



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:44 AM UTC

PDB ID : 1KSX / pdb\_00001ksx  
Title : Crystal Structures of Two Intermediates in the Assembly of the Papillomavirus Replication Initiation Complex  
Authors : Enemark, E.J.; Stenlund, A.; Joshua-Tor, L.  
Deposited on : 2002-01-14  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
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

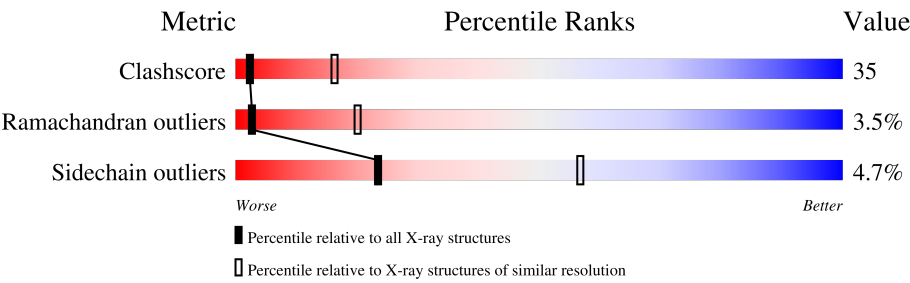
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 1573 (3.20-3.20)                                      |
| Ramachandran outliers | 187476                      | 1548 (3.20-3.20)                                      |
| Sidechain outliers    | 187428                      | 1547 (3.20-3.20)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain                                        |
|-----|-------|--------|---------------------------------------------------------|
| 1   | C     | 21     | <div><div>33%</div><div>62%</div><div>5%</div></div>    |
| 1   | G     | 21     | <div><div>33%</div><div>62%</div><div>5%</div></div>    |
| 1   | K     | 21     | <div><div>33%</div><div>62%</div><div>5%</div></div>    |
| 1   | O     | 21     | <div><div>33%</div><div>62%</div><div>5%</div></div>    |
| 2   | A     | 148    | <div><div>48%</div><div>46%</div><div>..</div></div>    |
| 2   | B     | 148    | <div><div>39%</div><div>51%</div><div>7% ..</div></div> |
| 2   | E     | 148    | <div><div>50%</div><div>44%</div><div>..</div></div>    |
| 2   | F     | 148    | <div><div>41%</div><div>50%</div><div>7% ..</div></div> |

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| Mol | Chain | Length | Quality of chain                                                           |
|-----|-------|--------|----------------------------------------------------------------------------|
| 2   | I     | 148    | <div><div></div><div>48%46%<div><div></div><div></div></div></div></div>   |
| 2   | J     | 148    | <div><div></div><div>39%51%7%<div><div></div><div></div></div></div></div> |
| 2   | M     | 148    | <div><div></div><div>49%45%<div><div></div><div></div></div></div></div>   |
| 2   | N     | 148    | <div><div></div><div>39%52%7%<div><div></div><div></div></div></div></div> |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11044 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 DNA chain called E1 Recognition Sequence.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 1   | C     | 21       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 428   | 208 | 77 | 123 | 20 |         |         |       |
| 1   | G     | 21       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 428   | 208 | 77 | 123 | 20 |         |         |       |
| 1   | K     | 21       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 428   | 208 | 77 | 123 | 20 |         |         |       |
| 1   | O     | 21       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 428   | 208 | 77 | 123 | 20 |         |         |       |

- Molecule 2 is a protein called REPLICATION PROTEIN E1.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | A     | 145      | Total | C   | N   | O   | S | 7       | 0       | 0     |
|     |       |          | 1164  | 754 | 200 | 201 | 9 |         |         |       |
| 2   | B     | 145      | Total | C   | N   | O   | S | 7       | 0       | 0     |
|     |       |          | 1164  | 754 | 200 | 201 | 9 |         |         |       |
| 2   | E     | 145      | Total | C   | N   | O   | S | 7       | 0       | 0     |
|     |       |          | 1164  | 754 | 200 | 201 | 9 |         |         |       |
| 2   | F     | 145      | Total | C   | N   | O   | S | 7       | 0       | 0     |
|     |       |          | 1164  | 754 | 200 | 201 | 9 |         |         |       |
| 2   | I     | 145      | Total | C   | N   | O   | S | 7       | 0       | 0     |
|     |       |          | 1164  | 754 | 200 | 201 | 9 |         |         |       |
| 2   | J     | 145      | Total | C   | N   | O   | S | 7       | 0       | 0     |
|     |       |          | 1164  | 754 | 200 | 201 | 9 |         |         |       |
| 2   | M     | 145      | Total | C   | N   | O   | S | 7       | 0       | 0     |
|     |       |          | 1164  | 754 | 200 | 201 | 9 |         |         |       |
| 2   | N     | 145      | Total | C   | N   | O   | S | 7       | 0       | 0     |
|     |       |          | 1164  | 754 | 200 | 201 | 9 |         |         |       |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 156     | GLY      | -      | cloning artifact | UNP P03116 |

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| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 157     | SER      | -      | cloning artifact | UNP P03116 |
| A     | 158     | ARG      | -      | cloning artifact | UNP P03116 |
| B     | 156     | GLY      | -      | cloning artifact | UNP P03116 |
| B     | 157     | SER      | -      | cloning artifact | UNP P03116 |
| B     | 158     | ARG      | -      | cloning artifact | UNP P03116 |
| E     | 156     | GLY      | -      | cloning artifact | UNP P03116 |
| E     | 157     | SER      | -      | cloning artifact | UNP P03116 |
| E     | 158     | ARG      | -      | cloning artifact | UNP P03116 |
| F     | 156     | GLY      | -      | cloning artifact | UNP P03116 |
| F     | 157     | SER      | -      | cloning artifact | UNP P03116 |
| F     | 158     | ARG      | -      | cloning artifact | UNP P03116 |
| I     | 156     | GLY      | -      | cloning artifact | UNP P03116 |
| I     | 157     | SER      | -      | cloning artifact | UNP P03116 |
| I     | 158     | ARG      | -      | cloning artifact | UNP P03116 |
| J     | 156     | GLY      | -      | cloning artifact | UNP P03116 |
| J     | 157     | SER      | -      | cloning artifact | UNP P03116 |
| J     | 158     | ARG      | -      | cloning artifact | UNP P03116 |
| M     | 156     | GLY      | -      | cloning artifact | UNP P03116 |
| M     | 157     | SER      | -      | cloning artifact | UNP P03116 |
| M     | 158     | ARG      | -      | cloning artifact | UNP P03116 |
| N     | 156     | GLY      | -      | cloning artifact | UNP P03116 |
| N     | 157     | SER      | -      | cloning artifact | UNP P03116 |
| N     | 158     | ARG      | -      | cloning artifact | UNP P03116 |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 3   | O     | 1        | Total O<br>1 1 | 0       | 0       |
| 3   | A     | 2        | Total O<br>2 2 | 0       | 0       |
| 3   | B     | 3        | Total O<br>3 3 | 0       | 0       |
| 3   | E     | 2        | Total O<br>2 2 | 0       | 0       |
| 3   | F     | 3        | Total O<br>3 3 | 0       | 0       |
| 3   | I     | 1        | Total O<br>1 1 | 0       | 0       |
| 3   | J     | 3        | Total O<br>3 3 | 0       | 0       |
| 3   | M     | 2        | Total O<br>2 2 | 0       | 0       |

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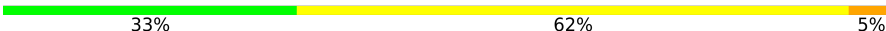
| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3   | N     | 3        | Total | O | 0       | 0       |
|     |       |          | 3     | 3 |         |         |

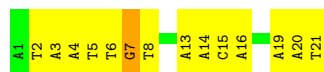
### 3 Residue-property plots [i](#)

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: E1 Recognition Sequence

Chain C: 



#### • Molecule 1: E1 Recognition Sequence

Chain G: 

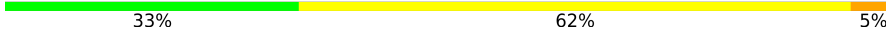


#### • Molecule 1: E1 Recognition Sequence

Chain K: 



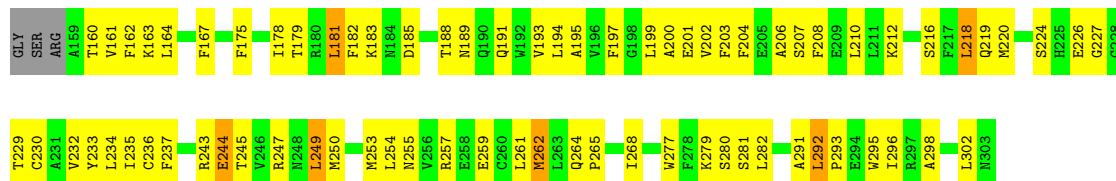
#### • Molecule 1: E1 Recognition Sequence

Chain O: 

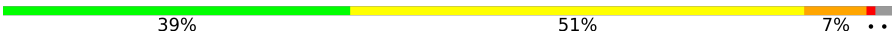
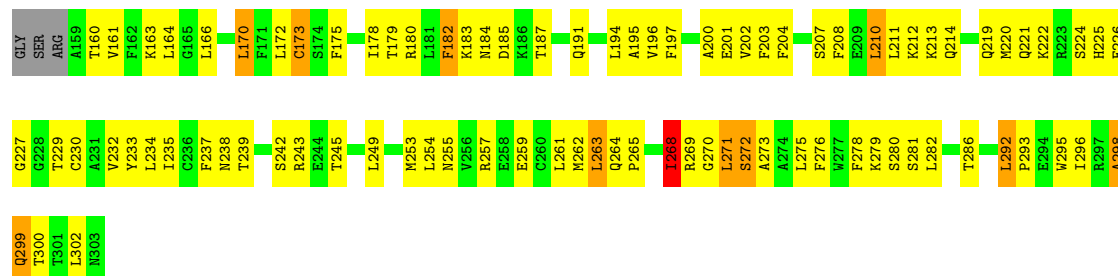


#### • Molecule 2: REPLICATION PROTEIN E1

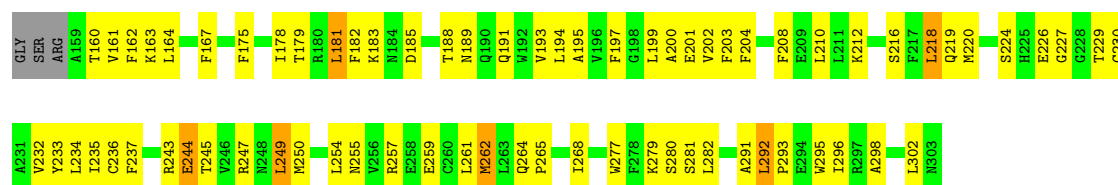
Chain A: 



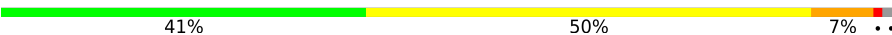
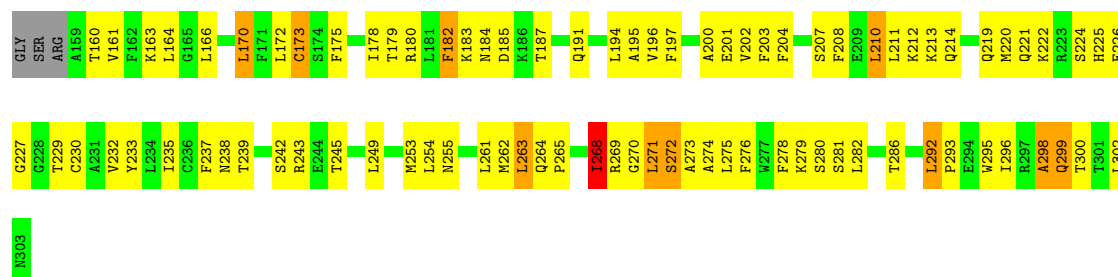
## • Molecule 2: REPLICATION PROTEIN E1

Chain B:  39% 51% 7% ..

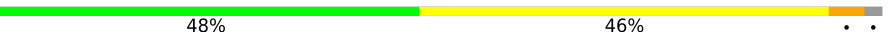
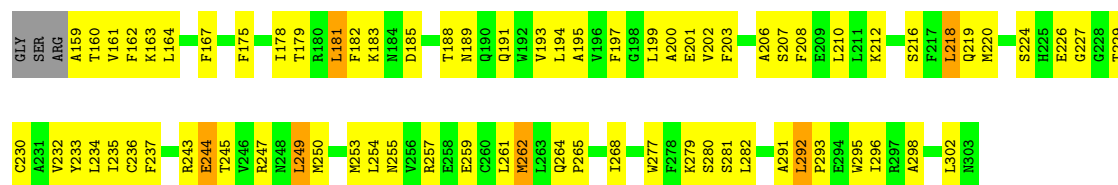
## • Molecule 2: REPLICATION PROTEIN E1

Chain E:  50% 44% 6% ..

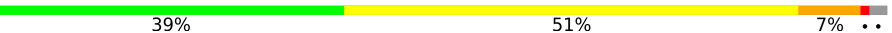
## • Molecule 2: REPLICATION PROTEIN E1

Chain F:  41% 50% 7% ..

## • Molecule 2: REPLICATION PROTEIN E1

Chain I:  48% 46% 6% ..

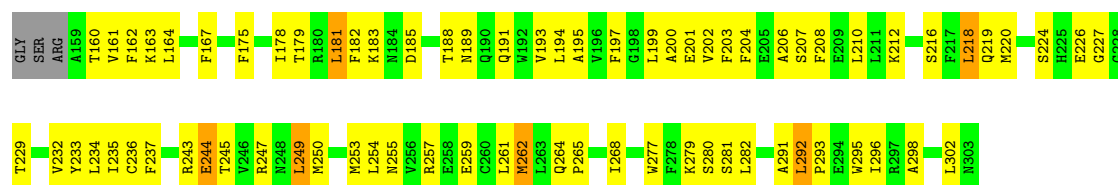
## • Molecule 2: REPLICATION PROTEIN E1

Chain J:  39% 51% 7% ..

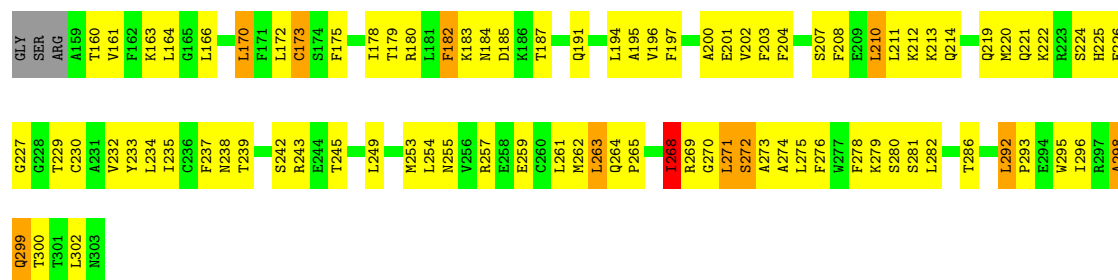




• Molecule 2: REPLICATION PROTEIN E1



• Molecule 2: REPLICATION PROTEIN E1



## 4 Data and refinement statistics

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

| Property                                                 | Value                                          | Source    |
|----------------------------------------------------------|------------------------------------------------|-----------|
| Space group                                              | P 1 21 1                                       | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 84.25Å 103.65Å 125.00Å<br>90.00° 99.53° 90.00° | Depositor |
| Resolution (Å)                                           | 42.62 – 3.20                                   | Depositor |
| % Data completeness<br>(in resolution range)             | 90.5 (42.62-3.20)                              | Depositor |
| $R_{merge}$                                              | 0.20                                           | Depositor |
| $R_{sym}$                                                | (Not available)                                | Depositor |
| Refinement program                                       | CNS 1.0                                        | Depositor |
| R, $R_{free}$                                            | 0.263 , 0.285                                  | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtrriage  |
| Total number of atoms                                    | 11044                                          | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 59.0                                           | 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     | 0.44         | 0/480       | 0.90        | 1/739 (0.1%)    |
| 1   | G     | 0.44         | 0/480       | 0.90        | 1/739 (0.1%)    |
| 1   | K     | 0.44         | 0/480       | 0.90        | 1/739 (0.1%)    |
| 1   | O     | 0.44         | 0/480       | 0.90        | 1/739 (0.1%)    |
| 2   | A     | 0.47         | 0/1190      | 0.92        | 3/1602 (0.2%)   |
| 2   | B     | 0.46         | 0/1190      | 1.04        | 6/1602 (0.4%)   |
| 2   | E     | 0.47         | 0/1190      | 0.92        | 3/1602 (0.2%)   |
| 2   | F     | 0.46         | 0/1190      | 1.04        | 6/1602 (0.4%)   |
| 2   | I     | 0.47         | 0/1190      | 0.92        | 3/1602 (0.2%)   |
| 2   | J     | 0.46         | 0/1190      | 1.04        | 6/1602 (0.4%)   |
| 2   | M     | 0.47         | 0/1190      | 0.92        | 3/1602 (0.2%)   |
| 2   | N     | 0.46         | 0/1190      | 1.04        | 6/1602 (0.4%)   |
| All | All   | 0.46         | 0/11440     | 0.97        | 40/15772 (0.3%) |

There are no bond length outliers.

All (40) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | J     | 292 | LEU  | CA-C-N      | 9.28  | 129.36      | 119.90   |
| 2   | J     | 292 | LEU  | C-N-CA      | 9.28  | 129.36      | 119.90   |
| 2   | B     | 292 | LEU  | CA-C-N      | 9.26  | 129.34      | 119.90   |
| 2   | B     | 292 | LEU  | C-N-CA      | 9.26  | 129.34      | 119.90   |
| 2   | F     | 292 | LEU  | CA-C-N      | 9.24  | 129.33      | 119.90   |
| 2   | F     | 292 | LEU  | C-N-CA      | 9.24  | 129.33      | 119.90   |
| 2   | N     | 292 | LEU  | CA-C-N      | 9.24  | 129.32      | 119.90   |
| 2   | N     | 292 | LEU  | C-N-CA      | 9.24  | 129.32      | 119.90   |
| 1   | K     | 7   | DG   | C5'-C4'-C3' | -5.93 | 106.00      | 114.90   |
| 1   | O     | 7   | DG   | C5'-C4'-C3' | -5.93 | 106.01      | 114.90   |
| 1   | C     | 7   | DG   | C5'-C4'-C3' | -5.91 | 106.03      | 114.90   |
| 1   | G     | 7   | DG   | C5'-C4'-C3' | -5.90 | 106.06      | 114.90   |
| 2   | E     | 216 | SER  | N-CA-C      | -5.88 | 105.00      | 111.82   |
| 2   | A     | 216 | SER  | N-CA-C      | -5.86 | 105.02      | 111.82   |
| 2   | I     | 216 | SER  | N-CA-C      | -5.85 | 105.04      | 111.82   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | M     | 216 | SER  | N-CA-C | -5.84 | 105.05      | 111.82   |
| 2   | J     | 263 | LEU  | N-CA-C | 5.68  | 117.65      | 108.34   |
| 2   | F     | 263 | LEU  | N-CA-C | 5.67  | 117.63      | 108.34   |
| 2   | B     | 263 | LEU  | N-CA-C | 5.66  | 117.63      | 108.34   |
| 2   | N     | 263 | LEU  | N-CA-C | 5.66  | 117.61      | 108.34   |
| 2   | I     | 181 | LEU  | N-CA-C | 5.45  | 118.81      | 110.20   |
| 2   | A     | 181 | LEU  | N-CA-C | 5.44  | 118.80      | 110.20   |
| 2   | E     | 181 | LEU  | N-CA-C | 5.44  | 118.79      | 110.20   |
| 2   | M     | 181 | LEU  | N-CA-C | 5.44  | 118.79      | 110.20   |
| 2   | E     | 224 | SER  | N-CA-C | 5.35  | 116.27      | 108.14   |
| 2   | A     | 224 | SER  | N-CA-C | 5.34  | 116.26      | 108.14   |
| 2   | M     | 224 | SER  | N-CA-C | 5.33  | 116.25      | 108.14   |
| 2   | I     | 224 | SER  | N-CA-C | 5.32  | 116.22      | 108.14   |
| 2   | J     | 268 | ILE  | N-CA-C | 5.28  | 116.06      | 110.72   |
| 2   | N     | 268 | ILE  | N-CA-C | 5.27  | 116.05      | 110.72   |
| 2   | B     | 268 | ILE  | N-CA-C | 5.25  | 116.03      | 110.72   |
| 2   | F     | 268 | ILE  | N-CA-C | 5.24  | 116.01      | 110.72   |
| 2   | N     | 175 | PHE  | N-CA-C | -5.23 | 105.69      | 111.71   |
| 2   | F     | 175 | PHE  | N-CA-C | -5.22 | 105.71      | 111.71   |
| 2   | B     | 175 | PHE  | N-CA-C | -5.21 | 105.72      | 111.71   |
| 2   | J     | 175 | PHE  | N-CA-C | -5.19 | 105.74      | 111.71   |
| 2   | B     | 170 | LEU  | N-CA-C | 5.06  | 117.91      | 111.69   |
| 2   | N     | 170 | LEU  | N-CA-C | 5.06  | 117.91      | 111.69   |
| 2   | F     | 170 | LEU  | N-CA-C | 5.05  | 117.91      | 111.69   |
| 2   | J     | 170 | LEU  | N-CA-C | 5.04  | 117.88      | 111.69   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | C     | 428   | 0        | 241      | 37      | 0            |
| 1   | G     | 428   | 0        | 241      | 59      | 0            |
| 1   | K     | 428   | 0        | 241      | 39      | 0            |
| 1   | O     | 428   | 0        | 241      | 41      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | A     | 1164  | 0        | 1189     | 70      | 0            |
| 2   | B     | 1164  | 0        | 1189     | 87      | 0            |
| 2   | E     | 1164  | 0        | 1189     | 68      | 0            |
| 2   | F     | 1164  | 0        | 1189     | 86      | 0            |
| 2   | I     | 1164  | 0        | 1189     | 92      | 0            |
| 2   | J     | 1164  | 0        | 1189     | 88      | 0            |
| 2   | M     | 1164  | 0        | 1189     | 70      | 0            |
| 2   | N     | 1164  | 0        | 1189     | 92      | 0            |
| 3   | A     | 2     | 0        | 0        | 0       | 0            |
| 3   | B     | 3     | 0        | 0        | 0       | 0            |
| 3   | E     | 2     | 0        | 0        | 0       | 0            |
| 3   | F     | 3     | 0        | 0        | 0       | 0            |
| 3   | I     | 1     | 0        | 0        | 0       | 0            |
| 3   | J     | 3     | 0        | 0        | 0       | 0            |
| 3   | M     | 2     | 0        | 0        | 0       | 0            |
| 3   | N     | 3     | 0        | 0        | 0       | 0            |
| 3   | O     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 11044 | 0        | 10476    | 757     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (757) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:G:21:DT:H71  | 2:I:162:PHE:CE2 | 1.40                     | 1.56              |
| 1:G:21:DT:C7   | 2:I:162:PHE:CZ  | 2.07                     | 1.38              |
| 1:G:21:DT:H73  | 2:I:162:PHE:CZ  | 1.64                     | 1.30              |
| 1:G:21:DT:C7   | 2:I:162:PHE:CE2 | 2.16                     | 1.26              |
| 1:O:3:DA:H2''  | 1:O:4:DA:C8     | 1.95                     | 1.02              |
| 1:G:3:DA:H2''  | 1:G:4:DA:C8     | 1.95                     | 1.02              |
| 1:K:3:DA:H2''  | 1:K:4:DA:C8     | 1.95                     | 1.01              |
| 1:C:3:DA:H2''  | 1:C:4:DA:C8     | 1.95                     | 1.00              |
| 1:G:21:DT:OP2  | 2:I:159:ALA:HA  | 1.63                     | 0.98              |
| 1:G:21:DT:H71  | 2:I:162:PHE:HE2 | 1.27                     | 0.96              |
| 1:O:20:DA:H2'' | 1:O:21:DT:H5''  | 1.51                     | 0.93              |
| 1:G:20:DA:H2'' | 1:G:21:DT:H5''  | 1.51                     | 0.92              |
| 1:K:20:DA:H2'' | 1:K:21:DT:H5''  | 1.51                     | 0.92              |
| 1:G:20:DA:H2'  | 2:I:162:PHE:CD2 | 2.04                     | 0.92              |
| 1:C:20:DA:H2'' | 1:C:21:DT:H5''  | 1.51                     | 0.92              |
| 1:C:19:DA:H2'' | 1:C:20:DA:H5'   | 1.52                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:4:DA:H2''    | 1:G:5:DT:C5'     | 2.01                     | 0.91              |
| 1:K:4:DA:H2''    | 1:K:5:DT:C5'     | 2.01                     | 0.91              |
| 1:K:19:DA:H2''   | 1:K:20:DA:H5'    | 1.52                     | 0.91              |
| 1:G:19:DA:H2''   | 1:G:20:DA:H5'    | 1.52                     | 0.91              |
| 1:C:4:DA:H2''    | 1:C:5:DT:C5'     | 2.01                     | 0.90              |
| 1:O:7:DG:H2''    | 1:O:8:DT:H5'     | 1.53                     | 0.90              |
| 1:O:4:DA:H2''    | 1:O:5:DT:C5'     | 2.01                     | 0.90              |
| 1:G:7:DG:H2''    | 1:G:8:DT:H5'     | 1.53                     | 0.90              |
| 1:K:7:DG:H2''    | 1:K:8:DT:H5'     | 1.53                     | 0.90              |
| 1:C:7:DG:H2''    | 1:C:8:DT:H5'     | 1.53                     | 0.90              |
| 1:G:21:DT:OP2    | 2:I:161:VAL:HG12 | 1.70                     | 0.90              |
| 2:A:218:LEU:HD11 | 2:A:220:MET:HG3  | 1.54                     | 0.90              |
| 2:I:218:LEU:HD11 | 2:I:220:MET:HG3  | 1.54                     | 0.89              |
| 1:O:19:DA:H2''   | 1:O:20:DA:H5'    | 1.52                     | 0.89              |
| 1:G:21:DT:H73    | 2:I:162:PHE:HZ   | 0.99                     | 0.89              |
| 2:E:218:LEU:HD11 | 2:E:220:MET:HG3  | 1.54                     | 0.88              |
| 2:M:218:LEU:HD11 | 2:M:220:MET:HG3  | 1.54                     | 0.88              |
| 1:C:6:DT:H2''    | 1:C:7:DG:H8      | 1.40                     | 0.87              |
| 1:K:6:DT:H2''    | 1:K:7:DG:H8      | 1.40                     | 0.87              |
| 2:B:210:LEU:HD13 | 2:B:253:MET:HE2  | 1.57                     | 0.86              |
| 2:J:210:LEU:HD13 | 2:J:253:MET:HE2  | 1.57                     | 0.85              |
| 2:N:210:LEU:HD13 | 2:N:253:MET:HE2  | 1.57                     | 0.85              |
| 1:G:21:DT:H71    | 2:I:162:PHE:CZ   | 1.85                     | 0.85              |
| 2:F:210:LEU:HD13 | 2:F:253:MET:HE2  | 1.57                     | 0.84              |
| 1:G:6:DT:H2''    | 1:G:7:DG:H8      | 1.40                     | 0.84              |
| 1:O:6:DT:H2''    | 1:O:7:DG:H8      | 1.40                     | 0.83              |
| 1:G:21:DT:OP2    | 2:I:161:VAL:CG1  | 2.25                     | 0.83              |
| 1:K:15:DC:H2''   | 1:K:16:DA:C8     | 2.15                     | 0.81              |
| 1:C:15:DC:H2''   | 1:C:16:DA:C8     | 2.15                     | 0.81              |
| 1:G:20:DA:H2'    | 2:I:162:PHE:CE2  | 2.15                     | 0.81              |
| 1:K:4:DA:H2''    | 1:K:5:DT:H5'     | 1.62                     | 0.81              |
| 1:C:4:DA:H2''    | 1:C:5:DT:H5'     | 1.62                     | 0.81              |
| 1:G:15:DC:H2''   | 1:G:16:DA:C8     | 2.15                     | 0.81              |
| 1:O:4:DA:H2''    | 1:O:5:DT:H5'     | 1.62                     | 0.81              |
| 1:O:15:DC:H2''   | 1:O:16:DA:C8     | 2.15                     | 0.80              |
| 1:G:4:DA:H2''    | 1:G:5:DT:H5'     | 1.62                     | 0.80              |
| 2:A:292:LEU:HD13 | 2:A:293:PRO:HD2  | 1.64                     | 0.79              |
| 2:I:292:LEU:HD13 | 2:I:293:PRO:HD2  | 1.64                     | 0.79              |
| 1:G:21:DT:O5'    | 2:I:161:VAL:HG11 | 1.81                     | 0.79              |
| 1:G:7:DG:H2''    | 1:G:8:DT:C5'     | 2.13                     | 0.79              |
| 1:O:7:DG:H2''    | 1:O:8:DT:C5'     | 2.13                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:7:DG:H2''    | 1:C:8:DT:C5'     | 2.13                     | 0.78              |
| 1:K:7:DG:H2''    | 1:K:8:DT:C5'     | 2.13                     | 0.78              |
| 2:M:292:LEU:HD13 | 2:M:293:PRO:HD2  | 1.64                     | 0.78              |
| 2:J:195:ALA:HB3  | 2:J:262:MET:HB2  | 1.66                     | 0.78              |
| 2:B:195:ALA:HB3  | 2:B:262:MET:HB2  | 1.66                     | 0.78              |
| 1:C:6:DT:H2''    | 1:C:7:DG:C8      | 2.19                     | 0.77              |
| 1:O:6:DT:H2''    | 1:O:7:DG:C8      | 2.19                     | 0.77              |
| 1:G:6:DT:H2''    | 1:G:7:DG:C8      | 2.19                     | 0.77              |
| 1:O:4:DA:H2''    | 1:O:5:DT:H5''    | 1.67                     | 0.77              |
| 1:G:4:DA:H2''    | 1:G:5:DT:H5''    | 1.67                     | 0.77              |
| 2:F:194:LEU:HB3  | 2:F:233:TYR:HB2  | 1.67                     | 0.77              |
| 1:K:6:DT:H2''    | 1:K:7:DG:C8      | 2.19                     | 0.77              |
| 2:F:195:ALA:HB3  | 2:F:262:MET:HB2  | 1.66                     | 0.77              |
| 2:N:194:LEU:HB3  | 2:N:233:TYR:HB2  | 1.67                     | 0.77              |
| 2:E:292:LEU:HD13 | 2:E:293:PRO:HD2  | 1.64                     | 0.77              |
| 2:F:292:LEU:HD11 | 2:F:296:ILE:CG2  | 2.15                     | 0.77              |
| 2:N:195:ALA:HB3  | 2:N:262:MET:HB2  | 1.66                     | 0.77              |
| 2:N:292:LEU:HD11 | 2:N:296:ILE:CG2  | 2.15                     | 0.77              |
| 2:J:292:LEU:HD11 | 2:J:296:ILE:CG2  | 2.15                     | 0.76              |
| 2:N:292:LEU:HD11 | 2:N:296:ILE:HG22 | 1.67                     | 0.76              |
| 2:B:292:LEU:HD11 | 2:B:296:ILE:CG2  | 2.15                     | 0.76              |
| 1:C:4:DA:H2''    | 1:C:5:DT:H5''    | 1.67                     | 0.75              |
| 2:B:194:LEU:HB3  | 2:B:233:TYR:HB2  | 1.67                     | 0.75              |
| 2:F:292:LEU:HD11 | 2:F:296:ILE:HG22 | 1.67                     | 0.75              |
| 1:K:2:DT:H2''    | 1:K:3:DA:O5'     | 1.86                     | 0.75              |
| 2:B:292:LEU:HD11 | 2:B:296:ILE:HG22 | 1.67                     | 0.75              |
| 2:J:194:LEU:HB3  | 2:J:233:TYR:HB2  | 1.67                     | 0.75              |
| 1:C:2:DT:H2''    | 1:C:3:DA:O5'     | 1.86                     | 0.75              |
| 1:O:2:DT:H2''    | 1:O:3:DA:O5'     | 1.86                     | 0.75              |
| 2:J:292:LEU:HD11 | 2:J:296:ILE:HG22 | 1.67                     | 0.75              |
| 1:K:4:DA:H2''    | 1:K:5:DT:H5''    | 1.67                     | 0.74              |
| 1:G:2:DT:H2''    | 1:G:3:DA:O5'     | 1.86                     | 0.74              |
| 2:J:182:PHE:CD1  | 2:J:265:PRO:HG3  | 2.23                     | 0.74              |
| 2:B:182:PHE:CD1  | 2:B:265:PRO:HG3  | 2.23                     | 0.74              |
| 1:O:7:DG:H5'     | 2:N:184:ASN:HB2  | 1.70                     | 0.73              |
| 2:F:182:PHE:CD1  | 2:F:265:PRO:HG3  | 2.23                     | 0.73              |
| 2:N:182:PHE:CD1  | 2:N:265:PRO:HG3  | 2.23                     | 0.73              |
| 1:O:4:DA:OP1     | 2:M:183:LYS:N    | 2.22                     | 0.73              |
| 1:G:4:DA:OP1     | 2:E:183:LYS:N    | 2.22                     | 0.73              |
| 1:K:5:DT:O2      | 1:O:20:DA:H2     | 1.72                     | 0.72              |
| 2:N:170:LEU:HD13 | 2:N:230:CYS:HB3  | 1.72                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:4:DA:OP1     | 2:A:183:LYS:N    | 2.22                     | 0.72              |
| 1:K:4:DA:OP1     | 2:I:183:LYS:N    | 2.22                     | 0.72              |
| 2:F:170:LEU:HD13 | 2:F:230:CYS:HB3  | 1.72                     | 0.72              |
| 1:G:7:DG:H5'     | 2:F:184:ASN:HB2  | 1.71                     | 0.72              |
| 1:C:7:DG:H5'     | 2:B:184:ASN:HB2  | 1.70                     | 0.71              |
| 2:M:179:THR:HG22 | 2:M:193:VAL:HG21 | 1.72                     | 0.71              |
| 2:A:194:LEU:HB3  | 2:A:233:TYR:HB2  | 1.73                     | 0.71              |
| 2:J:170:LEU:HD13 | 2:J:230:CYS:HB3  | 1.72                     | 0.71              |
| 1:K:7:DG:H5'     | 2:J:184:ASN:HB2  | 1.71                     | 0.71              |
| 2:I:194:LEU:HB3  | 2:I:233:TYR:HB2  | 1.73                     | 0.71              |
| 2:E:179:THR:HG22 | 2:E:193:VAL:HG21 | 1.72                     | 0.70              |
| 2:E:194:LEU:HB3  | 2:E:233:TYR:HB2  | 1.73                     | 0.70              |
| 2:M:194:LEU:HB3  | 2:M:233:TYR:HB2  | 1.73                     | 0.70              |
| 2:B:170:LEU:HD13 | 2:B:230:CYS:HB3  | 1.72                     | 0.70              |
| 2:I:179:THR:HG22 | 2:I:193:VAL:HG21 | 1.72                     | 0.70              |
| 2:A:179:THR:HG22 | 2:A:193:VAL:HG21 | 1.72                     | 0.70              |
| 2:M:185:ASP:OD1  | 2:M:243:ARG:HD2  | 1.93                     | 0.69              |
| 2:A:185:ASP:OD1  | 2:A:243:ARG:HD2  | 1.93                     | 0.69              |
| 2:E:185:ASP:OD1  | 2:E:243:ARG:HD2  | 1.93                     | 0.69              |
| 2:I:185:ASP:OD1  | 2:I:243:ARG:HD2  | 1.93                     | 0.69              |
| 1:G:21:DT:OP2    | 2:I:159:ALA:CA   | 2.41                     | 0.69              |
| 1:O:4:DA:C2'     | 1:O:5:DT:H5''    | 2.23                     | 0.69              |
| 1:G:4:DA:C2'     | 1:G:5:DT:H5''    | 2.23                     | 0.69              |
| 1:C:4:DA:C2'     | 1:C:5:DT:H5''    | 2.23                     | 0.68              |
| 2:F:302:LEU:HD22 | 2:F:302:LEU:H    | 1.58                     | 0.68              |
| 2:B:302:LEU:HD22 | 2:B:302:LEU:H    | 1.58                     | 0.68              |
| 1:K:4:DA:C2'     | 1:K:5:DT:H5''    | 2.23                     | 0.68              |
| 2:J:302:LEU:H    | 2:J:302:LEU:HD22 | 1.58                     | 0.68              |
| 2:N:302:LEU:HD22 | 2:N:302:LEU:H    | 1.58                     | 0.68              |
| 2:I:268:ILE:HG22 | 2:I:295:TRP:CD2  | 2.30                     | 0.67              |
| 2:E:268:ILE:HG22 | 2:E:295:TRP:CD2  | 2.30                     | 0.66              |
| 2:B:268:ILE:HD13 | 2:B:269:ARG:H    | 1.61                     | 0.66              |
| 2:J:268:ILE:HD13 | 2:J:269:ARG:H    | 1.61                     | 0.66              |
| 2:N:268:ILE:HD13 | 2:N:269:ARG:H    | 1.61                     | 0.66              |
| 2:A:200:ALA:HB3  | 2:A:203:PHE:HD2  | 1.61                     | 0.66              |
| 2:M:200:ALA:HB3  | 2:M:203:PHE:HD2  | 1.61                     | 0.66              |
| 2:A:268:ILE:HG22 | 2:A:295:TRP:CD2  | 2.30                     | 0.66              |
| 2:E:200:ALA:HB3  | 2:E:203:PHE:HD2  | 1.61                     | 0.66              |
| 2:I:200:ALA:HB3  | 2:I:203:PHE:HD2  | 1.61                     | 0.66              |
| 1:C:3:DA:H5'     | 2:A:182:PHE:CE1  | 2.31                     | 0.66              |
| 2:F:268:ILE:HD13 | 2:F:269:ARG:H    | 1.61                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:16:DA:O5'    | 2:I:245:THR:HG23 | 1.96                     | 0.65              |
| 1:O:3:DA:H5'     | 2:M:182:PHE:CE1  | 2.31                     | 0.65              |
| 1:K:3:DA:H5'     | 2:I:182:PHE:CE1  | 2.31                     | 0.65              |
| 2:M:268:ILE:HG22 | 2:M:295:TRP:CD2  | 2.30                     | 0.65              |
| 1:G:3:DA:H5'     | 2:E:182:PHE:CE1  | 2.31                     | 0.65              |
| 1:G:20:DA:C2'    | 2:I:162:PHE:CD2  | 2.78                     | 0.64              |
| 2:B:182:PHE:CE1  | 2:B:265:PRO:HG3  | 2.34                     | 0.63              |
| 1:C:6:DT:C2'     | 1:C:7:DG:C8      | 2.82                     | 0.63              |
| 1:K:6:DT:C2'     | 1:K:7:DG:C8      | 2.81                     | 0.63              |
| 2:J:182:PHE:CE1  | 2:J:265:PRO:HG3  | 2.33                     | 0.63              |
| 2:F:224:SER:CB   | 2:F:229:THR:HG22 | 2.29                     | 0.63              |
| 2:M:182:PHE:CD1  | 2:M:265:PRO:HG3  | 2.34                     | 0.63              |
| 2:B:224:SER:CB   | 2:B:229:THR:HG22 | 2.29                     | 0.63              |
| 2:J:224:SER:CB   | 2:J:229:THR:HG22 | 2.29                     | 0.62              |
| 2:M:292:LEU:HD13 | 2:M:293:PRO:CD   | 2.29                     | 0.62              |
| 2:N:224:SER:CB   | 2:N:229:THR:HG22 | 2.29                     | 0.62              |
| 2:E:182:PHE:CD1  | 2:E:265:PRO:HG3  | 2.34                     | 0.62              |
| 2:N:225:HIS:HD2  | 2:N:227:GLY:H    | 1.47                     | 0.62              |
| 1:G:20:DA:C2'    | 1:G:21:DT:H5''   | 2.28                     | 0.62              |
| 2:A:167:PHE:HE2  | 2:A:232:VAL:HG11 | 1.64                     | 0.62              |
| 2:A:182:PHE:CD1  | 2:A:265:PRO:HG3  | 2.34                     | 0.62              |
| 1:K:5:DT:O2      | 1:O:20:DA:C2     | 2.51                     | 0.62              |
| 2:A:181:LEU:C    | 2:A:181:LEU:HD23 | 2.25                     | 0.62              |
| 2:E:292:LEU:HD13 | 2:E:293:PRO:CD   | 2.29                     | 0.62              |
| 2:I:167:PHE:HE2  | 2:I:232:VAL:HG11 | 1.64                     | 0.62              |
| 2:I:182:PHE:CD1  | 2:I:265:PRO:HG3  | 2.34                     | 0.62              |
| 1:G:6:DT:C2'     | 1:G:7:DG:C8      | 2.82                     | 0.62              |
| 1:O:6:DT:C2'     | 1:O:7:DG:C8      | 2.81                     | 0.62              |
| 2:A:292:LEU:HD13 | 2:A:293:PRO:CD   | 2.29                     | 0.62              |
| 2:N:182:PHE:CE1  | 2:N:265:PRO:HG3  | 2.34                     | 0.62              |
| 1:G:20:DA:C2'    | 2:I:162:PHE:CE2  | 2.83                     | 0.62              |
| 2:E:167:PHE:HE2  | 2:E:232:VAL:HG11 | 1.64                     | 0.62              |
| 2:F:182:PHE:CE1  | 2:F:265:PRO:HG3  | 2.33                     | 0.62              |
| 2:F:220:MET:HE3  | 2:F:233:TYR:CE2  | 2.35                     | 0.62              |
| 2:I:181:LEU:HD23 | 2:I:181:LEU:C    | 2.25                     | 0.62              |
| 1:O:14:DA:H2''   | 1:O:15:DC:O5'    | 2.00                     | 0.62              |
| 2:F:225:HIS:HD2  | 2:F:227:GLY:H    | 1.47                     | 0.62              |
| 2:I:292:LEU:HD13 | 2:I:293:PRO:CD   | 2.29                     | 0.62              |
| 2:J:220:MET:HE3  | 2:J:233:TYR:CE2  | 2.35                     | 0.62              |
| 2:N:220:MET:HE3  | 2:N:233:TYR:CE2  | 2.35                     | 0.62              |
| 2:B:220:MET:HE3  | 2:B:233:TYR:CE2  | 2.35                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:167:PHE:HE2  | 2:M:232:VAL:HG11 | 1.64                     | 0.61              |
| 2:M:181:LEU:C    | 2:M:181:LEU:HD23 | 2.25                     | 0.61              |
| 1:C:14:DA:H2''   | 1:C:15:DC:O5'    | 2.00                     | 0.61              |
| 2:A:264:GLN:OE1  | 2:A:265:PRO:HD2  | 2.00                     | 0.61              |
| 2:E:264:GLN:OE1  | 2:E:265:PRO:HD2  | 2.00                     | 0.61              |
| 2:I:264:GLN:OE1  | 2:I:265:PRO:HD2  | 2.00                     | 0.61              |
| 2:J:225:HIS:HD2  | 2:J:227:GLY:H    | 1.47                     | 0.61              |
| 2:M:264:GLN:OE1  | 2:M:265:PRO:HD2  | 2.00                     | 0.61              |
| 2:I:249:LEU:HD12 | 2:I:249:LEU:O    | 2.01                     | 0.61              |
| 1:O:20:DA:C2'    | 1:O:21:DT:H5''   | 2.28                     | 0.61              |
| 2:I:292:LEU:HD11 | 2:I:296:ILE:HB   | 1.83                     | 0.61              |
| 2:A:292:LEU:HD11 | 2:A:296:ILE:HB   | 1.83                     | 0.61              |
| 1:G:14:DA:H2''   | 1:G:15:DC:O5'    | 2.00                     | 0.61              |
| 2:A:249:LEU:HD12 | 2:A:249:LEU:O    | 2.01                     | 0.61              |
| 1:K:20:DA:C2'    | 1:K:21:DT:H5''   | 2.28                     | 0.61              |
| 1:K:14:DA:H2''   | 1:K:15:DC:O5'    | 2.00                     | 0.61              |
| 2:E:181:LEU:C    | 2:E:181:LEU:HD23 | 2.25                     | 0.61              |
| 2:B:225:HIS:HD2  | 2:B:227:GLY:H    | 1.47                     | 0.61              |
| 2:F:202:VAL:HG13 | 2:F:203:PHE:H    | 1.66                     | 0.60              |
| 1:G:3:DA:H2''    | 1:G:4:DA:H8      | 1.62                     | 0.60              |
| 2:E:249:LEU:O    | 2:E:249:LEU:HD12 | 2.01                     | 0.60              |
| 1:O:3:DA:H2''    | 1:O:4:DA:H8      | 1.62                     | 0.60              |
| 2:F:243:ARG:NH2  | 2:F:264:GLN:HE22 | 2.00                     | 0.60              |
| 1:C:20:DA:C2'    | 1:C:21:DT:H5''   | 2.28                     | 0.60              |
| 1:C:7:DG:OP1     | 2:B:183:LYS:HG2  | 2.02                     | 0.60              |
| 2:E:292:LEU:HD11 | 2:E:296:ILE:HB   | 1.83                     | 0.60              |
| 2:B:243:ARG:NH2  | 2:B:264:GLN:HE22 | 2.00                     | 0.60              |
| 2:M:292:LEU:HD11 | 2:M:296:ILE:HB   | 1.83                     | 0.60              |
| 2:N:243:ARG:NH2  | 2:N:264:GLN:HE22 | 2.00                     | 0.60              |
| 2:B:224:SER:HB2  | 2:B:229:THR:HG22 | 1.84                     | 0.60              |
| 2:N:202:VAL:HG13 | 2:N:203:PHE:H    | 1.66                     | 0.60              |
| 2:N:224:SER:HB2  | 2:N:229:THR:HG22 | 1.84                     | 0.60              |
| 1:K:3:DA:H2''    | 1:K:4:DA:H8      | 1.62                     | 0.59              |
| 1:K:7:DG:OP1     | 2:J:183:LYS:HG2  | 2.02                     | 0.59              |
| 2:F:224:SER:HB2  | 2:F:229:THR:HG22 | 1.84                     | 0.59              |
| 2:M:249:LEU:HD12 | 2:M:249:LEU:O    | 2.01                     | 0.59              |
| 2:J:202:VAL:HG13 | 2:J:203:PHE:H    | 1.66                     | 0.59              |
| 2:J:224:SER:HB2  | 2:J:229:THR:HG22 | 1.84                     | 0.59              |
| 2:J:243:ARG:NH2  | 2:J:264:GLN:HE22 | 2.00                     | 0.59              |
| 1:C:19:DA:C2'    | 1:C:20:DA:H5'    | 2.31                     | 0.59              |
| 2:A:249:LEU:HD12 | 2:A:249:LEU:C    | 2.28                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:167:PHE:HE2  | 2:A:232:VAL:CG1  | 2.15                     | 0.59              |
| 2:B:194:LEU:HD13 | 2:B:263:LEU:HD21 | 1.84                     | 0.59              |
| 2:E:167:PHE:HE2  | 2:E:232:VAL:CG1  | 2.15                     | 0.59              |
| 2:I:249:LEU:HD12 | 2:I:249:LEU:C    | 2.28                     | 0.59              |
| 2:J:194:LEU:HD13 | 2:J:263:LEU:HD21 | 1.84                     | 0.59              |
| 2:J:202:VAL:HG13 | 2:J:203:PHE:N    | 2.18                     | 0.59              |
| 1:K:3:DA:H2''    | 1:K:4:DA:N7      | 2.18                     | 0.59              |
| 1:K:7:DG:C5'     | 2:J:184:ASN:HB2  | 2.33                     | 0.59              |
| 2:B:202:VAL:HG13 | 2:B:203:PHE:H    | 1.66                     | 0.59              |
| 1:G:7:DG:OP1     | 2:F:183:LYS:HG2  | 2.02                     | 0.59              |
| 2:N:202:VAL:HG13 | 2:N:203:PHE:N    | 2.18                     | 0.59              |
| 1:C:7:DG:C5'     | 2:B:184:ASN:HB2  | 2.33                     | 0.59              |
| 1:G:7:DG:C5'     | 2:F:184:ASN:HB2  | 2.33                     | 0.59              |
| 2:I:167:PHE:HE2  | 2:I:232:VAL:CG1  | 2.15                     | 0.59              |
| 1:C:3:DA:H2''    | 1:C:4:DA:N7      | 2.18                     | 0.58              |
| 1:K:19:DA:C2'    | 1:K:20:DA:H5'    | 2.31                     | 0.58              |
| 2:B:202:VAL:HG13 | 2:B:203:PHE:N    | 2.18                     | 0.58              |
| 2:M:167:PHE:HE2  | 2:M:232:VAL:CG1  | 2.15                     | 0.58              |
| 2:N:194:LEU:HD13 | 2:N:263:LEU:HD21 | 1.84                     | 0.58              |
| 1:O:7:DG:C5'     | 2:N:184:ASN:HB2  | 2.33                     | 0.58              |
| 1:O:3:DA:H2''    | 1:O:4:DA:N7      | 2.18                     | 0.58              |
| 2:F:194:LEU:HD13 | 2:F:263:LEU:HD21 | 1.84                     | 0.58              |
| 2:M:249:LEU:HD12 | 2:M:249:LEU:C    | 2.28                     | 0.58              |
| 1:G:3:DA:H2''    | 1:G:4:DA:N7      | 2.18                     | 0.58              |
| 1:K:13:DA:H5'    | 2:N:245:THR:HG23 | 1.84                     | 0.58              |
| 1:O:7:DG:OP1     | 2:N:183:LYS:HG2  | 2.02                     | 0.58              |
| 2:A:218:LEU:HD11 | 2:A:220:MET:CG   | 2.32                     | 0.58              |
| 2:E:249:LEU:HD12 | 2:E:249:LEU:C    | 2.28                     | 0.58              |
| 2:F:202:VAL:HG13 | 2:F:203:PHE:N    | 2.18                     | 0.58              |
| 2:J:302:LEU:HD22 | 2:J:302:LEU:N    | 2.18                     | 0.58              |
| 2:I:218:LEU:HD11 | 2:I:220:MET:CG   | 2.32                     | 0.58              |
| 1:C:3:DA:H2''    | 1:C:4:DA:H8      | 1.62                     | 0.58              |
| 2:J:185:ASP:OD1  | 2:J:243:ARG:NH1  | 2.38                     | 0.57              |
| 2:B:185:ASP:OD1  | 2:B:243:ARG:NH1  | 2.38                     | 0.57              |
| 2:B:302:LEU:HD22 | 2:B:302:LEU:N    | 2.18                     | 0.57              |
| 2:F:302:LEU:HD22 | 2:F:302:LEU:N    | 2.18                     | 0.57              |
| 2:N:302:LEU:HD22 | 2:N:302:LEU:N    | 2.18                     | 0.57              |
| 2:M:220:MET:HG2  | 2:M:233:TYR:CD2  | 2.40                     | 0.57              |
| 2:I:220:MET:HG2  | 2:I:233:TYR:CD2  | 2.40                     | 0.57              |
| 1:G:6:DT:H5'     | 2:F:182:PHE:CE1  | 2.40                     | 0.57              |
| 1:O:6:DT:H5'     | 2:N:182:PHE:CE1  | 2.40                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:220:MET:HG2  | 2:E:233:TYR:CD2  | 2.40                     | 0.57              |
| 2:M:208:PHE:CZ   | 2:M:212:LYS:HD3  | 2.40                     | 0.57              |
| 2:A:220:MET:HG2  | 2:A:233:TYR:CD2  | 2.40                     | 0.57              |
| 1:C:4:DA:H5''    | 2:A:183:LYS:HG3  | 1.87                     | 0.57              |
| 1:K:4:DA:H5''    | 2:I:183:LYS:HG3  | 1.87                     | 0.57              |
| 2:E:208:PHE:CZ   | 2:E:212:LYS:HD3  | 2.40                     | 0.57              |
| 2:E:244:GLU:O    | 2:E:245:THR:C    | 2.48                     | 0.57              |
| 2:F:184:ASN:HB3  | 2:F:187:THR:OG1  | 2.05                     | 0.57              |
| 2:I:208:PHE:CZ   | 2:I:212:LYS:HD3  | 2.40                     | 0.57              |
| 2:M:244:GLU:O    | 2:M:245:THR:C    | 2.48                     | 0.57              |
| 2:A:208:PHE:CZ   | 2:A:212:LYS:HD3  | 2.40                     | 0.56              |
| 2:E:194:LEU:O    | 2:E:232:VAL:HA   | 2.05                     | 0.56              |
| 1:O:4:DA:H5''    | 2:M:183:LYS:HG3  | 1.87                     | 0.56              |
| 2:N:184:ASN:HB3  | 2:N:187:THR:OG1  | 2.05                     | 0.56              |
| 1:C:6:DT:H5'     | 2:B:182:PHE:CE1  | 2.40                     | 0.56              |
| 1:K:6:DT:H5'     | 2:J:182:PHE:CE1  | 2.40                     | 0.56              |
| 2:A:194:LEU:O    | 2:A:232:VAL:HA   | 2.05                     | 0.56              |
| 2:I:194:LEU:O    | 2:I:232:VAL:HA   | 2.05                     | 0.56              |
| 2:M:194:LEU:O    | 2:M:232:VAL:HA   | 2.05                     | 0.56              |
| 1:G:4:DA:H5''    | 2:E:183:LYS:HG3  | 1.87                     | 0.56              |
| 1:G:19:DA:C2'    | 1:G:20:DA:H5'    | 2.31                     | 0.56              |
| 2:E:178:ILE:HG13 | 2:E:179:THR:HG23 | 1.87                     | 0.56              |
| 2:A:178:ILE:HG13 | 2:A:179:THR:HG23 | 1.87                     | 0.56              |
| 2:B:184:ASN:HB3  | 2:B:187:THR:OG1  | 2.05                     | 0.56              |
| 2:J:184:ASN:HB3  | 2:J:187:THR:OG1  | 2.05                     | 0.56              |
| 2:J:278:PHE:CE2  | 2:J:282:LEU:HD11 | 2.41                     | 0.56              |
| 1:K:6:DT:H2''    | 1:K:7:DG:O5'     | 2.06                     | 0.56              |
| 1:K:13:DA:C5'    | 2:N:245:THR:HG23 | 2.36                     | 0.56              |
| 1:O:6:DT:H2''    | 1:O:7:DG:O5'     | 2.06                     | 0.56              |
| 2:B:207:SER:O    | 2:B:211:LEU:HG   | 2.06                     | 0.56              |
| 2:F:243:ARG:HH21 | 2:F:264:GLN:NE2  | 2.04                     | 0.56              |
| 2:N:207:SER:O    | 2:N:211:LEU:HG   | 2.06                     | 0.56              |
| 2:B:278:PHE:CE2  | 2:B:282:LEU:HD11 | 2.41                     | 0.55              |
| 2:F:207:SER:O    | 2:F:211:LEU:HG   | 2.06                     | 0.55              |
| 2:F:278:PHE:CE2  | 2:F:282:LEU:HD11 | 2.41                     | 0.55              |
| 2:N:243:ARG:HH21 | 2:N:264:GLN:NE2  | 2.05                     | 0.55              |
| 2:A:182:PHE:CE1  | 2:A:265:PRO:HG3  | 2.42                     | 0.55              |
| 2:B:243:ARG:HH21 | 2:B:264:GLN:NE2  | 2.04                     | 0.55              |
| 2:E:182:PHE:CE1  | 2:E:265:PRO:HG3  | 2.42                     | 0.55              |
| 2:F:194:LEU:HD11 | 2:F:261:LEU:HD22 | 1.88                     | 0.55              |
| 2:I:182:PHE:CE1  | 2:I:265:PRO:HG3  | 2.42                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:178:ILE:HG13 | 2:M:179:THR:HG23 | 1.87                     | 0.55              |
| 2:M:182:PHE:CE1  | 2:M:265:PRO:HG3  | 2.42                     | 0.55              |
| 1:C:6:DT:H2''    | 1:C:7:DG:O5'     | 2.06                     | 0.55              |
| 1:G:6:DT:H2''    | 1:G:7:DG:O5'     | 2.06                     | 0.55              |
| 2:I:178:ILE:HG13 | 2:I:179:THR:HG23 | 1.87                     | 0.55              |
| 2:N:185:ASP:OD1  | 2:N:243:ARG:NH1  | 2.38                     | 0.55              |
| 2:N:278:PHE:CE2  | 2:N:282:LEU:HD11 | 2.41                     | 0.55              |
| 2:E:218:LEU:HD11 | 2:E:220:MET:CG   | 2.32                     | 0.55              |
| 2:J:207:SER:O    | 2:J:211:LEU:HG   | 2.06                     | 0.55              |
| 2:N:194:LEU:HD11 | 2:N:261:LEU:HD22 | 1.88                     | 0.55              |
| 1:O:19:DA:C2'    | 1:O:20:DA:H5'    | 2.30                     | 0.55              |
| 2:J:243:ARG:HH21 | 2:J:264:GLN:NE2  | 2.04                     | 0.55              |
| 1:O:13:DA:C5'    | 2:J:245:THR:HG23 | 2.37                     | 0.54              |
| 1:O:13:DA:H5''   | 2:J:245:THR:HG23 | 1.88                     | 0.54              |
| 2:M:218:LEU:HD11 | 2:M:220:MET:CG   | 2.32                     | 0.54              |
| 2:B:243:ARG:NH2  | 2:B:264:GLN:NE2  | 2.56                     | 0.54              |
| 2:J:243:ARG:NH2  | 2:J:264:GLN:NE2  | 2.56                     | 0.54              |
| 2:A:244:GLU:O    | 2:A:245:THR:C    | 2.48                     | 0.54              |
| 2:A:254:LEU:O    | 2:A:255:ASN:HB3  | 2.08                     | 0.54              |
| 2:M:254:LEU:O    | 2:M:255:ASN:HB3  | 2.08                     | 0.54              |
| 2:E:194:LEU:HD11 | 2:E:261:LEU:HD22 | 1.90                     | 0.54              |
| 2:F:185:ASP:OD1  | 2:F:243:ARG:NH1  | 2.38                     | 0.54              |
| 2:F:220:MET:HE3  | 2:F:233:TYR:CZ   | 2.42                     | 0.54              |
| 2:F:243:ARG:NH2  | 2:F:264:GLN:NE2  | 2.56                     | 0.54              |
| 2:I:254:LEU:O    | 2:I:255:ASN:HB3  | 2.08                     | 0.54              |
| 2:N:220:MET:HE3  | 2:N:233:TYR:CZ   | 2.42                     | 0.54              |
| 2:E:254:LEU:O    | 2:E:255:ASN:HB3  | 2.08                     | 0.54              |
| 2:I:244:GLU:O    | 2:I:245:THR:C    | 2.48                     | 0.54              |
| 2:M:194:LEU:HD11 | 2:M:261:LEU:HD22 | 1.90                     | 0.54              |
| 2:B:220:MET:HE3  | 2:B:233:TYR:CZ   | 2.42                     | 0.54              |
| 2:J:194:LEU:HD11 | 2:J:261:LEU:HD22 | 1.88                     | 0.54              |
| 2:B:194:LEU:HD11 | 2:B:261:LEU:HD22 | 1.88                     | 0.54              |
| 2:J:220:MET:HE3  | 2:J:233:TYR:CZ   | 2.42                     | 0.54              |
| 1:G:20:DA:C8     | 2:I:162:PHE:CE2  | 2.96                     | 0.53              |
| 2:A:162:PHE:O    | 2:A:163:LYS:C    | 2.51                     | 0.53              |
| 2:E:162:PHE:O    | 2:E:163:LYS:C    | 2.51                     | 0.53              |
| 2:M:162:PHE:O    | 2:M:163:LYS:C    | 2.51                     | 0.53              |
| 2:B:211:LEU:HD23 | 2:B:253:MET:HE1  | 1.91                     | 0.53              |
| 2:J:211:LEU:HD23 | 2:J:253:MET:HE1  | 1.91                     | 0.53              |
| 2:N:243:ARG:NH2  | 2:N:264:GLN:NE2  | 2.56                     | 0.53              |
| 1:C:16:DA:O5'    | 2:E:245:THR:HG23 | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:21:DT:C7     | 2:I:162:PHE:HE2  | 1.95                     | 0.53              |
| 2:B:220:MET:HG2  | 2:B:233:TYR:CD2  | 2.43                     | 0.53              |
| 2:I:162:PHE:O    | 2:I:163:LYS:C    | 2.51                     | 0.53              |
| 2:J:220:MET:HG2  | 2:J:233:TYR:CD2  | 2.43                     | 0.53              |
| 2:N:220:MET:HG2  | 2:N:233:TYR:CD2  | 2.43                     | 0.53              |
| 2:M:292:LEU:CD1  | 2:M:296:ILE:HB   | 2.38                     | 0.53              |
| 2:F:220:MET:HG2  | 2:F:233:TYR:CD2  | 2.43                     | 0.53              |
| 2:I:194:LEU:HD11 | 2:I:261:LEU:HD22 | 1.90                     | 0.53              |
| 1:G:20:DA:H2'    | 2:I:162:PHE:HD2  | 1.69                     | 0.52              |
| 2:A:194:LEU:HD11 | 2:A:261:LEU:HD22 | 1.90                     | 0.52              |
| 2:B:160:THR:O    | 2:B:163:LYS:HB2  | 2.10                     | 0.52              |
| 1:G:2:DT:C2'     | 1:G:3:DA:O5'     | 2.57                     | 0.52              |
| 2:A:292:LEU:CD1  | 2:A:296:ILE:HB   | 2.38                     | 0.52              |
| 2:J:160:THR:O    | 2:J:163:LYS:HB2  | 2.10                     | 0.52              |
| 1:K:2:DT:C2'     | 1:K:3:DA:O5'     | 2.57                     | 0.52              |
| 2:E:191:GLN:HG2  | 2:E:236:CYS:SG   | 2.50                     | 0.52              |
| 2:E:292:LEU:CD1  | 2:E:296:ILE:HB   | 2.38                     | 0.52              |
| 2:F:160:THR:O    | 2:F:163:LYS:HB2  | 2.10                     | 0.52              |
| 2:I:164:LEU:HD23 | 2:I:262:MET:HE1  | 1.92                     | 0.52              |
| 2:N:160:THR:O    | 2:N:163:LYS:HB2  | 2.10                     | 0.52              |
| 2:M:191:GLN:HG2  | 2:M:236:CYS:SG   | 2.50                     | 0.52              |
| 2:A:164:LEU:HD23 | 2:A:262:MET:HE1  | 1.92                     | 0.52              |
| 2:B:302:LEU:H    | 2:B:302:LEU:CD2  | 2.23                     | 0.52              |
| 2:F:211:LEU:HD23 | 2:F:253:MET:HE1  | 1.91                     | 0.52              |
| 2:I:292:LEU:CD1  | 2:I:296:ILE:HB   | 2.38                     | 0.52              |
| 2:J:302:LEU:H    | 2:J:302:LEU:CD2  | 2.23                     | 0.52              |
| 2:N:211:LEU:HD23 | 2:N:253:MET:HE1  | 1.91                     | 0.52              |
| 1:G:21:DT:P      | 2:I:161:VAL:CG1  | 2.98                     | 0.52              |
| 2:A:191:GLN:HG2  | 2:A:236:CYS:SG   | 2.50                     | 0.52              |
| 2:M:234:LEU:HD22 | 2:M:277:TRP:CD2  | 2.45                     | 0.52              |
| 2:E:234:LEU:HD22 | 2:E:277:TRP:CD2  | 2.45                     | 0.51              |
| 2:I:191:GLN:HG2  | 2:I:236:CYS:SG   | 2.50                     | 0.51              |
| 2:I:268:ILE:HA   | 2:I:295:TRP:CE3  | 2.45                     | 0.51              |
| 2:J:225:HIS:CD2  | 2:J:227:GLY:H    | 2.28                     | 0.51              |
| 1:C:7:DG:H3'     | 2:B:184:ASN:HD22 | 1.75                     | 0.51              |
| 2:E:167:PHE:CE1  | 2:E:175:PHE:HA   | 2.46                     | 0.51              |
| 2:M:164:LEU:HD23 | 2:M:262:MET:HE1  | 1.92                     | 0.51              |
| 2:N:225:HIS:CD2  | 2:N:227:GLY:H    | 2.28                     | 0.51              |
| 2:I:234:LEU:HD22 | 2:I:277:TRP:CD2  | 2.45                     | 0.51              |
| 2:M:167:PHE:CE1  | 2:M:175:PHE:HA   | 2.46                     | 0.51              |
| 2:M:268:ILE:HA   | 2:M:295:TRP:CE3  | 2.45                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:268:ILE:HA   | 2:A:295:TRP:CE3  | 2.45                     | 0.51              |
| 2:B:225:HIS:CD2  | 2:B:227:GLY:H    | 2.28                     | 0.51              |
| 2:N:302:LEU:H    | 2:N:302:LEU:CD2  | 2.22                     | 0.51              |
| 2:A:234:LEU:HD22 | 2:A:277:TRP:CD2  | 2.45                     | 0.51              |
| 2:A:291:ALA:O    | 2:A:292:LEU:C    | 2.54                     | 0.51              |
| 2:E:164:LEU:HD23 | 2:E:262:MET:HE1  | 1.92                     | 0.51              |
| 2:E:268:ILE:HA   | 2:E:295:TRP:CE3  | 2.45                     | 0.51              |
| 2:F:225:HIS:CD2  | 2:F:227:GLY:H    | 2.28                     | 0.51              |
| 2:F:302:LEU:H    | 2:F:302:LEU:CD2  | 2.23                     | 0.51              |
| 2:I:291:ALA:O    | 2:I:292:LEU:C    | 2.54                     | 0.51              |
| 1:G:7:DG:H3'     | 2:F:184:ASN:HD22 | 1.75                     | 0.51              |
| 1:K:7:DG:H3'     | 2:J:184:ASN:HD22 | 1.75                     | 0.50              |
| 1:O:7:DG:H3'     | 2:N:184:ASN:HD22 | 1.75                     | 0.50              |
| 2:A:235:ILE:HG21 | 2:A:237:PHE:CZ   | 2.47                     | 0.50              |
| 2:A:167:PHE:CE1  | 2:A:175:PHE:HA   | 2.46                     | 0.50              |
| 2:E:291:ALA:O    | 2:E:292:LEU:C    | 2.54                     | 0.50              |
| 2:I:167:PHE:CE1  | 2:I:175:PHE:HA   | 2.46                     | 0.50              |
| 2:I:199:LEU:HD11 | 2:I:254:LEU:HD22 | 1.94                     | 0.50              |
| 2:I:235:ILE:HG21 | 2:I:237:PHE:CZ   | 2.47                     | 0.50              |
| 1:G:20:DA:C2'    | 2:I:162:PHE:HD2  | 2.23                     | 0.50              |
| 2:A:199:LEU:HD11 | 2:A:254:LEU:HD22 | 1.94                     | 0.50              |
| 2:E:235:ILE:HG21 | 2:E:237:PHE:CZ   | 2.47                     | 0.50              |
| 2:B:268:ILE:CD1  | 2:B:268:ILE:H    | 2.25                     | 0.50              |
| 2:B:271:LEU:HD13 | 2:B:299:GLN:O    | 2.12                     | 0.50              |
| 2:F:163:LYS:HD3  | 2:F:197:PHE:HE2  | 1.77                     | 0.50              |
| 2:J:268:ILE:H    | 2:J:268:ILE:CD1  | 2.25                     | 0.50              |
| 2:J:268:ILE:HA   | 2:J:295:TRP:CE3  | 2.46                     | 0.50              |
| 2:B:268:ILE:HA   | 2:B:295:TRP:CE3  | 2.46                     | 0.50              |
| 2:F:268:ILE:H    | 2:F:268:ILE:CD1  | 2.25                     | 0.50              |
| 2:B:194:LEU:O    | 2:B:232:VAL:HA   | 2.12                     | 0.50              |
| 2:M:291:ALA:O    | 2:M:292:LEU:C    | 2.54                     | 0.50              |
| 2:N:163:LYS:HD3  | 2:N:197:PHE:HE2  | 1.77                     | 0.50              |
| 2:F:268:ILE:HA   | 2:F:295:TRP:CE3  | 2.46                     | 0.49              |
| 2:M:235:ILE:HG21 | 2:M:237:PHE:CZ   | 2.47                     | 0.49              |
| 2:N:268:ILE:HA   | 2:N:295:TRP:CE3  | 2.46                     | 0.49              |
| 1:O:6:DT:C2'     | 1:O:7:DG:H8      | 2.15                     | 0.49              |
| 2:A:189:ASN:ND2  | 2:A:191:GLN:O    | 2.45                     | 0.49              |
| 2:B:163:LYS:HD3  | 2:B:197:PHE:HE2  | 1.77                     | 0.49              |
| 2:E:218:LEU:CD1  | 2:E:220:MET:HG3  | 2.35                     | 0.49              |
| 2:M:161:VAL:HG13 | 2:M:162:PHE:N    | 2.27                     | 0.49              |
| 2:J:163:LYS:HD3  | 2:J:197:PHE:HE2  | 1.77                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:271:LEU:HD13 | 2:J:299:GLN:O    | 2.12                     | 0.49              |
| 2:N:268:ILE:CD1  | 2:N:268:ILE:H    | 2.25                     | 0.49              |
| 2:E:161:VAL:HG13 | 2:E:162:PHE:N    | 2.27                     | 0.49              |
| 2:J:194:LEU:O    | 2:J:232:VAL:HA   | 2.12                     | 0.49              |
| 1:G:6:DT:C2'     | 1:G:7:DG:H8      | 2.15                     | 0.49              |
| 2:F:194:LEU:O    | 2:F:232:VAL:HA   | 2.12                     | 0.49              |
| 2:F:271:LEU:HD13 | 2:F:299:GLN:O    | 2.12                     | 0.49              |
| 2:I:161:VAL:HG13 | 2:I:162:PHE:N    | 2.27                     | 0.49              |
| 2:M:218:LEU:CD1  | 2:M:220:MET:HG3  | 2.35                     | 0.49              |
| 2:A:161:VAL:HG13 | 2:A:162:PHE:N    | 2.27                     | 0.49              |
| 2:I:189:ASN:ND2  | 2:I:191:GLN:O    | 2.45                     | 0.49              |
| 2:N:219:GLN:HE22 | 2:N:281:SER:HB3  | 1.78                     | 0.49              |
| 2:N:292:LEU:HD22 | 2:N:293:PRO:HD2  | 1.95                     | 0.49              |
| 2:E:199:LEU:HD11 | 2:E:254:LEU:HD22 | 1.94                     | 0.49              |
| 1:O:6:DT:OP2     | 2:N:180:ARG:NE   | 2.46                     | 0.48              |
| 2:M:199:LEU:HD11 | 2:M:254:LEU:HD22 | 1.94                     | 0.48              |
| 2:B:219:GLN:HE22 | 2:B:281:SER:HB3  | 1.78                     | 0.48              |
| 2:I:195:ALA:HB3  | 2:I:262:MET:HB2  | 1.95                     | 0.48              |
| 1:K:6:DT:OP2     | 2:J:180:ARG:NE   | 2.46                     | 0.48              |
| 2:A:218:LEU:HD12 | 2:A:219:GLN:N    | 2.29                     | 0.48              |
| 2:I:218:LEU:HD12 | 2:I:219:GLN:N    | 2.29                     | 0.48              |
| 2:J:273:ALA:O    | 2:J:276:PHE:N    | 2.46                     | 0.48              |
| 2:F:219:GLN:HE22 | 2:F:281:SER:HB3  | 1.78                     | 0.48              |
| 2:J:219:GLN:HE22 | 2:J:281:SER:HB3  | 1.78                     | 0.48              |
| 2:N:271:LEU:HD13 | 2:N:299:GLN:O    | 2.12                     | 0.48              |
| 2:A:195:ALA:HB3  | 2:A:262:MET:HB2  | 1.95                     | 0.48              |
| 2:F:292:LEU:HD22 | 2:F:293:PRO:HD2  | 1.95                     | 0.48              |
| 2:N:194:LEU:O    | 2:N:232:VAL:HA   | 2.12                     | 0.48              |
| 1:G:6:DT:OP2     | 2:F:180:ARG:NE   | 2.46                     | 0.48              |
| 1:C:6:DT:OP2     | 2:B:180:ARG:NE   | 2.46                     | 0.48              |
| 2:B:292:LEU:HD22 | 2:B:293:PRO:HD2  | 1.95                     | 0.48              |
| 2:E:195:ALA:HB3  | 2:E:262:MET:HB2  | 1.95                     | 0.48              |
| 2:E:218:LEU:HD12 | 2:E:219:GLN:N    | 2.29                     | 0.48              |
| 2:J:201:GLU:HA   | 2:J:222:LYS:NZ   | 2.29                     | 0.48              |
| 2:M:163:LYS:HB3  | 2:M:197:PHE:CE2  | 2.48                     | 0.48              |
| 2:M:218:LEU:HD12 | 2:M:219:GLN:N    | 2.29                     | 0.48              |
| 2:J:292:LEU:HD22 | 2:J:293:PRO:HD2  | 1.95                     | 0.48              |
| 2:B:273:ALA:O    | 2:B:276:PHE:N    | 2.46                     | 0.48              |
| 2:F:254:LEU:O    | 2:F:255:ASN:HB3  | 2.14                     | 0.48              |
| 1:C:4:DA:C2'     | 1:C:5:DT:C5'     | 2.82                     | 0.48              |
| 2:A:163:LYS:HB3  | 2:A:197:PHE:CE2  | 2.49                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:201:GLU:HA   | 2:B:222:LYS:NZ   | 2.29                     | 0.47              |
| 2:E:189:ASN:ND2  | 2:E:191:GLN:O    | 2.45                     | 0.47              |
| 2:F:201:GLU:HA   | 2:F:222:LYS:NZ   | 2.29                     | 0.47              |
| 2:M:189:ASN:ND2  | 2:M:191:GLN:O    | 2.45                     | 0.47              |
| 2:N:201:GLU:HA   | 2:N:222:LYS:NZ   | 2.29                     | 0.47              |
| 2:N:254:LEU:O    | 2:N:255:ASN:HB3  | 2.14                     | 0.47              |
| 2:N:272:SER:O    | 2:N:275:LEU:HB2  | 2.14                     | 0.47              |
| 2:E:163:LYS:HB3  | 2:E:197:PHE:CE2  | 2.49                     | 0.47              |
| 2:F:272:SER:O    | 2:F:275:LEU:HB2  | 2.14                     | 0.47              |
| 2:I:163:LYS:HB3  | 2:I:197:PHE:CE2  | 2.49                     | 0.47              |
| 2:M:257:ARG:HB2  | 2:M:257:ARG:NH1  | 2.30                     | 0.47              |
| 2:B:272:SER:O    | 2:B:275:LEU:HB2  | 2.14                     | 0.47              |
| 2:E:257:ARG:NH1  | 2:E:257:ARG:HB2  | 2.30                     | 0.47              |
| 2:J:272:SER:O    | 2:J:275:LEU:HB2  | 2.14                     | 0.47              |
| 1:K:6:DT:C2'     | 1:K:7:DG:H8      | 2.15                     | 0.47              |
| 2:M:195:ALA:HB3  | 2:M:262:MET:HB2  | 1.95                     | 0.47              |
| 1:C:6:DT:H4'     | 1:C:6:DT:OP1     | 2.15                     | 0.47              |
| 1:K:6:DT:H4'     | 1:K:6:DT:OP1     | 2.15                     | 0.47              |
| 2:B:170:LEU:HD21 | 2:B:224:SER:HA   | 1.97                     | 0.47              |
| 2:B:178:ILE:HG13 | 2:B:179:THR:HG23 | 1.97                     | 0.47              |
| 2:I:280:SER:O    | 2:I:282:LEU:N    | 2.47                     | 0.47              |
| 2:J:178:ILE:HG13 | 2:J:179:THR:HG23 | 1.97                     | 0.47              |
| 1:K:4:DA:C2'     | 1:K:5:DT:C5'     | 2.82                     | 0.47              |
| 2:E:280:SER:O    | 2:E:282:LEU:N    | 2.47                     | 0.47              |
| 2:J:170:LEU:HD21 | 2:J:224:SER:HA   | 1.97                     | 0.47              |
| 2:M:280:SER:O    | 2:M:282:LEU:N    | 2.47                     | 0.47              |
| 1:C:6:DT:C2'     | 1:C:7:DG:H8      | 2.15                     | 0.47              |
| 2:N:273:ALA:O    | 2:N:276:PHE:N    | 2.46                     | 0.47              |
| 2:B:254:LEU:O    | 2:B:255:ASN:HB3  | 2.14                     | 0.46              |
| 2:F:273:ALA:O    | 2:F:276:PHE:N    | 2.46                     | 0.46              |
| 2:I:257:ARG:HB2  | 2:I:257:ARG:NH1  | 2.30                     | 0.46              |
| 2:N:173:CYS:O    | 2:N:173:CYS:SG   | 2.73                     | 0.46              |
| 1:O:2:DT:C2'     | 1:O:3:DA:O5'     | 2.57                     | 0.46              |
| 2:A:257:ARG:HB2  | 2:A:257:ARG:NH1  | 2.30                     | 0.46              |
| 2:A:280:SER:O    | 2:A:282:LEU:N    | 2.47                     | 0.46              |
| 2:F:173:CYS:O    | 2:F:173:CYS:SG   | 2.73                     | 0.46              |
| 2:J:254:LEU:O    | 2:J:255:ASN:HB3  | 2.14                     | 0.46              |
| 2:J:279:LYS:O    | 2:J:282:LEU:HB2  | 2.15                     | 0.46              |
| 1:G:6:DT:H4'     | 1:G:6:DT:OP1     | 2.15                     | 0.46              |
| 2:A:302:LEU:H    | 2:A:302:LEU:HD22 | 1.81                     | 0.46              |
| 2:E:277:TRP:HB2  | 2:E:296:ILE:HD13 | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:279:LYS:O    | 2:F:282:LEU:HB2  | 2.15                     | 0.46              |
| 2:I:302:LEU:HD22 | 2:I:302:LEU:H    | 1.81                     | 0.46              |
| 2:B:279:LYS:O    | 2:B:282:LEU:HB2  | 2.15                     | 0.46              |
| 2:M:277:TRP:HB2  | 2:M:296:ILE:HD13 | 1.98                     | 0.46              |
| 2:N:279:LYS:O    | 2:N:282:LEU:HB2  | 2.15                     | 0.46              |
| 2:E:235:ILE:HG22 | 2:E:236:CYS:N    | 2.31                     | 0.46              |
| 2:N:170:LEU:HD21 | 2:N:224:SER:HA   | 1.97                     | 0.46              |
| 1:O:6:DT:H4'     | 1:O:6:DT:OP1     | 2.15                     | 0.46              |
| 2:F:161:VAL:HA   | 2:F:164:LEU:HD12 | 1.98                     | 0.46              |
| 2:J:161:VAL:HA   | 2:J:164:LEU:HD12 | 1.98                     | 0.46              |
| 2:N:166:LEU:HD12 | 2:N:166:LEU:O    | 2.16                     | 0.46              |
| 2:N:178:ILE:HG13 | 2:N:179:THR:HG23 | 1.97                     | 0.46              |
| 2:J:166:LEU:HD12 | 2:J:166:LEU:O    | 2.16                     | 0.46              |
| 2:M:235:ILE:HG22 | 2:M:236:CYS:N    | 2.31                     | 0.46              |
| 2:N:280:SER:C    | 2:N:282:LEU:H    | 2.24                     | 0.46              |
| 1:O:3:DA:C2'     | 1:O:4:DA:C8      | 2.85                     | 0.45              |
| 2:A:235:ILE:HG22 | 2:A:236:CYS:N    | 2.31                     | 0.45              |
| 2:F:178:ILE:HG13 | 2:F:179:THR:HG23 | 1.97                     | 0.45              |
| 2:F:166:LEU:O    | 2:F:166:LEU:HD12 | 2.16                     | 0.45              |
| 2:F:280:SER:C    | 2:F:282:LEU:H    | 2.24                     | 0.45              |
| 2:N:161:VAL:HA   | 2:N:164:LEU:HD12 | 1.98                     | 0.45              |
| 2:I:279:LYS:O    | 2:I:282:LEU:HB2  | 2.17                     | 0.45              |
| 2:M:302:LEU:H    | 2:M:302:LEU:HD22 | 1.81                     | 0.45              |
| 2:B:161:VAL:HA   | 2:B:164:LEU:HD12 | 1.98                     | 0.45              |
| 2:B:280:SER:C    | 2:B:282:LEU:H    | 2.24                     | 0.45              |
| 2:F:170:LEU:HD21 | 2:F:224:SER:HA   | 1.97                     | 0.45              |
| 2:I:235:ILE:HG22 | 2:I:236:CYS:N    | 2.31                     | 0.45              |
| 2:J:280:SER:C    | 2:J:282:LEU:H    | 2.24                     | 0.45              |
| 2:A:250:MET:HE3  | 2:A:254:LEU:HG   | 1.99                     | 0.45              |
| 2:I:250:MET:HE3  | 2:I:254:LEU:HG   | 1.99                     | 0.45              |
| 2:B:166:LEU:HD12 | 2:B:166:LEU:O    | 2.16                     | 0.45              |
| 1:G:3:DA:C2'     | 1:G:4:DA:C8      | 2.85                     | 0.45              |
| 2:A:279:LYS:O    | 2:A:282:LEU:HB2  | 2.16                     | 0.45              |
| 2:F:220:MET:O    | 2:F:286:THR:HG23 | 2.17                     | 0.45              |
| 2:B:268:ILE:HD13 | 2:B:268:ILE:N    | 2.32                     | 0.45              |
| 2:E:302:LEU:H    | 2:E:302:LEU:HD22 | 1.81                     | 0.45              |
| 2:N:220:MET:O    | 2:N:286:THR:HG23 | 2.17                     | 0.45              |
| 2:J:173:CYS:O    | 2:J:173:CYS:SG   | 2.73                     | 0.45              |
| 2:J:200:ALA:O    | 2:J:201:GLU:C    | 2.61                     | 0.45              |
| 2:M:250:MET:HE3  | 2:M:254:LEU:HG   | 1.99                     | 0.45              |
| 2:B:200:ALA:O    | 2:B:201:GLU:C    | 2.60                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:220:MET:O    | 2:B:286:THR:HG23 | 2.17                     | 0.44              |
| 2:E:244:GLU:O    | 2:E:247:ARG:N    | 2.50                     | 0.44              |
| 2:J:268:ILE:HD13 | 2:J:268:ILE:N    | 2.32                     | 0.44              |
| 1:C:13:DA:C5'    | 2:F:245:THR:HG23 | 2.47                     | 0.44              |
| 2:B:173:CYS:O    | 2:B:173:CYS:SG   | 2.73                     | 0.44              |
| 2:E:279:LYS:O    | 2:E:282:LEU:HB2  | 2.17                     | 0.44              |
| 2:M:244:GLU:O    | 2:M:247:ARG:N    | 2.50                     | 0.44              |
| 2:I:244:GLU:O    | 2:I:247:ARG:N    | 2.50                     | 0.44              |
| 2:F:197:PHE:CE1  | 2:F:230:CYS:SG   | 3.09                     | 0.44              |
| 2:I:160:THR:O    | 2:I:161:VAL:C    | 2.60                     | 0.44              |
| 2:J:220:MET:O    | 2:J:286:THR:HG23 | 2.17                     | 0.44              |
| 2:A:277:TRP:HB2  | 2:A:296:ILE:HD13 | 1.98                     | 0.44              |
| 2:E:160:THR:O    | 2:E:161:VAL:C    | 2.60                     | 0.44              |
| 2:E:250:MET:HE3  | 2:E:254:LEU:HG   | 1.99                     | 0.44              |
| 2:N:197:PHE:CE1  | 2:N:230:CYS:SG   | 3.09                     | 0.44              |
| 2:A:160:THR:O    | 2:A:161:VAL:C    | 2.60                     | 0.44              |
| 2:I:277:TRP:HB2  | 2:I:296:ILE:HD13 | 1.98                     | 0.44              |
| 2:M:279:LYS:O    | 2:M:282:LEU:HB2  | 2.17                     | 0.44              |
| 2:A:244:GLU:O    | 2:A:247:ARG:N    | 2.50                     | 0.44              |
| 2:B:163:LYS:O    | 2:B:164:LEU:C    | 2.61                     | 0.44              |
| 2:F:200:ALA:HB3  | 2:F:203:PHE:HD2  | 1.83                     | 0.44              |
| 2:I:218:LEU:CD1  | 2:I:220:MET:HG3  | 2.35                     | 0.44              |
| 2:M:160:THR:O    | 2:M:161:VAL:C    | 2.60                     | 0.44              |
| 2:N:268:ILE:HD13 | 2:N:268:ILE:N    | 2.32                     | 0.44              |
| 1:C:3:DA:C2'     | 1:C:4:DA:C8      | 2.85                     | 0.44              |
| 2:B:172:LEU:O    | 2:B:173:CYS:HB3  | 2.17                     | 0.44              |
| 2:F:163:LYS:O    | 2:F:164:LEU:C    | 2.61                     | 0.44              |
| 2:M:226:GLU:HG2  | 2:M:227:GLY:N    | 2.33                     | 0.44              |
| 2:N:200:ALA:HB3  | 2:N:203:PHE:HD2  | 1.83                     | 0.44              |
| 2:N:200:ALA:O    | 2:N:201:GLU:C    | 2.60                     | 0.44              |
| 1:G:21:DT:P      | 2:I:161:VAL:HG11 | 2.58                     | 0.43              |
| 2:E:167:PHE:CE2  | 2:E:232:VAL:HG11 | 2.51                     | 0.43              |
| 2:N:172:LEU:O    | 2:N:173:CYS:HB3  | 2.17                     | 0.43              |
| 2:A:179:THR:HG22 | 2:A:193:VAL:CG2  | 2.47                     | 0.43              |
| 2:E:226:GLU:HG2  | 2:E:227:GLY:N    | 2.33                     | 0.43              |
| 2:F:200:ALA:O    | 2:F:201:GLU:C    | 2.61                     | 0.43              |
| 2:J:172:LEU:O    | 2:J:173:CYS:HB3  | 2.17                     | 0.43              |
| 2:B:191:GLN:HA   | 2:B:235:ILE:O    | 2.18                     | 0.43              |
| 2:B:292:LEU:HA   | 2:B:293:PRO:HD3  | 1.79                     | 0.43              |
| 2:J:200:ALA:HB3  | 2:J:203:PHE:HD2  | 1.83                     | 0.43              |
| 2:F:172:LEU:O    | 2:F:173:CYS:HB3  | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:163:LYS:O    | 2:J:164:LEU:C    | 2.61                     | 0.43              |
| 2:J:191:GLN:HA   | 2:J:235:ILE:O    | 2.18                     | 0.43              |
| 2:M:167:PHE:CE2  | 2:M:232:VAL:HG11 | 2.51                     | 0.43              |
| 2:N:210:LEU:CD1  | 2:N:253:MET:HE2  | 2.40                     | 0.43              |
| 2:F:191:GLN:HA   | 2:F:235:ILE:O    | 2.18                     | 0.43              |
| 2:F:268:ILE:HD13 | 2:F:268:ILE:N    | 2.32                     | 0.43              |
| 2:I:226:GLU:HG2  | 2:I:227:GLY:N    | 2.33                     | 0.43              |
| 1:G:13:DA:C5'    | 2:B:245:THR:HG23 | 2.49                     | 0.43              |
| 2:A:226:GLU:HG2  | 2:A:227:GLY:N    | 2.33                     | 0.43              |
| 2:E:163:LYS:HE2  | 2:E:259:GLU:O    | 2.19                     | 0.43              |
| 2:E:280:SER:C    | 2:E:282:LEU:N    | 2.77                     | 0.43              |
| 2:N:279:LYS:HA   | 2:N:282:LEU:HD12 | 2.01                     | 0.43              |
| 2:B:196:VAL:HG21 | 2:B:254:LEU:CD1  | 2.49                     | 0.43              |
| 2:F:279:LYS:HA   | 2:F:282:LEU:HD12 | 2.01                     | 0.43              |
| 2:I:179:THR:HG22 | 2:I:193:VAL:CG2  | 2.47                     | 0.43              |
| 2:N:163:LYS:O    | 2:N:164:LEU:C    | 2.61                     | 0.43              |
| 2:N:191:GLN:HA   | 2:N:235:ILE:O    | 2.18                     | 0.43              |
| 2:N:234:LEU:HD12 | 2:N:234:LEU:HA   | 1.82                     | 0.43              |
| 2:A:218:LEU:CD1  | 2:A:220:MET:HG3  | 2.35                     | 0.43              |
| 2:B:197:PHE:CE1  | 2:B:230:CYS:SG   | 3.09                     | 0.43              |
| 2:B:200:ALA:HB3  | 2:B:203:PHE:HD2  | 1.83                     | 0.43              |
| 2:M:280:SER:C    | 2:M:282:LEU:N    | 2.77                     | 0.43              |
| 1:K:16:DA:O5'    | 2:M:245:THR:HG23 | 2.19                     | 0.43              |
| 2:M:206:ALA:O    | 2:M:207:SER:C    | 2.62                     | 0.43              |
| 2:N:196:VAL:HG21 | 2:N:254:LEU:CD1  | 2.49                     | 0.43              |
| 2:N:214:GLN:C    | 2:N:238:ASN:ND2  | 2.77                     | 0.43              |
| 2:J:292:LEU:HA   | 2:J:293:PRO:HD3  | 1.79                     | 0.42              |
| 2:J:196:VAL:HG21 | 2:J:254:LEU:CD1  | 2.49                     | 0.42              |
| 1:O:3:DA:C2'     | 1:O:4:DA:N7      | 2.82                     | 0.42              |
| 2:B:210:LEU:HD23 | 2:B:210:LEU:HA   | 1.83                     | 0.42              |
| 2:F:214:GLN:C    | 2:F:238:ASN:ND2  | 2.77                     | 0.42              |
| 2:I:163:LYS:HE2  | 2:I:259:GLU:O    | 2.19                     | 0.42              |
| 2:J:210:LEU:CD1  | 2:J:253:MET:HE2  | 2.40                     | 0.42              |
| 2:M:163:LYS:HE2  | 2:M:259:GLU:O    | 2.18                     | 0.42              |
| 2:F:163:LYS:HD3  | 2:F:197:PHE:CE2  | 2.54                     | 0.42              |
| 2:J:210:LEU:HD23 | 2:J:210:LEU:HA   | 1.83                     | 0.42              |
| 2:E:210:LEU:HD23 | 2:E:210:LEU:HA   | 1.84                     | 0.42              |
| 2:A:206:ALA:O    | 2:A:207:SER:C    | 2.62                     | 0.42              |
| 2:B:234:LEU:HA   | 2:B:234:LEU:HD12 | 1.82                     | 0.42              |
| 2:F:292:LEU:HD13 | 2:F:293:PRO:HD2  | 2.02                     | 0.42              |
| 2:I:280:SER:C    | 2:I:282:LEU:N    | 2.77                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:268:ILE:CD1  | 2:J:268:ILE:N    | 2.83                     | 0.42              |
| 2:N:163:LYS:HD3  | 2:N:197:PHE:CE2  | 2.54                     | 0.42              |
| 2:N:211:LEU:O    | 2:N:212:LYS:C    | 2.63                     | 0.42              |
| 2:B:214:GLN:C    | 2:B:238:ASN:ND2  | 2.77                     | 0.42              |
| 2:B:257:ARG:C    | 2:B:259:GLU:N    | 2.77                     | 0.42              |
| 2:E:179:THR:HG22 | 2:E:193:VAL:CG2  | 2.47                     | 0.42              |
| 2:F:196:VAL:HG21 | 2:F:254:LEU:CD1  | 2.49                     | 0.42              |
| 2:F:211:LEU:O    | 2:F:212:LYS:C    | 2.63                     | 0.42              |
| 2:J:197:PHE:CE1  | 2:J:230:CYS:SG   | 3.09                     | 0.42              |
| 2:J:210:LEU:CD2  | 2:J:213:LYS:HE2  | 2.50                     | 0.42              |
| 1:G:16:DA:O5'    | 2:A:245:THR:HG23 | 2.19                     | 0.42              |
| 2:B:210:LEU:CD2  | 2:B:213:LYS:HE2  | 2.50                     | 0.42              |
| 2:I:210:LEU:HB3  | 2:I:253:MET:HE2  | 2.02                     | 0.42              |
| 2:A:210:LEU:HD23 | 2:A:210:LEU:HA   | 1.84                     | 0.42              |
| 2:B:268:ILE:CD1  | 2:B:268:ILE:N    | 2.83                     | 0.42              |
| 2:F:185:ASP:O    | 2:F:242:SER:HB2  | 2.20                     | 0.42              |
| 2:F:210:LEU:CD2  | 2:F:213:LYS:HE2  | 2.50                     | 0.42              |
| 2:F:224:SER:HB3  | 2:F:229:THR:HA   | 2.02                     | 0.42              |
| 2:N:268:ILE:CD1  | 2:N:268:ILE:N    | 2.83                     | 0.42              |
| 1:C:3:DA:C2'     | 1:C:4:DA:N7      | 2.82                     | 0.41              |
| 2:A:210:LEU:HB3  | 2:A:253:MET:HE2  | 2.02                     | 0.41              |
| 2:B:204:PHE:CE1  | 2:B:220:MET:HE2  | 2.55                     | 0.41              |
| 2:B:249:LEU:HD12 | 2:B:249:LEU:O    | 2.20                     | 0.41              |
| 2:J:214:GLN:C    | 2:J:238:ASN:ND2  | 2.77                     | 0.41              |
| 2:N:194:LEU:HG   | 2:N:196:VAL:HG23 | 2.02                     | 0.41              |
| 2:N:224:SER:HB3  | 2:N:229:THR:HA   | 2.02                     | 0.41              |
| 2:A:163:LYS:HE2  | 2:A:259:GLU:O    | 2.19                     | 0.41              |
| 2:A:302:LEU:HD22 | 2:A:302:LEU:N    | 2.36                     | 0.41              |
| 2:B:225:HIS:CD2  | 2:B:227:GLY:N    | 2.88                     | 0.41              |
| 2:F:268:ILE:CD1  | 2:F:268:ILE:N    | 2.83                     | 0.41              |
| 2:N:292:LEU:HD13 | 2:N:293:PRO:HD2  | 2.02                     | 0.41              |
| 1:K:3:DA:C2'     | 1:K:4:DA:N7      | 2.82                     | 0.41              |
| 2:B:279:LYS:HA   | 2:B:282:LEU:HD12 | 2.01                     | 0.41              |
| 2:I:206:ALA:O    | 2:I:207:SER:C    | 2.62                     | 0.41              |
| 2:I:302:LEU:HD22 | 2:I:302:LEU:N    | 2.36                     | 0.41              |
| 2:N:210:LEU:CD2  | 2:N:213:LYS:HE2  | 2.50                     | 0.41              |
| 2:A:160:THR:HG22 | 2:A:164:LEU:CD1  | 2.51                     | 0.41              |
| 2:J:204:PHE:CE1  | 2:J:220:MET:HE2  | 2.55                     | 0.41              |
| 2:J:225:HIS:CD2  | 2:J:227:GLY:N    | 2.88                     | 0.41              |
| 2:N:185:ASP:O    | 2:N:242:SER:HB2  | 2.20                     | 0.41              |
| 2:N:208:PHE:O    | 2:N:212:LYS:HG3  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:208:PHE:O    | 2:B:212:LYS:HG3  | 2.21                     | 0.41              |
| 2:F:194:LEU:HG   | 2:F:196:VAL:HG23 | 2.02                     | 0.41              |
| 2:F:204:PHE:CE1  | 2:F:220:MET:HE2  | 2.55                     | 0.41              |
| 2:J:279:LYS:HA   | 2:J:282:LEU:HD12 | 2.01                     | 0.41              |
| 2:M:160:THR:HG22 | 2:M:164:LEU:CD1  | 2.51                     | 0.41              |
| 2:N:273:ALA:O    | 2:N:274:ALA:C    | 2.64                     | 0.41              |
| 2:A:280:SER:C    | 2:A:282:LEU:N    | 2.77                     | 0.41              |
| 2:B:185:ASP:O    | 2:B:242:SER:HB2  | 2.20                     | 0.41              |
| 2:B:220:MET:SD   | 2:B:233:TYR:CE2  | 3.14                     | 0.41              |
| 2:F:273:ALA:O    | 2:F:274:ALA:C    | 2.64                     | 0.41              |
| 2:M:203:PHE:O    | 2:M:204:PHE:C    | 2.64                     | 0.41              |
| 1:C:14:DA:C2'    | 1:C:15:DC:O5'    | 2.68                     | 0.41              |
| 1:O:4:DA:C2'     | 1:O:5:DT:C5'     | 2.82                     | 0.41              |
| 2:A:167:PHE:CE2  | 2:A:232:VAL:HG11 | 2.51                     | 0.41              |
| 2:F:208:PHE:O    | 2:F:212:LYS:HG3  | 2.21                     | 0.41              |
| 2:F:249:LEU:HD12 | 2:F:249:LEU:O    | 2.20                     | 0.41              |
| 2:J:163:LYS:HD3  | 2:J:197:PHE:CE2  | 2.54                     | 0.41              |
| 2:J:220:MET:SD   | 2:J:233:TYR:CE2  | 3.14                     | 0.41              |
| 2:M:302:LEU:HD22 | 2:M:302:LEU:N    | 2.36                     | 0.41              |
| 2:N:225:HIS:CD2  | 2:N:227:GLY:N    | 2.88                     | 0.41              |
| 2:B:211:LEU:O    | 2:B:212:LYS:C    | 2.63                     | 0.41              |
| 2:B:292:LEU:HD13 | 2:B:293:PRO:HD2  | 2.01                     | 0.41              |
| 2:E:163:LYS:HB3  | 2:E:197:PHE:HE2  | 1.86                     | 0.41              |
| 2:I:160:THR:HG22 | 2:I:164:LEU:CD1  | 2.51                     | 0.41              |
| 2:J:249:LEU:HD12 | 2:J:249:LEU:O    | 2.20                     | 0.41              |
| 2:J:257:ARG:C    | 2:J:259:GLU:N    | 2.77                     | 0.41              |
| 2:J:273:ALA:O    | 2:J:274:ALA:C    | 2.64                     | 0.41              |
| 2:N:257:ARG:C    | 2:N:259:GLU:N    | 2.77                     | 0.41              |
| 1:G:3:DA:C2'     | 1:G:4:DA:N7      | 2.82                     | 0.41              |
| 2:A:197:PHE:CE1  | 2:A:230:CYS:SG   | 3.14                     | 0.41              |
| 2:B:163:LYS:HD3  | 2:B:197:PHE:CE2  | 2.54                     | 0.41              |
| 2:B:235:ILE:HG21 | 2:B:237:PHE:CZ   | 2.56                     | 0.41              |
| 2:E:203:PHE:O    | 2:E:204:PHE:C    | 2.64                     | 0.41              |
| 2:E:277:TRP:CB   | 2:E:296:ILE:HD13 | 2.51                     | 0.41              |
| 2:E:302:LEU:HD22 | 2:E:302:LEU:N    | 2.36                     | 0.41              |
| 2:J:185:ASP:O    | 2:J:242:SER:HB2  | 2.20                     | 0.41              |
| 2:J:208:PHE:O    | 2:J:212:LYS:HG3  | 2.21                     | 0.41              |
| 2:J:292:LEU:HD13 | 2:J:293:PRO:HD2  | 2.01                     | 0.41              |
| 2:M:163:LYS:HB3  | 2:M:197:PHE:HE2  | 1.86                     | 0.41              |
| 2:M:179:THR:HG22 | 2:M:193:VAL:CG2  | 2.47                     | 0.41              |
| 2:M:210:LEU:HA   | 2:M:210:LEU:HD23 | 1.84                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:218:LEU:HD13 | 2:M:235:ILE:HD13 | 2.03                     | 0.41              |
| 2:M:277:TRP:CB   | 2:M:296:ILE:HD13 | 2.51                     | 0.41              |
| 2:N:204:PHE:CE1  | 2:N:220:MET:HE2  | 2.55                     | 0.41              |
| 2:E:160:THR:HG22 | 2:E:164:LEU:CD1  | 2.51                     | 0.41              |
| 2:F:220:MET:SD   | 2:F:233:TYR:CE2  | 3.14                     | 0.41              |
| 2:J:224:SER:HB3  | 2:J:229:THR:HA   | 2.02                     | 0.41              |
| 2:J:235:ILE:HG21 | 2:J:237:PHE:CZ   | 2.56                     | 0.41              |
| 2:N:220:MET:SD   | 2:N:233:TYR:CE2  | 3.14                     | 0.41              |
| 2:N:235:ILE:HG21 | 2:N:237:PHE:CZ   | 2.56                     | 0.41              |
| 2:N:298:ALA:O    | 2:N:300:THR:N    | 2.54                     | 0.41              |
| 2:A:163:LYS:HB3  | 2:A:197:PHE:HE2  | 1.86                     | 0.40              |
| 2:A:200:ALA:O    | 2:A:201:GLU:C    | 2.64                     | 0.40              |
| 2:A:218:LEU:HD13 | 2:A:235:ILE:HD13 | 2.03                     | 0.40              |
| 2:B:224:SER:HB3  | 2:B:229:THR:HA   | 2.02                     | 0.40              |
| 2:E:200:ALA:O    | 2:E:201:GLU:C    | 2.64                     | 0.40              |
| 2:I:197:PHE:CE1  | 2:I:230:CYS:SG   | 3.14                     | 0.40              |
| 2:I:210:LEU:HD23 | 2:I:210:LEU:HA   | 1.84                     | 0.40              |
| 2:I:277:TRP:CB   | 2:I:296:ILE:HD13 | 2.51                     | 0.40              |
| 2:M:200:ALA:O    | 2:M:201:GLU:C    | 2.64                     | 0.40              |
| 2:N:254:LEU:HD23 | 2:N:254:LEU:HA   | 1.91                     | 0.40              |
| 2:N:292:LEU:HA   | 2:N:293:PRO:HD3  | 1.79                     | 0.40              |
| 2:A:203:PHE:O    | 2:A:204:PHE:C    | 2.64                     | 0.40              |
| 2:E:197:PHE:CE1  | 2:E:230:CYS:SG   | 3.14                     | 0.40              |
| 2:E:218:LEU:HD13 | 2:E:235:ILE:HD13 | 2.03                     | 0.40              |
| 2:F:235:ILE:HG21 | 2:F:237:PHE:CZ   | 2.56                     | 0.40              |
| 2:F:298:ALA:O    | 2:F:300:THR:N    | 2.55                     | 0.40              |
| 2:I:218:LEU:HD13 | 2:I:235:ILE:HD13 | 2.03                     | 0.40              |
| 2:M:282:LEU:HD23 | 2:M:282:LEU:HA   | 1.86                     | 0.40              |
| 2:N:249:LEU:O    | 2:N:249:LEU:HD12 | 2.20                     | 0.40              |
| 2:B:194:LEU:HG   | 2:B:196:VAL:HG23 | 2.02                     | 0.40              |
| 2:F:225:HIS:C    | 2:F:227:GLY:H    | 2.30                     | 0.40              |
| 2:I:200:ALA:O    | 2:I:201:GLU:C    | 2.64                     | 0.40              |
| 2:I:206:ALA:HB1  | 2:N:203:PHE:CE1  | 2.56                     | 0.40              |
| 2:J:298:ALA:O    | 2:J:300:THR:N    | 2.55                     | 0.40              |
| 2:N:225:HIS:C    | 2:N:227:GLY:H    | 2.30                     | 0.40              |
| 1:G:21:DT:P      | 2:I:159:ALA:HA   | 2.58                     | 0.40              |
| 1:O:14:DA:C2'    | 1:O:15:DC:O5'    | 2.68                     | 0.40              |
| 2:F:292:LEU:HA   | 2:F:293:PRO:HD3  | 1.79                     | 0.40              |
| 2:I:167:PHE:CE2  | 2:I:232:VAL:HG11 | 2.51                     | 0.40              |
| 2:M:210:LEU:HB3  | 2:M:253:MET:HE2  | 2.02                     | 0.40              |
| 2:A:277:TRP:CB   | 2:A:296:ILE:HD13 | 2.51                     | 0.40              |

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| Atom-1          | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|---------------|--------------------------|-------------------|
| 2:B:298:ALA:O   | 2:B:300:THR:N | 2.55                     | 0.40              |
| 2:F:225:HIS:CD2 | 2:F:227:GLY:N | 2.88                     | 0.40              |
| 2:J:211:LEU:O   | 2:J:212:LYS:C | 2.63                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured  | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|-----------|-----------|----------|-------------|----|
| 2   | A     | 143/148 (97%)   | 119 (83%) | 21 (15%)  | 3 (2%)   | 5           | 31 |
| 2   | B     | 143/148 (97%)   | 121 (85%) | 15 (10%)  | 7 (5%)   | 1           | 13 |
| 2   | E     | 143/148 (97%)   | 119 (83%) | 21 (15%)  | 3 (2%)   | 5           | 31 |
| 2   | F     | 143/148 (97%)   | 121 (85%) | 15 (10%)  | 7 (5%)   | 1           | 13 |
| 2   | I     | 143/148 (97%)   | 119 (83%) | 21 (15%)  | 3 (2%)   | 5           | 31 |
| 2   | J     | 143/148 (97%)   | 121 (85%) | 15 (10%)  | 7 (5%)   | 1           | 13 |
| 2   | M     | 143/148 (97%)   | 119 (83%) | 21 (15%)  | 3 (2%)   | 5           | 31 |
| 2   | N     | 143/148 (97%)   | 121 (85%) | 15 (10%)  | 7 (5%)   | 1           | 13 |
| All | All   | 1144/1184 (97%) | 960 (84%) | 144 (13%) | 40 (4%)  | 3           | 20 |

All (40) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 271 | LEU  |
| 2   | B     | 299 | GLN  |
| 2   | F     | 271 | LEU  |
| 2   | F     | 299 | GLN  |
| 2   | J     | 271 | LEU  |
| 2   | J     | 299 | GLN  |
| 2   | N     | 271 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 299 | GLN  |
| 2   | A     | 244 | GLU  |
| 2   | A     | 281 | SER  |
| 2   | E     | 244 | GLU  |
| 2   | E     | 281 | SER  |
| 2   | I     | 244 | GLU  |
| 2   | I     | 281 | SER  |
| 2   | M     | 244 | GLU  |
| 2   | M     | 281 | SER  |
| 2   | B     | 270 | GLY  |
| 2   | F     | 270 | GLY  |
| 2   | J     | 270 | GLY  |
| 2   | N     | 270 | GLY  |
| 2   | A     | 298 | ALA  |
| 2   | B     | 173 | CYS  |
| 2   | B     | 226 | GLU  |
| 2   | B     | 272 | SER  |
| 2   | E     | 298 | ALA  |
| 2   | F     | 173 | CYS  |
| 2   | F     | 226 | GLU  |
| 2   | F     | 272 | SER  |
| 2   | I     | 298 | ALA  |
| 2   | J     | 173 | CYS  |
| 2   | J     | 226 | GLU  |
| 2   | J     | 272 | SER  |
| 2   | M     | 298 | ALA  |
| 2   | N     | 173 | CYS  |
| 2   | N     | 226 | GLU  |
| 2   | N     | 272 | SER  |
| 2   | B     | 298 | ALA  |
| 2   | F     | 298 | ALA  |
| 2   | J     | 298 | ALA  |
| 2   | N     | 298 | ALA  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric | Outliers | Percentiles |    |
|-----|-------|-----------------|-----------|----------|-------------|----|
| 2   | A     | 127/129 (98%)   | 120 (94%) | 7 (6%)   | 19          | 52 |
| 2   | B     | 127/129 (98%)   | 122 (96%) | 5 (4%)   | 28          | 62 |
| 2   | E     | 127/129 (98%)   | 120 (94%) | 7 (6%)   | 19          | 52 |
| 2   | F     | 127/129 (98%)   | 122 (96%) | 5 (4%)   | 28          | 62 |
| 2   | I     | 127/129 (98%)   | 120 (94%) | 7 (6%)   | 19          | 52 |
| 2   | J     | 127/129 (98%)   | 122 (96%) | 5 (4%)   | 28          | 62 |
| 2   | M     | 127/129 (98%)   | 120 (94%) | 7 (6%)   | 19          | 52 |
| 2   | N     | 127/129 (98%)   | 122 (96%) | 5 (4%)   | 28          | 62 |
| All | All   | 1016/1032 (98%) | 968 (95%) | 48 (5%)  | 23          | 57 |

All (48) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 188 | THR  |
| 2   | A     | 202 | VAL  |
| 2   | A     | 218 | LEU  |
| 2   | A     | 229 | THR  |
| 2   | A     | 249 | LEU  |
| 2   | A     | 262 | MET  |
| 2   | A     | 292 | LEU  |
| 2   | B     | 182 | PHE  |
| 2   | B     | 210 | LEU  |
| 2   | B     | 221 | GLN  |
| 2   | B     | 239 | THR  |
| 2   | B     | 268 | ILE  |
| 2   | E     | 188 | THR  |
| 2   | E     | 202 | VAL  |
| 2   | E     | 218 | LEU  |
| 2   | E     | 229 | THR  |
| 2   | E     | 249 | LEU  |
| 2   | E     | 262 | MET  |
| 2   | E     | 292 | LEU  |
| 2   | F     | 182 | PHE  |
| 2   | F     | 210 | LEU  |
| 2   | F     | 221 | GLN  |
| 2   | F     | 239 | THR  |
| 2   | F     | 268 | ILE  |
| 2   | I     | 188 | THR  |
| 2   | I     | 202 | VAL  |
| 2   | I     | 218 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | I     | 229 | THR  |
| 2   | I     | 249 | LEU  |
| 2   | I     | 262 | MET  |
| 2   | I     | 292 | LEU  |
| 2   | J     | 182 | PHE  |
| 2   | J     | 210 | LEU  |
| 2   | J     | 221 | GLN  |
| 2   | J     | 239 | THR  |
| 2   | J     | 268 | ILE  |
| 2   | M     | 188 | THR  |
| 2   | M     | 202 | VAL  |
| 2   | M     | 218 | LEU  |
| 2   | M     | 229 | THR  |
| 2   | M     | 249 | LEU  |
| 2   | M     | 262 | MET  |
| 2   | M     | 292 | LEU  |
| 2   | N     | 182 | PHE  |
| 2   | N     | 210 | LEU  |
| 2   | N     | 221 | GLN  |
| 2   | N     | 239 | THR  |
| 2   | N     | 268 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 225 | HIS  |
| 2   | B     | 191 | GLN  |
| 2   | B     | 219 | GLN  |
| 2   | B     | 225 | HIS  |
| 2   | B     | 238 | ASN  |
| 2   | B     | 255 | ASN  |
| 2   | B     | 289 | HIS  |
| 2   | E     | 225 | HIS  |
| 2   | F     | 191 | GLN  |
| 2   | F     | 219 | GLN  |
| 2   | F     | 225 | HIS  |
| 2   | F     | 238 | ASN  |
| 2   | F     | 289 | HIS  |
| 2   | I     | 225 | HIS  |
| 2   | J     | 191 | GLN  |
| 2   | J     | 219 | GLN  |
| 2   | J     | 225 | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | J     | 238 | ASN  |
| 2   | J     | 255 | ASN  |
| 2   | J     | 289 | HIS  |
| 2   | M     | 225 | HIS  |
| 2   | N     | 191 | GLN  |
| 2   | N     | 219 | GLN  |
| 2   | N     | 225 | HIS  |
| 2   | N     | 238 | ASN  |
| 2   | N     | 289 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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.