  |
| 1   | A     | 135 | ASP  |
| 1   | A     | 146 | SER  |
| 1   | A     | 271 | PHE  |
| 1   | B     | 135 | ASP  |
| 1   | B     | 146 | SER  |
| 1   | B     | 271 | PHE  |
| 1   | C     | 135 | ASP  |
| 1   | C     | 146 | SER  |
| 1   | C     | 271 | PHE  |
| 1   | A     | 63  | LYS  |
| 1   | A     | 189 | VAL  |
| 1   | B     | 63  | LYS  |
| 1   | B     | 189 | VAL  |
| 1   | C     | 63  | LYS  |
| 1   | C     | 189 | VAL  |
| 1   | A     | 117 | LYS  |
| 1   | B     | 117 | LYS  |
| 1   | C     | 117 | LYS  |
| 1   | A     | 186 | GLY  |
| 1   | B     | 186 | GLY  |
| 1   | C     | 186 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 219/240 (91%) | 192 (88%) | 27 (12%) | 4           | 21 |
| 1   | B     | 219/240 (91%) | 192 (88%) | 27 (12%) | 4           | 21 |
| 1   | C     | 219/240 (91%) | 192 (88%) | 27 (12%) | 4           | 21 |
| All | All   | 657/720 (91%) | 576 (88%) | 81 (12%) | 4           | 21 |

All (81) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 20  | VAL  |
| 1   | A     | 41  | LEU  |
| 1   | A     | 53  | LEU  |
| 1   | A     | 54  | SER  |
| 1   | A     | 56  | ARG  |
| 1   | A     | 62  | LYS  |
| 1   | A     | 86  | SER  |
| 1   | A     | 106 | VAL  |
| 1   | A     | 113 | LYS  |
| 1   | A     | 115 | GLN  |
| 1   | A     | 133 | ASP  |
| 1   | A     | 136 | LEU  |
| 1   | A     | 143 | ILE  |
| 1   | A     | 145 | ARG  |
| 1   | A     | 147 | HIS  |
| 1   | A     | 167 | LEU  |
| 1   | A     | 179 | ILE  |
| 1   | A     | 187 | ARG  |
| 1   | A     | 189 | VAL  |
| 1   | A     | 202 | ASP  |
| 1   | A     | 204 | LEU  |
| 1   | A     | 205 | THR  |
| 1   | A     | 227 | ASP  |
| 1   | A     | 245 | GLU  |
| 1   | A     | 249 | LYS  |
| 1   | A     | 266 | LEU  |
| 1   | A     | 275 | THR  |
| 1   | B     | 20  | VAL  |
| 1   | B     | 41  | LEU  |
| 1   | B     | 53  | LEU  |
| 1   | B     | 54  | SER  |
| 1   | B     | 56  | ARG  |
| 1   | B     | 62  | LYS  |
| 1   | B     | 86  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 106 | VAL  |
| 1   | B     | 113 | LYS  |
| 1   | B     | 115 | GLN  |
| 1   | B     | 133 | ASP  |
| 1   | B     | 136 | LEU  |
| 1   | B     | 143 | ILE  |
| 1   | B     | 145 | ARG  |
| 1   | B     | 147 | HIS  |
| 1   | B     | 167 | LEU  |
| 1   | B     | 179 | ILE  |
| 1   | B     | 187 | ARG  |
| 1   | B     | 189 | VAL  |
| 1   | B     | 202 | ASP  |
| 1   | B     | 204 | LEU  |
| 1   | B     | 205 | THR  |
| 1   | B     | 227 | ASP  |
| 1   | B     | 245 | GLU  |
| 1   | B     | 249 | LYS  |
| 1   | B     | 266 | LEU  |
| 1   | B     | 275 | THR  |
| 1   | C     | 20  | VAL  |
| 1   | C     | 41  | LEU  |
| 1   | C     | 53  | LEU  |
| 1   | C     | 54  | SER  |
| 1   | C     | 56  | ARG  |
| 1   | C     | 62  | LYS  |
| 1   | C     | 86  | SER  |
| 1   | C     | 106 | VAL  |
| 1   | C     | 113 | LYS  |
| 1   | C     | 115 | GLN  |
| 1   | C     | 133 | ASP  |
| 1   | C     | 136 | LEU  |
| 1   | C     | 143 | ILE  |
| 1   | C     | 145 | ARG  |
| 1   | C     | 147 | HIS  |
| 1   | C     | 167 | LEU  |
| 1   | C     | 179 | ILE  |
| 1   | C     | 187 | ARG  |
| 1   | C     | 189 | VAL  |
| 1   | C     | 202 | ASP  |
| 1   | C     | 204 | LEU  |
| 1   | C     | 205 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 227 | ASP  |
| 1   | C     | 245 | GLU  |
| 1   | C     | 249 | LYS  |
| 1   | C     | 266 | LEU  |
| 1   | C     | 275 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 31  | HIS  |
| 1   | A     | 48  | ASN  |
| 1   | A     | 147 | HIS  |
| 1   | A     | 190 | ASN  |
| 1   | A     | 224 | ASN  |
| 1   | A     | 273 | GLN  |
| 1   | B     | 31  | HIS  |
| 1   | B     | 48  | ASN  |
| 1   | B     | 190 | ASN  |
| 1   | B     | 224 | ASN  |
| 1   | B     | 273 | GLN  |
| 1   | C     | 31  | HIS  |
| 1   | C     | 48  | ASN  |
| 1   | C     | 147 | HIS  |
| 1   | C     | 190 | ASN  |
| 1   | C     | 220 | ASN  |
| 1   | C     | 224 | ASN  |
| 1   | C     | 273 | 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

There are no ligands in this entry.

## 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.