



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Sep 5, 2017 – 04:53 AM EDT

PDB ID : 5XON  
EMDB ID: : EMD-6747  
Title : RNA Polymerase II elongation complex bound with Spt4/5 and TFIIS  
Authors : Ehara, H.; Yokoyama, T.; Shigematsu, H.; Shirouzu, M.; Sekine, S.  
Deposited on : unknown  
Resolution : 3.83 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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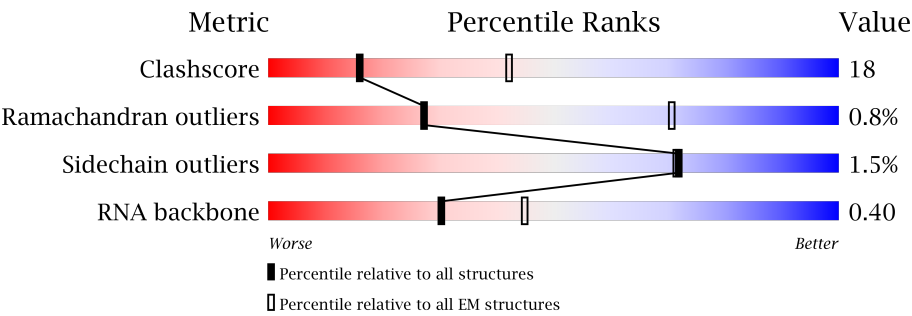
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.83 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) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 125131                      | 1336                        |
| Ramachandran outliers | 121729                      | 1120                        |
| Sidechain outliers    | 121581                      | 1026                        |
| RNA backbone          | 3398                        | 335                         |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

| Mol | Chain | Length | Quality of chain                |
|-----|-------|--------|---------------------------------|
| 1   | A     | 1743   | <div><div>61%19%18%</div></div> |
| 2   | B     | 1227   | <div><div>75%19%5%</div></div>  |
| 3   | C     | 304    | <div><div>69%16%13%</div></div> |
| 4   | D     | 186    | <div><div>52%37%10%</div></div> |
| 5   | E     | 214    | <div><div>78%20%</div></div>    |
| 6   | F     | 155    | <div><div>47%6%46%</div></div>  |
| 7   | G     | 171    | <div><div>49%49%</div></div>    |
| 8   | H     | 145    | <div><div>74%17%8%</div></div>  |

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| Mol | Chain | Length | Quality of chain                              |
|-----|-------|--------|---|
| 9   | I     | 115    | <div><div></div><div>78%17%••</div></div>     |
| 10  | J     | 72     | <div><div></div><div>72%19%8%</div></div>     |
| 11  | K     | 118    | <div><div></div><div>82%14%•</div></div>      |
| 12  | L     | 72     | <div><div></div><div>43%17%•38%</div></div>   |
| 13  | P     | 30     | <div><div></div><div>23%10%20%47%</div></div> |
| 14  | T     | 48     | <div><div></div><div>38%56%6%</div></div>     |
| 15  | N     | 48     | <div><div></div><div>33%50%6%10%</div></div>  |
| 16  | U     | 190    | <div><div></div><div>39%33%8%•18%</div></div> |
| 17  | V     | 108    | <div><div></div><div>81%12%•6%</div></div>    |
| 18  | W     | 612    | <div><div></div><div>35%16%•46%</div></div>   |

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 38369 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 1427     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11239 | 7089 | 1958 | 2122 | 70 |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | B     | 1161     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9261  | 5835 | 1636 | 1732 | 58 |         |       |

- Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 263      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2098  | 1319 | 354 | 413 | 12 |         |       |

- Molecule 4 is a protein called RNA polymerase II subunit B32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 168      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1314  | 812 | 237 | 263 | 2 |         |       |

- Molecule 5 is a protein called RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | E     | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1740  | 1094 | 312 | 324 | 10 |         |       |

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 677   | 429 | 114 | 131 | 3 |         |       |

- Molecule 7 is a protein called RNA polymerase II subunit.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | G     | 171      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1324  | 858 | 214 | 247 | 5 |         |       |

- Molecule 8 is a protein called RNA polymerase subunit ABC14.5, common to RNA polymerases I, II, and III.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1052  | 671 | 169 | 208 | 4 |         |       |

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 9   | I     | 111      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 917   | 565 | 161 | 180 | 11 |         |       |

There are 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment              | Reference  |
|-------|---------|----------|--------|----------------------|------------|
| I     | 1       | MET      | -      | see sequence details | UNP C4QY79 |
| I     | 2       | ALA      | -      | see sequence details | UNP C4QY79 |
| I     | 3       | SER      | MET    | see sequence details | UNP C4QY79 |
| I     | 4       | PHE      | THR    | see sequence details | UNP C4QY79 |
| I     | 5       | ARG      | ASN    | see sequence details | UNP C4QY79 |
| I     | 6       | PHE      | VAL    | see sequence details | UNP C4QY79 |
| I     | 7       | CYS      | ASN    | see sequence details | UNP C4QY79 |
| I     | 8       | LEU      | SER    | see sequence details | UNP C4QY79 |
| I     | 9       | GLU      | LEU    | see sequence details | UNP C4QY79 |
| I     | 10      | CYS      | SER    | see sequence details | UNP C4QY79 |

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10  | J     | 66       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 545   | 349 | 95 | 95 | 6 |         |       |

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | K     | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 932   | 599 | 160 | 169 | 4 |         |       |

- Molecule 12 is a protein called RNA polymerase subunit, found in RNA polymerase complexes I, II, and III.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12  | L     | 45       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 359   | 221 | 72 | 61 | 5 |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment              | Reference  |
|-------|---------|----------|--------|----------------------|------------|
| L     | 67      | ILE      | SER    | see sequence details | UNP C4QWA8 |
| L     | 68      | GLN      | LYS    | see sequence details | UNP C4QWA8 |
| L     | 70      | ASP      | LEU    | see sequence details | UNP C4QWA8 |
| L     | 71      | ALA      | THR    | see sequence details | UNP C4QWA8 |
| L     | 72      | ARG      | THR    | see sequence details | UNP C4QWA8 |

- Molecule 13 is a RNA chain called RNA (30-MER).

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 13  | P     | 16       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 338   | 151 | 55 | 116 | 16 |         |       |

- Molecule 14 is a DNA chain called DNA (48-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 14  | T     | 48       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 975   | 463 | 179 | 285 | 48 |         |       |

- Molecule 15 is a DNA chain called DNA (48-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 15  | N     | 43       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 889   | 422 | 163 | 261 | 43 |         |       |

- Molecule 16 is a protein called General transcription elongation factor TFIIS.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 16  | U     | 155      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1239  | 774 | 223 | 232 | 10 |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| U     | 96      | GLY      | -      | expression tag | UNP C4R2R6 |
| U     | 97      | PRO      | -      | expression tag | UNP C4R2R6 |
| U     | 98      | GLY      | -      | expression tag | UNP C4R2R6 |
| U     | 266     | ALA      | ASP    | conflict       | UNP C4R2R6 |
| U     | 267     | ALA      | GLU    | conflict       | UNP C4R2R6 |

- Molecule 17 is a protein called Transcription elongation factor SPT4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | V     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 792   | 492 | 143 | 150 | 7 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| V     | 7       | MET      | -      | expression tag | UNP C4R0E6 |

- Molecule 18 is a protein called Protein that forms a complex with Spt4p.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 18  | W     | 329      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2667  | 1698 | 483 | 485 | 1 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| W     | 204     | GLY      | -      | expression tag | UNP C4R370 |
| W     | 205     | PRO      | -      | expression tag | UNP C4R370 |

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 19  | J     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 19  | B     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 19  | I     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 19  | C     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 19  | V     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 19  | A     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 19  | U     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 19  | L     | 1        | Total<br>1 | Zn<br>1 | 0       |

- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

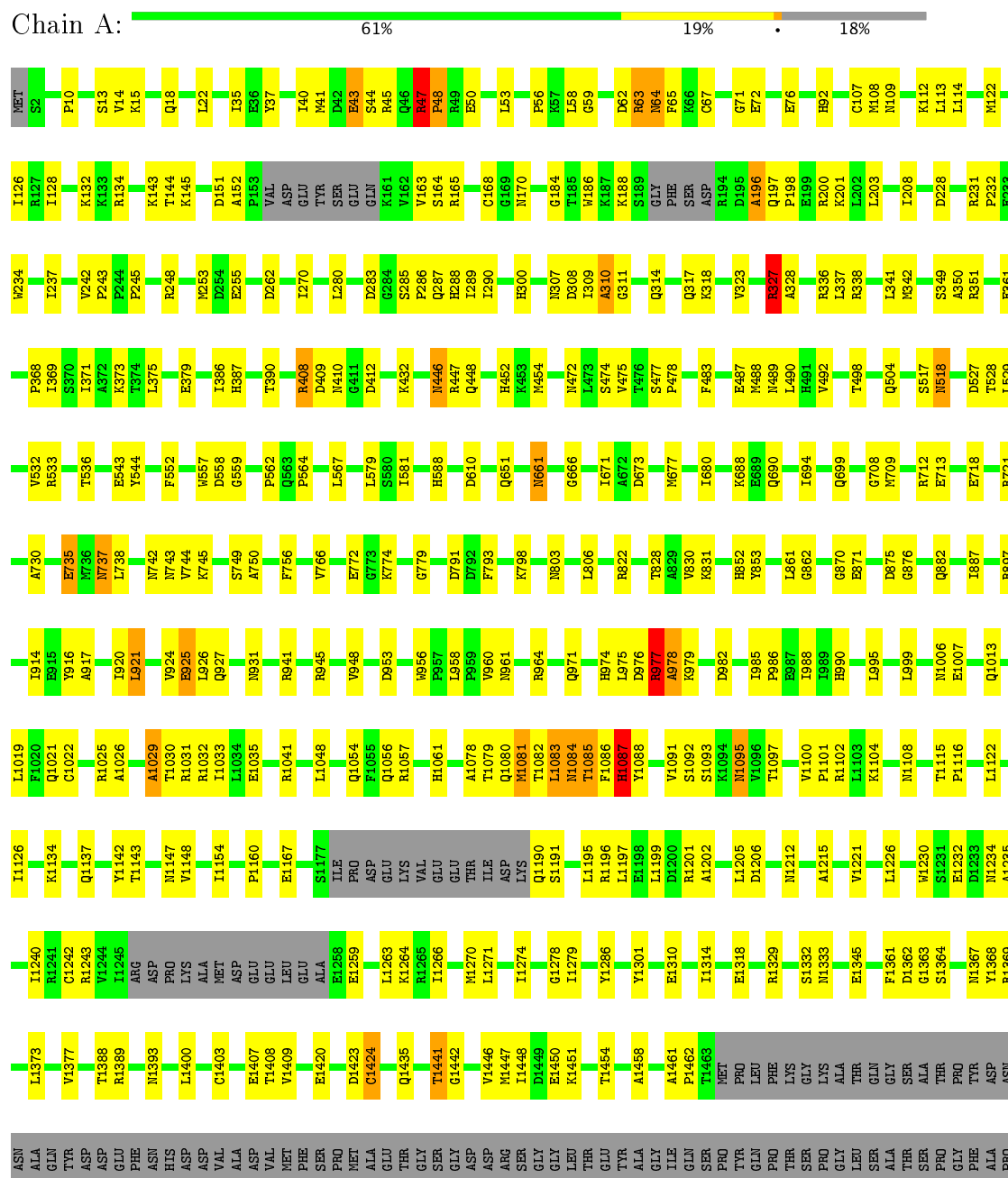
| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 20  | A     | 1        | Total<br>1 | Mg<br>1 | 0       |



### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

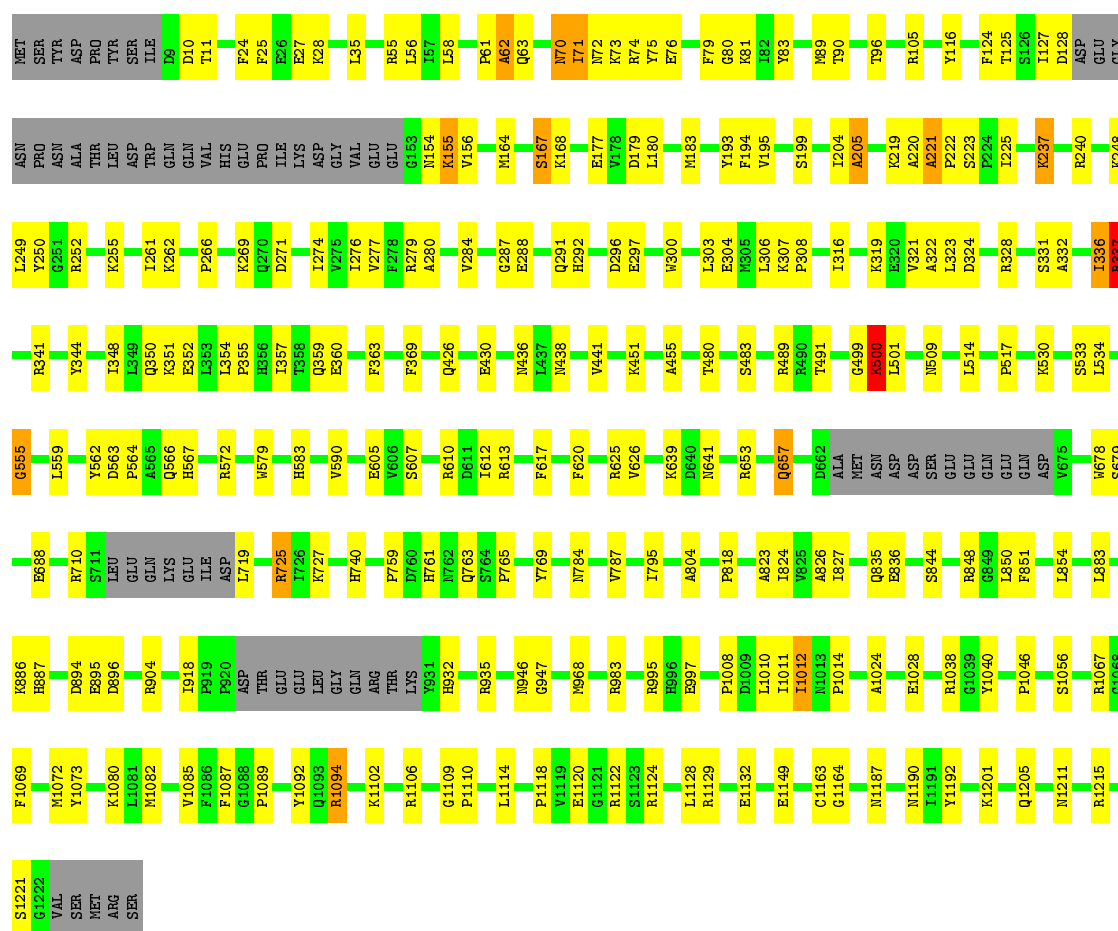
- Molecule 1: DNA-directed RNA polymerase subunit





- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:  75% 19% • 5%



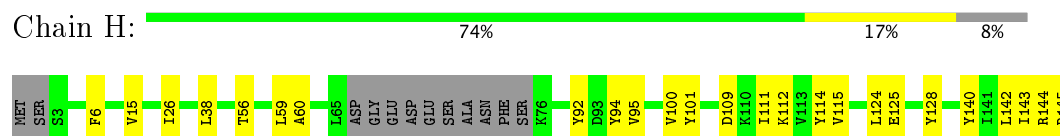
- Molecule 3: RNA polymerase II third largest subunit B44, part of central core

Chain C:  69% 16% • 13%

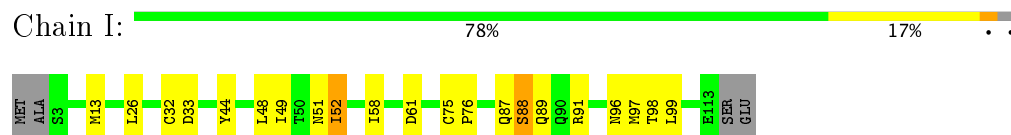




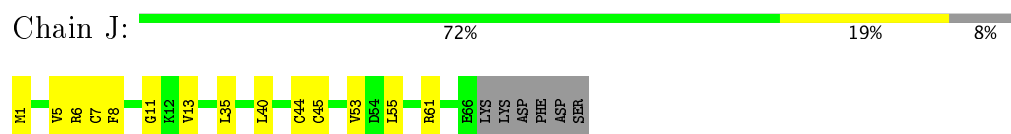
- Molecule 8: RNA polymerase subunit ABC14.5, common to RNA polymerases I, II, and III



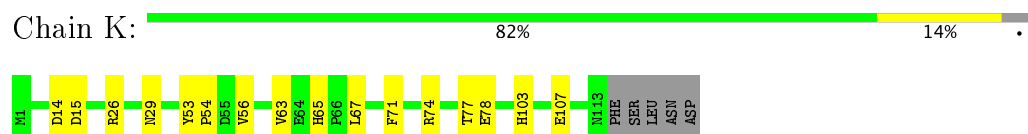
- Molecule 9: DNA-directed RNA polymerase subunit



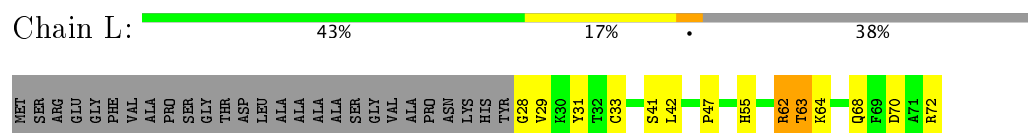
- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III



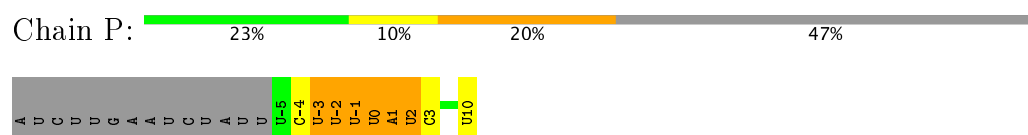
- Molecule 11: RNA polymerase II subunit B12.5



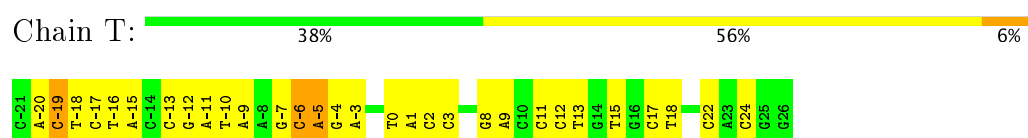
- Molecule 12: RNA polymerase subunit, found in RNA polymerase complexes I, II, and III



- Molecule 13: RNA (30-MER)



- Molecule 14: DNA (48-MER)



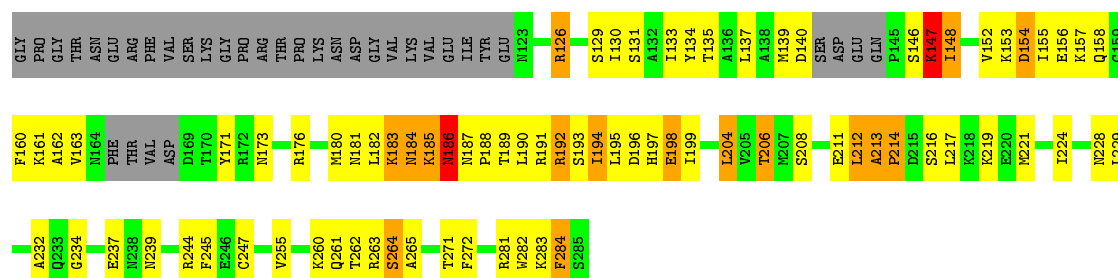
- Molecule 15: DNA (48-MER)

Chain N: 




- Molecule 16: General transcription elongation factor TFIIS

Chain U: 




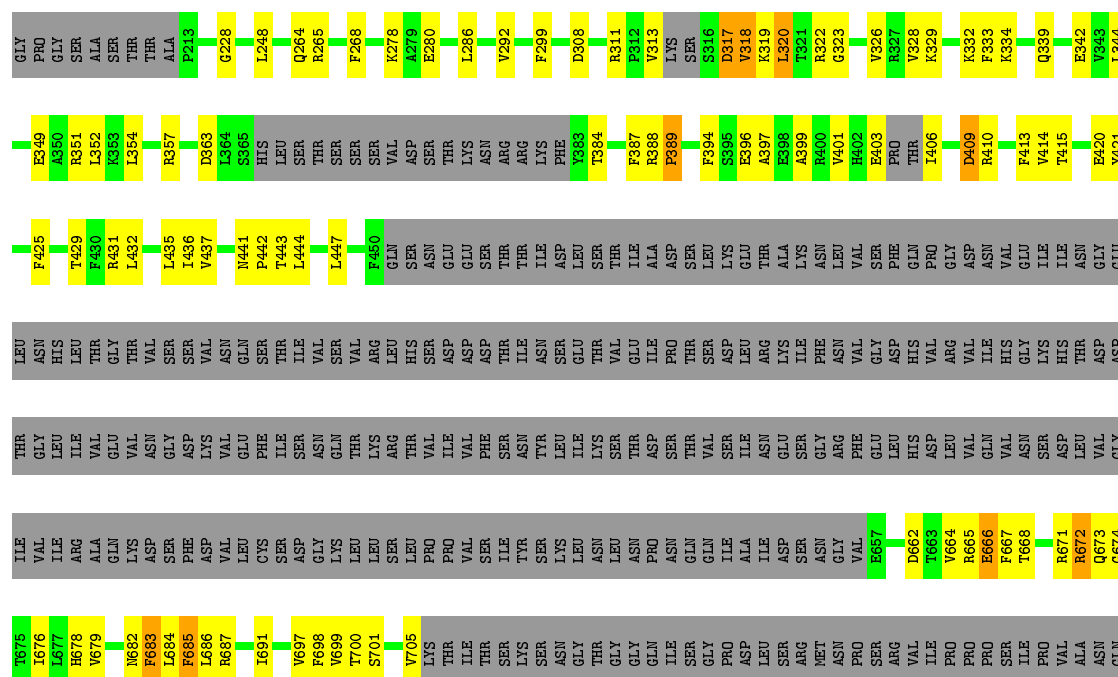
- Molecule 17: Transcription elongation factor SPT4

Chain V: 



- Molecule 18: Protein that forms a complex with Spt4p

Chain W: 



|     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |
|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|
| ARG | MET | THR | G747 | R748 | D749 | L752 | V756 | K757 | I758 | R759 | I767 | G775 | D776 | R777 | E781 | N784 | P785 | I786 | C793 | L796 | E799 | H802 | G803 | Y804 | Y805 | P806 | G807 | E808 | D809 | PHE | VAL | ALA | SER | ASP | ARG |
|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|

## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| Reconstruction method                | SINGLE PARTICLE           | Depositor |
| Imposed symmetry                     | POINT, C1                 | Depositor |
| Number of particles used             | 682749                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF         | Depositor |
| CTF correction method                | NONE                      | Depositor |
| Microscope                           | FEI TECNAI ARCTICA        | Depositor |
| Voltage (kV)                         | 200                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                        | Depositor |
| Minimum defocus (nm)                 | Not provided              | Depositor |
| Maximum defocus (nm)                 | Not provided              | Depositor |
| Magnification                        | Not provided              | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k) | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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         | $\# Z  > 2$     | RMSZ        | $\# Z  > 2$      |
| 1   | A     | 0.26         | 0/11449         | 0.69        | 42/15474 (0.3%)  |
| 10  | J     | 0.25         | 0/554           | 0.44        | 0/742            |
| 11  | K     | 0.26         | 0/953           | 0.44        | 0/1291           |
| 12  | L     | 0.25         | 0/365           | 0.70        | 2/484 (0.4%)     |
| 13  | P     | 0.28         | 0/376           | 0.85        | 0/583            |
| 14  | T     | 0.99         | 9/1092 (0.8%)   | 1.22        | 3/1680 (0.2%)    |
| 15  | N     | 0.89         | 10/996 (1.0%)   | 1.21        | 6/1535 (0.4%)    |
| 16  | U     | 0.29         | 0/1255          | 0.71        | 7/1677 (0.4%)    |
| 17  | V     | 0.46         | 0/808           | 0.60        | 0/1097           |
| 18  | W     | 0.40         | 0/2713          | 0.61        | 5/3646 (0.1%)    |
| 2   | B     | 0.26         | 0/9441          | 0.62        | 28/12732 (0.2%)  |
| 3   | C     | 0.25         | 0/2139          | 0.50        | 2/2895 (0.1%)    |
| 4   | D     | 0.31         | 0/1326          | 0.54        | 3/1788 (0.2%)    |
| 5   | E     | 0.25         | 0/1772          | 0.56        | 1/2385 (0.0%)    |
| 6   | F     | 0.24         | 0/687           | 0.52        | 1/931 (0.1%)     |
| 7   | G     | 0.33         | 0/1353          | 0.60        | 4/1837 (0.2%)    |
| 8   | H     | 0.25         | 0/1069          | 0.45        | 0/1444           |
| 9   | I     | 0.22         | 0/934           | 0.40        | 0/1257           |
| All | All   | 0.35         | 19/39282 (0.0%) | 0.67        | 104/53478 (0.2%) |

All (19) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | T     | -6  | DC   | C3'-O3' | -6.37 | 1.35        | 1.44     |
| 15  | N     | 2   | DT   | C1'-N1  | 6.00  | 1.57        | 1.49     |
| 15  | N     | -24 | DC   | C1'-N1  | 5.26  | 1.56        | 1.49     |
| 15  | N     | -19 | DC   | C1'-N1  | 5.24  | 1.56        | 1.49     |
| 15  | N     | -25 | DC   | C1'-N1  | 5.24  | 1.56        | 1.49     |
| 14  | T     | 15  | DT   | C1'-N1  | 5.24  | 1.56        | 1.49     |
| 14  | T     | 13  | DT   | C1'-N1  | 5.23  | 1.56        | 1.49     |
| 15  | N     | -22 | DT   | C1'-N1  | 5.23  | 1.56        | 1.49     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 14  | T     | 22  | DC   | C1'-N1 | 5.21 | 1.56        | 1.49     |
| 14  | T     | 24  | DC   | C1'-N1 | 5.19 | 1.56        | 1.49     |
| 14  | T     | 12  | DC   | C1'-N1 | 5.19 | 1.55        | 1.49     |
| 15  | N     | -13 | DC   | C1'-N1 | 5.18 | 1.55        | 1.49     |
| 15  | N     | -15 | DC   | C1'-N1 | 5.16 | 1.55        | 1.49     |
| 15  | N     | -20 | DT   | C1'-N1 | 5.15 | 1.55        | 1.49     |
| 14  | T     | 17  | DC   | C1'-N1 | 5.15 | 1.55        | 1.49     |
| 14  | T     | 18  | DT   | C1'-N1 | 5.14 | 1.55        | 1.49     |
| 15  | N     | -18 | DT   | C1'-N1 | 5.14 | 1.55        | 1.49     |
| 14  | T     | 11  | DC   | C1'-N1 | 5.11 | 1.55        | 1.49     |
| 15  | N     | -5  | DT   | C1'-N1 | 5.03 | 1.55        | 1.49     |

All (104) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | A     | 310  | ALA  | CB-CA-C | 16.63  | 135.04      | 110.10   |
| 2   | B     | 221  | ALA  | N-CA-CB | -14.50 | 89.80       | 110.10   |
| 2   | B     | 167  | SER  | CB-CA-C | 14.38  | 137.42      | 110.10   |
| 1   | A     | 47   | ARG  | C-N-CD  | -13.03 | 91.93       | 120.60   |
| 1   | A     | 861  | LEU  | CB-CA-C | -12.61 | 86.24       | 110.20   |
| 16  | U     | 198  | GLU  | CB-CA-C | 12.18  | 134.75      | 110.40   |
| 1   | A     | 1368 | TYR  | N-CA-CB | -12.14 | 88.74       | 110.60   |
| 1   | A     | 1367 | ASN  | CB-CA-C | -11.81 | 86.78       | 110.40   |
| 5   | E     | 104  | PHE  | CB-CA-C | -11.77 | 86.86       | 110.40   |
| 1   | A     | 328  | ALA  | N-CA-CB | -11.64 | 93.80       | 110.10   |
| 1   | A     | 1029 | ALA  | CB-CA-C | -11.45 | 92.93       | 110.10   |
| 1   | A     | 361  | GLU  | CB-CA-C | -11.20 | 88.01       | 110.40   |
| 1   | A     | 978  | ALA  | N-CA-CB | -11.08 | 94.59       | 110.10   |
| 1   | A     | 196  | ALA  | CB-CA-C | -10.87 | 93.80       | 110.10   |
| 1   | A     | 310  | ALA  | N-CA-C  | -10.73 | 82.03       | 111.00   |
| 1   | A     | 925  | GLU  | CB-CA-C | 10.60  | 131.60      | 110.40   |
| 1   | A     | 58   | LEU  | N-CA-C  | 10.59  | 139.58      | 111.00   |
| 1   | A     | 978  | ALA  | N-CA-C  | 10.46  | 139.24      | 111.00   |
| 2   | B     | 168  | LYS  | N-CA-CB | -10.31 | 92.05       | 110.60   |
| 1   | A     | 64   | ASN  | N-CA-CB | -10.17 | 92.29       | 110.60   |
| 2   | B     | 337  | ARG  | N-CA-CB | -10.15 | 92.33       | 110.60   |
| 1   | A     | 59   | GLY  | N-CA-C  | -9.81  | 88.58       | 113.10   |
| 1   | A     | 408  | ARG  | CB-CA-C | -9.79  | 90.82       | 110.40   |
| 2   | B     | 80   | GLY  | N-CA-C  | 9.60   | 137.10      | 113.10   |
| 2   | B     | 62   | ALA  | N-CA-CB | 9.58   | 123.51      | 110.10   |
| 1   | A     | 63   | ARG  | CB-CA-C | 9.56   | 129.52      | 110.40   |
| 2   | B     | 167  | SER  | N-CA-C  | -9.50  | 85.35       | 111.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 926  | LEU  | N-CA-CB    | -9.21 | 91.98       | 110.40   |
| 1   | A     | 977  | ARG  | CB-CA-C    | 9.00  | 128.41      | 110.40   |
| 2   | B     | 79   | PHE  | CB-CA-C    | -8.95 | 92.50       | 110.40   |
| 2   | B     | 887  | HIS  | N-CA-CB    | -8.63 | 95.06       | 110.60   |
| 18  | W     | 389  | PRO  | CA-N-CD    | -8.53 | 99.56       | 111.50   |
| 2   | B     | 886  | LYS  | CB-CA-C    | -8.37 | 93.66       | 110.40   |
| 1   | A     | 1030 | THR  | N-CA-C     | 8.21  | 133.16      | 111.00   |
| 2   | B     | 237  | LYS  | N-CA-C     | -8.13 | 89.05       | 111.00   |
| 2   | B     | 657  | GLN  | CB-CA-C    | -8.07 | 94.26       | 110.40   |
| 1   | A     | 1368 | TYR  | N-CA-C     | 8.04  | 132.71      | 111.00   |
| 15  | N     | 17   | DA   | O4'-C1'-N9 | 7.89  | 113.53      | 108.00   |
| 12  | L     | 47   | PRO  | CB-CA-C    | -7.85 | 92.38       | 112.00   |
| 2   | B     | 81   | LYS  | N-CA-CB    | 7.83  | 124.70      | 110.60   |
| 15  | N     | 16   | DT   | O4'-C1'-N1 | -7.68 | 102.62      | 108.00   |
| 2   | B     | 61   | PRO  | N-CA-C     | 7.67  | 132.04      | 112.10   |
| 14  | T     | -5   | DA   | O4'-C1'-N9 | 7.55  | 113.28      | 108.00   |
| 1   | A     | 1030 | THR  | N-CA-CB    | -7.54 | 95.97       | 110.30   |
| 2   | B     | 220  | ALA  | N-CA-C     | -7.53 | 90.67       | 111.00   |
| 2   | B     | 205  | ALA  | CB-CA-C    | 7.50  | 121.36      | 110.10   |
| 2   | B     | 221  | ALA  | N-CA-C     | 7.40  | 130.97      | 111.00   |
| 4   | D     | 53   | LEU  | N-CA-C     | 7.38  | 130.94      | 111.00   |
| 2   | B     | 887  | HIS  | N-CA-C     | 7.32  | 130.76      | 111.00   |
| 2   | B     | 351  | LYS  | N-CA-C     | 7.27  | 130.62      | 111.00   |
| 4   | D     | 19   | VAL  | CB-CA-C    | -7.26 | 97.61       | 111.40   |
| 1   | A     | 862  | GLY  | N-CA-C     | 7.24  | 131.20      | 113.10   |
| 7   | G     | 50   | ASP  | N-CA-C     | 7.09  | 130.15      | 111.00   |
| 2   | B     | 895  | GLU  | N-CA-C     | 7.01  | 129.92      | 111.00   |
| 16  | U     | 199  | ILE  | N-CA-C     | -6.92 | 92.32       | 111.00   |
| 16  | U     | 214  | PRO  | CB-CA-C    | -6.92 | 94.70       | 112.00   |
| 1   | A     | 311  | GLY  | N-CA-C     | 6.87  | 130.28      | 113.10   |
| 1   | A     | 1393 | ASN  | CB-CA-C    | 6.75  | 123.89      | 110.40   |
| 2   | B     | 79   | PHE  | N-CA-C     | 6.72  | 129.15      | 111.00   |
| 1   | A     | 921  | LEU  | N-CA-C     | -6.70 | 92.91       | 111.00   |
| 1   | A     | 197  | GLN  | N-CA-C     | 6.68  | 129.03      | 111.00   |
| 2   | B     | 657  | GLN  | N-CA-C     | 6.43  | 128.36      | 111.00   |
| 16  | U     | 183  | LYS  | CB-CA-C    | -6.42 | 97.55       | 110.40   |
| 2   | B     | 895  | GLU  | N-CA-CB    | -6.40 | 99.08       | 110.60   |
| 14  | T     | -6   | DC   | O4'-C1'-N1 | -6.37 | 103.54      | 108.00   |
| 2   | B     | 1012 | ILE  | CB-CA-C    | -6.29 | 99.02       | 111.60   |
| 12  | L     | 63   | THR  | CB-CA-C    | -6.27 | 94.67       | 111.60   |
| 6   | F     | 140  | ASP  | CB-CA-C    | -6.26 | 97.88       | 110.40   |
| 1   | A     | 58   | LEU  | CB-CA-C    | -6.26 | 98.31       | 110.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 543  | GLU  | CB-CA-C     | -6.22 | 97.95       | 110.40   |
| 7   | G     | 164  | LYS  | O-C-N       | -6.18 | 112.81      | 122.70   |
| 1   | A     | 338  | ARG  | CB-CA-C     | 6.08  | 122.57      | 110.40   |
| 1   | A     | 64   | ASN  | N-CA-C      | 6.08  | 127.42      | 111.00   |
| 1   | A     | 921  | LEU  | CB-CA-C     | 6.02  | 121.63      | 110.20   |
| 1   | A     | 1441 | THR  | CB-CA-C     | 5.99  | 127.77      | 111.60   |
| 3   | C     | 205  | LYS  | CB-CA-C     | 5.99  | 122.37      | 110.40   |
| 7   | G     | 163  | ILE  | CB-CA-C     | -5.97 | 99.66       | 111.60   |
| 2   | B     | 220  | ALA  | CB-CA-C     | -5.92 | 101.21      | 110.10   |
| 1   | A     | 1442 | GLY  | N-CA-C      | 5.91  | 127.87      | 113.10   |
| 1   | A     | 197  | GLN  | N-CA-CB     | -5.90 | 99.98       | 110.60   |
| 3   | C     | 206  | TYR  | N-CA-CB     | -5.88 | 100.02      | 110.60   |
| 1   | A     | 1029 | ALA  | N-CA-C      | -5.86 | 95.19       | 111.00   |
| 14  | T     | -19  | DC   | O4'-C1'-N1  | 5.81  | 112.06      | 108.00   |
| 7   | G     | 165  | GLU  | N-CA-CB     | -5.76 | 100.22      | 110.60   |
| 15  | N     | 16   | DT   | O4'-C4'-C3' | 5.71  | 109.43      | 106.00   |
| 2   | B     | 61   | PRO  | CB-CA-C     | -5.62 | 97.95       | 112.00   |
| 16  | U     | 199  | ILE  | N-CA-CB     | 5.53  | 123.53      | 110.80   |
| 4   | D     | 52   | SER  | CB-CA-C     | -5.52 | 99.61       | 110.10   |
| 15  | N     | 16   | DT   | P-O3'-C3'   | -5.48 | 113.13      | 119.70   |
| 1   | A     | 977  | ARG  | C-N-CA      | 5.46  | 135.36      | 121.70   |
| 1   | A     | 327  | ARG  | CB-CA-C     | 5.41  | 121.23      | 110.40   |
| 1   | A     | 1424 | CYS  | CB-CA-C     | -5.41 | 99.58       | 110.40   |
| 16  | U     | 184  | ASN  | N-CA-C      | -5.37 | 96.49       | 111.00   |
| 1   | A     | 774  | LYS  | CB-CA-C     | -5.32 | 99.77       | 110.40   |
| 2   | B     | 894  | ASP  | N-CA-C      | -5.30 | 96.69       | 111.00   |
| 18  | W     | 317  | ASP  | CB-CG-OD2   | 5.25  | 123.03      | 118.30   |
| 18  | W     | 409  | ASP  | CB-CG-OD2   | 5.23  | 123.01      | 118.30   |
| 18  | W     | 363  | ASP  | CB-CG-OD2   | 5.22  | 123.00      | 118.30   |
| 16  | U     | 154  | ASP  | CB-CG-OD2   | 5.21  | 122.98      | 118.30   |
| 18  | W     | 662  | ASP  | CB-CG-OD2   | 5.20  | 122.98      | 118.30   |
| 15  | N     | 16   | DT   | O4'-C1'-C2' | -5.12 | 101.81      | 105.90   |
| 2   | B     | 205  | ALA  | N-CA-C      | -5.10 | 97.23       | 111.00   |
| 15  | N     | 16   | DT   | N3-C4-O4    | 5.04  | 122.92      | 119.90   |
| 1   | A     | 544  | TYR  | N-CA-C      | 5.01  | 124.53      | 111.00   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 11239 | 0        | 11263    | 452     | 0            |
| 2   | B     | 9261  | 0        | 9267     | 204     | 0            |
| 3   | C     | 2098  | 0        | 2058     | 32      | 0            |
| 4   | D     | 1314  | 0        | 1314     | 153     | 0            |
| 5   | E     | 1740  | 0        | 1754     | 28      | 0            |
| 6   | F     | 677   | 0        | 693      | 11      | 0            |
| 7   | G     | 1324  | 0        | 1342     | 222     | 0            |
| 8   | H     | 1052  | 0        | 1050     | 15      | 0            |
| 9   | I     | 917   | 0        | 865      | 30      | 0            |
| 10  | J     | 545   | 0        | 560      | 9       | 0            |
| 11  | K     | 932   | 0        | 944      | 9       | 0            |
| 12  | L     | 359   | 0        | 360      | 16      | 0            |
| 13  | P     | 338   | 0        | 169      | 25      | 0            |
| 14  | T     | 975   | 0        | 538      | 43      | 0            |
| 15  | N     | 889   | 0        | 487      | 35      | 0            |
| 16  | U     | 1239  | 0        | 1263     | 264     | 0            |
| 17  | V     | 792   | 0        | 757      | 7       | 0            |
| 18  | W     | 2667  | 0        | 2712     | 250     | 0            |
| 19  | A     | 2     | 0        | 0        | 0       | 0            |
| 19  | B     | 1     | 0        | 0        | 0       | 0            |
| 19  | C     | 1     | 0        | 0        | 0       | 0            |
| 19  | I     | 2     | 0        | 0        | 0       | 0            |
| 19  | J     | 1     | 0        | 0        | 0       | 0            |
| 19  | L     | 1     | 0        | 0        | 0       | 0            |
| 19  | U     | 1     | 0        | 0        | 1       | 0            |
| 19  | V     | 1     | 0        | 0        | 0       | 0            |
| 20  | A     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 38369 | 0        | 37396    | 1359    | 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 18.

All (1359) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1363:GLY:CA   | 16:U:282:TRP:HA   | 1.30                     | 1.62              |
| 7:G:100:PHE:HZ    | 18:W:698:PHE:CE1  | 1.21                     | 1.54              |
| 7:G:100:PHE:CZ    | 18:W:698:PHE:CE1  | 1.94                     | 1.53              |
| 16:U:133:ILE:HG21 | 16:U:155:ILE:CG2  | 1.38                     | 1.49              |
| 1:A:1232:GLU:HG3  | 16:U:180:MET:CB   | 1.43                     | 1.48              |
| 1:A:1232:GLU:CG   | 16:U:180:MET:CB   | 1.91                     | 1.46              |
| 4:D:34:PHE:CE1    | 7:G:3:PHE:CD2     | 2.06                     | 1.42              |
| 1:A:1232:GLU:CG   | 16:U:180:MET:HB3  | 1.45                     | 1.41              |
| 4:D:34:PHE:CE1    | 7:G:3:PHE:CG      | 2.10                     | 1.40              |
| 1:A:1080:GLN:C    | 16:U:262:THR:HG21 | 1.42                     | 1.40              |
| 1:A:831:LYS:NZ    | 16:U:262:THR:HA   | 1.09                     | 1.39              |
| 16:U:133:ILE:CG2  | 16:U:155:ILE:HG21 | 1.52                     | 1.38              |
| 1:A:708:GLY:O     | 1:A:1093:SER:CB   | 1.68                     | 1.38              |
| 1:A:1085:THR:HA   | 16:U:260:LYS:NZ   | 1.32                     | 1.34              |
| 16:U:140:ASP:OD1  | 16:U:191:ARG:HB2  | 1.29                     | 1.31              |
| 1:A:1450:GLU:OE2  | 7:G:58:LYS:HE2    | 1.10                     | 1.27              |
| 2:B:336:ILE:O     | 2:B:341:ARG:HB2   | 1.14                     | 1.27              |
| 4:D:24:ASN:HA     | 7:G:83:LYS:O      | 1.29                     | 1.26              |
| 1:A:1080:GLN:C    | 16:U:262:THR:CG2  | 2.03                     | 1.26              |
| 4:D:158:THR:HG21  | 7:G:167:PHE:CD2   | 1.71                     | 1.25              |
| 2:B:70:ASN:O      | 2:B:127:ILE:HG22  | 1.18                     | 1.24              |
| 7:G:100:PHE:CZ    | 18:W:698:PHE:CZ   | 2.24                     | 1.24              |
| 7:G:100:PHE:CE1   | 18:W:698:PHE:CZ   | 2.24                     | 1.24              |
| 1:A:831:LYS:NZ    | 16:U:262:THR:CA   | 1.99                     | 1.23              |
| 4:D:33:GLU:OE1    | 7:G:42:PHE:CZ     | 1.92                     | 1.23              |
| 18:W:333:PHE:CD1  | 18:W:354:LEU:HD21 | 1.73                     | 1.22              |
| 18:W:409:ASP:HB2  | 18:W:413:PHE:CD2  | 1.73                     | 1.22              |
| 13:P:3:C:O2       | 14:T:8:DG:N2      | 1.74                     | 1.21              |
| 16:U:162:ALA:HB1  | 16:U:171:TYR:CD2  | 1.77                     | 1.19              |
| 16:U:133:ILE:HD13 | 16:U:155:ILE:CG2  | 1.72                     | 1.18              |
| 2:B:653:ARG:HD2   | 2:B:657:GLN:NE2   | 1.57                     | 1.18              |
| 1:A:50:GLU:OE2    | 18:W:444:LEU:CD1  | 1.90                     | 1.18              |
| 7:G:100:PHE:HZ    | 18:W:698:PHE:CD1  | 1.63                     | 1.16              |
| 4:D:5:THR:O       | 7:G:7:LEU:HD22    | 1.46                     | 1.16              |
| 4:D:25:ALA:HB3    | 7:G:85:GLU:HA     | 1.26                     | 1.16              |
| 4:D:23:GLU:CD     | 7:G:82:PHE:CD1    | 2.19                     | 1.15              |
| 1:A:831:LYS:HZ3   | 16:U:262:THR:CA   | 1.57                     | 1.15              |
| 1:A:1080:GLN:CA   | 16:U:262:THR:CG2  | 2.24                     | 1.15              |
| 2:B:307:LYS:NZ    | 9:I:13:MET:HE1    | 1.60                     | 1.14              |
| 18:W:333:PHE:CG   | 18:W:354:LEU:HD21 | 1.80                     | 1.14              |
| 4:D:34:PHE:CD1    | 7:G:3:PHE:CG      | 2.34                     | 1.14              |
| 16:U:162:ALA:HB3  | 16:U:171:TYR:CE2  | 1.82                     | 1.14              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:23:GLU:OE1    | 7:G:82:PHE:HA     | 1.42                     | 1.14              |
| 16:U:162:ALA:HB3  | 16:U:171:TYR:HE2  | 1.04                     | 1.13              |
| 16:U:162:ALA:CB   | 16:U:171:TYR:CE2  | 2.31                     | 1.13              |
| 1:A:1363:GLY:HA3  | 16:U:282:TRP:CA   | 1.77                     | 1.13              |
| 2:B:70:ASN:O      | 2:B:127:ILE:CG2   | 1.97                     | 1.13              |
| 1:A:1363:GLY:CA   | 16:U:282:TRP:CA   | 2.26                     | 1.13              |
| 1:A:1363:GLY:HA2  | 16:U:282:TRP:HA   | 1.24                     | 1.13              |
| 18:W:676:ILE:HG12 | 18:W:686:LEU:HD21 | 1.22                     | 1.13              |
| 1:A:1206:ASP:OD1  | 16:U:228:ASN:HB3  | 1.47                     | 1.12              |
| 4:D:34:PHE:CD1    | 7:G:3:PHE:CD2     | 2.37                     | 1.12              |
| 4:D:41:HIS:CE1    | 7:G:74:TYR:O      | 2.02                     | 1.12              |
| 18:W:409:ASP:HB2  | 18:W:413:PHE:HD2  | 1.04                     | 1.12              |
| 1:A:708:GLY:O     | 1:A:1093:SER:HB3  | 0.94                     | 1.12              |
| 1:A:50:GLU:OE2    | 18:W:444:LEU:HD11 | 0.94                     | 1.11              |
| 2:B:307:LYS:NZ    | 9:I:13:MET:CE     | 2.12                     | 1.11              |
| 1:A:1085:THR:CA   | 16:U:260:LYS:NZ   | 2.14                     | 1.11              |
| 18:W:684:LEU:HD12 | 18:W:699:VAL:HA   | 1.11                     | 1.10              |
| 13:P:3:C:N3       | 14:T:8:DG:N1      | 1.96                     | 1.10              |
| 4:D:23:GLU:O      | 7:G:83:LYS:HB3    | 1.52                     | 1.10              |
| 1:A:1461:ALA:HA   | 7:G:20:PRO:HD2    | 1.20                     | 1.10              |
| 4:D:7:THR:HG23    | 7:G:6:ASP:O       | 1.50                     | 1.10              |
| 1:A:1080:GLN:HA   | 16:U:262:THR:HG22 | 1.20                     | 1.09              |
| 1:A:1232:GLU:HG2  | 16:U:180:MET:HB3  | 1.32                     | 1.09              |
| 1:A:1271:LEU:HD13 | 9:I:48:LEU:HD11   | 1.33                     | 1.09              |
| 7:G:100:PHE:HE1   | 18:W:698:PHE:CE2  | 1.69                     | 1.09              |
| 4:D:23:GLU:CG     | 7:G:82:PHE:HD1    | 1.66                     | 1.08              |
| 15:N:15:DG:H2"    | 15:N:16:DT:H5"    | 1.31                     | 1.08              |
| 18:W:684:LEU:CD1  | 18:W:699:VAL:HA   | 1.81                     | 1.08              |
| 18:W:332:LYS:HD2  | 18:W:389:PRO:HD3  | 1.24                     | 1.08              |
| 1:A:1080:GLN:HA   | 16:U:262:THR:CG2  | 1.82                     | 1.08              |
| 4:D:34:PHE:CZ     | 7:G:3:PHE:CD2     | 2.41                     | 1.08              |
| 16:U:130:ILE:HG23 | 16:U:134:TYR:CZ   | 1.87                     | 1.08              |
| 1:A:47:ARG:HB3    | 1:A:48:PRO:HD2    | 1.28                     | 1.07              |
| 1:A:1202:ALA:HA   | 16:U:224:ILE:CG2  | 1.82                     | 1.07              |
| 1:A:1461:ALA:CA   | 7:G:20:PRO:HD2    | 1.83                     | 1.07              |
| 1:A:1450:GLU:OE2  | 7:G:58:LYS:CE     | 2.00                     | 1.07              |
| 1:A:1085:THR:CA   | 16:U:260:LYS:HZ3  | 1.64                     | 1.07              |
| 1:A:1202:ALA:HA   | 16:U:224:ILE:HG21 | 1.10                     | 1.07              |
| 18:W:664:VAL:HG21 | 18:W:686:LEU:CD1  | 1.84                     | 1.07              |
| 16:U:216:SER:O    | 16:U:219:LYS:HG2  | 1.55                     | 1.06              |
| 18:W:399:ALA:HB1  | 18:W:406:ILE:HD11 | 1.27                     | 1.06              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:48:LEU:HD21   | 7:G:3:PHE:HE1     | 1.20                     | 1.06              |
| 18:W:317:ASP:O    | 18:W:319:LYS:HG3  | 1.52                     | 1.06              |
| 18:W:352:LEU:HD11 | 18:W:435:LEU:HD11 | 1.31                     | 1.06              |
| 1:A:1232:GLU:HG3  | 16:U:180:MET:HB2  | 1.29                     | 1.06              |
| 1:A:1232:GLU:CG   | 16:U:180:MET:HB2  | 1.78                     | 1.05              |
| 15:N:-8:DA:H4'    | 15:N:-7:DA:OP1    | 1.51                     | 1.05              |
| 1:A:286:PRO:HG2   | 18:W:268:PHE:CE1  | 1.91                     | 1.05              |
| 16:U:187:ASN:HD21 | 16:U:214:PRO:HB3  | 1.11                     | 1.05              |
| 7:G:100:PHE:CE1   | 18:W:698:PHE:CE2  | 2.44                     | 1.05              |
| 12:L:62:ARG:HD3   | 12:L:63:THR:O     | 1.55                     | 1.05              |
| 1:A:1448:ILE:HB   | 7:G:61:ILE:CD1    | 1.86                     | 1.05              |
| 2:B:307:LYS:HZ3   | 9:I:13:MET:CE     | 1.71                     | 1.04              |
| 1:A:831:LYS:HB3   | 1:A:1083:LEU:CD2  | 1.88                     | 1.04              |
| 18:W:676:ILE:CG1  | 18:W:686:LEU:HD21 | 1.86                     | 1.04              |
| 7:G:95:SER:HB3    | 18:W:682:ASN:HD22 | 1.21                     | 1.04              |
| 16:U:185:LYS:O    | 16:U:187:ASN:N    | 1.91                     | 1.04              |
| 1:A:1447:MET:HE1  | 7:G:60:ARG:HA     | 1.40                     | 1.03              |
| 4:D:112:PHE:CE1   | 7:G:142:LYS:HD3   | 1.93                     | 1.03              |
| 2:B:70:ASN:ND2    | 2:B:128:ASP:C     | 2.12                     | 1.03              |
| 1:A:1234:ASN:ND2  | 16:U:213:ALA:O    | 1.90                     | 1.03              |
| 16:U:130:ILE:CG2  | 16:U:134:TYR:CZ   | 2.42                     | 1.03              |
| 18:W:320:LEU:HD22 | 18:W:432:LEU:CD1  | 1.88                     | 1.02              |
| 15:N:13:DC:H2''   | 15:N:14:DG:O4'    | 1.59                     | 1.02              |
| 18:W:664:VAL:HG11 | 18:W:676:ILE:HD11 | 1.37                     | 1.02              |
| 1:A:1448:ILE:CB   | 7:G:61:ILE:HD11   | 1.90                     | 1.02              |
| 2:B:653:ARG:HD2   | 2:B:657:GLN:CD    | 1.79                     | 1.02              |
| 18:W:320:LEU:HD22 | 18:W:432:LEU:HD13 | 1.37                     | 1.02              |
| 1:A:1361:PHE:CE1  | 16:U:281:ARG:NH1  | 2.27                     | 1.02              |
| 4:D:41:HIS:NE2    | 7:G:74:TYR:O      | 1.91                     | 1.02              |
| 16:U:130:ILE:CG2  | 16:U:134:TYR:CE1  | 2.43                     | 1.02              |
| 18:W:664:VAL:CG2  | 18:W:686:LEU:CD1  | 2.38                     | 1.01              |
| 2:B:336:ILE:O     | 2:B:341:ARG:CB    | 2.08                     | 1.01              |
| 18:W:399:ALA:CB   | 18:W:406:ILE:HD11 | 1.90                     | 1.01              |
| 14:T:-7:DG:H2''   | 14:T:-6:DC:H5''   | 1.36                     | 1.01              |
| 1:A:1447:MET:CE   | 7:G:60:ARG:HG3    | 1.89                     | 1.01              |
| 12:L:68:GLN:CD    | 18:W:767:ILE:HG12 | 1.80                     | 1.01              |
| 16:U:196:ASP:OD1  | 16:U:197:HIS:N    | 1.94                     | 1.01              |
| 16:U:162:ALA:CB   | 16:U:171:TYR:HE2  | 1.69                     | 1.00              |
| 4:D:6:SER:HA      | 7:G:7:LEU:HD23    | 1.43                     | 1.00              |
| 1:A:37:TYR:CE1    | 18:W:441:ASN:ND2  | 2.30                     | 1.00              |
| 1:A:831:LYS:CB    | 1:A:1083:LEU:HD22 | 1.92                     | 0.99              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:653:ARG:HD3   | 2:B:657:GLN:OE1   | 1.61                     | 0.99              |
| 18:W:664:VAL:HG21 | 18:W:686:LEU:HD11 | 1.41                     | 0.99              |
| 4:D:23:GLU:CD     | 7:G:82:PHE:HD1    | 1.60                     | 0.98              |
| 15:N:-7:DA:H2"    | 15:N:-6:DA:N7     | 1.78                     | 0.98              |
| 4:D:34:PHE:HE1    | 7:G:3:PHE:CB      | 1.76                     | 0.98              |
| 2:B:71:ILE:HG12   | 2:B:73:LYS:HE3    | 1.41                     | 0.98              |
| 1:A:1232:GLU:HG2  | 16:U:180:MET:CB   | 1.81                     | 0.98              |
| 1:A:1448:ILE:HB   | 7:G:61:ILE:HD11   | 0.98                     | 0.97              |
| 2:B:653:ARG:CD    | 2:B:657:GLN:NE2   | 2.26                     | 0.97              |
| 4:D:34:PHE:CE1    | 7:G:3:PHE:CB      | 2.48                     | 0.97              |
| 1:A:1447:MET:CE   | 7:G:60:ARG:HA     | 1.94                     | 0.97              |
| 1:A:1137:GLN:NE2  | 16:U:232:ALA:HB1  | 1.78                     | 0.97              |
| 18:W:396:GLU:OE2  | 18:W:414:VAL:HG23 | 1.64                     | 0.97              |
| 2:B:904:ARG:HH21  | 18:W:786:ASN:HA   | 1.30                     | 0.97              |
| 4:D:158:THR:CG2   | 7:G:167:PHE:CD2   | 2.48                     | 0.96              |
| 16:U:162:ALA:HB1  | 16:U:171:TYR:HD2  | 1.23                     | 0.96              |
| 18:W:664:VAL:CG2  | 18:W:686:LEU:HD13 | 1.95                     | 0.96              |
| 1:A:1363:GLY:HA3  | 16:U:282:TRP:HA   | 1.00                     | 0.96              |
| 1:A:186:TRP:O     | 1:A:198:PRO:HA    | 1.66                     | 0.96              |
| 15:N:-7:DA:H2"    | 15:N:-6:DA:C8     | 2.00                     | 0.96              |
| 4:D:40:ASP:HA     | 7:G:6:ASP:OD2     | 1.65                     | 0.96              |
| 16:U:183:LYS:O    | 16:U:183:LYS:HG3  | 1.62                     | 0.96              |
| 18:W:664:VAL:HG23 | 18:W:686:LEU:HD13 | 1.46                     | 0.96              |
| 18:W:399:ALA:HB1  | 18:W:406:ILE:CD1  | 1.95                     | 0.96              |
| 4:D:19:VAL:O      | 4:D:19:VAL:HG12   | 1.65                     | 0.96              |
| 1:A:1080:GLN:O    | 16:U:262:THR:HG21 | 1.66                     | 0.95              |
| 2:B:653:ARG:CD    | 2:B:657:GLN:CD    | 2.35                     | 0.95              |
| 4:D:24:ASN:CA     | 7:G:83:LYS:O      | 2.15                     | 0.95              |
| 1:A:253:MET:HG3   | 13:P:1:A:C2       | 2.01                     | 0.95              |
| 1:A:1234:ASN:OD1  | 16:U:217:LEU:HD23 | 1.66                     | 0.94              |
| 18:W:409:ASP:CB   | 18:W:413:PHE:CD2  | 2.50                     | 0.94              |
| 1:A:253:MET:HG3   | 13:P:1:A:N1       | 1.80                     | 0.94              |
| 4:D:34:PHE:CD1    | 7:G:3:PHE:CD1     | 2.55                     | 0.94              |
| 1:A:1206:ASP:HB2  | 16:U:228:ASN:ND2  | 1.82                     | 0.94              |
| 1:A:1134:LYS:HE3  | 16:U:229:LEU:HA   | 1.50                     | 0.94              |
| 18:W:676:ILE:HG12 | 18:W:686:LEU:CD2  | 1.96                     | 0.94              |
| 16:U:130:ILE:HA   | 16:U:155:ILE:HD12 | 1.50                     | 0.94              |
| 18:W:409:ASP:CB   | 18:W:413:PHE:HD2  | 1.80                     | 0.93              |
| 2:B:287:GLY:O     | 2:B:291:GLN:HB2   | 1.67                     | 0.93              |
| 1:A:831:LYS:HZ1   | 16:U:262:THR:HA   | 1.24                     | 0.93              |
| 1:A:1447:MET:SD   | 7:G:60:ARG:HA     | 2.08                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:72:ASN:O      | 2:B:125:THR:HA    | 1.69                     | 0.93              |
| 4:D:6:SER:CA      | 7:G:7:LEU:HD23    | 1.98                     | 0.92              |
| 18:W:684:LEU:HD12 | 18:W:699:VAL:CA   | 1.99                     | 0.92              |
| 18:W:684:LEU:HD11 | 18:W:699:VAL:HG13 | 1.48                     | 0.92              |
| 1:A:50:GLU:CD     | 18:W:444:LEU:HD11 | 1.90                     | 0.92              |
| 1:A:47:ARG:HB3    | 1:A:48:PRO:CD     | 1.97                     | 0.92              |
| 1:A:37:TYR:CZ     | 18:W:441:ASN:ND2  | 2.38                     | 0.92              |
| 4:D:34:PHE:CG     | 7:G:3:PHE:CE2     | 2.58                     | 0.91              |
| 1:A:1232:GLU:HG2  | 16:U:180:MET:CG   | 2.01                     | 0.91              |
| 4:D:112:PHE:CZ    | 7:G:142:LYS:HD3   | 2.05                     | 0.90              |
| 1:A:1080:GLN:CA   | 16:U:262:THR:HG22 | 1.95                     | 0.90              |
| 1:A:1100:VAL:HB   | 1:A:1101:PRO:HD3  | 1.51                     | 0.90              |
| 1:A:1232:GLU:HG3  | 16:U:180:MET:HB3  | 1.02                     | 0.90              |
| 1:A:713:GLU:OE2   | 1:A:1092:SER:OG   | 1.87                     | 0.90              |
| 14:T:-18:DT:H3    | 15:N:19:DA:H2     | 0.94                     | 0.90              |
| 16:U:130:ILE:HG22 | 16:U:134:TYR:CE1  | 2.07                     | 0.90              |
| 1:A:1361:PHE:CE1  | 16:U:281:ARG:CZ   | 2.55                     | 0.90              |
| 1:A:831:LYS:HZ1   | 16:U:262:THR:CA   | 1.77                     | 0.89              |
| 16:U:140:ASP:HB2  | 16:U:191:ARG:HD2  | 1.55                     | 0.89              |
| 16:U:183:LYS:NZ   | 16:U:185:LYS:HE3  | 1.87                     | 0.89              |
| 4:D:6:SER:CB      | 7:G:7:LEU:HD23    | 2.02                     | 0.89              |
| 18:W:394:PHE:HE2  | 18:W:396:GLU:HG2  | 1.37                     | 0.89              |
| 1:A:831:LYS:HE3   | 16:U:262:THR:O    | 1.71                     | 0.89              |
| 14:T:-18:DT:N3    | 15:N:19:DA:C2     | 2.26                     | 0.88              |
| 1:A:1446:VAL:O    | 7:G:61:ILE:HB     | 1.74                     | 0.88              |
| 16:U:247:CYS:HG   | 19:U:301:ZN:ZN    | 0.64                     | 0.88              |
| 1:A:1461:ALA:HA   | 7:G:20:PRO:CD     | 2.04                     | 0.88              |
| 16:U:130:ILE:HA   | 16:U:155:ILE:CD1  | 2.03                     | 0.88              |
| 1:A:1081:MET:N    | 16:U:262:THR:HG23 | 1.88                     | 0.88              |
| 13:P:3:C:N4       | 14:T:8:DG:O6      | 2.06                     | 0.87              |
| 4:D:48:LEU:HD21   | 7:G:3:PHE:CE1     | 2.07                     | 0.87              |
| 14:T:-18:DT:H2"   | 14:T:-17:DC:H5'   | 1.55                     | 0.87              |
| 1:A:831:LYS:CB    | 1:A:1083:LEU:CD2  | 2.48                     | 0.87              |
| 17:V:85:ARG:NH1   | 17:V:87:ASP:OD1   | 2.07                     | 0.87              |
| 18:W:684:LEU:CD1  | 18:W:699:VAL:HG22 | 2.04                     | 0.87              |
| 16:U:133:ILE:HD13 | 16:U:155:ILE:HG22 | 1.56                     | 0.87              |
| 1:A:1234:ASN:CG   | 16:U:213:ALA:O    | 2.12                     | 0.87              |
| 2:B:500:LYS:HG2   | 2:B:501:LEU:H     | 1.39                     | 0.86              |
| 4:D:34:PHE:CD1    | 7:G:3:PHE:CE2     | 2.62                     | 0.86              |
| 16:U:187:ASN:ND2  | 16:U:214:PRO:HB3  | 1.89                     | 0.86              |
| 18:W:399:ALA:C    | 18:W:406:ILE:CD1  | 2.43                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1447:MET:HE3  | 7:G:60:ARG:HG3    | 1.57                     | 0.86              |
| 1:A:1232:GLU:OE2  | 16:U:180:MET:HG3  | 1.76                     | 0.86              |
| 18:W:666:GLU:OE1  | 18:W:671:ARG:HB2  | 1.76                     | 0.86              |
| 14:T:-15:DA:N6    | 15:N:16:DT:O4     | 2.07                     | 0.86              |
| 2:B:769:TYR:OH    | 16:U:265:ALA:CB   | 2.23                     | 0.86              |
| 16:U:162:ALA:CB   | 16:U:171:TYR:CD2  | 2.53                     | 0.86              |
| 2:B:337:ARG:O     | 2:B:341:ARG:HB3   | 1.76                     | 0.86              |
| 18:W:320:LEU:CD2  | 18:W:432:LEU:HD13 | 2.04                     | 0.86              |
| 1:A:1447:MET:HE1  | 7:G:60:ARG:HG3    | 1.56                     | 0.86              |
| 2:B:769:TYR:OH    | 16:U:265:ALA:O    | 1.92                     | 0.86              |
| 18:W:684:LEU:HG   | 18:W:699:VAL:HG22 | 1.58                     | 0.86              |
| 16:U:140:ASP:OD1  | 16:U:191:ARG:CB   | 2.22                     | 0.86              |
| 1:A:1271:LEU:CD1  | 9:I:48:LEU:HD11   | 2.06                     | 0.85              |
| 2:B:769:TYR:OH    | 16:U:265:ALA:HB1  | 1.76                     | 0.85              |
| 16:U:162:ALA:HB1  | 16:U:171:TYR:CE2  | 2.04                     | 0.85              |
| 4:D:158:THR:HG21  | 7:G:167:PHE:HD2   | 1.10                     | 0.85              |
| 4:D:98:ALA:O      | 4:D:102:VAL:HB    | 1.77                     | 0.85              |
| 18:W:409:ASP:O    | 18:W:410:ARG:HG3  | 1.75                     | 0.85              |
| 1:A:37:TYR:OH     | 18:W:441:ASN:ND2  | 2.10                     | 0.85              |
| 18:W:667:PHE:HB3  | 18:W:701:SER:O    | 1.77                     | 0.85              |
| 4:D:25:ALA:CB     | 7:G:85:GLU:HA     | 2.05                     | 0.85              |
| 1:A:1264:LYS:HE2  | 9:I:44:TYR:CG     | 2.11                     | 0.84              |
| 1:A:1206:ASP:OD1  | 16:U:228:ASN:CB   | 2.25                     | 0.84              |
| 16:U:181:ASN:ND2  | 16:U:212:LEU:CD1  | 2.41                     | 0.84              |
| 2:B:769:TYR:OH    | 16:U:265:ALA:C    | 2.16                     | 0.84              |
| 18:W:333:PHE:CG   | 18:W:354:LEU:CD2  | 2.59                     | 0.84              |
| 4:D:112:PHE:CZ    | 7:G:142:LYS:CD    | 2.60                     | 0.84              |
| 16:U:184:ASN:O    | 16:U:185:LYS:O    | 1.94                     | 0.84              |
| 4:D:106:LEU:O     | 4:D:110:ASN:HB2   | 1.78                     | 0.84              |
| 1:A:1232:GLU:CD   | 16:U:180:MET:HB2  | 1.98                     | 0.84              |
| 18:W:666:GLU:OE1  | 18:W:671:ARG:N    | 2.10                     | 0.84              |
| 4:D:158:THR:CG2   | 7:G:167:PHE:HD2   | 1.85                     | 0.84              |
| 16:U:185:LYS:HG2  | 16:U:191:ARG:NH2  | 1.91                     | 0.84              |
| 1:A:1286:TYR:HD1  | 16:U:234:GLY:HA3  | 1.43                     | 0.84              |
| 2:B:63:GLN:HE22   | 18:W:248:LEU:HB3  | 1.41                     | 0.83              |
| 18:W:352:LEU:HD11 | 18:W:435:LEU:CD1  | 2.07                     | 0.83              |
| 18:W:665:ARG:HA   | 18:W:673:GLN:HA   | 1.58                     | 0.83              |
| 16:U:216:SER:O    | 16:U:219:LYS:CG   | 2.25                     | 0.83              |
| 1:A:1447:MET:HE1  | 7:G:60:ARG:CA     | 2.08                     | 0.83              |
| 1:A:40:ILE:HG22   | 1:A:41:MET:HE3    | 1.60                     | 0.83              |
| 1:A:831:LYS:HB3   | 1:A:1083:LEU:HD23 | 1.59                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:U:189:THR:O    | 16:U:193:SER:N    | 2.12                     | 0.83              |
| 4:D:48:LEU:HD11   | 7:G:3:PHE:CD1     | 2.14                     | 0.83              |
| 1:A:735:GLU:OE1   | 16:U:244:ARG:NH1  | 2.11                     | 0.83              |
| 18:W:329:LYS:HD2  | 18:W:436:ILE:HG13 | 1.60                     | 0.83              |
| 4:D:23:GLU:CG     | 7:G:82:PHE:CD1    | 2.58                     | 0.83              |
| 18:W:684:LEU:CG   | 18:W:699:VAL:HG22 | 2.09                     | 0.82              |
| 16:U:133:ILE:HD13 | 16:U:155:ILE:HG21 | 1.62                     | 0.82              |
| 18:W:676:ILE:CG1  | 18:W:686:LEU:CD2  | 2.55                     | 0.82              |
| 16:U:185:LYS:HG2  | 16:U:191:ARG:HH22 | 1.43                     | 0.82              |
| 4:D:23:GLU:HB3    | 7:G:82:PHE:HB3    | 1.61                     | 0.82              |
| 4:D:25:ALA:HB3    | 7:G:85:GLU:CA     | 2.09                     | 0.82              |
| 1:A:286:PRO:HG2   | 18:W:268:PHE:CZ   | 2.14                     | 0.81              |
| 15:N:14:DG:H4'    | 15:N:14:DG:OP1    | 1.78                     | 0.81              |
| 2:B:653:ARG:CD    | 2:B:657:GLN:OE1   | 2.28                     | 0.81              |
| 2:B:769:TYR:HH    | 16:U:265:ALA:C    | 1.82                     | 0.81              |
| 4:D:158:THR:HG21  | 7:G:167:PHE:CE2   | 2.15                     | 0.81              |
| 2:B:73:LYS:HA     | 2:B:124:PHE:O     | 1.79                     | 0.81              |
| 18:W:399:ALA:CB   | 18:W:406:ILE:CD1  | 2.55                     | 0.81              |
| 4:D:23:GLU:HG2    | 7:G:82:PHE:HD1    | 1.44                     | 0.81              |
| 7:G:95:SER:HB3    | 18:W:682:ASN:ND2  | 1.95                     | 0.81              |
| 12:L:68:GLN:NE2   | 18:W:767:ILE:HD11 | 1.95                     | 0.81              |
| 1:A:1137:GLN:NE2  | 16:U:232:ALA:CB   | 2.43                     | 0.81              |
| 18:W:676:ILE:HA   | 18:W:686:LEU:HD23 | 1.62                     | 0.80              |
| 1:A:831:LYS:CA    | 1:A:1083:LEU:CD2  | 2.59                     | 0.80              |
| 1:A:1361:PHE:HE1  | 16:U:281:ARG:CZ   | 1.94                     | 0.80              |
| 16:U:133:ILE:HD13 | 16:U:155:ILE:CB   | 2.11                     | 0.80              |
| 1:A:828:THR:OG1   | 16:U:261:GLN:CG   | 2.29                     | 0.80              |
| 18:W:357:ARG:HB3  | 18:W:389:PRO:HD2  | 1.64                     | 0.80              |
| 1:A:286:PRO:CG    | 18:W:268:PHE:CZ   | 2.65                     | 0.80              |
| 13:P:-1:U:O2'     | 13:P:0:U:OP1      | 2.00                     | 0.80              |
| 1:A:1461:ALA:N    | 7:G:20:PRO:HD2    | 1.95                     | 0.80              |
| 1:A:1081:MET:N    | 16:U:262:THR:CG2  | 2.44                     | 0.80              |
| 8:H:56:THR:HB     | 8:H:144:ARG:HB3   | 1.64                     | 0.80              |
| 1:A:828:THR:OG1   | 16:U:261:GLN:HG3  | 1.82                     | 0.79              |
| 18:W:357:ARG:C    | 18:W:389:PRO:HG2  | 2.02                     | 0.79              |
| 18:W:399:ALA:C    | 18:W:406:ILE:HD11 | 2.02                     | 0.79              |
| 18:W:328:VAL:HA   | 18:W:435:LEU:HD23 | 1.64                     | 0.79              |
| 1:A:772:GLU:HA    | 1:A:1086:PHE:CZ   | 2.17                     | 0.79              |
| 1:A:831:LYS:HZ1   | 16:U:262:THR:HG23 | 1.47                     | 0.79              |
| 2:B:74:ARG:HB2    | 2:B:124:PHE:HB2   | 1.64                     | 0.79              |
| 1:A:1137:GLN:NE2  | 16:U:232:ALA:O    | 2.16                     | 0.79              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:337:ARG:O    | 2:B:341:ARG:CB    | 2.31                     | 0.79              |
| 1:A:1232:GLU:CG  | 16:U:180:MET:CG   | 2.58                     | 0.78              |
| 4:D:49:ILE:HG21  | 7:G:4:LEU:HD12    | 1.65                     | 0.78              |
| 16:U:140:ASP:CG  | 16:U:191:ARG:HB2  | 2.03                     | 0.78              |
| 1:A:1202:ALA:CA  | 16:U:224:ILE:HG21 | 2.04                     | 0.78              |
| 1:A:1462:PRO:HG3 | 7:G:19:GLY:H      | 1.47                     | 0.78              |
| 18:W:394:PHE:CE2 | 18:W:396:GLU:HG2  | 2.18                     | 0.78              |
| 1:A:1206:ASP:HB2 | 16:U:228:ASN:CG   | 2.04                     | 0.78              |
| 16:U:133:ILE:CG2 | 16:U:155:ILE:CG2  | 2.32                     | 0.78              |
| 1:A:831:LYS:CE   | 16:U:262:THR:HA   | 2.13                     | 0.78              |
| 1:A:1085:THR:CA  | 16:U:260:LYS:HZ1  | 1.93                     | 0.78              |
| 1:A:285:SER:HB2  | 1:A:290:ILE:HD11  | 1.65                     | 0.78              |
| 4:D:34:PHE:CZ    | 7:G:3:PHE:HD2     | 2.02                     | 0.78              |
| 14:T:-7:DG:C2'   | 14:T:-6:DC:H5''   | 2.14                     | 0.78              |
| 14:T:-18:DT:N3   | 15:N:19:DA:H2     | 1.73                     | 0.78              |
| 1:A:831:LYS:HZ1  | 16:U:262:THR:CG2  | 1.96                     | 0.78              |
| 4:D:5:THR:O      | 7:G:7:LEU:CD2     | 2.30                     | 0.77              |
| 18:W:664:VAL:CG2 | 18:W:686:LEU:HD11 | 2.08                     | 0.77              |
| 12:L:68:GLN:OE1  | 18:W:767:ILE:HG12 | 1.84                     | 0.77              |
| 4:D:19:VAL:O     | 4:D:19:VAL:CG1    | 2.32                     | 0.77              |
| 18:W:679:VAL:HA  | 18:W:684:LEU:HD23 | 1.66                     | 0.77              |
| 2:B:288:GLU:O    | 2:B:292:HIS:ND1   | 2.17                     | 0.77              |
| 18:W:319:LYS:O   | 18:W:320:LEU:CB   | 2.33                     | 0.77              |
| 1:A:41:MET:HA    | 1:A:41:MET:CE     | 2.15                     | 0.76              |
| 4:D:34:PHE:HE1   | 7:G:3:PHE:HB2     | 1.50                     | 0.76              |
| 16:U:176:ARG:O   | 16:U:180:MET:HG2  | 1.85                     | 0.76              |
| 1:A:831:LYS:HA   | 1:A:1083:LEU:CD2  | 2.14                     | 0.76              |
| 1:A:831:LYS:CE   | 16:U:262:THR:O    | 2.33                     | 0.76              |
| 2:B:904:ARG:NH2  | 18:W:786:ASN:HA   | 2.00                     | 0.76              |
| 2:B:70:ASN:ND2   | 2:B:128:ASP:O     | 2.19                     | 0.76              |
| 2:B:55:ARG:HD2   | 2:B:76:GLU:OE2    | 1.85                     | 0.76              |
| 4:D:34:PHE:CG    | 7:G:3:PHE:CZ      | 2.74                     | 0.76              |
| 7:G:8:SER:HA     | 7:G:72:VAL:O      | 1.86                     | 0.76              |
| 14:T:-20:DA:H2'' | 14:T:-19:DC:O5'   | 1.82                     | 0.76              |
| 18:W:317:ASP:O   | 18:W:319:LYS:N    | 2.18                     | 0.76              |
| 1:A:1286:TYR:HD1 | 16:U:234:GLY:CA   | 1.99                     | 0.76              |
| 1:A:48:PRO:CG    | 1:A:56:PRO:HD3    | 2.14                     | 0.76              |
| 7:G:100:PHE:CZ   | 18:W:698:PHE:CD1  | 2.52                     | 0.76              |
| 18:W:674:GLY:CA  | 18:W:687:ARG:O    | 2.33                     | 0.76              |
| 1:A:1085:THR:HA  | 16:U:260:LYS:HZ3  | 0.72                     | 0.75              |
| 15:N:16:DT:H2'   | 15:N:17:DA:C8     | 2.21                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1364:SER:OG   | 16:U:283:LYS:HD3  | 1.85                     | 0.75              |
| 1:A:1154:ILE:HD12 | 9:I:44:TYR:HB3    | 1.68                     | 0.75              |
| 5:E:158:GLY:O     | 5:E:161:SER:N     | 2.18                     | 0.75              |
| 18:W:664:VAL:HG11 | 18:W:676:ILE:CD1  | 2.15                     | 0.75              |
| 4:D:30:LEU:O      | 7:G:82:PHE:CE1    | 2.39                     | 0.75              |
| 16:U:133:ILE:HG21 | 16:U:155:ILE:HG23 | 1.61                     | 0.75              |
| 16:U:245:PHE:HB2  | 16:U:255:VAL:HG11 | 1.66                     | 0.75              |
| 1:A:1080:GLN:CA   | 16:U:262:THR:HG21 | 1.99                     | 0.74              |
| 5:E:102:LYS:O     | 5:E:103:ASN:OD1   | 2.04                     | 0.74              |
| 1:A:831:LYS:CA    | 1:A:1083:LEU:HD22 | 2.16                     | 0.74              |
| 2:B:83:TYR:HB2    | 2:B:116:TYR:HB2   | 1.70                     | 0.74              |
| 1:A:1206:ASP:CB   | 16:U:228:ASN:ND2  | 2.51                     | 0.74              |
| 7:G:132:SER:HB2   | 7:G:135:GLU:HB2   | 1.69                     | 0.74              |
| 16:U:148:ILE:O    | 16:U:152:VAL:HG23 | 1.88                     | 0.74              |
| 12:L:62:ARG:CD    | 12:L:63:THR:O     | 2.35                     | 0.74              |
| 1:A:1202:ALA:CA   | 16:U:224:ILE:CG2  | 2.64                     | 0.74              |
| 18:W:333:PHE:CD1  | 18:W:354:LEU:CD2  | 2.65                     | 0.74              |
| 18:W:684:LEU:HD11 | 18:W:699:VAL:CG1  | 2.17                     | 0.73              |
| 18:W:396:GLU:OE2  | 18:W:414:VAL:CG2  | 2.36                     | 0.73              |
| 4:D:34:PHE:CE1    | 7:G:3:PHE:HB2     | 2.21                     | 0.73              |
| 18:W:328:VAL:HG22 | 18:W:435:LEU:HD21 | 1.70                     | 0.73              |
| 2:B:946:ASN:HB3   | 18:W:786:ASN:HB3  | 1.70                     | 0.73              |
| 16:U:133:ILE:CB   | 16:U:155:ILE:HG21 | 2.18                     | 0.73              |
| 8:H:112:LYS:HG2   | 8:H:125:GLU:HG2   | 1.70                     | 0.73              |
| 16:U:133:ILE:CD1  | 16:U:155:ILE:CG2  | 2.61                     | 0.73              |
| 1:A:1363:GLY:HA2  | 16:U:281:ARG:O    | 1.89                     | 0.73              |
| 2:B:307:LYS:HZ1   | 9:I:13:MET:CE     | 2.01                     | 0.73              |
| 15:N:-7:DA:C2'    | 15:N:-6:DA:N7     | 2.51                     | 0.73              |
| 4:D:7:THR:HG21    | 7:G:6:ASP:HB2     | 1.70                     | 0.72              |
| 1:A:1447:MET:CE   | 7:G:60:ARG:CG     | 2.65                     | 0.72              |
| 1:A:1362:ASP:O    | 16:U:283:LYS:HD2  | 1.90                     | 0.72              |
| 18:W:326:VAL:HG21 | 18:W:435:LEU:HD13 | 1.71                     | 0.72              |
| 2:B:1221:SER:CB   | 4:D:12:ARG:HH12   | 2.02                     | 0.72              |
| 12:L:68:GLN:CD    | 18:W:767:ILE:CG1  | 2.57                     | 0.71              |
| 15:N:14:DG:H2''   | 15:N:15:DG:H5'    | 1.71                     | 0.71              |
| 1:A:43:GLU:OE1    | 18:W:443:THR:HG21 | 1.90                     | 0.71              |
| 2:B:58:LEU:HB2    | 2:B:75:TYR:HB2    | 1.73                     | 0.71              |
| 1:A:699:GLN:O     | 9:I:98:THR:HG22   | 1.90                     | 0.71              |
| 13:P:1:A:N7       | 13:P:2:U:C4       | 2.58                     | 0.71              |
| 2:B:307:LYS:HZ2   | 9:I:13:MET:HE1    | 1.51                     | 0.71              |
| 2:B:818:PRO:HG3   | 10:J:53:VAL:HG21  | 1.72                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:W:684:LEU:HD11 | 18:W:699:VAL:HG22 | 1.71                     | 0.71              |
| 4:D:34:PHE:CD1    | 7:G:3:PHE:CE1     | 2.79                     | 0.71              |
| 1:A:310:ALA:CB    | 14:T:-4:DG:H5'    | 2.21                     | 0.71              |
| 18:W:323:GLY:HA2  | 18:W:339:GLN:HE21 | 1.55                     | 0.71              |
| 1:A:1232:GLU:CD   | 16:U:180:MET:CB   | 2.57                     | 0.70              |
| 18:W:682:ASN:O    | 18:W:698:PHE:HD1  | 1.72                     | 0.70              |
| 1:A:1447:MET:HE1  | 7:G:60:ARG:CG     | 2.20                     | 0.70              |
| 1:A:1232:GLU:HG2  | 16:U:180:MET:HG3  | 1.70                     | 0.70              |
| 18:W:666:GLU:OE1  | 18:W:671:ARG:CB   | 2.39                     | 0.70              |
| 5:E:100:GLN:HE21  | 5:E:126:VAL:HA    | 1.57                     | 0.70              |
| 1:A:974:HIS:O     | 1:A:977:ARG:NH1   | 2.24                     | 0.70              |
| 4:D:52:SER:O      | 4:D:56:SER:OG     | 2.05                     | 0.70              |
| 4:D:6:SER:HB2     | 7:G:5:LYS:HE3     | 1.73                     | 0.70              |
| 16:U:189:THR:O    | 16:U:193:SER:CB   | 2.39                     | 0.70              |
| 1:A:1232:GLU:OE2  | 16:U:180:MET:CG   | 2.39                     | 0.70              |
| 2:B:489:ARG:NH2   | 2:B:533:SER:O     | 2.24                     | 0.70              |
| 4:D:140:PHE:HE1   | 7:G:1:MET:SD      | 2.14                     | 0.70              |
| 7:G:39:THR:O      | 7:G:43:GLY:N      | 2.24                     | 0.70              |
| 4:D:23:GLU:HG2    | 7:G:82:PHE:CD1    | 2.26                     | 0.70              |
| 18:W:320:LEU:HD22 | 18:W:432:LEU:HD11 | 1.74                     | 0.70              |
| 16:U:184:ASN:O    | 16:U:185:LYS:C    | 2.30                     | 0.70              |
| 1:A:1447:MET:CE   | 7:G:60:ARG:CA     | 2.69                     | 0.69              |
| 7:G:91:VAL:HA     | 7:G:101:ALA:HA    | 1.73                     | 0.69              |
| 18:W:674:GLY:HA2  | 18:W:687:ARG:O    | 1.92                     | 0.69              |
| 1:A:184:GLY:O     | 1:A:200:ARG:HA    | 1.91                     | 0.69              |
| 4:D:6:SER:HB3     | 7:G:7:LEU:CD2     | 2.22                     | 0.69              |
| 2:B:1221:SER:HB3  | 4:D:12:ARG:HH22   | 1.57                     | 0.69              |
| 3:C:88:GLU:OE2    | 18:W:759:ARG:NH1  | 2.26                     | 0.69              |
| 3:C:90:TYR:OH     | 3:C:156:ARG:NH2   | 2.24                     | 0.69              |
| 18:W:748:ARG:O    | 18:W:749:ASP:HB2  | 1.92                     | 0.69              |
| 1:A:1462:PRO:HD3  | 7:G:19:GLY:C      | 2.13                     | 0.69              |
| 16:U:133:ILE:HD13 | 16:U:155:ILE:HB   | 1.74                     | 0.69              |
| 1:A:831:LYS:HZ1   | 16:U:262:THR:CB   | 2.04                     | 0.69              |
| 1:A:1134:LYS:HG2  | 16:U:229:LEU:HD13 | 1.74                     | 0.69              |
| 1:A:1226:LEU:HD11 | 1:A:1242:CYS:HB3  | 1.74                     | 0.69              |
| 2:B:653:ARG:CD    | 2:B:657:GLN:HE22  | 2.05                     | 0.69              |
| 3:C:49:GLU:HG2    | 12:L:68:GLN:HG2   | 1.73                     | 0.69              |
| 16:U:140:ASP:HB2  | 16:U:191:ARG:CD   | 2.23                     | 0.69              |
| 18:W:664:VAL:HG21 | 18:W:686:LEU:CD2  | 2.22                     | 0.69              |
| 1:A:588:HIS:NE2   | 1:A:971:GLN:OE1   | 2.24                     | 0.69              |
| 15:N:15:DG:H1'    | 15:N:16:DT:O4'    | 1.93                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:W:332:LYS:HG3  | 18:W:388:ARG:CB   | 2.22                     | 0.69              |
| 18:W:357:ARG:HB3  | 18:W:389:PRO:CD   | 2.22                     | 0.69              |
| 18:W:666:GLU:OE1  | 18:W:671:ARG:CA   | 2.41                     | 0.69              |
| 16:U:137:LEU:HD11 | 16:U:182:LEU:HD13 | 1.75                     | 0.69              |
| 16:U:173:ASN:OD1  | 16:U:176:ARG:NH1  | 2.26                     | 0.69              |
| 18:W:684:LEU:CD1  | 18:W:699:VAL:CA   | 2.64                     | 0.69              |
| 1:A:1450:GLU:CD   | 7:G:58:LYS:HE2    | 2.07                     | 0.68              |
| 18:W:357:ARG:HB3  | 18:W:389:PRO:HG2  | 1.75                     | 0.68              |
| 1:A:831:LYS:HA    | 1:A:1083:LEU:HD22 | 1.74                     | 0.68              |
| 4:D:23:GLU:OE2    | 7:G:82:PHE:CD1    | 2.46                     | 0.68              |
| 15:N:16:DT:H2'    | 15:N:17:DA:H8     | 1.55                     | 0.68              |
| 3:C:90:TYR:HH     | 3:C:156:ARG:HH22  | 1.42                     | 0.68              |
| 18:W:667:PHE:CB   | 18:W:701:SER:O    | 2.41                     | 0.68              |
| 1:A:41:MET:HA     | 1:A:41:MET:HE2    | 1.74                     | 0.68              |
| 18:W:357:ARG:O    | 18:W:389:PRO:HG2  | 1.94                     | 0.68              |
| 2:B:1106:ARG:HE   | 2:B:1109:GLY:H    | 1.39                     | 0.68              |
| 16:U:183:LYS:O    | 16:U:183:LYS:CG   | 2.34                     | 0.68              |
| 18:W:318:VAL:O    | 18:W:318:VAL:HG12 | 1.94                     | 0.68              |
| 1:A:48:PRO:HG2    | 1:A:56:PRO:HD3    | 1.75                     | 0.67              |
| 4:D:112:PHE:CE1   | 7:G:142:LYS:CD    | 2.76                     | 0.67              |
| 4:D:34:PHE:CD2    | 7:G:3:PHE:CE2     | 2.82                     | 0.67              |
| 18:W:329:LYS:CD   | 18:W:436:ILE:HG13 | 2.24                     | 0.67              |
| 4:D:112:PHE:HE1   | 7:G:142:LYS:HD3   | 1.56                     | 0.67              |
| 1:A:1462:PRO:CD   | 7:G:21:GLN:H      | 2.07                     | 0.67              |
| 1:A:1363:GLY:N    | 16:U:282:TRP:HA   | 2.06                     | 0.67              |
| 5:E:19:LYS:NZ     | 5:E:33:GLU:O      | 2.26                     | 0.67              |
| 4:D:41:HIS:HE2    | 7:G:74:TYR:C      | 1.98                     | 0.67              |
| 16:U:130:ILE:HG23 | 16:U:134:TYR:CE2  | 2.30                     | 0.67              |
| 2:B:324:ASP:OD2   | 2:B:328:ARG:NE    | 2.28                     | 0.67              |
| 16:U:189:THR:O    | 16:U:193:SER:OG   | 2.13                     | 0.67              |
| 18:W:399:ALA:CA   | 18:W:406:ILE:HD11 | 2.23                     | 0.67              |
| 4:D:41:HIS:HE1    | 7:G:74:TYR:O      | 1.76                     | 0.67              |
| 2:B:995:ARG:NH1   | 2:B:997:GLU:OE2   | 2.27                     | 0.67              |
| 4:D:34:PHE:CD1    | 7:G:3:PHE:CZ      | 2.83                     | 0.67              |
| 4:D:6:SER:HA      | 7:G:7:LEU:HA      | 1.77                     | 0.67              |
| 18:W:352:LEU:CD1  | 18:W:435:LEU:HD11 | 2.19                     | 0.66              |
| 1:A:1286:TYR:CD1  | 16:U:234:GLY:HA3  | 2.29                     | 0.66              |
| 7:G:46:VAL:HG12   | 7:G:47:THR:HG23   | 1.78                     | 0.66              |
| 18:W:329:LYS:HD2  | 18:W:436:ILE:CG1  | 2.25                     | 0.66              |
| 1:A:1446:VAL:O    | 7:G:61:ILE:CB     | 2.42                     | 0.66              |
| 7:G:97:ILE:HG22   | 7:G:97:ILE:O      | 1.95                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:U:183:LYS:HZ2  | 16:U:185:LYS:HE3  | 1.60                     | 0.66              |
| 1:A:995:LEU:HD22  | 1:A:1048:LEU:HD22 | 1.76                     | 0.66              |
| 1:A:132:LYS:NZ    | 1:A:1420:GLU:OE2  | 2.28                     | 0.66              |
| 1:A:557:TRP:O     | 11:K:26:ARG:NH1   | 2.27                     | 0.66              |
| 16:U:133:ILE:CD1  | 16:U:155:ILE:HB   | 2.25                     | 0.66              |
| 1:A:1264:LYS:HE2  | 9:I:44:TYR:CD1    | 2.30                     | 0.66              |
| 2:B:607:SER:HB2   | 2:B:620:PHE:HB2   | 1.77                     | 0.66              |
| 4:D:34:PHE:HD1    | 7:G:3:PHE:CD1     | 2.10                     | 0.66              |
| 18:W:409:ASP:O    | 18:W:410:ARG:CG   | 2.43                     | 0.66              |
| 14:T:-13:DC:H2'   | 14:T:-12:DG:C8    | 2.31                     | 0.66              |
| 1:A:999:LEU:O     | 1:A:1013:GLN:NE2  | 2.28                     | 0.66              |
| 5:E:181:ASP:O     | 5:E:184:ALA:N     | 2.24                     | 0.66              |
| 16:U:133:ILE:HB   | 16:U:155:ILE:HD13 | 1.77                     | 0.66              |
| 1:A:887:ILE:O     | 1:A:945:ARG:NH2   | 2.29                     | 0.65              |
| 2:B:70:ASN:O      | 2:B:127:ILE:CB    | 2.43                     | 0.65              |
| 1:A:948:VAL:HA    | 5:E:200:ARG:HD2   | 1.78                     | 0.65              |
| 16:U:183:LYS:HZ1  | 16:U:185:LYS:HE3  | 1.60                     | 0.65              |
| 1:A:831:LYS:HB3   | 1:A:1083:LEU:HB2  | 1.78                     | 0.65              |
| 4:D:140:PHE:CE1   | 7:G:1:MET:SD      | 2.89                     | 0.65              |
| 4:D:95:GLY:O      | 4:D:99:ASN:ND2    | 2.29                     | 0.65              |
| 16:U:134:TYR:OH   | 16:U:152:VAL:HG22 | 1.96                     | 0.65              |
| 18:W:664:VAL:HG23 | 18:W:686:LEU:CD1  | 2.14                     | 0.65              |
| 1:A:1447:MET:SD   | 7:G:60:ARG:CA     | 2.83                     | 0.65              |
| 16:U:133:ILE:HG21 | 16:U:155:ILE:HG21 | 0.67                     | 0.65              |
| 16:U:194:ILE:O    | 16:U:198:GLU:OE2  | 2.15                     | 0.65              |
| 1:A:1363:GLY:HA2  | 16:U:282:TRP:CA   | 2.07                     | 0.65              |
| 16:U:133:ILE:CD1  | 16:U:155:ILE:HG21 | 2.25                     | 0.65              |
| 2:B:352:GLU:O     | 2:B:355:PRO:HD3   | 1.97                     | 0.65              |
| 2:B:63:GLN:NE2    | 18:W:248:LEU:HB3  | 2.09                     | 0.65              |
| 13:P:-2:U:O5'     | 13:P:-2:U:H6      | 1.79                     | 0.65              |
| 1:A:1205:LEU:HD21 | 16:U:221:MET:O    | 1.97                     | 0.65              |
| 1:A:1085:THR:HA   | 16:U:260:LYS:CE   | 2.27                     | 0.65              |
| 1:A:828:THR:OG1   | 16:U:261:GLN:HG2  | 1.97                     | 0.64              |
| 16:U:156:GLU:O    | 16:U:160:PHE:HD2  | 1.79                     | 0.64              |
| 18:W:332:LYS:HG3  | 18:W:388:ARG:HB3  | 1.78                     | 0.64              |
| 1:A:48:PRO:HG3    | 1:A:56:PRO:HD3    | 1.79                     | 0.64              |
| 14:T:1:DA:H2'     | 14:T:2:DC:H6      | 1.61                     | 0.64              |
| 2:B:287:GLY:O     | 2:B:291:GLN:CB    | 2.44                     | 0.64              |
| 2:B:688:GLU:OE2   | 2:B:740:HIS:NE2   | 2.19                     | 0.64              |
| 3:C:91:CYS:SG     | 3:C:92:ASP:N      | 2.70                     | 0.64              |
| 15:N:15:DG:H2''   | 15:N:16:DT:C5'    | 2.20                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:U:154:ASP:O    | 16:U:158:GLN:HG3  | 1.97                     | 0.64              |
| 18:W:351:ARG:HG2  | 18:W:429:THR:HG22 | 1.77                     | 0.64              |
| 18:W:409:ASP:CB   | 18:W:413:PHE:CE2  | 2.80                     | 0.64              |
| 18:W:666:GLU:N    | 18:W:672:ARG:O    | 2.30                     | 0.64              |
| 1:A:1286:TYR:HB2  | 1:A:1310:GLU:O    | 1.97                     | 0.64              |
| 1:A:43:GLU:OE1    | 18:W:443:THR:CG2  | 2.45                     | 0.64              |
| 5:E:61:ALA:HB3    | 5:E:77:LEU:HB3    | 1.80                     | 0.64              |
| 1:A:1462:PRO:HD3  | 7:G:19:GLY:CA     | 2.28                     | 0.64              |
| 18:W:664:VAL:CG1  | 18:W:676:ILE:HD11 | 2.21                     | 0.64              |
| 1:A:828:THR:HG23  | 16:U:263:ARG:O    | 1.99                     | 0.63              |
| 1:A:1234:ASN:HA   | 16:U:217:LEU:CD2  | 2.29                     | 0.63              |
| 1:A:1447:MET:CE   | 7:G:60:ARG:CB     | 2.76                     | 0.63              |
| 1:A:37:TYR:HE1    | 18:W:441:ASN:ND2  | 1.93                     | 0.63              |
| 15:N:-11:DG:OP1   | 18:W:334:LYS:HE3  | 1.98                     | 0.63              |
| 13:P:1:A:N7       | 13:P:2:U:C5       | 2.67                     | 0.63              |
| 1:A:446:ASN:HD22  | 1:A:447:ARG:H     | 1.45                     | 0.63              |
| 4:D:33:GLU:OE1    | 7:G:42:PHE:HZ     | 1.73                     | 0.63              |
| 7:G:97:ILE:HG13   | 18:W:683:PHE:CD1  | 2.34                     | 0.63              |
| 12:L:68:GLN:NE2   | 18:W:767:ILE:CD1  | 2.60                     | 0.63              |
| 4:D:128:LEU:HD11  | 4:D:146:SER:HB2   | 1.80                     | 0.63              |
| 1:A:1206:ASP:CA   | 16:U:228:ASN:ND2  | 2.61                     | 0.63              |
| 14:T:1:DA:H2'     | 14:T:2:DC:C6      | 2.33                     | 0.63              |
| 18:W:437:VAL:O    | 18:W:437:VAL:HG22 | 1.98                     | 0.63              |
| 1:A:40:ILE:HG22   | 1:A:41:MET:CE     | 2.28                     | 0.63              |
| 2:B:1187:ASN:HD21 | 2:B:1190:ASN:HB3  | 1.64                     | 0.63              |
| 4:D:108:TYR:OH    | 7:G:88:ASP:HB2    | 1.99                     | 0.63              |
| 14:T:-19:DC:H2'   | 14:T:-18:DT:C6    | 2.34                     | 0.63              |
| 18:W:784:ASN:HB2  | 18:W:785:PRO:HD3  | 1.81                     | 0.63              |
| 18:W:317:ASP:O    | 18:W:318:VAL:C    | 2.37                     | 0.62              |
| 1:A:791:ASP:CG    | 9:I:87:GLN:HE21   | 2.02                     | 0.62              |
| 7:G:158:TYR:CE1   | 18:W:700:THR:HG21 | 2.35                     | 0.62              |
| 1:A:982:ASP:O     | 1:A:1041:ARG:NH2  | 2.33                     | 0.62              |
| 1:A:151:ASP:HA    | 1:A:164:SER:HA    | 1.81                     | 0.62              |
| 2:B:279:ARG:NH1   | 2:B:316:ILE:O     | 2.32                     | 0.62              |
| 18:W:676:ILE:HA   | 18:W:686:LEU:CD2  | 2.29                     | 0.62              |
| 3:C:74:GLU:O      | 3:C:246:ARG:NH2   | 2.32                     | 0.62              |
| 15:N:-6:DA:OP2    | 15:N:-5:DT:H72    | 2.00                     | 0.62              |
| 18:W:329:LYS:CG   | 18:W:436:ILE:HG13 | 2.29                     | 0.62              |
| 1:A:1078:ALA:HA   | 1:A:1081:MET:HE3  | 1.82                     | 0.62              |
| 1:A:1084:ASN:O    | 1:A:1086:PHE:N    | 2.31                     | 0.62              |
| 2:B:316:ILE:HG21  | 2:B:322:ALA:HB2   | 1.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:W:672:ARG:HH12 | 18:W:691:ILE:HG13 | 1.63                     | 0.62              |
| 1:A:113:LEU:O     | 1:A:165:ARG:NH2   | 2.33                     | 0.62              |
| 4:D:23:GLU:OE2    | 7:G:82:PHE:CE1    | 2.53                     | 0.62              |
| 14:T:-5:DA:H8     | 14:T:-5:DA:H5"    | 1.63                     | 0.62              |
| 1:A:1201:ARG:CZ   | 16:U:217:LEU:HD11 | 2.30                     | 0.62              |
| 8:H:95:VAL:HG22   | 8:H:142:LEU:HG    | 1.82                     | 0.61              |
| 1:A:1134:LYS:CE   | 16:U:229:LEU:HA   | 2.27                     | 0.61              |
| 1:A:53:LEU:O      | 1:A:248:ARG:NH2   | 2.32                     | 0.61              |
| 4:D:112:PHE:HZ    | 7:G:142:LYS:CG    | 2.13                     | 0.61              |
| 4:D:41:HIS:NE2    | 7:G:74:TYR:C      | 2.53                     | 0.61              |
| 2:B:307:LYS:HZ1   | 9:I:13:MET:HE3    | 1.64                     | 0.61              |
| 16:U:185:LYS:C    | 16:U:187:ASN:H    | 1.98                     | 0.61              |
| 7:G:158:TYR:HB2   | 18:W:667:PHE:CE2  | 2.36                     | 0.61              |
| 18:W:684:LEU:HD11 | 18:W:699:VAL:CB   | 2.30                     | 0.61              |
| 1:A:610:ASP:OD1   | 1:A:971:GLN:NE2   | 2.32                     | 0.61              |
| 2:B:71:ILE:HG12   | 2:B:73:LYS:CE     | 2.23                     | 0.61              |
| 4:D:6:SER:HA      | 7:G:7:LEU:CD2     | 2.25                     | 0.61              |
| 18:W:328:VAL:HG22 | 18:W:435:LEU:CD2  | 2.30                     | 0.61              |
| 1:A:1079:THR:O    | 1:A:1079:THR:HG22 | 2.01                     | 0.61              |
| 1:A:186:TRP:HZ3   | 1:A:201:LYS:HG2   | 1.64                     | 0.61              |
| 4:D:6:SER:CB      | 7:G:7:LEU:CD2     | 2.75                     | 0.61              |
| 1:A:1447:MET:HE3  | 7:G:60:ARG:CG     | 2.26                     | 0.61              |
| 2:B:303:LEU:HD23  | 2:B:306:LEU:HD12  | 1.82                     | 0.61              |
| 1:A:308:ASP:OD1   | 1:A:314:GLN:NE2   | 2.33                     | 0.61              |
| 2:B:1038:ARG:HD2  | 2:B:1040:TYR:HE1  | 1.65                     | 0.61              |
| 2:B:70:ASN:HD21   | 2:B:128:ASP:C     | 2.02                     | 0.61              |
| 14:T:-20:DA:H61   | 15:N:21:DT:H3     | 1.47                     | 0.61              |
| 2:B:1106:ARG:NH2  | 2:B:1110:PRO:O    | 2.32                     | 0.61              |
| 1:A:1423:ASP:O    | 1:A:1424:CYS:HB2  | 2.02                     | 0.60              |
| 1:A:708:GLY:O     | 1:A:1093:SER:OG   | 2.19                     | 0.60              |
| 1:A:791:ASP:OD2   | 9:I:87:GLN:HG2    | 2.01                     | 0.60              |
| 16:U:216:SER:C    | 16:U:219:LYS:HG2  | 2.21                     | 0.60              |
| 1:A:286:PRO:HG3   | 18:W:268:PHE:CZ   | 2.36                     | 0.60              |
| 1:A:114:LEU:HB3   | 1:A:145:LYS:HG2   | 1.82                     | 0.60              |
| 2:B:262:LYS:HB3   | 2:B:271:ASP:HB3   | 1.83                     | 0.60              |
| 2:B:291:GLN:NE2   | 2:B:563:ASP:OD1   | 2.34                     | 0.60              |
| 4:D:23:GLU:HB2    | 7:G:83:LYS:H      | 1.65                     | 0.60              |
| 1:A:255:GLU:HG2   | 2:B:935:ARG:HH12  | 1.67                     | 0.60              |
| 1:A:307:ASN:ND2   | 1:A:323:VAL:O     | 2.34                     | 0.60              |
| 3:C:217:GLU:HG2   | 3:C:218:VAL:O     | 2.02                     | 0.60              |
| 16:U:135:THR:O    | 16:U:139:MET:HG2  | 2.00                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 18:W:394:PHE:HE2 | 18:W:396:GLU:CG   | 2.14                     | 0.60              |
| 1:A:708:GLY:C    | 1:A:1093:SER:CB   | 2.63                     | 0.60              |
| 2:B:613:ARG:O    | 9:I:58:ILE:HD12   | 2.01                     | 0.60              |
| 1:A:1083:LEU:O   | 1:A:1083:LEU:HD12 | 2.01                     | 0.60              |
| 16:U:216:SER:CB  | 16:U:219:LYS:HE2  | 2.31                     | 0.60              |
| 1:A:228:ASP:OD1  | 4:D:15:ALA:HB2    | 2.02                     | 0.60              |
| 11:K:56:VAL:HG22 | 11:K:77:THR:HG22  | 1.82                     | 0.60              |
| 1:A:831:LYS:CA   | 1:A:1083:LEU:HD23 | 2.32                     | 0.60              |
| 2:B:1129:ARG:HD3 | 14:T:2:DC:H5'     | 1.83                     | 0.60              |
| 18:W:357:ARG:HB3 | 18:W:389:PRO:CG   | 2.31                     | 0.60              |
| 4:D:34:PHE:HB3   | 7:G:3:PHE:CZ      | 2.37                     | 0.60              |
| 14:T:0:DT:C2     | 14:T:1:DA:C8      | 2.89                     | 0.60              |
| 18:W:319:LYS:O   | 18:W:320:LEU:HB3  | 2.02                     | 0.60              |
| 7:G:158:TYR:CE1  | 18:W:700:THR:CG2  | 2.84                     | 0.60              |
| 16:U:192:ARG:O   | 16:U:192:ARG:HD2  | 2.02                     | 0.59              |
| 18:W:396:GLU:CD  | 18:W:414:VAL:CG2  | 2.70                     | 0.59              |
| 2:B:653:ARG:HD3  | 2:B:657:GLN:CD    | 2.10                     | 0.59              |
| 4:D:66:ALA:O     | 4:D:70:ALA:HB2    | 2.01                     | 0.59              |
| 16:U:129:SER:O   | 16:U:133:ILE:HG13 | 2.02                     | 0.59              |
| 1:A:286:PRO:CG   | 18:W:268:PHE:CE1  | 2.76                     | 0.59              |
| 18:W:413:PHE:CE1 | 18:W:420:GLU:HB3  | 2.38                     | 0.59              |
| 2:B:759:PRO:HD2  | 2:B:1046:PRO:HB3  | 1.83                     | 0.59              |
| 3:C:18:GLU:OE2   | 3:C:206:TYR:OH    | 2.15                     | 0.59              |
| 4:D:121:CYS:O    | 4:D:125:ASP:HB2   | 2.02                     | 0.59              |
| 7:G:100:PHE:HB3  | 7:G:107:ASN:HD21  | 1.67                     | 0.59              |
| 11:K:29:ASN:ND2  | 11:K:78:GLU:O     | 2.35                     | 0.59              |
| 16:U:131:SER:O   | 16:U:135:THR:HG23 | 2.01                     | 0.59              |
| 17:V:44:ALA:O    | 17:V:48:GLU:HG2   | 2.01                     | 0.59              |
| 4:D:112:PHE:CZ   | 7:G:142:LYS:CE    | 2.86                     | 0.59              |
| 4:D:96:ALA:HA    | 4:D:99:ASN:HD22   | 1.67                     | 0.59              |
| 7:G:4:LEU:HA     | 7:G:76:ALA:O      | 2.02                     | 0.59              |
| 16:U:185:LYS:C   | 16:U:187:ASN:N    | 2.56                     | 0.59              |
| 5:E:213:CYS:SG   | 5:E:214:LEU:N     | 2.75                     | 0.59              |
| 1:A:1462:PRO:HG3 | 7:G:19:GLY:N      | 2.16                     | 0.59              |
| 8:H:15:VAL:HG22  | 8:H:26:ILE:HG22   | 1.85                     | 0.59              |
| 1:A:504:GLN:OE1  | 6:F:90:ARG:NH1    | 2.33                     | 0.59              |
| 1:A:1462:PRO:HD2 | 7:G:21:GLN:H      | 1.67                     | 0.59              |
| 1:A:1054:GLN:HG2 | 1:A:1057:ARG:HH21 | 1.67                     | 0.59              |
| 13:P:2:U:H2'     | 13:P:3:C:C6       | 2.36                     | 0.59              |
| 1:A:1363:GLY:HA3 | 16:U:282:TRP:C    | 2.23                     | 0.59              |
| 14:T:-18:DT:H2'  | 14:T:-17:DC:C6    | 2.38                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:W:397:ALA:O    | 18:W:401:VAL:HG23 | 2.03                     | 0.59              |
| 1:A:270:ILE:HG12  | 1:A:300:HIS:HB3   | 1.84                     | 0.58              |
| 2:B:823:ALA:O     | 2:B:1089:PRO:HA   | 2.03                     | 0.58              |
| 18:W:399:ALA:O    | 18:W:406:ILE:CD1  | 2.50                     | 0.58              |
| 7:G:4:LEU:HD22    | 7:G:49:LEU:HD11   | 1.84                     | 0.58              |
| 1:A:1462:PRO:HD3  | 7:G:19:GLY:HA3    | 1.85                     | 0.58              |
| 2:B:276:ILE:O     | 2:B:280:ALA:HB2   | 2.04                     | 0.58              |
| 16:U:208:SER:HB3  | 16:U:211:GLU:HB3  | 1.84                     | 0.58              |
| 18:W:698:PHE:CE2  | 18:W:700:THR:HB   | 2.38                     | 0.58              |
| 1:A:709:MET:CG    | 1:A:1091:VAL:HG13 | 2.32                     | 0.58              |
| 2:B:451:LYS:O     | 2:B:455:ALA:HB2   | 2.03                     | 0.58              |
| 4:D:112:PHE:HZ    | 7:G:142:LYS:HG2   | 1.67                     | 0.58              |
| 4:D:7:THR:CG2     | 7:G:6:ASP:O       | 2.40                     | 0.58              |
| 9:I:88:SER:O      | 9:I:89:GLN:NE2    | 2.37                     | 0.58              |
| 16:U:160:PHE:HA   | 16:U:163:VAL:HG23 | 1.86                     | 0.58              |
| 1:A:286:PRO:HG3   | 18:W:268:PHE:HZ   | 1.67                     | 0.58              |
| 18:W:328:VAL:HA   | 18:W:435:LEU:CD2  | 2.33                     | 0.58              |
| 18:W:684:LEU:HD11 | 18:W:699:VAL:CG2  | 2.32                     | 0.58              |
| 16:U:126:ARG:O    | 16:U:130:ILE:HD12 | 2.03                     | 0.58              |
| 16:U:160:PHE:O    | 16:U:163:VAL:HB   | 2.04                     | 0.58              |
| 2:B:500:LYS:HG2   | 2:B:501:LEU:N     | 2.15                     | 0.58              |
| 10:J:7:CYS:SG     | 10:J:8:PHE:N      | 2.77                     | 0.58              |
| 18:W:389:PRO:HD2  | 18:W:389:PRO:O    | 2.04                     | 0.58              |
| 4:D:33:GLU:HG3    | 7:G:41:GLN:O      | 2.04                     | 0.57              |
| 4:D:112:PHE:CZ    | 7:G:142:LYS:HE3   | 2.39                     | 0.57              |
| 1:A:1446:VAL:O    | 7:G:61:ILE:CG1    | 2.51                     | 0.57              |
| 1:A:1361:PHE:CZ   | 16:U:281:ARG:NH1  | 2.70                     | 0.57              |
| 1:A:128:ILE:O     | 1:A:134:ARG:NH2   | 2.37                     | 0.57              |
| 2:B:761:HIS:HB2   | 2:B:1024:ALA:HB2  | 1.84                     | 0.57              |
| 18:W:394:PHE:CE2  | 18:W:396:GLU:CG   | 2.86                     | 0.57              |
| 16:U:133:ILE:O    | 16:U:137:LEU:HB2  | 2.04                     | 0.57              |
| 16:U:137:LEU:CD1  | 16:U:182:LEU:HD13 | 2.33                     | 0.57              |
| 2:B:1201:LYS:HE2  | 2:B:1205:GLN:NE2  | 2.20                     | 0.57              |
| 2:B:279:ARG:HG2   | 2:B:284:VAL:HA    | 1.85                     | 0.57              |
| 2:B:71:ILE:HG23   | 2:B:71:ILE:O      | 2.03                     | 0.57              |
| 1:A:47:ARG:CB     | 1:A:48:PRO:HD2    | 2.14                     | 0.57              |
| 2:B:105:ARG:NH2   | 2:B:193:TYR:OH    | 2.37                     | 0.57              |
| 1:A:22:LEU:HD12   | 2:B:1211:ASN:HA   | 1.87                     | 0.57              |
| 1:A:35:ILE:HG13   | 1:A:242:VAL:HG21  | 1.87                     | 0.57              |
| 1:A:446:ASN:HD22  | 1:A:447:ARG:N     | 2.02                     | 0.57              |
| 2:B:590:VAL:HG12  | 2:B:617:PHE:CE1   | 2.39                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:T:-16:DT:H2"   | 14:T:-15:DA:C8    | 2.40                     | 0.57              |
| 18:W:674:GLY:HA3  | 18:W:687:ARG:O    | 2.04                     | 0.57              |
| 2:B:164:MET:HB2   | 2:B:194:PHE:HE1   | 1.70                     | 0.57              |
| 1:A:1235:ALA:HA   | 16:U:184:ASN:HD21 | 1.70                     | 0.57              |
| 1:A:369:ILE:HG22  | 1:A:373:LYS:HE2   | 1.86                     | 0.57              |
| 1:A:1232:GLU:CG   | 16:U:180:MET:HG3  | 2.30                     | 0.57              |
| 18:W:319:LYS:O    | 18:W:320:LEU:HB2  | 2.03                     | 0.57              |
| 4:D:169:VAL:HG12  | 4:D:171:LEU:H     | 1.69                     | 0.56              |
| 4:D:33:GLU:HB3    | 7:G:42:PHE:CE1    | 2.40                     | 0.56              |
| 1:A:1286:TYR:CD1  | 16:U:234:GLY:CA   | 2.85                     | 0.56              |
| 18:W:317:ASP:O    | 18:W:319:LYS:CG   | 2.42                     | 0.56              |
| 1:A:977:ARG:HA    | 1:A:978:ALA:HB3   | 1.87                     | 0.56              |
| 2:B:90:THR:HA     | 2:B:96:THR:HG22   | 1.87                     | 0.56              |
| 7:G:97:ILE:CG1    | 18:W:683:PHE:CD1  | 2.88                     | 0.56              |
| 1:A:745:LYS:O     | 1:A:749:SER:CB    | 2.54                     | 0.56              |
| 1:A:1403:CYS:HB2  | 1:A:1408:THR:HG23 | 1.87                     | 0.56              |
| 1:A:738:LEU:HD22  | 1:A:742:ASN:HD22  | 1.71                     | 0.56              |
| 2:B:177:GLU:O     | 2:B:180:LEU:N     | 2.38                     | 0.56              |
| 2:B:336:ILE:O     | 2:B:341:ARG:NE    | 2.39                     | 0.56              |
| 4:D:138:HIS:HB3   | 4:D:141:GLU:HG2   | 1.87                     | 0.56              |
| 4:D:86:ASP:OD2    | 4:D:110:ASN:ND2   | 2.36                     | 0.56              |
| 2:B:55:ARG:CD     | 2:B:76:GLU:OE2    | 2.53                     | 0.56              |
| 2:B:918:ILE:HD11  | 2:B:935:ARG:HB2   | 1.87                     | 0.56              |
| 3:C:145:CYS:SG    | 3:C:146:LYS:N     | 2.79                     | 0.56              |
| 18:W:664:VAL:HG21 | 18:W:686:LEU:HD21 | 1.87                     | 0.56              |
| 1:A:483:PHE:HD2   | 2:B:836:GLU:HB2   | 1.70                     | 0.56              |
| 18:W:332:LYS:HG3  | 18:W:388:ARG:HB2  | 1.86                     | 0.56              |
| 7:G:12:THR:HA     | 7:G:68:ALA:O      | 2.06                     | 0.56              |
| 16:U:194:ILE:HA   | 16:U:198:GLU:CD   | 2.26                     | 0.56              |
| 1:A:1451:LYS:O    | 1:A:1454:THR:OG1  | 2.20                     | 0.56              |
| 1:A:168:CYS:SG    | 1:A:170:ASN:ND2   | 2.79                     | 0.56              |
| 18:W:666:GLU:CD   | 18:W:671:ARG:HB2  | 2.26                     | 0.56              |
| 1:A:350:ALA:O     | 1:A:489:ASN:HA    | 2.07                     | 0.55              |
| 1:A:974:HIS:O     | 1:A:976:ASP:N     | 2.38                     | 0.55              |
| 16:U:181:ASN:ND2  | 16:U:212:LEU:HD11 | 2.19                     | 0.55              |
| 7:G:97:ILE:HG13   | 18:W:683:PHE:CG   | 2.41                     | 0.55              |
| 1:A:1137:GLN:NE2  | 16:U:232:ALA:C    | 2.59                     | 0.55              |
| 18:W:683:PHE:N    | 18:W:683:PHE:CD2  | 2.73                     | 0.55              |
| 1:A:1100:VAL:HB   | 1:A:1101:PRO:CD   | 2.30                     | 0.55              |
| 1:A:1202:ALA:CB   | 16:U:224:ILE:HG23 | 2.35                     | 0.55              |
| 1:A:15:LYS:O      | 1:A:1424:CYS:HB2  | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:T:-17:DC:H2"   | 14:T:-16:DT:OP1   | 2.06                     | 0.55              |
| 16:U:183:LYS:NZ   | 16:U:185:LYS:CE   | 2.63                     | 0.55              |
| 16:U:190:LEU:O    | 16:U:194:ILE:HB   | 2.07                     | 0.55              |
| 1:A:337:LEU:HD23  | 1:A:341:LEU:HD12  | 1.88                     | 0.55              |
| 16:U:134:TYR:CZ   | 16:U:152:VAL:HG22 | 2.41                     | 0.55              |
| 1:A:47:ARG:CB     | 1:A:48:PRO:CD     | 2.61                     | 0.55              |
| 2:B:904:ARG:HH21  | 18:W:786:ASN:CA   | 2.09                     | 0.55              |
| 16:U:216:SER:OG   | 16:U:219:LYS:HE2  | 2.06                     | 0.55              |
| 18:W:409:ASP:HB2  | 18:W:413:PHE:CE2  | 2.35                     | 0.55              |
| 1:A:1271:LEU:HD13 | 9:I:48:LEU:CD1    | 2.23                     | 0.55              |
| 18:W:344:LEU:CD1  | 18:W:349:GLU:HB2  | 2.35                     | 0.55              |
| 1:A:317:GLN:HG3   | 1:A:318:LYS:H     | 1.71                     | 0.55              |
| 1:A:1447:MET:HE1  | 7:G:60:ARG:CB     | 2.36                     | 0.55              |
| 18:W:396:GLU:CD   | 18:W:414:VAL:HG21 | 2.27                     | 0.55              |
| 18:W:748:ARG:O    | 18:W:749:ASP:CB   | 2.54                     | 0.55              |
| 1:A:1389:ARG:NH1  | 1:A:1407:GLU:OE2  | 2.40                     | 0.54              |
| 1:A:828:THR:CG2   | 16:U:264:SER:HA   | 2.36                     | 0.54              |
| 1:A:831:LYS:CB    | 1:A:1083:LEU:HD23 | 2.26                     | 0.54              |
| 4:D:33:GLU:OE1    | 7:G:42:PHE:CE1    | 2.58                     | 0.54              |
| 1:A:41:MET:CA     | 1:A:41:MET:CE     | 2.86                     | 0.54              |
| 7:G:125:ASN:HD22  | 7:G:126:SER:H     | 1.55                     | 0.54              |
| 14:T:-6:DC:C2'    | 14:T:-5:DA:C8     | 2.91                     | 0.54              |
| 1:A:941:ARG:HH21  | 1:A:945:ARG:HH22  | 1.55                     | 0.54              |
| 2:B:223:SER:O     | 2:B:252:ARG:NH2   | 2.36                     | 0.54              |
| 3:C:79:MET:O      | 3:C:161:LYS:NZ    | 2.34                     | 0.54              |
| 18:W:684:LEU:CD1  | 18:W:699:VAL:CG2  | 2.80                     | 0.54              |
| 1:A:243:PRO:O     | 1:A:248:ARG:NH1   | 2.41                     | 0.54              |
| 1:A:1361:PHE:O    | 16:U:281:ARG:HD3  | 2.07                     | 0.54              |
| 1:A:831:LYS:HB3   | 1:A:1083:LEU:CB   | 2.38                     | 0.54              |
| 1:A:1362:ASP:HB2  | 16:U:272:PHE:CD1  | 2.43                     | 0.54              |
| 1:A:1462:PRO:HD3  | 7:G:21:GLN:H      | 1.71                     | 0.54              |
| 1:A:379:GLU:O     | 1:A:432:LYS:HA    | 2.07                     | 0.54              |
| 16:U:147:LYS:H    | 16:U:147:LYS:HD2  | 1.72                     | 0.54              |
| 1:A:286:PRO:HG2   | 18:W:268:PHE:HE1  | 1.67                     | 0.54              |
| 4:D:112:PHE:HZ    | 7:G:142:LYS:CD    | 2.20                     | 0.54              |
| 18:W:352:LEU:HD11 | 18:W:435:LEU:HD21 | 1.90                     | 0.54              |
| 1:A:564:PRO:HG2   | 1:A:567:LEU:HD23  | 1.89                     | 0.54              |
| 1:A:661:ASN:ND2   | 2:B:1082:MET:HB3  | 2.23                     | 0.54              |
| 1:A:941:ARG:HH21  | 1:A:945:ARG:NH2   | 2.05                     | 0.54              |
| 2:B:1010:LEU:HD22 | 2:B:1092:TYR:HE2  | 1.72                     | 0.54              |
| 2:B:804:ALA:HB3   | 2:B:983:ARG:HH22  | 1.72                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:71:TYR:OH     | 5:E:154:ARG:O     | 2.23                     | 0.54              |
| 8:H:38:LEU:HD13   | 8:H:124:LEU:HD13  | 1.90                     | 0.54              |
| 4:D:99:ASN:O      | 4:D:103:LYS:HB2   | 2.07                     | 0.54              |
| 6:F:140:ASP:OD1   | 6:F:141:GLY:N     | 2.41                     | 0.54              |
| 16:U:140:ASP:CB   | 16:U:191:ARG:HB2  | 2.37                     | 0.54              |
| 16:U:214:PRO:HD2  | 16:U:217:LEU:HB3  | 1.90                     | 0.54              |
| 18:W:676:ILE:HG13 | 18:W:686:LEU:HD21 | 1.80                     | 0.54              |
| 1:A:1148:VAL:HG23 | 1:A:1199:LEU:HD22 | 1.90                     | 0.54              |
| 2:B:27:GLU:OE1    | 2:B:678:TRP:HB3   | 2.07                     | 0.54              |
| 7:G:151:ARG:HG2   | 18:W:667:PHE:O    | 2.08                     | 0.54              |
| 1:A:1078:ALA:HA   | 1:A:1081:MET:CE   | 2.38                     | 0.53              |
| 4:D:34:PHE:CE2    | 7:G:3:PHE:CD2     | 2.96                     | 0.53              |
| 13:P:-1:U:O2      | 13:P:-1:U:H2'     | 2.07                     | 0.53              |
| 11:K:14:ASP:OD1   | 11:K:15:ASP:N     | 2.42                     | 0.53              |
| 15:N:-8:DA:C4'    | 15:N:-7:DA:OP1    | 2.39                     | 0.53              |
| 1:A:1363:GLY:HA3  | 16:U:283:LYS:N    | 2.24                     | 0.53              |
| 4:D:87:ASP:OD1    | 4:D:103:LYS:HG3   | 2.09                     | 0.53              |
| 4:D:34:PHE:CB     | 7:G:3:PHE:CZ      | 2.91                     | 0.53              |
| 7:G:95:SER:O      | 7:G:130:TYR:OH    | 2.26                     | 0.53              |
| 1:A:109:ASN:HD22  | 1:A:170:ASN:ND2   | 2.06                     | 0.53              |
| 13:P:-3:U:H3'     | 13:P:-2:U:C5      | 2.44                     | 0.53              |
| 18:W:665:ARG:HB2  | 18:W:705:VAL:HG11 | 1.90                     | 0.53              |
| 1:A:351:ARG:HB2   | 2:B:1128:LEU:HD11 | 1.89                     | 0.53              |
| 6:F:107:VAL:HB    | 6:F:111:ILE:HD11  | 1.91                     | 0.53              |
| 7:G:30:LEU:HD22   | 7:G:72:VAL:HG11   | 1.89                     | 0.53              |
| 8:H:60:ALA:O      | 8:H:140:TYR:HB2   | 2.09                     | 0.53              |
| 2:B:195:VAL:HA    | 2:B:199:SER:O     | 2.09                     | 0.53              |
| 1:A:1056:GLN:HB3  | 6:F:84:TYR:HE2    | 1.74                     | 0.53              |
| 4:D:23:GLU:O      | 7:G:83:LYS:CB     | 2.41                     | 0.53              |
| 1:A:852:HIS:HB3   | 6:F:139:PRO:HG3   | 1.91                     | 0.53              |
| 18:W:409:ASP:OD2  | 18:W:415:THR:OG1  | 2.21                     | 0.53              |
| 18:W:682:ASN:O    | 18:W:698:PHE:CD1  | 2.59                     | 0.53              |
| 16:U:183:LYS:HZ2  | 16:U:185:LYS:CE   | 2.22                     | 0.53              |
| 1:A:109:ASN:HD22  | 1:A:170:ASN:HD21  | 1.57                     | 0.53              |
| 2:B:300:TRP:HA    | 2:B:303:LEU:HB2   | 1.91                     | 0.53              |
| 16:U:216:SER:CA   | 16:U:219:LYS:HE2  | 2.39                     | 0.53              |
| 17:V:43:GLN:NE2   | 17:V:47:ASN:OD1   | 2.39                     | 0.53              |
| 1:A:1137:GLN:HE21 | 16:U:232:ALA:HB1  | 1.68                     | 0.52              |
| 18:W:664:VAL:CG1  | 18:W:676:ILE:CD1  | 2.85                     | 0.52              |
| 2:B:946:ASN:CB    | 18:W:786:ASN:HB3  | 2.36                     | 0.52              |
| 2:B:354:LEU:HB3   | 2:B:357:ILE:HD12  | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:100:VAL:HG22  | 8:H:115:VAL:HG22  | 1.92                     | 0.52              |
| 2:B:983:ARG:NH2   | 2:B:1028:GLU:OE2  | 2.36                     | 0.52              |
| 2:B:316:ILE:HG23  | 2:B:321:VAL:HG23  | 1.92                     | 0.52              |
| 2:B:451:LYS:O     | 2:B:455:ALA:CB    | 2.57                     | 0.52              |
| 4:D:6:SER:CA      | 7:G:7:LEU:CD2     | 2.81                     | 0.52              |
| 1:A:1088:TYR:OH   | 16:U:237:GLU:CG   | 2.58                     | 0.52              |
| 1:A:1232:GLU:OE2  | 16:U:176:ARG:O    | 2.28                     | 0.52              |
| 1:A:680:ILE:HG23  | 1:A:730:ALA:HB1   | 1.90                     | 0.52              |
| 15:N:15:DG:H1'    | 15:N:16:DT:C4'    | 2.39                     | 0.52              |
| 1:A:1160:PRO:HB3  | 1:A:1190:GLN:HE21 | 1.75                     | 0.52              |
| 2:B:827:ILE:HG22  | 2:B:1014:PRO:HG3  | 1.92                     | 0.52              |
| 4:D:49:ILE:HG21   | 7:G:4:LEU:CD1     | 2.38                     | 0.52              |
| 14:T:-15:DA:OP2   | 14:T:-15:DA:H8    | 1.92                     | 0.52              |
| 17:V:41:SER:HB2   | 17:V:45:THR:HB    | 1.91                     | 0.52              |
| 18:W:672:ARG:NH1  | 18:W:691:ILE:HG13 | 2.24                     | 0.52              |
| 2:B:563:ASP:HB3   | 2:B:566:GLN:HB3   | 1.91                     | 0.52              |
| 2:B:883:LEU:HB3   | 2:B:932:HIS:CE1   | 2.45                     | 0.52              |
| 4:D:137:LEU:HB3   | 4:D:142:ILE:HD11  | 1.91                     | 0.52              |
| 4:D:176:ASP:O     | 4:D:180:ARG:HB2   | 2.09                     | 0.52              |
| 4:D:48:LEU:HD11   | 7:G:3:PHE:CE1     | 2.45                     | 0.52              |
| 3:C:148:ARG:NH1   | 10:J:61:ARG:HA    | 2.25                     | 0.52              |
| 1:A:1206:ASP:CB   | 16:U:228:ASN:CG   | 2.76                     | 0.52              |
| 2:B:332:ALA:HB2   | 2:B:344:TYR:CZ    | 2.45                     | 0.52              |
| 2:B:369:PHE:HB3   | 2:B:579:TRP:HZ3   | 1.74                     | 0.52              |
| 2:B:826:ALA:O     | 2:B:1011:ILE:HA   | 2.10                     | 0.52              |
| 1:A:10:PRO:HG2    | 2:B:1192:TYR:CD1  | 2.46                     | 0.51              |
| 1:A:803:ASN:ND2   | 2:B:725:ARG:HB2   | 2.25                     | 0.51              |
| 2:B:72:ASN:O      | 2:B:125:THR:CA    | 2.53                     | 0.51              |
| 5:E:126:VAL:HG11  | 5:E:131:ILE:HG12  | 1.92                     | 0.51              |
| 4:D:23:GLU:HB3    | 7:G:82:PHE:CB     | 2.34                     | 0.51              |
| 18:W:332:LYS:CG   | 18:W:388:ARG:HB2  | 2.39                     | 0.51              |
| 1:A:713:GLU:CD    | 1:A:1092:SER:OG   | 2.49                     | 0.51              |
| 1:A:447:ARG:HB2   | 1:A:488:MET:HE3   | 1.91                     | 0.51              |
| 1:A:699:GLN:CD    | 9:I:99:LEU:HD11   | 2.30                     | 0.51              |
| 7:G:89:ALA:HB2    | 7:G:103:VAL:HG22  | 1.92                     | 0.51              |
| 16:U:181:ASN:HD22 | 16:U:212:LEU:HD13 | 1.75                     | 0.51              |
| 1:A:1362:ASP:O    | 16:U:283:LYS:CD   | 2.58                     | 0.51              |
| 7:G:97:ILE:CG1    | 18:W:683:PHE:CG   | 2.93                     | 0.51              |
| 16:U:176:ARG:O    | 16:U:180:MET:CG   | 2.58                     | 0.51              |
| 1:A:1104:LYS:O    | 1:A:1108:ASN:ND2  | 2.43                     | 0.51              |
| 1:A:1373:LEU:O    | 1:A:1377:VAL:HG23 | 2.11                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:349:SER:HB2   | 2:B:1128:LEU:HD12 | 1.93                     | 0.51              |
| 1:A:1197:LEU:HD11 | 1:A:1240:ILE:HD12 | 1.92                     | 0.51              |
| 14:T:-16:DT:H2"   | 14:T:-15:DA:N7    | 2.26                     | 0.51              |
| 16:U:130:ILE:HG22 | 16:U:134:TYR:CD1  | 2.45                     | 0.51              |
| 1:A:1085:THR:C    | 16:U:260:LYS:HZ1  | 2.13                     | 0.51              |
| 16:U:271:THR:HB   | 16:U:284:PHE:HB2  | 1.93                     | 0.51              |
| 5:E:158:GLY:O     | 5:E:160:LYS:N     | 2.44                     | 0.51              |
| 13:P:1:A:C5       | 13:P:2:U:C4       | 2.99                     | 0.51              |
| 1:A:831:LYS:NZ    | 16:U:262:THR:CB   | 2.68                     | 0.51              |
| 2:B:156:VAL:HG11  | 2:B:441:VAL:HG21  | 1.93                     | 0.51              |
| 2:B:500:LYS:CG    | 2:B:501:LEU:H     | 2.15                     | 0.51              |
| 7:G:153:ASP:O     | 7:G:155:ASN:N     | 2.42                     | 0.51              |
| 12:L:68:GLN:NE2   | 18:W:767:ILE:CG1  | 2.73                     | 0.51              |
| 1:A:671:ILE:HG12  | 1:A:806:LEU:HD21  | 1.93                     | 0.51              |
| 4:D:112:PHE:CZ    | 7:G:142:LYS:CG    | 2.92                     | 0.51              |
| 4:D:34:PHE:HE2    | 7:G:80:LYS:HB3    | 1.74                     | 0.51              |
| 13:P:-2:U:OP2     | 13:P:-2:U:H5      | 1.94                     | 0.51              |
| 18:W:805:VAL:HG12 | 18:W:808:GLU:HG2  | 1.93                     | 0.51              |
| 7:G:149:GLY:O     | 7:G:159:ALA:HA    | 2.11                     | 0.51              |
| 7:G:49:LEU:N      | 7:G:75:ARG:O      | 2.33                     | 0.51              |
| 18:W:349:GLU:HG2  | 18:W:431:ARG:HA   | 1.92                     | 0.51              |
| 18:W:679:VAL:HG13 | 18:W:684:LEU:HD21 | 1.92                     | 0.51              |
| 1:A:871:GLU:OE1   | 5:E:201:SER:OG    | 2.21                     | 0.50              |
| 4:D:148:LEU:HD13  | 4:D:159:LEU:HD13  | 1.93                     | 0.50              |
| 18:W:805:VAL:CG1  | 18:W:808:GLU:HG2  | 2.41                     | 0.50              |
| 1:A:1361:PHE:O    | 16:U:281:ARG:HB3  | 2.10                     | 0.50              |
| 2:B:336:ILE:O     | 2:B:337:ARG:O     | 2.29                     | 0.50              |
| 6:F:92:ARG:HH22   | 7:G:63:PRO:HG3    | 1.76                     | 0.50              |
| 16:U:186:ASN:OD1  | 16:U:187:ASN:OD1  | 2.28                     | 0.50              |
| 16:U:181:ASN:HD22 | 16:U:212:LEU:CD1  | 2.22                     | 0.50              |
| 3:C:9:ILE:HG21    | 3:C:12:ALA:HB2    | 1.94                     | 0.50              |
| 4:D:66:ALA:O      | 4:D:70:ALA:CB     | 2.58                     | 0.50              |
| 7:G:1:MET:N       | 7:G:80:LYS:O      | 2.35                     | 0.50              |
| 2:B:10:ASP:OD1    | 2:B:11:THR:N      | 2.43                     | 0.50              |
| 1:A:1458:ALA:HA   | 7:G:20:PRO:HG3    | 1.92                     | 0.50              |
| 8:H:111:ILE:HD12  | 8:H:128:TYR:HA    | 1.92                     | 0.50              |
| 13:P:1:A:C8       | 13:P:2:U:C5       | 3.00                     | 0.50              |
| 1:A:336:ARG:HH22  | 2:B:1114:LEU:HD21 | 1.76                     | 0.50              |
| 14:T:-6:DC:H2'    | 14:T:-5:DA:C8     | 2.45                     | 0.50              |
| 1:A:1232:GLU:CD   | 16:U:180:MET:HG3  | 2.32                     | 0.50              |
| 18:W:286:LEU:HD22 | 18:W:292:VAL:HG21 | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:W:676:ILE:HG13 | 18:W:686:LEU:CD2  | 2.37                     | 0.50              |
| 3:C:88:GLU:HG2    | 18:W:759:ARG:HD2  | 1.94                     | 0.50              |
| 1:A:114:LEU:HD13  | 1:A:145:LYS:HB3   | 1.93                     | 0.50              |
| 2:B:225:ILE:HD13  | 2:B:248:LYS:HD3   | 1.93                     | 0.50              |
| 2:B:337:ARG:O     | 2:B:341:ARG:HB2   | 2.09                     | 0.50              |
| 1:A:1448:ILE:N    | 7:G:61:ILE:HG12   | 2.26                     | 0.50              |
| 16:U:153:LYS:O    | 16:U:157:LYS:HG3  | 2.12                     | 0.50              |
| 18:W:678:HIS:HB2  | 18:W:685:PHE:HB2  | 1.93                     | 0.50              |
| 2:B:70:ASN:ND2    | 2:B:128:ASP:CA    | 2.74                     | 0.50              |
| 7:G:125:ASN:HD22  | 7:G:126:SER:N     | 2.09                     | 0.50              |
| 1:A:958:LEU:HD21  | 1:A:1019:LEU:HD23 | 1.92                     | 0.50              |
| 1:A:830:VAL:HG12  | 1:A:1083:LEU:HD21 | 1.92                     | 0.50              |
| 1:A:122:MET:O     | 1:A:126:ILE:HG12  | 2.11                     | 0.50              |
| 1:A:920:ILE:O     | 1:A:921:LEU:C     | 2.49                     | 0.50              |
| 1:A:977:ARG:HG3   | 1:A:979:LYS:HB2   | 1.94                     | 0.50              |
| 2:B:307:LYS:HB3   | 2:B:308:PRO:HD3   | 1.94                     | 0.50              |
| 2:B:563:ASP:O     | 2:B:567:HIS:N     | 2.44                     | 0.50              |
| 16:U:160:PHE:HA   | 16:U:163:VAL:CG2  | 2.40                     | 0.50              |
| 16:U:181:ASN:ND2  | 16:U:212:LEU:HD13 | 2.24                     | 0.50              |
| 16:U:187:ASN:HD21 | 16:U:214:PRO:CB   | 2.03                     | 0.50              |
| 2:B:328:ARG:HA    | 2:B:341:ARG:HD3   | 1.94                     | 0.49              |
| 2:B:56:LEU:O      | 2:B:76:GLU:HA     | 2.12                     | 0.49              |
| 5:E:160:LYS:NZ    | 5:E:192:GLY:O     | 2.42                     | 0.49              |
| 16:U:134:TYR:CE2  | 16:U:152:VAL:HG22 | 2.46                     | 0.49              |
| 1:A:528:THR:HG21  | 1:A:651:GLN:HG2   | 1.94                     | 0.49              |
| 3:C:241:ASN:OD1   | 3:C:242:GLN:N     | 2.44                     | 0.49              |
| 5:E:99:ILE:HG13   | 5:E:131:ILE:HD11  | 1.94                     | 0.49              |
| 1:A:712:ARG:HH12  | 9:I:91:ARG:HD2    | 1.77                     | 0.49              |
| 1:A:1230:TRP:HZ2  | 16:U:176:ARG:NH1  | 2.10                     | 0.49              |
| 1:A:1085:THR:O    | 16:U:260:LYS:CE   | 2.60                     | 0.49              |
| 3:C:40:VAL:HB     | 3:C:172:PRO:HG3   | 1.94                     | 0.49              |
| 18:W:357:ARG:CB   | 18:W:389:PRO:HG2  | 2.42                     | 0.49              |
| 12:L:68:GLN:NE2   | 18:W:767:ILE:HG12 | 2.27                     | 0.49              |
| 1:A:1279:ILE:HD12 | 1:A:1318:GLU:HB3  | 1.94                     | 0.49              |
| 1:A:694:ILE:HD13  | 1:A:718:GLU:HG3   | 1.95                     | 0.49              |
| 2:B:896:ASP:OD2   | 12:L:31:TYR:OH    | 2.31                     | 0.49              |
| 1:A:791:ASP:OD1   | 9:I:87:GLN:NE2    | 2.36                     | 0.49              |
| 4:D:6:SER:HB2     | 7:G:5:LYS:CE      | 2.41                     | 0.49              |
| 1:A:831:LYS:HB2   | 1:A:1083:LEU:HD22 | 1.91                     | 0.49              |
| 1:A:1264:LYS:HE2  | 9:I:44:TYR:CB     | 2.43                     | 0.49              |
| 1:A:112:LYS:HB3   | 1:A:165:ARG:HH22  | 1.77                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:245:PRO:HA    | 1:A:248:ARG:HG2   | 1.95                     | 0.49              |
| 1:A:673:ASP:OD2   | 1:A:737:ASN:OD1   | 2.30                     | 0.49              |
| 2:B:76:GLU:OE1    | 2:B:124:PHE:HE2   | 1.95                     | 0.49              |
| 2:B:250:TYR:HE2   | 2:B:262:LYS:HB2   | 1.78                     | 0.49              |
| 1:A:92:HIS:CD2    | 1:A:237:ILE:HD11  | 2.48                     | 0.49              |
| 5:E:102:LYS:HB2   | 5:E:104:PHE:CE2   | 2.47                     | 0.49              |
| 16:U:194:ILE:HD13 | 16:U:194:ILE:O    | 2.12                     | 0.49              |
| 18:W:775:GLY:O    | 18:W:777:ARG:N    | 2.42                     | 0.49              |
| 1:A:1202:ALA:HB1  | 16:U:224:ILE:HG23 | 1.95                     | 0.49              |
| 1:A:673:ASP:O     | 1:A:677:MET:HG2   | 2.12                     | 0.49              |
| 16:U:216:SER:HA   | 16:U:219:LYS:HE2  | 1.94                     | 0.49              |
| 18:W:403:GLU:O    | 18:W:403:GLU:HG3  | 2.12                     | 0.49              |
| 18:W:684:LEU:CD1  | 18:W:699:VAL:CB   | 2.91                     | 0.49              |
| 1:A:472:ASN:O     | 1:A:475:VAL:HG22  | 2.13                     | 0.49              |
| 3:C:50:ILE:HA     | 3:C:155:ILE:HG22  | 1.93                     | 0.49              |
| 18:W:399:ALA:O    | 18:W:406:ILE:HD12 | 2.13                     | 0.49              |
| 18:W:409:ASP:OD2  | 18:W:413:PHE:CE2  | 2.66                     | 0.49              |
| 18:W:678:HIS:HD2  | 18:W:685:PHE:HD2  | 1.60                     | 0.49              |
| 1:A:953:ASP:O     | 1:A:956:TRP:NE1   | 2.46                     | 0.48              |
| 1:A:1088:TYR:OH   | 16:U:237:GLU:HG3  | 2.13                     | 0.48              |
| 1:A:350:ALA:HB3   | 1:A:490:LEU:HB3   | 1.95                     | 0.48              |
| 1:A:745:LYS:O     | 1:A:749:SER:HB2   | 2.14                     | 0.48              |
| 3:C:32:LEU:HD21   | 3:C:244:PHE:CE1   | 2.48                     | 0.48              |
| 15:N:17:DA:C2     | 15:N:18:DG:C4     | 3.00                     | 0.48              |
| 7:G:96:PRO:HD2    | 18:W:683:PHE:CE2  | 2.47                     | 0.48              |
| 1:A:742:ASN:O     | 1:A:744:VAL:N     | 2.46                     | 0.48              |
| 2:B:266:PRO:CG    | 2:B:352:GLU:HB3   | 2.43                     | 0.48              |
| 4:D:112:PHE:CZ    | 7:G:142:LYS:HG2   | 2.46                     | 0.48              |
| 7:G:38:CYS:HB2    | 7:G:44:TYR:CE1    | 2.48                     | 0.48              |
| 12:L:70:ASP:C     | 12:L:72:ARG:H     | 2.16                     | 0.48              |
| 1:A:742:ASN:O     | 1:A:745:LYS:N     | 2.38                     | 0.48              |
| 2:B:1163:CYS:SG   | 2:B:1164:GLY:N    | 2.86                     | 0.48              |
| 2:B:555:GLY:O     | 2:B:583:HIS:CD2   | 2.66                     | 0.48              |
| 7:G:100:PHE:HE1   | 18:W:698:PHE:CD2  | 2.23                     | 0.48              |
| 1:A:310:ALA:HB1   | 14:T:-4:DG:H5'    | 1.94                     | 0.48              |
| 1:A:1085:THR:CB   | 16:U:260:LYS:NZ   | 2.77                     | 0.48              |
| 18:W:399:ALA:O    | 18:W:406:ILE:HD11 | 2.14                     | 0.48              |
| 1:A:1142:TYR:HA   | 1:A:1278:GLY:HA3  | 1.95                     | 0.48              |
| 2:B:653:ARG:O     | 2:B:657:GLN:HG3   | 2.14                     | 0.48              |
| 8:H:94:TYR:HD2    | 8:H:143:ILE:HD12  | 1.79                     | 0.48              |
| 1:A:253:MET:HA    | 13:P:1:A:C2       | 2.49                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:69:ILE:HD11  | 3:C:144:LEU:HD21  | 1.95                     | 0.48              |
| 7:G:42:PHE:HA    | 7:G:80:LYS:HD2    | 1.95                     | 0.48              |
| 15:N:16:DT:H2"   | 15:N:17:DA:C5'    | 2.44                     | 0.48              |
| 14:T:8:DG:H2"    | 14:T:9:DA:C8      | 2.48                     | 0.48              |
| 16:U:188:PRO:O   | 16:U:192:ARG:CB   | 2.62                     | 0.48              |
| 1:A:1362:ASP:HB2 | 16:U:272:PHE:CE1  | 2.47                     | 0.48              |
| 14:T:2:DC:H2'    | 14:T:3:DC:H6      | 1.78                     | 0.48              |
| 18:W:308:ASP:HA  | 18:W:311:ARG:HG3  | 1.96                     | 0.48              |
| 18:W:678:HIS:HD2 | 18:W:685:PHE:CD2  | 2.31                     | 0.48              |
| 1:A:286:PRO:O    | 1:A:288:HIS:N     | 2.47                     | 0.48              |
| 3:C:135:ARG:NH2  | 3:C:139:ASP:OD1   | 2.46                     | 0.48              |
| 4:D:41:HIS:CE1   | 7:G:74:TYR:N      | 2.81                     | 0.48              |
| 14:T:-18:DT:H2'  | 14:T:-17:DC:C5    | 2.48                     | 0.48              |
| 14:T:-5:DA:C8    | 14:T:-5:DA:H5"    | 2.45                     | 0.48              |
| 1:A:327:ARG:HG2  | 1:A:1409:VAL:HG21 | 1.95                     | 0.48              |
| 2:B:291:GLN:O    | 2:B:564:PRO:HG3   | 2.14                     | 0.48              |
| 14:T:-4:DG:H2"   | 14:T:-3:DA:C8     | 2.49                     | 0.48              |
| 2:B:319:LYS:HE2  | 2:B:323:LEU:HD11  | 1.96                     | 0.48              |
| 2:B:610:ARG:NE   | 2:B:612:ILE:HG12  | 2.29                     | 0.48              |
| 4:D:49:ILE:CG2   | 7:G:4:LEU:HD12    | 2.40                     | 0.48              |
| 10:J:1:MET:HA    | 10:J:55:LEU:HB2   | 1.95                     | 0.48              |
| 17:V:91:PRO:HB2  | 17:V:93:ASP:OD1   | 2.14                     | 0.48              |
| 1:A:1202:ALA:HA  | 16:U:224:ILE:HG23 | 1.89                     | 0.47              |
| 1:A:1400:LEU:HA  | 1:A:1403:CYS:SG   | 2.53                     | 0.47              |
| 1:A:924:VAL:O    | 1:A:925:GLU:C     | 2.52                     | 0.47              |
| 1:A:985:ILE:HA   | 1:A:988:ILE:HD12  | 1.96                     | 0.47              |
| 3:C:174:SER:OG   | 3:C:175:ALA:N     | 2.47                     | 0.47              |
| 7:G:148:VAL:HG22 | 7:G:161:GLY:HA2   | 1.95                     | 0.47              |
| 16:U:157:LYS:O   | 16:U:161:LYS:HB2  | 2.14                     | 0.47              |
| 1:A:699:GLN:NE2  | 9:I:99:LEU:HD21   | 2.29                     | 0.47              |
| 2:B:70:ASN:CG    | 2:B:128:ASP:N     | 2.67                     | 0.47              |
| 2:B:25:PHE:HZ    | 2:B:534:LEU:HG    | 1.79                     | 0.47              |
| 4:D:38:GLN:HE21  | 7:G:5:LYS:HZ2     | 1.61                     | 0.47              |
| 16:U:214:PRO:HD2 | 16:U:217:LEU:CB   | 2.44                     | 0.47              |
| 18:W:384:THR:OG1 | 18:W:387:PHE:HD2  | 1.97                     | 0.47              |
| 5:E:60:LEU:HD12  | 5:E:77:LEU:O      | 2.14                     | 0.47              |
| 7:G:158:TYR:HB2  | 18:W:667:PHE:HE2  | 1.76                     | 0.47              |
| 7:G:3:PHE:O      | 7:G:77:VAL:HA     | 2.14                     | 0.47              |
| 18:W:437:VAL:O   | 18:W:437:VAL:CG2  | 2.61                     | 0.47              |
| 5:E:54:ARG:HB2   | 5:E:83:ASP:OD1    | 2.14                     | 0.47              |
| 18:W:413:PHE:HE1 | 18:W:420:GLU:HB3  | 1.78                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:W:678:HIS:HB2  | 18:W:685:PHE:CB   | 2.45                     | 0.47              |
| 1:A:487:GLU:OE2   | 2:B:1102:LYS:HD3  | 2.15                     | 0.47              |
| 4:D:64:LEU:HB3    | 4:D:89:LEU:HG     | 1.95                     | 0.47              |
| 13:P:1:A:N6       | 13:P:2:U:N3       | 2.63                     | 0.47              |
| 1:A:1137:GLN:HE22 | 16:U:232:ALA:C    | 2.18                     | 0.47              |
| 1:A:1362:ASP:O    | 16:U:283:LYS:CG   | 2.63                     | 0.47              |
| 2:B:1072:MET:SD   | 2:B:1085:VAL:HB   | 2.55                     | 0.47              |
| 2:B:514:LEU:HD22  | 2:B:626:VAL:HG12  | 1.97                     | 0.47              |
| 4:D:23:GLU:OE1    | 7:G:82:PHE:CD1    | 2.65                     | 0.47              |
| 12:L:29:VAL:O     | 12:L:41:SER:HA    | 2.14                     | 0.47              |
| 18:W:396:GLU:CD   | 18:W:414:VAL:HG23 | 2.30                     | 0.47              |
| 1:A:558:ASP:OD1   | 1:A:559:GLY:N     | 2.46                     | 0.47              |
| 1:A:342:MET:HB3   | 2:B:1132:GLU:HG2  | 1.97                     | 0.47              |
| 7:G:97:ILE:CG2    | 7:G:97:ILE:O      | 2.63                     | 0.47              |
| 18:W:684:LEU:N    | 18:W:697:VAL:O    | 2.47                     | 0.47              |
| 1:A:1061:HIS:ND1  | 6:F:87:LYS:HE3    | 2.30                     | 0.47              |
| 1:A:831:LYS:HB3   | 1:A:1083:LEU:HD22 | 1.62                     | 0.47              |
| 2:B:179:ASP:O     | 2:B:183:MET:HG2   | 2.15                     | 0.47              |
| 8:H:144:ARG:HG3   | 8:H:145:ARG:HG2   | 1.97                     | 0.47              |
| 1:A:1097:THR:HG22 | 1:A:1102:ARG:HB2  | 1.96                     | 0.47              |
| 2:B:219:LYS:HA    | 2:B:219:LYS:HD3   | 1.69                     | 0.47              |
| 4:D:85:ASP:OD1    | 4:D:86:ASP:N      | 2.48                     | 0.47              |
| 5:E:158:GLY:O     | 5:E:159:GLU:C     | 2.52                     | 0.47              |
| 1:A:914:ILE:HG13  | 1:A:917:ALA:HB2   | 1.96                     | 0.46              |
| 7:G:22:MET:O      | 7:G:26:LEU:HG     | 2.15                     | 0.46              |
| 14:T:-10:DT:H2'   | 14:T:-9:DA:C8     | 2.50                     | 0.46              |
| 16:U:206:THR:HG22 | 16:U:208:SER:HB2  | 1.97                     | 0.46              |
| 1:A:1205:LEU:HD23 | 16:U:224:ILE:HB   | 1.97                     | 0.46              |
| 1:A:831:LYS:HZ3   | 16:U:262:THR:HA   | 0.64                     | 0.46              |
| 1:A:793:PHE:CD1   | 1:A:798:LYS:HD2   | 2.51                     | 0.46              |
| 11:K:65:HIS:HE1   | 11:K:67:LEU:HD12  | 1.79                     | 0.46              |
| 15:N:15:DG:C2'    | 15:N:16:DT:H5''   | 2.23                     | 0.46              |
| 1:A:18:GLN:HB3    | 2:B:1215:ARG:HB2  | 1.96                     | 0.46              |
| 1:A:474:SER:OG    | 1:A:651:GLN:NE2   | 2.47                     | 0.46              |
| 2:B:559:LEU:O     | 2:B:562:TYR:N     | 2.45                     | 0.46              |
| 4:D:25:ALA:CB     | 7:G:85:GLU:CA     | 2.83                     | 0.46              |
| 10:J:6:ARG:HD3    | 10:J:13:VAL:HG22  | 1.96                     | 0.46              |
| 1:A:1234:ASN:ND2  | 16:U:212:LEU:O    | 2.48                     | 0.46              |
| 1:A:766:VAL:HG23  | 1:A:803:ASN:O     | 2.15                     | 0.46              |
| 2:B:336:ILE:HD12  | 2:B:336:ILE:H     | 1.80                     | 0.46              |
| 15:N:5:DC:H2''    | 15:N:6:DT:H5'     | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:W:413:PHE:HZ   | 18:W:420:GLU:CD   | 2.17                     | 0.46              |
| 2:B:480:THR:HG23  | 2:B:483:SER:H     | 1.80                     | 0.46              |
| 3:C:68:LEU:O      | 10:J:5:VAL:HG11   | 2.15                     | 0.46              |
| 1:A:735:GLU:CB    | 1:A:756:PHE:HE1   | 2.28                     | 0.46              |
| 2:B:300:TRP:O     | 2:B:304:GLU:HB2   | 2.15                     | 0.46              |
| 1:A:1202:ALA:CA   | 16:U:224:ILE:HG23 | 2.45                     | 0.46              |
| 1:A:92:HIS:HD2    | 1:A:237:ILE:HD11  | 1.80                     | 0.46              |
| 1:A:408:ARG:HD3   | 1:A:412:ASP:HB2   | 1.97                     | 0.46              |
| 1:A:666:GLY:HA3   | 2:B:1069:PHE:CZ   | 2.51                     | 0.46              |
| 3:C:149:ASN:OD1   | 3:C:150:HIS:CD2   | 2.68                     | 0.46              |
| 4:D:7:THR:CG2     | 7:G:6:ASP:HB2     | 2.44                     | 0.46              |
| 1:A:452:HIS:CE1   | 1:A:454:MET:HB2   | 2.50                     | 0.46              |
| 1:A:745:LYS:O     | 1:A:749:SER:HB3   | 2.16                     | 0.46              |
| 2:B:725:ARG:HD3   | 2:B:727:LYS:HE3   | 1.97                     | 0.46              |
| 5:E:82:CYS:SG     | 5:E:83:ASP:N      | 2.89                     | 0.46              |
| 15:N:13:DC:H2'    | 15:N:14:DG:C8     | 2.50                     | 0.46              |
| 1:A:152:ALA:N     | 1:A:163:VAL:O     | 2.45                     | 0.46              |
| 13:P:-3:U:H3'     | 13:P:-2:U:C6      | 2.50                     | 0.46              |
| 14:T:-20:DA:C8    | 14:T:-19:DC:C5    | 3.04                     | 0.46              |
| 1:A:280:LEU:HD13  | 1:A:289:ILE:HG22  | 1.98                     | 0.46              |
| 2:B:491:THR:OG1   | 2:B:530:LYS:HB2   | 2.16                     | 0.46              |
| 1:A:1022:CYS:O    | 1:A:1026:ALA:HB2  | 2.15                     | 0.45              |
| 1:A:985:ILE:N     | 1:A:986:PRO:HD2   | 2.31                     | 0.45              |
| 7:G:5:LYS:HE2     | 7:G:42:PHE:CZ     | 2.51                     | 0.45              |
| 12:L:28:GLY:HA3   | 12:L:42:LEU:O     | 2.16                     | 0.45              |
| 16:U:188:PRO:O    | 16:U:192:ARG:N    | 2.38                     | 0.45              |
| 18:W:388:ARG:HB2  | 18:W:389:PRO:CD   | 2.46                     | 0.45              |
| 18:W:664:VAL:CG2  | 18:W:686:LEU:CD2  | 2.93                     | 0.45              |
| 1:A:1085:THR:C    | 16:U:260:LYS:NZ   | 2.69                     | 0.45              |
| 1:A:977:ARG:HB2   | 1:A:978:ALA:HB3   | 1.96                     | 0.45              |
| 2:B:851:PHE:O     | 2:B:1094:ARG:NH1  | 2.50                     | 0.45              |
| 2:B:332:ALA:HB2   | 2:B:344:TYR:CE2   | 2.51                     | 0.45              |
| 4:D:176:ASP:O     | 4:D:180:ARG:CB    | 2.64                     | 0.45              |
| 16:U:146:SER:C    | 16:U:148:ILE:H    | 2.19                     | 0.45              |
| 18:W:322:ARG:HD3  | 18:W:342:GLU:HA   | 1.99                     | 0.45              |
| 18:W:352:LEU:CD1  | 18:W:435:LEU:HD21 | 2.46                     | 0.45              |
| 18:W:672:ARG:HH12 | 18:W:691:ILE:CG1  | 2.29                     | 0.45              |
| 1:A:1100:VAL:CB   | 1:A:1101:PRO:HD3  | 2.34                     | 0.45              |
| 2:B:499:GLY:C     | 2:B:500:LYS:HD2   | 2.36                     | 0.45              |
| 4:D:55:GLU:HG2    | 4:D:121:CYS:SG    | 2.57                     | 0.45              |
| 15:N:-6:DA:OP2    | 15:N:-5:DT:C7     | 2.64                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 16:U:146:SER:O   | 16:U:148:ILE:HG22 | 2.17                     | 0.45              |
| 1:A:203:LEU:HB3  | 1:A:208:ILE:HD11  | 1.99                     | 0.45              |
| 1:A:386:ILE:O    | 1:A:390:THR:HG23  | 2.17                     | 0.45              |
| 2:B:1120:GLU:O   | 2:B:1124:ARG:NH2  | 2.33                     | 0.45              |
| 4:D:72:ASN:HB3   | 4:D:75:VAL:HB     | 1.98                     | 0.45              |
| 13:P:3:C:N3      | 14:T:8:DG:C2      | 2.81                     | 0.45              |
| 1:A:1232:GLU:CD  | 16:U:180:MET:CG   | 2.83                     | 0.45              |
| 1:A:309:ILE:C    | 1:A:310:ALA:O     | 2.40                     | 0.45              |
| 1:A:1085:THR:O   | 16:U:260:LYS:NZ   | 2.50                     | 0.45              |
| 1:A:713:GLU:OE2  | 1:A:1092:SER:CB   | 2.64                     | 0.45              |
| 1:A:1082:THR:CB  | 16:U:260:LYS:HZ3  | 2.30                     | 0.45              |
| 1:A:1388:THR:OG1 | 1:A:1389:ARG:N    | 2.49                     | 0.45              |
| 1:A:1462:PRO:HD2 | 7:G:21:GLN:N      | 2.31                     | 0.45              |
| 2:B:252:ARG:HB3  | 2:B:255:LYS:HB3   | 1.99                     | 0.45              |
| 4:D:30:LEU:O     | 7:G:82:PHE:CZ     | 2.70                     | 0.45              |
| 9:I:51:ASN:HB3   | 9:I:52:ILE:H      | 1.58                     | 0.45              |
| 15:N:4:DT:H2'    | 15:N:5:DC:C6      | 2.51                     | 0.45              |
| 1:A:1195:LEU:HB2 | 1:A:1263:LEU:HD11 | 1.98                     | 0.45              |
| 1:A:1191:SER:OG  | 1:A:1259:GLU:OE1  | 2.21                     | 0.45              |
| 1:A:67:CYS:O     | 1:A:71:GLY:N      | 2.45                     | 0.45              |
| 2:B:1008:PRO:HB3 | 2:B:1087:PHE:HE1  | 1.81                     | 0.45              |
| 1:A:661:ASN:HD21 | 2:B:1082:MET:HB3  | 1.80                     | 0.45              |
| 2:B:555:GLY:O    | 2:B:583:HIS:HD2   | 2.00                     | 0.45              |
| 3:C:173:CYS:SG   | 3:C:243:VAL:HG11  | 2.57                     | 0.45              |
| 4:D:6:SER:HB3    | 7:G:7:LEU:HD21    | 1.98                     | 0.45              |
| 7:G:56:VAL:HG12  | 7:G:72:VAL:HG22   | 1.99                     | 0.45              |
| 7:G:98:GLY:HA3   | 7:G:110:VAL:O     | 2.17                     | 0.45              |
| 16:U:133:ILE:CD1 | 16:U:155:ILE:CB   | 2.84                     | 0.45              |
| 4:D:57:ARG:HD2   | 4:D:110:ASN:HA    | 1.99                     | 0.45              |
| 5:E:24:ASP:OD2   | 5:E:186:TYR:OH    | 2.28                     | 0.45              |
| 1:A:231:ARG:HB3  | 1:A:234:TRP:CD2   | 2.52                     | 0.44              |
| 1:A:387:HIS:O    | 1:A:390:THR:OG1   | 2.24                     | 0.44              |
| 2:B:1073:TYR:CE1 | 2:B:1080:LYS:HG2  | 2.52                     | 0.44              |
| 2:B:269:LYS:HE2  | 2:B:331:SER:HA    | 1.98                     | 0.44              |
| 2:B:276:ILE:O    | 2:B:280:ALA:CB    | 2.64                     | 0.44              |
| 2:B:795:ILE:HB   | 2:B:854:LEU:HB2   | 1.99                     | 0.44              |
| 1:A:1264:LYS:CE  | 9:I:44:TYR:CD1    | 2.99                     | 0.44              |
| 15:N:-6:DA:C8    | 15:N:-6:DA:O5'    | 2.71                     | 0.44              |
| 13:P:-2:U:C5     | 13:P:-2:U:OP2     | 2.70                     | 0.44              |
| 16:U:183:LYS:C   | 16:U:185:LYS:H    | 2.19                     | 0.44              |
| 1:A:1206:ASP:HA  | 16:U:228:ASN:ND2  | 2.32                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:41:MET:HE3    | 1:A:41:MET:N      | 2.32                     | 0.44              |
| 2:B:154:ASN:OD1   | 2:B:155:LYS:N     | 2.45                     | 0.44              |
| 2:B:947:GLY:HA3   | 2:B:968:MET:SD    | 2.57                     | 0.44              |
| 1:A:699:GLN:NE2   | 9:I:99:LEU:HD11   | 2.32                     | 0.44              |
| 16:U:182:LEU:O    | 16:U:191:ARG:HD3  | 2.17                     | 0.44              |
| 18:W:409:ASP:OD2  | 18:W:413:PHE:HE2  | 2.00                     | 0.44              |
| 18:W:664:VAL:HG21 | 18:W:686:LEU:CG   | 2.45                     | 0.44              |
| 1:A:1116:PRO:HB3  | 1:A:1314:ILE:HG23 | 1.99                     | 0.44              |
| 2:B:824:ILE:HD13  | 2:B:1089:PRO:HB3  | 2.00                     | 0.44              |
| 2:B:436:ASN:O     | 2:B:438:ASN:N     | 2.39                     | 0.44              |
| 4:D:23:GLU:OE1    | 7:G:82:PHE:CA     | 2.36                     | 0.44              |
| 1:A:1441:THR:HG23 | 6:F:88:TYR:HD1    | 1.82                     | 0.44              |
| 8:H:92:TYR:CD1    | 8:H:144:ARG:HB2   | 2.52                     | 0.44              |
| 17:V:28:GLY:HA3   | 17:V:33:ASP:CG    | 2.38                     | 0.44              |
| 1:A:875:ASP:CG    | 1:A:876:GLY:H     | 2.21                     | 0.44              |
| 4:D:68:SER:HB2    | 4:D:92:VAL:HG21   | 1.99                     | 0.44              |
| 7:G:116:PRO:HA    | 7:G:164:LYS:HD3   | 1.98                     | 0.44              |
| 15:N:20:DG:H2"    | 15:N:21:DT:H5"    | 1.99                     | 0.44              |
| 1:A:64:ASN:OD1    | 1:A:65:PHE:N      | 2.51                     | 0.44              |
| 1:A:772:GLU:HA    | 1:A:1086:PHE:CE2  | 2.53                     | 0.44              |
| 1:A:882:GLN:NE2   | 1:A:961:ASN:HA    | 2.33                     | 0.44              |
| 7:G:151:ARG:HG3   | 18:W:667:PHE:CD1  | 2.40                     | 0.44              |
| 1:A:375:LEU:HD13  | 1:A:492:VAL:HG21  | 1.99                     | 0.44              |
| 1:A:1345:GLU:OE1  | 5:E:199:ARG:HD3   | 2.17                     | 0.44              |
| 1:A:62:ASP:OD1    | 1:A:63:ARG:N      | 2.47                     | 0.44              |
| 4:D:169:VAL:HG12  | 4:D:170:ASN:N     | 2.31                     | 0.44              |
| 7:G:151:ARG:HG2   | 18:W:668:THR:HG23 | 2.00                     | 0.44              |
| 7:G:95:SER:HB3    | 18:W:682:ASN:CB   | 2.48                     | 0.44              |
| 8:H:109:ASP:OD1   | 8:H:128:TYR:N     | 2.50                     | 0.44              |
| 1:A:1226:LEU:HD12 | 1:A:1243:ARG:O    | 2.18                     | 0.44              |
| 1:A:1446:VAL:O    | 7:G:61:ILE:HG12   | 2.18                     | 0.44              |
| 1:A:735:GLU:HG3   | 1:A:756:PHE:CE1   | 2.52                     | 0.44              |
| 1:A:1447:MET:HB2  | 6:F:133:VAL:HB    | 2.00                     | 0.44              |
| 12:L:63:THR:OG1   | 12:L:64:LYS:N     | 2.49                     | 0.44              |
| 1:A:107:CYS:SG    | 1:A:108:MET:N     | 2.91                     | 0.44              |
| 1:A:231:ARG:HH11  | 1:A:232:PRO:HD2   | 1.83                     | 0.43              |
| 1:A:248:ARG:O     | 1:A:248:ARG:HG3   | 2.18                     | 0.43              |
| 2:B:237:LYS:HD3   | 2:B:237:LYS:HA    | 1.90                     | 0.43              |
| 2:B:344:TYR:CE2   | 2:B:348:ILE:HD11  | 2.53                     | 0.43              |
| 2:B:763:GLN:HG2   | 2:B:765:PRO:HD2   | 1.99                     | 0.43              |
| 4:D:151:GLU:N     | 4:D:155:GLU:OE1   | 2.46                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:85:GLU:HG2    | 7:G:87:VAL:HG13   | 2.00                     | 0.43              |
| 14:T:-6:DC:H2"    | 14:T:-5:DA:C8     | 2.53                     | 0.43              |
| 16:U:189:THR:O    | 16:U:193:SER:CA   | 2.66                     | 0.43              |
| 1:A:1205:LEU:HD22 | 16:U:221:MET:HA   | 2.00                     | 0.43              |
| 16:U:284:PHE:HD2  | 16:U:284:PHE:HA   | 1.72                     | 0.43              |
| 1:A:1212:ASN:O    | 1:A:1215:ALA:N    | 2.50                     | 0.43              |
| 1:A:536:THR:HG21  | 1:A:579:LEU:HD22  | 2.00                     | 0.43              |
| 1:A:533:ARG:HD3   | 1:A:750:ALA:HA    | 2.00                     | 0.43              |
| 1:A:986:PRO:O     | 1:A:990:HIS:HB2   | 2.19                     | 0.43              |
| 2:B:35:LEU:HD22   | 2:B:167:SER:HB3   | 1.99                     | 0.43              |
| 2:B:426:GLN:O     | 2:B:430:GLU:HG3   | 2.18                     | 0.43              |
| 2:B:1221:SER:HB2  | 4:D:12:ARG:HH12   | 1.82                     | 0.43              |
| 16:U:156:GLU:O    | 16:U:160:PHE:CD2  | 2.64                     | 0.43              |
| 18:W:442:PRO:HB2  | 18:W:447:LEU:CD1  | 2.48                     | 0.43              |
| 1:A:1095:ASN:O    | 1:A:1115:THR:HG21 | 2.18                     | 0.43              |
| 1:A:1329:ARG:HG2  | 5:E:147:GLU:OE2   | 2.17                     | 0.43              |
| 1:A:735:GLU:HG3   | 1:A:756:PHE:CD1   | 2.54                     | 0.43              |
| 1:A:779:GLY:HA3   | 2:B:509:ASN:HB2   | 2.00                     | 0.43              |
| 4:D:52:SER:O      | 4:D:56:SER:CB     | 2.66                     | 0.43              |
| 4:D:158:THR:CG2   | 7:G:167:PHE:CE2   | 2.94                     | 0.43              |
| 12:L:33:CYS:SG    | 12:L:55:HIS:HB3   | 2.59                     | 0.43              |
| 15:N:-6:DA:O5'    | 15:N:-6:DA:H8     | 2.01                     | 0.43              |
| 1:A:253:MET:CG    | 13:P:1:A:C2       | 2.89                     | 0.43              |
| 13:P:-1:U:C5      | 13:P:-1:U:OP2     | 2.71                     | 0.43              |
| 18:W:333:PHE:CD2  | 18:W:354:LEU:CD2  | 3.00                     | 0.43              |
| 1:A:1122:LEU:HD13 | 1:A:1126:ILE:HG22 | 2.00                     | 0.43              |
| 1:A:143:LYS:HG3   | 1:A:144:THR:HG23  | 2.00                     | 0.43              |
| 3:C:4:GLU:HB3     | 3:C:5:PRO:HD3     | 2.00                     | 0.43              |
| 7:G:50:ASP:OD1    | 7:G:50:ASP:C      | 2.56                     | 0.43              |
| 18:W:344:LEU:HD12 | 18:W:349:GLU:HB2  | 2.00                     | 0.43              |
| 1:A:897:ARG:HD3   | 1:A:1032:ARG:HD2  | 2.01                     | 0.43              |
| 1:A:1143:THR:HG23 | 1:A:1147:ASN:HB2  | 1.99                     | 0.43              |
| 1:A:337:LEU:HD12  | 1:A:1408:THR:HG21 | 2.01                     | 0.43              |
| 1:A:961:ASN:HD22  | 1:A:964:ARG:CZ    | 2.32                     | 0.43              |
| 2:B:204:ILE:O     | 2:B:205:ALA:C     | 2.56                     | 0.43              |
| 3:C:103:ARG:HH21  | 3:C:152:GLU:CD    | 2.21                     | 0.43              |
| 1:A:1061:HIS:CE1  | 6:F:87:LYS:HE3    | 2.53                     | 0.43              |
| 13:P:-2:U:H6      | 13:P:-2:U:C5'     | 2.31                     | 0.43              |
| 18:W:265:ARG:HD2  | 18:W:265:ARG:HA   | 1.71                     | 0.43              |
| 1:A:527:ASP:HB2   | 2:B:835:GLN:NE2   | 2.34                     | 0.43              |
| 7:G:152:THR:HG22  | 7:G:154:VAL:H     | 1.83                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:34:PHE:CE2    | 7:G:80:LYS:HB3    | 2.53                     | 0.43              |
| 9:I:87:GLN:O      | 9:I:88:SER:HB2    | 2.18                     | 0.43              |
| 1:A:368:PRO:HD2   | 1:A:371:ILE:HD12  | 2.01                     | 0.43              |
| 1:A:50:GLU:OE1    | 18:W:444:LEU:HD21 | 2.19                     | 0.43              |
| 2:B:249:LEU:HD13  | 2:B:261:ILE:HG12  | 2.00                     | 0.43              |
| 3:C:13:GLN:HE21   | 3:C:16:GLU:HG2    | 1.84                     | 0.43              |
| 10:J:7:CYS:HB3    | 10:J:11:GLY:H     | 1.84                     | 0.43              |
| 14:T:0:DT:C2      | 14:T:1:DA:N7      | 2.87                     | 0.43              |
| 1:A:1332:SER:OG   | 1:A:1333:ASN:N    | 2.51                     | 0.43              |
| 1:A:317:GLN:HG3   | 1:A:318:LYS:N     | 2.33                     | 0.43              |
| 2:B:769:TYR:OH    | 16:U:265:ALA:CA   | 2.66                     | 0.43              |
| 4:D:114:ARG:NH2   | 4:D:178:LEU:HB3   | 2.33                     | 0.43              |
| 7:G:84:GLY:N      | 7:G:147:VAL:O     | 2.45                     | 0.43              |
| 9:I:96:ASN:OD1    | 9:I:97:MET:N      | 2.52                     | 0.43              |
| 18:W:344:LEU:HD11 | 18:W:349:GLU:HB2  | 2.01                     | 0.43              |
| 1:A:961:ASN:HD22  | 1:A:964:ARG:NH2   | 2.17                     | 0.43              |
| 4:D:30:LEU:C      | 7:G:82:PHE:CE1    | 2.92                     | 0.43              |
| 1:A:409:ASP:OD1   | 1:A:410:ASN:N     | 2.52                     | 0.43              |
| 2:B:605:GLU:O     | 2:B:625:ARG:NH2   | 2.31                     | 0.43              |
| 5:E:143:ILE:HG13  | 5:E:143:ILE:H     | 1.66                     | 0.43              |
| 4:D:101:VAL:HG13  | 7:G:105:PRO:HA    | 2.00                     | 0.43              |
| 1:A:37:TYR:HE1    | 18:W:441:ASN:HD21 | 1.51                     | 0.42              |
| 1:A:529:LEU:O     | 1:A:532:VAL:HG12  | 2.18                     | 0.42              |
| 7:G:10:ILE:HA     | 7:G:70:PHE:O      | 2.19                     | 0.42              |
| 17:V:15:CYS:HB3   | 17:V:32:CYS:SG    | 2.59                     | 0.42              |
| 1:A:831:LYS:N     | 1:A:1083:LEU:HD23 | 2.35                     | 0.42              |
| 2:B:1106:ARG:NH1  | 2:B:1118:PRO:HB3  | 2.34                     | 0.42              |
| 7:G:45:ILE:HG23   | 7:G:78:VAL:HG12   | 2.00                     | 0.42              |
| 18:W:421:TYR:HA   | 18:W:425:PHE:O    | 2.19                     | 0.42              |
| 1:A:1100:VAL:CB   | 1:A:1101:PRO:CD   | 2.95                     | 0.42              |
| 1:A:13:SER:HB2    | 1:A:1435:GLN:NE2  | 2.34                     | 0.42              |
| 5:E:123:ILE:HB    | 5:E:124:PRO:HD3   | 2.01                     | 0.42              |
| 8:H:101:TYR:CZ    | 8:H:114:TYR:HB3   | 2.55                     | 0.42              |
| 14:T:2:DC:H2'     | 14:T:3:DC:C6      | 2.54                     | 0.42              |
| 16:U:129:SER:O    | 16:U:133:ILE:CG1  | 2.66                     | 0.42              |
| 18:W:388:ARG:HB2  | 18:W:389:PRO:HD3  | 2.01                     | 0.42              |
| 1:A:1031:ARG:O    | 1:A:1035:GLU:HB2  | 2.18                     | 0.42              |
| 4:D:33:GLU:OE1    | 7:G:42:PHE:CE2    | 2.63                     | 0.42              |
| 7:G:79:TRP:CZ3    | 7:G:81:PRO:HD3    | 2.54                     | 0.42              |
| 18:W:749:ASP:HB3  | 18:W:752:LEU:HD11 | 2.01                     | 0.42              |
| 1:A:562:PRO:HG3   | 1:A:581:ILE:HD11  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:572:ARG:HB3   | 2:B:579:TRP:HE1   | 1.84                     | 0.42              |
| 6:F:92:ARG:NH2    | 7:G:63:PRO:HB3    | 2.34                     | 0.42              |
| 18:W:799:GLU:HB3  | 18:W:804:TRP:CZ3  | 2.55                     | 0.42              |
| 1:A:1080:GLN:OE1  | 16:U:283:LYS:HE2  | 2.20                     | 0.42              |
| 2:B:296:ASP:OD1   | 2:B:297:GLU:N     | 2.52                     | 0.42              |
| 3:C:104:HIS:HD2   | 3:C:149:ASN:HA    | 1.85                     | 0.42              |
| 2:B:1073:TYR:HE2  | 3:C:179:GLU:HA    | 1.84                     | 0.42              |
| 7:G:112:THR:HA    | 7:G:115:ILE:HD12  | 2.01                     | 0.42              |
| 9:I:75:CYS:HA     | 9:I:76:PRO:HD3    | 1.93                     | 0.42              |
| 10:J:44:CYS:SG    | 10:J:45:CYS:N     | 2.93                     | 0.42              |
| 18:W:278:LYS:HD2  | 18:W:280:GLU:OE2  | 2.20                     | 0.42              |
| 18:W:332:LYS:HE3  | 18:W:357:ARG:HB2  | 2.01                     | 0.42              |
| 1:A:1361:PHE:O    | 16:U:281:ARG:CB   | 2.68                     | 0.42              |
| 1:A:72:GLU:HB3    | 1:A:76:GLU:HB2    | 2.02                     | 0.42              |
| 4:D:23:GLU:CB     | 7:G:83:LYS:H      | 2.31                     | 0.42              |
| 7:G:97:ILE:HG13   | 18:W:683:PHE:CB   | 2.50                     | 0.42              |
| 18:W:352:LEU:HD21 | 18:W:435:LEU:CD1  | 2.50                     | 0.42              |
| 18:W:676:ILE:CA   | 18:W:686:LEU:CD2  | 2.97                     | 0.42              |
| 2:B:639:LYS:HG3   | 2:B:641:ASN:H     | 1.85                     | 0.42              |
| 5:E:55:LYS:HG3    | 5:E:56:LEU:HD12   | 2.01                     | 0.42              |
| 11:K:63:VAL:HG22  | 11:K:71:PHE:HB3   | 2.02                     | 0.42              |
| 15:N:16:DT:C2'    | 15:N:17:DA:C8     | 2.96                     | 0.42              |
| 16:U:161:LYS:HD3  | 16:U:204:LEU:HG   | 2.02                     | 0.42              |
| 3:C:89:ASP:OD1    | 18:W:757:LYS:HD3  | 2.20                     | 0.42              |
| 2:B:127:ILE:O     | 2:B:127:ILE:HG13  | 2.20                     | 0.42              |
| 2:B:710:ARG:NH1   | 2:B:719:LEU:HG    | 2.35                     | 0.42              |
| 4:D:144:GLN:HA    | 4:D:147:SER:HB2   | 2.02                     | 0.42              |
| 5:E:87:VAL:HG11   | 5:E:109:PHE:HE2   | 1.83                     | 0.42              |
| 2:B:24:PHE:CE1    | 2:B:28:LYS:HD2    | 2.55                     | 0.42              |
| 4:D:178:LEU:O     | 4:D:182:GLU:HB2   | 2.20                     | 0.42              |
| 4:D:41:HIS:HE1    | 7:G:7:LEU:O       | 2.03                     | 0.42              |
| 18:W:672:ARG:HH22 | 18:W:691:ILE:HD11 | 1.85                     | 0.42              |
| 1:A:1082:THR:CB   | 16:U:260:LYS:NZ   | 2.82                     | 0.41              |
| 1:A:1202:ALA:HA   | 16:U:224:ILE:HD13 | 2.02                     | 0.41              |
| 2:B:784:ASN:HB2   | 2:B:787:VAL:HG22  | 2.02                     | 0.41              |
| 2:B:844:SER:HB3   | 2:B:848:ARG:NH1   | 2.35                     | 0.41              |
| 4:D:46:HIS:CD2    | 4:D:47:ASP:H      | 2.37                     | 0.41              |
| 9:I:32:CYS:HB3    | 9:I:33:ASP:H      | 1.73                     | 0.41              |
| 14:T:12:DG:N2     | 15:N:14:DG:N3     | 2.68                     | 0.41              |
| 1:A:1266:ILE:O    | 1:A:1270:MET:HG3  | 2.19                     | 0.41              |
| 1:A:552:PHE:CE1   | 11:K:74:ARG:HB2   | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:W:352:LEU:HD11 | 18:W:435:LEU:CD2  | 2.49                     | 0.41              |
| 1:A:1006:ASN:OD1  | 1:A:1007:GLU:N    | 2.51                     | 0.41              |
| 1:A:408:ARG:HB3   | 1:A:409:ASP:H     | 1.74                     | 0.41              |
| 7:G:100:PHE:CE1   | 18:W:698:PHE:CD2  | 3.02                     | 0.41              |
| 7:G:23:ASN:HA     | 7:G:26:LEU:HD12   | 2.02                     | 0.41              |
| 16:U:133:ILE:CG1  | 16:U:155:ILE:HG21 | 2.49                     | 0.41              |
| 18:W:806:PRO:O    | 18:W:808:GLU:N    | 2.45                     | 0.41              |
| 1:A:1134:LYS:HD3  | 16:U:229:LEU:HD12 | 2.02                     | 0.41              |
| 2:B:221:ALA:HB3   | 2:B:222:PRO:HD3   | 2.02                     | 0.41              |
| 4:D:34:PHE:HD2    | 7:G:82:PHE:HZ     | 1.69                     | 0.41              |
| 4:D:38:GLN:HE21   | 7:G:5:LYS:NZ      | 2.18                     | 0.41              |
| 8:H:6:PHE:HB3     | 8:H:59:LEU:HB2    | 2.01                     | 0.41              |
| 1:A:1221:VAL:HG21 | 1:A:1274:ILE:HD12 | 2.03                     | 0.41              |
| 1:A:188:LYS:HB2   | 1:A:196:ALA:HB3   | 2.02                     | 0.41              |
| 2:B:827:ILE:HG12  | 2:B:1012:ILE:HD11 | 2.02                     | 0.41              |
| 2:B:274:ILE:O     | 2:B:277:VAL:HG22  | 2.21                     | 0.41              |
| 2:B:89:MET:O      | 2:B:96:THR:HA     | 2.20                     | 0.41              |
| 3:C:220:ASP:OD1   | 3:C:221:TYR:N     | 2.50                     | 0.41              |
| 14:T:-20:DA:N1    | 15:N:22:DG:N2     | 2.68                     | 0.41              |
| 14:T:-12:DG:H3'   | 14:T:-11:DA:C8    | 2.55                     | 0.41              |
| 1:A:1201:ARG:NE   | 16:U:217:LEU:HD11 | 2.36                     | 0.41              |
| 18:W:756:VAL:HG11 | 18:W:796:LEU:HD22 | 2.02                     | 0.41              |
| 1:A:1206:ASP:OD1  | 16:U:228:ASN:CG   | 2.59                     | 0.41              |
| 1:A:1286:TYR:CD1  | 16:U:234:GLY:HA2  | 2.54                     | 0.41              |
| 1:A:517:SER:O     | 1:A:518:ASN:CG    | 2.59                     | 0.41              |
| 1:A:945:ARG:HG3   | 1:A:1301:TYR:OH   | 2.20                     | 0.41              |
| 2:B:850:LEU:HG    | 2:B:851:PHE:CD2   | 2.55                     | 0.41              |
| 4:D:141:GLU:HA    | 4:D:144:GLN:HB2   | 2.01                     | 0.41              |
| 16:U:213:ALA:HA   | 16:U:214:PRO:HA   | 1.80                     | 0.41              |
| 1:A:1082:THR:HB   | 16:U:260:LYS:HZ3  | 1.86                     | 0.41              |
| 1:A:1167:GLU:OE1  | 1:A:1196:ARG:NH2  | 2.53                     | 0.41              |
| 1:A:448:GLN:HE22  | 1:A:489:ASN:HD22  | 1.68                     | 0.41              |
| 1:A:870:GLY:HA3   | 1:A:1369:ARG:NH1  | 2.35                     | 0.41              |
| 2:B:1056:SER:OG   | 2:B:1067:ARG:NH1  | 2.53                     | 0.41              |
| 2:B:904:ARG:NH1   | 18:W:781:GLU:CG   | 2.83                     | 0.41              |
| 2:B:266:PRO:HG2   | 2:B:352:GLU:HB3   | 2.03                     | 0.41              |
| 4:D:24:ASN:OD1    | 7:G:84:GLY:HA3    | 2.21                     | 0.41              |
| 7:G:97:ILE:HG12   | 18:W:683:PHE:CD1  | 2.56                     | 0.41              |
| 18:W:749:ASP:HB3  | 18:W:752:LEU:CD1  | 2.51                     | 0.41              |
| 1:A:1021:GLN:HB3  | 1:A:1025:ARG:NH1  | 2.36                     | 0.41              |
| 1:A:831:LYS:CB    | 1:A:1083:LEU:HB2  | 2.48                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:10:PRO:HG2    | 2:B:1192:TYR:HD1  | 1.85                     | 0.41              |
| 1:A:14:VAL:H      | 1:A:1435:GLN:HE22 | 1.68                     | 0.41              |
| 2:B:350:GLN:NE2   | 2:B:359:GLN:O     | 2.54                     | 0.41              |
| 11:K:103:HIS:NE2  | 11:K:107:GLU:OE2  | 2.54                     | 0.41              |
| 13:P:-3:U:H2'     | 13:P:-3:U:O2      | 2.19                     | 0.41              |
| 1:A:1206:ASP:HA   | 16:U:228:ASN:HD22 | 1.86                     | 0.41              |
| 18:W:399:ALA:CB   | 18:W:406:ILE:HD13 | 2.44                     | 0.41              |
| 10:J:35:LEU:HD22  | 10:J:40:LEU:HD12  | 2.02                     | 0.41              |
| 2:B:826:ALA:HB3   | 2:B:1011:ILE:HG12 | 2.03                     | 0.41              |
| 4:D:106:LEU:O     | 4:D:110:ASN:CB    | 2.58                     | 0.41              |
| 2:B:307:LYS:HZ3   | 9:I:13:MET:HE1    | 1.39                     | 0.41              |
| 14:T:-20:DA:N1    | 15:N:21:DT:O2     | 2.53                     | 0.41              |
| 13:P:1:A:C6       | 13:P:2:U:N3       | 2.89                     | 0.41              |
| 16:U:146:SER:O    | 16:U:148:ILE:N    | 2.54                     | 0.41              |
| 18:W:322:ARG:CD   | 18:W:342:GLU:HA   | 2.51                     | 0.41              |
| 18:W:322:ARG:CD   | 18:W:342:GLU:HG3  | 2.51                     | 0.41              |
| 1:A:1458:ALA:HA   | 7:G:20:PRO:CG     | 2.51                     | 0.40              |
| 1:A:262:ASP:OD1   | 1:A:317:GLN:NE2   | 2.45                     | 0.40              |
| 1:A:822:ARG:NH2   | 2:B:517:PRO:O     | 2.54                     | 0.40              |
| 1:A:927:GLN:HG3   | 1:A:931:ASN:HD21  | 1.86                     | 0.40              |
| 2:B:27:GLU:OE2    | 2:B:679:SER:OG    | 2.39                     | 0.40              |
| 2:B:844:SER:HB3   | 2:B:848:ARG:HH12  | 1.86                     | 0.40              |
| 3:C:13:GLN:HE21   | 3:C:16:GLU:CG     | 2.33                     | 0.40              |
| 5:E:152:HIS:CD2   | 5:E:197:ILE:HG12  | 2.57                     | 0.40              |
| 4:D:34:PHE:CE2    | 7:G:3:PHE:CE2     | 3.09                     | 0.40              |
| 11:K:53:TYR:HA    | 11:K:54:PRO:HD3   | 1.95                     | 0.40              |
| 1:A:1134:LYS:CD   | 16:U:229:LEU:HD12 | 2.52                     | 0.40              |
| 3:C:32:LEU:HD21   | 3:C:244:PHE:HE1   | 1.85                     | 0.40              |
| 7:G:86:VAL:HA     | 7:G:146:LYS:HA    | 2.02                     | 0.40              |
| 16:U:146:SER:C    | 16:U:148:ILE:N    | 2.74                     | 0.40              |
| 16:U:186:ASN:OD1  | 16:U:187:ASN:CG   | 2.60                     | 0.40              |
| 18:W:228:GLY:HA3  | 18:W:299:PHE:CZ   | 2.55                     | 0.40              |
| 18:W:409:ASP:C    | 18:W:410:ARG:HG3  | 2.37                     | 0.40              |
| 1:A:498:THR:HG21  | 2:B:1149:GLU:OE1  | 2.21                     | 0.40              |
| 2:B:360:GLU:HG3   | 2:B:363:PHE:CD2   | 2.56                     | 0.40              |
| 5:E:14:SER:O      | 5:E:18:VAL:HG23   | 2.21                     | 0.40              |
| 16:U:194:ILE:HA   | 16:U:198:GLU:OE1  | 2.19                     | 0.40              |
| 18:W:389:PRO:O    | 18:W:389:PRO:CD   | 2.68                     | 0.40              |
| 18:W:664:VAL:O    | 18:W:673:GLN:HA   | 2.21                     | 0.40              |
| 18:W:684:LEU:HD11 | 18:W:699:VAL:CA   | 2.49                     | 0.40              |
| 1:A:1029:ALA:O    | 1:A:1033:ILE:HG13 | 2.21                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1087:HIS:O   | 1:A:1088:TYR:HB2  | 2.22                     | 0.40              |
| 2:B:71:ILE:CG2   | 2:B:71:ILE:O      | 2.69                     | 0.40              |
| 1:A:477:SER:H    | 1:A:478:PRO:HD2   | 1.86                     | 0.40              |
| 8:H:94:TYR:HB3   | 8:H:143:ILE:HB    | 2.03                     | 0.40              |
| 18:W:667:PHE:CD2 | 18:W:668:THR:HG23 | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 1417/1743 (81%) | 1235 (87%) | 169 (12%) | 13 (1%)  | 20          | 63  |
| 2   | B     | 1151/1227 (94%) | 987 (86%)  | 159 (14%) | 5 (0%)   | 38          | 77  |
| 3   | C     | 261/304 (86%)   | 231 (88%)  | 27 (10%)  | 3 (1%)   | 17          | 60  |
| 4   | D     | 162/186 (87%)   | 141 (87%)  | 20 (12%)  | 1 (1%)   | 28          | 70  |
| 5   | E     | 211/214 (99%)   | 190 (90%)  | 19 (9%)   | 2 (1%)   | 20          | 63  |
| 6   | F     | 82/155 (53%)    | 70 (85%)   | 12 (15%)  | 0        | 100         | 100 |
| 7   | G     | 169/171 (99%)   | 150 (89%)  | 19 (11%)  | 0        | 100         | 100 |
| 8   | H     | 129/145 (89%)   | 111 (86%)  | 18 (14%)  | 0        | 100         | 100 |
| 9   | I     | 109/115 (95%)   | 93 (85%)   | 14 (13%)  | 2 (2%)   | 10          | 51  |
| 10  | J     | 64/72 (89%)     | 62 (97%)   | 2 (3%)    | 0        | 100         | 100 |
| 11  | K     | 111/118 (94%)   | 99 (89%)   | 12 (11%)  | 0        | 100         | 100 |
| 12  | L     | 43/72 (60%)     | 37 (86%)   | 6 (14%)   | 0        | 100         | 100 |
| 16  | U     | 149/190 (78%)   | 120 (80%)  | 24 (16%)  | 5 (3%)   | 4           | 39  |
| 17  | V     | 100/108 (93%)   | 97 (97%)   | 3 (3%)    | 0        | 100         | 100 |
| 18  | W     | 317/612 (52%)   | 288 (91%)  | 26 (8%)   | 3 (1%)   | 20          | 63  |
| All | All   | 4475/5432 (82%) | 3911 (87%) | 530 (12%) | 34 (1%)  | 27          | 65  |

All (34) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 47   | ARG  |
| 1   | A     | 48   | PRO  |
| 1   | A     | 743  | ASN  |
| 1   | A     | 1085 | THR  |
| 2   | B     | 62   | ALA  |
| 2   | B     | 337  | ARG  |
| 4   | D     | 169  | VAL  |
| 16  | U     | 185  | LYS  |
| 16  | U     | 186  | ASN  |
| 18  | W     | 318  | VAL  |
| 18  | W     | 320  | LEU  |
| 1   | A     | 975  | LEU  |
| 9   | I     | 88   | SER  |
| 18  | W     | 749  | ASP  |
| 1   | A     | 327  | ARG  |
| 1   | A     | 853  | TYR  |
| 1   | A     | 1084 | ASN  |
| 1   | A     | 1087 | HIS  |
| 2   | B     | 155  | LYS  |
| 3   | C     | 205  | LYS  |
| 5   | E     | 159  | GLU  |
| 16  | U     | 147  | LYS  |
| 1   | A     | 287  | GLN  |
| 2   | B     | 500  | LYS  |
| 9   | I     | 52   | ILE  |
| 1   | A     | 283  | ASP  |
| 1   | A     | 960  | VAL  |
| 3   | C     | 172  | PRO  |
| 5   | E     | 123  | ILE  |
| 16  | U     | 239  | ASN  |
| 1   | A     | 916  | TYR  |
| 2   | B     | 555  | GLY  |
| 16  | U     | 213  | ALA  |
| 3   | C     | 182  | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | A     | 1238/1528 (81%) | 1222 (99%) | 16 (1%)  | 73          | 88  |
| 2   | B     | 1016/1077 (94%) | 1008 (99%) | 8 (1%)   | 85          | 93  |
| 3   | C     | 236/264 (89%)   | 235 (100%) | 1 (0%)   | 93          | 96  |
| 4   | D     | 143/160 (89%)   | 142 (99%)  | 1 (1%)   | 87          | 94  |
| 5   | E     | 196/197 (100%)  | 193 (98%)  | 3 (2%)   | 70          | 87  |
| 6   | F     | 75/137 (55%)    | 75 (100%)  | 0        | 100         | 100 |
| 7   | G     | 148/148 (100%)  | 145 (98%)  | 3 (2%)   | 60          | 83  |
| 8   | H     | 120/130 (92%)   | 120 (100%) | 0        | 100         | 100 |
| 9   | I     | 106/109 (97%)   | 103 (97%)  | 3 (3%)   | 49          | 76  |
| 10  | J     | 60/66 (91%)     | 60 (100%)  | 0        | 100         | 100 |
| 11  | K     | 104/109 (95%)   | 104 (100%) | 0        | 100         | 100 |
| 12  | L     | 38/56 (68%)     | 37 (97%)   | 1 (3%)   | 51          | 78  |
| 16  | U     | 139/171 (81%)   | 127 (91%)  | 12 (9%)  | 12          | 47  |
| 17  | V     | 86/92 (94%)     | 85 (99%)   | 1 (1%)   | 75          | 88  |
| 18  | W     | 290/548 (53%)   | 279 (96%)  | 11 (4%)  | 38          | 70  |
| All | All   | 3995/4792 (83%) | 3935 (98%) | 60 (2%)  | 72          | 87  |

All (60) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 43   | GLU  |
| 1   | A     | 44   | SER  |
| 1   | A     | 45   | ARG  |
| 1   | A     | 446  | ASN  |
| 1   | A     | 518  | ASN  |
| 1   | A     | 661  | ASN  |
| 1   | A     | 688  | LYS  |
| 1   | A     | 690  | GLN  |
| 1   | A     | 721  | ARG  |
| 1   | A     | 735  | GLU  |
| 1   | A     | 737  | ASN  |
| 1   | A     | 977  | ARG  |
| 1   | A     | 1081 | MET  |
| 1   | A     | 1083 | LEU  |
| 1   | A     | 1087 | HIS  |
| 1   | A     | 1095 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 70   | ASN  |
| 2   | B     | 71   | ILE  |
| 2   | B     | 240  | ARG  |
| 2   | B     | 336  | ILE  |
| 2   | B     | 500  | LYS  |
| 2   | B     | 725  | ARG  |
| 2   | B     | 1094 | ARG  |
| 2   | B     | 1122 | ARG  |
| 3   | C     | 8    | ASN  |
| 4   | D     | 11   | ARG  |
| 5   | E     | 4    | ASN  |
| 5   | E     | 120  | ASN  |
| 5   | E     | 166  | ARG  |
| 7   | G     | 106  | LEU  |
| 7   | G     | 125  | ASN  |
| 7   | G     | 151  | ARG  |
| 9   | I     | 26   | LEU  |
| 9   | I     | 49   | ILE  |
| 9   | I     | 61   | ASP  |
| 12  | L     | 62   | ARG  |
| 16  | U     | 126  | ARG  |
| 16  | U     | 147  | LYS  |
| 16  | U     | 148  | ILE  |
| 16  | U     | 186  | ASN  |
| 16  | U     | 192  | ARG  |
| 16  | U     | 194  | ILE  |
| 16  | U     | 195  | LEU  |
| 16  | U     | 204  | LEU  |
| 16  | U     | 206  | THR  |
| 16  | U     | 212  | LEU  |
| 16  | U     | 264  | SER  |
| 16  | U     | 284  | PHE  |
| 17  | V     | 33   | ASP  |
| 18  | W     | 264  | GLN  |
| 18  | W     | 313  | VAL  |
| 18  | W     | 666  | GLU  |
| 18  | W     | 672  | ARG  |
| 18  | W     | 683  | PHE  |
| 18  | W     | 685  | PHE  |
| 18  | W     | 777  | ARG  |
| 18  | W     | 784  | ASN  |
| 18  | W     | 793  | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | W     | 802 | HIS  |
| 18  | W     | 809 | ASP  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 3    | GLN  |
| 1   | A     | 170  | ASN  |
| 1   | A     | 214  | HIS  |
| 1   | A     | 359  | ASN  |
| 1   | A     | 446  | ASN  |
| 1   | A     | 448  | GLN  |
| 1   | A     | 489  | ASN  |
| 1   | A     | 661  | ASN  |
| 1   | A     | 699  | GLN  |
| 1   | A     | 768  | GLN  |
| 1   | A     | 787  | HIS  |
| 1   | A     | 927  | GLN  |
| 1   | A     | 931  | ASN  |
| 1   | A     | 961  | ASN  |
| 1   | A     | 968  | ASN  |
| 1   | A     | 1137 | GLN  |
| 1   | A     | 1190 | GLN  |
| 1   | A     | 1435 | GLN  |
| 2   | B     | 63   | GLN  |
| 2   | B     | 97   | HIS  |
| 2   | B     | 102  | GLN  |
| 2   | B     | 206  | GLN  |
| 2   | B     | 426  | GLN  |
| 2   | B     | 651  | HIS  |
| 2   | B     | 657  | GLN  |
| 2   | B     | 794  | ASN  |
| 2   | B     | 1093 | GLN  |
| 3   | C     | 8    | ASN  |
| 3   | C     | 13   | GLN  |
| 3   | C     | 150  | HIS  |
| 4   | D     | 17   | GLN  |
| 4   | D     | 38   | GLN  |
| 4   | D     | 46   | HIS  |
| 4   | D     | 99   | ASN  |
| 5   | E     | 4    | ASN  |
| 5   | E     | 100  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 120 | ASN  |
| 5   | E     | 145 | HIS  |
| 7   | G     | 125 | ASN  |
| 8   | H     | 44  | ASN  |
| 9   | I     | 87  | GLN  |
| 16  | U     | 181 | ASN  |
| 16  | U     | 184 | ASN  |
| 16  | U     | 187 | ASN  |
| 18  | W     | 339 | GLN  |
| 18  | W     | 402 | HIS  |
| 18  | W     | 434 | ASN  |
| 18  | W     | 441 | ASN  |
| 18  | W     | 678 | HIS  |
| 18  | W     | 682 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 13  | P     | 15/30 (50%) | 7 (46%)           | 1 (6%)          |

All (7) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | P     | -4  | C    |
| 13  | P     | -3  | U    |
| 13  | P     | -2  | U    |
| 13  | P     | 0   | U    |
| 13  | P     | 1   | A    |
| 13  | P     | 2   | U    |
| 13  | P     | 10  | U    |

All (1) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | P     | -1  | U    |

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.