



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:33 PM UTC

PDB ID : 1HVU / pdb\_00001hvu  
Title : HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE COMPLEXED WITH A 33-BASE NUCLEOTIDE RNA PSEUDO-KNOT  
Authors : Jaeger, J.; Restle, T.; Steitz, T.A.  
Deposited on : 1998-06-30  
Resolution : 4.75 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                                                             |

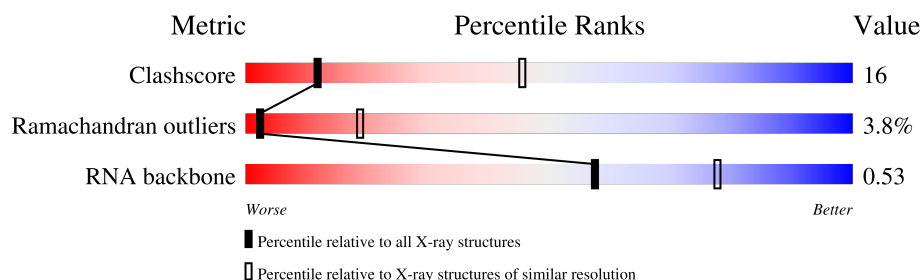
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.75 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                      | 1039 (5.56-3.96)                                      |
| Ramachandran outliers | 187476                      | 1100 (5.58-3.90)                                      |
| RNA backbone          | 3983                        | 1042 (6.22-3.10)                                      |

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   | C     | 30     | 23% 53% 17% 7%   |
| 1   | F     | 30     | 23% 53% 17% 7%   |
| 1   | I     | 30     | 23% 53% 17% 7%   |
| 1   | L     | 30     | 23% 53% 17% 7%   |
| 2   | A     | 554    | 78% 19% .        |
| 2   | D     | 554    | 78% 19% .        |
| 2   | G     | 554    | 78% 19% .        |
| 2   | J     | 554    | 78% 19% .        |

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| Mol | Chain | Length | Quality of chain                                                                              |
|-----|-------|--------|-----------------------------------------------------------------------------------------------|
| 3   | B     | 423    |  72%21%• 5% |
| 3   | E     | 423    |  72%21%• 5% |
| 3   | H     | 423    |  72%21%• 5% |
| 3   | K     | 423    |  72%21%• 5% |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21416 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 RNA chain called RNA (33 NUCLEOTIDE RNA PSEUDOKNOT).

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 1   | C     | 30       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 638   | 287 | 116 | 206 | 29 |         |         |       |
| 1   | F     | 30       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 638   | 287 | 116 | 206 | 29 |         |         |       |
| 1   | I     | 30       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 638   | 287 | 116 | 206 | 29 |         |         |       |
| 1   | L     | 30       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 638   | 287 | 116 | 206 | 29 |         |         |       |

- Molecule 2 is a protein called PROTEIN (HIV-1 REVERSE TRANSCRIPTASE).

| Mol | Chain | Residues | Atoms |      |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|---------|-------|
| 2   | A     | 554      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2737  | 1629 | 554 | 554 |         |         |       |
| 2   | D     | 554      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2737  | 1629 | 554 | 554 |         |         |       |
| 2   | G     | 554      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2737  | 1629 | 554 | 554 |         |         |       |
| 2   | J     | 554      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2737  | 1629 | 554 | 554 |         |         |       |

- Molecule 3 is a protein called PROTEIN (HIV-1 REVERSE TRANSCRIPTASE).

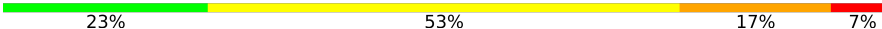
| Mol | Chain | Residues | Atoms |      |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|---------|-------|
| 3   | B     | 400      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 1979  | 1179 | 400 | 400 |         |         |       |
| 3   | E     | 400      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 1979  | 1179 | 400 | 400 |         |         |       |
| 3   | H     | 400      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 1979  | 1179 | 400 | 400 |         |         |       |
| 3   | K     | 400      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 1979  | 1179 | 400 | 400 |         |         |       |

### 3 Residue-property plots

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

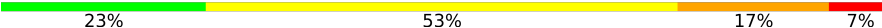
Note EDS was not executed.

- Molecule 1: RNA (33 NUCLEOTIDE RNA PSEUDOKNOT)

Chain C: 

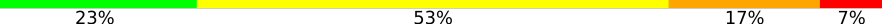


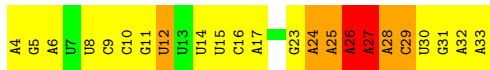
- Molecule 1: RNA (33 NUCLEOTIDE RNA PSEUDOKNOT)

Chain F: 

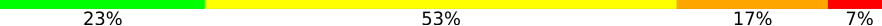


- Molecule 1: RNA (33 NUCLEOTIDE RNA PSEUDOKNOT)

Chain I: 



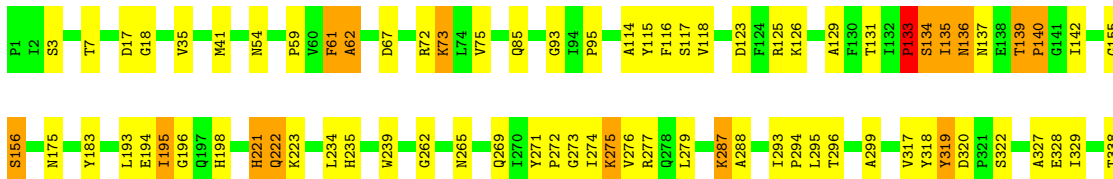
- Molecule 1: RNA (33 NUCLEOTIDE RNA PSEUDOKNOT)

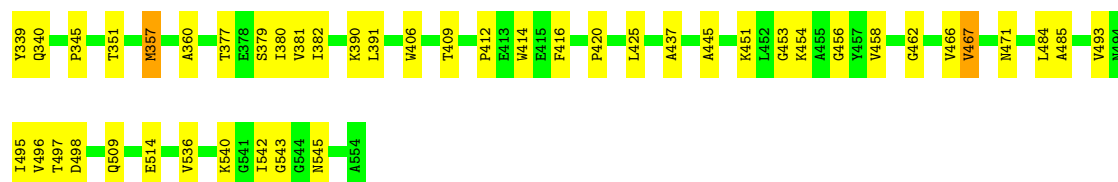
Chain L: 



- Molecule 2: PROTEIN (HIV-1 REVERSE TRANSCRIPTASE)

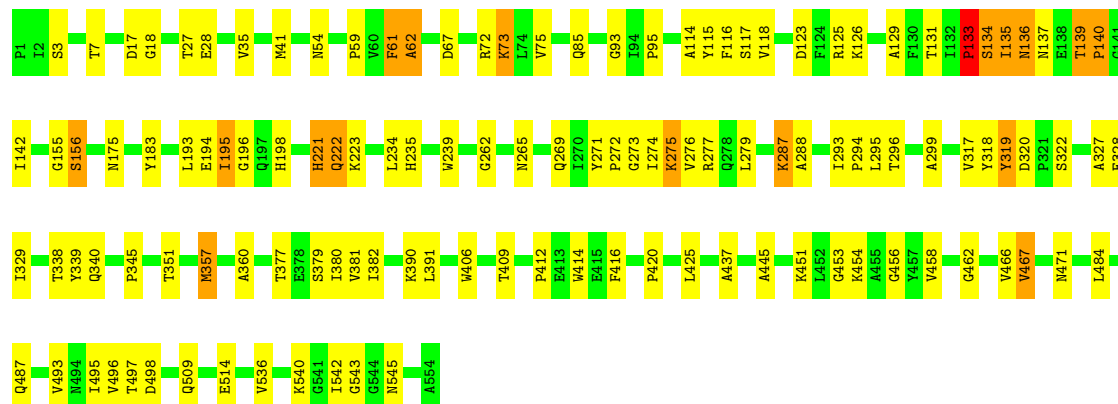
Chain A: 





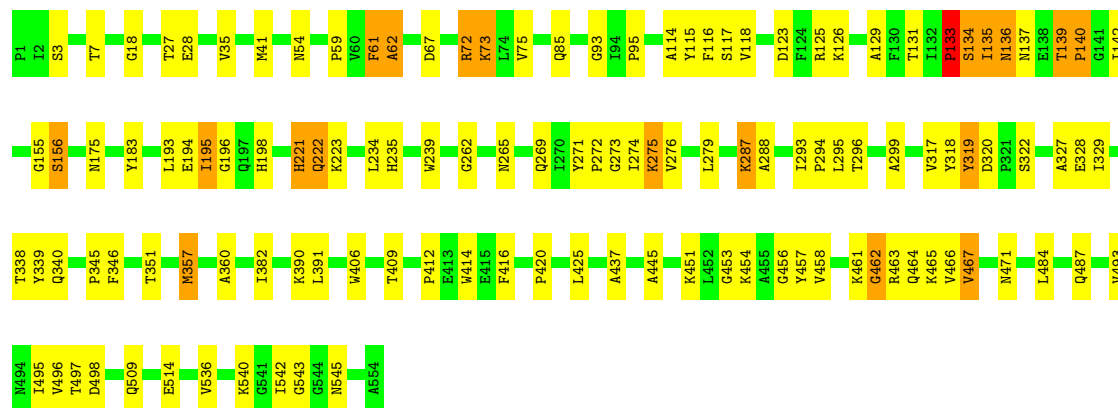
• Molecule 2: PROTEIN (HIV-1 REVERSE TRANSCRIPTASE)

Chain D: 78% 19% .



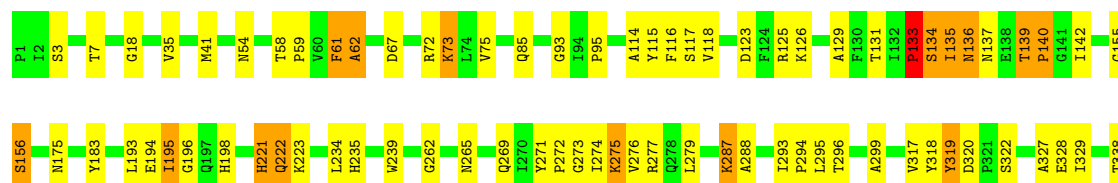
• Molecule 2: PROTEIN (HIV-1 REVERSE TRANSCRIPTASE)

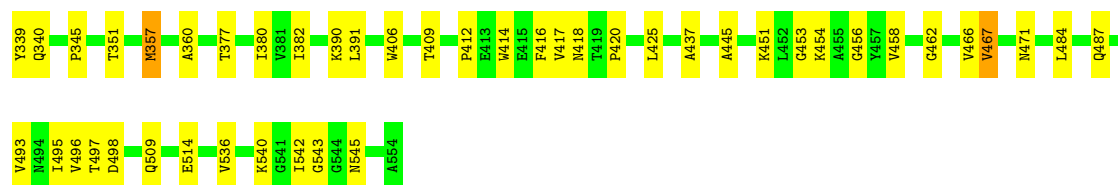
Chain G: 78% 19% .



• Molecule 2: PROTEIN (HIV-1 REVERSE TRANSCRIPTASE)

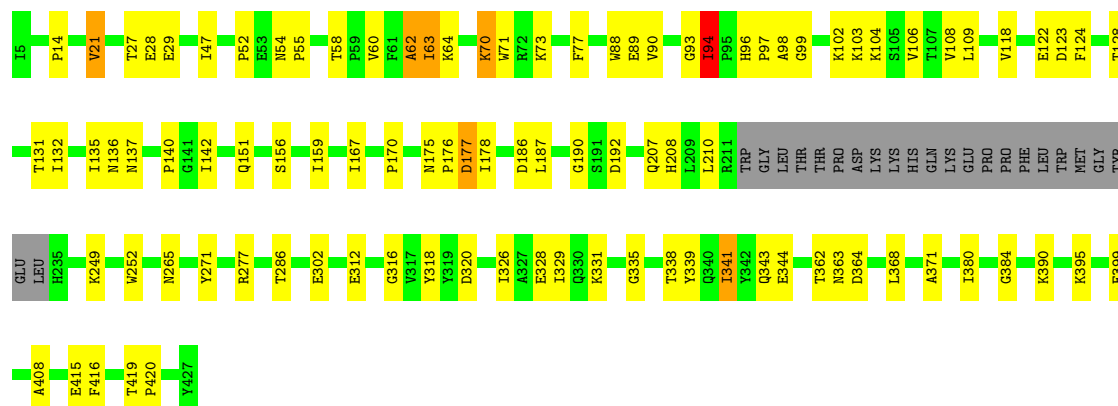
Chain J: 78% 19% .





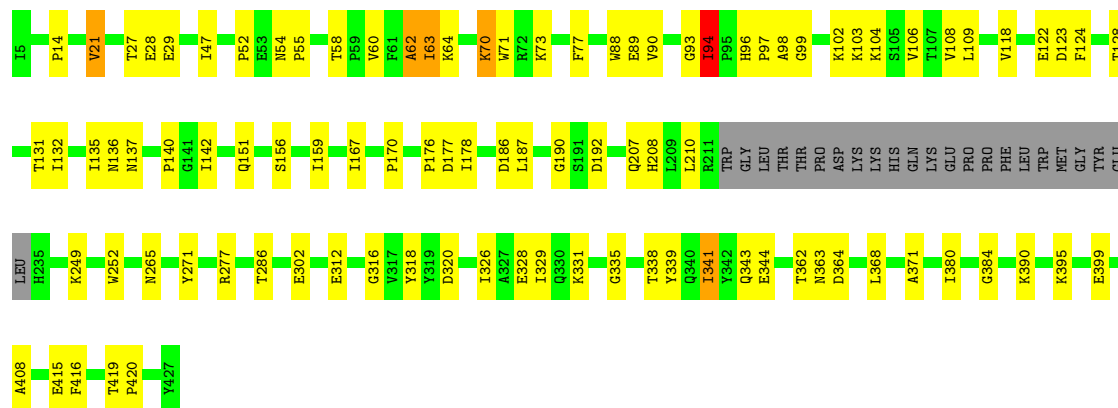
• Molecule 3: PROTEIN (HIV-1 REVERSE TRANSCRIPTASE)

Chain B: 72% 21% 5%



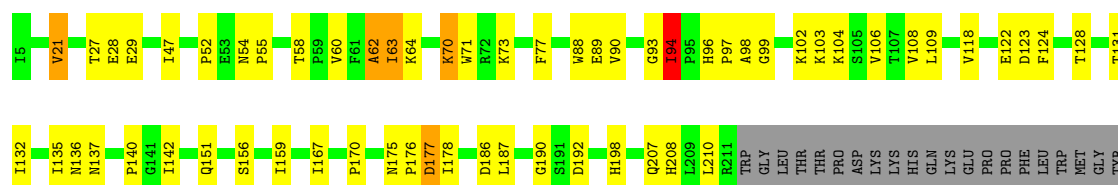
• Molecule 3: PROTEIN (HIV-1 REVERSE TRANSCRIPTASE)

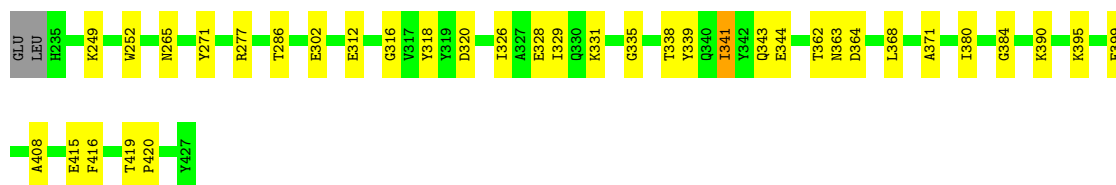
Chain E: 72% 21% 5%



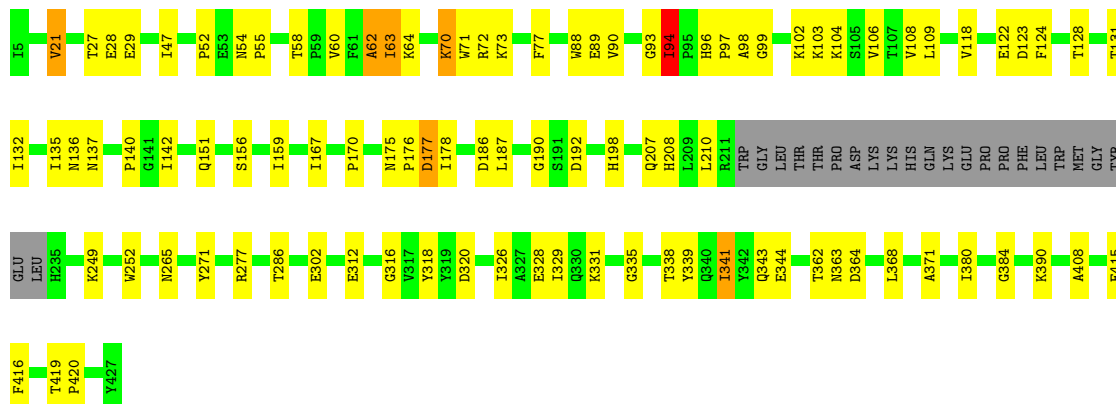
• Molecule 3: PROTEIN (HIV-1 REVERSE TRANSCRIPTASE)

Chain H: 72% 21% 5%





- Molecule 3: PROTEIN (HIV-1 REVERSE TRANSCRIPTASE)



## 4 Data and refinement statistics

Xtriage (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, $\alpha$ , $\beta$ , $\gamma$ | 166.70Å 169.20Å 331.40Å<br>90.00° 104.50° 90.00° | Depositor |
| Resolution (Å)                                           | 30.00 – 4.75                                     | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (30.00-4.75)                     | Depositor |
| $R_{merge}$                                              | (Not available)                                  | Depositor |
| $R_{sym}$                                                | 0.06                                             | Depositor |
| Refinement program                                       | X-PLOR 3.853                                     | Depositor |
| R, $R_{free}$                                            | 0.340 , 0.413                                    | Depositor |
| Estimated twinning fraction                              | No twinning to report.                           | Xtriage   |
| Total number of atoms                                    | 21416                                            | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 52.0                                             | wwPDB-VP  |

## 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   | C     | 0.95         | 1/714 (0.1%)    | 0.69        | 2/1111 (0.2%)    |
| 1   | F     | 0.95         | 1/714 (0.1%)    | 0.69        | 2/1111 (0.2%)    |
| 1   | I     | 0.95         | 1/714 (0.1%)    | 0.69        | 2/1111 (0.2%)    |
| 1   | L     | 0.95         | 1/714 (0.1%)    | 0.69        | 2/1111 (0.2%)    |
| 2   | A     | 1.15         | 9/2736 (0.3%)   | 1.70        | 64/3809 (1.7%)   |
| 2   | D     | 1.15         | 9/2736 (0.3%)   | 1.70        | 64/3809 (1.7%)   |
| 2   | G     | 1.15         | 9/2736 (0.3%)   | 1.70        | 65/3809 (1.7%)   |
| 2   | J     | 1.15         | 9/2736 (0.3%)   | 1.70        | 66/3809 (1.7%)   |
| 3   | B     | 1.63         | 7/1977 (0.4%)   | 1.79        | 57/2752 (2.1%)   |
| 3   | E     | 1.63         | 7/1977 (0.4%)   | 1.79        | 57/2752 (2.1%)   |
| 3   | H     | 1.63         | 7/1977 (0.4%)   | 1.78        | 58/2752 (2.1%)   |
| 3   | K     | 1.62         | 7/1977 (0.4%)   | 1.79        | 58/2752 (2.1%)   |
| All | All   | 1.32         | 68/21708 (0.3%) | 1.63        | 497/30688 (1.6%) |

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 |
|-----|-------|---------------------|---------------------|
| 2   | A     | 0                   | 1                   |
| 2   | D     | 0                   | 1                   |
| 2   | G     | 0                   | 1                   |
| 2   | J     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

All (68) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | E     | 70  | LYS  | C-N   | 41.70 | 1.90        | 1.33     |
| 3   | H     | 70  | LYS  | C-N   | 41.67 | 1.90        | 1.33     |
| 3   | B     | 70  | LYS  | C-N   | 41.66 | 1.90        | 1.33     |
| 3   | K     | 70  | LYS  | C-N   | 41.60 | 1.90        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | B     | 62  | ALA  | C-N   | 27.19 | 1.70        | 1.33     |
| 3   | E     | 62  | ALA  | C-N   | 27.17 | 1.70        | 1.33     |
| 3   | K     | 62  | ALA  | C-N   | 27.15 | 1.70        | 1.33     |
| 3   | H     | 62  | ALA  | C-N   | 27.14 | 1.70        | 1.33     |
| 3   | H     | 64  | LYS  | C-N   | 22.76 | 1.66        | 1.33     |
| 3   | B     | 64  | LYS  | C-N   | 22.74 | 1.66        | 1.33     |
| 3   | K     | 64  | LYS  | C-N   | 22.69 | 1.66        | 1.33     |
| 3   | E     | 64  | LYS  | C-N   | 22.69 | 1.66        | 1.33     |
| 1   | L     | 26  | A    | O3'-P | 21.99 | 1.94        | 1.61     |
| 1   | C     | 26  | A    | O3'-P | 21.99 | 1.94        | 1.61     |
| 1   | F     | 26  | A    | O3'-P | 21.99 | 1.94        | 1.61     |
| 1   | I     | 26  | A    | O3'-P | 21.96 | 1.94        | 1.61     |
| 2   | D     | 319 | TYR  | C-N   | 14.77 | 1.59        | 1.33     |
| 2   | J     | 319 | TYR  | C-N   | 14.76 | 1.59        | 1.33     |
| 2   | A     | 319 | TYR  | C-N   | 14.76 | 1.59        | 1.33     |
| 2   | G     | 319 | TYR  | C-N   | 14.72 | 1.59        | 1.33     |
| 2   | G     | 61  | PHE  | C-N   | 13.49 | 1.52        | 1.33     |
| 2   | A     | 61  | PHE  | C-N   | 13.45 | 1.52        | 1.33     |
| 2   | J     | 61  | PHE  | C-N   | 13.44 | 1.52        | 1.33     |
| 2   | D     | 61  | PHE  | C-N   | 13.40 | 1.52        | 1.33     |
| 2   | J     | 73  | LYS  | N-CA  | 8.71  | 1.56        | 1.46     |
| 2   | G     | 73  | LYS  | N-CA  | 8.69  | 1.56        | 1.46     |
| 2   | D     | 73  | LYS  | N-CA  | 8.65  | 1.56        | 1.46     |
| 2   | A     | 73  | LYS  | N-CA  | 8.64  | 1.56        | 1.46     |
| 2   | J     | 222 | GLN  | C-O   | 7.61  | 1.33        | 1.24     |
| 2   | G     | 222 | GLN  | C-O   | 7.60  | 1.33        | 1.24     |
| 2   | A     | 222 | GLN  | C-O   | 7.58  | 1.33        | 1.24     |
| 2   | D     | 222 | GLN  | C-O   | 7.56  | 1.33        | 1.24     |
| 2   | D     | 118 | VAL  | CA-C  | -6.26 | 1.48        | 1.53     |
| 2   | G     | 118 | VAL  | CA-C  | -6.26 | 1.48        | 1.53     |
| 2   | A     | 118 | VAL  | CA-C  | -6.24 | 1.48        | 1.53     |
| 2   | J     | 118 | VAL  | CA-C  | -6.19 | 1.48        | 1.53     |
| 3   | H     | 21  | VAL  | CA-CB | -6.12 | 1.46        | 1.54     |
| 3   | K     | 21  | VAL  | CA-CB | -6.10 | 1.46        | 1.54     |
| 3   | E     | 21  | VAL  | CA-CB | -6.09 | 1.46        | 1.54     |
| 3   | B     | 21  | VAL  | CA-CB | -6.08 | 1.46        | 1.54     |
| 2   | G     | 269 | GLN  | C-N   | -5.69 | 1.25        | 1.33     |
| 2   | A     | 269 | GLN  | C-N   | -5.68 | 1.25        | 1.33     |
| 2   | D     | 269 | GLN  | C-N   | -5.64 | 1.25        | 1.33     |
| 2   | J     | 269 | GLN  | C-N   | -5.63 | 1.25        | 1.33     |
| 3   | H     | 362 | THR  | C-O   | 5.58  | 1.31        | 1.24     |
| 3   | K     | 362 | THR  | C-O   | 5.56  | 1.30        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | B     | 362 | THR  | C-O   | 5.55  | 1.30        | 1.24     |
| 3   | E     | 362 | THR  | C-O   | 5.54  | 1.30        | 1.24     |
| 3   | K     | 159 | ILE  | CA-CB | -5.52 | 1.48        | 1.54     |
| 3   | B     | 159 | ILE  | CA-CB | -5.52 | 1.48        | 1.54     |
| 3   | H     | 159 | ILE  | CA-CB | -5.52 | 1.48        | 1.54     |
| 2   | D     | 61  | PHE  | C-O   | -5.47 | 1.17        | 1.23     |
| 3   | E     | 159 | ILE  | CA-CB | -5.47 | 1.48        | 1.54     |
| 2   | G     | 61  | PHE  | C-O   | -5.46 | 1.17        | 1.23     |
| 2   | A     | 61  | PHE  | C-O   | -5.46 | 1.17        | 1.23     |
| 2   | J     | 61  | PHE  | C-O   | -5.45 | 1.17        | 1.23     |
| 3   | K     | 341 | ILE  | CA-CB | -5.26 | 1.48        | 1.54     |
| 3   | H     | 341 | ILE  | CA-CB | -5.24 | 1.48        | 1.54     |
| 3   | B     | 341 | ILE  | CA-CB | -5.22 | 1.48        | 1.54     |
| 3   | E     | 341 | ILE  | CA-CB | -5.20 | 1.48        | 1.54     |
| 2   | J     | 183 | TYR  | CA-C  | -5.19 | 1.48        | 1.53     |
| 2   | G     | 183 | TYR  | CA-C  | -5.18 | 1.48        | 1.53     |
| 2   | D     | 279 | LEU  | C-O   | -5.17 | 1.17        | 1.24     |
| 2   | A     | 183 | TYR  | CA-C  | -5.15 | 1.48        | 1.53     |
| 2   | A     | 279 | LEU  | C-O   | -5.15 | 1.17        | 1.24     |
| 2   | G     | 279 | LEU  | C-O   | -5.15 | 1.17        | 1.24     |
| 2   | J     | 279 | LEU  | C-O   | -5.11 | 1.17        | 1.24     |
| 2   | D     | 183 | TYR  | CA-C  | -5.04 | 1.49        | 1.53     |

All (497) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 3   | K     | 64  | LYS  | CA-C-N | 14.88  | 151.97      | 122.07   |
| 3   | K     | 64  | LYS  | C-N-CA | 14.88  | 151.97      | 122.07   |
| 3   | B     | 64  | LYS  | CA-C-N | 14.87  | 151.96      | 122.07   |
| 3   | B     | 64  | LYS  | C-N-CA | 14.87  | 151.96      | 122.07   |
| 3   | E     | 64  | LYS  | CA-C-N | 14.87  | 151.95      | 122.07   |
| 3   | E     | 64  | LYS  | C-N-CA | 14.87  | 151.95      | 122.07   |
| 3   | H     | 64  | LYS  | CA-C-N | 14.85  | 151.92      | 122.07   |
| 3   | H     | 64  | LYS  | C-N-CA | 14.85  | 151.92      | 122.07   |
| 3   | K     | 94  | ILE  | CA-C-N | -13.18 | 106.54      | 119.85   |
| 3   | K     | 94  | ILE  | C-N-CA | -13.18 | 106.54      | 119.85   |
| 3   | E     | 94  | ILE  | CA-C-N | -13.15 | 106.57      | 119.85   |
| 3   | E     | 94  | ILE  | C-N-CA | -13.15 | 106.57      | 119.85   |
| 3   | B     | 94  | ILE  | CA-C-N | -13.15 | 106.57      | 119.85   |
| 3   | B     | 94  | ILE  | C-N-CA | -13.15 | 106.57      | 119.85   |
| 3   | H     | 94  | ILE  | CA-C-N | -13.10 | 106.62      | 119.85   |
| 3   | H     | 94  | ILE  | C-N-CA | -13.10 | 106.62      | 119.85   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | H     | 54  | ASN  | CA-C-N | 12.51 | 135.48      | 119.84   |
| 3   | H     | 54  | ASN  | C-N-CA | 12.51 | 135.48      | 119.84   |
| 3   | B     | 54  | ASN  | CA-C-N | 12.51 | 135.47      | 119.84   |
| 3   | B     | 54  | ASN  | C-N-CA | 12.51 | 135.47      | 119.84   |
| 3   | E     | 54  | ASN  | CA-C-N | 12.51 | 135.47      | 119.84   |
| 3   | E     | 54  | ASN  | C-N-CA | 12.51 | 135.47      | 119.84   |
| 3   | K     | 54  | ASN  | CA-C-N | 12.46 | 135.42      | 119.84   |
| 3   | K     | 54  | ASN  | C-N-CA | 12.46 | 135.42      | 119.84   |
| 2   | J     | 118 | VAL  | CA-C-N | 11.75 | 131.88      | 119.90   |
| 2   | J     | 118 | VAL  | C-N-CA | 11.75 | 131.88      | 119.90   |
| 2   | D     | 118 | VAL  | CA-C-N | 11.74 | 131.88      | 119.90   |
| 2   | D     | 118 | VAL  | C-N-CA | 11.74 | 131.88      | 119.90   |
| 2   | A     | 118 | VAL  | CA-C-N | 11.72 | 131.85      | 119.90   |
| 2   | A     | 118 | VAL  | C-N-CA | 11.72 | 131.85      | 119.90   |
| 2   | G     | 118 | VAL  | CA-C-N | 11.71 | 131.84      | 119.90   |
| 2   | G     | 118 | VAL  | C-N-CA | 11.71 | 131.84      | 119.90   |
| 2   | J     | 271 | TYR  | CA-C-N | 10.74 | 133.27      | 119.84   |
| 2   | J     | 271 | TYR  | C-N-CA | 10.74 | 133.27      | 119.84   |
| 2   | A     | 271 | TYR  | CA-C-N | 10.74 | 133.26      | 119.84   |
| 2   | A     | 271 | TYR  | C-N-CA | 10.74 | 133.26      | 119.84   |
| 2   | G     | 271 | TYR  | CA-C-N | 10.71 | 133.23      | 119.84   |
| 2   | G     | 271 | TYR  | C-N-CA | 10.71 | 133.23      | 119.84   |
| 2   | D     | 271 | TYR  | CA-C-N | 10.71 | 133.22      | 119.84   |
| 2   | D     | 271 | TYR  | C-N-CA | 10.71 | 133.22      | 119.84   |
| 3   | H     | 70  | LYS  | O-C-N  | 10.58 | 136.66      | 122.59   |
| 3   | K     | 70  | LYS  | O-C-N  | 10.58 | 136.66      | 122.59   |
| 3   | B     | 70  | LYS  | O-C-N  | 10.56 | 136.63      | 122.59   |
| 3   | E     | 70  | LYS  | O-C-N  | 10.52 | 136.58      | 122.59   |
| 2   | D     | 319 | TYR  | CA-C-N | -9.53 | 105.73      | 121.17   |
| 2   | D     | 319 | TYR  | C-N-CA | -9.53 | 105.73      | 121.17   |
| 2   | A     | 319 | TYR  | CA-C-N | -9.51 | 105.77      | 121.17   |
| 2   | A     | 319 | TYR  | C-N-CA | -9.51 | 105.77      | 121.17   |
| 2   | G     | 319 | TYR  | CA-C-N | -9.50 | 105.77      | 121.17   |
| 2   | G     | 319 | TYR  | C-N-CA | -9.50 | 105.77      | 121.17   |
| 2   | J     | 319 | TYR  | CA-C-N | -9.50 | 105.79      | 121.17   |
| 2   | J     | 319 | TYR  | C-N-CA | -9.50 | 105.79      | 121.17   |
| 2   | D     | 382 | ILE  | N-CA-C | 9.13  | 119.11      | 110.53   |
| 2   | A     | 382 | ILE  | N-CA-C | 9.10  | 119.09      | 110.53   |
| 2   | J     | 382 | ILE  | N-CA-C | 9.10  | 119.08      | 110.53   |
| 2   | G     | 382 | ILE  | N-CA-C | 9.08  | 119.06      | 110.53   |
| 3   | H     | 102 | LYS  | N-CA-C | 9.04  | 124.11      | 112.89   |
| 3   | B     | 102 | LYS  | N-CA-C | 9.01  | 124.06      | 112.89   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | K     | 102 | LYS  | N-CA-C  | 8.99  | 124.04      | 112.89   |
| 3   | E     | 102 | LYS  | N-CA-C  | 8.98  | 124.03      | 112.89   |
| 3   | E     | 312 | GLU  | CA-C-N  | 8.87  | 130.93      | 119.84   |
| 3   | E     | 312 | GLU  | C-N-CA  | 8.87  | 130.93      | 119.84   |
| 3   | H     | 312 | GLU  | CA-C-N  | 8.87  | 130.93      | 119.84   |
| 3   | H     | 312 | GLU  | C-N-CA  | 8.87  | 130.93      | 119.84   |
| 3   | B     | 312 | GLU  | CA-C-N  | 8.86  | 130.92      | 119.84   |
| 3   | B     | 312 | GLU  | C-N-CA  | 8.86  | 130.92      | 119.84   |
| 3   | K     | 312 | GLU  | CA-C-N  | 8.83  | 130.88      | 119.84   |
| 3   | K     | 312 | GLU  | C-N-CA  | 8.83  | 130.88      | 119.84   |
| 3   | H     | 60  | VAL  | CB-CA-C | -8.18 | 99.12       | 110.90   |
| 3   | B     | 60  | VAL  | CB-CA-C | -8.17 | 99.14       | 110.90   |
| 3   | E     | 60  | VAL  | CB-CA-C | -8.15 | 99.16       | 110.90   |
| 3   | K     | 60  | VAL  | CB-CA-C | -8.14 | 99.17       | 110.90   |
| 2   | D     | 118 | VAL  | N-CA-C  | 8.14  | 114.97      | 107.56   |
| 2   | G     | 118 | VAL  | N-CA-C  | 8.14  | 114.97      | 107.56   |
| 2   | A     | 118 | VAL  | N-CA-C  | 8.13  | 114.96      | 107.56   |
| 2   | J     | 118 | VAL  | N-CA-C  | 8.10  | 114.93      | 107.56   |
| 2   | A     | 221 | HIS  | CA-C-N  | 8.08  | 136.97      | 121.54   |
| 2   | A     | 221 | HIS  | C-N-CA  | 8.08  | 136.97      | 121.54   |
| 2   | D     | 221 | HIS  | CA-C-N  | 8.07  | 136.96      | 121.54   |
| 2   | D     | 221 | HIS  | C-N-CA  | 8.07  | 136.96      | 121.54   |
| 2   | G     | 221 | HIS  | CA-C-N  | 8.07  | 136.96      | 121.54   |
| 2   | G     | 221 | HIS  | C-N-CA  | 8.07  | 136.96      | 121.54   |
| 2   | J     | 221 | HIS  | CA-C-N  | 8.06  | 136.93      | 121.54   |
| 2   | J     | 221 | HIS  | C-N-CA  | 8.06  | 136.93      | 121.54   |
| 3   | K     | 118 | VAL  | CA-C-N  | 8.04  | 127.80      | 119.76   |
| 3   | K     | 118 | VAL  | C-N-CA  | 8.04  | 127.80      | 119.76   |
| 3   | B     | 118 | VAL  | CA-C-N  | 8.03  | 127.79      | 119.76   |
| 3   | B     | 118 | VAL  | C-N-CA  | 8.03  | 127.79      | 119.76   |
| 3   | H     | 118 | VAL  | CA-C-N  | 8.01  | 127.77      | 119.76   |
| 3   | H     | 118 | VAL  | C-N-CA  | 8.01  | 127.77      | 119.76   |
| 3   | B     | 90  | VAL  | N-CA-C  | -7.99 | 97.66       | 106.21   |
| 3   | E     | 118 | VAL  | CA-C-N  | 7.99  | 127.75      | 119.76   |
| 3   | E     | 118 | VAL  | C-N-CA  | 7.99  | 127.75      | 119.76   |
| 3   | K     | 90  | VAL  | N-CA-C  | -7.99 | 97.67       | 106.21   |
| 3   | E     | 90  | VAL  | N-CA-C  | -7.98 | 97.67       | 106.21   |
| 3   | H     | 90  | VAL  | N-CA-C  | -7.98 | 97.67       | 106.21   |
| 2   | G     | 351 | THR  | N-CA-C  | -7.82 | 98.65       | 110.14   |
| 2   | J     | 351 | THR  | N-CA-C  | -7.80 | 98.67       | 110.14   |
| 2   | A     | 351 | THR  | N-CA-C  | -7.79 | 98.68       | 110.14   |
| 2   | D     | 351 | THR  | N-CA-C  | -7.77 | 98.72       | 110.14   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | G     | 498 | ASP  | N-CA-C  | -7.70 | 101.78      | 112.25   |
| 2   | J     | 498 | ASP  | N-CA-C  | -7.69 | 101.79      | 112.25   |
| 2   | D     | 498 | ASP  | N-CA-C  | -7.68 | 101.81      | 112.25   |
| 3   | B     | 103 | LYS  | N-CA-C  | 7.68  | 120.79      | 110.35   |
| 3   | H     | 103 | LYS  | N-CA-C  | 7.67  | 120.79      | 110.35   |
| 2   | A     | 498 | ASP  | N-CA-C  | -7.67 | 101.82      | 112.25   |
| 3   | K     | 103 | LYS  | N-CA-C  | 7.67  | 120.78      | 110.35   |
| 3   | E     | 103 | LYS  | N-CA-C  | 7.64  | 120.74      | 110.35   |
| 2   | J     | 59  | PRO  | CB-CA-C | -7.50 | 101.16      | 110.98   |
| 2   | A     | 59  | PRO  | CB-CA-C | -7.49 | 101.17      | 110.98   |
| 2   | D     | 59  | PRO  | CB-CA-C | -7.49 | 101.17      | 110.98   |
| 2   | G     | 59  | PRO  | CB-CA-C | -7.49 | 101.17      | 110.98   |
| 2   | D     | 3   | SER  | CA-C-N  | 7.38  | 129.56      | 121.00   |
| 2   | D     | 3   | SER  | C-N-CA  | 7.38  | 129.56      | 121.00   |
| 2   | A     | 18  | GLY  | CA-C-N  | 7.37  | 127.33      | 120.03   |
| 2   | A     | 18  | GLY  | C-N-CA  | 7.37  | 127.33      | 120.03   |
| 2   | J     | 3   | SER  | CA-C-N  | 7.37  | 129.54      | 121.00   |
| 2   | J     | 3   | SER  | C-N-CA  | 7.37  | 129.54      | 121.00   |
| 2   | D     | 18  | GLY  | CA-C-N  | 7.36  | 127.31      | 120.03   |
| 2   | D     | 18  | GLY  | C-N-CA  | 7.36  | 127.31      | 120.03   |
| 2   | G     | 18  | GLY  | CA-C-N  | 7.34  | 127.30      | 120.03   |
| 2   | G     | 18  | GLY  | C-N-CA  | 7.34  | 127.30      | 120.03   |
| 2   | A     | 3   | SER  | CA-C-N  | 7.34  | 129.52      | 121.00   |
| 2   | A     | 3   | SER  | C-N-CA  | 7.34  | 129.52      | 121.00   |
| 2   | J     | 18  | GLY  | CA-C-N  | 7.33  | 127.28      | 120.03   |
| 2   | J     | 18  | GLY  | C-N-CA  | 7.33  | 127.28      | 120.03   |
| 2   | G     | 3   | SER  | CA-C-N  | 7.31  | 129.49      | 121.00   |
| 2   | G     | 3   | SER  | C-N-CA  | 7.31  | 129.49      | 121.00   |
| 2   | J     | 536 | VAL  | CA-C-N  | 7.13  | 128.76      | 119.84   |
| 2   | J     | 536 | VAL  | C-N-CA  | 7.13  | 128.76      | 119.84   |
| 2   | D     | 536 | VAL  | CA-C-N  | 7.13  | 128.75      | 119.84   |
| 2   | D     | 536 | VAL  | C-N-CA  | 7.13  | 128.75      | 119.84   |
| 2   | A     | 536 | VAL  | CA-C-N  | 7.12  | 128.73      | 119.84   |
| 2   | A     | 536 | VAL  | C-N-CA  | 7.12  | 128.73      | 119.84   |
| 2   | G     | 536 | VAL  | CA-C-N  | 7.10  | 128.72      | 119.84   |
| 2   | G     | 536 | VAL  | C-N-CA  | 7.10  | 128.72      | 119.84   |
| 2   | J     | 497 | THR  | N-CA-C  | 6.87  | 120.79      | 110.14   |
| 2   | J     | 129 | ALA  | CA-C-N  | 6.87  | 134.00      | 121.85   |
| 2   | J     | 129 | ALA  | C-N-CA  | 6.87  | 134.00      | 121.85   |
| 2   | D     | 497 | THR  | N-CA-C  | 6.86  | 120.77      | 110.14   |
| 2   | A     | 129 | ALA  | CA-C-N  | 6.86  | 133.99      | 121.85   |
| 2   | A     | 129 | ALA  | C-N-CA  | 6.86  | 133.99      | 121.85   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 35  | VAL  | CB-CA-C | -6.85 | 103.25      | 111.81   |
| 2   | J     | 35  | VAL  | CB-CA-C | -6.85 | 103.24      | 111.81   |
| 2   | A     | 497 | THR  | N-CA-C  | 6.85  | 120.76      | 110.14   |
| 2   | G     | 497 | THR  | N-CA-C  | 6.85  | 120.75      | 110.14   |
| 2   | A     | 35  | VAL  | CB-CA-C | -6.84 | 103.25      | 111.81   |
| 2   | D     | 129 | ALA  | CA-C-N  | 6.84  | 133.96      | 121.85   |
| 2   | D     | 129 | ALA  | C-N-CA  | 6.84  | 133.96      | 121.85   |
| 2   | G     | 129 | ALA  | CA-C-N  | 6.84  | 133.96      | 121.85   |
| 2   | G     | 129 | ALA  | C-N-CA  | 6.84  | 133.96      | 121.85   |
| 2   | D     | 54  | ASN  | CA-C-N  | 6.83  | 127.40      | 119.47   |
| 2   | D     | 54  | ASN  | C-N-CA  | 6.83  | 127.40      | 119.47   |
| 2   | G     | 54  | ASN  | CA-C-N  | 6.83  | 127.39      | 119.47   |
| 2   | G     | 54  | ASN  | C-N-CA  | 6.83  | 127.39      | 119.47   |
| 2   | A     | 54  | ASN  | CA-C-N  | 6.82  | 127.38      | 119.47   |
| 2   | A     | 54  | ASN  | C-N-CA  | 6.82  | 127.38      | 119.47   |
| 2   | G     | 35  | VAL  | CB-CA-C | -6.81 | 103.30      | 111.81   |
| 2   | J     | 54  | ASN  | CA-C-N  | 6.78  | 127.33      | 119.47   |
| 2   | J     | 54  | ASN  | C-N-CA  | 6.78  | 127.33      | 119.47   |
| 2   | J     | 140 | PRO  | N-CA-CB | 6.75  | 110.34      | 103.25   |
| 2   | A     | 140 | PRO  | N-CA-CB | 6.71  | 110.30      | 103.25   |
| 2   | D     | 140 | PRO  | N-CA-CB | 6.69  | 110.27      | 103.25   |
| 2   | G     | 140 | PRO  | N-CA-CB | 6.69  | 110.27      | 103.25   |
| 3   | B     | 47  | ILE  | CB-CA-C | -6.61 | 100.45      | 111.29   |
| 3   | H     | 89  | GLU  | N-CA-C  | -6.60 | 103.70      | 111.03   |
| 3   | E     | 47  | ILE  | CB-CA-C | -6.60 | 100.47      | 111.29   |
| 3   | K     | 47  | ILE  | CB-CA-C | -6.59 | 100.48      | 111.29   |
| 3   | H     | 47  | ILE  | CB-CA-C | -6.59 | 100.48      | 111.29   |
| 2   | D     | 133 | PRO  | N-CA-CB | 6.59  | 110.17      | 103.25   |
| 3   | K     | 89  | GLU  | N-CA-C  | -6.58 | 103.73      | 111.03   |
| 2   | J     | 133 | PRO  | N-CA-CB | 6.58  | 110.16      | 103.25   |
| 3   | B     | 89  | GLU  | N-CA-C  | -6.57 | 103.73      | 111.03   |
| 2   | D     | 391 | LEU  | CA-C-N  | 6.57  | 128.06      | 119.84   |
| 2   | D     | 391 | LEU  | C-N-CA  | 6.57  | 128.06      | 119.84   |
| 2   | G     | 133 | PRO  | N-CA-CB | 6.57  | 110.15      | 103.25   |
| 3   | E     | 89  | GLU  | N-CA-C  | -6.57 | 103.74      | 111.03   |
| 2   | A     | 133 | PRO  | N-CA-CB | 6.56  | 110.14      | 103.25   |
| 2   | A     | 514 | GLU  | N-CA-C  | -6.54 | 103.98      | 112.23   |
| 2   | J     | 514 | GLU  | N-CA-C  | -6.54 | 103.99      | 112.23   |
| 2   | G     | 514 | GLU  | N-CA-C  | -6.54 | 103.99      | 112.23   |
| 2   | G     | 294 | PRO  | N-CA-CB | 6.53  | 110.11      | 103.25   |
| 2   | A     | 391 | LEU  | CA-C-N  | 6.53  | 128.00      | 119.84   |
| 2   | A     | 391 | LEU  | C-N-CA  | 6.53  | 128.00      | 119.84   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 514 | GLU  | N-CA-C  | -6.52 | 104.01      | 112.23   |
| 2   | G     | 391 | LEU  | CA-C-N  | 6.52  | 127.99      | 119.84   |
| 2   | G     | 391 | LEU  | C-N-CA  | 6.52  | 127.99      | 119.84   |
| 2   | J     | 294 | PRO  | N-CA-CB | 6.50  | 110.08      | 103.25   |
| 2   | D     | 509 | GLN  | CA-C-N  | 6.50  | 127.96      | 119.84   |
| 2   | D     | 509 | GLN  | C-N-CA  | 6.50  | 127.96      | 119.84   |
| 2   | J     | 391 | LEU  | CA-C-N  | 6.49  | 127.96      | 119.84   |
| 2   | J     | 391 | LEU  | C-N-CA  | 6.49  | 127.96      | 119.84   |
| 2   | G     | 509 | GLN  | CA-C-N  | 6.49  | 127.95      | 119.84   |
| 2   | G     | 509 | GLN  | C-N-CA  | 6.49  | 127.95      | 119.84   |
| 2   | A     | 294 | PRO  | N-CA-CB | 6.49  | 110.06      | 103.25   |
| 3   | B     | 132 | ILE  | CA-C-N  | 6.48  | 127.37      | 120.11   |
| 3   | B     | 132 | ILE  | C-N-CA  | 6.48  | 127.37      | 120.11   |
| 3   | H     | 132 | ILE  | CA-C-N  | 6.47  | 127.36      | 120.11   |
| 3   | H     | 132 | ILE  | C-N-CA  | 6.47  | 127.36      | 120.11   |
| 2   | D     | 294 | PRO  | N-CA-CB | 6.47  | 110.04      | 103.25   |
| 2   | A     | 509 | GLN  | CA-C-N  | 6.46  | 127.91      | 119.84   |
| 2   | A     | 509 | GLN  | C-N-CA  | 6.46  | 127.91      | 119.84   |
| 3   | E     | 132 | ILE  | CA-C-N  | 6.46  | 127.34      | 120.11   |
| 3   | E     | 132 | ILE  | C-N-CA  | 6.46  | 127.34      | 120.11   |
| 2   | J     | 509 | GLN  | CA-C-N  | 6.45  | 127.91      | 119.84   |
| 2   | J     | 509 | GLN  | C-N-CA  | 6.45  | 127.91      | 119.84   |
| 3   | K     | 132 | ILE  | CA-C-N  | 6.45  | 127.33      | 120.11   |
| 3   | K     | 132 | ILE  | C-N-CA  | 6.45  | 127.33      | 120.11   |
| 2   | D     | 496 | VAL  | N-CA-C  | 6.42  | 118.28      | 107.18   |
| 2   | G     | 287 | LYS  | CA-C-O  | -6.40 | 114.54      | 121.14   |
| 2   | A     | 496 | VAL  | N-CA-C  | 6.40  | 118.25      | 107.18   |
| 2   | G     | 496 | VAL  | N-CA-C  | 6.39  | 118.24      | 107.18   |
| 2   | J     | 496 | VAL  | N-CA-C  | 6.38  | 118.22      | 107.18   |
| 2   | A     | 272 | PRO  | N-CA-CB | 6.38  | 109.95      | 103.25   |
| 2   | A     | 287 | LYS  | CA-C-O  | -6.37 | 114.58      | 121.14   |
| 2   | J     | 272 | PRO  | N-CA-CB | 6.37  | 109.94      | 103.25   |
| 2   | J     | 287 | LYS  | CA-C-O  | -6.36 | 114.59      | 121.14   |
| 3   | H     | 249 | LYS  | N-CA-C  | 6.36  | 119.53      | 109.81   |
| 2   | D     | 272 | PRO  | N-CA-CB | 6.35  | 109.92      | 103.25   |
| 2   | G     | 272 | PRO  | N-CA-CB | 6.35  | 109.92      | 103.25   |
| 3   | E     | 249 | LYS  | N-CA-C  | 6.35  | 119.52      | 109.81   |
| 3   | E     | 96  | HIS  | CA-C-N  | 6.34  | 127.76      | 119.84   |
| 3   | E     | 96  | HIS  | C-N-CA  | 6.34  | 127.76      | 119.84   |
| 3   | B     | 249 | LYS  | N-CA-C  | 6.33  | 119.50      | 109.81   |
| 2   | D     | 287 | LYS  | CA-C-O  | -6.33 | 114.62      | 121.14   |
| 3   | K     | 96  | HIS  | CA-C-N  | 6.33  | 127.75      | 119.84   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | K     | 96  | HIS  | C-N-CA | 6.33  | 127.75      | 119.84   |
| 3   | K     | 249 | LYS  | N-CA-C | 6.33  | 119.49      | 109.81   |
| 3   | B     | 96  | HIS  | CA-C-N | 6.32  | 127.75      | 119.84   |
| 3   | B     | 96  | HIS  | C-N-CA | 6.32  | 127.75      | 119.84   |
| 3   | H     | 96  | HIS  | CA-C-N | 6.32  | 127.73      | 119.84   |
| 3   | H     | 96  | HIS  | C-N-CA | 6.32  | 127.73      | 119.84   |
| 3   | B     | 156 | SER  | CA-C-N | 6.19  | 125.68      | 119.24   |
| 3   | B     | 156 | SER  | C-N-CA | 6.19  | 125.68      | 119.24   |
| 3   | K     | 156 | SER  | CA-C-N | 6.19  | 125.68      | 119.24   |
| 3   | K     | 156 | SER  | C-N-CA | 6.19  | 125.68      | 119.24   |
| 3   | H     | 156 | SER  | CA-C-N | 6.17  | 125.66      | 119.24   |
| 3   | H     | 156 | SER  | C-N-CA | 6.17  | 125.66      | 119.24   |
| 3   | E     | 156 | SER  | CA-C-N | 6.17  | 125.65      | 119.24   |
| 3   | E     | 156 | SER  | C-N-CA | 6.17  | 125.65      | 119.24   |
| 2   | J     | 357 | MET  | N-CA-C | -6.14 | 97.71       | 110.80   |
| 3   | K     | 128 | THR  | N-CA-C | -6.14 | 104.28      | 112.94   |
| 2   | A     | 357 | MET  | N-CA-C | -6.14 | 97.72       | 110.80   |
| 2   | G     | 357 | MET  | N-CA-C | -6.14 | 97.72       | 110.80   |
| 3   | E     | 128 | THR  | N-CA-C | -6.14 | 104.28      | 112.94   |
| 3   | H     | 128 | THR  | N-CA-C | -6.14 | 104.28      | 112.94   |
| 2   | D     | 357 | MET  | N-CA-C | -6.14 | 97.73       | 110.80   |
| 3   | B     | 128 | THR  | N-CA-C | -6.13 | 104.29      | 112.94   |
| 2   | J     | 416 | PHE  | N-CA-C | 6.07  | 119.06      | 109.96   |
| 2   | A     | 416 | PHE  | N-CA-C | 6.06  | 119.05      | 109.96   |
| 2   | G     | 416 | PHE  | N-CA-C | 6.06  | 119.05      | 109.96   |
| 2   | D     | 416 | PHE  | N-CA-C | 6.05  | 119.04      | 109.96   |
| 2   | G     | 293 | ILE  | CA-C-N | 6.00  | 127.33      | 119.84   |
| 2   | G     | 293 | ILE  | C-N-CA | 6.00  | 127.33      | 119.84   |
| 2   | J     | 293 | ILE  | CA-C-N | 5.99  | 127.33      | 119.84   |
| 2   | J     | 293 | ILE  | C-N-CA | 5.99  | 127.33      | 119.84   |
| 2   | A     | 293 | ILE  | CA-C-N | 5.97  | 127.30      | 119.84   |
| 2   | A     | 293 | ILE  | C-N-CA | 5.97  | 127.30      | 119.84   |
| 2   | D     | 293 | ILE  | CA-C-N | 5.95  | 127.28      | 119.84   |
| 2   | D     | 293 | ILE  | C-N-CA | 5.95  | 127.28      | 119.84   |
| 2   | J     | 41  | MET  | N-CA-C | -5.94 | 104.88      | 111.71   |
| 2   | D     | 41  | MET  | N-CA-C | -5.92 | 104.90      | 111.71   |
| 3   | H     | 64  | LYS  | O-C-N  | -5.92 | 117.58      | 123.62   |
| 2   | A     | 41  | MET  | N-CA-C | -5.92 | 104.91      | 111.71   |
| 3   | B     | 64  | LYS  | O-C-N  | -5.91 | 117.59      | 123.62   |
| 2   | G     | 41  | MET  | N-CA-C | -5.91 | 104.91      | 111.71   |
| 3   | E     | 64  | LYS  | O-C-N  | -5.89 | 117.61      | 123.62   |
| 3   | E     | 63  | ILE  | N-CA-C | -5.87 | 97.12       | 109.34   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | H     | 63  | ILE  | N-CA-C  | -5.87 | 97.14       | 109.34   |
| 3   | B     | 63  | ILE  | N-CA-C  | -5.86 | 97.14       | 109.34   |
| 3   | K     | 63  | ILE  | N-CA-C  | -5.86 | 97.15       | 109.34   |
| 3   | K     | 64  | LYS  | O-C-N   | -5.86 | 117.64      | 123.62   |
| 2   | J     | 317 | VAL  | CA-C-O  | -5.85 | 117.06      | 121.68   |
| 2   | G     | 317 | VAL  | CA-C-O  | -5.84 | 117.06      | 121.68   |
| 3   | E     | 140 | PRO  | N-CA-C  | -5.84 | 102.09      | 111.38   |
| 2   | G     | 198 | HIS  | N-CA-C  | -5.83 | 104.56      | 111.03   |
| 3   | K     | 140 | PRO  | N-CA-C  | -5.83 | 102.11      | 111.38   |
| 3   | B     | 140 | PRO  | N-CA-C  | -5.82 | 102.12      | 111.38   |
| 3   | H     | 140 | PRO  | N-CA-C  | -5.82 | 102.12      | 111.38   |
| 2   | A     | 198 | HIS  | N-CA-C  | -5.82 | 104.57      | 111.03   |
| 2   | A     | 317 | VAL  | CA-C-O  | -5.81 | 117.09      | 121.68   |
| 3   | B     | 52  | PRO  | N-CA-C  | -5.81 | 106.43      | 114.27   |
| 3   | K     | 52  | PRO  | N-CA-C  | -5.80 | 106.44      | 114.27   |
| 2   | D     | 198 | HIS  | N-CA-C  | -5.80 | 104.59      | 111.03   |
| 3   | E     | 52  | PRO  | N-CA-C  | -5.80 | 106.44      | 114.27   |
| 2   | D     | 317 | VAL  | CA-C-O  | -5.79 | 117.10      | 121.68   |
| 2   | J     | 198 | HIS  | N-CA-C  | -5.79 | 104.60      | 111.03   |
| 3   | E     | 58  | THR  | CA-C-N  | -5.78 | 114.01      | 120.14   |
| 3   | E     | 58  | THR  | C-N-CA  | -5.78 | 114.01      | 120.14   |
| 3   | B     | 58  | THR  | CA-C-N  | -5.78 | 114.01      | 120.14   |
| 3   | B     | 58  | THR  | C-N-CA  | -5.78 | 114.01      | 120.14   |
| 3   | H     | 52  | PRO  | N-CA-C  | -5.78 | 106.47      | 114.27   |
| 3   | K     | 58  | THR  | CA-C-N  | -5.77 | 114.02      | 120.14   |
| 3   | K     | 58  | THR  | C-N-CA  | -5.77 | 114.02      | 120.14   |
| 3   | H     | 408 | ALA  | N-CA-C  | 5.76  | 119.48      | 110.32   |
| 2   | G     | 239 | TRP  | N-CA-C  | -5.76 | 101.16      | 110.32   |
| 2   | A     | 239 | TRP  | N-CA-C  | -5.76 | 101.16      | 110.32   |
| 2   | J     | 382 | ILE  | CB-CA-C | -5.75 | 104.48      | 112.02   |
| 3   | B     | 408 | ALA  | N-CA-C  | 5.75  | 119.46      | 110.32   |
| 3   | E     | 408 | ALA  | N-CA-C  | 5.75  | 119.47      | 110.32   |
| 2   | G     | 390 | LYS  | N-CA-C  | -5.75 | 97.79       | 108.02   |
| 2   | J     | 239 | TRP  | N-CA-C  | -5.75 | 101.18      | 110.32   |
| 2   | A     | 382 | ILE  | CB-CA-C | -5.75 | 104.50      | 112.02   |
| 2   | J     | 390 | LYS  | N-CA-C  | -5.75 | 97.80       | 108.02   |
| 3   | H     | 58  | THR  | CA-C-N  | -5.75 | 114.05      | 120.14   |
| 3   | H     | 58  | THR  | C-N-CA  | -5.75 | 114.05      | 120.14   |
| 2   | G     | 382 | ILE  | CB-CA-C | -5.74 | 104.50      | 112.02   |
| 2   | A     | 390 | LYS  | N-CA-C  | -5.74 | 97.81       | 108.02   |
| 3   | K     | 408 | ALA  | N-CA-C  | 5.74  | 119.44      | 110.32   |
| 2   | D     | 239 | TRP  | N-CA-C  | -5.73 | 101.21      | 110.32   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 390 | LYS  | N-CA-C  | -5.73 | 97.81       | 108.02   |
| 2   | D     | 382 | ILE  | CB-CA-C | -5.73 | 104.52      | 112.02   |
| 2   | A     | 360 | ALA  | N-CA-C  | -5.68 | 106.18      | 113.23   |
| 2   | D     | 360 | ALA  | N-CA-C  | -5.67 | 106.19      | 113.23   |
| 2   | G     | 360 | ALA  | N-CA-C  | -5.66 | 106.21      | 113.23   |
| 2   | J     | 360 | ALA  | N-CA-C  | -5.65 | 106.22      | 113.23   |
| 2   | A     | 75  | VAL  | N-CA-C  | 5.63  | 117.43      | 108.87   |
| 2   | D     | 75  | VAL  | N-CA-C  | 5.63  | 117.43      | 108.87   |
| 2   | G     | 75  | VAL  | N-CA-C  | 5.62  | 117.41      | 108.87   |
| 2   | J     | 75  | VAL  | N-CA-C  | 5.59  | 117.37      | 108.87   |
| 3   | H     | 344 | GLU  | CA-C-N  | 5.58  | 125.90      | 119.93   |
| 3   | H     | 344 | GLU  | C-N-CA  | 5.58  | 125.90      | 119.93   |
| 3   | K     | 344 | GLU  | CA-C-N  | 5.56  | 125.88      | 119.93   |
| 3   | K     | 344 | GLU  | C-N-CA  | 5.56  | 125.88      | 119.93   |
| 3   | H     | 131 | THR  | N-CA-C  | 5.56  | 117.45      | 108.34   |
| 3   | K     | 335 | GLY  | N-CA-C  | -5.56 | 105.26      | 114.48   |
| 3   | B     | 344 | GLU  | CA-C-N  | 5.55  | 125.87      | 119.93   |
| 3   | B     | 344 | GLU  | C-N-CA  | 5.55  | 125.87      | 119.93   |
| 3   | E     | 335 | GLY  | N-CA-C  | -5.54 | 105.28      | 114.48   |
| 3   | K     | 21  | VAL  | N-CA-C  | 5.54  | 116.56      | 108.58   |
| 3   | B     | 335 | GLY  | N-CA-C  | -5.54 | 105.28      | 114.48   |
| 3   | E     | 21  | VAL  | N-CA-C  | 5.54  | 116.56      | 108.58   |
| 2   | A     | 7   | THR  | N-CA-C  | 5.54  | 118.95      | 110.20   |
| 3   | B     | 131 | THR  | N-CA-C  | 5.54  | 117.42      | 108.34   |
| 2   | J     | 7   | THR  | N-CA-C  | 5.54  | 118.95      | 110.20   |
| 3   | H     | 21  | VAL  | N-CA-C  | 5.53  | 116.55      | 108.58   |
| 2   | D     | 7   | THR  | N-CA-C  | 5.53  | 118.94      | 110.20   |
| 2   | J     | 458 | VAL  | N-CA-C  | -5.53 | 100.32      | 108.23   |
| 3   | K     | 131 | THR  | N-CA-C  | 5.53  | 117.41      | 108.34   |
| 3   | E     | 131 | THR  | N-CA-C  | 5.53  | 117.40      | 108.34   |
| 3   | B     | 21  | VAL  | N-CA-C  | 5.52  | 116.53      | 108.58   |
| 2   | A     | 458 | VAL  | N-CA-C  | -5.52 | 100.34      | 108.23   |
| 2   | G     | 7   | THR  | N-CA-C  | 5.52  | 118.92      | 110.20   |
| 3   | H     | 335 | GLY  | N-CA-C  | -5.51 | 105.33      | 114.48   |
| 2   | D     | 458 | VAL  | N-CA-C  | -5.51 | 100.35      | 108.23   |
| 2   | G     | 458 | VAL  | N-CA-C  | -5.51 | 100.35      | 108.23   |
| 3   | E     | 344 | GLU  | CA-C-N  | 5.51  | 125.82      | 119.93   |
| 3   | E     | 344 | GLU  | C-N-CA  | 5.51  | 125.82      | 119.93   |
| 2   | A     | 318 | TYR  | CA-C-N  | -5.50 | 115.00      | 123.14   |
| 2   | A     | 318 | TYR  | C-N-CA  | -5.50 | 115.00      | 123.14   |
| 2   | J     | 175 | ASN  | CA-C-N  | 5.50  | 126.71      | 119.84   |
| 2   | J     | 175 | ASN  | C-N-CA  | 5.50  | 126.71      | 119.84   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | A     | 175 | ASN  | CA-C-N  | 5.50  | 126.71      | 119.84   |
| 2   | A     | 175 | ASN  | C-N-CA  | 5.50  | 126.71      | 119.84   |
| 3   | E     | 419 | THR  | N-CA-C  | 5.50  | 117.39      | 109.48   |
| 2   | G     | 318 | TYR  | CA-C-N  | -5.49 | 115.01      | 123.14   |
| 2   | G     | 318 | TYR  | C-N-CA  | -5.49 | 115.01      | 123.14   |
| 2   | G     | 175 | ASN  | CA-C-N  | 5.49  | 126.70      | 119.84   |
| 2   | G     | 175 | ASN  | C-N-CA  | 5.49  | 126.70      | 119.84   |
| 3   | H     | 419 | THR  | N-CA-C  | 5.49  | 117.38      | 109.48   |
| 2   | D     | 175 | ASN  | CA-C-N  | 5.48  | 126.69      | 119.84   |
| 2   | D     | 175 | ASN  | C-N-CA  | 5.48  | 126.69      | 119.84   |
| 2   | J     | 318 | TYR  | CA-C-N  | -5.48 | 115.04      | 123.14   |
| 2   | J     | 318 | TYR  | C-N-CA  | -5.48 | 115.04      | 123.14   |
| 3   | B     | 419 | THR  | N-CA-C  | 5.47  | 117.35      | 109.48   |
| 3   | K     | 419 | THR  | N-CA-C  | 5.47  | 117.35      | 109.48   |
| 2   | D     | 318 | TYR  | CA-C-N  | -5.45 | 115.07      | 123.14   |
| 2   | D     | 318 | TYR  | C-N-CA  | -5.45 | 115.07      | 123.14   |
| 2   | G     | 234 | LEU  | N-CA-C  | 5.44  | 118.03      | 108.56   |
| 2   | A     | 234 | LEU  | N-CA-C  | 5.44  | 118.03      | 108.56   |
| 2   | J     | 234 | LEU  | N-CA-C  | 5.43  | 118.01      | 108.56   |
| 3   | H     | 252 | TRP  | N-CA-C  | 5.43  | 117.32      | 108.63   |
| 2   | D     | 234 | LEU  | N-CA-C  | 5.43  | 118.00      | 108.56   |
| 2   | D     | 139 | THR  | O-C-N   | 5.42  | 126.88      | 121.30   |
| 2   | D     | 495 | ILE  | CB-CA-C | 5.42  | 119.36      | 110.69   |
| 3   | E     | 252 | TRP  | N-CA-C  | 5.42  | 117.30      | 108.63   |
| 2   | G     | 495 | ILE  | CB-CA-C | 5.41  | 119.35      | 110.69   |
| 3   | H     | 343 | GLN  | N-CA-C  | -5.41 | 105.48      | 112.68   |
| 2   | A     | 495 | ILE  | CB-CA-C | 5.41  | 119.35      | 110.69   |
| 3   | E     | 265 | ASN  | N-CA-C  | -5.41 | 105.02      | 111.03   |
| 3   | B     | 343 | GLN  | N-CA-C  | -5.41 | 105.49      | 112.68   |
| 3   | B     | 265 | ASN  | N-CA-C  | -5.41 | 105.03      | 111.03   |
| 2   | A     | 139 | THR  | O-C-N   | 5.40  | 126.86      | 121.30   |
| 3   | H     | 265 | ASN  | N-CA-C  | -5.40 | 105.03      | 111.03   |
| 3   | B     | 252 | TRP  | N-CA-C  | 5.40  | 117.27      | 108.63   |
| 3   | E     | 343 | GLN  | N-CA-C  | -5.40 | 105.50      | 112.68   |
| 2   | J     | 495 | ILE  | CB-CA-C | 5.40  | 119.32      | 110.69   |
| 3   | K     | 252 | TRP  | N-CA-C  | 5.39  | 117.26      | 108.63   |
| 3   | K     | 265 | ASN  | N-CA-C  | -5.39 | 105.05      | 111.03   |
| 3   | K     | 343 | GLN  | N-CA-C  | -5.39 | 105.51      | 112.68   |
| 2   | G     | 139 | THR  | O-C-N   | 5.39  | 126.85      | 121.30   |
| 2   | J     | 139 | THR  | O-C-N   | 5.38  | 126.84      | 121.30   |
| 2   | J     | 317 | VAL  | CB-CA-C | -5.34 | 103.76      | 112.03   |
| 2   | D     | 317 | VAL  | CB-CA-C | -5.33 | 103.77      | 112.03   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | G     | 317 | VAL  | CB-CA-C   | -5.33 | 103.78      | 112.03   |
| 3   | H     | 167 | ILE  | CB-CA-C   | -5.32 | 104.96      | 112.14   |
| 1   | L     | 26  | A    | OP2-P-O3' | -5.31 | 92.07       | 108.00   |
| 2   | A     | 317 | VAL  | CB-CA-C   | -5.31 | 103.80      | 112.03   |
| 1   | C     | 26  | A    | OP2-P-O3' | -5.31 | 92.08       | 108.00   |
| 1   | F     | 26  | A    | OP2-P-O3' | -5.30 | 92.10       | 108.00   |
| 3   | E     | 167 | ILE  | CB-CA-C   | -5.30 | 104.98      | 112.14   |
| 1   | I     | 26  | A    | OP2-P-O3' | -5.30 | 92.10       | 108.00   |
| 3   | K     | 167 | ILE  | CB-CA-C   | -5.30 | 104.98      | 112.14   |
| 3   | H     | 177 | ASP  | N-CA-C    | 5.29  | 119.47      | 108.53   |
| 3   | B     | 167 | ILE  | CB-CA-C   | -5.29 | 105.00      | 112.14   |
| 3   | K     | 177 | ASP  | N-CA-C    | 5.28  | 119.47      | 108.53   |
| 3   | B     | 177 | ASP  | N-CA-C    | 5.27  | 119.44      | 108.53   |
| 3   | E     | 177 | ASP  | N-CA-C    | 5.26  | 119.42      | 108.53   |
| 2   | D     | 467 | VAL  | CB-CA-C   | -5.23 | 101.85      | 111.36   |
| 2   | A     | 467 | VAL  | CB-CA-C   | -5.22 | 101.86      | 111.36   |
| 3   | H     | 419 | THR  | CA-C-N    | 5.22  | 125.75      | 120.38   |
| 3   | H     | 419 | THR  | C-N-CA    | 5.22  | 125.75      | 120.38   |
| 2   | D     | 414 | TRP  | N-CA-CB   | -5.21 | 102.31      | 109.97   |
| 2   | G     | 467 | VAL  | CB-CA-C   | -5.21 | 101.88      | 111.36   |
| 2   | G     | 414 | TRP  | N-CA-CB   | -5.20 | 102.32      | 109.97   |
| 2   | J     | 467 | VAL  | CB-CA-C   | -5.20 | 101.89      | 111.36   |
| 2   | J     | 414 | TRP  | N-CA-CB   | -5.20 | 102.32      | 109.97   |
| 3   | B     | 419 | THR  | CA-C-N    | 5.20  | 125.74      | 120.38   |
| 3   | B     | 419 | THR  | C-N-CA    | 5.20  | 125.74      | 120.38   |
| 2   | A     | 414 | TRP  | N-CA-CB   | -5.20 | 102.33      | 109.97   |
| 3   | K     | 142 | ILE  | N-CA-C    | -5.19 | 101.11      | 108.58   |
| 3   | E     | 142 | ILE  | N-CA-C    | -5.18 | 101.11      | 108.58   |
| 3   | H     | 142 | ILE  | N-CA-C    | -5.18 | 101.11      | 108.58   |
| 3   | B     | 142 | ILE  | N-CA-C    | -5.18 | 101.12      | 108.58   |
| 3   | K     | 419 | THR  | CA-C-N    | 5.17  | 125.71      | 120.38   |
| 3   | K     | 419 | THR  | C-N-CA    | 5.17  | 125.71      | 120.38   |
| 3   | E     | 419 | THR  | CA-C-N    | 5.16  | 125.70      | 120.38   |
| 3   | E     | 419 | THR  | C-N-CA    | 5.16  | 125.70      | 120.38   |
| 3   | K     | 318 | TYR  | CA-C-N    | -5.16 | 114.83      | 122.41   |
| 3   | K     | 318 | TYR  | C-N-CA    | -5.16 | 114.83      | 122.41   |
| 2   | D     | 319 | TYR  | N-CA-C    | 5.15  | 117.77      | 107.62   |
| 3   | H     | 302 | GLU  | N-CA-C    | 5.15  | 116.58      | 111.07   |
| 3   | B     | 318 | TYR  | CA-C-N    | -5.15 | 114.85      | 122.41   |
| 3   | B     | 318 | TYR  | C-N-CA    | -5.15 | 114.85      | 122.41   |
| 3   | H     | 118 | VAL  | CB-CA-C   | -5.14 | 104.76      | 110.68   |
| 3   | E     | 320 | ASP  | CA-C-N    | 5.13  | 126.26      | 119.84   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | E     | 320 | ASP  | C-N-CA    | 5.13  | 126.26      | 119.84   |
| 3   | E     | 318 | TYR  | CA-C-N    | -5.13 | 114.86      | 122.41   |
| 3   | E     | 318 | TYR  | C-N-CA    | -5.13 | 114.86      | 122.41   |
| 2   | A     | 319 | TYR  | N-CA-C    | 5.13  | 117.73      | 107.62   |
| 3   | H     | 318 | TYR  | CA-C-N    | -5.13 | 114.87      | 122.41   |
| 3   | H     | 318 | TYR  | C-N-CA    | -5.13 | 114.87      | 122.41   |
| 3   | K     | 302 | GLU  | N-CA-C    | 5.13  | 116.56      | 111.07   |
| 3   | B     | 302 | GLU  | N-CA-C    | 5.13  | 116.56      | 111.07   |
| 2   | G     | 319 | TYR  | N-CA-C    | 5.12  | 117.71      | 107.62   |
| 2   | J     | 319 | TYR  | N-CA-C    | 5.12  | 117.71      | 107.62   |
| 3   | E     | 271 | TYR  | CA-C-N    | 5.12  | 126.24      | 119.84   |
| 3   | E     | 271 | TYR  | C-N-CA    | 5.12  | 126.24      | 119.84   |
| 3   | B     | 118 | VAL  | CB-CA-C   | -5.11 | 104.80      | 110.68   |
| 3   | K     | 271 | TYR  | CA-C-N    | 5.11  | 126.23      | 119.84   |
| 3   | K     | 271 | TYR  | C-N-CA    | 5.11  | 126.23      | 119.84   |
| 3   | B     | 151 | GLN  | N-CA-C    | 5.11  | 117.25      | 111.02   |
| 3   | K     | 151 | GLN  | N-CA-C    | 5.11  | 117.25      | 111.02   |
| 3   | E     | 118 | VAL  | CB-CA-C   | -5.10 | 104.81      | 110.68   |
| 3   | K     | 118 | VAL  | CB-CA-C   | -5.10 | 104.81      | 110.68   |
| 3   | E     | 151 | GLN  | N-CA-C    | 5.09  | 117.24      | 111.02   |
| 3   | E     | 302 | GLU  | N-CA-C    | 5.09  | 116.52      | 111.07   |
| 3   | H     | 151 | GLN  | N-CA-C    | 5.09  | 117.23      | 111.02   |
| 2   | J     | 193 | LEU  | N-CA-C    | 5.09  | 116.72      | 109.14   |
| 3   | E     | 73  | LYS  | N-CA-C    | -5.09 | 102.16      | 110.20   |
| 3   | B     | 320 | ASP  | CA-C-N    | 5.08  | 126.20      | 119.84   |
| 3   | B     | 320 | ASP  | C-N-CA    | 5.08  | 126.20      | 119.84   |
| 3   | H     | 271 | TYR  | CA-C-N    | 5.08  | 126.19      | 119.84   |
| 3   | H     | 271 | TYR  | C-N-CA    | 5.08  | 126.19      | 119.84   |
| 1   | C     | 27  | A    | O5'-P-OP1 | 5.08  | 123.24      | 108.00   |
| 1   | L     | 27  | A    | O5'-P-OP1 | 5.08  | 123.24      | 108.00   |
| 1   | I     | 27  | A    | O5'-P-OP1 | 5.08  | 123.23      | 108.00   |
| 3   | B     | 271 | TYR  | CA-C-N    | 5.08  | 126.18      | 119.84   |
| 3   | B     | 271 | TYR  | C-N-CA    | 5.08  | 126.18      | 119.84   |
| 3   | H     | 320 | ASP  | CA-C-N    | 5.07  | 126.18      | 119.84   |
| 3   | H     | 320 | ASP  | C-N-CA    | 5.07  | 126.18      | 119.84   |
| 3   | K     | 178 | ILE  | N-CA-C    | -5.07 | 98.79       | 109.34   |
| 1   | F     | 27  | A    | O5'-P-OP1 | 5.07  | 123.21      | 108.00   |
| 2   | D     | 235 | HIS  | N-CA-C    | -5.07 | 102.90      | 110.20   |
| 3   | K     | 73  | LYS  | N-CA-C    | -5.07 | 102.19      | 110.20   |
| 2   | A     | 235 | HIS  | N-CA-C    | -5.07 | 102.91      | 110.20   |
| 3   | B     | 73  | LYS  | N-CA-C    | -5.07 | 102.20      | 110.20   |
| 3   | K     | 320 | ASP  | CA-C-N    | 5.06  | 126.17      | 119.84   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | K     | 320 | ASP  | C-N-CA | 5.06  | 126.17      | 119.84   |
| 2   | A     | 193 | LEU  | N-CA-C | 5.06  | 116.68      | 109.14   |
| 3   | H     | 73  | LYS  | N-CA-C | -5.06 | 102.21      | 110.20   |
| 3   | B     | 178 | ILE  | N-CA-C | -5.06 | 98.82       | 109.34   |
| 2   | D     | 193 | LEU  | N-CA-C | 5.06  | 116.68      | 109.14   |
| 2   | D     | 425 | LEU  | N-CA-C | -5.06 | 100.54      | 108.63   |
| 2   | G     | 235 | HIS  | N-CA-C | -5.06 | 102.92      | 110.20   |
| 3   | H     | 178 | ILE  | N-CA-C | -5.06 | 98.82       | 109.34   |
| 2   | J     | 235 | HIS  | N-CA-C | -5.05 | 102.92      | 110.20   |
| 2   | A     | 425 | LEU  | N-CA-C | -5.05 | 100.55      | 108.63   |
| 3   | E     | 178 | ILE  | N-CA-C | -5.05 | 98.84       | 109.34   |
| 2   | G     | 193 | LEU  | N-CA-C | 5.05  | 116.66      | 109.14   |
| 2   | J     | 425 | LEU  | N-CA-C | -5.04 | 100.56      | 108.63   |
| 2   | J     | 58  | THR  | CA-C-N | 5.03  | 124.93      | 119.85   |
| 2   | J     | 58  | THR  | C-N-CA | 5.03  | 124.93      | 119.85   |
| 2   | G     | 72  | ARG  | O-C-N  | -5.02 | 116.70      | 122.87   |
| 3   | K     | 198 | HIS  | N-CA-C | -5.02 | 104.77      | 111.24   |
| 2   | G     | 425 | LEU  | N-CA-C | -5.01 | 100.61      | 108.63   |
| 3   | H     | 198 | HIS  | N-CA-C | -5.01 | 104.78      | 111.24   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | A     | 319 | TYR  | Mainchain |
| 2   | D     | 319 | TYR  | Mainchain |
| 2   | G     | 319 | TYR  | Mainchain |
| 2   | J     | 319 | TYR  | Mainchain |

## 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   | C     | 638   | 0        | 323      | 38      | 0            |
| 1   | F     | 638   | 0        | 323      | 39      | 0            |
| 1   | I     | 638   | 0        | 323      | 37      | 0            |
| 1   | L     | 638   | 0        | 323      | 37      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | A     | 2737  | 0        | 1181     | 58      | 0            |
| 2   | D     | 2737  | 0        | 1181     | 61      | 0            |
| 2   | G     | 2737  | 0        | 1181     | 56      | 30           |
| 2   | J     | 2737  | 0        | 1181     | 58      | 3            |
| 3   | B     | 1979  | 0        | 832      | 39      | 0            |
| 3   | E     | 1979  | 0        | 832      | 38      | 0            |
| 3   | H     | 1979  | 0        | 832      | 38      | 0            |
| 3   | K     | 1979  | 0        | 832      | 38      | 0            |
| All | All   | 21416 | 0        | 9344     | 486     | 30           |

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 16.

All (486) 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) |
|----------------|---------------|--------------------------|-------------------|
| 2:J:62:ALA:CB  | 2:J:73:LYS:HA | 1.14                     | 1.62              |
| 2:A:62:ALA:CB  | 2:A:73:LYS:HA | 1.14                     | 1.59              |
| 2:D:62:ALA:CB  | 2:D:73:LYS:HA | 1.14                     | 1.57              |
| 2:G:62:ALA:CB  | 2:G:73:LYS:HA | 1.14                     | 1.55              |
| 3:H:62:ALA:C   | 3:H:63:ILE:N  | 1.70                     | 1.49              |
| 3:E:62:ALA:C   | 3:E:63:ILE:N  | 1.70                     | 1.49              |
| 3:K:62:ALA:C   | 3:K:63:ILE:N  | 1.70                     | 1.46              |
| 3:B:62:ALA:C   | 3:B:63:ILE:N  | 1.70                     | 1.45              |
| 2:A:62:ALA:CB  | 2:A:73:LYS:CA | 2.01                     | 1.36              |
| 2:G:62:ALA:CB  | 2:G:73:LYS:CA | 2.01                     | 1.35              |
| 2:J:62:ALA:CB  | 2:J:73:LYS:CA | 2.01                     | 1.35              |
| 2:D:62:ALA:CB  | 2:D:73:LYS:CA | 2.01                     | 1.35              |
| 2:G:62:ALA:HB1 | 2:G:72:ARG:O  | 1.25                     | 1.34              |
| 2:D:62:ALA:HB1 | 2:D:72:ARG:O  | 1.25                     | 1.33              |
| 3:E:70:LYS:C   | 3:E:71:TRP:N  | 1.90                     | 1.29              |
| 3:B:70:LYS:C   | 3:B:71:TRP:N  | 1.90                     | 1.29              |
| 2:A:62:ALA:HB1 | 2:A:72:ARG:O  | 1.25                     | 1.29              |
| 3:H:70:LYS:C   | 3:H:71:TRP:N  | 1.90                     | 1.29              |
| 3:K:70:LYS:C   | 3:K:71:TRP:N  | 1.90                     | 1.28              |
| 2:J:62:ALA:HB1 | 2:J:72:ARG:O  | 1.25                     | 1.24              |
| 2:D:62:ALA:HB2 | 2:D:73:LYS:CA | 1.67                     | 1.20              |
| 2:J:62:ALA:HB2 | 2:J:73:LYS:CA | 1.67                     | 1.19              |
| 2:G:62:ALA:HB2 | 2:G:73:LYS:CA | 1.67                     | 1.19              |
| 2:G:62:ALA:HB1 | 2:G:72:ARG:C  | 1.69                     | 1.18              |
| 2:J:62:ALA:HB1 | 2:J:72:ARG:C  | 1.69                     | 1.17              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 2:A:62:ALA:HB1 | 2:A:72:ARG:C   | 1.69                     | 1.17              |
| 2:D:62:ALA:HB1 | 2:D:72:ARG:C   | 1.69                     | 1.16              |
| 2:A:62:ALA:HB2 | 2:A:73:LYS:CA  | 1.67                     | 1.16              |
| 2:G:62:ALA:HB3 | 2:G:73:LYS:HA  | 1.36                     | 1.08              |
| 2:D:62:ALA:HB3 | 2:D:73:LYS:HA  | 1.36                     | 1.07              |
| 2:A:62:ALA:HB3 | 2:A:73:LYS:HA  | 1.36                     | 1.06              |
| 1:I:17:A:O2'   | 2:G:275:LYS:CB | 2.04                     | 1.06              |
| 1:L:17:A:O2'   | 2:J:275:LYS:CB | 2.04                     | 1.06              |
| 2:J:62:ALA:HB3 | 2:J:73:LYS:HA  | 1.36                     | 1.06              |
| 1:C:17:A:O2'   | 2:A:275:LYS:CB | 2.04                     | 1.05              |
| 1:F:17:A:O2'   | 2:D:275:LYS:CB | 2.04                     | 1.04              |
| 2:D:62:ALA:CB  | 2:D:72:ARG:O   | 2.06                     | 1.04              |
| 2:A:62:ALA:CB  | 2:A:72:ARG:O   | 2.06                     | 1.03              |
| 1:C:32:A:O2'   | 2:A:265:ASN:CB | 2.06                     | 1.03              |
| 1:L:32:A:O2'   | 2:J:265:ASN:CB | 2.06                     | 1.03              |
| 1:F:32:A:O2'   | 2:D:265:ASN:CB | 2.06                     | 1.02              |
| 1:I:32:A:O2'   | 2:G:265:ASN:CB | 2.06                     | 1.02              |
| 2:G:62:ALA:CB  | 2:G:72:ARG:O   | 2.06                     | 1.02              |
| 2:J:62:ALA:CB  | 2:J:72:ARG:O   | 2.06                     | 1.02              |
| 2:G:133:PRO:O  | 2:G:135:ILE:N  | 2.03                     | 0.91              |
| 2:D:133:PRO:O  | 2:D:135:ILE:N  | 2.03                     | 0.91              |
| 2:A:133:PRO:O  | 2:A:135:ILE:N  | 2.03                     | 0.90              |
| 2:J:133:PRO:O  | 2:J:135:ILE:N  | 2.03                     | 0.90              |
| 1:C:25:A:HO2'  | 1:C:26:A:H8    | 0.95                     | 0.90              |
| 1:I:25:A:HO2'  | 1:I:26:A:H8    | 0.94                     | 0.90              |
| 1:L:25:A:HO2'  | 1:L:26:A:H8    | 0.96                     | 0.90              |
| 1:F:25:A:HO2'  | 1:F:26:A:H8    | 0.93                     | 0.90              |
| 2:D:62:ALA:HB1 | 2:D:73:LYS:HA  | 1.55                     | 0.88              |
| 1:I:23:G:H1'   | 1:I:26:A:C2    | 2.10                     | 0.87              |
| 1:C:23:G:H1'   | 1:C:26:A:C2    | 2.10                     | 0.86              |
| 1:F:23:G:H1'   | 1:F:26:A:C2    | 2.10                     | 0.86              |
| 1:L:23:G:H1'   | 1:L:26:A:C2    | 2.10                     | 0.86              |
| 2:G:62:ALA:HB1 | 2:G:73:LYS:HA  | 1.55                     | 0.85              |
| 3:B:70:LYS:CB  | 3:B:71:TRP:N   | 2.40                     | 0.85              |
| 3:H:70:LYS:CB  | 3:H:71:TRP:N   | 2.40                     | 0.84              |
| 3:K:70:LYS:CB  | 3:K:71:TRP:N   | 2.40                     | 0.84              |
| 3:E:70:LYS:CB  | 3:E:71:TRP:N   | 2.40                     | 0.84              |
| 1:C:23:G:O2'   | 1:C:24:A:H5'   | 1.77                     | 0.83              |
| 1:L:23:G:O2'   | 1:L:24:A:H5'   | 1.77                     | 0.83              |
| 1:F:25:A:O2'   | 1:F:26:A:H5''  | 1.79                     | 0.83              |
| 1:I:23:G:O2'   | 1:I:24:A:H5'   | 1.77                     | 0.83              |

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| Atom-1         | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|---------------|--------------------------|-------------------|
| 1:I:25:A:O2'   | 1:I:26:A:H5'' | 1.79                     | 0.82              |
| 2:J:62:ALA:HB1 | 2:J:73:LYS:HA | 1.56                     | 0.82              |
| 1:F:23:G:O2'   | 1:F:24:A:H5'  | 1.77                     | 0.82              |
| 1:C:25:A:O2'   | 1:C:26:A:H5'' | 1.79                     | 0.82              |
| 1:L:25:A:O2'   | 1:L:26:A:H5'' | 1.78                     | 0.82              |
| 2:D:62:ALA:HB1 | 2:D:73:LYS:N  | 2.00                     | 0.77              |
| 2:A:62:ALA:HB1 | 2:A:73:LYS:N  | 2.00                     | 0.77              |
| 2:G:62:ALA:HB1 | 2:G:73:LYS:N  | 2.00                     | 0.77              |
| 2:D:95:PRO:CA  | 3:E:136:ASN:O | 2.33                     | 0.76              |
| 2:G:62:ALA:HB1 | 2:G:73:LYS:CA | 2.10                     | 0.76              |
| 2:A:95:PRO:CA  | 3:B:136:ASN:O | 2.33                     | 0.76              |
| 2:G:62:ALA:HB2 | 2:G:73:LYS:HA | 0.76                     | 0.76              |
| 2:J:62:ALA:HB2 | 2:J:73:LYS:HA | 0.76                     | 0.76              |
| 2:D:62:ALA:HB2 | 2:D:73:LYS:HA | 0.76                     | 0.76              |
| 2:G:62:ALA:HB3 | 2:G:73:LYS:CA | 2.00                     | 0.76              |
| 2:A:95:PRO:HA  | 3:B:136:ASN:O | 1.86                     | 0.75              |
| 2:G:95:PRO:CA  | 3:H:136:ASN:O | 2.33                     | 0.75              |
| 2:J:62:ALA:HB1 | 2:J:73:LYS:N  | 2.00                     | 0.75              |
| 2:J:95:PRO:CA  | 3:K:136:ASN:O | 2.33                     | 0.75              |
| 2:G:95:PRO:HA  | 3:H:136:ASN:O | 1.86                     | 0.75              |
| 2:A:62:ALA:HB2 | 2:A:73:LYS:HA | 0.76                     | 0.75              |
| 2:D:95:PRO:HA  | 3:E:136:ASN:O | 1.86                     | 0.75              |
| 2:J:95:PRO:HA  | 3:K:136:ASN:O | 1.86                     | 0.75              |
| 2:A:137:ASN:C  | 2:A:139:THR:H | 1.96                     | 0.73              |
| 2:G:137:ASN:C  | 2:G:139:THR:H | 1.96                     | 0.73              |
| 2:D:137:ASN:C  | 2:D:139:THR:H | 1.96                     | 0.73              |
| 2:J:137:ASN:C  | 2:J:139:THR:H | 1.96                     | 0.73              |
| 2:A:62:ALA:HB3 | 2:A:73:LYS:CA | 2.00                     | 0.72              |
| 2:G:135:ILE:O  | 2:G:137:ASN:N | 2.24                     | 0.71              |
| 2:J:135:ILE:O  | 2:J:137:ASN:N | 2.24                     | 0.71              |
| 2:G:95:PRO:CB  | 3:H:136:ASN:O | 2.39                     | 0.71              |
| 2:D:135:ILE:O  | 2:D:137:ASN:N | 2.24                     | 0.70              |
| 1:C:25:A:O2'   | 1:C:26:A:H8   | 1.73                     | 0.70              |
| 2:A:135:ILE:O  | 2:A:137:ASN:N | 2.24                     | 0.70              |
| 2:D:95:PRO:CB  | 3:E:136:ASN:O | 2.39                     | 0.70              |
| 2:J:95:PRO:CB  | 3:K:136:ASN:O | 2.39                     | 0.70              |
| 2:A:95:PRO:CB  | 3:B:136:ASN:O | 2.39                     | 0.70              |
| 2:J:62:ALA:HB3 | 2:J:73:LYS:CA | 2.00                     | 0.69              |
| 1:C:10:C:H1'   | 1:C:27:A:N6   | 2.08                     | 0.69              |
| 1:L:25:A:O2'   | 1:L:26:A:H8   | 1.73                     | 0.69              |
| 2:D:62:ALA:HB3 | 2:D:73:LYS:CA | 2.00                     | 0.68              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 2:D:221:HIS:O  | 2:D:223:LYS:N  | 2.26                     | 0.68              |
| 1:L:10:C:H1'   | 1:L:27:A:N6    | 2.08                     | 0.68              |
| 2:J:62:ALA:CB  | 2:J:73:LYS:N   | 2.57                     | 0.68              |
| 1:F:10:C:H1'   | 1:F:27:A:N6    | 2.08                     | 0.68              |
| 1:I:10:C:H1'   | 1:I:27:A:N6    | 2.08                     | 0.68              |
| 2:G:221:HIS:O  | 2:G:223:LYS:N  | 2.26                     | 0.68              |
| 2:G:62:ALA:CB  | 2:G:73:LYS:N   | 2.57                     | 0.68              |
| 2:A:221:HIS:O  | 2:A:223:LYS:N  | 2.27                     | 0.68              |
| 2:A:62:ALA:CB  | 2:A:73:LYS:N   | 2.57                     | 0.67              |
| 2:J:221:HIS:O  | 2:J:223:LYS:N  | 2.27                     | 0.67              |
| 1:I:25:A:O2'   | 1:I:26:A:H8    | 1.73                     | 0.67              |
| 1:I:32:A:HO2'  | 2:G:265:ASN:CB | 2.09                     | 0.66              |
| 1:F:25:A:O2'   | 1:F:26:A:H8    | 1.73                     | 0.65              |
| 2:D:62:ALA:CB  | 2:D:73:LYS:N   | 2.57                     | 0.65              |
| 2:A:328:GLU:O  | 2:A:339:TYR:HA | 1.97                     | 0.65              |
| 2:J:328:GLU:O  | 2:J:339:TYR:HA | 1.97                     | 0.65              |
| 2:D:328:GLU:O  | 2:D:339:TYR:HA | 1.97                     | 0.64              |
| 2:G:328:GLU:O  | 2:G:339:TYR:HA | 1.97                     | 0.64              |
| 2:D:62:ALA:HB3 | 2:D:73:LYS:CB  | 2.28                     | 0.64              |
| 1:C:5:G:H2'    | 1:C:6:A:O4'    | 1.99                     | 0.63              |
| 1:L:5:G:H2'    | 1:L:6:A:O4'    | 1.99                     | 0.63              |
| 2:G:62:ALA:HB3 | 2:G:73:LYS:CB  | 2.29                     | 0.63              |
| 2:A:62:ALA:HB3 | 2:A:73:LYS:CB  | 2.29                     | 0.63              |
| 2:J:61:PHE:O   | 2:J:62:ALA:HB2 | 1.99                     | 0.63              |
| 1:F:5:G:H2'    | 1:F:6:A:O4'    | 1.99                     | 0.62              |
| 2:D:62:ALA:HB1 | 2:D:73:LYS:CA  | 2.10                     | 0.62              |
| 2:G:61:PHE:O   | 2:G:62:ALA:HB2 | 1.99                     | 0.62              |
| 2:G:93:GLY:O   | 3:H:137:ASN:CB | 2.47                     | 0.62              |
| 2:D:61:PHE:O   | 2:D:62:ALA:HB2 | 1.99                     | 0.62              |
| 2:J:93:GLY:O   | 3:K:137:ASN:CB | 2.47                     | 0.62              |
| 2:A:93:GLY:O   | 3:B:137:ASN:CB | 2.47                     | 0.62              |
| 1:I:5:G:H2'    | 1:I:6:A:O4'    | 1.99                     | 0.62              |
| 2:J:62:ALA:HB3 | 2:J:73:LYS:CB  | 2.29                     | 0.62              |
| 2:A:61:PHE:O   | 2:A:62:ALA:HB2 | 1.99                     | 0.61              |
| 2:D:93:GLY:O   | 3:E:137:ASN:CB | 2.47                     | 0.61              |
| 2:A:61:PHE:O   | 2:A:62:ALA:CB  | 2.49                     | 0.61              |
| 1:I:8:U:H3     | 1:I:23:G:H1    | 1.49                     | 0.61              |
| 1:L:8:U:H3     | 1:L:23:G:H1    | 1.49                     | 0.61              |
| 3:H:70:LYS:CA  | 3:H:71:TRP:N   | 2.64                     | 0.61              |
| 2:J:61:PHE:O   | 2:J:62:ALA:CB  | 2.49                     | 0.61              |
| 2:D:61:PHE:O   | 2:D:62:ALA:CB  | 2.49                     | 0.60              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:C:9:C:OP1    | 3:B:416:PHE:O   | 2.20                     | 0.60              |
| 3:B:14:PRO:CB  | 2:D:17:ASP:CB   | 2.80                     | 0.60              |
| 3:B:328:GLU:O  | 3:B:339:TYR:HA  | 2.02                     | 0.60              |
| 1:I:9:C:OP1    | 3:H:416:PHE:O   | 2.20                     | 0.60              |
| 1:L:9:C:OP1    | 3:K:416:PHE:O   | 2.20                     | 0.60              |
| 2:G:61:PHE:O   | 2:G:62:ALA:CB   | 2.49                     | 0.60              |
| 3:H:328:GLU:O  | 3:H:339:TYR:HA  | 2.02                     | 0.60              |
| 3:K:70:LYS:CA  | 3:K:71:TRP:N    | 2.64                     | 0.60              |
| 3:K:328:GLU:O  | 3:K:339:TYR:HA  | 2.02                     | 0.60              |
| 1:F:8:U:H3     | 1:F:23:G:H1     | 1.49                     | 0.60              |
| 1:L:32:A:HO2'  | 2:J:265:ASN:CB  | 2.13                     | 0.60              |
| 3:B:70:LYS:CA  | 3:B:71:TRP:N    | 2.64                     | 0.60              |
| 1:C:8:U:H3     | 1:C:23:G:H1     | 1.49                     | 0.59              |
| 3:E:328:GLU:O  | 3:E:339:TYR:HA  | 2.02                     | 0.59              |
| 2:D:295:LEU:CB | 2:D:299:ALA:HB2 | 2.33                     | 0.59              |
| 3:E:70:LYS:CA  | 3:E:71:TRP:N    | 2.64                     | 0.59              |
| 1:F:9:C:OP1    | 3:E:416:PHE:O   | 2.20                     | 0.59              |
| 2:G:295:LEU:CB | 2:G:299:ALA:HB2 | 2.33                     | 0.59              |
| 2:D:406:TRP:O  | 3:E:331:LYS:CB  | 2.51                     | 0.59              |
| 2:J:295:LEU:CB | 2:J:299:ALA:HB2 | 2.33                     | 0.59              |
| 3:H:97:PRO:C   | 3:H:99:GLY:H    | 2.11                     | 0.59              |
| 2:A:406:TRP:O  | 3:B:331:LYS:CB  | 2.51                     | 0.58              |
| 2:J:406:TRP:O  | 3:K:331:LYS:CB  | 2.51                     | 0.58              |
| 1:F:23:G:H1'   | 1:F:26:A:N1     | 2.18                     | 0.58              |
| 1:I:33:A:OP1   | 2:G:262:GLY:HA2 | 2.04                     | 0.58              |
| 2:G:134:SER:O  | 2:G:136:ASN:N   | 2.37                     | 0.58              |
| 2:G:406:TRP:O  | 3:H:331:LYS:CB  | 2.51                     | 0.58              |
| 3:E:106:VAL:HA | 3:E:190:GLY:HA2 | 1.85                     | 0.58              |
| 1:C:23:G:H1'   | 1:C:26:A:N1     | 2.18                     | 0.58              |
| 1:I:23:G:H1'   | 1:I:26:A:N1     | 2.18                     | 0.58              |
| 3:H:106:VAL:HA | 3:H:190:GLY:HA2 | 1.85                     | 0.58              |
| 1:F:33:A:OP1   | 2:D:262:GLY:HA2 | 2.04                     | 0.58              |
| 1:L:33:A:OP1   | 2:J:262:GLY:HA2 | 2.04                     | 0.58              |
| 2:A:295:LEU:CB | 2:A:299:ALA:HB2 | 2.33                     | 0.57              |
| 2:J:134:SER:O  | 2:J:136:ASN:N   | 2.37                     | 0.57              |
| 3:K:106:VAL:HA | 3:K:190:GLY:HA2 | 1.85                     | 0.57              |
| 1:C:14:U:OP2   | 3:B:21:VAL:HA   | 2.05                     | 0.57              |
| 1:F:14:U:OP2   | 3:E:21:VAL:HA   | 2.05                     | 0.57              |
| 1:F:32:A:HO2'  | 2:D:265:ASN:CB  | 2.15                     | 0.57              |
| 1:L:23:G:H1'   | 1:L:26:A:N1     | 2.18                     | 0.57              |
| 1:I:14:U:OP2   | 3:H:21:VAL:HA   | 2.05                     | 0.57              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:L:4:A:H2'    | 1:L:5:G:C8      | 2.40                     | 0.57              |
| 3:B:106:VAL:HA | 3:B:190:GLY:HA2 | 1.85                     | 0.57              |
| 1:L:14:U:OP2   | 3:K:21:VAL:HA   | 2.04                     | 0.57              |
| 2:A:134:SER:O  | 2:A:136:ASN:N   | 2.37                     | 0.57              |
| 2:D:134:SER:O  | 2:D:136:ASN:N   | 2.37                     | 0.57              |
| 2:J:62:ALA:HB1 | 2:J:73:LYS:CA   | 2.10                     | 0.57              |
| 1:C:4:A:H2'    | 1:C:5:G:C8      | 2.40                     | 0.57              |
| 1:C:33:A:OP1   | 2:A:262:GLY:HA2 | 2.04                     | 0.57              |
| 3:E:97:PRO:C   | 3:E:99:GLY:H    | 2.11                     | 0.57              |
| 2:A:409:THR:O  | 3:B:364:ASP:CB  | 2.54                     | 0.56              |
| 2:D:409:THR:O  | 3:E:364:ASP:CB  | 2.54                     | 0.56              |
| 2:J:409:THR:O  | 3:K:364:ASP:CB  | 2.54                     | 0.56              |
| 1:F:4:A:H2'    | 1:F:5:G:C8      | 2.40                     | 0.56              |
| 1:I:4:A:H2'    | 1:I:5:G:C8      | 2.40                     | 0.56              |
| 3:K:97:PRO:C   | 3:K:99:GLY:H    | 2.11                     | 0.56              |
| 2:G:409:THR:O  | 3:H:364:ASP:CB  | 2.54                     | 0.56              |
| 1:F:23:G:H1'   | 1:F:26:A:H2     | 1.66                     | 0.56              |
| 3:B:97:PRO:C   | 3:B:99:GLY:H    | 2.11                     | 0.56              |
| 1:C:32:A:HO2'  | 2:A:265:ASN:CB  | 2.13                     | 0.55              |
| 3:B:368:LEU:O  | 3:B:371:ALA:HB3 | 2.07                     | 0.55              |
| 3:K:368:LEU:O  | 3:K:371:ALA:HB3 | 2.07                     | 0.55              |
| 3:B:27:THR:C   | 3:B:29:GLU:H    | 2.15                     | 0.55              |
| 3:H:97:PRO:O   | 3:H:98:ALA:HB3  | 2.07                     | 0.55              |
| 3:K:97:PRO:O   | 3:K:98:ALA:HB3  | 2.07                     | 0.55              |
| 1:I:23:G:H1'   | 1:I:26:A:H2     | 1.65                     | 0.54              |
| 3:E:97:PRO:O   | 3:E:98:ALA:HB3  | 2.07                     | 0.54              |
| 3:B:27:THR:O   | 3:B:29:GLU:N    | 2.41                     | 0.54              |
| 3:E:27:THR:C   | 3:E:29:GLU:H    | 2.15                     | 0.54              |
| 3:K:93:GLY:O   | 3:K:94:ILE:O    | 2.26                     | 0.54              |
| 3:E:93:GLY:O   | 3:E:94:ILE:O    | 2.26                     | 0.54              |
| 3:H:93:GLY:O   | 3:H:94:ILE:O    | 2.26                     | 0.54              |
| 3:H:27:THR:C   | 3:H:29:GLU:H    | 2.15                     | 0.54              |
| 3:K:27:THR:C   | 3:K:29:GLU:H    | 2.14                     | 0.54              |
| 3:K:27:THR:O   | 3:K:29:GLU:N    | 2.41                     | 0.54              |
| 1:F:12:U:OP1   | 1:F:28:A:N7     | 2.41                     | 0.54              |
| 3:B:97:PRO:O   | 3:B:98:ALA:HB3  | 2.07                     | 0.53              |
| 1:L:5:G:H2'    | 1:L:6:A:C8      | 2.43                     | 0.53              |
| 3:E:27:THR:O   | 3:E:29:GLU:N    | 2.41                     | 0.53              |
| 3:H:27:THR:O   | 3:H:29:GLU:N    | 2.41                     | 0.53              |
| 3:H:368:LEU:O  | 3:H:371:ALA:HB3 | 2.07                     | 0.53              |
| 3:B:93:GLY:O   | 3:B:94:ILE:O    | 2.26                     | 0.53              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:F:5:G:H2'    | 1:F:6:A:C8      | 2.43                     | 0.53              |
| 1:I:5:G:H2'    | 1:I:6:A:C8      | 2.43                     | 0.53              |
| 1:C:5:G:H2'    | 1:C:6:A:C8      | 2.43                     | 0.53              |
| 1:I:12:U:OP1   | 1:I:28:A:N7     | 2.41                     | 0.53              |
| 3:H:27:THR:C   | 3:H:29:GLU:N    | 2.66                     | 0.53              |
| 3:E:368:LEU:O  | 3:E:371:ALA:HB3 | 2.07                     | 0.53              |
| 1:L:12:U:OP1   | 1:L:28:A:N7     | 2.41                     | 0.53              |
| 1:L:23:G:H1'   | 1:L:26:A:H2     | 1.66                     | 0.53              |
| 1:I:23:G:C1'   | 1:I:26:A:C2     | 2.91                     | 0.52              |
| 2:G:454:LYS:HA | 2:G:467:VAL:O   | 2.10                     | 0.52              |
| 2:D:454:LYS:HA | 2:D:467:VAL:O   | 2.10                     | 0.52              |
| 3:E:27:THR:C   | 3:E:29:GLU:N    | 2.66                     | 0.52              |
| 3:B:27:THR:C   | 3:B:29:GLU:N    | 2.66                     | 0.52              |
| 1:C:12:U:OP1   | 1:C:28:A:N7     | 2.41                     | 0.52              |
| 2:A:454:LYS:HA | 2:A:467:VAL:O   | 2.10                     | 0.52              |
| 3:K:329:ILE:HA | 3:K:338:THR:O   | 2.10                     | 0.52              |
| 1:C:5:G:H2'    | 1:C:6:A:H8      | 1.75                     | 0.52              |
| 3:B:329:ILE:HA | 3:B:338:THR:O   | 2.10                     | 0.52              |
| 2:J:454:LYS:HA | 2:J:467:VAL:O   | 2.10                     | 0.52              |
| 3:E:326:ILE:O  | 3:E:341:ILE:HA  | 2.10                     | 0.51              |
| 1:L:8:U:H2'    | 1:L:9:C:C6      | 2.46                     | 0.51              |
| 3:K:27:THR:C   | 3:K:29:GLU:N    | 2.66                     | 0.51              |
| 1:C:8:U:H2'    | 1:C:9:C:C6      | 2.46                     | 0.51              |
| 1:C:23:G:H1'   | 1:C:26:A:H2     | 1.66                     | 0.51              |
| 3:K:326:ILE:O  | 3:K:341:ILE:HA  | 2.10                     | 0.51              |
| 1:F:8:U:H2'    | 1:F:9:C:C6      | 2.46                     | 0.51              |
| 1:I:30:U:H2'   | 1:I:31:G:C8     | 2.46                     | 0.51              |
| 1:F:5:G:H2'    | 1:F:6:A:H8      | 1.75                     | 0.51              |
| 3:E:329:ILE:HA | 3:E:338:THR:O   | 2.10                     | 0.51              |
| 1:I:6:A:H2'    | 1:I:6:A:N3      | 2.25                     | 0.51              |
| 3:B:326:ILE:O  | 3:B:341:ILE:HA  | 2.10                     | 0.51              |
| 1:C:6:A:N3     | 1:C:6:A:H2'     | 2.25                     | 0.51              |
| 1:I:5:G:H2'    | 1:I:6:A:H8      | 1.75                     | 0.51              |
| 1:I:8:U:H2'    | 1:I:9:C:C6      | 2.46                     | 0.51              |
| 2:J:451:LYS:O  | 2:J:471:ASN:HA  | 2.11                     | 0.51              |
| 1:F:6:A:N3     | 1:F:6:A:H2'     | 2.25                     | 0.51              |
| 1:L:5:G:H2'    | 1:L:6:A:H8      | 1.75                     | 0.51              |
| 1:L:6:A:N3     | 1:L:6:A:H2'     | 2.25                     | 0.51              |
| 2:A:451:LYS:O  | 2:A:471:ASN:HA  | 2.11                     | 0.51              |
| 3:H:329:ILE:HA | 3:H:338:THR:O   | 2.10                     | 0.51              |
| 3:H:135:ILE:C  | 3:H:137:ASN:H   | 2.19                     | 0.50              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 3:H:326:ILE:O  | 3:H:341:ILE:HA | 2.10                     | 0.50              |
| 2:G:451:LYS:O  | 2:G:471:ASN:HA | 2.11                     | 0.50              |
| 1:F:30:U:H2'   | 1:F:31:G:C8    | 2.46                     | 0.50              |
| 2:D:125:ARG:O  | 2:D:126:LYS:C  | 2.55                     | 0.50              |
| 2:J:194:GLU:O  | 2:J:196:GLY:N  | 2.45                     | 0.50              |
| 1:L:30:U:H2'   | 1:L:31:G:C8    | 2.46                     | 0.50              |
| 2:A:125:ARG:O  | 2:A:126:LYS:C  | 2.55                     | 0.50              |
| 2:G:540:LYS:C  | 2:G:542:ILE:H  | 2.20                     | 0.49              |
| 3:K:135:ILE:C  | 3:K:137:ASN:H  | 2.19                     | 0.49              |
| 2:G:125:ARG:O  | 2:G:126:LYS:C  | 2.55                     | 0.49              |
| 1:C:30:U:H2'   | 1:C:31:G:C8    | 2.46                     | 0.49              |
| 1:I:23:G:O2'   | 1:I:26:A:C2    | 2.64                     | 0.49              |
| 2:A:194:GLU:O  | 2:A:196:GLY:N  | 2.45                     | 0.49              |
| 3:B:104:LYS:CB | 3:B:192:ASP:HA | 2.43                     | 0.49              |
| 2:D:451:LYS:O  | 2:D:471:ASN:HA | 2.11                     | 0.49              |
| 2:J:540:LYS:C  | 2:J:542:ILE:H  | 2.20                     | 0.49              |
| 1:F:23:G:C1'   | 1:F:26:A:C2    | 2.91                     | 0.49              |
| 2:D:194:GLU:O  | 2:D:196:GLY:N  | 2.45                     | 0.49              |
| 3:K:104:LYS:CB | 3:K:192:ASP:HA | 2.43                     | 0.49              |
| 3:B:135:ILE:C  | 3:B:137:ASN:H  | 2.19                     | 0.49              |
| 2:G:194:GLU:O  | 2:G:196:GLY:N  | 2.45                     | 0.49              |
| 3:E:104:LYS:CB | 3:E:192:ASP:HA | 2.43                     | 0.49              |
| 3:E:207:GLN:O  | 3:E:208:HIS:C  | 2.56                     | 0.49              |
| 3:E:207:GLN:O  | 3:E:210:LEU:N  | 2.46                     | 0.49              |
| 3:E:135:ILE:C  | 3:E:137:ASN:H  | 2.19                     | 0.49              |
| 3:K:207:GLN:O  | 3:K:210:LEU:N  | 2.46                     | 0.49              |
| 2:J:125:ARG:O  | 2:J:126:LYS:C  | 2.55                     | 0.49              |
| 2:A:540:LYS:C  | 2:A:542:ILE:H  | 2.20                     | 0.49              |
| 1:F:24:A:O2'   | 1:F:25:A:OP2   | 2.31                     | 0.48              |
| 3:B:207:GLN:O  | 3:B:210:LEU:N  | 2.46                     | 0.48              |
| 3:H:207:GLN:O  | 3:H:210:LEU:N  | 2.46                     | 0.48              |
| 3:H:62:ALA:CA  | 3:H:63:ILE:N   | 2.69                     | 0.48              |
| 1:L:29:C:H2'   | 1:L:30:U:C6    | 2.49                     | 0.48              |
| 2:J:543:GLY:C  | 2:J:545:ASN:H  | 2.22                     | 0.48              |
| 1:C:23:G:C1'   | 1:C:26:A:C2    | 2.91                     | 0.48              |
| 2:D:543:GLY:C  | 2:D:545:ASN:H  | 2.22                     | 0.48              |
| 2:G:543:GLY:C  | 2:G:545:ASN:H  | 2.22                     | 0.48              |
| 3:E:62:ALA:CA  | 3:E:63:ILE:N   | 2.68                     | 0.48              |
| 2:A:543:GLY:C  | 2:A:545:ASN:H  | 2.22                     | 0.48              |
| 3:H:104:LYS:CB | 3:H:192:ASP:HA | 2.43                     | 0.48              |
| 3:K:62:ALA:C   | 3:K:63:ILE:CA  | 2.78                     | 0.48              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:29:C:H2'    | 1:C:30:U:C6     | 2.49                     | 0.48              |
| 1:F:29:C:H2'    | 1:F:30:U:C6     | 2.49                     | 0.48              |
| 1:I:29:C:H2'    | 1:I:30:U:C6     | 2.49                     | 0.48              |
| 3:K:207:GLN:O   | 3:K:208:HIS:C   | 2.56                     | 0.47              |
| 3:H:207:GLN:O   | 3:H:208:HIS:C   | 2.56                     | 0.47              |
| 2:A:17:ASP:CB   | 3:E:14:PRO:CB   | 2.92                     | 0.47              |
| 3:B:207:GLN:O   | 3:B:208:HIS:C   | 2.56                     | 0.47              |
| 2:D:540:LYS:C   | 2:D:542:ILE:H   | 2.21                     | 0.47              |
| 3:B:108:VAL:HA  | 3:B:187:LEU:O   | 2.15                     | 0.47              |
| 3:H:108:VAL:HA  | 3:H:187:LEU:O   | 2.15                     | 0.47              |
| 3:E:108:VAL:HA  | 3:E:187:LEU:O   | 2.15                     | 0.47              |
| 3:K:108:VAL:HA  | 3:K:187:LEU:O   | 2.15                     | 0.47              |
| 1:F:15:U:H2'    | 1:F:16:C:C6     | 2.50                     | 0.47              |
| 1:C:15:U:H2'    | 1:C:16:C:C6     | 2.50                     | 0.47              |
| 3:H:62:ALA:C    | 3:H:63:ILE:CA   | 2.78                     | 0.46              |
| 1:L:15:U:H2'    | 1:L:16:C:C6     | 2.50                     | 0.46              |
| 3:B:62:ALA:C    | 3:B:63:ILE:CA   | 2.78                     | 0.46              |
| 3:E:62:ALA:C    | 3:E:63:ILE:CA   | 2.78                     | 0.46              |
| 3:K:62:ALA:CA   | 3:K:63:ILE:N    | 2.68                     | 0.46              |
| 1:I:15:U:H2'    | 1:I:16:C:C6     | 2.50                     | 0.46              |
| 1:L:23:G:C1'    | 1:L:26:A:C2     | 2.91                     | 0.46              |
| 2:D:437:ALA:HB1 | 2:D:493:VAL:HA  | 1.97                     | 0.46              |
| 2:G:445:ALA:O   | 2:G:453:GLY:HA3 | 2.16                     | 0.46              |
| 1:I:24:A:O2'    | 1:I:25:A:OP2    | 2.31                     | 0.46              |
| 2:A:445:ALA:O   | 2:A:453:GLY:HA3 | 2.16                     | 0.45              |
| 2:A:115:TYR:O   | 2:A:117:SER:N   | 2.50                     | 0.45              |
| 2:G:437:ALA:HB1 | 2:G:493:VAL:HA  | 1.97                     | 0.45              |
| 2:J:437:ALA:HB1 | 2:J:493:VAL:HA  | 1.97                     | 0.45              |
| 2:J:445:ALA:O   | 2:J:453:GLY:HA3 | 2.16                     | 0.45              |
| 1:L:4:A:H2'     | 1:L:5:G:H8      | 1.81                     | 0.45              |
| 2:D:115:TYR:O   | 2:D:117:SER:N   | 2.50                     | 0.45              |
| 3:E:390:LYS:HA  | 3:E:415:GLU:O   | 2.17                     | 0.45              |
| 2:A:437:ALA:HB1 | 2:A:493:VAL:HA  | 1.97                     | 0.45              |
| 2:D:445:ALA:O   | 2:D:453:GLY:HA3 | 2.16                     | 0.45              |
| 2:J:115:TYR:O   | 2:J:117:SER:N   | 2.50                     | 0.45              |
| 2:D:327:ALA:HA  | 2:D:340:GLN:O   | 2.17                     | 0.45              |
| 3:H:390:LYS:HA  | 3:H:415:GLU:O   | 2.17                     | 0.45              |
| 1:C:4:A:H2'     | 1:C:5:G:H8      | 1.81                     | 0.45              |
| 2:D:329:ILE:HA  | 2:D:338:THR:O   | 2.17                     | 0.45              |
| 2:J:327:ALA:HA  | 2:J:340:GLN:O   | 2.17                     | 0.45              |
| 1:C:24:A:O2'    | 1:C:25:A:OP2    | 2.31                     | 0.45              |

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| Atom-1         | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|---------------|--------------------------|-------------------|
| 3:B:390:LYS:HA | 3:B:415:GLU:O | 2.17                     | 0.45              |
| 2:A:135:ILE:O  | 2:A:136:ASN:C | 2.60                     | 0.45              |
| 2:A:327:ALA:HA | 2:A:340:GLN:O | 2.17                     | 0.45              |
| 2:D:135:ILE:O  | 2:D:136:ASN:C | 2.60                     | 0.45              |
| 2:G:115:TYR:O  | 2:G:117:SER:N | 2.50                     | 0.45              |
| 2:G:131:THR:HA | 2:G:142:ILE:O | 2.17                     | 0.45              |
| 2:G:135:ILE:O  | 2:G:136:ASN:C | 2.60                     | 0.45              |
| 1:F:23:G:O2'   | 1:F:26:A:C2   | 2.64                     | 0.44              |
| 1:F:4:A:H2'    | 1:F:5:G:H8    | 1.81                     | 0.44              |
| 2:D:194:GLU:C  | 2:D:196:GLY:N | 2.76                     | 0.44              |
| 2:J:131:THR:HA | 2:J:142:ILE:O | 2.17                     | 0.44              |
| 2:A:329:ILE:HA | 2:A:338:THR:O | 2.17                     | 0.44              |
| 3:B:62:ALA:CA  | 3:B:63:ILE:N  | 2.69                     | 0.44              |
| 2:D:131:THR:HA | 2:D:142:ILE:O | 2.17                     | 0.44              |
| 2:G:329:ILE:HA | 2:G:338:THR:O | 2.17                     | 0.44              |
| 2:G:327:ALA:HA | 2:G:340:GLN:O | 2.17                     | 0.44              |
| 3:K:390:LYS:HA | 3:K:415:GLU:O | 2.16                     | 0.44              |
| 2:A:131:THR:HA | 2:A:142:ILE:O | 2.17                     | 0.44              |
| 2:J:135:ILE:O  | 2:J:136:ASN:C | 2.60                     | 0.44              |
| 2:J:329:ILE:HA | 2:J:338:THR:O | 2.17                     | 0.44              |
| 2:A:155:GLY:O  | 2:A:156:SER:C | 2.60                     | 0.44              |
| 2:A:451:LYS:O  | 2:A:471:ASN:N | 2.51                     | 0.44              |
| 2:A:194:GLU:C  | 2:A:196:GLY:N | 2.76                     | 0.44              |
| 1:F:30:U:H2'   | 1:F:31:G:H8   | 1.83                     | 0.43              |
| 2:D:137:ASN:C  | 2:D:139:THR:N | 2.66                     | 0.43              |
| 1:F:11:G:H2'   | 1:F:12:U:OP1  | 2.18                     | 0.43              |
| 1:I:11:G:H2'   | 1:I:12:U:OP1  | 2.18                     | 0.43              |
| 3:B:97:PRO:C   | 3:B:99:GLY:N  | 2.76                     | 0.43              |
| 2:G:155:GLY:O  | 2:G:156:SER:C | 2.60                     | 0.43              |
| 2:J:155:GLY:O  | 2:J:156:SER:C | 2.60                     | 0.43              |
| 2:D:451:LYS:O  | 2:D:471:ASN:N | 2.51                     | 0.43              |
| 2:J:133:PRO:C  | 2:J:135:ILE:N | 2.75                     | 0.43              |
| 1:L:24:A:O2'   | 1:L:25:A:OP2  | 2.31                     | 0.43              |
| 2:G:194:GLU:C  | 2:G:196:GLY:N | 2.76                     | 0.43              |
| 2:J:194:GLU:C  | 2:J:196:GLY:N | 2.76                     | 0.43              |
| 2:J:451:LYS:O  | 2:J:471:ASN:N | 2.51                     | 0.43              |
| 3:K:97:PRO:C   | 3:K:99:GLY:N  | 2.76                     | 0.43              |
| 3:E:97:PRO:C   | 3:E:99:GLY:N  | 2.76                     | 0.43              |
| 3:H:122:GLU:C  | 3:H:124:PHE:H | 2.27                     | 0.43              |
| 1:C:11:G:H2'   | 1:C:12:U:OP1  | 2.18                     | 0.43              |
| 1:L:30:U:H2'   | 1:L:31:G:H8   | 1.83                     | 0.43              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:23:G:O2'    | 1:C:26:A:C2     | 2.64                     | 0.43              |
| 2:A:133:PRO:C   | 2:A:135:ILE:N   | 2.75                     | 0.43              |
| 3:H:363:ASN:O   | 3:H:364:ASP:C   | 2.62                     | 0.43              |
| 3:K:122:GLU:C   | 3:K:124:PHE:H   | 2.27                     | 0.43              |
| 3:K:363:ASN:O   | 3:K:364:ASP:C   | 2.62                     | 0.43              |
| 1:C:30:U:H2'    | 1:C:31:G:H8     | 1.83                     | 0.43              |
| 1:L:11:G:H2'    | 1:L:12:U:OP1    | 2.18                     | 0.43              |
| 3:B:395:LYS:O   | 3:B:399:GLU:N   | 2.48                     | 0.43              |
| 2:D:155:GLY:O   | 2:D:156:SER:C   | 2.60                     | 0.43              |
| 2:D:287:LYS:O   | 2:D:288:ALA:C   | 2.62                     | 0.43              |
| 3:E:363:ASN:O   | 3:E:364:ASP:C   | 2.62                     | 0.43              |
| 1:F:24:A:O2'    | 1:F:25:A:P      | 2.77                     | 0.42              |
| 1:L:23:G:O2'    | 1:L:26:A:C2     | 2.64                     | 0.42              |
| 2:A:287:LYS:O   | 2:A:288:ALA:C   | 2.62                     | 0.42              |
| 2:D:133:PRO:C   | 2:D:135:ILE:N   | 2.75                     | 0.42              |
| 2:G:194:GLU:O   | 2:G:195:ILE:C   | 2.62                     | 0.42              |
| 2:G:287:LYS:O   | 2:G:288:ALA:C   | 2.62                     | 0.42              |
| 2:G:451:LYS:O   | 2:G:471:ASN:N   | 2.51                     | 0.42              |
| 1:L:24:A:O2'    | 1:L:25:A:P      | 2.77                     | 0.42              |
| 3:B:122:GLU:C   | 3:B:124:PHE:H   | 2.27                     | 0.42              |
| 1:F:14:U:O2'    | 1:F:15:U:H5'    | 2.20                     | 0.42              |
| 2:A:194:GLU:O   | 2:A:195:ILE:C   | 2.62                     | 0.42              |
| 2:J:287:LYS:O   | 2:J:288:ALA:C   | 2.62                     | 0.42              |
| 1:I:24:A:O2'    | 1:I:25:A:P      | 2.77                     | 0.42              |
| 2:G:133:PRO:C   | 2:G:135:ILE:N   | 2.75                     | 0.42              |
| 2:J:194:GLU:O   | 2:J:195:ILE:C   | 2.62                     | 0.42              |
| 3:B:380:ILE:O   | 3:B:384:GLY:HA2 | 2.20                     | 0.42              |
| 3:E:122:GLU:C   | 3:E:124:PHE:H   | 2.27                     | 0.42              |
| 3:H:395:LYS:O   | 3:H:399:GLU:N   | 2.48                     | 0.42              |
| 3:K:380:ILE:O   | 3:K:384:GLY:HA2 | 2.20                     | 0.42              |
| 1:I:4:A:H2'     | 1:I:5:G:H8      | 1.81                     | 0.42              |
| 2:D:194:GLU:O   | 2:D:195:ILE:C   | 2.62                     | 0.42              |
| 2:D:275:LYS:C   | 2:D:277:ARG:H   | 2.28                     | 0.42              |
| 1:C:24:A:O2'    | 1:C:25:A:P      | 2.77                     | 0.42              |
| 1:I:30:U:H2'    | 1:I:31:G:H8     | 1.83                     | 0.42              |
| 1:F:26:A:O2'    | 1:F:27:A:OP1    | 2.35                     | 0.41              |
| 1:I:14:U:O2'    | 1:I:15:U:H5'    | 2.20                     | 0.41              |
| 3:E:380:ILE:O   | 3:E:384:GLY:HA2 | 2.20                     | 0.41              |
| 1:F:10:C:H2'    | 1:F:11:G:C8     | 2.55                     | 0.41              |
| 2:D:456:GLY:HA3 | 2:D:466:VAL:HA  | 2.02                     | 0.41              |
| 1:C:14:U:O2'    | 1:C:15:U:H5'    | 2.20                     | 0.41              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:G:456:GLY:HA3 | 2:G:466:VAL:HA  | 2.02                     | 0.41              |
| 1:L:14:U:O2'    | 1:L:15:U:H5'    | 2.20                     | 0.41              |
| 2:A:275:LYS:C   | 2:A:277:ARG:H   | 2.28                     | 0.41              |
| 2:J:456:GLY:HA3 | 2:J:466:VAL:HA  | 2.02                     | 0.41              |
| 3:H:109:LEU:O   | 3:H:186:ASP:HA  | 2.20                     | 0.41              |
| 1:C:15:U:H2'    | 1:C:16:C:H6     | 1.86                     | 0.41              |
| 1:F:9:C:O2'     | 1:F:10:C:H5'    | 2.20                     | 0.41              |
| 1:F:24:A:C2'    | 1:F:25:A:OP2    | 2.68                     | 0.41              |
| 1:I:9:C:O2'     | 1:I:10:C:H5'    | 2.20                     | 0.41              |
| 1:I:15:U:H2'    | 1:I:16:C:H6     | 1.85                     | 0.41              |
| 3:B:109:LEU:O   | 3:B:186:ASP:HA  | 2.20                     | 0.41              |
| 3:B:363:ASN:O   | 3:B:364:ASP:C   | 2.62                     | 0.41              |
| 2:D:484:LEU:O   | 2:D:487:GLN:N   | 2.54                     | 0.41              |
| 2:J:275:LYS:C   | 2:J:277:ARG:H   | 2.28                     | 0.41              |
| 3:E:395:LYS:O   | 3:E:399:GLU:N   | 2.48                     | 0.41              |
| 1:F:15:U:H2'    | 1:F:16:C:H6     | 1.86                     | 0.41              |
| 1:F:23:G:C2'    | 1:F:24:A:H5'    | 2.51                     | 0.41              |
| 1:I:24:A:C2'    | 1:I:25:A:OP2    | 2.68                     | 0.41              |
| 1:L:33:A:OP1    | 2:J:262:GLY:CA  | 2.69                     | 0.41              |
| 2:G:320:ASP:C   | 2:G:322:SER:H   | 2.29                     | 0.41              |
| 2:G:484:LEU:O   | 2:G:487:GLN:N   | 2.54                     | 0.41              |
| 2:J:484:LEU:O   | 2:J:487:GLN:N   | 2.54                     | 0.41              |
| 1:L:9:C:O2'     | 1:L:10:C:H5'    | 2.20                     | 0.41              |
| 2:A:379:SER:C   | 2:A:381:VAL:N   | 2.79                     | 0.41              |
| 3:B:175:ASN:O   | 3:B:177:ASP:N   | 2.54                     | 0.41              |
| 3:H:380:ILE:O   | 3:H:384:GLY:HA2 | 2.20                     | 0.41              |
| 1:C:9:C:O2'     | 1:C:10:C:H5'    | 2.20                     | 0.40              |
| 1:C:26:A:O2'    | 1:C:27:A:OP1    | 2.35                     | 0.40              |
| 1:I:10:C:H2'    | 1:I:11:G:C8     | 2.56                     | 0.40              |
| 1:L:24:A:C2'    | 1:L:25:A:OP2    | 2.68                     | 0.40              |
| 2:A:320:ASP:C   | 2:A:322:SER:H   | 2.29                     | 0.40              |
| 2:D:320:ASP:C   | 2:D:322:SER:H   | 2.29                     | 0.40              |
| 3:H:97:PRO:C    | 3:H:99:GLY:N    | 2.76                     | 0.40              |
| 2:A:377:THR:O   | 2:A:380:ILE:N   | 2.54                     | 0.40              |
| 2:D:377:THR:O   | 2:D:380:ILE:N   | 2.54                     | 0.40              |
| 2:J:377:THR:O   | 2:J:380:ILE:N   | 2.55                     | 0.40              |
| 3:E:109:LEU:O   | 3:E:186:ASP:HA  | 2.20                     | 0.40              |
| 3:H:175:ASN:O   | 3:H:177:ASP:N   | 2.54                     | 0.40              |
| 3:K:109:LEU:O   | 3:K:186:ASP:HA  | 2.20                     | 0.40              |
| 2:A:456:GLY:HA3 | 2:A:466:VAL:HA  | 2.02                     | 0.40              |
| 2:G:27:THR:O    | 2:G:28:GLU:C    | 2.65                     | 0.40              |

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| Atom-1        | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|---------------|--------------------------|-------------------|
| 3:K:62:ALA:HA | 3:K:72:ARG:O  | 2.22                     | 0.40              |
| 1:C:24:A:C2'  | 1:C:25:A:OP2  | 2.68                     | 0.40              |
| 1:L:15:U:H2'  | 1:L:16:C:H6   | 1.85                     | 0.40              |
| 2:A:137:ASN:C | 2:A:139:THR:N | 2.66                     | 0.40              |
| 2:D:379:SER:C | 2:D:381:VAL:N | 2.79                     | 0.40              |
| 2:J:320:ASP:C | 2:J:322:SER:H | 2.29                     | 0.40              |
| 3:K:175:ASN:O | 3:K:177:ASP:N | 2.54                     | 0.40              |
| 1:C:10:C:H2'  | 1:C:11:G:C8   | 2.55                     | 0.40              |
| 2:A:484:LEU:O | 2:A:485:ALA:C | 2.64                     | 0.40              |
| 2:D:27:THR:O  | 2:D:28:GLU:C  | 2.65                     | 0.40              |

All (30) 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) |
|----------------|-----------------------|--------------------------|-------------------|
| 2:G:463:ARG:N  | 2:G:465:LYS:N[2_656]  | 0.58                     | 1.62              |
| 2:G:463:ARG:C  | 2:G:464:GLN:N[2_656]  | 0.70                     | 1.50              |
| 2:G:464:GLN:N  | 2:G:464:GLN:N[2_656]  | 0.73                     | 1.47              |
| 2:G:463:ARG:N  | 2:G:464:GLN:C[2_656]  | 0.89                     | 1.31              |
| 2:G:463:ARG:C  | 2:G:464:GLN:CA[2_656] | 1.01                     | 1.19              |
| 2:G:463:ARG:CA | 2:G:465:LYS:N[2_656]  | 1.26                     | 0.94              |
| 2:G:461:LYS:O  | 2:G:466:VAL:CB[2_656] | 1.38                     | 0.82              |
| 2:G:463:ARG:CA | 2:G:464:GLN:C[2_656]  | 1.40                     | 0.80              |
| 2:G:462:GLY:C  | 2:G:464:GLN:C[2_656]  | 1.43                     | 0.77              |
| 2:G:463:ARG:O  | 2:G:464:GLN:N[2_656]  | 1.56                     | 0.64              |
| 2:G:463:ARG:N  | 2:G:465:LYS:CA[2_656] | 1.59                     | 0.61              |
| 2:G:463:ARG:O  | 2:G:464:GLN:CA[2_656] | 1.60                     | 0.60              |
| 2:G:346:PHE:CB | 2:J:418:ASN:N[1_455]  | 1.62                     | 0.58              |
| 2:G:463:ARG:C  | 2:G:464:GLN:C[2_656]  | 1.70                     | 0.50              |
| 2:G:463:ARG:N  | 2:G:464:GLN:O[2_656]  | 1.72                     | 0.48              |
| 2:G:462:GLY:C  | 2:G:465:LYS:N[2_656]  | 1.73                     | 0.47              |
| 2:G:464:GLN:N  | 2:G:464:GLN:CA[2_656] | 1.73                     | 0.47              |
| 2:G:461:LYS:CB | 2:G:466:VAL:O[2_656]  | 1.77                     | 0.43              |
| 2:G:463:ARG:CA | 2:G:464:GLN:CA[2_656] | 1.78                     | 0.42              |
| 2:G:346:PHE:CB | 2:J:417:VAL:C[1_455]  | 1.85                     | 0.35              |
| 2:G:462:GLY:O  | 2:G:464:GLN:CA[2_656] | 1.86                     | 0.34              |
| 2:G:346:PHE:CB | 2:J:417:VAL:CA[1_455] | 1.89                     | 0.31              |
| 2:G:463:ARG:C  | 2:G:463:ARG:C[2_656]  | 1.98                     | 0.22              |
| 2:G:462:GLY:CA | 2:G:465:LYS:O[2_656]  | 1.99                     | 0.21              |
| 2:G:462:GLY:C  | 2:G:464:GLN:O[2_656]  | 1.99                     | 0.21              |

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| Atom-1        | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------------|--------------------------|-------------------|
| 2:G:462:GLY:O | 2:G:464:GLN:CB[2_656] | 2.02                     | 0.18              |
| 2:G:462:GLY:N | 2:G:465:LYS:C[2_656]  | 2.04                     | 0.16              |
| 2:G:462:GLY:O | 2:G:464:GLN:C[2_656]  | 2.04                     | 0.16              |
| 2:G:461:LYS:C | 2:G:466:VAL:CB[2_656] | 2.09                     | 0.11              |
| 2:G:457:TYR:O | 2:G:462:GLY:O[2_656]  | 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 |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 2   | A     | 552/554 (100%)  | 449 (81%)  | 79 (14%)  | 24 (4%)  | 2           | 17 |
| 2   | D     | 552/554 (100%)  | 449 (81%)  | 79 (14%)  | 24 (4%)  | 2           | 17 |
| 2   | G     | 552/554 (100%)  | 449 (81%)  | 79 (14%)  | 24 (4%)  | 2           | 17 |
| 2   | J     | 552/554 (100%)  | 450 (82%)  | 78 (14%)  | 24 (4%)  | 2           | 17 |
| 3   | B     | 396/423 (94%)   | 322 (81%)  | 62 (16%)  | 12 (3%)  | 3           | 22 |
| 3   | E     | 396/423 (94%)   | 322 (81%)  | 62 (16%)  | 12 (3%)  | 3           | 22 |
| 3   | H     | 396/423 (94%)   | 322 (81%)  | 62 (16%)  | 12 (3%)  | 3           | 22 |
| 3   | K     | 396/423 (94%)   | 322 (81%)  | 62 (16%)  | 12 (3%)  | 3           | 22 |
| All | All   | 3792/3908 (97%) | 3085 (81%) | 563 (15%) | 144 (4%) | 2           | 19 |

All (144) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 62  | ALA  |
| 2   | A     | 134 | SER  |
| 2   | A     | 135 | ILE  |
| 2   | A     | 136 | ASN  |
| 2   | A     | 140 | PRO  |
| 2   | A     | 222 | GLN  |
| 2   | A     | 345 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B     | 94  | ILE  |
| 2   | D     | 62  | ALA  |
| 2   | D     | 134 | SER  |
| 2   | D     | 135 | ILE  |
| 2   | D     | 136 | ASN  |
| 2   | D     | 140 | PRO  |
| 2   | D     | 222 | GLN  |
| 2   | D     | 345 | PRO  |
| 2   | G     | 62  | ALA  |
| 2   | G     | 134 | SER  |
| 2   | G     | 135 | ILE  |
| 2   | G     | 136 | ASN  |
| 2   | G     | 140 | PRO  |
| 2   | G     | 222 | GLN  |
| 2   | G     | 345 | PRO  |
| 2   | J     | 62  | ALA  |
| 2   | J     | 134 | SER  |
| 2   | J     | 135 | ILE  |
| 2   | J     | 136 | ASN  |
| 2   | J     | 140 | PRO  |
| 2   | J     | 222 | GLN  |
| 2   | J     | 345 | PRO  |
| 3   | E     | 94  | ILE  |
| 3   | H     | 94  | ILE  |
| 3   | K     | 94  | ILE  |
| 2   | A     | 67  | ASP  |
| 2   | A     | 85  | GLN  |
| 2   | A     | 273 | GLY  |
| 2   | A     | 412 | PRO  |
| 2   | D     | 67  | ASP  |
| 2   | D     | 85  | GLN  |
| 2   | D     | 273 | GLY  |
| 2   | D     | 412 | PRO  |
| 2   | G     | 67  | ASP  |
| 2   | G     | 85  | GLN  |
| 2   | G     | 273 | GLY  |
| 2   | G     | 412 | PRO  |
| 2   | J     | 67  | ASP  |
| 2   | J     | 85  | GLN  |
| 2   | J     | 273 | GLY  |
| 2   | J     | 412 | PRO  |
| 2   | A     | 123 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 156 | SER  |
| 2   | A     | 296 | THR  |
| 2   | A     | 420 | PRO  |
| 3   | B     | 28  | GLU  |
| 3   | B     | 123 | ASP  |
| 3   | B     | 176 | PRO  |
| 3   | B     | 286 | THR  |
| 2   | D     | 123 | ASP  |
| 2   | D     | 156 | SER  |
| 2   | D     | 296 | THR  |
| 2   | D     | 420 | PRO  |
| 2   | G     | 123 | ASP  |
| 2   | G     | 156 | SER  |
| 2   | G     | 296 | THR  |
| 2   | G     | 420 | PRO  |
| 2   | J     | 123 | ASP  |
| 2   | J     | 156 | SER  |
| 2   | J     | 296 | THR  |
| 2   | J     | 420 | PRO  |
| 3   | E     | 28  | GLU  |
| 3   | E     | 123 | ASP  |
| 3   | E     | 176 | PRO  |
| 3   | E     | 286 | THR  |
| 3   | H     | 28  | GLU  |
| 3   | H     | 123 | ASP  |
| 3   | H     | 176 | PRO  |
| 3   | H     | 286 | THR  |
| 3   | K     | 28  | GLU  |
| 3   | K     | 123 | ASP  |
| 3   | K     | 176 | PRO  |
| 3   | K     | 286 | THR  |
| 2   | A     | 114 | ALA  |
| 2   | A     | 195 | ILE  |
| 2   | A     | 274 | ILE  |
| 2   | A     | 275 | LYS  |
| 3   | B     | 277 | ARG  |
| 3   | B     | 316 | GLY  |
| 2   | D     | 114 | ALA  |
| 2   | D     | 195 | ILE  |
| 2   | D     | 274 | ILE  |
| 2   | D     | 275 | LYS  |
| 2   | G     | 114 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | G     | 195 | ILE  |
| 2   | G     | 274 | ILE  |
| 2   | G     | 275 | LYS  |
| 2   | J     | 114 | ALA  |
| 2   | J     | 195 | ILE  |
| 2   | J     | 274 | ILE  |
| 2   | J     | 275 | LYS  |
| 3   | E     | 277 | ARG  |
| 3   | E     | 316 | GLY  |
| 3   | H     | 277 | ARG  |
| 3   | H     | 316 | GLY  |
| 3   | K     | 277 | ARG  |
| 3   | K     | 316 | GLY  |
| 2   | A     | 116 | PHE  |
| 2   | A     | 276 | VAL  |
| 2   | A     | 357 | MET  |
| 3   | B     | 77  | PHE  |
| 3   | B     | 88  | TRP  |
| 2   | D     | 116 | PHE  |
| 2   | D     | 276 | VAL  |
| 2   | D     | 357 | MET  |
| 2   | G     | 116 | PHE  |
| 2   | G     | 276 | VAL  |
| 2   | G     | 357 | MET  |
| 2   | J     | 116 | PHE  |
| 2   | J     | 276 | VAL  |
| 2   | J     | 357 | MET  |
| 3   | E     | 77  | PHE  |
| 3   | E     | 88  | TRP  |
| 3   | H     | 77  | PHE  |
| 3   | H     | 88  | TRP  |
| 3   | K     | 88  | TRP  |
| 2   | A     | 133 | PRO  |
| 2   | A     | 462 | GLY  |
| 3   | B     | 55  | PRO  |
| 2   | D     | 133 | PRO  |
| 2   | D     | 462 | GLY  |
| 2   | G     | 133 | PRO  |
| 2   | G     | 462 | GLY  |
| 2   | J     | 133 | PRO  |
| 2   | J     | 462 | GLY  |
| 3   | E     | 55  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | H     | 55  | PRO  |
| 3   | K     | 55  | PRO  |
| 3   | K     | 77  | PHE  |
| 3   | B     | 170 | PRO  |
| 3   | E     | 170 | PRO  |
| 3   | H     | 170 | PRO  |
| 3   | K     | 170 | PRO  |
| 3   | B     | 420 | PRO  |
| 3   | E     | 420 | PRO  |
| 3   | H     | 420 | PRO  |
| 3   | K     | 420 | PRO  |

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed      | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 1   | C     | 29/30 (96%)   | 6 (20%)           | 2 (6%)          |
| 1   | F     | 29/30 (96%)   | 6 (20%)           | 2 (6%)          |
| 1   | I     | 29/30 (96%)   | 6 (20%)           | 2 (6%)          |
| 1   | L     | 29/30 (96%)   | 6 (20%)           | 2 (6%)          |
| All | All   | 116/120 (96%) | 24 (20%)          | 8 (6%)          |

All (24) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 12  | U    |
| 1   | C     | 25  | A    |
| 1   | C     | 26  | A    |
| 1   | C     | 27  | A    |
| 1   | C     | 28  | A    |
| 1   | C     | 29  | C    |
| 1   | F     | 12  | U    |
| 1   | F     | 25  | A    |
| 1   | F     | 26  | A    |
| 1   | F     | 27  | A    |
| 1   | F     | 28  | A    |
| 1   | F     | 29  | C    |
| 1   | I     | 12  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 25  | A    |
| 1   | I     | 26  | A    |
| 1   | I     | 27  | A    |
| 1   | I     | 28  | A    |
| 1   | I     | 29  | C    |
| 1   | L     | 12  | U    |
| 1   | L     | 25  | A    |
| 1   | L     | 26  | A    |
| 1   | L     | 27  | A    |
| 1   | L     | 28  | A    |
| 1   | L     | 29  | C    |

All (8) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 24  | A    |
| 1   | C     | 26  | A    |
| 1   | F     | 24  | A    |
| 1   | F     | 26  | A    |
| 1   | I     | 24  | A    |
| 1   | I     | 26  | A    |
| 1   | L     | 24  | A    |
| 1   | L     | 26  | A    |

## 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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 3   | B     | 3                |
| 3   | E     | 3                |
| 3   | H     | 3                |
| 3   | K     | 3                |
| 1   | C     | 1                |
| 1   | F     | 1                |
| 1   | I     | 1                |
| 1   | L     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | C     | 26:A      | O3'    | 27:A      | P      | 1.94         |
| 1     | F     | 26:A      | O3'    | 27:A      | P      | 1.94         |
| 1     | I     | 26:A      | O3'    | 27:A      | P      | 1.94         |
| 1     | L     | 26:A      | O3'    | 27:A      | P      | 1.94         |
| 1     | B     | 70:LYS    | C      | 71:TRP    | N      | 1.90         |
| 1     | E     | 70:LYS    | C      | 71:TRP    | N      | 1.90         |
| 1     | H     | 70:LYS    | C      | 71:TRP    | N      | 1.90         |
| 1     | K     | 70:LYS    | C      | 71:TRP    | N      | 1.90         |
| 1     | B     | 62:ALA    | C      | 63:ILE    | N      | 1.70         |
| 1     | E     | 62:ALA    | C      | 63:ILE    | N      | 1.70         |
| 1     | H     | 62:ALA    | C      | 63:ILE    | N      | 1.70         |
| 1     | K     | 62:ALA    | C      | 63:ILE    | N      | 1.70         |
| 1     | B     | 64:LYS    | C      | 65:LYS    | N      | 1.66         |
| 1     | E     | 64:LYS    | C      | 65:LYS    | N      | 1.66         |
| 1     | H     | 64:LYS    | C      | 65:LYS    | N      | 1.66         |
| 1     | K     | 64:LYS    | C      | 65:LYS    | N      | 1.66         |

## 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.