



## Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 10:42 AM UTC

PDB ID : 6AWC / pdb\_00006awc  
EMDB ID : EMD-7015  
Title : Structure of 30S ribosomal subunit and RNA polymerase complex in rotated state  
Authors : Demo, G.; Rasouly, A.; Vasilyev, N.; Loveland, A.B.; Diaz-Avalos, R.; Grigorieff, N.; Nudler, E.; Korostelev, A.A.  
Deposited on : 2017-09-05  
Resolution : 7.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

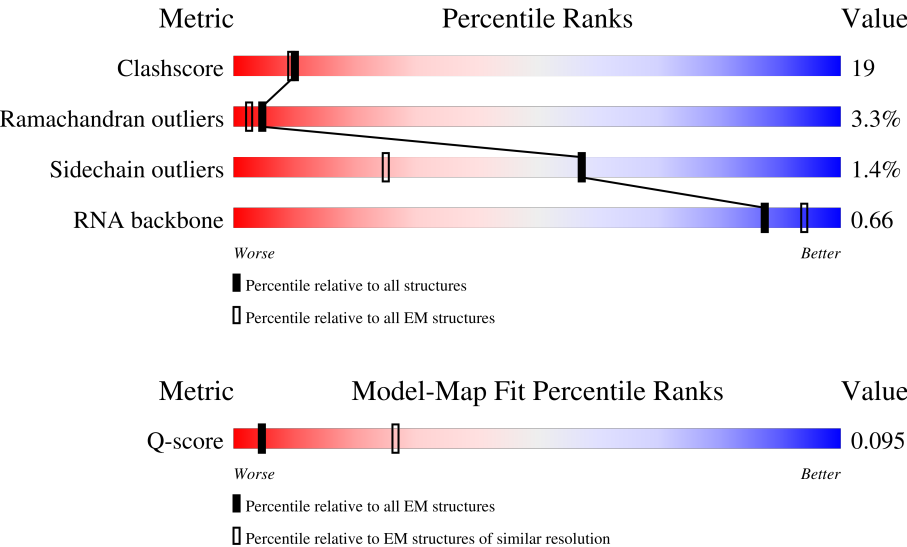
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 7.90 Å.

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



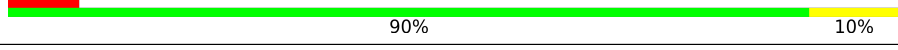
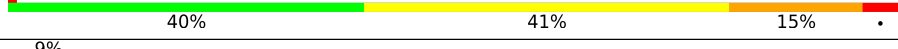
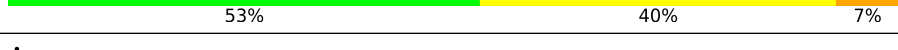
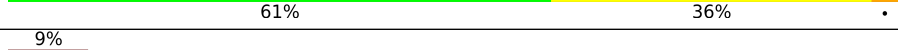
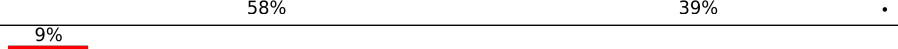
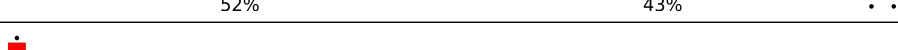
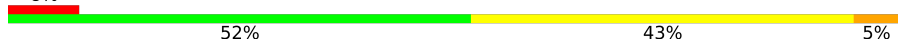
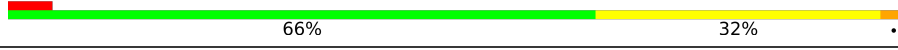
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 366 ( 7.40 - 8.40 )                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1539   |                  |
| 2   | 01    | 229    |                  |
| 2   | 02    | 229    |                  |

Continued on next page...

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 3   | 03    | 1340   |    |
| 4   | 04    | 1369   |    |
| 5   | 05    | 59     |    |
| 6   | B     | 153    |    |
| 7   | E     | 218    |    |
| 8   | F     | 206    |    |
| 9   | G     | 205    |    |
| 10  | H     | 157    |    |
| 11  | I     | 100    |    |
| 12  | J     | 151    |    |
| 13  | K     | 129    |    |
| 14  | L     | 127    |  |
| 15  | M     | 98     |  |
| 16  | N     | 116    |  |
| 17  | O     | 123    |  |
| 18  | P     | 114    |  |
| 19  | Q     | 100    |  |
| 20  | R     | 88     |  |
| 21  | S     | 82     |  |
| 22  | T     | 80     |  |
| 23  | U     | 65     |  |
| 24  | V     | 79     |  |
| 25  | W     | 85     |  |
| 26  | X     | 65     |  |

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 75169 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 RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | A     | 1443     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 30955 | 13808 | 5681 | 10024 | 1442 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | 01    | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1753  | 1091 | 311 | 345 | 6 |         |       |
| 2   | 02    | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1757  | 1094 | 311 | 346 | 6 |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 3   | 03    | 1327     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10272 | 6441 | 1787 | 2001 | 43 |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta'.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 4   | 04    | 1345     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10372 | 6508 | 1853 | 1962 | 49 |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | 05    | 59       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 458   | 283 | 86 | 88 | 1 |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S1.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 6   | B     | 153      | Total | C   | N   | O   |         |       |
|     |       |          | 774   | 463 | 154 | 157 | 0       | 0     |

- Molecule 7 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | E     | 218      | Total | C    | N   | O   | S |         |       |
|     |       |          | 1705  | 1081 | 305 | 312 | 7 | 0       | 0     |

- Molecule 8 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | F     | 206      | Total | C    | N   | O   | S |         |       |
|     |       |          | 1625  | 1028 | 305 | 289 | 3 | 0       | 0     |

- Molecule 9 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | G     | 205      | Total | C    | N   | O   | S |         |       |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 | 0       | 0     |

- Molecule 10 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | H     | 157      | Total | C   | N   | O   | S |         |       |
|     |       |          | 1157  | 719 | 218 | 214 | 6 | 0       | 0     |

- Molecule 11 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | I     | 100      | Total | C   | N   | O   | S |         |       |
|     |       |          | 818   | 515 | 148 | 149 | 6 | 0       | 0     |

- Molecule 12 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | J     | 151      | Total | C   | N   | O   | S |         |       |
|     |       |          | 1182  | 735 | 227 | 216 | 4 | 0       | 0     |

- Molecule 13 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | K     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | L     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | M     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 787   | 493 | 150 | 143 | 1 |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | N     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 870   | 535 | 173 | 159 | 3 |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | O     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | P     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 884   | 546 | 178 | 157 | 3 |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | Q     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | R     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |       |

- Molecule 21 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | S     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |       |

- Molecule 22 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | T     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 411 | 121 | 114 | 3 |         |       |

- Molecule 23 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 23  | U     | 65       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 536   | 339 | 100 | 96 | 1 |         |       |

- Molecule 24 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | V     | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 638   | 408 | 120 | 108 | 2 |         |       |

- Molecule 25 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | W     | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |       |

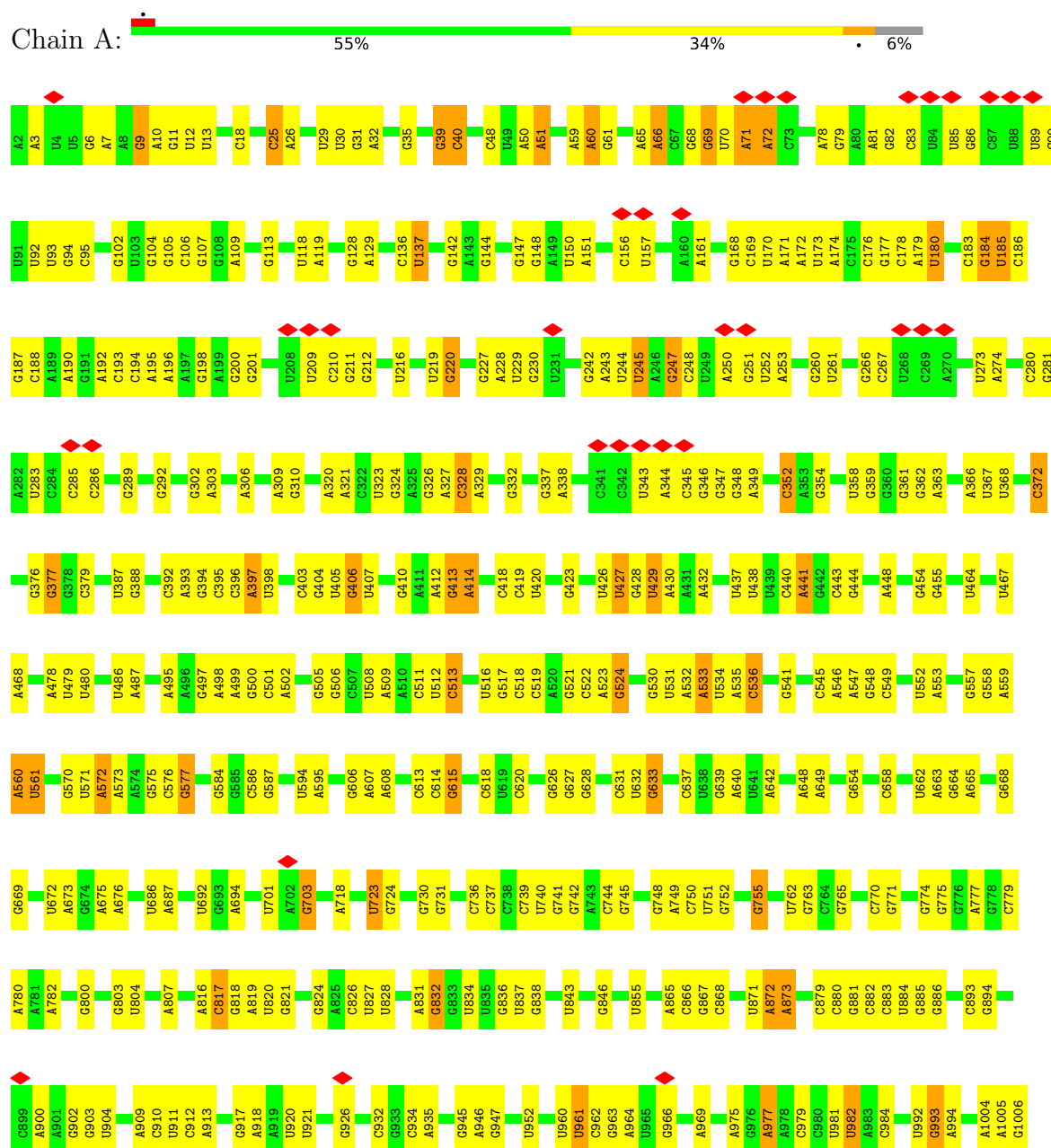
- Molecule 26 is a protein called 30S ribosomal protein S21.

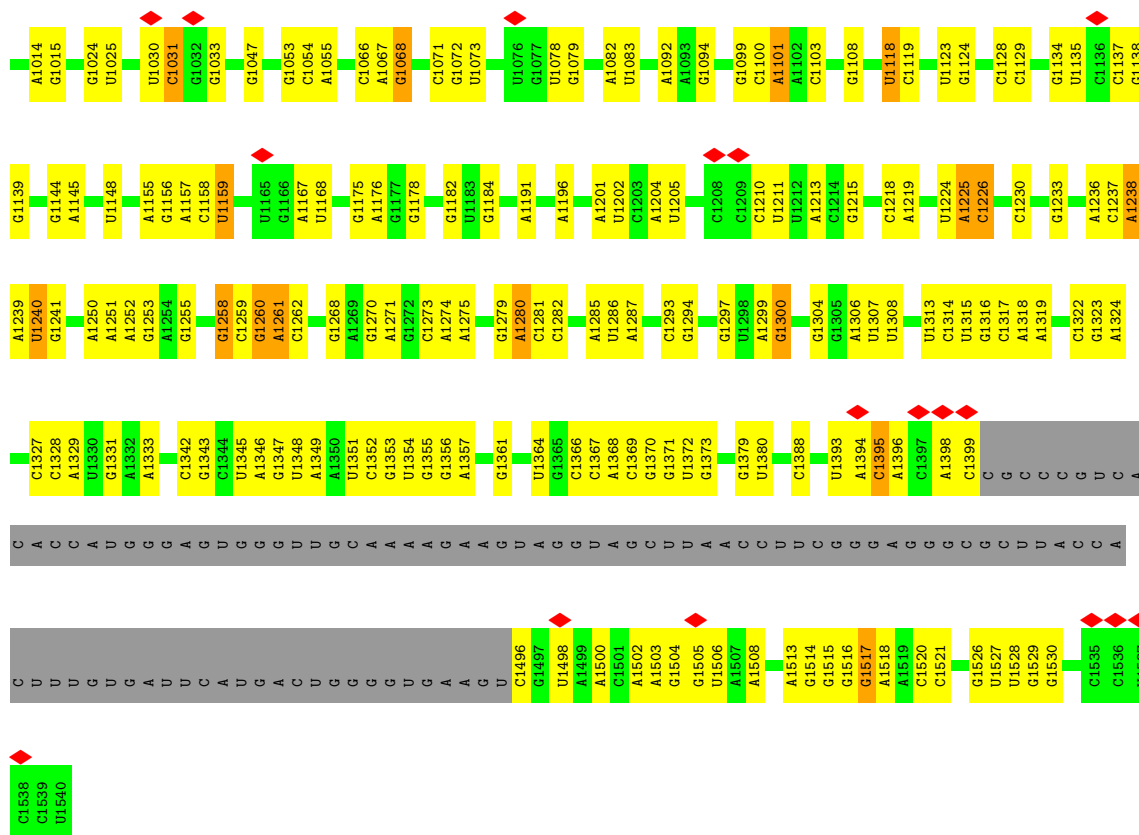
| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 26  | X     | 65       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 545   | 335 | 117 | 92 | 1 |         |       |

### 3 Residue-property plots

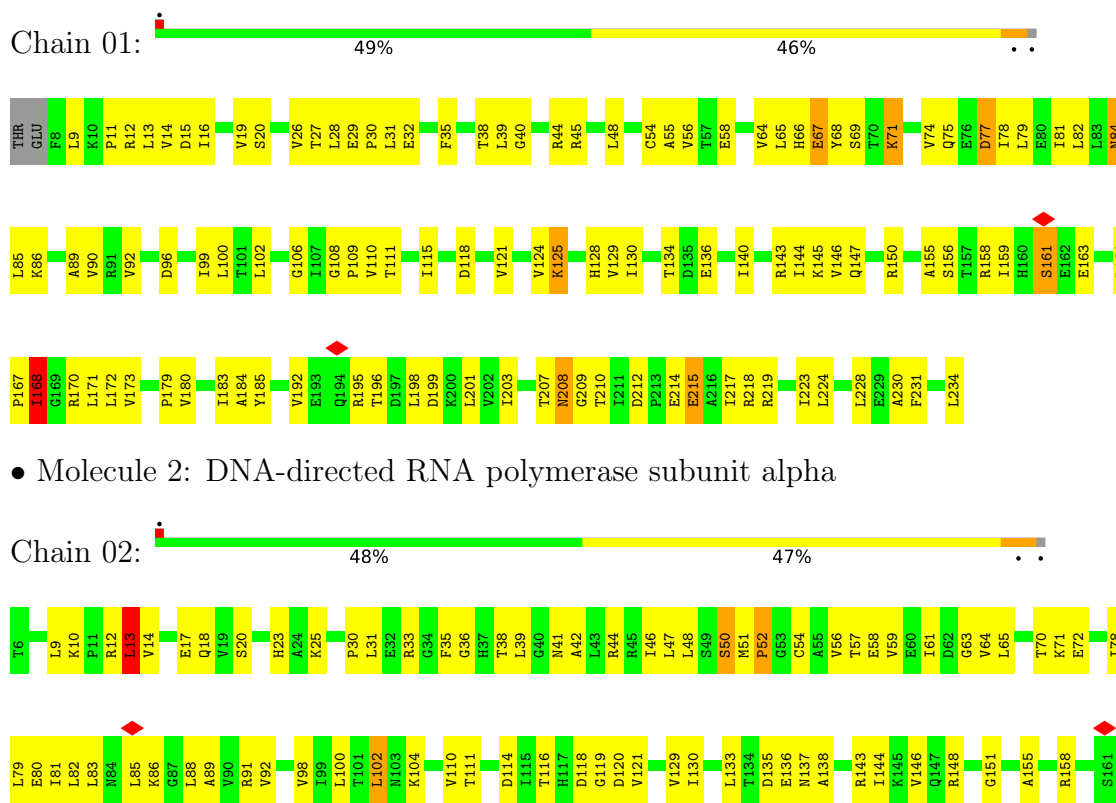
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: 16S rRNA

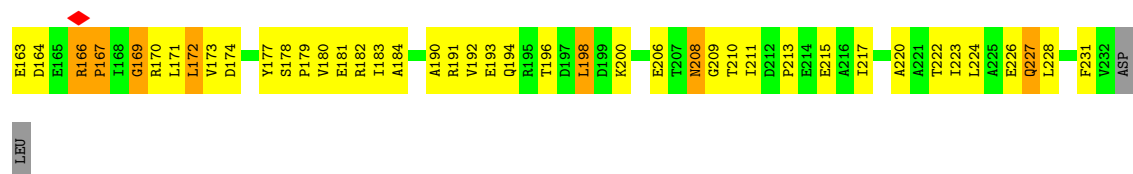




- Molecule 2: DNA-directed RNA polymerase subunit alpha

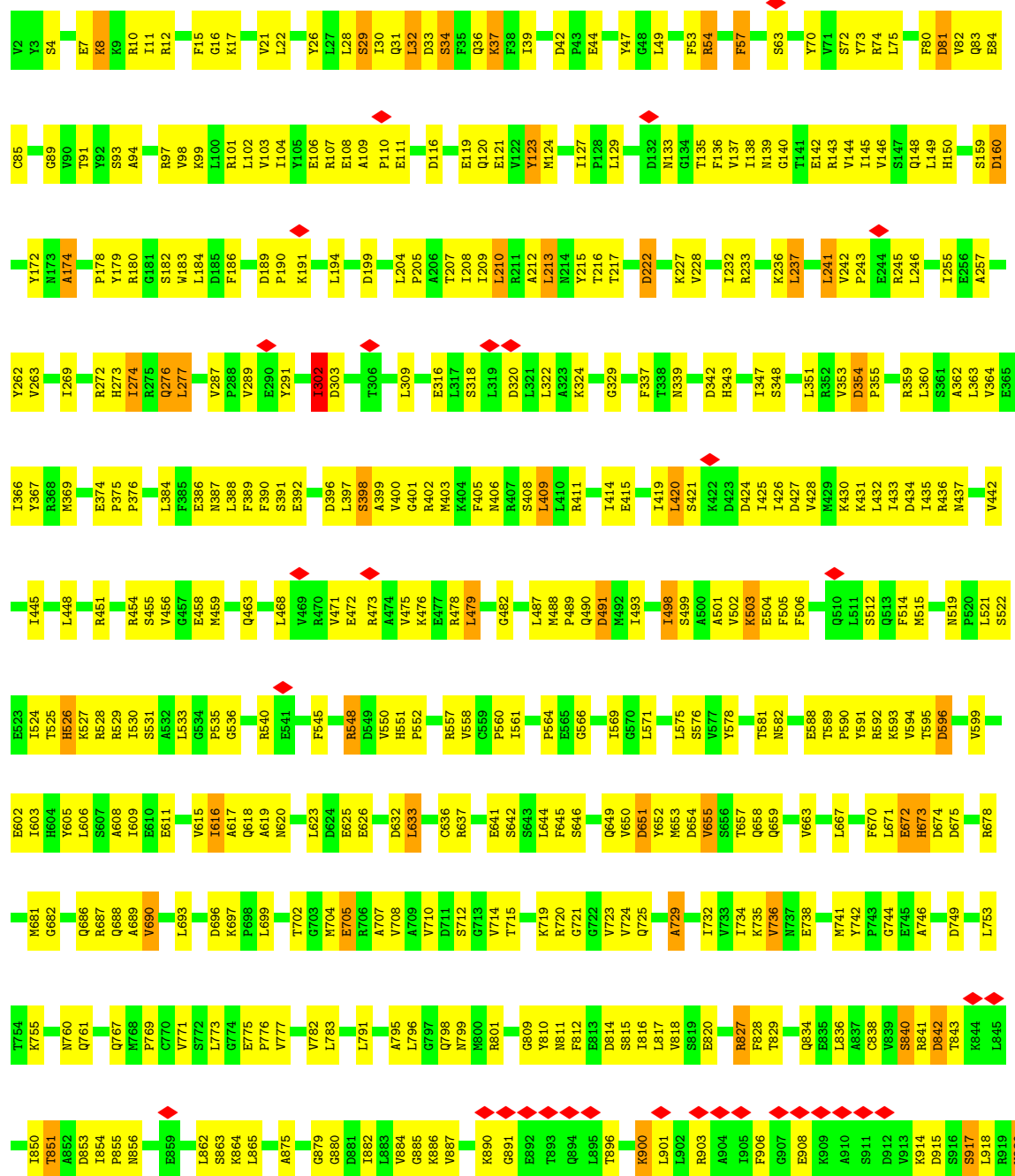


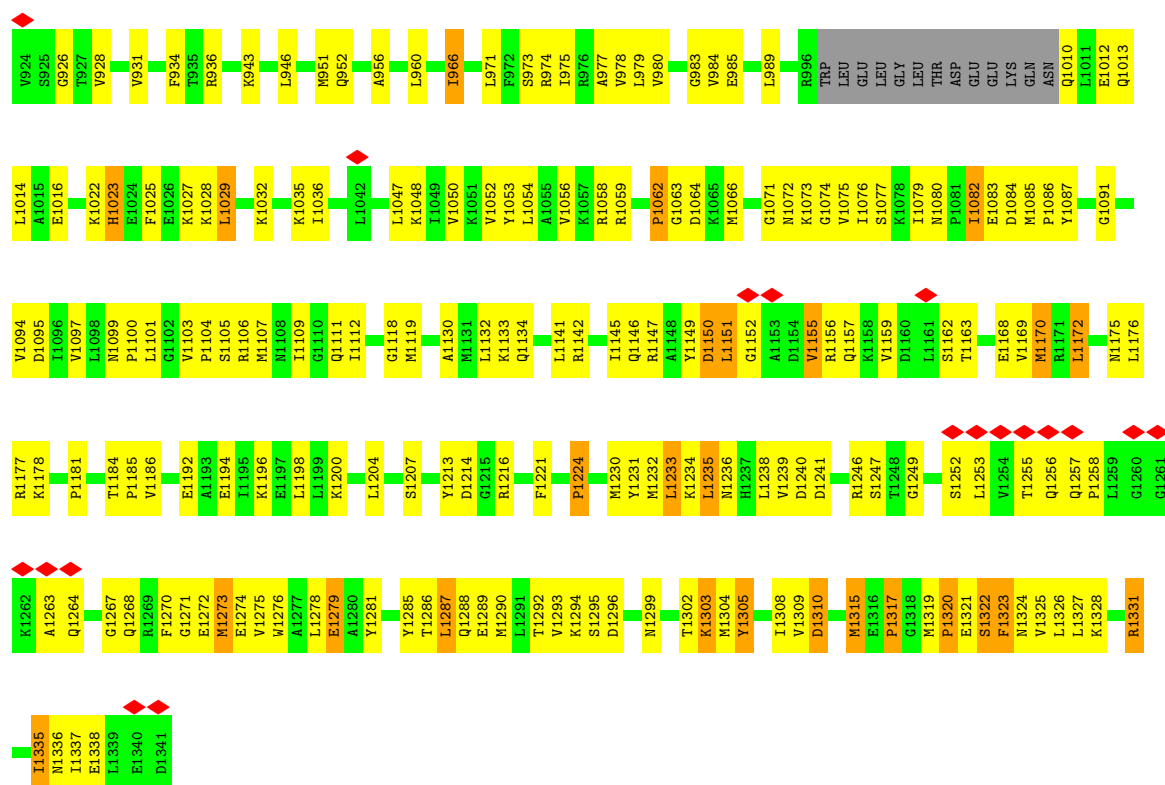
- Molecule 2: DNA-directed RNA polymerase subunit alpha



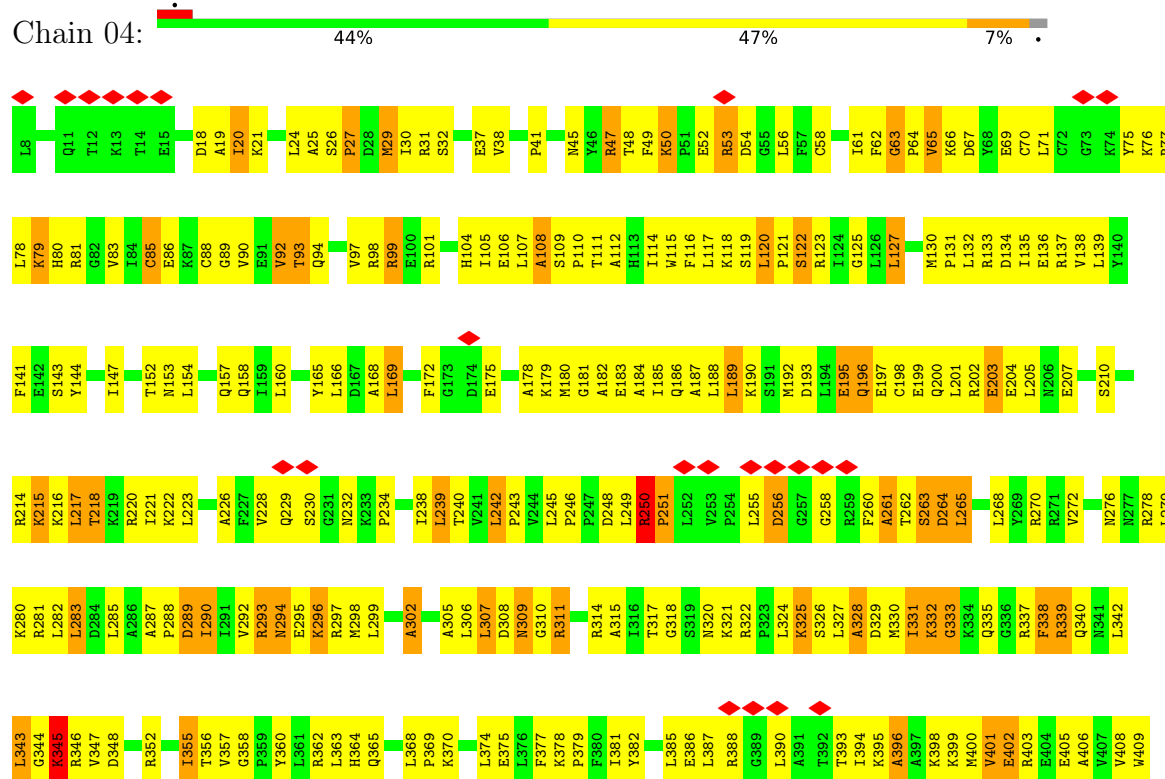
• Molecule 3: DNA-directed RNA polymerase subunit beta

Chain 03: 52% 41% 5%

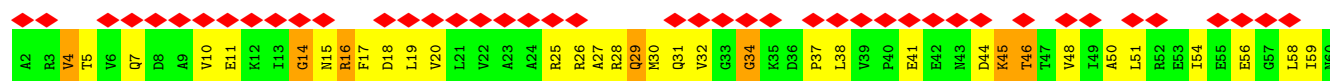




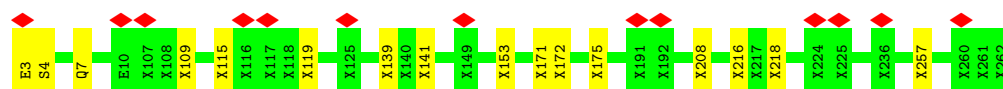
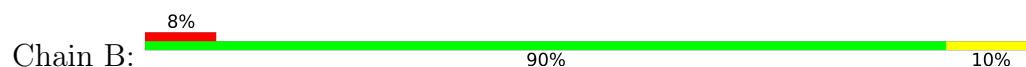
• Molecule 4: DNA-directed RNA polymerase subunit beta'



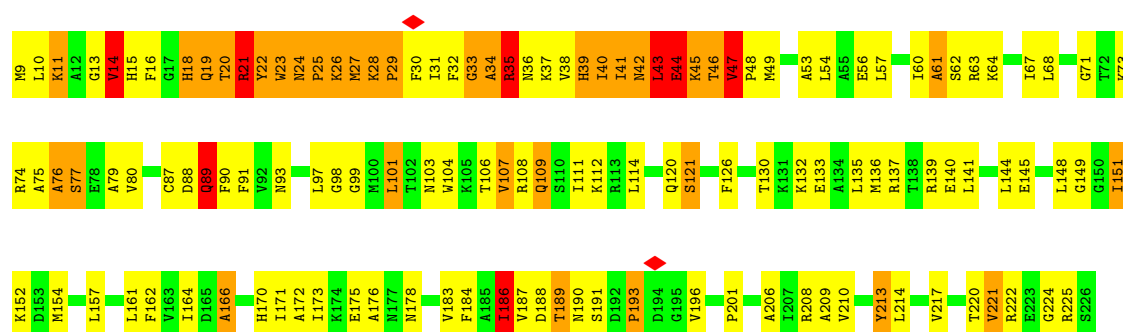




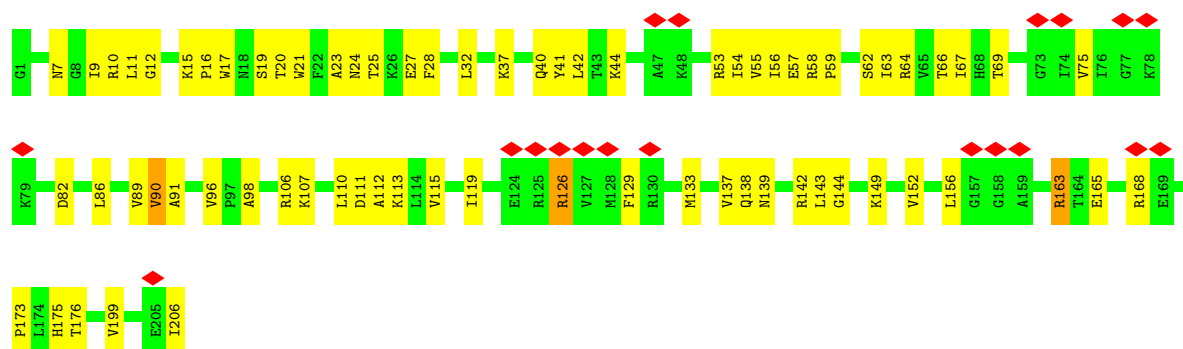
• Molecule 6: 30S ribosomal protein S1



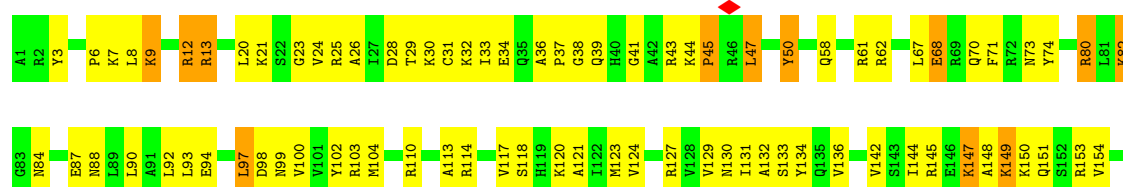
• Molecule 7: 30S ribosomal protein S2



• Molecule 8: 30S ribosomal protein S3

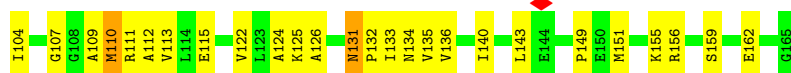
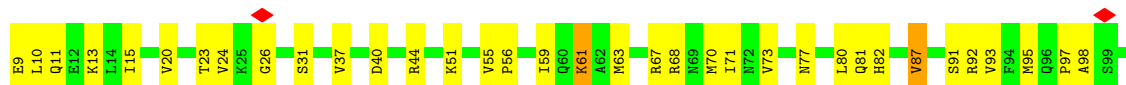


• Molecule 9: 30S ribosomal protein S4

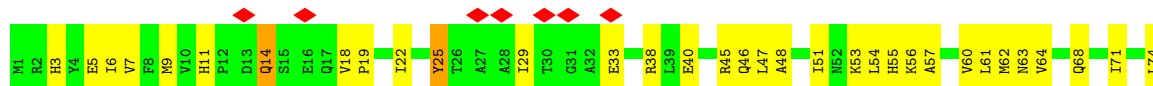




- Molecule 10: 30S ribosomal protein S5



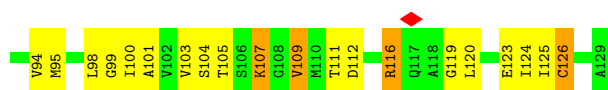
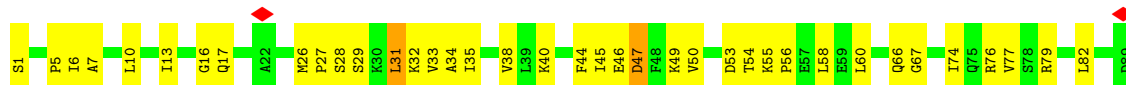
- Molecule 11: 30S ribosomal protein S6



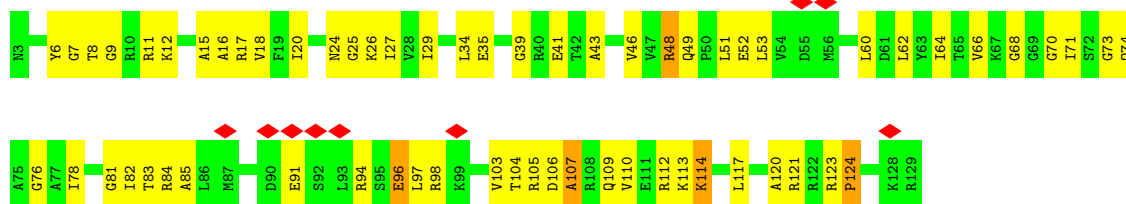
- Molecule 12: 30S ribosomal protein S7



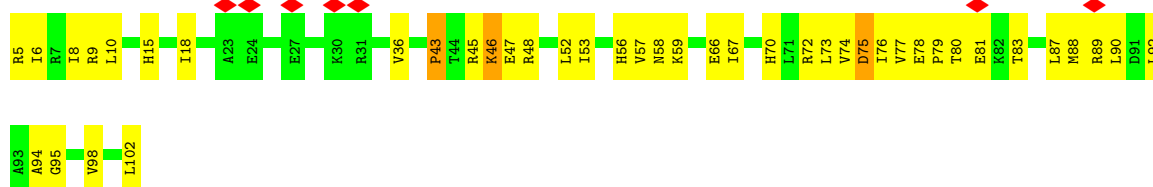
- Molecule 13: 30S ribosomal protein S8



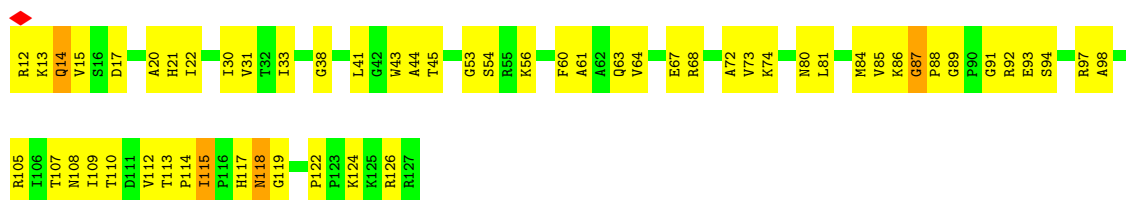
- Molecule 14: 30S ribosomal protein S9



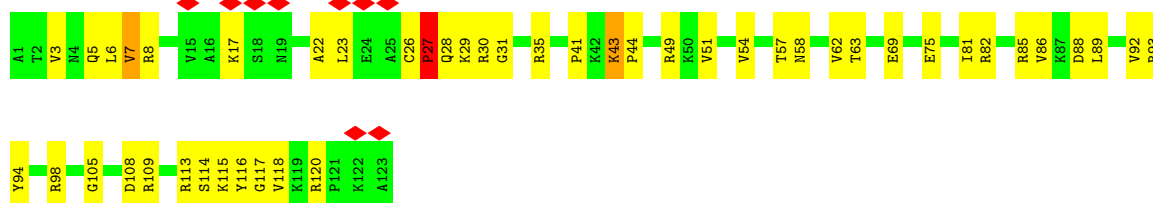
- Molecule 15: 30S ribosomal protein S10



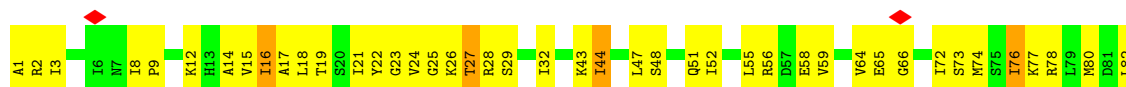
- Molecule 16: 30S ribosomal protein S11

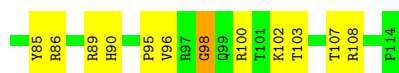


- Molecule 17: 30S ribosomal protein S12

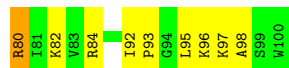


- Molecule 18: 30S ribosomal protein S13

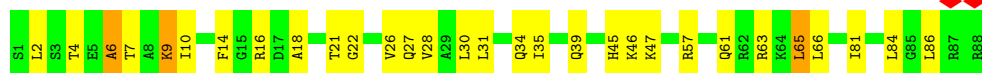




- Molecule 19: 30S ribosomal protein S14



- Molecule 20: 30S ribosomal protein S15



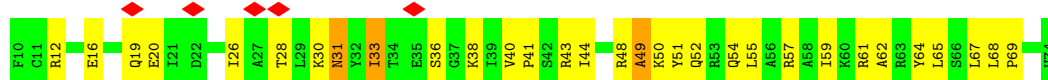
- Molecule 21: 30S ribosomal protein S16



- Molecule 22: 30S ribosomal protein S17

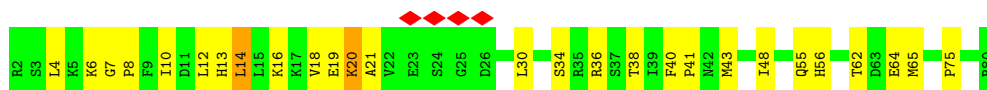


- Molecule 23: 30S ribosomal protein S18

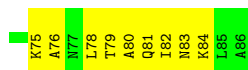
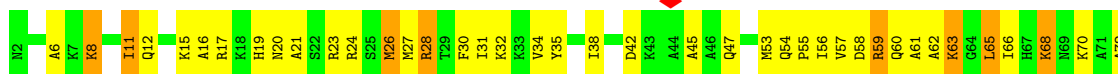


- Molecule 24: 30S ribosomal protein S19

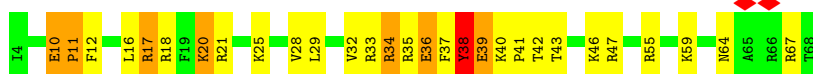




- Molecule 25: 30S ribosomal protein S20



- Molecule 26: 30S ribosomal protein S21



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 10090                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40.0                                    | Depositor |
| Minimum defocus (nm)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | 25000                                   | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 9.739                                   | Depositor |
| Minimum map value                    | -3.633                                  | Depositor |
| Average map value                    | -0.011                                  | Depositor |
| Map value standard deviation         | 0.655                                   | Depositor |
| Recommended contour level            | 2                                       | Depositor |
| Map size (Å)                         | 459.98398, 459.98398, 459.98398         | wwPDB     |
| Map dimensions                       | 280, 280, 280                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.6428, 1.6428, 1.6428                  | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |             | Bond angles |                   |
|-----|-------|--------------|-------------|-------------|-------------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$       |
| 1   | A     | 0.39         | 0/34660     | 0.51        | 3/54067 (0.0%)    |
| 2   | 01    | 0.31         | 0/1774      | 1.01        | 14/2405 (0.6%)    |
| 2   | 02    | 0.37         | 0/1779      | 1.07        | 12/2411 (0.5%)    |
| 3   | 03    | 0.33         | 0/10433     | 1.14        | 106/14101 (0.8%)  |
| 4   | 04    | 0.34         | 0/10528     | 1.15        | 117/14224 (0.8%)  |
| 5   | 05    | 0.33         | 0/460       | 1.26        | 8/620 (1.3%)      |
| 6   | B     | 0.34         | 0/65        | 0.87        | 0/86              |
| 7   | E     | 0.44         | 0/1736      | 1.44        | 33/2338 (1.4%)    |
| 8   | F     | 0.31         | 0/1652      | 1.01        | 5/2225 (0.2%)     |
| 9   | G     | 0.29         | 0/1665      | 1.01        | 9/2227 (0.4%)     |
| 10  | H     | 0.32         | 0/1170      | 0.92        | 3/1573 (0.2%)     |
| 11  | I     | 0.32         | 0/836       | 1.04        | 6/1128 (0.5%)     |
| 12  | J     | 0.32         | 0/1196      | 1.08        | 15/1602 (0.9%)    |
| 13  | K     | 0.36         | 0/989       | 1.12        | 13/1326 (1.0%)    |
| 14  | L     | 0.28         | 0/1034      | 0.92        | 3/1375 (0.2%)     |
| 15  | M     | 0.33         | 0/797       | 0.93        | 2/1077 (0.2%)     |
| 16  | N     | 0.33         | 0/886       | 1.14        | 10/1195 (0.8%)    |
| 17  | O     | 0.35         | 0/969       | 1.07        | 7/1300 (0.5%)     |
| 18  | P     | 0.32         | 0/893       | 0.98        | 4/1193 (0.3%)     |
| 19  | Q     | 0.30         | 0/817       | 1.00        | 7/1088 (0.6%)     |
| 20  | R     | 0.30         | 0/722       | 1.07        | 6/964 (0.6%)      |
| 21  | S     | 0.34         | 0/659       | 0.95        | 3/884 (0.3%)      |
| 22  | T     | 0.31         | 0/658       | 0.97        | 2/881 (0.2%)      |
| 23  | U     | 0.38         | 0/545       | 1.14        | 4/731 (0.5%)      |
| 24  | V     | 0.34         | 0/653       | 1.09        | 7/877 (0.8%)      |
| 25  | W     | 0.34         | 0/671       | 1.11        | 8/888 (0.9%)      |
| 26  | X     | 0.45         | 0/551       | 1.04        | 4/728 (0.5%)      |
| All | All   | 0.36         | 0/78798     | 0.87        | 411/113514 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 3                   |
| 7   | E     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

There are no bond length outliers.

All (411) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 7   | E     | 26   | LYS  | N-CA-C | -23.23 | 86.05       | 111.14   |
| 7   | E     | 109  | GLN  | N-CA-C | -11.96 | 98.23       | 111.14   |
| 17  | O     | 114  | SER  | N-CA-C | -11.39 | 98.55       | 110.97   |
| 7   | E     | 23   | TRP  | N-CA-C | -10.78 | 100.26      | 113.41   |
| 3   | 03    | 374  | GLU  | CA-C-N | 10.68  | 131.38      | 120.38   |
| 3   | 03    | 374  | GLU  | C-N-CA | 10.68  | 131.38      | 120.38   |
| 5   | 05    | 14   | GLY  | N-CA-C | 10.59  | 126.15      | 114.40   |
| 12  | J     | 5    | VAL  | N-CA-C | -10.54 | 103.20      | 113.53   |
| 4   | 04    | 309  | ASN  | N-CA-C | -10.51 | 99.75       | 112.58   |
| 25  | W     | 63   | LYS  | N-CA-C | -10.25 | 99.88       | 114.12   |
| 7   | E     | 24   | ASN  | CA-C-N | 10.21  | 132.60      | 119.84   |
| 7   | E     | 24   | ASN  | C-N-CA | 10.21  | 132.60      | 119.84   |
| 4   | 04    | 329  | ASP  | N-CA-C | -10.16 | 102.20      | 112.97   |
| 4   | 04    | 328  | ALA  | N-CA-C | -9.91  | 99.50       | 111.69   |
| 7   | E     | 41   | ILE  | N-CA-C | 9.80   | 122.12      | 107.51   |
| 16  | N     | 115  | ILE  | N-CA-C | 9.79   | 118.07      | 107.60   |
| 24  | V     | 7    | GLY  | CA-C-N | 9.72   | 132.00      | 119.84   |
| 24  | V     | 7    | GLY  | C-N-CA | 9.72   | 132.00      | 119.84   |
| 20  | R     | 6    | ALA  | N-CA-C | -9.70  | 101.32      | 113.55   |
| 4   | 04    | 347  | VAL  | N-CA-C | 9.56   | 121.83      | 109.30   |
| 3   | 03    | 1150 | ASP  | N-CA-C | -9.45  | 101.76      | 113.38   |
| 19  | Q     | 39   | ASP  | N-CA-C | -9.15  | 102.26      | 113.97   |
| 4   | 04    | 511  | TYR  | N-CA-C | -8.99  | 100.91      | 112.23   |
| 4   | 04    | 50   | LYS  | CA-C-N | 8.97   | 131.06      | 119.84   |
| 4   | 04    | 50   | LYS  | C-N-CA | 8.97   | 131.06      | 119.84   |
| 3   | 03    | 375  | PRO  | N-CA-C | 8.93   | 121.60      | 110.70   |
| 4   | 04    | 904  | ALA  | N-CA-C | -8.93  | 100.98      | 112.23   |
| 4   | 04    | 338  | PHE  | N-CA-C | 8.81   | 122.77      | 112.72   |
| 3   | 03    | 133  | ASN  | N-CA-C | -8.81  | 104.58      | 114.62   |
| 3   | 03    | 1147 | ARG  | N-CA-C | -8.79  | 101.78      | 111.36   |
| 3   | 03    | 34   | SER  | N-CA-C | -8.73  | 101.23      | 112.23   |
| 4   | 04    | 339  | ARG  | N-CA-C | -8.69  | 93.70       | 110.56   |
| 13  | K     | 28   | SER  | N-CA-C | 8.69   | 124.01      | 109.76   |
| 8   | F     | 106  | ARG  | N-CA-C | 8.68   | 120.74      | 111.28   |
| 4   | 04    | 987  | GLU  | N-CA-C | -8.66  | 102.15      | 112.89   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4   | 04    | 228  | VAL  | N-CA-C | -8.62 | 102.02      | 110.72   |
| 7   | E     | 166  | ALA  | N-CA-C | -8.55 | 102.84      | 113.28   |
| 2   | 02    | 36   | GLY  | N-CA-C | -8.50 | 104.19      | 115.32   |
| 3   | 03    | 478  | ARG  | N-CA-C | -8.44 | 102.98      | 113.28   |
| 17  | O     | 43   | LYS  | N-CA-C | 8.27  | 124.68      | 113.77   |
| 2   | 01    | 208  | ASN  | N-CA-C | -8.27 | 101.82      | 112.23   |
| 3   | 03    | 274  | ILE  | N-CA-C | -8.26 | 102.38      | 110.72   |
| 4   | 04    | 283  | LEU  | N-CA-C | -8.25 | 103.16      | 113.55   |
| 3   | 03    | 316  | GLU  | N-CA-C | 8.18  | 121.15      | 110.43   |
| 13  | K     | 116  | ARG  | N-CA-C | -8.17 | 102.34      | 111.82   |
| 4   | 04    | 196  | GLN  | N-CA-C | -7.95 | 102.69      | 111.36   |
| 4   | 04    | 326  | SER  | N-CA-C | 7.93  | 122.03      | 107.99   |
| 3   | 03    | 1029 | LEU  | N-CA-C | -7.90 | 102.61      | 111.14   |
| 7   | E     | 46   | THR  | N-CA-C | -7.87 | 102.29      | 111.03   |
| 7   | E     | 93   | ASN  | N-CA-C | -7.84 | 103.84      | 113.41   |
| 4   | 04    | 99   | ARG  | N-CA-C | -7.84 | 102.79      | 113.30   |
| 21  | S     | 57   | ILE  | N-CA-C | -7.82 | 103.07      | 110.42   |
| 7   | E     | 178  | ASN  | N-CA-C | -7.76 | 103.63      | 113.72   |
| 3   | 03    | 81   | ASP  | N-CA-C | -7.76 | 98.46       | 110.17   |
| 3   | 03    | 1156 | ARG  | N-CA-C | 7.76  | 118.22      | 108.45   |
| 25  | W     | 21   | ALA  | N-CA-C | -7.72 | 103.32      | 112.89   |
| 4   | 04    | 632  | ALA  | N-CA-C | -7.71 | 102.95      | 111.36   |
| 4   | 04    | 215  | LYS  | N-CA-C | -7.69 | 102.23      | 111.69   |
| 3   | 03    | 1331 | ARG  | N-CA-C | -7.67 | 103.38      | 112.89   |
| 3   | 03    | 651  | ASP  | N-CA-C | -7.64 | 101.18      | 111.96   |
| 4   | 04    | 682  | VAL  | N-CA-C | -7.64 | 103.08      | 110.42   |
| 3   | 03    | 32   | LEU  | N-CA-C | 7.62  | 119.22      | 111.07   |
| 4   | 04    | 1090 | ILE  | N-CA-C | 7.61  | 116.40      | 108.95   |
| 5   | 05    | 34   | GLY  | N-CA-C | -7.57 | 103.64      | 112.73   |
| 4   | 04    | 387  | LEU  | N-CA-C | -7.57 | 102.99      | 112.90   |
| 7   | E     | 79   | ALA  | N-CA-C | -7.55 | 103.53      | 112.89   |
| 4   | 04    | 250  | ARG  | CA-C-N | 7.53  | 129.25      | 119.84   |
| 4   | 04    | 250  | ARG  | C-N-CA | 7.53  | 129.25      | 119.84   |
| 4   | 04    | 1010 | GLN  | N-CA-C | 7.51  | 121.13      | 110.23   |
| 4   | 04    | 533  | ALA  | N-CA-C | -7.45 | 103.24      | 111.36   |
| 3   | 03    | 843  | THR  | N-CA-C | -7.41 | 98.66       | 110.14   |
| 3   | 03    | 1162 | SER  | N-CA-C | -7.39 | 103.26      | 112.72   |
| 3   | 03    | 1247 | SER  | N-CA-C | -7.39 | 102.85      | 112.68   |
| 4   | 04    | 1146 | GLU  | N-CA-C | -7.38 | 102.54      | 113.61   |
| 9   | G     | 50   | TYR  | N-CA-C | -7.37 | 102.63      | 111.69   |
| 3   | 03    | 827  | ARG  | N-CA-C | -7.34 | 104.30      | 113.18   |
| 7   | E     | 34   | ALA  | N-CA-C | -7.32 | 97.31       | 109.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | 02    | 119  | GLY  | N-CA-C      | -7.31 | 105.32      | 114.16   |
| 3   | 03    | 1303 | LYS  | N-CA-C      | -7.30 | 103.84      | 112.89   |
| 3   | 03    | 901  | LEU  | N-CA-C      | -7.24 | 104.08      | 113.12   |
| 4   | 04    | 910  | ASN  | N-CA-C      | 7.21  | 120.05      | 110.53   |
| 26  | X     | 39   | GLU  | N-CA-C      | 7.21  | 121.33      | 112.54   |
| 3   | 03    | 8    | LYS  | N-CA-C      | -7.20 | 104.49      | 113.28   |
| 7   | E     | 44   | GLU  | N-CA-C      | 7.19  | 126.12      | 110.80   |
| 3   | 03    | 1273 | MET  | N-CA-C      | -7.16 | 103.51      | 111.82   |
| 3   | 03    | 1170 | MET  | N-CA-C      | -7.14 | 103.54      | 111.82   |
| 4   | 04    | 65   | VAL  | N-CA-C      | -7.13 | 105.83      | 112.96   |
| 20  | R     | 18   | ALA  | N-CA-C      | -7.13 | 104.61      | 113.38   |
| 3   | 03    | 374  | GLU  | N-CA-C      | 7.10  | 119.02      | 110.07   |
| 9   | G     | 192  | ALA  | N-CA-C      | 7.09  | 121.03      | 111.24   |
| 4   | 04    | 704  | GLU  | N-CA-C      | 7.09  | 121.03      | 112.38   |
| 13  | K     | 29   | SER  | N-CA-C      | -7.08 | 97.86       | 109.40   |
| 18  | P     | 44   | ILE  | N-CA-C      | -7.04 | 102.72      | 112.50   |
| 3   | 03    | 705  | GLU  | N-CA-C      | -7.03 | 103.54      | 111.14   |
| 7   | E     | 172  | ALA  | N-CA-C      | -7.02 | 103.67      | 111.82   |
| 25  | W     | 26   | MET  | N-CA-C      | -7.01 | 103.57      | 111.07   |
| 3   | 03    | 15   | PHE  | N-CA-C      | -7.00 | 103.58      | 111.14   |
| 4   | 04    | 851  | PRO  | N-CA-C      | -6.96 | 104.26      | 113.65   |
| 3   | 03    | 1310 | ASP  | N-CA-C      | -6.93 | 103.97      | 113.18   |
| 23  | U     | 31   | ASN  | N-CA-C      | -6.92 | 103.83      | 112.90   |
| 2   | 01    | 86   | LYS  | N-CA-C      | -6.84 | 103.61      | 112.23   |
| 1   | A     | 69   | G    | C2'-C3'-O3' | 6.83  | 119.75      | 109.50   |
| 3   | 03    | 337  | PHE  | N-CA-C      | 6.82  | 120.36      | 109.24   |
| 3   | 03    | 690  | VAL  | N-CA-C      | 6.81  | 115.36      | 109.02   |
| 3   | 03    | 966  | ILE  | N-CA-C      | 6.81  | 119.56      | 111.05   |
| 4   | 04    | 296  | LYS  | N-CA-C      | -6.81 | 103.79      | 111.14   |
| 3   | 03    | 1322 | SER  | N-CA-C      | -6.81 | 104.24      | 112.54   |
| 3   | 03    | 1315 | MET  | N-CA-C      | 6.80  | 117.25      | 108.34   |
| 2   | 02    | 227  | GLN  | N-CA-C      | 6.79  | 120.44      | 111.75   |
| 4   | 04    | 1192 | LYS  | N-CA-C      | -6.76 | 104.90      | 113.01   |
| 4   | 04    | 1243 | LEU  | N-CA-C      | -6.74 | 105.02      | 113.18   |
| 2   | 02    | 198  | LEU  | N-CA-C      | -6.74 | 99.59       | 109.63   |
| 18  | P     | 76   | ILE  | N-CA-C      | -6.73 | 103.96      | 110.42   |
| 16  | N     | 54   | SER  | N-CA-C      | -6.67 | 105.13      | 113.20   |
| 9   | G     | 9    | LYS  | N-CA-C      | -6.66 | 103.84      | 112.23   |
| 3   | 03    | 561  | ILE  | N-CA-C      | 6.64  | 117.33      | 110.36   |
| 3   | 03    | 900  | LYS  | N-CA-C      | -6.62 | 104.42      | 113.30   |
| 20  | R     | 4    | THR  | N-CA-C      | 6.62  | 119.32      | 111.71   |
| 3   | 03    | 1326 | LEU  | N-CA-C      | -6.62 | 104.15      | 111.36   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 9   | G     | 147  | LYS  | N-CA-C | -6.59 | 104.72      | 112.89   |
| 19  | Q     | 57   | SER  | N-CA-C | -6.53 | 105.47      | 113.50   |
| 4   | 04    | 216  | LYS  | N-CA-C | -6.51 | 103.29      | 111.11   |
| 4   | 04    | 1367 | GLN  | N-CA-C | -6.50 | 104.12      | 111.14   |
| 21  | S     | 61   | VAL  | N-CA-C | -6.50 | 103.47      | 112.50   |
| 7   | E     | 53   | ALA  | N-CA-C | -6.48 | 104.14      | 111.14   |
| 4   | 04    | 120  | LEU  | N-CA-C | -6.48 | 104.83      | 113.25   |
| 10  | H     | 61   | LYS  | N-CA-C | -6.47 | 104.08      | 112.23   |
| 16  | N     | 117  | HIS  | N-CA-C | -6.46 | 102.51      | 111.81   |
| 4   | 04    | 539  | SER  | N-CA-C | -6.45 | 105.05      | 113.12   |
| 23  | U     | 33   | ILE  | N-CA-C | -6.44 | 100.97      | 108.82   |
| 3   | 03    | 409  | LEU  | N-CA-C | -6.41 | 104.72      | 113.30   |
| 7   | E     | 28   | LYS  | CA-C-N | -6.40 | 111.84      | 119.84   |
| 7   | E     | 28   | LYS  | C-N-CA | -6.40 | 111.84      | 119.84   |
| 3   | 03    | 550  | VAL  | N-CA-C | 6.38  | 117.10      | 108.17   |
| 11  | I     | 25   | TYR  | N-CA-C | 6.37  | 118.23      | 111.28   |
| 4   | 04    | 265  | LEU  | N-CA-C | -6.36 | 104.44      | 111.82   |
| 4   | 04    | 1302 | TYR  | N-CA-C | 6.36  | 119.81      | 110.59   |
| 5   | 05    | 18   | ASP  | N-CA-C | -6.35 | 104.79      | 112.54   |
| 4   | 04    | 27   | PRO  | N-CA-C | -6.35 | 105.92      | 113.86   |
| 14  | L     | 96   | GLU  | N-CA-C | -6.35 | 104.45      | 111.82   |
| 4   | 04    | 1330 | ARG  | N-CA-C | -6.34 | 104.29      | 111.14   |
| 12  | J     | 109  | LYS  | N-CA-C | -6.33 | 101.41      | 110.59   |
| 4   | 04    | 458  | ASN  | N-CA-C | -6.33 | 102.74      | 111.28   |
| 4   | 04    | 769  | VAL  | N-CA-C | 6.33  | 118.96      | 111.05   |
| 15  | M     | 45   | ARG  | N-CA-C | -6.31 | 96.89       | 107.99   |
| 2   | 02    | 88   | LEU  | N-CA-C | 6.30  | 118.85      | 109.59   |
| 4   | 04    | 203  | GLU  | N-CA-C | -6.29 | 104.35      | 111.14   |
| 2   | 02    | 116  | THR  | N-CA-C | 6.29  | 119.33      | 109.96   |
| 3   | 03    | 1279 | GLU  | N-CA-C | -6.28 | 105.77      | 113.50   |
| 4   | 04    | 294  | ASN  | N-CA-C | -6.27 | 104.33      | 112.23   |
| 4   | 04    | 532  | GLU  | N-CA-C | -6.26 | 105.61      | 113.18   |
| 4   | 04    | 18   | ASP  | N-CA-C | 6.26  | 120.22      | 108.65   |
| 7   | E     | 187  | VAL  | N-CA-C | 6.25  | 116.15      | 108.53   |
| 23  | U     | 16   | GLU  | N-CA-C | -6.23 | 105.32      | 113.17   |
| 16  | N     | 98   | ALA  | N-CA-C | -6.22 | 104.04      | 111.69   |
| 16  | N     | 89   | GLY  | CA-C-N | 6.22  | 125.44      | 118.97   |
| 16  | N     | 89   | GLY  | C-N-CA | 6.22  | 125.44      | 118.97   |
| 4   | 04    | 311  | ARG  | N-CA-C | -6.21 | 103.37      | 113.19   |
| 12  | J     | 145  | GLU  | N-CA-C | 6.21  | 119.70      | 111.75   |
| 4   | 04    | 302  | ALA  | N-CA-C | -6.18 | 104.45      | 111.07   |
| 4   | 04    | 667  | GLN  | N-CA-C | -6.18 | 105.23      | 112.89   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 25  | W     | 28   | ARG  | N-CA-C | 6.15  | 119.62      | 111.75   |
| 26  | X     | 20   | LYS  | N-CA-C | -6.15 | 104.58      | 111.28   |
| 4   | 04    | 166  | LEU  | N-CA-C | -6.14 | 104.69      | 111.82   |
| 3   | 03    | 1163 | THR  | N-CA-C | -6.14 | 100.41      | 109.81   |
| 4   | 04    | 754  | ILE  | N-CA-C | 6.14  | 116.85      | 107.77   |
| 7   | E     | 47   | VAL  | CA-C-N | -6.12 | 113.37      | 119.56   |
| 7   | E     | 47   | VAL  | C-N-CA | -6.12 | 113.37      | 119.56   |
| 4   | 04    | 836  | ARG  | N-CA-C | 6.10  | 118.44      | 111.11   |
| 3   | 03    | 29   | SER  | N-CA-C | -6.10 | 104.55      | 112.23   |
| 25  | W     | 70   | LYS  | N-CA-C | -6.09 | 104.19      | 111.69   |
| 20  | R     | 46   | LYS  | N-CA-C | 6.09  | 123.77      | 110.80   |
| 3   | 03    | 526  | HIS  | N-CA-C | -6.09 | 104.56      | 112.23   |
| 9   | G     | 198  | LEU  | N-CA-C | -6.08 | 106.84      | 114.56   |
| 4   | 04    | 218  | THR  | N-CA-C | 6.06  | 117.88      | 111.28   |
| 7   | E     | 63   | ARG  | N-CA-C | -6.04 | 105.83      | 112.72   |
| 3   | 03    | 611  | GLU  | N-CA-C | -6.03 | 104.79      | 111.36   |
| 2   | 02    | 208  | ASN  | N-CA-C | 6.01  | 117.64      | 111.14   |
| 4   | 04    | 63   | GLY  | CA-C-N | 6.01  | 127.35      | 119.84   |
| 4   | 04    | 63   | GLY  | C-N-CA | 6.01  | 127.35      | 119.84   |
| 3   | 03    | 548  | ARG  | N-CA-C | 6.00  | 118.78      | 111.82   |
| 19  | Q     | 49   | THR  | N-CA-C | -6.00 | 104.87      | 111.82   |
| 16  | N     | 118  | ASN  | N-CA-C | -5.97 | 103.17      | 111.52   |
| 3   | 03    | 242  | VAL  | CA-C-N | 5.95  | 126.37      | 119.47   |
| 3   | 03    | 242  | VAL  | C-N-CA | 5.95  | 126.37      | 119.47   |
| 3   | 03    | 210  | LEU  | N-CA-C | -5.95 | 104.88      | 111.36   |
| 2   | 01    | 212  | ASP  | CA-C-N | 5.94  | 127.26      | 119.84   |
| 2   | 01    | 212  | ASP  | C-N-CA | 5.94  | 127.26      | 119.84   |
| 24  | V     | 20   | LYS  | N-CA-C | -5.94 | 106.02      | 113.20   |
| 4   | 04    | 63   | GLY  | N-CA-C | 5.93  | 124.44      | 112.34   |
| 3   | 03    | 57   | PHE  | N-CA-C | -5.92 | 102.13      | 110.31   |
| 4   | 04    | 358  | GLY  | CA-C-N | 5.92  | 125.62      | 119.82   |
| 4   | 04    | 358  | GLY  | C-N-CA | 5.92  | 125.62      | 119.82   |
| 21  | S     | 69   | ASP  | N-CA-C | 5.91  | 118.48      | 111.33   |
| 19  | Q     | 18   | LYS  | N-CA-C | -5.91 | 104.79      | 112.23   |
| 12  | J     | 105  | GLU  | N-CA-C | -5.89 | 105.58      | 112.89   |
| 4   | 04    | 988  | PHE  | N-CA-C | -5.89 | 104.78      | 111.14   |
| 3   | 03    | 241  | LEU  | N-CA-C | 5.88  | 119.12      | 110.30   |
| 3   | 03    | 213  | LEU  | N-CA-C | -5.87 | 98.30       | 110.80   |
| 3   | 03    | 482  | GLY  | N-CA-C | -5.86 | 104.55      | 112.57   |
| 16  | N     | 61   | ALA  | N-CA-C | -5.85 | 104.86      | 112.23   |
| 4   | 04    | 1303 | SER  | N-CA-C | -5.85 | 98.88       | 108.76   |
| 4   | 04    | 85   | CYS  | N-CA-C | -5.83 | 97.73       | 107.99   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | 03    | 856  | ASN  | N-CA-C | 5.83  | 120.20      | 113.38   |
| 23  | U     | 67   | LEU  | N-CA-C | -5.82 | 104.30      | 111.40   |
| 3   | 03    | 123  | TYR  | N-CA-C | 5.82  | 117.52      | 109.15   |
| 12  | J     | 22   | LEU  | N-CA-C | -5.82 | 105.68      | 112.89   |
| 12  | J     | 71   | THR  | N-CA-C | -5.82 | 104.33      | 112.12   |
| 25  | W     | 59   | ARG  | N-CA-C | -5.81 | 104.58      | 111.03   |
| 26  | X     | 64   | ASN  | N-CA-C | 5.81  | 120.43      | 113.23   |
| 8   | F     | 67   | ILE  | N-CA-C | 5.80  | 116.22      | 107.75   |
| 18  | P     | 27   | THR  | N-CA-C | 5.80  | 117.60      | 111.28   |
| 25  | W     | 58   | ASP  | N-CA-C | -5.80 | 106.36      | 113.50   |
| 4   | 04    | 1293 | GLU  | N-CA-C | 5.78  | 118.84      | 110.28   |
| 3   | 03    | 842  | ASP  | N-CA-C | 5.78  | 123.10      | 110.80   |
| 9   | G     | 13   | ARG  | N-CA-C | -5.78 | 106.07      | 113.23   |
| 17  | O     | 7    | VAL  | N-CA-C | -5.77 | 104.89      | 110.72   |
| 3   | 03    | 1023 | HIS  | N-CA-C | -5.77 | 104.89      | 111.07   |
| 3   | 03    | 408  | SER  | N-CA-C | -5.77 | 106.24      | 113.28   |
| 5   | 05    | 19   | LEU  | N-CA-C | -5.77 | 104.90      | 111.07   |
| 3   | 03    | 302  | ILE  | CA-C-N | -5.77 | 113.93      | 122.41   |
| 3   | 03    | 302  | ILE  | C-N-CA | -5.77 | 113.93      | 122.41   |
| 3   | 03    | 891  | GLY  | N-CA-C | 5.76  | 123.23      | 110.66   |
| 7   | E     | 121  | SER  | N-CA-C | -5.76 | 106.29      | 113.38   |
| 3   | 03    | 736  | VAL  | N-CA-C | 5.76  | 117.01      | 109.58   |
| 24  | V     | 36   | ARG  | N-CA-C | 5.76  | 120.03      | 112.89   |
| 4   | 04    | 388  | ARG  | N-CA-C | -5.75 | 103.85      | 111.96   |
| 10  | H     | 87   | VAL  | N-CA-C | 5.75  | 116.43      | 108.84   |
| 4   | 04    | 1296 | GLY  | N-CA-C | -5.74 | 99.57       | 113.18   |
| 5   | 05    | 29   | GLN  | N-CA-C | -5.74 | 105.16      | 111.82   |
| 4   | 04    | 263  | SER  | N-CA-C | -5.74 | 99.78       | 108.67   |
| 7   | E     | 221  | VAL  | N-CA-C | -5.73 | 103.76      | 111.44   |
| 19  | Q     | 9    | GLU  | N-CA-C | -5.73 | 102.16      | 111.04   |
| 4   | 04    | 345  | LYS  | N-CA-C | 5.73  | 123.00      | 110.80   |
| 12  | J     | 144  | ALA  | N-CA-C | 5.71  | 117.37      | 111.03   |
| 3   | 03    | 37   | LYS  | N-CA-C | -5.71 | 105.81      | 112.89   |
| 3   | 03    | 920  | VAL  | CA-C-O | 5.71  | 122.32      | 119.12   |
| 3   | 03    | 536  | GLY  | N-CA-C | -5.71 | 105.06      | 114.76   |
| 4   | 04    | 402  | GLU  | N-CA-C | -5.71 | 105.14      | 111.36   |
| 4   | 04    | 195  | GLU  | N-CA-C | 5.70  | 119.50      | 112.54   |
| 20  | R     | 65   | LEU  | N-CA-C | -5.70 | 104.99      | 111.14   |
| 13  | K     | 66   | GLN  | N-CA-C | -5.69 | 106.32      | 113.72   |
| 3   | 03    | 609  | ILE  | N-CA-C | -5.69 | 105.07      | 110.42   |
| 3   | 03    | 148  | GLN  | N-CA-C | 5.68  | 118.80      | 109.72   |
| 4   | 04    | 169  | LEU  | N-CA-C | -5.67 | 106.03      | 113.12   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 12  | J     | 42   | VAL  | N-CA-C | -5.67 | 104.84      | 110.62   |
| 17  | O     | 5    | GLN  | N-CA-C | -5.67 | 105.62      | 112.54   |
| 2   | 01    | 77   | ASP  | N-CA-C | -5.67 | 103.05      | 110.53   |
| 8   | F     | 15   | LYS  | N-CA-C | 5.67  | 117.83      | 109.50   |
| 11  | I     | 83   | ALA  | N-CA-C | -5.67 | 103.93      | 111.24   |
| 12  | J     | 61   | PHE  | N-CA-C | -5.67 | 106.50      | 113.41   |
| 3   | 03    | 237  | LEU  | N-CA-C | 5.66  | 117.44      | 108.67   |
| 4   | 04    | 289  | ASP  | N-CA-C | 5.66  | 117.45      | 111.28   |
| 12  | J     | 122  | GLU  | N-CA-C | 5.65  | 119.69      | 112.34   |
| 11  | I     | 90   | MET  | N-CA-C | 5.65  | 119.41      | 109.80   |
| 4   | 04    | 411  | ILE  | N-CA-C | -5.65 | 104.65      | 112.50   |
| 7   | E     | 30   | PHE  | N-CA-C | 5.65  | 119.91      | 113.19   |
| 3   | 03    | 160  | ASP  | N-CA-C | -5.64 | 104.31      | 110.91   |
| 13  | K     | 67   | GLY  | N-CA-C | -5.64 | 99.81       | 113.18   |
| 13  | K     | 123  | GLU  | N-CA-C | 5.64  | 117.27      | 109.15   |
| 2   | 02    | 135  | ASP  | N-CA-C | 5.62  | 118.22      | 110.35   |
| 4   | 04    | 79   | LYS  | N-CA-C | -5.61 | 105.16      | 112.23   |
| 4   | 04    | 1311 | LYS  | N-CA-C | -5.61 | 106.60      | 113.50   |
| 2   | 01    | 84   | ASN  | N-CA-C | -5.60 | 105.94      | 112.89   |
| 3   | 03    | 303  | ASP  | N-CA-C | 5.60  | 117.84      | 107.99   |
| 7   | E     | 107  | VAL  | N-CA-C | -5.59 | 103.95      | 111.44   |
| 4   | 04    | 1145 | PHE  | N-CA-C | 5.58  | 119.72      | 113.02   |
| 2   | 02    | 50   | SER  | N-CA-C | 5.57  | 117.31      | 107.61   |
| 18  | P     | 107  | THR  | N-CA-C | -5.56 | 105.23      | 112.23   |
| 17  | O     | 81   | ILE  | N-CA-C | 5.56  | 115.65      | 107.15   |
| 7   | E     | 61   | ALA  | N-CA-C | -5.55 | 106.67      | 113.50   |
| 3   | 03    | 106  | GLU  | N-CA-C | 5.55  | 117.57      | 108.52   |
| 4   | 04    | 93   | THR  | N-CA-C | 5.55  | 115.61      | 108.34   |
| 3   | 03    | 54   | ARG  | N-CA-C | -5.54 | 104.06      | 112.04   |
| 3   | 03    | 1207 | SER  | N-CA-C | 5.54  | 118.08      | 111.71   |
| 4   | 04    | 52   | GLU  | N-CA-C | 5.54  | 118.22      | 109.96   |
| 4   | 04    | 771  | GLN  | N-CA-C | -5.53 | 105.25      | 111.28   |
| 3   | 03    | 1302 | THR  | N-CA-C | -5.53 | 105.66      | 112.90   |
| 4   | 04    | 518  | VAL  | N-CA-C | 5.53  | 116.30      | 110.72   |
| 4   | 04    | 20   | ILE  | N-CA-C | 5.52  | 116.68      | 108.46   |
| 3   | 03    | 277  | LEU  | N-CA-C | -5.51 | 105.68      | 112.90   |
| 5   | 05    | 45   | LYS  | N-CA-C | -5.51 | 103.22      | 110.43   |
| 2   | 01    | 125  | LYS  | CA-C-N | 5.50  | 126.72      | 119.84   |
| 2   | 01    | 125  | LYS  | C-N-CA | 5.50  | 126.72      | 119.84   |
| 20  | R     | 47   | LYS  | N-CA-C | 5.50  | 117.58      | 110.65   |
| 4   | 04    | 452  | LEU  | N-CA-C | 5.50  | 119.09      | 112.38   |
| 3   | 03    | 503  | LYS  | N-CA-C | -5.49 | 105.31      | 112.23   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4   | 04    | 450  | HIS  | CA-C-N | 5.49  | 126.71      | 119.84   |
| 4   | 04    | 450  | HIS  | C-N-CA | 5.49  | 126.71      | 119.84   |
| 4   | 04    | 919  | ALA  | N-CA-C | -5.49 | 105.21      | 111.14   |
| 7   | E     | 112  | LYS  | N-CA-C | -5.49 | 106.08      | 112.89   |
| 7   | E     | 208  | ARG  | N-CA-C | -5.49 | 104.70      | 111.40   |
| 9   | G     | 12   | ARG  | N-CA-C | -5.49 | 106.54      | 113.18   |
| 19  | Q     | 78   | LEU  | N-CA-C | 5.48  | 115.52      | 108.34   |
| 3   | 03    | 291  | TYR  | N-CA-C | 5.48  | 117.96      | 111.33   |
| 3   | 03    | 1287 | LEU  | N-CA-C | -5.46 | 104.86      | 112.45   |
| 5   | 05    | 56   | GLU  | N-CA-C | -5.46 | 105.36      | 112.23   |
| 7   | E     | 151  | ILE  | N-CA-C | -5.45 | 104.66      | 112.35   |
| 4   | 04    | 1291 | GLU  | N-CA-C | -5.44 | 106.64      | 113.28   |
| 13  | K     | 40   | LYS  | N-CA-C | -5.44 | 104.89      | 112.45   |
| 8   | F     | 90   | VAL  | N-CA-C | -5.43 | 105.23      | 110.72   |
| 7   | E     | 186  | ILE  | N-CA-C | -5.40 | 101.76      | 108.89   |
| 3   | 03    | 1305 | TYR  | N-CA-C | -5.39 | 105.32      | 111.14   |
| 8   | F     | 27   | GLU  | N-CA-C | 5.39  | 119.55      | 112.92   |
| 17  | O     | 75   | GLU  | N-CA-C | -5.39 | 106.21      | 112.89   |
| 4   | 04    | 189  | LEU  | N-CA-C | -5.39 | 105.57      | 111.82   |
| 13  | K     | 16   | GLY  | N-CA-C | -5.38 | 105.88      | 112.77   |
| 4   | 04    | 355  | ILE  | N-CA-C | 5.37  | 116.91      | 109.29   |
| 4   | 04    | 577  | ALA  | N-CA-C | -5.36 | 105.51      | 111.36   |
| 4   | 04    | 1074 | LEU  | N-CA-C | 5.36  | 117.56      | 109.41   |
| 7   | E     | 62   | SER  | N-CA-C | -5.36 | 105.48      | 112.23   |
| 2   | 02    | 70   | THR  | N-CA-C | 5.35  | 117.69      | 109.07   |
| 4   | 04    | 322  | ARG  | CA-C-N | -5.34 | 114.27      | 119.78   |
| 4   | 04    | 322  | ARG  | C-N-CA | -5.34 | 114.27      | 119.78   |
| 14  | L     | 48   | ARG  | N-CA-C | -5.34 | 106.89      | 113.41   |
| 26  | X     | 36   | GLU  | N-CA-C | 5.34  | 117.52      | 111.11   |
| 4   | 04    | 1220 | ILE  | N-CA-C | -5.34 | 104.41      | 111.09   |
| 11  | I     | 68   | GLN  | N-CA-C | 5.34  | 117.85      | 111.71   |
| 2   | 01    | 161  | SER  | N-CA-C | -5.33 | 105.38      | 111.14   |
| 3   | 03    | 179  | TYR  | N-CA-C | -5.33 | 104.97      | 112.12   |
| 19  | Q     | 80   | ARG  | N-CA-C | 5.33  | 116.77      | 111.07   |
| 4   | 04    | 183  | GLU  | N-CA-C | -5.31 | 104.54      | 111.02   |
| 3   | 03    | 626  | GLU  | N-CA-C | 5.31  | 117.97      | 111.82   |
| 4   | 04    | 47   | ARG  | N-CA-C | -5.31 | 99.50       | 110.80   |
| 4   | 04    | 1372 | ARG  | N-CA-C | -5.30 | 106.83      | 113.72   |
| 3   | 03    | 427  | ASP  | N-CA-C | -5.29 | 105.59      | 111.36   |
| 3   | 03    | 354  | ASP  | N-CA-C | -5.29 | 98.11       | 109.81   |
| 4   | 04    | 870  | ASP  | N-CA-C | -5.29 | 105.68      | 111.82   |
| 13  | K     | 103  | VAL  | N-CA-C | 5.29  | 116.21      | 108.53   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | 03    | 1118 | GLY  | N-CA-C | -5.29 | 105.92      | 113.86   |
| 4   | 04    | 293  | ARG  | N-CA-C | -5.29 | 106.82      | 113.28   |
| 3   | 03    | 222  | ASP  | N-CA-C | -5.28 | 107.49      | 114.04   |
| 11  | I     | 81   | ASN  | N-CA-C | -5.28 | 98.78       | 108.02   |
| 2   | 01    | 212  | ASP  | N-CA-C | 5.28  | 116.53      | 109.83   |
| 4   | 04    | 806  | ASP  | N-CA-C | 5.27  | 119.42      | 113.15   |
| 14  | L     | 114  | LYS  | N-CA-C | 5.27  | 118.24      | 110.59   |
| 9   | G     | 21   | LYS  | N-CA-C | -5.27 | 105.57      | 113.89   |
| 4   | 04    | 152  | THR  | N-CA-C | -5.27 | 101.78      | 109.63   |
| 12  | J     | 124  | SER  | N-CA-C | -5.26 | 105.72      | 111.82   |
| 22  | T     | 32   | ILE  | N-CA-C | 5.26  | 115.53      | 110.74   |
| 2   | 01    | 168  | ILE  | N-CA-C | 5.26  | 120.28      | 109.34   |
| 13  | K     | 31   | LEU  | N-CA-C | -5.25 | 105.24      | 111.69   |
| 3   | 03    | 812  | PHE  | N-CA-C | 5.24  | 117.76      | 109.96   |
| 4   | 04    | 544  | LEU  | N-CA-C | -5.24 | 106.48      | 112.92   |
| 4   | 04    | 261  | ALA  | N-CA-C | -5.24 | 106.12      | 112.88   |
| 15  | M     | 46   | LYS  | N-CA-C | 5.23  | 116.83      | 108.41   |
| 24  | V     | 41   | PRO  | N-CA-C | -5.23 | 107.81      | 114.35   |
| 4   | 04    | 1052 | GLU  | N-CA-C | -5.23 | 106.91      | 113.28   |
| 7   | E     | 43   | LEU  | N-CA-C | 5.22  | 121.92      | 110.80   |
| 3   | 03    | 906  | PHE  | N-CA-C | 5.22  | 116.65      | 111.07   |
| 4   | 04    | 127  | LEU  | N-CA-C | -5.21 | 105.20      | 112.45   |
| 3   | 03    | 479  | LEU  | N-CA-C | -5.21 | 106.77      | 113.23   |
| 4   | 04    | 417  | ARG  | N-CA-C | 5.21  | 121.90      | 110.80   |
| 4   | 04    | 980  | THR  | N-CA-C | 5.21  | 115.92      | 107.23   |
| 17  | O     | 115  | LYS  | N-CA-C | -5.21 | 103.27      | 110.35   |
| 9   | G     | 97   | LEU  | N-CA-C | 5.20  | 117.35      | 111.11   |
| 4   | 04    | 665  | GLN  | N-CA-C | -5.20 | 106.45      | 112.89   |
| 2   | 01    | 215  | GLU  | N-CA-C | -5.19 | 105.52      | 111.07   |
| 3   | 03    | 353  | VAL  | N-CA-C | -5.19 | 104.48      | 111.44   |
| 3   | 03    | 632  | ASP  | N-CA-C | -5.19 | 106.90      | 113.18   |
| 13  | K     | 126  | CYS  | N-CA-C | 5.19  | 117.62      | 108.75   |
| 3   | 03    | 755  | LYS  | N-CA-C | 5.18  | 117.88      | 107.41   |
| 4   | 04    | 902  | ASP  | N-CA-C | 5.18  | 117.82      | 110.10   |
| 2   | 01    | 230  | ALA  | N-CA-C | 5.18  | 116.92      | 111.28   |
| 24  | V     | 14   | LEU  | N-CA-C | -5.18 | 105.08      | 111.40   |
| 3   | 03    | 1186 | VAL  | N-CA-C | 5.18  | 120.11      | 113.07   |
| 4   | 04    | 450  | HIS  | N-CA-C | -5.18 | 102.04      | 109.24   |
| 3   | 03    | 348  | SER  | N-CA-C | -5.17 | 105.72      | 111.36   |
| 4   | 04    | 325  | LYS  | N-CA-C | 5.17  | 117.73      | 110.23   |
| 3   | 03    | 1325 | VAL  | N-CA-C | -5.17 | 105.46      | 113.16   |
| 25  | W     | 11   | ILE  | N-CA-C | -5.17 | 106.04      | 110.74   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | 04    | 396  | ALA  | N-CA-C      | -5.16 | 106.49      | 112.89   |
| 3   | 03    | 473  | ARG  | N-CA-C      | -5.16 | 106.94      | 113.18   |
| 4   | 04    | 679  | TYR  | N-CA-C      | -5.16 | 105.31      | 111.03   |
| 3   | 03    | 863  | SER  | N-CA-C      | -5.15 | 106.94      | 113.18   |
| 2   | 01    | 96   | ASP  | N-CA-C      | -5.15 | 107.05      | 113.38   |
| 3   | 03    | 687  | ARG  | N-CA-C      | -5.14 | 107.03      | 113.15   |
| 2   | 02    | 110  | VAL  | N-CA-C      | 5.14  | 115.73      | 109.30   |
| 4   | 04    | 401  | VAL  | N-CA-C      | -5.13 | 106.09      | 113.07   |
| 1   | A     | 184  | G    | N9-C1'-C2'  | 5.13  | 119.69      | 112.00   |
| 24  | V     | 19   | GLU  | N-CA-C      | -5.12 | 105.88      | 111.82   |
| 2   | 02    | 18   | GLN  | N-CA-C      | 5.10  | 117.72      | 109.40   |
| 4   | 04    | 700  | ASN  | N-CA-C      | -5.10 | 105.61      | 111.07   |
| 4   | 04    | 412  | LEU  | N-CA-C      | -5.10 | 105.91      | 111.82   |
| 3   | 03    | 276  | GLN  | N-CA-C      | -5.10 | 107.01      | 113.18   |
| 3   | 03    | 729  | ALA  | N-CA-C      | -5.09 | 107.20      | 113.41   |
| 16  | N     | 73   | VAL  | N-CA-C      | -5.08 | 108.32      | 113.20   |
| 10  | H     | 55   | VAL  | N-CA-C      | 5.08  | 118.44      | 112.35   |
| 12  | J     | 95   | ARG  | N-CA-C      | 5.08  | 116.51      | 110.97   |
| 4   | 04    | 29   | MET  | N-CA-C      | -5.08 | 105.83      | 112.23   |
| 3   | 03    | 174  | ALA  | N-CA-C      | 5.07  | 116.95      | 108.99   |
| 13  | K     | 27   | PRO  | N-CA-C      | -5.06 | 103.24      | 111.14   |
| 16  | N     | 94   | SER  | N-CA-C      | -5.06 | 105.95      | 111.82   |
| 11  | I     | 63   | ASN  | N-CA-C      | -5.05 | 105.00      | 110.91   |
| 4   | 04    | 1276 | GLU  | N-CA-C      | 5.05  | 117.01      | 109.59   |
| 12  | J     | 89   | GLU  | N-CA-C      | -5.05 | 102.44      | 109.96   |
| 22  | T     | 20   | ILE  | N-CA-C      | 5.05  | 115.24      | 108.17   |
| 4   | 04    | 242  | LEU  | N-CA-C      | 5.04  | 116.02      | 109.72   |
| 3   | 03    | 93   | SER  | N-CA-C      | 5.04  | 116.47      | 108.96   |
| 3   | 03    | 1133 | LYS  | N-CA-C      | -5.04 | 106.64      | 112.89   |
| 3   | 03    | 973  | SER  | N-CA-C      | -5.03 | 105.98      | 111.82   |
| 12  | J     | 24   | LYS  | N-CA-C      | -5.03 | 105.99      | 111.82   |
| 1   | A     | 1399 | C    | C2'-C3'-O3' | 5.02  | 117.03      | 109.50   |
| 3   | 03    | 633  | LEU  | N-CA-C      | 5.02  | 117.50      | 109.81   |
| 3   | 03    | 1323 | PHE  | N-CA-C      | -5.02 | 105.99      | 111.82   |
| 12  | J     | 60   | ALA  | N-CA-C      | -5.02 | 107.12      | 113.20   |
| 5   | 05    | 46   | THR  | N-CA-C      | 5.02  | 118.50      | 112.38   |
| 3   | 03    | 98   | VAL  | N-CA-C      | 5.01  | 115.80      | 108.58   |
| 7   | E     | 35   | ARG  | N-CA-C      | 5.01  | 117.98      | 109.76   |
| 13  | K     | 109  | VAL  | N-CA-C      | 5.00  | 115.52      | 108.36   |
| 3   | 03    | 420  | LEU  | N-CA-C      | 5.00  | 117.55      | 110.50   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 25  | C    | Sidechain |
| 1   | A     | 872 | A    | Sidechain |
| 1   | A     | 9   | G    | Sidechain |
| 7   | E     | 22  | TYR  | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 30955 | 0        | 15586    | 430     | 0            |
| 2   | 01    | 1753  | 0        | 1780     | 100     | 0            |
| 2   | 02    | 1757  | 0        | 1778     | 101     | 0            |
| 3   | 03    | 10272 | 0        | 10138    | 502     | 0            |
| 4   | 04    | 10372 | 0        | 10512    | 643     | 0            |
| 5   | 05    | 458   | 0        | 476      | 33      | 0            |
| 6   | B     | 774   | 0        | 201      | 9       | 0            |
| 7   | E     | 1705  | 0        | 1732     | 168     | 0            |
| 8   | F     | 1625  | 0        | 1699     | 50      | 0            |
| 9   | G     | 1643  | 0        | 1710     | 77      | 0            |
| 10  | H     | 1157  | 0        | 1199     | 48      | 0            |
| 11  | I     | 818   | 0        | 808      | 40      | 0            |
| 12  | J     | 1182  | 0        | 1240     | 53      | 0            |
| 13  | K     | 979   | 0        | 1034     | 40      | 0            |
| 14  | L     | 1022  | 0        | 1070     | 63      | 0            |
| 15  | M     | 787   | 0        | 828      | 35      | 0            |
| 16  | N     | 870   | 0        | 878      | 39      | 0            |
| 17  | O     | 955   | 0        | 1019     | 32      | 0            |
| 18  | P     | 884   | 0        | 944      | 53      | 0            |
| 19  | Q     | 805   | 0        | 847      | 54      | 0            |
| 20  | R     | 714   | 0        | 737      | 23      | 0            |
| 21  | S     | 649   | 0        | 666      | 26      | 0            |
| 22  | T     | 649   | 0        | 691      | 21      | 0            |
| 23  | U     | 536   | 0        | 552      | 22      | 0            |
| 24  | V     | 638   | 0        | 665      | 27      | 0            |
| 25  | W     | 665   | 0        | 714      | 61      | 0            |
| 26  | X     | 545   | 0        | 579      | 40      | 0            |
| All | All   | 75169 | 0        | 60083    | 2604    | 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 19.

All (2604) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:E:25:PRO:HB2    | 7:E:28:LYS:HB2     | 1.30                     | 1.13              |
| 25:W:54:GLN:HA    | 25:W:57:VAL:HG12   | 1.39                     | 1.03              |
| 7:E:23:TRP:CZ3    | 7:E:25:PRO:HB3     | 1.96                     | 1.00              |
| 3:03:979:LEU:HD21 | 3:03:989:LEU:HD22  | 1.43                     | 0.99              |
| 7:E:19:GLN:H      | 7:E:40:ILE:HA      | 1.27                     | 0.98              |
| 1:A:1304:G:H21    | 1:A:1333:A:H62     | 1.08                     | 0.97              |
| 7:E:39:HIS:O      | 7:E:40:ILE:HG23    | 1.63                     | 0.97              |
| 7:E:87:CYS:HB2    | 7:E:89:GLN:HE22    | 1.30                     | 0.97              |
| 25:W:38:ILE:HG21  | 25:W:81:GLN:HE21   | 1.28                     | 0.96              |
| 4:04:705:THR:HG21 | 4:04:719:PHE:H     | 1.32                     | 0.94              |
| 4:04:94:GLN:HB2   | 4:04:97:VAL:HG23   | 1.50                     | 0.94              |
| 7:E:47:VAL:HB     | 7:E:48:PRO:HD3     | 1.49                     | 0.94              |
| 3:03:1267:GLY:H   | 4:04:346:ARG:HH21  | 1.14                     | 0.93              |
| 7:E:11:LYS:HB2    | 7:E:15:HIS:HB3     | 1.50                     | 0.92              |
| 2:01:11:PRO:HA    | 2:01:30:PRO:HB2    | 1.52                     | 0.92              |
| 4:04:327:LEU:HA   | 4:04:330:MET:HB2   | 1.49                     | 0.92              |
| 3:03:397:LEU:HB3  | 3:03:401:GLY:HA3   | 1.51                     | 0.92              |
| 3:03:588:GLU:HB3  | 3:03:605:TYR:HB3   | 1.52                     | 0.91              |
| 4:04:290:ILE:H    | 4:04:290:ILE:HD12  | 1.36                     | 0.91              |
| 4:04:845:ALA:HA   | 4:04:883:ARG:HG3   | 1.50                     | 0.91              |
| 7:E:26:LYS:O      | 7:E:29:PRO:HD2     | 1.71                     | 0.91              |
| 1:A:427:U:H1'     | 1:A:541:G:H5''     | 1.50                     | 0.90              |
| 2:02:35:PHE:HA    | 2:02:38:THR:HG22   | 1.53                     | 0.90              |
| 3:03:1058:ARG:HD2 | 3:03:1238:LEU:HD13 | 1.52                     | 0.90              |
| 7:E:19:GLN:N      | 7:E:40:ILE:HA      | 1.88                     | 0.89              |
| 3:03:137:VAL:HG22 | 3:03:142:GLU:HG3   | 1.55                     | 0.88              |
| 3:03:1149:TYR:HB3 | 3:03:1159:VAL:HG12 | 1.54                     | 0.88              |
| 1:A:961:U:H3      | 1:A:1201:A:H61     | 1.23                     | 0.87              |
| 3:03:1082:ILE:H   | 3:03:1082:ILE:HD12 | 1.38                     | 0.87              |
| 3:03:241:LEU:HD21 | 3:03:277:LEU:HD13  | 1.56                     | 0.86              |
| 3:03:1320:PRO:HG2 | 3:03:1323:PHE:HB2  | 1.55                     | 0.86              |
| 4:04:109:SER:HB2  | 4:04:279:LEU:HD13  | 1.55                     | 0.86              |
| 3:03:149:LEU:HD11 | 3:03:451:ARG:HB3   | 1.57                     | 0.86              |
| 2:02:83:LEU:HB3   | 4:04:528:THR:HB    | 1.58                     | 0.86              |
| 19:Q:60:ARG:HG2   | 19:Q:62:ARG:HH21   | 1.40                     | 0.86              |
| 18:P:3:ILE:HD13   | 18:P:21:ILE:HD11   | 1.58                     | 0.85              |
| 24:V:62:THR:H     | 24:V:65:MET:HE3    | 1.38                     | 0.85              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:E:90:PHE:HB3     | 7:E:151:ILE:HA    | 1.58                     | 0.85              |
| 4:04:909:ILE:HD11  | 4:04:913:GLU:HG2  | 1.59                     | 0.85              |
| 5:05:27:ALA:HA     | 5:05:30:MET:HE3   | 1.57                     | 0.85              |
| 2:02:51:MET:HE1    | 2:02:220:ALA:HB2  | 1.58                     | 0.85              |
| 1:A:363:A:H5'      | 17:O:30:ARG:HB2   | 1.57                     | 0.84              |
| 3:03:502:VAL:HG13  | 3:03:503:LYS:HD2  | 1.59                     | 0.84              |
| 14:L:24:ASN:HB3    | 14:L:26:LYS:HE2   | 1.59                     | 0.83              |
| 1:A:1259:C:H3'     | 1:A:1260:G:H5''   | 1.61                     | 0.83              |
| 3:03:673:HIS:HA    | 4:04:763:PHE:O    | 1.78                     | 0.83              |
| 10:H:133:ILE:HD12  | 10:H:133:ILE:H    | 1.41                     | 0.83              |
| 10:H:24:VAL:HG23   | 10:H:26:GLY:H     | 1.44                     | 0.83              |
| 3:03:420:LEU:HB3   | 3:03:425:ILE:HD11 | 1.62                     | 0.82              |
| 3:03:1255:THR:HG22 | 3:03:1256:GLN:H   | 1.42                     | 0.82              |
| 4:04:20:ILE:O      | 4:04:1343:GLU:HA  | 1.80                     | 0.82              |
| 25:W:8:LYS:NZ      | 25:W:8:LYS:HB3    | 1.93                     | 0.81              |
| 3:03:237:LEU:HD12  | 3:03:289:VAL:HA   | 1.63                     | 0.81              |
| 1:A:1230:C:H41     | 18:P:103:THR:HG21 | 1.46                     | 0.80              |
| 4:04:1366:HIS:HA   | 4:04:1369:ARG:HB2 | 1.63                     | 0.80              |
| 12:J:24:LYS:HA     | 12:J:27:ASN:HD22  | 1.44                     | 0.80              |
| 4:04:1191:PRO:HB2  | 4:04:1194:ARG:HD3 | 1.64                     | 0.80              |
| 1:A:92:U:H2'       | 1:A:93:U:H4'      | 1.63                     | 0.80              |
| 4:04:272:VAL:HG22  | 4:04:302:ALA:HB1  | 1.64                     | 0.80              |
| 17:O:43:LYS:HG3    | 17:O:44:PRO:HD3   | 1.63                     | 0.80              |
| 3:03:519:ASN:ND2   | 3:03:521:LEU:HB3  | 1.97                     | 0.79              |
| 1:A:1329:A:H5''    | 18:P:25:GLY:H     | 1.47                     | 0.79              |
| 3:03:190:PRO:HG3   | 3:03:436:ARG:HH21 | 1.45                     | 0.79              |
| 3:03:723:VAL:HG22  | 3:03:776:PRO:HG3  | 1.65                     | 0.79              |
| 4:04:19:ALA:HB1    | 4:04:1343:GLU:HB3 | 1.63                     | 0.79              |
| 3:03:74:ARG:HB2    | 3:03:99:LYS:HE3   | 1.65                     | 0.78              |
| 2:02:65:LEU:HB3    | 2:02:169:GLY:HA2  | 1.66                     | 0.78              |
| 3:03:1258:PRO:HB3  | 4:04:346:ARG:HH11 | 1.49                     | 0.78              |
| 4:04:337:ARG:H     | 4:04:337:ARG:HD2  | 1.48                     | 0.78              |
| 4:04:844:THR:HG23  | 4:04:864:LEU:HD11 | 1.64                     | 0.78              |
| 2:01:180:VAL:HB    | 2:01:183:ILE:HD11 | 1.65                     | 0.78              |
| 9:G:129:VAL:HG12   | 9:G:131:ILE:H     | 1.49                     | 0.78              |
| 2:01:100:LEU:HD21  | 2:01:121:VAL:HG11 | 1.66                     | 0.78              |
| 2:02:166:ARG:HB2   | 2:02:167:PRO:HD3  | 1.63                     | 0.78              |
| 1:A:1103:C:H4'     | 7:E:97:LEU:HD22   | 1.65                     | 0.77              |
| 2:02:193:GLU:HB3   | 4:04:406:ALA:HB1  | 1.66                     | 0.77              |
| 4:04:1242:ARG:HH12 | 4:04:1247:LYS:HG2 | 1.49                     | 0.77              |
| 7:E:33:GLY:HA2     | 7:E:41:ILE:O      | 1.84                     | 0.77              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:E:54:LEU:HD22    | 7:E:220:THR:HG21   | 1.63                     | 0.77              |
| 18:P:16:ILE:HD12   | 18:P:16:ILE:H      | 1.48                     | 0.77              |
| 18:P:72:ILE:O      | 18:P:76:ILE:HG13   | 1.83                     | 0.77              |
| 2:01:207:THR:HG22  | 2:01:209:GLY:H     | 1.48                     | 0.77              |
| 4:04:1327:GLU:HB3  | 4:04:1330:ARG:HG3  | 1.67                     | 0.77              |
| 4:04:849:LEU:HD23  | 4:04:849:LEU:H     | 1.49                     | 0.77              |
| 3:03:241:LEU:HD11  | 3:03:246:LEU:HD11  | 1.64                     | 0.77              |
| 3:03:729:ALA:HA    | 3:03:769:PRO:HG2   | 1.67                     | 0.77              |
| 4:04:958:ILE:HD12  | 4:04:982:LEU:HD11  | 1.65                     | 0.77              |
| 2:01:29:GLU:HB3    | 2:01:30:PRO:HD3    | 1.67                     | 0.77              |
| 3:03:1109:ILE:HG21 | 4:04:764:ARG:HA    | 1.66                     | 0.77              |
| 7:E:166:ALA:HB3    | 7:E:191:SER:HB3    | 1.67                     | 0.77              |
| 10:H:80:LEU:HG     | 10:H:81:GLN:H      | 1.49                     | 0.77              |
| 14:L:114:LYS:HB2   | 14:L:117:LEU:HD12  | 1.67                     | 0.77              |
| 1:A:419:C:H5'      | 1:A:513:C:H4'      | 1.67                     | 0.76              |
| 3:03:592:ARG:HG3   | 3:03:655:VAL:HG22  | 1.66                     | 0.76              |
| 3:03:1063:GLY:H    | 3:03:1076:ILE:HG23 | 1.50                     | 0.76              |
| 4:04:526:VAL:HG12  | 4:04:549:LYS:HB2   | 1.67                     | 0.76              |
| 14:L:18:VAL:HG21   | 14:L:81:GLY:HA3    | 1.68                     | 0.76              |
| 14:L:83:THR:HG21   | 14:L:103:VAL:HG22  | 1.67                     | 0.76              |
| 2:02:89:ALA:HB1    | 2:02:210:THR:HG23  | 1.67                     | 0.76              |
| 1:A:244:U:H4'      | 1:A:245:U:H5'      | 1.67                     | 0.76              |
| 5:05:4:VAL:HG13    | 5:05:5:THR:HG23    | 1.68                     | 0.76              |
| 1:A:1250:A:H4'     | 14:L:68:GLY:HA2    | 1.66                     | 0.76              |
| 4:04:130:MET:HE3   | 4:04:157:GLN:HA    | 1.68                     | 0.76              |
| 1:A:426:U:H1'      | 9:G:39:GLN:HE21    | 1.48                     | 0.76              |
| 3:03:1335:ILE:HA   | 4:04:24:LEU:HD13   | 1.68                     | 0.76              |
| 3:03:82:VAL:HG13   | 3:03:137:VAL:HG21  | 1.67                     | 0.76              |
| 6:B:109:UNK:HA     | 6:B:153:UNK:HA     | 1.65                     | 0.75              |
| 3:03:207:THR:HG21  | 3:03:351:LEU:HD23  | 1.69                     | 0.75              |
| 9:G:104:MET:HE1    | 9:G:170:LEU:HB3    | 1.69                     | 0.75              |
| 3:03:732:ILE:HG13  | 3:03:753:LEU:HD11  | 1.69                     | 0.75              |
| 9:G:84:ASN:HD22    | 9:G:87:GLU:HG3     | 1.51                     | 0.75              |
| 7:E:21:ARG:O       | 7:E:23:TRP:HD1     | 1.70                     | 0.75              |
| 1:A:614:C:H2'      | 1:A:615:G:H5''     | 1.68                     | 0.75              |
| 1:A:1158:C:H4'     | 7:E:132:LYS:HD3    | 1.69                     | 0.75              |
| 3:03:448:LEU:HB2   | 3:03:608:ALA:HB3   | 1.68                     | 0.75              |
| 7:E:23:TRP:HE3     | 7:E:189:THR:HB     | 1.52                     | 0.75              |
| 2:02:164:ASP:HB2   | 2:02:170:ARG:HB2   | 1.68                     | 0.74              |
| 1:A:161:A:H61      | 1:A:347:G:H21      | 1.35                     | 0.74              |
| 3:03:209:ILE:HA    | 3:03:212:ALA:HB3   | 1.69                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:04:1173:ARG:HH21 | 4:04:1196:LEU:HD23 | 1.51                     | 0.74              |
| 9:G:7:LYS:HE3      | 9:G:20:LEU:HD22    | 1.68                     | 0.74              |
| 1:A:1322:C:H5'     | 18:P:98:GLY:HA3    | 1.69                     | 0.74              |
| 8:F:9:ILE:HG13     | 19:Q:97:LYS:HD3    | 1.68                     | 0.74              |
| 3:03:1320:PRO:O    | 3:03:1322:SER:N    | 2.19                     | 0.74              |
| 21:S:54:LEU:HD23   | 21:S:57:ILE:HD12   | 1.67                     | 0.74              |
| 3:03:406:ASN:HB3   | 3:03:411:ARG:HB2   | 1.70                     | 0.74              |
| 4:04:814:CYS:HB2   | 4:04:889:ASP:HB3   | 1.67                     | 0.74              |
| 20:R:28:VAL:HG22   | 20:R:65:LEU:HD23   | 1.69                     | 0.74              |
| 1:A:396:C:O2'      | 1:A:397:A:H5'      | 1.86                     | 0.74              |
| 4:04:393:THR:HG23  | 4:04:396:ALA:H     | 1.51                     | 0.74              |
| 3:03:364:VAL:HG13  | 3:03:376:PRO:HG3   | 1.70                     | 0.74              |
| 4:04:555:TYR:HB3   | 4:04:563:LEU:HB3   | 1.68                     | 0.74              |
| 4:04:1314:LEU:HD12 | 4:04:1326:GLN:HE21 | 1.53                     | 0.74              |
| 4:04:925:GLU:HB3   | 4:04:926:PRO:HD3   | 1.68                     | 0.74              |
| 21:S:52:LEU:HD13   | 21:S:75:ILE:HD13   | 1.70                     | 0.74              |
| 11:I:6:ILE:HG12    | 11:I:89:VAL:HG12   | 1.69                     | 0.73              |
| 25:W:42:ASP:HB3    | 25:W:45:ALA:HB3    | 1.69                     | 0.73              |
| 2:02:190:ALA:HB2   | 2:02:200:LYS:HB2   | 1.68                     | 0.73              |
| 3:03:30:ILE:H      | 3:03:30:ILE:HD12   | 1.51                     | 0.73              |
| 4:04:80:HIS:HB3    | 4:04:92:VAL:HG21   | 1.70                     | 0.73              |
| 4:04:154:LEU:HD21  | 4:04:160:LEU:HD21  | 1.71                     | 0.73              |
| 11:I:29:ILE:HG21   | 11:I:64:VAL:HG21   | 1.70                     | 0.73              |
| 2:01:32:GLU:HB2    | 2:01:35:PHE:HD2    | 1.52                     | 0.73              |
| 2:02:23:HIS:HB3    | 2:02:206:GLU:HG2   | 1.70                     | 0.73              |
| 4:04:485:MET:HB3   | 4:04:488:ASN:HD22  | 1.52                     | 0.73              |
| 15:M:57:VAL:HG22   | 15:M:58:ASN:H      | 1.53                     | 0.73              |
| 8:F:163:ARG:H      | 8:F:163:ARG:HD3    | 1.53                     | 0.73              |
| 3:03:434:ASP:HA    | 3:03:437:ASN:HD22  | 1.53                     | 0.73              |
| 4:04:344:GLY:O     | 4:04:345:LYS:CB    | 2.37                     | 0.73              |
| 8:F:59:PRO:HB3     | 15:M:94:ALA:HA     | 1.71                     | 0.73              |
| 2:02:56:VAL:HG21   | 2:02:144:ILE:HD11  | 1.69                     | 0.73              |
| 3:03:1169:VAL:HA   | 3:03:1172:LEU:HB2  | 1.70                     | 0.73              |
| 1:A:1202:U:H4'     | 19:Q:68:ARG:HD2    | 1.69                     | 0.72              |
| 4:04:120:LEU:HB3   | 4:04:121:PRO:HD3   | 1.71                     | 0.72              |
| 7:E:89:GLN:NE2     | 7:E:89:GLN:H       | 1.86                     | 0.72              |
| 7:E:151:ILE:HG13   | 7:E:154:MET:HE2    | 1.70                     | 0.72              |
| 4:04:327:LEU:CA    | 4:04:330:MET:HB2   | 2.19                     | 0.72              |
| 4:04:342:LEU:O     | 4:04:343:LEU:HB2   | 1.88                     | 0.72              |
| 13:K:35:ILE:HG12   | 13:K:109:VAL:HG11  | 1.71                     | 0.72              |
| 1:A:1252:A:H61     | 1:A:1285:A:H61     | 1.35                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:04:490:ILE:HD12  | 4:04:491:LEU:HG    | 1.71                     | 0.72              |
| 1:A:1502:A:H8      | 1:A:1505:G:H22     | 1.38                     | 0.72              |
| 3:03:1331:ARG:HG2  | 4:04:243:PRO:HG2   | 1.71                     | 0.72              |
| 4:04:1190:ILE:HG21 | 4:04:1196:LEU:HD11 | 1.71                     | 0.72              |
| 4:04:1320:ILE:HB   | 4:04:1349:GLU:HG3  | 1.72                     | 0.72              |
| 1:A:414:A:H62      | 1:A:430:A:H61      | 1.37                     | 0.72              |
| 4:04:116:PHE:HE1   | 4:04:1333:THR:HA   | 1.53                     | 0.72              |
| 4:04:749:LYS:HD3   | 4:04:753:SER:HB2   | 1.69                     | 0.72              |
| 25:W:59:ARG:O      | 25:W:63:LYS:HB2    | 1.90                     | 0.72              |
| 24:V:40:PHE:H      | 24:V:43:MET:HE2    | 1.55                     | 0.71              |
| 4:04:108:ALA:HB1   | 4:04:283:LEU:HD11  | 1.70                     | 0.71              |
| 8:F:107:LYS:HD2    | 8:F:110:LEU:HD22   | 1.72                     | 0.71              |
| 19:Q:8:ARG:HB3     | 19:Q:12:ARG:HH12   | 1.54                     | 0.71              |
| 2:02:33:ARG:H      | 2:02:33:ARG:HD3    | 1.55                     | 0.71              |
| 3:03:1099:ASN:HD21 | 3:03:1101:LEU:HB2  | 1.55                     | 0.71              |
| 3:03:1101:LEU:HD21 | 4:04:508:LEU:HD22  | 1.72                     | 0.71              |
| 5:05:26:ARG:HG3    | 5:05:30:MET:HE2    | 1.70                     | 0.71              |
| 4:04:107:LEU:HD23  | 4:04:276:ASN:ND2   | 2.06                     | 0.71              |
| 4:04:425:ARG:HG2   | 4:04:427:PRO:HD2   | 1.73                     | 0.71              |
| 18:P:90:HIS:HA     | 18:P:108:ARG:HH22  | 1.55                     | 0.71              |
| 3:03:810:TYR:HB3   | 3:03:817:LEU:HD23  | 1.72                     | 0.71              |
| 4:04:114:ILE:HG13  | 4:04:118:LYS:HE2   | 1.73                     | 0.71              |
| 1:A:150:U:H3       | 1:A:171:A:H62      | 1.39                     | 0.70              |
| 1:A:1158:C:H2'     | 1:A:1159:U:H4'     | 1.71                     | 0.70              |
| 4:04:1344:LEU:HD12 | 4:04:1349:GLU:HB3  | 1.73                     | 0.70              |
| 3:03:39:ILE:HD11   | 3:03:75:LEU:HD21   | 1.73                     | 0.70              |
| 3:03:102:LEU:HD22  | 3:03:489:PRO:HD3   | 1.72                     | 0.70              |
| 3:03:479:LEU:HD23  | 3:03:487:LEU:HD13  | 1.73                     | 0.70              |
| 4:04:963:VAL:HG21  | 4:04:975:ILE:HG23  | 1.73                     | 0.70              |
| 9:G:33:ILE:HG13    | 9:G:34:GLU:HG3     | 1.72                     | 0.70              |
| 3:03:697:LYS:H     | 3:03:697:LYS:HD3   | 1.57                     | 0.70              |
| 4:04:328:ALA:C     | 4:04:330:MET:H     | 1.97                     | 0.70              |
| 21:S:23:ASP:HB2    | 21:S:26:ASN:ND2    | 2.06                     | 0.70              |
| 4:04:534:GLU:HG3   | 4:04:538:ARG:HD3   | 1.74                     | 0.70              |
| 7:E:23:TRP:HA      | 7:E:190:ASN:HB3    | 1.73                     | 0.70              |
| 4:04:246:PRO:HD2   | 4:04:249:LEU:HD12  | 1.72                     | 0.70              |
| 14:L:60:LEU:O      | 14:L:60:LEU:HD12   | 1.92                     | 0.70              |
| 1:A:831:A:H3'      | 1:A:832:G:H5''     | 1.73                     | 0.70              |
| 7:E:43:LEU:O       | 7:E:46:THR:HB      | 1.91                     | 0.70              |
| 15:M:102:LEU:HD23  | 15:M:102:LEU:H     | 1.55                     | 0.70              |
| 4:04:504:GLN:HE22  | 4:04:731:ARG:HD2   | 1.56                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:04:504:GLN:HA    | 4:04:507:VAL:HG22  | 1.74                     | 0.69              |
| 7:E:76:ALA:O       | 7:E:80:VAL:HG23    | 1.92                     | 0.69              |
| 3:03:548:ARG:HD3   | 3:03:569:ILE:HG13  | 1.74                     | 0.69              |
| 4:04:123:ARG:HD2   | 4:04:1337:VAL:HG21 | 1.74                     | 0.69              |
| 1:A:188:C:H5       | 25:W:83:ASN:HD22   | 1.40                     | 0.69              |
| 2:02:54:CYS:HB2    | 2:02:91:ARG:HA     | 1.74                     | 0.69              |
| 5:05:58:LEU:HG     | 5:05:59:ILE:HG12   | 1.74                     | 0.69              |
| 3:03:1319:MET:HE3  | 3:03:1324:ASN:HB2  | 1.74                     | 0.69              |
| 9:G:70:GLN:HA      | 9:G:73:ASN:HD22    | 1.55                     | 0.69              |
| 1:A:59:A:H3'       | 1:A:60:A:H5'       | 1.73                     | 0.69              |
| 1:A:770:C:H1'      | 1:A:900:A:H2       | 1.57                     | 0.69              |
| 2:02:56:VAL:HG22   | 2:02:146:VAL:HG22  | 1.73                     | 0.69              |
| 10:H:44:ARG:HE     | 10:H:70:MET:HB3    | 1.57                     | 0.69              |
| 2:02:30:PRO:C      | 2:02:31:LEU:HD22   | 2.18                     | 0.69              |
| 4:04:456:ALA:HB2   | 4:04:500:ILE:HD11  | 1.75                     | 0.69              |
| 4:04:472:LEU:HD23  | 4:04:472:LEU:H     | 1.56                     | 0.69              |
| 23:U:55:LEU:O      | 23:U:59:ILE:HG13   | 1.93                     | 0.69              |
| 1:A:410:G:H21      | 1:A:432:A:H62      | 1.39                     | 0.69              |
| 3:03:678:ARG:NH2   | 3:03:1106:ARG:HG2  | 2.07                     | 0.69              |
| 1:A:1219:A:H5''    | 19:Q:52:ARG:HG2    | 1.75                     | 0.68              |
| 3:03:263:VAL:HG11  | 3:03:269:ILE:HG12  | 1.74                     | 0.68              |
| 4:04:903:LEU:HG    | 4:04:904:ALA:H     | 1.56                     | 0.68              |
| 7:E:26:LYS:O       | 7:E:29:PRO:CD      | 2.41                     | 0.68              |
| 13:K:33:VAL:HG22   | 13:K:58:LEU:HD13   | 1.75                     | 0.68              |
| 1:A:1148:U:H1'     | 14:L:17:ARG:HD3    | 1.75                     | 0.68              |
| 2:02:80:GLU:HB3    | 4:04:551:ARG:HH21  | 1.58                     | 0.68              |
| 9:G:113:ALA:O      | 9:G:117:VAL:HG23   | 1.93                     | 0.68              |
| 1:A:321:A:H61      | 1:A:332:G:H1       | 1.40                     | 0.68              |
| 3:03:174:ALA:O     | 3:03:186:PHE:HB2   | 1.94                     | 0.68              |
| 2:02:118:ASP:H     | 2:02:121:VAL:HB    | 1.59                     | 0.68              |
| 4:04:260:PHE:HB3   | 4:04:262:THR:HG22  | 1.76                     | 0.68              |
| 7:E:21:ARG:O       | 7:E:23:TRP:CD1     | 2.47                     | 0.68              |
| 17:O:29:LYS:HG3    | 17:O:30:ARG:H      | 1.59                     | 0.68              |
| 1:A:12:U:H2'       | 1:A:13:U:H5''      | 1.76                     | 0.68              |
| 1:A:142:G:H1'      | 1:A:195:A:H61      | 1.57                     | 0.68              |
| 4:04:1067:ARG:HH12 | 4:04:1076:PRO:HD3  | 1.58                     | 0.68              |
| 7:E:23:TRP:CD2     | 7:E:25:PRO:HD3     | 2.29                     | 0.68              |
| 10:H:104:ILE:HG13  | 10:H:122:VAL:HG23  | 1.74                     | 0.68              |
| 12:J:40:SER:HA     | 12:J:43:TYR:HD2    | 1.57                     | 0.68              |
| 18:P:16:ILE:HD12   | 18:P:16:ILE:N      | 2.08                     | 0.68              |
| 1:A:410:G:H2'      | 1:A:429:U:C5       | 2.30                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:981:U:H3'      | 1:A:982:U:H5''     | 1.75                     | 0.67              |
| 3:03:673:HIS:CA    | 4:04:763:PHE:O     | 2.42                     | 0.67              |
| 4:04:527:LEU:HD13  | 4:04:548:VAL:HG11  | 1.75                     | 0.67              |
| 7:E:21:ARG:HD3     | 7:E:22:TYR:N       | 2.08                     | 0.67              |
| 12:J:103:ILE:HD13  | 12:J:123:LEU:HD13  | 1.75                     | 0.67              |
| 3:03:1082:ILE:HD12 | 3:03:1082:ILE:N    | 2.08                     | 0.67              |
| 20:R:84:LEU:HD23   | 20:R:86:LEU:HD23   | 1.76                     | 0.67              |
| 2:01:16:ILE:HG23   | 2:01:26:VAL:HA     | 1.77                     | 0.67              |
| 4:04:826:ILE:HA    | 4:04:831:VAL:HA    | 1.76                     | 0.67              |
| 2:01:228:LEU:HD21  | 2:02:224:LEU:HD22  | 1.75                     | 0.67              |
| 3:03:799:ASN:HB3   | 3:03:1231:TYR:HD1  | 1.58                     | 0.67              |
| 18:P:64:VAL:HG23   | 18:P:66:GLY:H      | 1.59                     | 0.67              |
| 3:03:851:THR:H     | 3:03:887:VAL:HG23  | 1.60                     | 0.67              |
| 13:K:77:VAL:HG23   | 13:K:126:CYS:HA    | 1.75                     | 0.67              |
| 17:O:51:VAL:HG11   | 17:O:89:LEU:HD22   | 1.76                     | 0.67              |
| 24:V:14:LEU:O      | 24:V:18:VAL:HG23   | 1.94                     | 0.67              |
| 4:04:364:HIS:HB3   | 5:05:4:VAL:HG23    | 1.75                     | 0.67              |
| 1:A:81:A:H2'       | 1:A:82:G:H4'       | 1.77                     | 0.67              |
| 1:A:1053:G:H4'     | 1:A:1054:C:H3'     | 1.75                     | 0.67              |
| 3:03:1292:THR:O    | 3:03:1296:ASP:HB3  | 1.95                     | 0.67              |
| 25:W:31:ILE:HG12   | 25:W:53:MET:HE3    | 1.75                     | 0.67              |
| 3:03:1336:ASN:HB3  | 4:04:25:ALA:HB3    | 1.77                     | 0.67              |
| 4:04:395:LYS:HA    | 4:04:398:LYS:HE2   | 1.76                     | 0.67              |
| 1:A:105:G:N2       | 1:A:379:C:H4'      | 2.09                     | 0.66              |
| 3:03:159:SER:HB2   | 3:03:442:VAL:HG21  | 1.77                     | 0.66              |
| 3:03:1335:ILE:N    | 3:03:1335:ILE:HD12 | 2.10                     | 0.66              |
| 7:E:31:ILE:HB      | 7:E:42:ASN:HA      | 1.76                     | 0.66              |
| 26:X:40:LYS:HB3    | 26:X:41:PRO:HD3    | 1.77                     | 0.66              |
| 1:A:186:C:H5'      | 25:W:72:ALA:HA     | 1.76                     | 0.66              |
| 2:01:184:ALA:HB2   | 3:03:1091:GLY:HA3  | 1.77                     | 0.66              |
| 12:J:49:LEU:HD22   | 12:J:123:LEU:HB3   | 1.76                     | 0.66              |
| 4:04:97:VAL:HG12   | 4:04:101:ARG:HH12  | 1.59                     | 0.66              |
| 1:A:1236:A:H4'     | 1:A:1304:G:H4'     | 1.77                     | 0.66              |
| 3:03:433:ILE:HG22  | 3:03:437:ASN:HD21  | 1.60                     | 0.66              |
| 3:03:1103:VAL:HB   | 3:03:1104:PRO:HD3  | 1.76                     | 0.66              |
| 20:R:28:VAL:HG11   | 20:R:66:LEU:HD21   | 1.77                     | 0.66              |
| 1:A:194:C:H4'      | 25:W:59:ARG:HG3    | 1.77                     | 0.66              |
| 1:A:831:A:C3'      | 1:A:832:G:H5''     | 2.26                     | 0.66              |
| 1:A:1226:C:N4      | 18:P:102:LYS:HE2   | 2.11                     | 0.66              |
| 3:03:966:ILE:H     | 3:03:966:ILE:HD12  | 1.61                     | 0.66              |
| 13:K:94:VAL:HG12   | 13:K:95:MET:HG3    | 1.78                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:L:18:VAL:HA     | 14:L:64:ILE:HG12   | 1.76                     | 0.66              |
| 16:N:88:PRO:HA     | 16:N:92:ARG:HH11   | 1.59                     | 0.66              |
| 26:X:28:VAL:O      | 26:X:32:VAL:HG22   | 1.96                     | 0.66              |
| 3:03:228:VAL:HG22  | 3:03:245:ARG:HH11  | 1.59                     | 0.66              |
| 3:03:1319:MET:HG3  | 3:03:1323:PHE:HD2  | 1.61                     | 0.66              |
| 4:04:1179:PRO:HD2  | 4:04:1184:ASP:HA   | 1.77                     | 0.66              |
| 4:04:1252:HIS:O    | 4:04:1255:VAL:HG22 | 1.95                     | 0.66              |
| 16:N:72:ALA:H      | 16:N:74:LYS:HZ2    | 1.43                     | 0.66              |
| 3:03:616:ILE:HD12  | 3:03:616:ILE:N     | 2.10                     | 0.66              |
| 4:04:609:TYR:HE1   | 4:04:614:LEU:HB2   | 1.59                     | 0.66              |
| 14:L:94:ARG:O      | 14:L:98:ARG:HG3    | 1.96                     | 0.66              |
| 1:A:440:C:H2'      | 1:A:441:A:H5''     | 1.77                     | 0.66              |
| 16:N:53:GLY:H      | 16:N:56:LYS:HG3    | 1.61                     | 0.66              |
| 3:03:498:ILE:H     | 3:03:498:ILE:HD12  | 1.61                     | 0.65              |
| 12:J:78:ARG:H      | 12:J:78:ARG:HD2    | 1.59                     | 0.65              |
| 9:G:88:ASN:O       | 9:G:92:LEU:HD13    | 1.97                     | 0.65              |
| 14:L:27:ILE:HG21   | 14:L:34:LEU:HD12   | 1.78                     | 0.65              |
| 1:A:718:A:H5'      | 16:N:118:ASN:HB2   | 1.78                     | 0.65              |
| 2:01:195:ARG:HG2   | 2:01:198:LEU:HG    | 1.78                     | 0.65              |
| 3:03:204:LEU:HD21  | 3:03:369:MET:HG3   | 1.78                     | 0.65              |
| 1:A:1280:A:O2'     | 1:A:1281:C:H5'     | 1.96                     | 0.65              |
| 5:05:58:LEU:HD23   | 5:05:58:LEU:H      | 1.62                     | 0.65              |
| 8:F:69:THR:HG21    | 8:F:75:VAL:HG21    | 1.79                     | 0.65              |
| 25:W:27:MET:O      | 25:W:31:ILE:HG13   | 1.96                     | 0.65              |
| 1:A:65:A:H4'       | 1:A:66:A:H5'       | 1.79                     | 0.65              |
| 3:03:761:GLN:HE22  | 3:03:1236:ASN:ND2  | 1.95                     | 0.65              |
| 3:03:1141:LEU:HD12 | 3:03:1142:ARG:N    | 2.11                     | 0.65              |
| 4:04:926:PRO:HG2   | 4:04:1248:ILE:HD11 | 1.79                     | 0.65              |
| 9:G:90:LEU:HD23    | 9:G:93:LEU:HD12    | 1.78                     | 0.65              |
| 1:A:1393:U:H2'     | 1:A:1395:C:H5      | 1.61                     | 0.65              |
| 9:G:121:ALA:HB1    | 9:G:148:ALA:HB2    | 1.77                     | 0.65              |
| 1:A:981:U:H4'      | 19:Q:62:ARG:HH22   | 1.61                     | 0.65              |
| 3:03:817:LEU:HB3   | 3:03:1097:VAL:HB   | 1.79                     | 0.65              |
| 10:H:73:VAL:HG21   | 10:H:143:LEU:HB3   | 1.77                     | 0.65              |
| 24:V:4:LEU:HD23    | 24:V:4:LEU:H       | 1.61                     | 0.65              |
| 1:A:25:C:H41       | 1:A:558:G:N2       | 1.95                     | 0.65              |
| 4:04:377:PHE:O     | 4:04:381:ILE:HG13  | 1.97                     | 0.65              |
| 1:A:252:U:O2       | 1:A:252:U:H2'      | 1.97                     | 0.64              |
| 4:04:141:PHE:HB3   | 4:04:180:MET:HE3   | 1.79                     | 0.64              |
| 4:04:1041:ILE:HD12 | 4:04:1041:ILE:N    | 2.12                     | 0.64              |
| 1:A:1285:A:H4'     | 1:A:1286:U:H5''    | 1.77                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:1526:G:OP2     | 26:X:39:GLU:HB2    | 1.97                     | 0.64              |
| 3:03:54:ARG:NH1    | 3:03:54:ARG:HB2    | 2.13                     | 0.64              |
| 4:04:86:GLU:HG3    | 7:E:74:ARG:HG3     | 1.79                     | 0.64              |
| 4:04:506:VAL:HG23  | 4:04:628:GLY:HA3   | 1.78                     | 0.64              |
| 1:A:179:A:H61      | 1:A:196:A:H62      | 1.45                     | 0.64              |
| 14:L:109:GLN:HG2   | 14:L:110:VAL:H     | 1.62                     | 0.64              |
| 1:A:885:G:H2'      | 1:A:886:G:C8       | 2.33                     | 0.64              |
| 4:04:1029:THR:HG23 | 4:04:1121:LEU:HD11 | 1.79                     | 0.64              |
| 7:E:18:HIS:HA      | 7:E:40:ILE:HG22    | 1.80                     | 0.64              |
| 11:I:47:LEU:HD12   | 11:I:55:HIS:HA     | 1.80                     | 0.64              |
| 3:03:54:ARG:HB2    | 3:03:54:ARG:HH11   | 1.63                     | 0.64              |
| 12:J:29:LEU:HD23   | 12:J:42:VAL:HG22   | 1.78                     | 0.64              |
| 1:A:614:C:C2'      | 1:A:615:G:H5''     | 2.28                     | 0.64              |
| 4:04:811:GLU:HA    | 4:04:911:LYS:HE2   | 1.78                     | 0.64              |
| 3:03:205:PRO:HD2   | 3:03:208:ILE:HB    | 1.80                     | 0.64              |
| 6:B:218:UNK:HA     | 6:B:257:UNK:O      | 1.98                     | 0.64              |
| 1:A:245:U:H3       | 1:A:283:U:H3       | 1.45                     | 0.64              |
| 13:K:79:ARG:HG3    | 13:K:82:LEU:H      | 1.61                     | 0.64              |
| 2:01:166:ARG:N     | 2:01:167:PRO:HD2   | 2.12                     | 0.63              |
| 7:E:27:MET:HE2     | 7:E:188:ASP:O      | 1.98                     | 0.63              |
| 17:O:28:GLN:HE22   | 17:O:82:ARG:HG3    | 1.62                     | 0.63              |
| 19:Q:2:LYS:HE2     | 19:Q:5:MET:HB2     | 1.80                     | 0.63              |
| 19:Q:9:GLU:O       | 19:Q:13:VAL:HG23   | 1.97                     | 0.63              |
| 25:W:76:ALA:C      | 25:W:78:LEU:H      | 2.05                     | 0.63              |
| 4:04:814:CYS:SG    | 4:04:816:THR:HG22  | 2.39                     | 0.63              |
| 7:E:41:ILE:HG22    | 7:E:43:LEU:H       | 1.62                     | 0.63              |
| 9:G:190:LEU:HD12   | 9:G:192:ALA:H      | 1.63                     | 0.63              |
| 19:Q:55:SER:HA     | 19:Q:57:SER:H      | 1.61                     | 0.63              |
| 1:A:1306:A:H61     | 1:A:1331:G:H1'     | 1.63                     | 0.63              |
| 4:04:45:ASN:C      | 4:04:47:ARG:H      | 2.06                     | 0.63              |
| 4:04:582:ILE:HD13  | 4:04:627:THR:HG21  | 1.81                     | 0.63              |
| 4:04:678:ARG:O     | 4:04:682:VAL:HG23  | 1.99                     | 0.63              |
| 4:04:812:ASP:HA    | 4:04:896:ALA:H     | 1.62                     | 0.63              |
| 1:A:292:G:H21      | 1:A:608:A:H61      | 1.46                     | 0.63              |
| 2:02:12:ARG:C      | 2:02:13:LEU:HD23   | 2.22                     | 0.63              |
| 2:02:80:GLU:HB3    | 4:04:551:ARG:NH2   | 2.13                     | 0.63              |
| 3:03:384:LEU:O     | 3:03:388:LEU:HG    | 1.97                     | 0.63              |
| 4:04:112:ALA:HB2   | 4:04:182:ALA:HB2   | 1.81                     | 0.63              |
| 4:04:195:GLU:HA    | 4:04:198:CYS:HB2   | 1.81                     | 0.63              |
| 4:04:525:MET:HE2   | 4:04:527:LEU:HD11  | 1.79                     | 0.63              |
| 18:P:74:MET:HA     | 18:P:74:MET:HE3    | 1.81                     | 0.63              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:522:C:H5''    | 17:O:109:ARG:HH22  | 1.62                     | 0.63              |
| 4:04:483:LEU:HD23 | 4:04:483:LEU:H     | 1.64                     | 0.63              |
| 2:01:183:ILE:HD12 | 2:01:183:ILE:N     | 2.14                     | 0.63              |
| 3:03:104:ILE:HD12 | 3:03:104:ILE:N     | 2.13                     | 0.63              |
| 3:03:397:LEU:O    | 3:03:398:SER:O     | 2.17                     | 0.63              |
| 7:E:13:GLY:O      | 7:E:14:VAL:HG13    | 1.99                     | 0.63              |
| 16:N:87:GLY:H     | 16:N:114:PRO:HD2   | 1.62                     | 0.63              |
| 24:V:40:PHE:H     | 24:V:43:MET:CE     | 2.12                     | 0.63              |
| 1:A:405:U:H1'     | 1:A:498:A:H2'      | 1.80                     | 0.63              |
| 1:A:884:U:H4'     | 1:A:885:G:H5''     | 1.81                     | 0.63              |
| 2:01:45:ARG:HB2   | 2:02:38:THR:HB     | 1.81                     | 0.63              |
| 4:04:520:ALA:HB3  | 4:04:523:GLU:HB2   | 1.81                     | 0.63              |
| 4:04:600:ALA:HA   | 4:04:603:LYS:NZ    | 2.14                     | 0.63              |
| 4:04:812:ASP:OD2  | 4:04:911:LYS:HE3   | 1.98                     | 0.63              |
| 16:N:107:THR:HG23 | 16:N:108:ASN:OD1   | 1.99                     | 0.63              |
| 17:O:98:ARG:HB3   | 17:O:105:GLY:HA2   | 1.81                     | 0.63              |
| 3:03:80:PHE:HB2   | 3:03:85:CYS:SG     | 2.39                     | 0.63              |
| 3:03:670:PHE:HB3  | 3:03:673:HIS:HD2   | 1.63                     | 0.63              |
| 7:E:35:ARG:HD3    | 7:E:35:ARG:H       | 1.64                     | 0.63              |
| 7:E:36:ASN:HB2    | 7:E:40:ILE:HD13    | 1.81                     | 0.63              |
| 1:A:501:C:H2'     | 1:A:502:A:H8       | 1.64                     | 0.62              |
| 3:03:836:LEU:HD13 | 3:03:1054:LEU:HD13 | 1.81                     | 0.62              |
| 4:04:697:MET:HE1  | 4:04:742:GLY:HA3   | 1.81                     | 0.62              |
| 21:S:61:VAL:HA    | 21:S:65:ALA:HB3    | 1.80                     | 0.62              |
| 1:A:523:A:H61     | 17:O:49:ARG:NH2    | 1.96                     | 0.62              |
| 1:A:1297:G:H21    | 12:J:113:LYS:HB3   | 1.64                     | 0.62              |
| 2:01:14:VAL:HG22  | 2:01:15:ASP:H      | 1.64                     | 0.62              |
| 3:03:672:GLU:HB2  | 4:04:766:GLY:HA2   | 1.80                     | 0.62              |
| 18:P:28:ARG:O     | 18:P:32:ILE:HG12   | 1.99                     | 0.62              |
| 4:04:579:LEU:HD12 | 4:04:582:ILE:HD12  | 1.81                     | 0.62              |
| 9:G:13:ARG:NH1    | 9:G:37:PRO:HB2     | 2.13                     | 0.62              |
| 25:W:24:ARG:HB3   | 25:W:28:ARG:HH22   | 1.64                     | 0.62              |
| 26:X:43:THR:HA    | 26:X:46:LYS:NZ     | 2.14                     | 0.62              |
| 3:03:1272:GLU:HA  | 3:03:1275:VAL:HG23 | 1.80                     | 0.62              |
| 5:05:25:ARG:HG2   | 5:05:28:ARG:HH21   | 1.65                     | 0.62              |
| 21:S:5:ARG:HD3    | 21:S:5:ARG:H       | 1.65                     | 0.62              |
| 1:A:501:C:H2'     | 1:A:502:A:C8       | 2.34                     | 0.62              |
| 1:A:1224:U:H4'    | 18:P:100:ARG:HH12  | 1.64                     | 0.62              |
| 3:03:979:LEU:HD13 | 3:03:985:GLU:HB2   | 1.81                     | 0.62              |
| 18:P:19:THR:HA    | 18:P:25:GLY:HA2    | 1.81                     | 0.62              |
| 1:A:59:A:H1'      | 1:A:354:G:N2       | 2.15                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:426:U:H1'     | 9:G:39:GLN:NE2     | 2.14                     | 0.62              |
| 1:A:883:C:O2'     | 1:A:884:U:H5'      | 2.00                     | 0.62              |
| 2:02:47:LEU:HD22  | 2:02:180:VAL:HG11  | 1.82                     | 0.62              |
| 3:03:401:GLY:O    | 3:03:405:PHE:HB2   | 1.98                     | 0.62              |
| 4:04:81:ARG:HB2   | 7:E:206:ALA:HB1    | 1.81                     | 0.62              |
| 4:04:527:LEU:HB2  | 4:04:550:VAL:HG12  | 1.81                     | 0.62              |
| 4:04:552:ILE:HD12 | 4:04:552:ILE:O     | 2.00                     | 0.62              |
| 7:E:188:ASP:C     | 7:E:190:ASN:H      | 2.08                     | 0.62              |
| 14:L:51:LEU:HD21  | 14:L:82:ILE:HG21   | 1.82                     | 0.62              |
| 25:W:68:LYS:HB2   | 25:W:68:LYS:NZ     | 2.15                     | 0.62              |
| 1:A:552:U:H2'     | 1:A:553:A:H8       | 1.64                     | 0.62              |
| 12:J:68:VAL:HG23  | 12:J:99:ALA:HB1    | 1.81                     | 0.62              |
| 1:A:151:A:H62     | 1:A:170:U:H3       | 1.46                     | 0.62              |
| 1:A:437:U:O2'     | 1:A:438:U:H5'      | 1.99                     | 0.62              |
| 2:02:41:ASN:HA    | 2:02:44:ARG:HG2    | 1.82                     | 0.62              |
| 3:03:499:SER:HA   | 3:03:503:LYS:HD3   | 1.82                     | 0.62              |
| 3:03:657:THR:HG23 | 3:03:658:GLN:HG3   | 1.81                     | 0.62              |
| 3:03:673:HIS:C    | 4:04:763:PHE:O     | 2.43                     | 0.62              |
| 16:N:92:ARG:HH21  | 26:X:20:LYS:HD3    | 1.64                     | 0.62              |
| 2:02:172:LEU:HD23 | 2:02:172:LEU:H     | 1.64                     | 0.62              |
| 2:01:48:LEU:HD21  | 2:01:183:ILE:HD13  | 1.82                     | 0.61              |
| 3:03:557:ARG:HG2  | 3:03:558:VAL:HG23  | 1.82                     | 0.61              |
| 3:03:886:LYS:HB3  | 3:03:917:SER:HA    | 1.82                     | 0.61              |
| 19:Q:68:ARG:HH22  | 19:Q:80:ARG:HH21   | 1.48                     | 0.61              |
| 1:A:614:C:C3'     | 1:A:615:G:H5''     | 2.30                     | 0.61              |
| 9:G:94:GLU:HG2    | 9:G:185:PRO:HG3    | 1.82                     | 0.61              |
| 13:K:34:ALA:O     | 13:K:38:VAL:HG23   | 2.00                     | 0.61              |
| 14:L:105:ARG:O    | 14:L:105:ARG:HD3   | 1.99                     | 0.61              |
| 19:Q:65:GLN:HE21  | 19:Q:82:LYS:HE2    | 1.66                     | 0.61              |
| 3:03:1010:GLN:O   | 3:03:1014:LEU:HD13 | 2.00                     | 0.61              |
| 4:04:64:PRO:HG2   | 4:04:93:THR:H      | 1.65                     | 0.61              |
| 16:N:86:LYS:HB3   | 16:N:114:PRO:HD3   | 1.82                     | 0.61              |
| 4:04:311:ARG:HH21 | 4:04:1329:THR:HB   | 1.64                     | 0.61              |
| 4:04:1167:LYS:HE3 | 4:04:1174:ARG:HG3  | 1.82                     | 0.61              |
| 5:05:32:VAL:C     | 5:05:34:GLY:H      | 2.08                     | 0.61              |
| 2:01:185:TYR:HB2  | 2:01:201:LEU:HD11  | 1.81                     | 0.61              |
| 4:04:97:VAL:HG12  | 4:04:101:ARG:NH1   | 2.14                     | 0.61              |
| 3:03:815:SER:OG   | 3:03:1077:SER:HB3  | 2.01                     | 0.61              |
| 3:03:884:VAL:HG11 | 3:03:1050:VAL:HG11 | 1.83                     | 0.61              |
| 5:05:7:GLN:O      | 5:05:11:GLU:HG2    | 2.01                     | 0.61              |
| 1:A:216:U:H4'     | 1:A:464:U:H4'      | 1.82                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:02:59:VAL:HG21   | 2:02:85:LEU:HD13   | 1.82                     | 0.61              |
| 3:03:838:CYS:HB3   | 3:03:1050:VAL:HB   | 1.82                     | 0.61              |
| 9:G:100:VAL:O      | 9:G:104:MET:HG2    | 1.99                     | 0.61              |
| 4:04:903:LEU:HB3   | 4:04:905:ARG:HG2   | 1.81                     | 0.61              |
| 4:04:1137:GLY:O    | 4:04:1141:VAL:HG23 | 2.01                     | 0.61              |
| 7:E:23:TRP:CE2     | 7:E:25:PRO:HD3     | 2.36                     | 0.61              |
| 1:A:326:G:H2'      | 1:A:327:A:H5'      | 1.82                     | 0.61              |
| 3:03:498:ILE:HD12  | 3:03:498:ILE:N     | 2.15                     | 0.61              |
| 4:04:66:LYS:NZ     | 4:04:78:LEU:HD11   | 2.16                     | 0.60              |
| 4:04:1159:ILE:HG21 | 4:04:1179:PRO:HG3  | 1.83                     | 0.60              |
| 9:G:117:VAL:O      | 9:G:130:ASN:HA     | 2.01                     | 0.60              |
| 13:K:45:ILE:HD11   | 13:K:60:LEU:HB3    | 1.83                     | 0.60              |
| 22:T:35:LYS:NZ     | 22:T:35:LYS:HB3    | 2.15                     | 0.60              |
| 1:A:516:U:H5       | 1:A:533:A:H62      | 1.47                     | 0.60              |
| 2:01:32:GLU:HB2    | 2:01:35:PHE:CD2    | 2.35                     | 0.60              |
| 3:03:26:TYR:HE2    | 3:03:32:LEU:HD13   | 1.66                     | 0.60              |
| 3:03:623:LEU:HD12  | 3:03:623:LEU:O     | 2.01                     | 0.60              |
| 4:04:117:LEU:HD22  | 4:04:139:LEU:HD12  | 1.82                     | 0.60              |
| 4:04:583:VAL:HG21  | 4:04:592:VAL:HG11  | 1.83                     | 0.60              |
| 25:W:26:MET:HG2    | 25:W:56:ILE:HG12   | 1.83                     | 0.60              |
| 1:A:1343:G:H4'     | 14:L:123:ARG:HB3   | 1.83                     | 0.60              |
| 9:G:36:ALA:HB1     | 9:G:38:GLY:O       | 2.01                     | 0.60              |
| 18:P:15:VAL:HB     | 18:P:16:ILE:HD12   | 1.82                     | 0.60              |
| 2:01:89:ALA:HB1    | 2:01:208:ASN:HD22  | 1.64                     | 0.60              |
| 14:L:20:ILE:HG21   | 14:L:60:LEU:HD22   | 1.82                     | 0.60              |
| 15:M:6:ILE:HD11    | 15:M:79:PRO:HB3    | 1.83                     | 0.60              |
| 18:P:77:LYS:NZ     | 18:P:77:LYS:HB3    | 2.17                     | 0.60              |
| 3:03:671:LEU:O     | 3:03:673:HIS:N     | 2.34                     | 0.60              |
| 11:I:46:GLN:HA     | 11:I:56:LYS:HG2    | 1.81                     | 0.60              |
| 18:P:55:LEU:HD12   | 18:P:56:ARG:N      | 2.15                     | 0.60              |
| 12:J:41:ILE:HG23   | 12:J:116:ALA:HB2   | 1.84                     | 0.60              |
| 15:M:80:THR:H      | 15:M:83:THR:HB     | 1.65                     | 0.60              |
| 1:A:367:U:O2'      | 1:A:368:U:H4'      | 2.02                     | 0.60              |
| 3:03:646:SER:HB3   | 3:03:649:GLN:HG3   | 1.82                     | 0.60              |
| 4:04:1138:LEU:HB3  | 4:04:1139:PRO:HD3  | 1.84                     | 0.60              |
| 8:F:24:ASN:ND2     | 8:F:25:THR:H       | 1.99                     | 0.60              |
| 2:02:194:GLN:HG3   | 4:04:406:ALA:HB2   | 1.84                     | 0.60              |
| 4:04:214:ARG:HA    | 4:04:217:LEU:HB2   | 1.84                     | 0.60              |
| 7:E:11:LYS:CB      | 7:E:15:HIS:HB3     | 2.28                     | 0.60              |
| 8:F:63:ILE:HG23    | 8:F:98:ALA:HA      | 1.84                     | 0.60              |
| 25:W:79:THR:HA     | 25:W:82:ILE:HG12   | 1.84                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:01:31:LEU:HB2    | 2:01:199:ASP:O     | 2.02                     | 0.60              |
| 3:03:136:PHE:O     | 3:03:143:ARG:HD2   | 2.02                     | 0.60              |
| 3:03:616:ILE:HG13  | 3:03:652:TYR:HB2   | 1.84                     | 0.60              |
| 4:04:530:PRO:HB3   | 4:04:577:ALA:O     | 2.02                     | 0.60              |
| 4:04:554:GLU:HG3   | 4:04:566:LYS:HE3   | 1.83                     | 0.60              |
| 4:04:959:LYS:HB3   | 4:04:983:LYS:HB2   | 1.82                     | 0.60              |
| 1:A:244:U:H5'      | 1:A:894:G:N2       | 2.16                     | 0.60              |
| 1:A:1239:A:H5''    | 1:A:1240:U:H5      | 1.66                     | 0.60              |
| 3:03:74:ARG:HD2    | 3:03:75:LEU:N      | 2.17                     | 0.60              |
| 3:03:402:ARG:HG3   | 3:03:406:ASN:ND2   | 2.17                     | 0.60              |
| 3:03:488:MET:O     | 3:03:491:ASP:HB3   | 2.01                     | 0.60              |
| 3:03:931:VAL:HG13  | 3:03:1052:VAL:HG22 | 1.83                     | 0.60              |
| 4:04:99:ARG:HA     | 4:04:248:ASP:HB2   | 1.84                     | 0.60              |
| 4:04:1273:ASP:CG   | 4:04:1274:PHE:H    | 2.10                     | 0.60              |
| 7:E:15:HIS:CE1     | 7:E:47:VAL:HG22    | 2.37                     | 0.60              |
| 14:L:83:THR:HG23   | 14:L:97:LEU:HD23   | 1.84                     | 0.59              |
| 15:M:52:LEU:HB2    | 19:Q:80:ARG:HD2    | 1.84                     | 0.59              |
| 21:S:67:ILE:HD12   | 21:S:67:ILE:N      | 2.15                     | 0.59              |
| 3:03:524:ILE:HD12  | 3:03:708:VAL:HG13  | 1.84                     | 0.59              |
| 7:E:9:MET:HG3      | 7:E:10:LEU:HD23    | 1.84                     | 0.59              |
| 7:E:106:THR:HA     | 7:E:109:GLN:HG3    | 1.84                     | 0.59              |
| 16:N:88:PRO:HG2    | 26:X:29:LEU:HD22   | 1.85                     | 0.59              |
| 2:02:42:ALA:O      | 2:02:46:ILE:HG13   | 2.02                     | 0.59              |
| 3:03:34:SER:HA     | 3:03:37:LYS:NZ     | 2.18                     | 0.59              |
| 3:03:143:ARG:HD2   | 3:03:143:ARG:H     | 1.66                     | 0.59              |
| 3:03:1293:VAL:HG21 | 3:03:1315:MET:HE1  | 1.85                     | 0.59              |
| 12:J:113:LYS:HD2   | 12:J:117:LEU:CD2   | 2.33                     | 0.59              |
| 16:N:20:ALA:HB2    | 16:N:33:ILE:HG22   | 1.84                     | 0.59              |
| 4:04:86:GLU:HG2    | 26:X:67:ARG:HH22   | 1.67                     | 0.59              |
| 4:04:1252:HIS:O    | 4:04:1256:ILE:HG12 | 2.02                     | 0.59              |
| 1:A:885:G:H2'      | 1:A:886:G:H8       | 1.67                     | 0.59              |
| 3:03:1235:LEU:H    | 3:03:1235:LEU:HD12 | 1.68                     | 0.59              |
| 4:04:278:ARG:HD2   | 4:04:295:GLU:OE1   | 2.03                     | 0.59              |
| 4:04:426:ALA:HB3   | 4:04:427:PRO:HD3   | 1.84                     | 0.59              |
| 4:04:912:GLY:O     | 4:04:1359:ALA:HB1  | 2.03                     | 0.59              |
| 26:X:34:ARG:HD3    | 26:X:34:ARG:H      | 1.67                     | 0.59              |
| 4:04:483:LEU:HA    | 5:05:16:ARG:HH21   | 1.67                     | 0.59              |
| 9:G:25:ARG:HD3     | 9:G:28:ASP:HA      | 1.83                     | 0.59              |
| 1:A:1355:G:H2'     | 1:A:1356:G:C8      | 2.38                     | 0.59              |
| 22:T:63:CYS:SG     | 22:T:64:ARG:N      | 2.75                     | 0.59              |
| 1:A:71:A:H3'       | 1:A:72:A:H5''      | 1.85                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:03:575:LEU:HG    | 3:03:576:SER:H    | 1.68                     | 0.59              |
| 4:04:422:LEU:C     | 4:04:423:LEU:HD12 | 2.27                     | 0.59              |
| 7:E:25:PRO:C       | 7:E:28:LYS:H      | 2.11                     | 0.59              |
| 10:H:159:SER:HB3   | 10:H:162:GLU:HB2  | 1.84                     | 0.59              |
| 1:A:1047:G:H5''    | 19:Q:3:GLN:HG3    | 1.84                     | 0.59              |
| 4:04:415:VAL:HG23  | 4:04:416:ILE:HG13 | 1.85                     | 0.59              |
| 3:03:94:ALA:HB2    | 3:03:129:LEU:HD11 | 1.83                     | 0.58              |
| 4:04:342:LEU:O     | 4:04:343:LEU:CB   | 2.48                     | 0.58              |
| 4:04:1153:PRO:HA   | 4:04:1214:PRO:O   | 2.02                     | 0.58              |
| 1:A:1345:U:H4'     | 1:A:1346:A:C8     | 2.38                     | 0.58              |
| 2:01:45:ARG:CB     | 2:02:38:THR:HB    | 2.33                     | 0.58              |
| 2:01:48:LEU:HD23   | 2:01:180:VAL:HG21 | 1.85                     | 0.58              |
| 2:02:86:LYS:HG2    | 2:02:174:ASP:H    | 1.67                     | 0.58              |
| 3:03:1132:LEU:HD23 | 3:03:1132:LEU:O   | 2.02                     | 0.58              |
| 4:04:475:GLU:O     | 4:04:479:GLU:HG3  | 2.03                     | 0.58              |
| 4:04:797:THR:HG22  | 4:04:924:GLY:HA3  | 1.84                     | 0.58              |
| 8:F:59:PRO:HD3     | 15:M:94:ALA:HB1   | 1.84                     | 0.58              |
| 23:U:30:LYS:HA     | 23:U:33:ILE:HG12  | 1.85                     | 0.58              |
| 3:03:107:ARG:HG2   | 3:03:108:GLU:HG3  | 1.84                     | 0.58              |
| 3:03:702:THR:HG23  | 3:03:704:MET:H    | 1.67                     | 0.58              |
| 1:A:440:C:C3'      | 1:A:441:A:H5''    | 2.32                     | 0.58              |
| 2:02:155:ALA:HB1   | 2:02:172:LEU:HD12 | 1.86                     | 0.58              |
| 3:03:971:LEU:O     | 3:03:975:ILE:HG13 | 2.03                     | 0.58              |
| 4:04:356:THR:HG23  | 4:04:448:GLN:HG2  | 1.85                     | 0.58              |
| 1:A:750:C:H2'      | 1:A:751:U:C6      | 2.39                     | 0.58              |
| 1:A:1108:G:H5'     | 8:F:175:HIS:ND1   | 2.18                     | 0.58              |
| 3:03:426:ILE:HG22  | 3:03:430:LYS:HE3  | 1.86                     | 0.58              |
| 3:03:738:GLU:HA    | 3:03:741:MET:HB3  | 1.84                     | 0.58              |
| 9:G:103:ARG:HB3    | 9:G:167:PRO:HG2   | 1.86                     | 0.58              |
| 14:L:41:GLU:HG2    | 14:L:71:ILE:HG21  | 1.85                     | 0.58              |
| 18:P:16:ILE:H      | 18:P:16:ILE:CD1   | 2.17                     | 0.58              |
| 1:A:392:C:H2'      | 1:A:393:A:H8      | 1.68                     | 0.58              |
| 4:04:109:SER:CB    | 4:04:279:LEU:HD13 | 2.30                     | 0.58              |
| 4:04:120:LEU:O     | 4:04:122:SER:N    | 2.37                     | 0.58              |
| 25:W:30:PHE:HB3    | 25:W:53:MET:HA    | 1.86                     | 0.58              |
| 1:A:664:G:OP1      | 23:U:57:ARG:HD2   | 2.04                     | 0.58              |
| 2:01:71:LYS:O      | 2:01:74:VAL:HG12  | 2.04                     | 0.58              |
| 2:01:130:ILE:N     | 2:01:130:ILE:HD12 | 2.19                     | 0.58              |
| 3:03:31:GLN:HE22   | 3:03:456:VAL:HG21 | 1.68                     | 0.58              |
| 3:03:204:LEU:HD22  | 3:03:208:ILE:HD13 | 1.86                     | 0.58              |
| 3:03:796:LEU:H     | 3:03:796:LEU:HD12 | 1.68                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:04:360:TYR:HA    | 4:04:626:TYR:HE1   | 1.69                     | 0.58              |
| 4:04:847:ASP:HB3   | 4:04:856:ILE:HD13  | 1.85                     | 0.58              |
| 7:E:34:ALA:H       | 7:E:41:ILE:HB      | 1.68                     | 0.58              |
| 1:A:917:G:H2'      | 1:A:918:A:C8       | 2.39                     | 0.58              |
| 2:02:33:ARG:HD3    | 2:02:33:ARG:N      | 2.17                     | 0.58              |
| 4:04:1320:ILE:HG21 | 4:04:1349:GLU:HA   | 1.86                     | 0.58              |
| 10:H:44:ARG:HA     | 10:H:71:ILE:O      | 2.04                     | 0.58              |
| 17:O:89:LEU:HD12   | 17:O:89:LEU:N      | 2.18                     | 0.58              |
| 3:03:864:LYS:HZ1   | 3:03:882:ILE:H     | 1.50                     | 0.58              |
| 3:03:1141:LEU:O    | 3:03:1145:ILE:HG12 | 2.04                     | 0.58              |
| 4:04:1323:ALA:HA   | 4:04:1331:VAL:HG21 | 1.86                     | 0.58              |
| 3:03:17:LYS:HD3    | 3:03:1155:VAL:HG21 | 1.86                     | 0.57              |
| 3:03:322:LEU:O     | 3:03:322:LEU:HD23  | 2.04                     | 0.57              |
| 4:04:30:ILE:HD13   | 4:04:243:PRO:HG3   | 1.85                     | 0.57              |
| 4:04:520:ALA:HB1   | 4:04:546:ALA:HA    | 1.85                     | 0.57              |
| 14:L:11:ARG:HG2    | 14:L:76:GLY:HA3    | 1.86                     | 0.57              |
| 26:X:16:LEU:HA     | 26:X:18:ARG:HH11   | 1.67                     | 0.57              |
| 1:A:867:G:H2'      | 1:A:868:C:C6       | 2.38                     | 0.57              |
| 1:A:1304:G:N2      | 1:A:1333:A:H62     | 1.89                     | 0.57              |
| 1:A:1345:U:H4'     | 1:A:1346:A:H8      | 1.69                     | 0.57              |
| 3:03:10:ARG:HD3    | 3:03:1181:PRO:HG2  | 1.86                     | 0.57              |
| 4:04:1060:VAL:HG13 | 4:04:1106:ILE:HA   | 1.87                     | 0.57              |
| 12:J:68:VAL:HG21   | 12:J:103:ILE:HD11  | 1.86                     | 0.57              |
| 22:T:70:LYS:HB2    | 22:T:70:LYS:NZ     | 2.19                     | 0.57              |
| 1:A:1500:A:H5''    | 1:A:1508:A:H5''    | 1.84                     | 0.57              |
| 2:02:222:THR:O     | 2:02:226:GLU:HG2   | 2.04                     | 0.57              |
| 3:03:180:ARG:HB3   | 3:03:396:ASP:HB3   | 1.85                     | 0.57              |
| 1:A:687:A:H62      | 1:A:703:G:H21      | 1.50                     | 0.57              |
| 1:A:1225:A:H5'     | 1:A:1226:C:OP2     | 2.05                     | 0.57              |
| 3:03:74:ARG:HD2    | 3:03:75:LEU:H      | 1.69                     | 0.57              |
| 7:E:76:ALA:HB2     | 7:E:210:VAL:HG21   | 1.84                     | 0.57              |
| 9:G:190:LEU:CD1    | 9:G:192:ALA:H      | 2.17                     | 0.57              |
| 12:J:49:LEU:HD12   | 12:J:50:ALA:N      | 2.19                     | 0.57              |
| 1:A:1118:U:H4'     | 14:L:84:ARG:HH12   | 1.69                     | 0.57              |
| 2:01:111:THR:HA    | 2:01:129:VAL:HA    | 1.85                     | 0.57              |
| 3:03:30:ILE:HD12   | 3:03:30:ILE:N      | 2.20                     | 0.57              |
| 3:03:594:VAL:HG22  | 3:03:599:VAL:HG13  | 1.85                     | 0.57              |
| 4:04:107:LEU:HD11  | 4:04:239:LEU:HD12  | 1.85                     | 0.57              |
| 7:E:16:PHE:HD2     | 7:E:41:ILE:HG23    | 1.68                     | 0.57              |
| 3:03:405:PHE:HE2   | 3:03:424:ASP:HB3   | 1.70                     | 0.57              |
| 3:03:617:ALA:HB3   | 3:03:653:MET:HG3   | 1.86                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:04:1149:ARG:HD3  | 4:04:1150:PRO:O    | 2.05                     | 0.57              |
| 10:H:149:PRO:HG3   | 13:K:98:LEU:HD21   | 1.86                     | 0.57              |
| 14:L:91:GLU:HA     | 14:L:94:ARG:HB2    | 1.86                     | 0.57              |
| 19:Q:5:MET:HA      | 19:Q:5:MET:HE3     | 1.86                     | 0.57              |
| 3:03:53:PHE:O      | 3:03:57:PHE:HB2    | 2.04                     | 0.57              |
| 4:04:700:ASN:O     | 4:04:704:GLU:HB2   | 2.04                     | 0.57              |
| 8:F:163:ARG:HD3    | 8:F:163:ARG:N      | 2.18                     | 0.57              |
| 18:P:24:VAL:HG23   | 18:P:28:ARG:HB3    | 1.87                     | 0.57              |
| 20:R:21:THR:HA     | 20:R:26:VAL:HG11   | 1.86                     | 0.57              |
| 24:V:30:LEU:HD22   | 24:V:48:ILE:HG22   | 1.85                     | 0.57              |
| 26:X:18:ARG:HA     | 26:X:21:ARG:HH11   | 1.68                     | 0.57              |
| 2:02:100:LEU:HD21  | 2:02:121:VAL:HG21  | 1.85                     | 0.57              |
| 4:04:65:VAL:HG22   | 4:04:98:ARG:NH1    | 2.19                     | 0.57              |
| 4:04:597:GLY:H     | 4:04:600:ALA:HB3   | 1.68                     | 0.57              |
| 4:04:609:TYR:HA    | 4:04:613:GLY:O     | 2.05                     | 0.57              |
| 4:04:627:THR:HA    | 4:04:630:ALA:HB3   | 1.87                     | 0.57              |
| 7:E:21:ARG:C       | 7:E:23:TRP:HD1     | 2.13                     | 0.57              |
| 24:V:30:LEU:HD12   | 24:V:30:LEU:N      | 2.19                     | 0.57              |
| 3:03:1255:THR:HG22 | 3:03:1256:GLN:N    | 2.15                     | 0.57              |
| 7:E:103:ASN:O      | 7:E:107:VAL:HG23   | 2.05                     | 0.57              |
| 16:N:74:LYS:HD3    | 16:N:74:LYS:H      | 1.69                     | 0.57              |
| 21:S:4:ILE:HD12    | 21:S:67:ILE:HG13   | 1.87                     | 0.57              |
| 25:W:75:LYS:HA     | 25:W:78:LEU:HB3    | 1.86                     | 0.57              |
| 2:02:100:LEU:HD21  | 2:02:121:VAL:HG11  | 1.87                     | 0.57              |
| 3:03:1109:ILE:O    | 3:03:1112:ILE:HG22 | 2.04                     | 0.57              |
| 3:03:1275:VAL:O    | 3:03:1279:GLU:HG3  | 2.05                     | 0.57              |
| 4:04:378:LYS:HZ2   | 4:04:401:VAL:HG21  | 1.70                     | 0.57              |
| 4:04:778:GLY:O     | 4:04:781:LYS:HB3   | 2.05                     | 0.57              |
| 4:04:1157:ALA:HB2  | 4:04:1210:ILE:HD11 | 1.86                     | 0.57              |
| 10:H:15:ILE:N      | 10:H:15:ILE:HD12   | 2.20                     | 0.57              |
| 16:N:84:MET:HG2    | 16:N:110:THR:HB    | 1.86                     | 0.57              |
| 1:A:39:G:C3'       | 1:A:40:C:H5''      | 2.35                     | 0.56              |
| 1:A:632:U:H3'      | 1:A:633:G:H5'      | 1.85                     | 0.56              |
| 2:01:13:LEU:HD23   | 2:01:13:LEU:H      | 1.70                     | 0.56              |
| 2:02:102:LEU:C     | 2:02:102:LEU:HD13  | 2.30                     | 0.56              |
| 4:04:952:VAL:HG22  | 4:04:954:ASN:H     | 1.69                     | 0.56              |
| 4:04:1216:ALA:O    | 4:04:1220:ILE:HG12 | 2.05                     | 0.56              |
| 8:F:133:MET:O      | 8:F:137:VAL:HG23   | 2.05                     | 0.56              |
| 11:I:89:VAL:O      | 11:I:90:MET:HE2    | 2.04                     | 0.56              |
| 11:I:93:LYS:HB3    | 11:I:93:LYS:NZ     | 2.20                     | 0.56              |
| 21:S:71:VAL:O      | 21:S:75:ILE:HG12   | 2.05                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:W:20:ASN:O      | 25:W:24:ARG:HG3    | 2.04                     | 0.56              |
| 1:A:190:A:H2       | 25:W:47:GLN:HB3    | 1.69                     | 0.56              |
| 2:01:78:ILE:O      | 2:01:82:LEU:HG     | 2.05                     | 0.56              |
| 3:03:1082:ILE:H    | 3:03:1082:ILE:CD1  | 2.14                     | 0.56              |
| 4:04:511:TYR:O     | 4:04:515:ARG:HB2   | 2.05                     | 0.56              |
| 4:04:844:THR:CG2   | 4:04:864:LEU:HD11  | 2.35                     | 0.56              |
| 15:M:89:ARG:C      | 15:M:90:LEU:HD12   | 2.30                     | 0.56              |
| 1:A:50:A:H4'       | 1:A:51:A:H5'       | 1.87                     | 0.56              |
| 1:A:376:G:H2'      | 1:A:377:G:C5'      | 2.35                     | 0.56              |
| 1:A:1101:A:N7      | 7:E:171:ILE:HD13   | 2.19                     | 0.56              |
| 1:A:1308:U:H5''    | 18:P:96:VAL:HG22   | 1.87                     | 0.56              |
| 1:A:1323:G:H2'     | 1:A:1324:A:H8      | 1.68                     | 0.56              |
| 3:03:243:PRO:HB3   | 3:03:274:ILE:HG23  | 1.87                     | 0.56              |
| 3:03:405:PHE:O     | 3:03:409:LEU:HG    | 2.05                     | 0.56              |
| 4:04:449:LEU:HG    | 4:04:450:HIS:H     | 1.69                     | 0.56              |
| 4:04:865:HIS:HE1   | 4:04:867:GLN:HB2   | 1.70                     | 0.56              |
| 7:E:157:LEU:HD12   | 7:E:157:LEU:O      | 2.05                     | 0.56              |
| 15:M:77:VAL:HG12   | 15:M:78:GLU:N      | 2.21                     | 0.56              |
| 19:Q:43:ALA:O      | 19:Q:47:LEU:HB2    | 2.05                     | 0.56              |
| 21:S:43:ALA:HA     | 21:S:46:LYS:HZ3    | 1.69                     | 0.56              |
| 26:X:36:GLU:HG3    | 26:X:38:TYR:H      | 1.71                     | 0.56              |
| 1:A:1167:A:H2'     | 1:A:1167:A:N3      | 2.20                     | 0.56              |
| 3:03:387:ASN:HA    | 3:03:391:SER:HB2   | 1.86                     | 0.56              |
| 3:03:1109:ILE:HG12 | 4:04:764:ARG:HG3   | 1.87                     | 0.56              |
| 3:03:1317:PRO:HB3  | 4:04:1355:ARG:HG2  | 1.86                     | 0.56              |
| 4:04:205:LEU:HD23  | 4:04:217:LEU:HD12  | 1.88                     | 0.56              |
| 4:04:249:LEU:C     | 4:04:251:PRO:HD3   | 2.31                     | 0.56              |
| 4:04:418:GLU:HB3   | 5:05:45:LYS:HD3    | 1.87                     | 0.56              |
| 1:A:250:A:H4'      | 1:A:252:U:C6       | 2.40                     | 0.56              |
| 1:A:920:U:H2'      | 1:A:921:U:C6       | 2.39                     | 0.56              |
| 2:01:27:THR:C      | 2:01:28:LEU:HD12   | 2.31                     | 0.56              |
| 3:03:409:LEU:HD21  | 3:03:428:VAL:HG22  | 1.88                     | 0.56              |
| 3:03:431:LYS:O     | 3:03:435:ILE:HG13  | 2.06                     | 0.56              |
| 3:03:1192:GLU:O    | 3:03:1196:LYS:HG2  | 2.06                     | 0.56              |
| 3:03:1327:LEU:HG   | 3:03:1337:ILE:HG21 | 1.88                     | 0.56              |
| 4:04:333:GLY:HA3   | 4:04:338:PHE:CZ    | 2.41                     | 0.56              |
| 4:04:650:LYS:O     | 4:04:654:ILE:HG13  | 2.04                     | 0.56              |
| 1:A:39:G:H2'       | 1:A:40:C:H5''      | 1.88                     | 0.56              |
| 2:01:214:GLU:HA    | 2:01:217:ILE:HG22  | 1.88                     | 0.56              |
| 3:03:1151:LEU:HD12 | 3:03:1152:GLY:N    | 2.21                     | 0.56              |
| 4:04:530:PRO:O     | 4:04:533:ALA:HB3   | 2.06                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 16:N:22:ILE:HG23   | 16:N:31:VAL:HG22  | 1.87                     | 0.56              |
| 16:N:109:ILE:HD12  | 16:N:109:ILE:N    | 2.21                     | 0.56              |
| 2:01:231:PHE:CE2   | 2:02:39:LEU:HD11  | 2.40                     | 0.56              |
| 2:02:183:ILE:N     | 2:02:183:ILE:HD12 | 2.20                     | 0.56              |
| 3:03:519:ASN:HD21  | 3:03:521:LEU:HB3  | 1.69                     | 0.56              |
| 16:N:81:LEU:HD23   | 16:N:81:LEU:H     | 1.71                     | 0.56              |
| 2:02:56:VAL:HA     | 2:02:146:VAL:HA   | 1.88                     | 0.56              |
| 3:03:1221:PHE:HB3  | 4:04:636:GLY:HA2  | 1.88                     | 0.56              |
| 4:04:1327:GLU:HB3  | 4:04:1330:ARG:CG  | 2.34                     | 0.56              |
| 7:E:87:CYS:HB2     | 7:E:89:GLN:NE2    | 2.12                     | 0.56              |
| 9:G:118:SER:HA     | 9:G:130:ASN:HB2   | 1.88                     | 0.56              |
| 15:M:80:THR:HG22   | 15:M:81:GLU:H     | 1.70                     | 0.56              |
| 25:W:8:LYS:HB3     | 25:W:8:LYS:HZ2    | 1.68                     | 0.56              |
| 25:W:56:ILE:HD12   | 25:W:56:ILE:N     | 2.21                     | 0.56              |
| 3:03:127:ILE:O     | 3:03:127:ILE:HG13 | 2.06                     | 0.56              |
| 4:04:547:ARG:HH11  | 4:04:547:ARG:HG3  | 1.70                     | 0.56              |
| 4:04:1304:ARG:HH11 | 4:04:1304:ARG:HG3 | 1.71                     | 0.56              |
| 3:03:255:ILE:HB    | 3:03:263:VAL:HB   | 1.87                     | 0.56              |
| 3:03:476:LYS:HA    | 3:03:479:LEU:HD12 | 1.88                     | 0.56              |
| 3:03:490:GLN:H     | 3:03:493:ILE:HG22 | 1.71                     | 0.56              |
| 3:03:1084:ASP:O    | 3:03:1085:MET:HE2 | 2.05                     | 0.56              |
| 3:03:1150:ASP:O    | 3:03:1152:GLY:N   | 2.34                     | 0.56              |
| 4:04:37:GLU:HG3    | 4:04:105:ILE:HA   | 1.88                     | 0.56              |
| 4:04:417:ARG:HG2   | 4:04:417:ARG:HH11 | 1.71                     | 0.56              |
| 4:04:579:LEU:O     | 4:04:583:VAL:HG23 | 2.06                     | 0.56              |
| 7:E:39:HIS:O       | 7:E:40:ILE:CG2    | 2.47                     | 0.56              |
| 7:E:209:ALA:HB1    | 7:E:213:TYR:CE2   | 2.41                     | 0.56              |
| 19:Q:53:ASP:HA     | 19:Q:58:ARG:HD3   | 1.88                     | 0.56              |
| 26:X:17:ARG:HB2    | 26:X:20:LYS:HD2   | 1.88                     | 0.56              |
| 1:A:219:U:H2'      | 1:A:220:G:H5''    | 1.86                     | 0.55              |
| 3:03:414:ILE:HD12  | 3:03:415:GLU:N    | 2.21                     | 0.55              |
| 9:G:7:LYS:HB3      | 9:G:20:LEU:HD13   | 1.88                     | 0.55              |
| 14:L:43:ALA:HB1    | 14:L:46:VAL:HG21  | 1.87                     | 0.55              |
| 15:M:10:LEU:HD23   | 15:M:98:VAL:HA    | 1.88                     | 0.55              |
| 26:X:35:ARG:HD3    | 26:X:37:PHE:CE2   | 2.41                     | 0.55              |
| 3:03:30:ILE:H      | 3:03:30:ILE:CD1   | 2.20                     | 0.55              |
| 3:03:896:THR:O     | 3:03:900:LYS:HG3  | 2.06                     | 0.55              |
| 4:04:431:ARG:HD3   | 4:04:432:LEU:N    | 2.21                     | 0.55              |
| 1:A:39:G:H3'       | 1:A:40:C:H5''     | 1.88                     | 0.55              |
| 1:A:440:C:C2'      | 1:A:441:A:H5''    | 2.35                     | 0.55              |
| 4:04:205:LEU:HD13  | 4:04:205:LEU:O    | 2.07                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:E:13:GLY:C      | 7:E:14:VAL:HG22    | 2.31                     | 0.55              |
| 9:G:100:VAL:HG21  | 9:G:136:VAL:HG21   | 1.88                     | 0.55              |
| 1:A:1299:A:H2'    | 1:A:1300:G:H4'     | 1.87                     | 0.55              |
| 3:03:97:ARG:NH1   | 3:03:123:TYR:HB2   | 2.21                     | 0.55              |
| 3:03:560:PRO:HD3  | 4:04:773:PHE:HE1   | 1.70                     | 0.55              |
| 4:04:66:LYS:HD3   | 4:04:67:ASP:N      | 2.22                     | 0.55              |
| 4:04:306:LEU:O    | 4:04:327:LEU:HD12  | 2.06                     | 0.55              |
| 4:04:797:THR:HA   | 4:04:800:LEU:HB2   | 1.88                     | 0.55              |
| 5:05:28:ARG:HA    | 5:05:31:GLN:HG3    | 1.87                     | 0.55              |
| 7:E:44:GLU:C      | 7:E:46:THR:H       | 2.14                     | 0.55              |
| 13:K:10:LEU:HD22  | 13:K:74:ILE:HD11   | 1.89                     | 0.55              |
| 16:N:86:LYS:HA    | 16:N:113:THR:HA    | 1.88                     | 0.55              |
| 3:03:454:ARG:HH21 | 3:03:535:PRO:HG2   | 1.70                     | 0.55              |
| 4:04:1227:HIS:HA  | 4:04:1230:THR:HG22 | 1.88                     | 0.55              |
| 9:G:71:PHE:HE1    | 9:G:93:LEU:HD11    | 1.72                     | 0.55              |
| 25:W:8:LYS:HB3    | 25:W:8:LYS:HZ3     | 1.71                     | 0.55              |
| 3:03:22:LEU:HB2   | 3:03:655:VAL:HG11  | 1.89                     | 0.55              |
| 3:03:150:HIS:NE2  | 3:03:454:ARG:HG3   | 2.22                     | 0.55              |
| 3:03:943:LYS:HA   | 3:03:946:LEU:HD12  | 1.88                     | 0.55              |
| 4:04:77:ARG:HG2   | 7:E:20:THR:HG23    | 1.88                     | 0.55              |
| 7:E:23:TRP:CE3    | 7:E:25:PRO:HB3     | 2.41                     | 0.55              |
| 10:H:133:ILE:HD12 | 10:H:133:ILE:N     | 2.18                     | 0.55              |
| 1:A:1210:C:H2'    | 1:A:1211:U:H5'     | 1.87                     | 0.55              |
| 2:01:143:ARG:HD3  | 2:01:143:ARG:N     | 2.22                     | 0.55              |
| 3:03:499:SER:O    | 3:03:503:LYS:HB2   | 2.06                     | 0.55              |
| 4:04:202:ARG:HA   | 4:04:205:LEU:HB2   | 1.89                     | 0.55              |
| 4:04:572:THR:OG1  | 4:04:576:ARG:HB2   | 2.05                     | 0.55              |
| 4:04:746:LEU:HG   | 4:04:758:PRO:HG3   | 1.89                     | 0.55              |
| 4:04:850:LYS:HB3  | 4:04:851:PRO:HD2   | 1.88                     | 0.55              |
| 7:E:47:VAL:HB     | 7:E:48:PRO:CD      | 2.30                     | 0.55              |
| 14:L:20:ILE:HD12  | 14:L:85:ALA:HB3    | 1.88                     | 0.55              |
| 19:Q:22:LYS:C     | 19:Q:24:ALA:H      | 2.15                     | 0.55              |
| 3:03:796:LEU:HD12 | 3:03:796:LEU:N     | 2.22                     | 0.55              |
| 3:03:1150:ASP:O   | 3:03:1151:LEU:HG   | 2.07                     | 0.55              |
| 4:04:116:PHE:HB3  | 4:04:123:ARG:HB2   | 1.89                     | 0.55              |
| 4:04:800:LEU:O    | 4:04:803:VAL:HG12  | 2.06                     | 0.55              |
| 19:Q:68:ARG:HH22  | 19:Q:80:ARG:NH2    | 2.05                     | 0.55              |
| 20:R:2:LEU:HG     | 20:R:7:THR:OG1     | 2.07                     | 0.55              |
| 1:A:18:C:H4'      | 1:A:1078:U:O2      | 2.07                     | 0.55              |
| 1:A:765:G:H21     | 1:A:816:A:H61      | 1.54                     | 0.55              |
| 1:A:1496:C:H1'    | 1:A:1517:G:H1      | 1.71                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:01:9:LEU:HD23    | 2:01:9:LEU:H       | 1.71                     | 0.55              |
| 3:03:980:VAL:HA    | 3:03:984:VAL:HA    | 1.88                     | 0.55              |
| 3:03:1285:TYR:O    | 3:03:1288:GLN:HB3  | 2.07                     | 0.55              |
| 4:04:186:GLN:HB2   | 4:04:238:ILE:HG13  | 1.88                     | 0.55              |
| 4:04:294:ASN:O     | 4:04:298:MET:HG3   | 2.07                     | 0.55              |
| 7:E:42:ASN:HD22    | 7:E:189:THR:HG23   | 1.70                     | 0.55              |
| 7:E:121:SER:HA     | 7:E:126:PHE:HB3    | 1.89                     | 0.55              |
| 19:Q:26:LEU:HD22   | 19:Q:43:ALA:HA     | 1.88                     | 0.55              |
| 24:V:10:ILE:C      | 24:V:10:ILE:HD12   | 2.32                     | 0.55              |
| 1:A:1395:C:O2'     | 1:A:1396:A:H5'     | 2.07                     | 0.55              |
| 2:01:64:VAL:HG13   | 2:01:69:SER:OG     | 2.07                     | 0.55              |
| 2:02:57:THR:HG22   | 2:02:58:GLU:HG3    | 1.89                     | 0.55              |
| 4:04:693:VAL:HG12  | 4:04:697:MET:HE2   | 1.89                     | 0.55              |
| 15:M:80:THR:HG22   | 15:M:81:GLU:N      | 2.22                     | 0.55              |
| 18:P:76:ILE:O      | 18:P:80:MET:HG3    | 2.07                     | 0.55              |
| 3:03:1146:GLN:OE1  | 3:03:1146:GLN:HA   | 2.08                     | 0.54              |
| 4:04:255:LEU:HD23  | 4:04:261:ALA:HB2   | 1.88                     | 0.54              |
| 4:04:473:THR:HG23  | 4:04:476:ALA:H     | 1.72                     | 0.54              |
| 7:E:213:TYR:O      | 7:E:217:VAL:HG23   | 2.07                     | 0.54              |
| 9:G:97:LEU:HB2     | 9:G:134:TYR:HB3    | 1.88                     | 0.54              |
| 21:S:57:ILE:O      | 21:S:61:VAL:HG23   | 2.06                     | 0.54              |
| 23:U:50:LYS:O      | 23:U:54:GLN:HG2    | 2.07                     | 0.54              |
| 2:02:118:ASP:HB2   | 2:02:121:VAL:H     | 1.72                     | 0.54              |
| 3:03:1062:PRO:HG3  | 3:03:1079:ILE:HG22 | 1.89                     | 0.54              |
| 4:04:478:LEU:HD23  | 4:04:478:LEU:C     | 2.32                     | 0.54              |
| 4:04:485:MET:HB3   | 4:04:488:ASN:ND2   | 2.22                     | 0.54              |
| 10:H:132:PRO:HA    | 10:H:135:VAL:HG22  | 1.89                     | 0.54              |
| 17:O:29:LYS:NZ     | 17:O:58:ASN:ND2    | 2.55                     | 0.54              |
| 13:K:50:VAL:O      | 13:K:50:VAL:HG22   | 2.07                     | 0.54              |
| 23:U:36:SER:HB3    | 23:U:38:LYS:HE3    | 1.88                     | 0.54              |
| 2:01:82:LEU:HD23   | 2:01:85:LEU:HD12   | 1.89                     | 0.54              |
| 3:03:817:LEU:HD21  | 3:03:1080:ASN:ND2  | 2.23                     | 0.54              |
| 4:04:289:ASP:HA    | 4:04:292:VAL:HG22  | 1.88                     | 0.54              |
| 4:04:1218:HIS:O    | 4:04:1221:LEU:HB3  | 2.07                     | 0.54              |
| 4:04:1320:ILE:HD12 | 4:04:1349:GLU:HG3  | 1.88                     | 0.54              |
| 21:S:8:ARG:HH11    | 21:S:8:ARG:HG3     | 1.72                     | 0.54              |
| 22:T:70:LYS:HB2    | 22:T:70:LYS:HZ2    | 1.72                     | 0.54              |
| 1:A:78:A:H2'       | 1:A:79:G:H4'       | 1.89                     | 0.54              |
| 3:03:414:ILE:HD12  | 3:03:414:ILE:C     | 2.32                     | 0.54              |
| 3:03:840:SER:HA    | 3:03:886:LYS:NZ    | 2.23                     | 0.54              |
| 4:04:320:ASN:HD22  | 4:04:321:LYS:H     | 1.55                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:04:662:ALA:O     | 4:04:666:GLU:HG3   | 2.08                     | 0.54              |
| 10:H:44:ARG:HG2    | 10:H:70:MET:HE3    | 1.89                     | 0.54              |
| 15:M:77:VAL:HG12   | 15:M:78:GLU:H      | 1.71                     | 0.54              |
| 17:O:17:LYS:HB2    | 17:O:17:LYS:NZ     | 2.22                     | 0.54              |
| 19:Q:84:ARG:C      | 19:Q:84:ARG:HD3    | 2.32                     | 0.54              |
| 22:T:30:HIS:HB3    | 22:T:34:GLY:H      | 1.72                     | 0.54              |
| 3:03:966:ILE:HD12  | 3:03:966:ILE:N     | 2.22                     | 0.54              |
| 3:03:1106:ARG:N    | 3:03:1106:ARG:HD2  | 2.23                     | 0.54              |
| 4:04:71:LEU:O      | 4:04:71:LEU:HD13   | 2.06                     | 0.54              |
| 4:04:327:LEU:C     | 4:04:330:MET:HB2   | 2.33                     | 0.54              |
| 4:04:680:ASN:HA    | 4:04:683:ILE:HD12  | 1.89                     | 0.54              |
| 7:E:44:GLU:C       | 7:E:46:THR:N       | 2.63                     | 0.54              |
| 11:I:9:MET:HE1     | 23:U:65:LEU:O      | 2.07                     | 0.54              |
| 24:V:4:LEU:HG      | 24:V:6:LYS:H       | 1.72                     | 0.54              |
| 1:A:1329:A:H5'     | 18:P:25:GLY:N      | 2.19                     | 0.54              |
| 3:03:886:LYS:H     | 3:03:917:SER:HA    | 1.72                     | 0.54              |
| 4:04:187:ALA:HA    | 4:04:190:LYS:HZ2   | 1.72                     | 0.54              |
| 4:04:1221:LEU:HD13 | 4:04:1221:LEU:C    | 2.33                     | 0.54              |
| 4:04:1282:TYR:O    | 4:04:1285:VAL:HG12 | 2.06                     | 0.54              |
| 1:A:744:C:H2'      | 1:A:745:G:H8       | 1.73                     | 0.54              |
| 1:A:1253:G:OP1     | 15:M:46:LYS:HB2    | 2.07                     | 0.54              |
| 2:01:102:LEU:HD23  | 2:01:115:ILE:HG12  | 1.90                     | 0.54              |
| 4:04:76:LYS:HD3    | 4:04:76:LYS:N      | 2.23                     | 0.54              |
| 4:04:132:LEU:O     | 4:04:132:LEU:HD13  | 2.08                     | 0.54              |
| 4:04:532:GLU:O     | 4:04:536:LEU:HD23  | 2.07                     | 0.54              |
| 24:V:40:PHE:HB2    | 24:V:43:MET:HG3    | 1.89                     | 0.54              |
| 3:03:222:ASP:OD1   | 3:03:227:LYS:HE2   | 2.08                     | 0.54              |
| 3:03:445:ILE:HG12  | 3:03:451:ARG:HH21  | 1.72                     | 0.54              |
| 4:04:902:ASP:HB3   | 4:04:1251:LYS:HZ1  | 1.73                     | 0.54              |
| 4:04:1238:GLN:O    | 4:04:1242:ARG:HG2  | 2.08                     | 0.54              |
| 5:05:37:PRO:HG3    | 5:05:41:GLU:OE1    | 2.08                     | 0.54              |
| 1:A:1502:A:H5'     | 1:A:1504:G:N7      | 2.23                     | 0.54              |
| 3:03:454:ARG:HG2   | 3:03:458:GLU:OE2   | 2.08                     | 0.54              |
| 3:03:1255:THR:HB   | 3:03:1257:GLN:HG2  | 1.89                     | 0.54              |
| 4:04:1163:VAL:HG13 | 4:04:1200:GLU:HA   | 1.90                     | 0.54              |
| 16:N:85:VAL:HG11   | 16:N:92:ARG:HG2    | 1.90                     | 0.54              |
| 21:S:61:VAL:HG21   | 21:S:67:ILE:HD11   | 1.89                     | 0.54              |
| 25:W:54:GLN:N      | 25:W:55:PRO:CD     | 2.71                     | 0.54              |
| 1:A:675:A:H2'      | 1:A:676:A:H8       | 1.72                     | 0.53              |
| 1:A:1148:U:H5'     | 14:L:6:TYR:OH      | 2.08                     | 0.53              |
| 4:04:317:THR:HG23  | 4:04:320:ASN:HB3   | 1.90                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:04:418:GLU:O    | 4:04:420:PRO:HD3   | 2.08                     | 0.53              |
| 4:04:473:THR:O    | 4:04:477:GLN:HG3   | 2.07                     | 0.53              |
| 4:04:826:ILE:HG12 | 4:04:831:VAL:HB    | 1.88                     | 0.53              |
| 18:P:17:ALA:HB1   | 18:P:44:ILE:HD12   | 1.90                     | 0.53              |
| 1:A:309:A:H2'     | 1:A:310:G:H8       | 1.72                     | 0.53              |
| 1:A:626:G:H2'     | 1:A:627:G:H8       | 1.73                     | 0.53              |
| 1:A:1297:G:N2     | 12:J:113:LYS:HB3   | 2.23                     | 0.53              |
| 2:01:56:VAL:HA    | 2:01:146:VAL:HG22  | 1.89                     | 0.53              |
| 3:03:39:ILE:HA    | 3:03:49:LEU:HD12   | 1.90                     | 0.53              |
| 3:03:1328:LYS:NZ  | 4:04:245:LEU:HA    | 2.24                     | 0.53              |
| 4:04:619:ILE:O    | 4:04:623:GLN:HG2   | 2.08                     | 0.53              |
| 7:E:164:ILE:O     | 7:E:186:ILE:HG23   | 2.08                     | 0.53              |
| 9:G:9:LYS:O       | 9:G:13:ARG:HG2     | 2.07                     | 0.53              |
| 13:K:116:ARG:HB2  | 13:K:116:ARG:NH1   | 2.23                     | 0.53              |
| 16:N:33:ILE:HG13  | 16:N:41:LEU:HB2    | 1.91                     | 0.53              |
| 1:A:1268:G:H1'    | 1:A:1327:C:H5'     | 1.91                     | 0.53              |
| 1:A:1346:A:H2'    | 1:A:1346:A:N3      | 2.23                     | 0.53              |
| 2:02:65:LEU:HD22  | 2:02:65:LEU:N      | 2.24                     | 0.53              |
| 3:03:91:THR:HA    | 3:03:138:ILE:HA    | 1.89                     | 0.53              |
| 3:03:138:ILE:HB   | 3:03:143:ARG:CZ    | 2.38                     | 0.53              |
| 3:03:386:GLU:O    | 3:03:390:PHE:HB2   | 2.08                     | 0.53              |
| 4:04:210:SER:O    | 4:04:214:ARG:HG2   | 2.08                     | 0.53              |
| 4:04:345:LYS:O    | 4:04:346:ARG:HB2   | 2.07                     | 0.53              |
| 4:04:374:LEU:HD23 | 4:04:375:GLU:N     | 2.23                     | 0.53              |
| 7:E:21:ARG:HD3    | 7:E:22:TYR:H       | 1.72                     | 0.53              |
| 7:E:21:ARG:HB3    | 7:E:38:VAL:HA      | 1.91                     | 0.53              |
| 10:H:133:ILE:H    | 10:H:133:ILE:CD1   | 2.16                     | 0.53              |
| 10:H:136:VAL:O    | 10:H:140:ILE:HG12  | 2.08                     | 0.53              |
| 3:03:144:VAL:HG23 | 3:03:515:MET:HB2   | 1.90                     | 0.53              |
| 3:03:213:LEU:HD22 | 3:03:215:TYR:CZ    | 2.43                     | 0.53              |
| 3:03:479:LEU:HD23 | 3:03:487:LEU:CD1   | 2.37                     | 0.53              |
| 3:03:818:VAL:HG23 | 3:03:1076:ILE:HD13 | 1.91                     | 0.53              |
| 4:04:41:PRO:HB2   | 4:04:270:ARG:HG3   | 1.89                     | 0.53              |
| 7:E:99:GLY:HA3    | 7:E:103:ASN:HD22   | 1.72                     | 0.53              |
| 10:H:13:LYS:HG2   | 10:H:112:ALA:HB1   | 1.90                     | 0.53              |
| 11:I:51:ILE:HD12  | 11:I:86:ARG:HH21   | 1.72                     | 0.53              |
| 13:K:119:GLY:C    | 13:K:120:LEU:HD12  | 2.33                     | 0.53              |
| 1:A:440:C:H3'     | 1:A:441:A:H5''     | 1.90                     | 0.53              |
| 8:F:112:ALA:HB1   | 8:F:199:VAL:HG13   | 1.90                     | 0.53              |
| 10:H:56:PRO:HA    | 10:H:59:ILE:HG12   | 1.91                     | 0.53              |
| 12:J:24:LYS:HB2   | 12:J:24:LYS:NZ     | 2.23                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:U:61:ARG:O     | 23:U:65:LEU:HD13  | 2.09                     | 0.53              |
| 1:A:427:U:H1'     | 1:A:541:G:C5'     | 2.30                     | 0.53              |
| 1:A:570:G:H2'     | 1:A:571:U:C6      | 2.44                     | 0.53              |
| 1:A:584:G:H22     | 1:A:879:C:H4'     | 1.74                     | 0.53              |
| 1:A:1271:A:H5'    | 1:A:1314:C:H5''   | 1.91                     | 0.53              |
| 2:02:151:GLY:O    | 2:02:177:TYR:HB2  | 2.09                     | 0.53              |
| 3:03:1272:GLU:HA  | 3:03:1275:VAL:CG2 | 2.39                     | 0.53              |
| 4:04:659:ALA:O    | 4:04:663:GLU:HG2  | 2.08                     | 0.53              |
| 4:04:746:LEU:N    | 4:04:746:LEU:HD12 | 2.23                     | 0.53              |
| 1:A:260:G:H2'     | 1:A:261:U:C6      | 2.44                     | 0.53              |
| 1:A:1157:A:H61    | 1:A:1178:G:H1'    | 1.73                     | 0.53              |
| 2:01:45:ARG:HH22  | 3:03:1216:ARG:HA  | 1.74                     | 0.53              |
| 2:01:77:ASP:O     | 2:01:81:ILE:HG13  | 2.09                     | 0.53              |
| 2:02:83:LEU:HA    | 2:02:86:LYS:NZ    | 2.24                     | 0.53              |
| 3:03:682:GLY:O    | 3:03:686:GLN:HG3  | 2.09                     | 0.53              |
| 4:04:71:LEU:H     | 4:04:90:VAL:HG11  | 1.74                     | 0.53              |
| 4:04:612:LEU:HG   | 4:04:616:PRO:HG2  | 1.91                     | 0.53              |
| 4:04:646:ILE:HG12 | 4:04:764:ARG:HH21 | 1.74                     | 0.53              |
| 9:G:149:LYS:HB3   | 9:G:149:LYS:NZ    | 2.24                     | 0.53              |
| 12:J:55:LYS:HD2   | 12:J:59:GLU:OE2   | 2.09                     | 0.53              |
| 1:A:1118:U:OP1    | 14:L:105:ARG:HG3  | 2.09                     | 0.53              |
| 1:A:1315:U:H1'    | 1:A:1361:G:H4'    | 1.91                     | 0.53              |
| 3:03:243:PRO:HA   | 3:03:246:LEU:HD12 | 1.91                     | 0.53              |
| 3:03:263:VAL:HG22 | 3:03:273:HIS:HB3  | 1.90                     | 0.53              |
| 4:04:504:GLN:NE2  | 4:04:731:ARG:HD2  | 2.23                     | 0.53              |
| 1:A:686:U:O2'     | 1:A:687:A:H5'     | 2.09                     | 0.53              |
| 1:A:1369:C:H2'    | 1:A:1370:G:C8     | 2.44                     | 0.53              |
| 3:03:81:ASP:OD2   | 3:03:83:GLN:HB2   | 2.09                     | 0.53              |
| 3:03:103:VAL:C    | 3:03:104:ILE:HD12 | 2.33                     | 0.53              |
| 3:03:399:ALA:O    | 3:03:403:MET:HB2  | 2.09                     | 0.53              |
| 4:04:583:VAL:HG13 | 4:04:587:LEU:HD23 | 1.90                     | 0.53              |
| 4:04:705:THR:CG2  | 4:04:719:PHE:H    | 2.14                     | 0.53              |
| 19:Q:8:ARG:HB3    | 19:Q:12:ARG:NH1   | 2.22                     | 0.53              |
| 1:A:29:U:O2'      | 1:A:30:U:H5'      | 2.08                     | 0.53              |
| 2:01:155:ALA:HA   | 2:01:158:ARG:HE   | 1.74                     | 0.53              |
| 3:03:4:SER:H      | 3:03:7:GLU:HB2    | 1.74                     | 0.53              |
| 3:03:109:ALA:C    | 3:03:111:GLU:H    | 2.17                     | 0.53              |
| 3:03:605:TYR:C    | 3:03:606:LEU:HD12 | 2.33                     | 0.53              |
| 15:M:5:ARG:HH12   | 15:M:102:LEU:HB2  | 1.73                     | 0.53              |
| 18:P:74:MET:HE3   | 18:P:77:LYS:HB2   | 1.91                     | 0.53              |
| 24:V:4:LEU:HD23   | 24:V:4:LEU:N      | 2.24                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:1315:U:H2'     | 1:A:1316:G:O4'     | 2.10                     | 0.52              |
| 2:02:48:LEU:HD22   | 4:04:535:ARG:HA    | 1.91                     | 0.52              |
| 3:03:363:LEU:HD23  | 3:03:366:ILE:HD12  | 1.91                     | 0.52              |
| 4:04:130:MET:HB2   | 4:04:157:GLN:OE1   | 2.09                     | 0.52              |
| 4:04:141:PHE:CE1   | 4:04:181:GLY:HA3   | 2.44                     | 0.52              |
| 4:04:279:LEU:HD23  | 4:04:279:LEU:O     | 2.09                     | 0.52              |
| 4:04:487:THR:HG21  | 5:05:4:VAL:HG22    | 1.91                     | 0.52              |
| 7:E:140:GLU:O      | 7:E:144:LEU:HD23   | 2.09                     | 0.52              |
| 10:H:10:LEU:HD21   | 10:H:67:ARG:HE     | 1.74                     | 0.52              |
| 11:I:60:VAL:C      | 11:I:61:LEU:HD12   | 2.34                     | 0.52              |
| 25:W:15:LYS:O      | 25:W:19:HIS:HB3    | 2.09                     | 0.52              |
| 25:W:79:THR:HG23   | 25:W:82:ILE:HD11   | 1.90                     | 0.52              |
| 1:A:946:A:H1'      | 1:A:1333:A:C2      | 2.45                     | 0.52              |
| 4:04:53:ARG:O      | 4:04:53:ARG:HD3    | 2.10                     | 0.52              |
| 4:04:368:LEU:HD12  | 4:04:439:PRO:HB3   | 1.90                     | 0.52              |
| 12:J:40:SER:HA     | 12:J:43:TYR:CD2    | 2.42                     | 0.52              |
| 12:J:115:MET:SD    | 12:J:118:ARG:HD2   | 2.50                     | 0.52              |
| 18:P:44:ILE:HA     | 18:P:47:LEU:HG     | 1.89                     | 0.52              |
| 20:R:81:ILE:HG22   | 20:R:86:LEU:HD12   | 1.91                     | 0.52              |
| 1:A:511:C:O2'      | 1:A:512:U:H5'      | 2.09                     | 0.52              |
| 2:01:167:PRO:HG2   | 2:01:170:ARG:HE    | 1.73                     | 0.52              |
| 3:03:22:LEU:HB2    | 3:03:655:VAL:CG1   | 2.39                     | 0.52              |
| 3:03:838:CYS:HB2   | 3:03:918:LEU:HD22  | 1.91                     | 0.52              |
| 3:03:1308:ILE:HG22 | 3:03:1308:ILE:O    | 2.09                     | 0.52              |
| 4:04:531:LYS:O     | 4:04:534:GLU:HB3   | 2.10                     | 0.52              |
| 4:04:798:ARG:O     | 4:04:801:VAL:HG22  | 2.10                     | 0.52              |
| 9:G:82:LYS:HZ2     | 9:G:82:LYS:HA      | 1.74                     | 0.52              |
| 1:A:414:A:H2'      | 1:A:414:A:N3       | 2.24                     | 0.52              |
| 1:A:1369:C:H2'     | 1:A:1370:G:H8      | 1.73                     | 0.52              |
| 3:03:89:GLY:HA2    | 3:03:140:GLY:H     | 1.75                     | 0.52              |
| 3:03:1132:LEU:HD22 | 3:03:1177:ARG:NH1  | 2.25                     | 0.52              |
| 4:04:263:SER:C     | 4:04:265:LEU:H     | 2.16                     | 0.52              |
| 4:04:706:VAL:HG23  | 4:04:706:VAL:O     | 2.10                     | 0.52              |
| 4:04:767:LEU:HB2   | 4:04:771:GLN:OE1   | 2.10                     | 0.52              |
| 7:E:47:VAL:CB      | 7:E:48:PRO:HD3     | 2.32                     | 0.52              |
| 10:H:68:ARG:O      | 10:H:68:ARG:HD2    | 2.10                     | 0.52              |
| 18:P:48:SER:O      | 18:P:52:ILE:HG13   | 2.10                     | 0.52              |
| 2:01:82:LEU:HB3    | 2:01:173:VAL:HG11  | 1.92                     | 0.52              |
| 3:03:34:SER:HA     | 3:03:37:LYS:HZ1    | 1.75                     | 0.52              |
| 3:03:1053:TYR:C    | 3:03:1054:LEU:HD12 | 2.35                     | 0.52              |
| 3:03:1084:ASP:C    | 3:03:1085:MET:HE2  | 2.35                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:04:107:LEU:HD22  | 4:04:299:LEU:HD21  | 1.92                     | 0.52              |
| 4:04:820:ILE:HG12  | 4:04:884:SER:HB2   | 1.92                     | 0.52              |
| 11:I:47:LEU:HD21   | 11:I:57:ALA:CB     | 2.39                     | 0.52              |
| 12:J:22:LEU:O      | 12:J:26:VAL:HG23   | 2.10                     | 0.52              |
| 13:K:5:PRO:HB2     | 13:K:32:LYS:HE3    | 1.90                     | 0.52              |
| 14:L:117:LEU:HD21  | 14:L:123:ARG:HE    | 1.75                     | 0.52              |
| 22:T:30:HIS:HD2    | 22:T:33:TYR:H      | 1.58                     | 0.52              |
| 25:W:54:GLN:C      | 25:W:56:ILE:H      | 2.16                     | 0.52              |
| 1:A:637:C:H5''     | 22:T:3:LYS:HG3     | 1.92                     | 0.52              |
| 3:03:80:PHE:HB3    | 3:03:84:GLU:HB2    | 1.91                     | 0.52              |
| 3:03:502:VAL:CG1   | 3:03:503:LYS:HD2   | 2.35                     | 0.52              |
| 4:04:154:LEU:N     | 4:04:154:LEU:HD12  | 2.25                     | 0.52              |
| 9:G:184:LYS:HD3    | 9:G:185:PRO:HD2    | 1.91                     | 0.52              |
| 3:03:671:LEU:O     | 3:03:672:GLU:C     | 2.52                     | 0.52              |
| 4:04:600:ALA:HA    | 4:04:603:LYS:HZ3   | 1.74                     | 0.52              |
| 4:04:1306:LEU:C    | 4:04:1307:LEU:HD12 | 2.35                     | 0.52              |
| 5:05:28:ARG:HG2    | 5:05:31:GLN:OE1    | 2.10                     | 0.52              |
| 14:L:62:LEU:HD12   | 14:L:62:LEU:O      | 2.10                     | 0.52              |
| 18:P:82:LEU:HD11   | 24:V:65:MET:HG3    | 1.92                     | 0.52              |
| 19:Q:92:ILE:HD13   | 19:Q:95:LEU:HD22   | 1.91                     | 0.52              |
| 20:R:57:ARG:O      | 20:R:61:GLN:HG2    | 2.10                     | 0.52              |
| 22:T:35:LYS:HB3    | 22:T:35:LYS:HZ3    | 1.75                     | 0.52              |
| 1:A:328:C:H4'      | 1:A:329:A:H5'      | 1.91                     | 0.52              |
| 1:A:454:G:H22      | 1:A:478:A:H2       | 1.57                     | 0.52              |
| 1:A:1252:A:H61     | 1:A:1285:A:N6      | 2.07                     | 0.52              |
| 3:03:42:ASP:HB3    | 3:03:44:GLU:HG2    | 1.91                     | 0.52              |
| 3:03:1278:LEU:HD13 | 3:03:1287:LEU:HD13 | 1.91                     | 0.52              |
| 4:04:79:LYS:HD2    | 7:E:20:THR:OG1     | 2.09                     | 0.52              |
| 4:04:127:LEU:HG    | 4:04:192:MET:HE1   | 1.92                     | 0.52              |
| 4:04:165:TYR:O     | 4:04:169:LEU:HG    | 2.09                     | 0.52              |
| 8:F:138:GLN:O      | 8:F:142:ARG:HG2    | 2.10                     | 0.52              |
| 20:R:27:GLN:O      | 20:R:31:LEU:HG     | 2.10                     | 0.52              |
| 3:03:212:ALA:HA    | 3:03:359:ARG:HG3   | 1.92                     | 0.52              |
| 3:03:525:THR:O     | 3:03:529:ARG:HB2   | 2.10                     | 0.52              |
| 3:03:540:ARG:HB2   | 3:03:548:ARG:NH2   | 2.25                     | 0.52              |
| 3:03:690:VAL:CG1   | 3:03:1234:LYS:HB3  | 2.40                     | 0.52              |
| 3:03:724:VAL:HG22  | 3:03:775:GLU:H     | 1.75                     | 0.52              |
| 3:03:890:LYS:HE3   | 3:03:914:LYS:HB3   | 1.91                     | 0.52              |
| 4:04:362:ARG:HB2   | 4:04:365:GLN:HG2   | 1.92                     | 0.52              |
| 4:04:437:PHE:CE2   | 4:04:449:LEU:HD11  | 2.45                     | 0.52              |
| 1:A:109:A:H62      | 1:A:324:G:H21      | 1.57                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A:427:U:C1'      | 1:A:541:G:H5''    | 2.33                     | 0.52              |
| 3:03:119:GLU:HB2   | 3:03:489:PRO:HG2  | 1.92                     | 0.52              |
| 3:03:233:ARG:O     | 3:03:236:LYS:HG2  | 2.10                     | 0.52              |
| 3:03:753:LEU:N     | 3:03:753:LEU:HD12 | 2.23                     | 0.52              |
| 3:03:1308:ILE:C    | 3:03:1310:ASP:H   | 2.18                     | 0.52              |
| 4:04:531:LYS:HG2   | 4:04:581:MET:HE3  | 1.92                     | 0.52              |
| 4:04:1370:MET:HE3  | 4:04:1373:ARG:HB3 | 1.92                     | 0.52              |
| 8:F:9:ILE:HG23     | 8:F:10:ARG:HG3    | 1.92                     | 0.52              |
| 10:H:51:LYS:H      | 10:H:61:LYS:HD3   | 1.73                     | 0.52              |
| 17:O:22:ALA:HB2    | 17:O:94:TYR:OH    | 2.10                     | 0.52              |
| 19:Q:13:VAL:HA     | 19:Q:59:GLN:HE22  | 1.75                     | 0.52              |
| 1:A:403:C:H5'      | 9:G:114:ARG:HH21  | 1.75                     | 0.51              |
| 1:A:1099:G:H5''    | 26:X:67:ARG:CD    | 2.40                     | 0.51              |
| 2:02:181:GLU:HB3   | 4:04:531:LYS:HD3  | 1.91                     | 0.51              |
| 3:03:814:ASP:O     | 3:03:1074:GLY:HA2 | 2.10                     | 0.51              |
| 3:03:882:ILE:HD12  | 3:03:882:ILE:N    | 2.25                     | 0.51              |
| 3:03:1079:ILE:HG23 | 3:03:1079:ILE:O   | 2.10                     | 0.51              |
| 4:04:107:LEU:CD1   | 4:04:239:LEU:HD12 | 2.40                     | 0.51              |
| 19:Q:40:ARG:HD2    | 19:Q:40:ARG:O     | 2.10                     | 0.51              |
| 1:A:418:C:H2'      | 1:A:419:C:C6      | 2.45                     | 0.51              |
| 1:A:718:A:H5'      | 16:N:118:ASN:CB   | 2.40                     | 0.51              |
| 1:A:1099:G:H5''    | 26:X:67:ARG:HD3   | 1.92                     | 0.51              |
| 1:A:1259:C:H3'     | 1:A:1260:G:C5'    | 2.38                     | 0.51              |
| 2:02:78:ILE:HA     | 2:02:81:ILE:HD12  | 1.93                     | 0.51              |
| 3:03:241:LEU:CD1   | 3:03:246:LEU:HD11 | 2.37                     | 0.51              |
| 3:03:1100:PRO:HG2  | 4:04:638:SER:HB3  | 1.92                     | 0.51              |
| 4:04:264:ASP:O     | 4:04:268:LEU:HG   | 2.10                     | 0.51              |
| 4:04:305:ALA:HA    | 4:04:309:ASN:HA   | 1.92                     | 0.51              |
| 4:04:858:VAL:HG13  | 4:04:858:VAL:O    | 2.10                     | 0.51              |
| 7:E:31:ILE:O       | 7:E:32:PHE:HB3    | 2.11                     | 0.51              |
| 25:W:60:GLN:HB3    | 25:W:66:ILE:HG12  | 1.91                     | 0.51              |
| 1:A:193:C:H2'      | 1:A:194:C:C6      | 2.45                     | 0.51              |
| 2:01:28:LEU:HD12   | 2:01:28:LEU:N     | 2.25                     | 0.51              |
| 3:03:145:ILE:HG12  | 3:03:512:SER:HB2  | 1.91                     | 0.51              |
| 3:03:1235:LEU:HD12 | 3:03:1235:LEU:N   | 2.24                     | 0.51              |
| 9:G:71:PHE:HA      | 9:G:74:TYR:HD2    | 1.75                     | 0.51              |
| 14:L:105:ARG:HH11  | 14:L:107:ALA:HA   | 1.75                     | 0.51              |
| 2:01:79:LEU:HD13   | 2:01:79:LEU:C     | 2.35                     | 0.51              |
| 3:03:146:VAL:CG1   | 3:03:531:SER:HB2  | 2.41                     | 0.51              |
| 3:03:672:GLU:HB2   | 4:04:766:GLY:CA   | 2.40                     | 0.51              |
| 3:03:734:ILE:HB    | 3:03:749:ASP:HB2  | 1.91                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:04:688:ALA:O     | 4:04:692:ARG:HG3   | 2.10                     | 0.51              |
| 1:A:817:C:H5'      | 1:A:820:U:OP1      | 2.10                     | 0.51              |
| 1:A:1314:C:H2'     | 1:A:1315:U:C6      | 2.46                     | 0.51              |
| 2:02:191:ARG:NH1   | 2:02:191:ARG:HB3   | 2.26                     | 0.51              |
| 3:03:159:SER:O     | 3:03:160:ASP:HB2   | 2.11                     | 0.51              |
| 3:03:398:SER:C     | 3:03:400:VAL:H     | 2.18                     | 0.51              |
| 7:E:23:TRP:CD1     | 7:E:23:TRP:H       | 2.27                     | 0.51              |
| 7:E:67:ILE:HB      | 7:E:89:GLN:HG2     | 1.92                     | 0.51              |
| 14:L:66:VAL:HG21   | 14:L:74:GLN:HB3    | 1.92                     | 0.51              |
| 20:R:16:ARG:HD3    | 20:R:16:ARG:N      | 2.26                     | 0.51              |
| 1:A:102:G:O2'      | 1:A:151:A:H1'      | 2.11                     | 0.51              |
| 2:01:134:THR:OG1   | 3:03:773:LEU:HD22  | 2.11                     | 0.51              |
| 2:02:83:LEU:HA     | 2:02:86:LYS:HZ1    | 1.76                     | 0.51              |
| 4:04:108:ALA:HB2   | 4:04:280:LYS:HG2   | 1.91                     | 0.51              |
| 4:04:278:ARG:HG3   | 4:04:281:ARG:HH21  | 1.76                     | 0.51              |
| 9:G:37:PRO:HD2     | 9:G:41:GLY:HA2     | 1.92                     | 0.51              |
| 11:I:40:GLU:OE1    | 11:I:61:LEU:HD22   | 2.10                     | 0.51              |
| 15:M:8:ILE:HD12    | 15:M:74:VAL:HB     | 1.92                     | 0.51              |
| 15:M:57:VAL:HG22   | 15:M:58:ASN:N      | 2.24                     | 0.51              |
| 20:R:28:VAL:CG2    | 20:R:65:LEU:HD23   | 2.38                     | 0.51              |
| 24:V:10:ILE:HG21   | 24:V:40:PHE:CZ     | 2.45                     | 0.51              |
| 1:A:392:C:H2'      | 1:A:393:A:C8       | 2.45                     | 0.51              |
| 2:02:52:PRO:HD2    | 2:02:223:ILE:HD13  | 1.93                     | 0.51              |
| 3:03:798:GLN:NE2   | 3:03:827:ARG:HE    | 2.08                     | 0.51              |
| 3:03:983:GLY:O     | 3:03:985:GLU:HG3   | 2.10                     | 0.51              |
| 4:04:499:ILE:HG23  | 4:04:500:ILE:HG12  | 1.91                     | 0.51              |
| 12:J:55:LYS:NZ     | 12:J:63:VAL:HG21   | 2.26                     | 0.51              |
| 4:04:623:GLN:O     | 4:04:627:THR:HG22  | 2.11                     | 0.51              |
| 4:04:1029:THR:HG23 | 4:04:1121:LEU:HD21 | 1.93                     | 0.51              |
| 2:01:67:GLU:N      | 2:01:171:LEU:HD11  | 2.26                     | 0.51              |
| 3:03:514:PHE:HB3   | 3:03:760:ASN:HD22  | 1.76                     | 0.51              |
| 4:04:308:ASP:O     | 4:04:309:ASN:HB2   | 2.11                     | 0.51              |
| 4:04:483:LEU:HA    | 5:05:16:ARG:NH2    | 2.25                     | 0.51              |
| 4:04:1075:ARG:HG2  | 4:04:1075:ARG:HH11 | 1.75                     | 0.51              |
| 7:E:46:THR:HG23    | 7:E:201:PRO:O      | 2.11                     | 0.51              |
| 7:E:74:ARG:HH21    | 7:E:77:SER:CB      | 2.24                     | 0.51              |
| 7:E:141:LEU:O      | 7:E:145:GLU:HG3    | 2.11                     | 0.51              |
| 20:R:6:ALA:O       | 20:R:10:ILE:HG13   | 2.10                     | 0.51              |
| 1:A:981:U:C4'      | 19:Q:62:ARG:HH22   | 2.23                     | 0.51              |
| 1:A:1014:A:H5''    | 24:V:13:HIS:HB2    | 1.93                     | 0.51              |
| 4:04:189:LEU:HD13  | 4:04:234:PRO:O     | 2.10                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:04:660:GLU:O    | 4:04:664:ILE:HG12  | 2.10                     | 0.51              |
| 17:O:29:LYS:HE2   | 17:O:57:THR:HB     | 1.93                     | 0.51              |
| 1:A:774:G:H2'     | 1:A:775:G:H5'      | 1.93                     | 0.50              |
| 1:A:1371:G:H4'    | 14:L:70:GLY:HA3    | 1.93                     | 0.50              |
| 2:02:172:LEU:H    | 2:02:172:LEU:CD2   | 2.24                     | 0.50              |
| 4:04:27:PRO:HB2   | 4:04:31:ARG:HH12   | 1.75                     | 0.50              |
| 4:04:428:THR:HG21 | 4:04:433:GLY:HA3   | 1.92                     | 0.50              |
| 4:04:678:ARG:HA   | 4:04:681:LYS:HB3   | 1.92                     | 0.50              |
| 4:04:721:SER:HA   | 4:04:724:MET:HE2   | 1.94                     | 0.50              |
| 7:E:16:PHE:CD2    | 7:E:41:ILE:HD12    | 2.46                     | 0.50              |
| 11:I:5:GLU:HB2    | 11:I:90:MET:HB2    | 1.92                     | 0.50              |
| 25:W:53:MET:HE2   | 25:W:75:LYS:HD3    | 1.93                     | 0.50              |
| 1:A:105:G:N7      | 25:W:8:LYS:HE3     | 2.26                     | 0.50              |
| 1:A:762:U:H2'     | 1:A:763:G:C8       | 2.46                     | 0.50              |
| 1:A:1030:U:H3'    | 1:A:1031:C:H5'     | 1.94                     | 0.50              |
| 2:01:65:LEU:HD12  | 2:01:168:ILE:HG13  | 1.92                     | 0.50              |
| 3:03:678:ARG:HH21 | 3:03:1106:ARG:HG2  | 1.72                     | 0.50              |
| 3:03:1013:GLN:O   | 3:03:1016:GLU:HB2  | 2.11                     | 0.50              |
| 7:E:27:MET:C      | 7:E:29:PRO:HD2     | 2.36                     | 0.50              |
| 9:G:110:ARG:O     | 9:G:114:ARG:HG3    | 2.11                     | 0.50              |
| 10:H:59:ILE:O     | 10:H:63:MET:HG2    | 2.11                     | 0.50              |
| 10:H:156:ARG:HG2  | 13:K:44:PHE:CE1    | 2.46                     | 0.50              |
| 12:J:99:ALA:O     | 12:J:103:ILE:HG13  | 2.11                     | 0.50              |
| 19:Q:5:MET:HG2    | 19:Q:62:ARG:NH1    | 2.26                     | 0.50              |
| 1:A:516:U:H5      | 1:A:533:A:N6       | 2.10                     | 0.50              |
| 1:A:517:G:H4'     | 1:A:519:C:C2       | 2.47                     | 0.50              |
| 1:A:658:C:H1'     | 20:R:21:THR:HG21   | 1.91                     | 0.50              |
| 1:A:1123:U:O2'    | 1:A:1124:G:H5'     | 2.11                     | 0.50              |
| 3:03:12:ARG:HH22  | 3:03:705:GLU:HB2   | 1.75                     | 0.50              |
| 3:03:471:VAL:O    | 3:03:475:VAL:HG23  | 2.11                     | 0.50              |
| 4:04:749:LYS:HB3  | 4:04:755:ILE:HG13  | 1.93                     | 0.50              |
| 4:04:865:HIS:CE1  | 4:04:867:GLN:HB2   | 2.46                     | 0.50              |
| 4:04:1327:GLU:O   | 4:04:1330:ARG:HB2  | 2.11                     | 0.50              |
| 11:I:18:VAL:N     | 11:I:19:PRO:CD     | 2.75                     | 0.50              |
| 14:L:18:VAL:HG13  | 14:L:64:ILE:CD1    | 2.40                     | 0.50              |
| 1:A:879:C:H2'     | 1:A:880:C:C6       | 2.47                     | 0.50              |
| 4:04:1223:LEU:C   | 4:04:1223:LEU:HD13 | 2.36                     | 0.50              |
| 7:E:222:ARG:HA    | 7:E:225:ARG:HG2    | 1.94                     | 0.50              |
| 25:W:68:LYS:HB2   | 25:W:68:LYS:HZ2    | 1.75                     | 0.50              |
| 1:A:219:U:H2'     | 1:A:220:G:C4'      | 2.41                     | 0.50              |
| 1:A:1273:C:H2'    | 1:A:1274:A:H5'     | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:1527:U:O2'     | 1:A:1528:U:H5'     | 2.12                     | 0.50              |
| 3:03:725:GLN:HB2   | 3:03:735:LYS:HB2   | 1.94                     | 0.50              |
| 4:04:77:ARG:HB3    | 4:04:79:LYS:HG2    | 1.94                     | 0.50              |
| 4:04:311:ARG:NH2   | 4:04:1329:THR:HB   | 2.25                     | 0.50              |
| 4:04:1159:ILE:HG13 | 4:04:1160:SER:N    | 2.26                     | 0.50              |
| 4:04:1230:THR:O    | 4:04:1234:VAL:HG13 | 2.11                     | 0.50              |
| 8:F:19:SER:O       | 19:Q:93:PRO:HG3    | 2.12                     | 0.50              |
| 11:I:90:MET:SD     | 23:U:61:ARG:HD3    | 2.52                     | 0.50              |
| 12:J:96:ASN:HB3    | 12:J:100:MET:HE2   | 1.93                     | 0.50              |
| 1:A:613:C:P        | 9:G:80:ARG:HD3     | 2.52                     | 0.50              |
| 3:03:1230:MET:HB3  | 3:03:1232:MET:HE1  | 1.93                     | 0.50              |
| 4:04:179:LYS:HD2   | 4:04:293:ARG:HH22  | 1.77                     | 0.50              |
| 4:04:204:GLU:HA    | 4:04:207:GLU:HB2   | 1.92                     | 0.50              |
| 4:04:1040:MET:C    | 4:04:1041:ILE:HD12 | 2.37                     | 0.50              |
| 4:04:1221:LEU:HD23 | 4:04:1229:VAL:HG11 | 1.93                     | 0.50              |
| 4:04:1266:ILE:HG21 | 4:04:1300:ALA:HB1  | 1.93                     | 0.50              |
| 11:I:3:HIS:HB3     | 11:I:95:ALA:HB2    | 1.94                     | 0.50              |
| 22:T:10:ARG:HH11   | 22:T:10:ARG:HG3    | 1.75                     | 0.50              |
| 2:02:54:CYS:SG     | 2:02:92:VAL:HG22   | 2.52                     | 0.50              |
| 2:02:213:PRO:O     | 2:02:217:ILE:HG13  | 2.10                     | 0.50              |
| 3:03:615:VAL:HG12  | 3:03:651:ASP:OD2   | 2.11                     | 0.50              |
| 3:03:960:LEU:HG    | 3:03:1029:LEU:HD12 | 1.93                     | 0.50              |
| 3:03:1263:ALA:HB1  | 3:03:1264:GLN:OE1  | 2.12                     | 0.50              |
| 3:03:1335:ILE:HD12 | 3:03:1335:ILE:H    | 1.75                     | 0.50              |
| 7:E:20:THR:O       | 7:E:21:ARG:C       | 2.55                     | 0.50              |
| 7:E:23:TRP:CA      | 7:E:190:ASN:HB3    | 2.41                     | 0.50              |
| 24:V:8:PRO:HB2     | 24:V:38:THR:HG21   | 1.94                     | 0.50              |
| 24:V:30:LEU:HD12   | 24:V:30:LEU:H      | 1.76                     | 0.50              |
| 1:A:577:G:H1'      | 1:A:816:A:H2'      | 1.92                     | 0.50              |
| 1:A:1270:G:H2'     | 1:A:1271:A:C8      | 2.47                     | 0.50              |
| 1:A:1395:C:H2'     | 1:A:1396:A:C8      | 2.46                     | 0.50              |
| 2:01:82:LEU:HA     | 2:01:85:LEU:HD12   | 1.94                     | 0.50              |
| 3:03:139:ASN:HB2   | 3:03:143:ARG:NH2   | 2.26                     | 0.50              |
| 4:04:512:TYR:CD2   | 4:04:635:SER:HA    | 2.47                     | 0.50              |
| 7:E:21:ARG:H       | 7:E:38:VAL:HB      | 1.76                     | 0.50              |
| 7:E:27:MET:SD      | 7:E:191:SER:HB2    | 2.52                     | 0.50              |
| 7:E:36:ASN:HB2     | 7:E:40:ILE:CD1     | 2.41                     | 0.50              |
| 10:H:87:VAL:HB     | 10:H:92:ARG:NH1    | 2.27                     | 0.50              |
| 18:P:86:ARG:O      | 18:P:96:VAL:HG12   | 2.11                     | 0.50              |
| 25:W:27:MET:HG2    | 25:W:31:ILE:HD11   | 1.94                     | 0.50              |
| 1:A:443:C:H2'      | 1:A:444:G:C8       | 2.47                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:1366:C:H2'    | 1:A:1367:C:C6      | 2.46                     | 0.50              |
| 2:01:58:GLU:HB2   | 2:01:145:LYS:HB3   | 1.93                     | 0.50              |
| 3:03:1267:GLY:H   | 4:04:346:ARG:NH2   | 1.95                     | 0.50              |
| 4:04:70:CYS:SG    | 4:04:85:CYS:HB2    | 2.51                     | 0.50              |
| 4:04:429:LEU:HD12 | 4:04:430:HIS:N     | 2.26                     | 0.50              |
| 4:04:1271:SER:HB2 | 4:04:1299:GLY:HA2  | 1.93                     | 0.50              |
| 17:O:88:ASP:C     | 17:O:89:LEU:HD12   | 2.37                     | 0.50              |
| 19:Q:92:ILE:HD12  | 19:Q:92:ILE:N      | 2.27                     | 0.50              |
| 1:A:219:U:H2'     | 1:A:220:G:C5'      | 2.42                     | 0.49              |
| 3:03:97:ARG:HB3   | 3:03:121:GLU:HB2   | 1.94                     | 0.49              |
| 3:03:144:VAL:HG11 | 3:03:527:LYS:HA    | 1.94                     | 0.49              |
| 3:03:521:LEU:C    | 3:03:521:LEU:HD13  | 2.37                     | 0.49              |
| 4:04:355:ILE:HG23 | 4:04:464:ASP:O     | 2.12                     | 0.49              |
| 4:04:930:LEU:HD23 | 4:04:1244:GLN:HG3  | 1.94                     | 0.49              |
| 10:H:91:SER:OG    | 10:H:134:ASN:HB3   | 2.12                     | 0.49              |
| 12:J:24:LYS:HA    | 12:J:27:ASN:ND2    | 2.21                     | 0.49              |
| 14:L:34:LEU:C     | 14:L:34:LEU:HD23   | 2.36                     | 0.49              |
| 18:P:2:ARG:H      | 18:P:8:ILE:HG12    | 1.77                     | 0.49              |
| 3:03:362:ALA:O    | 3:03:366:ILE:HG13  | 2.11                     | 0.49              |
| 3:03:936:ARG:HA   | 3:03:1047:LEU:HB3  | 1.94                     | 0.49              |
| 12:J:52:ARG:HH22  | 12:J:117:LEU:HD11  | 1.77                     | 0.49              |
| 14:L:18:VAL:HG13  | 14:L:64:ILE:HD11   | 1.94                     | 0.49              |
| 1:A:508:U:H4'     | 9:G:50:TYR:CD2     | 2.47                     | 0.49              |
| 2:01:35:PHE:HA    | 2:01:38:THR:HB     | 1.95                     | 0.49              |
| 3:03:137:VAL:HG22 | 3:03:142:GLU:CG    | 2.37                     | 0.49              |
| 3:03:974:ARG:HH21 | 3:03:977:ALA:HB3   | 1.77                     | 0.49              |
| 3:03:1172:LEU:HA  | 3:03:1175:ASN:HD22 | 1.77                     | 0.49              |
| 3:03:1253:LEU:O   | 3:03:1253:LEU:HD13 | 2.12                     | 0.49              |
| 4:04:290:ILE:HD12 | 4:04:290:ILE:N     | 2.17                     | 0.49              |
| 4:04:588:PRO:O    | 4:04:591:ILE:HG22  | 2.13                     | 0.49              |
| 4:04:1173:ARG:NH2 | 4:04:1196:LEU:HD23 | 2.23                     | 0.49              |
| 10:H:104:ILE:HG23 | 10:H:104:ILE:O     | 2.11                     | 0.49              |
| 17:O:98:ARG:HB2   | 17:O:116:TYR:HA    | 1.95                     | 0.49              |
| 1:A:118:U:H2'     | 1:A:119:A:H5'      | 1.95                     | 0.49              |
| 1:A:675:A:H2'     | 1:A:676:A:C8       | 2.47                     | 0.49              |
| 2:01:69:SER:O     | 2:01:78:ILE:HG12   | 2.11                     | 0.49              |
| 3:03:498:ILE:H    | 3:03:498:ILE:CD1   | 2.24                     | 0.49              |
| 3:03:704:MET:HA   | 3:03:707:ALA:HB3   | 1.94                     | 0.49              |
| 3:03:820:GLU:HB3  | 3:03:1082:ILE:HD12 | 1.95                     | 0.49              |
| 4:04:137:ARG:HB3  | 4:04:143:SER:OG    | 2.12                     | 0.49              |
| 4:04:615:LYS:HB2  | 4:04:615:LYS:NZ    | 2.26                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:04:647:PRO:C    | 4:04:649:LYS:H    | 2.19                     | 0.49              |
| 4:04:821:MET:HG3  | 4:04:823:THR:HG23 | 1.93                     | 0.49              |
| 7:E:57:LEU:HD13   | 7:E:217:VAL:HG13  | 1.93                     | 0.49              |
| 14:L:35:GLU:HA    | 14:L:39:GLY:HA3   | 1.94                     | 0.49              |
| 19:Q:48:GLN:HB2   | 24:V:12:LEU:HD22  | 1.95                     | 0.49              |
| 1:A:664:G:H1      | 1:A:741:G:H1      | 1.60                     | 0.49              |
| 1:A:1304:G:H21    | 1:A:1333:A:N6     | 1.92                     | 0.49              |
| 3:03:1100:PRO:CG  | 4:04:638:SER:HB3  | 2.43                     | 0.49              |
| 4:04:199:GLU:O    | 4:04:203:GLU:HG3  | 2.13                     | 0.49              |
| 4:04:223:LEU:O    | 4:04:226:ALA:HB3  | 2.12                     | 0.49              |
| 7:E:126:PHE:HD1   | 7:E:126:PHE:H     | 1.59                     | 0.49              |
| 8:F:111:ASP:OD2   | 8:F:113:LYS:HB3   | 2.12                     | 0.49              |
| 15:M:47:GLU:HB2   | 15:M:67:ILE:HB    | 1.92                     | 0.49              |
| 15:M:57:VAL:O     | 15:M:58:ASN:HB2   | 2.12                     | 0.49              |
| 21:S:1:MET:HE2    | 21:S:3:THR:HB     | 1.94                     | 0.49              |
| 25:W:34:VAL:O     | 25:W:38:ILE:HG13  | 2.12                     | 0.49              |
| 4:04:83:VAL:HB    | 7:E:75:ALA:HB2    | 1.92                     | 0.49              |
| 4:04:242:LEU:HD23 | 4:04:242:LEU:C    | 2.37                     | 0.49              |
| 4:04:485:MET:HE3  | 4:04:486:SER:H    | 1.78                     | 0.49              |
| 7:E:28:LYS:O      | 7:E:29:PRO:C      | 2.53                     | 0.49              |
| 18:P:18:LEU:HD12  | 18:P:29:SER:OG    | 2.12                     | 0.49              |
| 20:R:9:LYS:NZ     | 20:R:9:LYS:HB3    | 2.27                     | 0.49              |
| 26:X:10:GLU:H     | 26:X:11:PRO:CD    | 2.26                     | 0.49              |
| 1:A:1024:G:O2'    | 1:A:1025:U:H5'    | 2.12                     | 0.49              |
| 1:A:1285:A:H4'    | 1:A:1286:U:C5'    | 2.43                     | 0.49              |
| 3:03:971:LEU:O    | 3:03:974:ARG:HB3  | 2.11                     | 0.49              |
| 3:03:1099:ASN:ND2 | 3:03:1101:LEU:HB2 | 2.27                     | 0.49              |
| 4:04:131:PRO:O    | 4:04:135:ILE:HG13 | 2.12                     | 0.49              |
| 4:04:141:PHE:HD2  | 4:04:297:ARG:HH11 | 1.61                     | 0.49              |
| 7:E:217:VAL:O     | 7:E:221:VAL:HG23  | 2.12                     | 0.49              |
| 8:F:42:LEU:O      | 8:F:42:LEU:HD23   | 2.12                     | 0.49              |
| 17:O:109:ARG:CB   | 17:O:118:VAL:HG21 | 2.43                     | 0.49              |
| 19:Q:5:MET:HG2    | 19:Q:62:ARG:HH11  | 1.78                     | 0.49              |
| 19:Q:56:PRO:HA    | 19:Q:59:GLN:HG2   | 1.95                     | 0.49              |
| 26:X:10:GLU:N     | 26:X:11:PRO:CD    | 2.75                     | 0.49              |
| 1:A:419:C:C5'     | 1:A:513:C:H4'     | 2.40                     | 0.49              |
| 2:01:67:GLU:H     | 2:01:171:LEU:HD11 | 1.78                     | 0.49              |
| 3:03:816:ILE:HG13 | 3:03:1074:GLY:HA3 | 1.93                     | 0.49              |
| 3:03:1235:LEU:H   | 3:03:1235:LEU:CD1 | 2.26                     | 0.49              |
| 7:E:21:ARG:HB3    | 7:E:38:VAL:HG12   | 1.94                     | 0.49              |
| 9:G:45:PRO:HB2    | 9:G:47:LEU:HD12   | 1.95                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:X:29:LEU:HG    | 26:X:33:ARG:HD3    | 1.95                     | 0.49              |
| 1:A:834:U:OP1     | 23:U:49:ALA:HB2    | 2.13                     | 0.49              |
| 3:03:208:ILE:HG13 | 3:03:354:ASP:OD1   | 2.13                     | 0.49              |
| 3:03:798:GLN:HE22 | 3:03:827:ARG:HE    | 1.59                     | 0.49              |
| 3:03:801:ARG:HG3  | 3:03:1094:VAL:HG23 | 1.95                     | 0.49              |
| 3:03:1319:MET:HG3 | 3:03:1323:PHE:CD2  | 2.45                     | 0.49              |
| 3:03:1338:GLU:HB2 | 4:04:21:LYS:NZ     | 2.27                     | 0.49              |
| 4:04:21:LYS:HD2   | 4:04:21:LYS:C      | 2.38                     | 0.49              |
| 4:04:430:HIS:HD2  | 4:04:432:LEU:HB2   | 1.76                     | 0.49              |
| 4:04:643:ASP:HB3  | 4:04:720:ASN:HD22  | 1.77                     | 0.49              |
| 4:04:1172:LYS:HD3 | 4:04:1189:MET:HB3  | 1.94                     | 0.49              |
| 10:H:15:ILE:HG23  | 10:H:109:ALA:HA    | 1.93                     | 0.49              |
| 10:H:111:ARG:O    | 10:H:115:GLU:HG3   | 2.13                     | 0.49              |
| 19:Q:16:ALA:HA    | 19:Q:55:SER:HB2    | 1.95                     | 0.49              |
| 25:W:28:ARG:HA    | 25:W:31:ILE:HD12   | 1.95                     | 0.49              |
| 1:A:751:U:H2'     | 1:A:752:G:H5'      | 1.95                     | 0.49              |
| 1:A:979:C:N3      | 19:Q:58:ARG:HG2    | 2.28                     | 0.49              |
| 3:03:302:ILE:HG21 | 3:03:309:LEU:HD12  | 1.95                     | 0.49              |
| 3:03:1285:TYR:HB2 | 4:04:1356:LEU:HD21 | 1.94                     | 0.49              |
| 4:04:88:CYS:O     | 4:04:90:VAL:HG23   | 2.13                     | 0.49              |
| 4:04:689:ALA:O    | 4:04:693:VAL:HG23  | 2.13                     | 0.49              |
| 4:04:795:TYR:O    | 4:04:798:ARG:HB3   | 2.12                     | 0.49              |
| 4:04:896:ALA:HA   | 4:04:909:ILE:CG2   | 2.42                     | 0.49              |
| 11:I:29:ILE:HD11  | 11:I:62:MET:CE     | 2.43                     | 0.49              |
| 24:V:16:LYS:O     | 24:V:20:LYS:HG3    | 2.12                     | 0.49              |
| 3:03:99:LYS:HA    | 3:03:120:GLN:HA    | 1.95                     | 0.48              |
| 3:03:721:GLY:HA2  | 3:03:777:VAL:HG23  | 1.95                     | 0.48              |
| 3:03:723:VAL:HA   | 3:03:776:PRO:HA    | 1.95                     | 0.48              |
| 3:03:1285:TYR:HE2 | 4:04:473:THR:HG21  | 1.78                     | 0.48              |
| 4:04:514:THR:HG21 | 4:04:596:LEU:HB2   | 1.94                     | 0.48              |
| 7:E:45:LYS:O      | 7:E:49:MET:HB2     | 2.13                     | 0.48              |
| 25:W:54:GLN:C     | 25:W:56:ILE:N      | 2.71                     | 0.48              |
| 1:A:361:G:H2'     | 1:A:362:G:O4'      | 2.13                     | 0.48              |
| 1:A:1319:A:H61    | 1:A:1361:G:H1'     | 1.78                     | 0.48              |
| 2:01:224:LEU:HD13 | 2:02:228:LEU:HD12  | 1.95                     | 0.48              |
| 2:02:179:PRO:HA   | 2:02:208:ASN:HD21  | 1.77                     | 0.48              |
| 3:03:8:LYS:HG3    | 3:03:1168:GLU:HG3  | 1.94                     | 0.48              |
| 3:03:809:GLY:N    | 4:04:629:PHE:HB3   | 2.28                     | 0.48              |
| 3:03:886:LYS:N    | 3:03:917:SER:HA    | 2.28                     | 0.48              |
| 4:04:222:LYS:HD3  | 4:04:222:LYS:C     | 2.39                     | 0.48              |
| 4:04:239:LEU:HD13 | 4:04:240:THR:N     | 2.28                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:04:1255:VAL:O    | 4:04:1259:GLN:HG2 | 2.13                     | 0.48              |
| 5:05:32:VAL:C      | 5:05:34:GLY:N     | 2.71                     | 0.48              |
| 7:E:87:CYS:SG      | 7:E:222:ARG:HD2   | 2.53                     | 0.48              |
| 8:F:21:TRP:HB3     | 8:F:58:ARG:HB3    | 1.94                     | 0.48              |
| 13:K:54:THR:C      | 13:K:56:PRO:HD3   | 2.37                     | 0.48              |
| 18:P:1:ALA:N       | 18:P:44:ILE:HD11  | 2.28                     | 0.48              |
| 21:S:31:ARG:HD3    | 21:S:31:ARG:C     | 2.39                     | 0.48              |
| 1:A:346:G:H2'      | 1:A:347:G:H5'     | 1.95                     | 0.48              |
| 1:A:663:A:H61      | 1:A:742:G:H1      | 1.61                     | 0.48              |
| 1:A:912:C:O2'      | 1:A:913:A:H5'     | 2.14                     | 0.48              |
| 3:03:589:THR:HG23  | 3:03:591:TYR:CE2  | 2.49                     | 0.48              |
| 4:04:365:GLN:HA    | 4:04:438:GLU:H    | 1.79                     | 0.48              |
| 4:04:369:PRO:HB3   | 4:04:444:GLY:O    | 2.13                     | 0.48              |
| 7:E:23:TRP:HB2     | 7:E:189:THR:OG1   | 2.13                     | 0.48              |
| 12:J:25:PHE:HD1    | 12:J:100:MET:HB3  | 1.78                     | 0.48              |
| 26:X:43:THR:HA     | 26:X:46:LYS:HZ1   | 1.78                     | 0.48              |
| 1:A:105:G:OP1      | 25:W:12:GLN:HG3   | 2.13                     | 0.48              |
| 1:A:762:U:H2'      | 1:A:763:G:H8      | 1.77                     | 0.48              |
| 1:A:946:A:H2'      | 1:A:947:G:H8      | 1.78                     | 0.48              |
| 1:A:1379:G:O2'     | 1:A:1380:U:H5'    | 2.12                     | 0.48              |
| 4:04:245:LEU:HD23  | 4:04:250:ARG:HD2  | 1.94                     | 0.48              |
| 4:04:848:VAL:HB    | 4:04:858:VAL:CG1  | 2.44                     | 0.48              |
| 4:04:850:LYS:HG2   | 4:04:857:LEU:HD23 | 1.95                     | 0.48              |
| 7:E:19:GLN:HG3     | 7:E:42:ASN:ND2    | 2.28                     | 0.48              |
| 7:E:35:ARG:HH11    | 7:E:35:ARG:HG3    | 1.79                     | 0.48              |
| 7:E:132:LYS:O      | 7:E:136:MET:HG3   | 2.13                     | 0.48              |
| 1:A:178:C:C2       | 1:A:179:A:H1'     | 2.48                     | 0.48              |
| 1:A:179:A:H3'      | 1:A:180:U:C5      | 2.49                     | 0.48              |
| 1:A:376:G:H2'      | 1:A:377:G:H5'     | 1.95                     | 0.48              |
| 2:01:12:ARG:H      | 2:01:30:PRO:HD2   | 1.78                     | 0.48              |
| 3:03:623:LEU:HD12  | 3:03:623:LEU:C    | 2.39                     | 0.48              |
| 3:03:1059:ARG:HH11 | 3:03:1059:ARG:HG3 | 1.78                     | 0.48              |
| 4:04:86:GLU:CG     | 26:X:67:ARG:HH22  | 2.26                     | 0.48              |
| 4:04:1242:ARG:NH1  | 4:04:1247:LYS:HG2 | 2.22                     | 0.48              |
| 5:05:32:VAL:O      | 5:05:34:GLY:N     | 2.46                     | 0.48              |
| 7:E:43:LEU:CD1     | 7:E:44:GLU:N      | 2.76                     | 0.48              |
| 12:J:65:LEU:HD21   | 12:J:96:ASN:ND2   | 2.28                     | 0.48              |
| 15:M:8:ILE:HB      | 15:M:74:VAL:HB    | 1.96                     | 0.48              |
| 15:M:36:VAL:HG23   | 15:M:76:ILE:HG12  | 1.93                     | 0.48              |
| 1:A:229:U:H2'      | 1:A:230:G:C8      | 2.48                     | 0.48              |
| 1:A:443:C:H2'      | 1:A:444:G:H8      | 1.78                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A:523:A:C2'      | 1:A:524:G:H5''    | 2.44                     | 0.48              |
| 3:03:885:GLY:HA2   | 3:03:917:SER:HB3  | 1.94                     | 0.48              |
| 3:03:1107:MET:HB3  | 4:04:740:LEU:HD13 | 1.96                     | 0.48              |
| 4:04:64:PRO:CG     | 4:04:93:THR:H     | 2.26                     | 0.48              |
| 4:04:115:TRP:CZ3   | 4:04:307:LEU:HD13 | 2.49                     | 0.48              |
| 4:04:378:LYS:HA    | 4:04:381:ILE:HD12 | 1.94                     | 0.48              |
| 4:04:396:ALA:O     | 4:04:400:MET:HG3  | 2.13                     | 0.48              |
| 4:04:399:LYS:HB3   | 4:04:403:ARG:HH12 | 1.79                     | 0.48              |
| 5:05:54:ILE:HD13   | 5:05:59:ILE:O     | 2.14                     | 0.48              |
| 7:E:18:HIS:HA      | 7:E:40:ILE:CA     | 2.44                     | 0.48              |
| 11:I:62:MET:HG2    | 11:I:64:VAL:HB    | 1.94                     | 0.48              |
| 1:A:946:A:H2'      | 1:A:947:G:C8      | 2.47                     | 0.48              |
| 1:A:1261:A:H2'     | 1:A:1262:C:H5'    | 1.94                     | 0.48              |
| 2:01:81:ILE:HA     | 2:01:84:ASN:HD22  | 1.78                     | 0.48              |
| 2:01:161:SER:C     | 2:01:163:GLU:H    | 2.21                     | 0.48              |
| 3:03:816:ILE:HD12  | 3:03:1066:MET:HB3 | 1.94                     | 0.48              |
| 3:03:1281:TYR:HE2  | 4:04:434:ILE:HB   | 1.78                     | 0.48              |
| 4:04:200:GLN:HA    | 4:04:203:GLU:OE1  | 2.13                     | 0.48              |
| 4:04:632:ALA:O     | 4:04:635:SER:HB3  | 2.14                     | 0.48              |
| 4:04:958:ILE:HD12  | 4:04:982:LEU:CD1  | 2.38                     | 0.48              |
| 8:F:152:VAL:HG23   | 8:F:165:GLU:HB3   | 1.95                     | 0.48              |
| 12:J:56:SER:OG     | 12:J:59:GLU:HG2   | 2.13                     | 0.48              |
| 14:L:104:THR:HG22  | 14:L:106:ASP:H    | 1.79                     | 0.48              |
| 19:Q:60:ARG:HG2    | 19:Q:62:ARG:NH2   | 2.19                     | 0.48              |
| 1:A:219:U:C3'      | 1:A:220:G:H5''    | 2.44                     | 0.48              |
| 3:03:815:SER:HA    | 3:03:1075:VAL:O   | 2.13                     | 0.48              |
| 4:04:133:ARG:HH21  | 4:04:136:GLU:CD   | 2.22                     | 0.48              |
| 10:H:87:VAL:O      | 10:H:87:VAL:HG13  | 2.12                     | 0.48              |
| 15:M:9:ARG:HA      | 15:M:72:ARG:O     | 2.13                     | 0.48              |
| 16:N:44:ALA:HB1    | 16:N:68:ARG:HB3   | 1.95                     | 0.48              |
| 17:O:29:LYS:HZ1    | 17:O:58:ASN:ND2   | 2.10                     | 0.48              |
| 17:O:43:LYS:CG     | 17:O:44:PRO:HD3   | 2.37                     | 0.48              |
| 26:X:10:GLU:HA     | 26:X:12:PHE:CE1   | 2.49                     | 0.48              |
| 2:01:26:VAL:CG2    | 2:01:203:ILE:HB   | 2.44                     | 0.48              |
| 3:03:39:ILE:HG23   | 3:03:39:ILE:O     | 2.14                     | 0.48              |
| 3:03:455:SER:O     | 3:03:459:MET:HG3  | 2.14                     | 0.48              |
| 3:03:960:LEU:HD11  | 3:03:1028:LYS:CB  | 2.43                     | 0.48              |
| 4:04:385:LEU:HD11  | 4:04:408:VAL:HG12 | 1.95                     | 0.48              |
| 4:04:1306:LEU:HD23 | 4:04:1307:LEU:N   | 2.29                     | 0.48              |
| 6:B:171:UNK:O      | 6:B:172:UNK:C     | 2.61                     | 0.48              |
| 7:E:16:PHE:CD1     | 7:E:16:PHE:N      | 2.79                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:E:18:HIS:HA      | 7:E:40:ILE:HA      | 1.96                     | 0.48              |
| 14:L:49:GLN:HA     | 14:L:52:GLU:OE1    | 2.12                     | 0.48              |
| 16:N:113:THR:O     | 16:N:115:ILE:HG13  | 2.14                     | 0.48              |
| 18:P:9:PRO:HG3     | 18:P:17:ALA:O      | 2.14                     | 0.48              |
| 19:Q:40:ARG:HD2    | 19:Q:40:ARG:C      | 2.38                     | 0.48              |
| 23:U:49:ALA:HA     | 23:U:52:GLN:HB3    | 1.96                     | 0.48              |
| 1:A:66:A:H1'       | 1:A:173:U:H2'      | 1.95                     | 0.48              |
| 1:A:105:G:H22      | 1:A:379:C:H4'      | 1.78                     | 0.48              |
| 1:A:557:G:H2'      | 1:A:558:G:O4'      | 2.13                     | 0.48              |
| 1:A:865:A:O2'      | 1:A:866:C:H5'      | 2.12                     | 0.48              |
| 1:A:1373:G:H5''    | 12:J:35:LYS:HD2    | 1.95                     | 0.48              |
| 3:03:678:ARG:NH2   | 3:03:1106:ARG:NH1  | 2.62                     | 0.48              |
| 4:04:1046:ILE:HD12 | 4:04:1059:LEU:HB3  | 1.94                     | 0.48              |
| 4:04:1358:PRO:HB3  | 4:04:1366:HIS:CD2  | 2.49                     | 0.48              |
| 5:05:38:LEU:N      | 5:05:38:LEU:HD12   | 2.28                     | 0.48              |
| 9:G:167:PRO:HB2    | 9:G:170:LEU:HB2    | 1.95                     | 0.48              |
| 11:I:40:GLU:HB3    | 11:I:61:LEU:HB2    | 1.95                     | 0.48              |
| 17:O:113:ARG:HH12  | 17:O:120:ARG:HH11  | 1.61                     | 0.48              |
| 25:W:35:TYR:CZ     | 25:W:78:LEU:HD13   | 2.49                     | 0.48              |
| 1:A:176:C:H5'      | 25:W:19:HIS:NE2    | 2.29                     | 0.47              |
| 1:A:571:U:H2'      | 1:A:572:A:H5''     | 1.96                     | 0.47              |
| 1:A:1356:G:H2'     | 1:A:1357:A:C8      | 2.49                     | 0.47              |
| 3:03:135:THR:HB    | 3:03:142:GLU:HB3   | 1.96                     | 0.47              |
| 3:03:557:ARG:HD2   | 3:03:557:ARG:N     | 2.29                     | 0.47              |
| 3:03:1196:LYS:HB3  | 3:03:1200:LYS:HZ3  | 1.77                     | 0.47              |
| 4:04:66:LYS:HB3    | 4:04:69:GLU:HB2    | 1.94                     | 0.47              |
| 4:04:153:ASN:HB3   | 4:04:154:LEU:HD12  | 1.96                     | 0.47              |
| 4:04:1253:ILE:O    | 4:04:1257:VAL:HG23 | 2.14                     | 0.47              |
| 4:04:1273:ASP:CG   | 4:04:1274:PHE:N    | 2.71                     | 0.47              |
| 7:E:183:VAL:HB     | 7:E:196:VAL:HA     | 1.95                     | 0.47              |
| 14:L:29:ILE:HG12   | 14:L:78:ILE:HD11   | 1.95                     | 0.47              |
| 1:A:1318:A:H2'     | 1:A:1319:A:H5'     | 1.96                     | 0.47              |
| 3:03:1258:PRO:HG3  | 4:04:346:ARG:HG2   | 1.96                     | 0.47              |
| 4:04:796:LEU:HD22  | 4:04:1138:LEU:HD11 | 1.96                     | 0.47              |
| 5:05:29:GLN:O      | 5:05:32:VAL:O      | 2.32                     | 0.47              |
| 7:E:73:LYS:HE3     | 26:X:67:ARG:HH11   | 1.79                     | 0.47              |
| 7:E:135:LEU:O      | 7:E:139:ARG:HG2    | 2.14                     | 0.47              |
| 9:G:37:PRO:HD2     | 9:G:41:GLY:CA      | 2.44                     | 0.47              |
| 10:H:40:ASP:OD1    | 10:H:44:ARG:HB3    | 2.14                     | 0.47              |
| 12:J:59:GLU:O      | 12:J:63:VAL:HG23   | 2.13                     | 0.47              |
| 15:M:6:ILE:HD13    | 15:M:87:LEU:HD11   | 1.96                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:02:79:LEU:HD11  | 4:04:526:VAL:HG11  | 1.96                     | 0.47              |
| 3:03:103:VAL:HG12 | 3:03:116:ASP:HA    | 1.96                     | 0.47              |
| 3:03:1323:PHE:O   | 3:03:1327:LEU:HD13 | 2.14                     | 0.47              |
| 4:04:66:LYS:HZ3   | 4:04:78:LEU:HD11   | 1.77                     | 0.47              |
| 4:04:168:ALA:O    | 4:04:172:PHE:HB2   | 2.15                     | 0.47              |
| 4:04:315:ALA:O    | 4:04:324:LEU:HG    | 2.14                     | 0.47              |
| 4:04:423:LEU:HD12 | 4:04:423:LEU:N     | 2.29                     | 0.47              |
| 4:04:857:LEU:HD12 | 4:04:858:VAL:HG12  | 1.96                     | 0.47              |
| 9:G:142:VAL:O     | 9:G:142:VAL:HG13   | 2.14                     | 0.47              |
| 14:L:117:LEU:HD13 | 14:L:120:ALA:O     | 2.14                     | 0.47              |
| 1:A:161:A:N6      | 1:A:347:G:H21      | 2.08                     | 0.47              |
| 1:A:837:U:H2'     | 1:A:838:G:H8       | 1.78                     | 0.47              |
| 1:A:1395:C:H2'    | 1:A:1396:A:H8      | 1.80                     | 0.47              |
| 2:01:215:GLU:O    | 2:01:219:ARG:HG3   | 2.13                     | 0.47              |
| 3:03:109:ALA:O    | 3:03:111:GLU:N     | 2.44                     | 0.47              |
| 3:03:811:ASN:HA   | 3:03:815:SER:O     | 2.14                     | 0.47              |
| 3:03:1273:MET:HA  | 3:03:1276:TRP:CE3  | 2.49                     | 0.47              |
| 4:04:47:ARG:HA    | 4:04:47:ARG:HE     | 1.78                     | 0.47              |
| 4:04:537:TYR:CD2  | 4:04:544:LEU:HD13  | 2.48                     | 0.47              |
| 7:E:108:ARG:HA    | 7:E:111:ILE:HB     | 1.97                     | 0.47              |
| 11:I:61:LEU:HD12  | 11:I:61:LEU:N      | 2.30                     | 0.47              |
| 19:Q:11:LYS:O     | 19:Q:15:LEU:HD13   | 2.15                     | 0.47              |
| 20:R:30:LEU:O     | 20:R:34:GLN:HB2    | 2.15                     | 0.47              |
| 26:X:36:GLU:C     | 26:X:38:TYR:H      | 2.22                     | 0.47              |
| 1:A:577:G:C1'     | 1:A:816:A:H2'      | 2.45                     | 0.47              |
| 1:A:626:G:H2'     | 1:A:627:G:C8       | 2.49                     | 0.47              |
| 1:A:826:C:H2'     | 1:A:827:U:C6       | 2.49                     | 0.47              |
| 1:A:1066:C:H2'    | 1:A:1067:A:O4'     | 2.15                     | 0.47              |
| 2:01:234:LEU:HD22 | 2:01:234:LEU:N     | 2.30                     | 0.47              |
| 3:03:414:ILE:HD12 | 3:03:415:GLU:HB3   | 1.95                     | 0.47              |
| 3:03:463:GLN:HG3  | 3:03:505:PHE:CD1   | 2.49                     | 0.47              |
| 3:03:1194:GLU:O   | 3:03:1198:LEU:HD23 | 2.15                     | 0.47              |
| 4:04:563:LEU:HD12 | 4:04:563:LEU:N     | 2.29                     | 0.47              |
| 4:04:721:SER:HA   | 4:04:724:MET:CE    | 2.45                     | 0.47              |
| 7:E:56:GLU:O      | 7:E:60:ILE:HG12    | 2.15                     | 0.47              |
| 13:K:13:ILE:O     | 13:K:17:GLN:HG2    | 2.14                     | 0.47              |
| 14:L:43:ALA:HB1   | 14:L:46:VAL:CG2    | 2.44                     | 0.47              |
| 1:A:187:G:H1'     | 25:W:79:THR:HG21   | 1.95                     | 0.47              |
| 2:01:218:ARG:NH1  | 2:02:231:PHE:HA    | 2.28                     | 0.47              |
| 3:03:138:ILE:HG22 | 3:03:139:ASN:ND2   | 2.28                     | 0.47              |
| 3:03:633:LEU:C    | 3:03:633:LEU:HD12  | 2.40                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:03:1176:LEU:C   | 3:03:1178:LYS:H   | 2.21                     | 0.47              |
| 4:04:147:ILE:HG22 | 4:04:188:LEU:HG   | 1.97                     | 0.47              |
| 4:04:568:SER:C    | 4:04:569:LEU:HD12 | 2.40                     | 0.47              |
| 4:04:680:ASN:O    | 4:04:683:ILE:HB   | 2.15                     | 0.47              |
| 7:E:41:ILE:HG21   | 7:E:43:LEU:HD23   | 1.96                     | 0.47              |
| 7:E:170:HIS:HA    | 7:E:173:ILE:HD12  | 1.96                     | 0.47              |
| 8:F:111:ASP:O     | 8:F:115:VAL:HG23  | 2.14                     | 0.47              |
| 17:O:63:THR:HG23  | 17:O:92:VAL:HA    | 1.96                     | 0.47              |
| 1:A:320:A:H2'     | 1:A:321:A:C8      | 2.50                     | 0.47              |
| 1:A:909:A:H2'     | 1:A:910:C:O4'     | 2.14                     | 0.47              |
| 1:A:1323:G:H2'    | 1:A:1324:A:C8     | 2.50                     | 0.47              |
| 1:A:1513:A:H2'    | 1:A:1514:G:C8     | 2.50                     | 0.47              |
| 2:01:54:CYS:SG    | 2:01:92:VAL:HG22  | 2.55                     | 0.47              |
| 3:03:145:ILE:HG12 | 3:03:512:SER:CB   | 2.44                     | 0.47              |
| 3:03:530:ILE:HD11 | 3:03:575:LEU:HD13 | 1.96                     | 0.47              |
| 3:03:1106:ARG:HD2 | 3:03:1106:ARG:H   | 1.78                     | 0.47              |
| 4:04:490:ILE:O    | 4:04:498:PRO:HA   | 2.13                     | 0.47              |
| 4:04:514:THR:HG23 | 4:04:514:THR:O    | 2.14                     | 0.47              |
| 4:04:859:PRO:HG2  | 4:04:862:THR:OG1  | 2.15                     | 0.47              |
| 5:05:26:ARG:O     | 5:05:30:MET:HG3   | 2.14                     | 0.47              |
| 5:05:50:ALA:O     | 5:05:54:ILE:HG12  | 2.15                     | 0.47              |
| 7:E:44:GLU:O      | 7:E:48:PRO:CD     | 2.62                     | 0.47              |
| 8:F:20:THR:HG22   | 15:M:95:GLY:HA3   | 1.96                     | 0.47              |
| 18:P:14:ALA:HB2   | 18:P:47:LEU:HD21  | 1.97                     | 0.47              |
| 19:Q:26:LEU:HD13  | 19:Q:43:ALA:O     | 2.14                     | 0.47              |
| 21:S:5:ARG:HD3    | 21:S:5:ARG:N      | 2.29                     | 0.47              |
| 1:A:39:G:C2'      | 1:A:40:C:H5''     | 2.44                     | 0.47              |
| 1:A:168:G:O2'     | 1:A:169:C:H5'     | 2.14                     | 0.47              |
| 1:A:545:C:O2'     | 1:A:546:A:H5'     | 2.15                     | 0.47              |
| 1:A:1128:C:O2'    | 1:A:1129:C:H5'    | 2.15                     | 0.47              |
| 2:01:150:ARG:HH11 | 2:01:150:ARG:HG3  | 1.79                     | 0.47              |
| 2:01:207:THR:HG22 | 2:01:208:ASN:N    | 2.29                     | 0.47              |
| 2:02:86:LYS:HG2   | 2:02:173:VAL:HB   | 1.97                     | 0.47              |
| 2:02:163:GLU:HA   | 2:02:167:PRO:HD2  | 1.97                     | 0.47              |
| 3:03:433:ILE:O    | 3:03:437:ASN:ND2  | 2.47                     | 0.47              |
| 3:03:619:ALA:HB2  | 3:03:654:ASP:HB3  | 1.96                     | 0.47              |
| 4:04:1179:PRO:HG2 | 4:04:1183:SER:O   | 2.14                     | 0.47              |
| 7:E:9:MET:C       | 7:E:11:LYS:N      | 2.71                     | 0.47              |
| 7:E:71:GLY:HA2    | 7:E:164:ILE:HB    | 1.96                     | 0.47              |
| 10:H:107:GLY:N    | 10:H:110:MET:HE2  | 2.30                     | 0.47              |
| 12:J:30:MET:HA    | 12:J:38:ALA:CB    | 2.45                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:J:113:LYS:HD2  | 12:J:117:LEU:HD23 | 1.97                     | 0.47              |
| 19:Q:12:ARG:HH11  | 19:Q:12:ARG:HG3   | 1.80                     | 0.47              |
| 1:A:614:C:H3'     | 1:A:615:G:H5''    | 1.96                     | 0.47              |
| 3:03:4:SER:HB2    | 3:03:7:GLU:HG2    | 1.96                     | 0.47              |
| 3:03:29:SER:C     | 3:03:31:GLN:N     | 2.72                     | 0.47              |
| 3:03:670:PHE:HB3  | 3:03:673:HIS:CD2  | 2.48                     | 0.47              |
| 4:04:48:THR:C     | 4:04:50:LYS:H     | 2.23                     | 0.47              |
| 4:04:409:TRP:O    | 4:04:412:LEU:HB3  | 2.15                     | 0.47              |
| 4:04:733:SER:O    | 4:04:737:ILE:HG12 | 2.14                     | 0.47              |
| 6:B:3:GLU:O       | 6:B:7:GLN:HG3     | 2.15                     | 0.47              |
| 7:E:39:HIS:C      | 7:E:40:ILE:HG12   | 2.40                     | 0.47              |
| 7:E:74:ARG:HA     | 7:E:74:ARG:HE     | 1.80                     | 0.47              |
| 9:G:123:MET:HE2   | 9:G:145:ARG:HB2   | 1.97                     | 0.47              |
| 13:K:26:MET:HE3   | 13:K:60:LEU:HD12  | 1.97                     | 0.47              |
| 3:03:1064:ASP:OD1 | 3:03:1234:LYS:HE3 | 2.15                     | 0.47              |
| 4:04:449:LEU:HG   | 4:04:450:HIS:N    | 2.30                     | 0.47              |
| 4:04:504:GLN:O    | 4:04:507:VAL:HG22 | 2.14                     | 0.47              |
| 4:04:631:TYR:HA   | 4:04:634:ARG:HB2  | 1.97                     | 0.47              |
| 7:E:145:GLU:O     | 7:E:149:GLY:HA3   | 2.14                     | 0.47              |
| 8:F:32:LEU:O      | 8:F:32:LEU:HD23   | 2.14                     | 0.47              |
| 12:J:72:VAL:HG21  | 12:J:144:ALA:HB2  | 1.97                     | 0.47              |
| 25:W:17:ARG:HD2   | 25:W:17:ARG:C     | 2.40                     | 0.47              |
| 2:01:102:LEU:HD13 | 2:01:102:LEU:C    | 2.39                     | 0.46              |
| 2:01:102:LEU:HD21 | 2:01:110:VAL:HG11 | 1.97                     | 0.46              |
| 2:02:98:VAL:HG13  | 2:02:100:LEU:HD11 | 1.96                     | 0.46              |
| 3:03:30:ILE:HA    | 3:03:581:THR:OG1  | 2.15                     | 0.46              |
| 3:03:719:LYS:HD2  | 3:03:719:LYS:N    | 2.31                     | 0.46              |
| 4:04:92:VAL:O     | 4:04:92:VAL:HG23  | 2.15                     | 0.46              |
| 4:04:506:VAL:HG13 | 4:04:507:VAL:N    | 2.29                     | 0.46              |
| 7:E:27:MET:HG3    | 7:E:191:SER:H     | 1.80                     | 0.46              |
| 7:E:44:GLU:O      | 7:E:46:THR:N      | 2.48                     | 0.46              |
| 8:F:21:TRP:CB     | 8:F:58:ARG:HB3    | 2.45                     | 0.46              |
| 9:G:130:ASN:O     | 9:G:131:ILE:HD13  | 2.15                     | 0.46              |
| 10:H:93:VAL:HG22  | 10:H:126:ALA:HA   | 1.97                     | 0.46              |
| 16:N:63:GLN:O     | 16:N:67:GLU:HG2   | 2.14                     | 0.46              |
| 1:A:505:G:H2'     | 1:A:506:G:H8      | 1.81                     | 0.46              |
| 1:A:618:C:H5''    | 1:A:620:C:OP2     | 2.14                     | 0.46              |
| 1:A:1218:C:H2'    | 1:A:1219:A:C8     | 2.50                     | 0.46              |
| 2:02:92:VAL:HA    | 2:02:120:ASP:O    | 2.15                     | 0.46              |
| 2:02:182:ARG:HH11 | 2:02:182:ARG:HG3  | 1.81                     | 0.46              |
| 3:03:101:ARG:HG2  | 3:03:103:VAL:HG13 | 1.96                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:04:502:PRO:HG2   | 4:04:601:ILE:CD1  | 2.45                     | 0.46              |
| 4:04:865:HIS:HA    | 4:04:901:ARG:HH21 | 1.80                     | 0.46              |
| 4:04:1184:ASP:N    | 4:04:1185:PRO:HD2 | 2.30                     | 0.46              |
| 9:G:120:LYS:O      | 9:G:147:LYS:HD3   | 2.15                     | 0.46              |
| 13:K:124:ILE:HG13  | 13:K:124:ILE:O    | 2.15                     | 0.46              |
| 15:M:70:HIS:HB3    | 15:M:72:ARG:HH12  | 1.78                     | 0.46              |
| 23:U:38:LYS:HB2    | 23:U:38:LYS:NZ    | 2.31                     | 0.46              |
| 25:W:38:ILE:HG21   | 25:W:81:GLN:NE2   | 2.12                     | 0.46              |
| 1:A:10:A:H2'       | 1:A:11:G:C8       | 2.50                     | 0.46              |
| 1:A:1210:C:C2'     | 1:A:1211:U:H5'    | 2.45                     | 0.46              |
| 1:A:1355:G:H2'     | 1:A:1356:G:H8     | 1.78                     | 0.46              |
| 1:A:1393:U:H2'     | 1:A:1395:C:C5     | 2.45                     | 0.46              |
| 1:A:1520:C:H2'     | 1:A:1521:C:C6     | 2.50                     | 0.46              |
| 2:02:79:LEU:HD13   | 2:02:79:LEU:C     | 2.40                     | 0.46              |
| 3:03:712:SER:HB3   | 3:03:714:VAL:HG22 | 1.97                     | 0.46              |
| 3:03:855:PRO:HD2   | 3:03:915:ASP:HB2  | 1.96                     | 0.46              |
| 3:03:1328:LYS:NZ   | 4:04:246:PRO:HD3  | 2.30                     | 0.46              |
| 7:E:188:ASP:O      | 7:E:190:ASN:N     | 2.48                     | 0.46              |
| 9:G:8:LEU:O        | 9:G:12:ARG:HG3    | 2.15                     | 0.46              |
| 9:G:148:ALA:O      | 9:G:154:VAL:HG21  | 2.15                     | 0.46              |
| 10:H:37:VAL:HG11   | 10:H:113:VAL:HG13 | 1.96                     | 0.46              |
| 13:K:107:LYS:NZ    | 13:K:107:LYS:HB3  | 2.29                     | 0.46              |
| 14:L:114:LYS:HE3   | 14:L:117:LEU:CD1  | 2.46                     | 0.46              |
| 17:O:85:ARG:HA     | 17:O:93:ARG:HA    | 1.97                     | 0.46              |
| 1:A:348:G:H2'      | 1:A:349:A:H8      | 1.79                     | 0.46              |
| 1:A:1258:G:H2'     | 1:A:1259:C:C6     | 2.51                     | 0.46              |
| 2:01:156:SER:O     | 2:01:159:ILE:HG22 | 2.15                     | 0.46              |
| 2:02:10:LYS:N      | 2:02:10:LYS:HD2   | 2.30                     | 0.46              |
| 3:03:29:SER:HB3    | 3:03:33:ASP:HB2   | 1.96                     | 0.46              |
| 3:03:720:ARG:HD2   | 3:03:736:VAL:HG11 | 1.97                     | 0.46              |
| 4:04:196:GLN:OE1   | 4:04:196:GLN:HA   | 2.15                     | 0.46              |
| 4:04:370:LYS:HD3   | 4:04:443:GLU:HG2  | 1.98                     | 0.46              |
| 4:04:1223:LEU:HD13 | 4:04:1223:LEU:O   | 2.14                     | 0.46              |
| 7:E:16:PHE:HD2     | 7:E:41:ILE:HD12   | 1.79                     | 0.46              |
| 7:E:101:LEU:HD23   | 7:E:175:GLU:O     | 2.14                     | 0.46              |
| 8:F:11:LEU:HB3     | 8:F:17:TRP:NE1    | 2.30                     | 0.46              |
| 25:W:76:ALA:C      | 25:W:78:LEU:N     | 2.70                     | 0.46              |
| 1:A:147:G:H2'      | 1:A:148:G:C8      | 2.50                     | 0.46              |
| 1:A:523:A:O2'      | 1:A:524:G:H5''    | 2.16                     | 0.46              |
| 1:A:879:C:H2'      | 1:A:880:C:H6      | 1.81                     | 0.46              |
| 2:01:11:PRO:HG3    | 2:02:227:GLN:HA   | 1.97                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:01:195:ARG:HE   | 2:01:196:THR:H     | 1.63                     | 0.46              |
| 2:02:65:LEU:HD22  | 2:02:65:LEU:H      | 1.80                     | 0.46              |
| 3:03:468:LEU:O    | 3:03:472:GLU:HB2   | 2.16                     | 0.46              |
| 3:03:926:GLY:HA2  | 3:03:1056:VAL:HG22 | 1.97                     | 0.46              |
| 3:03:934:PHE:O    | 3:03:1048:LYS:HA   | 2.15                     | 0.46              |
| 3:03:956:ALA:O    | 3:03:960:LEU:HD23  | 2.15                     | 0.46              |
| 3:03:1032:LYS:O   | 3:03:1036:ILE:HG13 | 2.16                     | 0.46              |
| 3:03:1286:THR:O   | 3:03:1290:MET:HB2  | 2.15                     | 0.46              |
| 7:E:40:ILE:HG13   | 7:E:41:ILE:HG12    | 1.97                     | 0.46              |
| 8:F:37:LYS:HD3    | 8:F:40:GLN:NE2     | 2.31                     | 0.46              |
| 8:F:82:ASP:O      | 8:F:86:LEU:HG      | 2.16                     | 0.46              |
| 21:S:36:VAL:HG13  | 21:S:36:VAL:O      | 2.15                     | 0.46              |
| 1:A:302:G:H2'     | 1:A:303:A:C8       | 2.51                     | 0.46              |
| 1:A:662:U:H2'     | 1:A:663:A:C8       | 2.50                     | 0.46              |
| 2:02:80:GLU:HG2   | 4:04:569:LEU:HD21  | 1.96                     | 0.46              |
| 2:02:172:LEU:HD23 | 2:02:172:LEU:N     | 2.30                     | 0.46              |
| 3:03:498:ILE:O    | 3:03:502:VAL:HG12  | 2.15                     | 0.46              |
| 3:03:593:LYS:HB3  | 3:03:602:GLU:HB2   | 1.98                     | 0.46              |
| 3:03:675:ASP:HB2  | 3:03:1107:MET:HB2  | 1.98                     | 0.46              |
| 4:04:195:GLU:HA   | 4:04:198:CYS:SG    | 2.55                     | 0.46              |
| 4:04:395:LYS:HA   | 4:04:398:LYS:CE    | 2.45                     | 0.46              |
| 4:04:909:ILE:CD1  | 4:04:913:GLU:HG2   | 2.39                     | 0.46              |
| 15:M:102:LEU:HD23 | 15:M:102:LEU:N     | 2.25                     | 0.46              |
| 16:N:122:PRO:HB3  | 26:X:32:VAL:HA     | 1.96                     | 0.46              |
| 1:A:252:U:O2      | 1:A:252:U:C2'      | 2.64                     | 0.46              |
| 1:A:346:G:C2'     | 1:A:347:G:H5'      | 2.46                     | 0.46              |
| 2:01:89:ALA:HB1   | 2:01:208:ASN:ND2   | 2.31                     | 0.46              |
| 3:03:392:GLU:OE1  | 3:03:419:ILE:HG23  | 2.16                     | 0.46              |
| 3:03:702:THR:HA   | 3:03:1184:THR:H    | 1.81                     | 0.46              |
| 4:04:255:LEU:HD13 | 4:04:256:ASP:N     | 2.31                     | 0.46              |
| 4:04:863:LEU:HD21 | 4:04:901:ARG:HD3   | 1.96                     | 0.46              |
| 4:04:871:LEU:C    | 4:04:871:LEU:HD23  | 2.41                     | 0.46              |
| 7:E:21:ARG:C      | 7:E:23:TRP:H       | 2.24                     | 0.46              |
| 8:F:57:GLU:HB2    | 8:F:64:ARG:HB3     | 1.97                     | 0.46              |
| 3:03:320:ASP:O    | 3:03:324:LYS:HG3   | 2.15                     | 0.46              |
| 3:03:360:LEU:O    | 3:03:364:VAL:HG23  | 2.16                     | 0.46              |
| 3:03:1087:TYR:HB2 | 3:03:1091:GLY:HA2  | 1.97                     | 0.46              |
| 3:03:1104:PRO:HB3 | 4:04:722:ILE:HG13  | 1.97                     | 0.46              |
| 4:04:220:ARG:HG2  | 4:04:220:ARG:HH11  | 1.80                     | 0.46              |
| 4:04:472:LEU:H    | 4:04:472:LEU:CD2   | 2.25                     | 0.46              |
| 4:04:767:LEU:HB2  | 4:04:771:GLN:CD    | 2.41                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:04:1233:ILE:O    | 4:04:1237:VAL:HG12 | 2.15                     | 0.46              |
| 4:04:1314:LEU:HD11 | 4:04:1330:ARG:HH12 | 1.81                     | 0.46              |
| 7:E:31:ILE:HG21    | 7:E:189:THR:HG22   | 1.98                     | 0.46              |
| 26:X:17:ARG:HE     | 26:X:21:ARG:HH22   | 1.64                     | 0.46              |
| 1:A:247:G:H2'      | 1:A:248:C:C6       | 2.51                     | 0.46              |
| 1:A:285:C:H2'      | 1:A:286:C:C6       | 2.51                     | 0.46              |
| 1:A:977:A:H4'      | 1:A:981:U:H3       | 1.81                     | 0.46              |
| 3:03:241:LEU:O     | 3:03:243:PRO:HD3   | 2.16                     | 0.46              |
| 3:03:696:ASP:HB3   | 3:03:798:GLN:HA    | 1.98                     | 0.46              |
| 3:03:1246:ARG:C    | 3:03:1246:ARG:HD3  | 2.41                     | 0.46              |
| 4:04:134:ASP:O     | 4:04:138:VAL:HG23  | 2.15                     | 0.46              |
| 4:04:290:ILE:H     | 4:04:290:ILE:CD1   | 2.14                     | 0.46              |
| 4:04:1323:ALA:N    | 4:04:1331:VAL:HG21 | 2.31                     | 0.46              |
| 9:G:36:ALA:HA      | 9:G:41:GLY:HA3     | 1.98                     | 0.46              |
| 9:G:149:LYS:HA     | 9:G:177:MET:HE1    | 1.98                     | 0.46              |
| 13:K:76:ARG:HA     | 13:K:126:CYS:HB3   | 1.97                     | 0.46              |
| 25:W:24:ARG:CB     | 25:W:28:ARG:HH22   | 2.27                     | 0.46              |
| 1:A:39:G:H2'       | 1:A:40:C:C5'       | 2.46                     | 0.46              |
| 1:A:751:U:C2'      | 1:A:752:G:H5'      | 2.46                     | 0.46              |
| 1:A:824:G:H1'      | 13:K:1:S:ER:HA     | 1.97                     | 0.46              |
| 1:A:1157:A:N6      | 1:A:1178:G:H1'     | 2.31                     | 0.46              |
| 2:01:124:VAL:HG13  | 2:01:125:LYS:HG2   | 1.98                     | 0.46              |
| 3:03:7:GLU:OE1     | 3:03:11:ILE:HD12   | 2.16                     | 0.46              |
| 3:03:434:ASP:HA    | 3:03:437:ASN:ND2   | 2.27                     | 0.46              |
| 3:03:880:GLY:HA2   | 3:03:920:VAL:O     | 2.16                     | 0.46              |
| 3:03:1105:S:ER:HB2 | 4:04:731:ARG:O     | 2.17                     | 0.46              |
| 4:04:555:TYR:HD2   | 4:04:585:LYS:HB3   | 1.81                     | 0.46              |
| 7:E:54:LEU:CD2     | 7:E:220:THR:HG21   | 2.39                     | 0.46              |
| 8:F:23:ALA:HB3     | 8:F:28:PHE:HD1     | 1.81                     | 0.46              |
| 10:H:104:ILE:HA    | 10:H:122:VAL:O     | 2.16                     | 0.46              |
| 13:K:54:THR:HG23   | 13:K:55:LYS:HG3    | 1.98                     | 0.46              |
| 21:S:32:PHE:H      | 21:S:32:PHE:HD1    | 1.64                     | 0.46              |
| 1:A:1368:A:O2'     | 1:A:1369:C:H5'     | 2.15                     | 0.45              |
| 2:01:45:ARG:HD3    | 3:03:1083:GLU:HB3  | 1.97                     | 0.45              |
| 3:03:124:MET:HG2   | 3:03:493:ILE:HG12  | 1.97                     | 0.45              |
| 3:03:533:LEU:HD11  | 3:03:571:LEU:HD13  | 1.97                     | 0.45              |
| 4:04:382:TYR:O     | 4:04:386:GLU:HG2   | 2.16                     | 0.45              |
| 15:M:52:LEU:HD21   | 15:M:59:LYS:HE2    | 1.98                     | 0.45              |
| 18:P:19:THR:HG22   | 18:P:25:GLY:C      | 2.41                     | 0.45              |
| 21:S:70:ARG:HG2    | 21:S:70:ARG:HH11   | 1.80                     | 0.45              |
| 23:U:40:VAL:HA     | 23:U:41:PRO:HD3    | 1.77                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:X:10:GLU:HA     | 26:X:12:PHE:HE1    | 1.81                     | 0.45              |
| 1:A:648:A:H2'      | 1:A:649:A:C8       | 2.52                     | 0.45              |
| 1:A:750:C:O2       | 20:R:22:GLY:HA3    | 2.16                     | 0.45              |
| 1:A:770:C:H2'      | 1:A:771:G:H8       | 1.81                     | 0.45              |
| 1:A:1372:U:OP1     | 14:L:73:GLY:N      | 2.49                     | 0.45              |
| 2:01:145:LYS:NZ    | 2:01:147:GLN:HB3   | 2.31                     | 0.45              |
| 2:01:166:ARG:N     | 2:01:167:PRO:CD    | 2.79                     | 0.45              |
| 2:02:111:THR:HA    | 2:02:129:VAL:HA    | 1.97                     | 0.45              |
| 3:03:33:ASP:HA     | 3:03:36:GLN:CB     | 2.46                     | 0.45              |
| 3:03:213:LEU:O     | 3:03:213:LEU:HD23  | 2.16                     | 0.45              |
| 3:03:515:MET:HA    | 3:03:526:HIS:ND1   | 2.32                     | 0.45              |
| 3:03:582:ASN:HB2   | 3:03:588:GLU:HG2   | 1.97                     | 0.45              |
| 3:03:753:LEU:HB3   | 3:03:767:GLN:HB2   | 1.97                     | 0.45              |
| 3:03:1025:PHE:O    | 3:03:1029:LEU:HD13 | 2.16                     | 0.45              |
| 4:04:399:LYS:O     | 4:04:402:GLU:HB3   | 2.16                     | 0.45              |
| 4:04:547:ARG:HG3   | 4:04:547:ARG:NH1   | 2.31                     | 0.45              |
| 4:04:661:VAL:HG12  | 4:04:685:ILE:HD11  | 1.99                     | 0.45              |
| 4:04:796:LEU:O     | 4:04:800:LEU:HD13  | 2.16                     | 0.45              |
| 4:04:1304:ARG:HG3  | 4:04:1304:ARG:NH1  | 2.30                     | 0.45              |
| 4:04:1353:VAL:HG22 | 4:04:1353:VAL:O    | 2.16                     | 0.45              |
| 12:J:78:ARG:HH11   | 12:J:78:ARG:HG3    | 1.81                     | 0.45              |
| 26:X:42:THR:HG22   | 26:X:46:LYS:HZ3    | 1.81                     | 0.45              |
| 1:A:194:C:O2       | 25:W:62:ALA:HB3    | 2.16                     | 0.45              |
| 1:A:376:G:H2'      | 1:A:377:G:H5'      | 1.98                     | 0.45              |
| 1:A:782:A:H62      | 1:A:800:G:H21      | 1.64                     | 0.45              |
| 1:A:981:U:H4'      | 19:Q:62:ARG:NH2    | 2.31                     | 0.45              |
| 2:02:158:ARG:HA    | 2:02:158:ARG:HE    | 1.80                     | 0.45              |
| 3:03:589:THR:HA    | 3:03:590:PRO:HD3   | 1.82                     | 0.45              |
| 3:03:738:GLU:HA    | 3:03:741:MET:CB    | 2.46                     | 0.45              |
| 3:03:817:LEU:HD21  | 3:03:1080:ASN:HD22 | 1.81                     | 0.45              |
| 4:04:86:GLU:HG2    | 26:X:67:ARG:NH2    | 2.31                     | 0.45              |
| 4:04:309:ASN:HB3   | 4:04:314:ARG:HA    | 1.98                     | 0.45              |
| 4:04:767:LEU:HD23  | 4:04:767:LEU:N     | 2.32                     | 0.45              |
| 7:E:20:THR:O       | 7:E:23:TRP:N       | 2.49                     | 0.45              |
| 7:E:130:THR:HG22   | 7:E:132:LYS:H      | 1.81                     | 0.45              |
| 9:G:58:GLN:O       | 9:G:62:ARG:HG2     | 2.16                     | 0.45              |
| 10:H:87:VAL:HA     | 10:H:91:SER:O      | 2.15                     | 0.45              |
| 12:J:30:MET:HG3    | 12:J:30:MET:O      | 2.17                     | 0.45              |
| 12:J:55:LYS:HZ2    | 12:J:63:VAL:HG21   | 1.82                     | 0.45              |
| 1:A:242:G:H2'      | 1:A:243:A:H5'      | 1.98                     | 0.45              |
| 1:A:881:G:O2'      | 1:A:882:C:H5'      | 2.17                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:1092:A:OP2     | 12:J:3:ARG:HD3     | 2.15                     | 0.45              |
| 3:03:182:SER:HB2   | 3:03:389:PHE:HE1   | 1.82                     | 0.45              |
| 3:03:367:TYR:HB3   | 3:03:376:PRO:HB3   | 1.97                     | 0.45              |
| 4:04:320:ASN:ND2   | 4:04:321:LYS:N     | 2.65                     | 0.45              |
| 4:04:769:VAL:O     | 4:04:772:TYR:HB3   | 2.17                     | 0.45              |
| 7:E:114:LEU:HD13   | 7:E:144:LEU:HB3    | 1.98                     | 0.45              |
| 10:H:151:MET:O     | 10:H:155:LYS:HG3   | 2.15                     | 0.45              |
| 14:L:83:THR:HG22   | 14:L:94:ARG:HH22   | 1.82                     | 0.45              |
| 19:Q:77:GLY:O      | 19:Q:78:LEU:HD23   | 2.16                     | 0.45              |
| 1:A:961:U:H2'      | 1:A:962:C:O4'      | 2.17                     | 0.45              |
| 1:A:1066:C:H42     | 1:A:1191:A:H62     | 1.63                     | 0.45              |
| 3:03:402:ARG:HG3   | 3:03:406:ASN:HD21  | 1.81                     | 0.45              |
| 4:04:53:ARG:O      | 4:04:54:ASP:HB2    | 2.16                     | 0.45              |
| 4:04:405:GLU:O     | 4:04:408:VAL:HG22  | 2.17                     | 0.45              |
| 4:04:1196:LEU:HD12 | 4:04:1210:ILE:HG22 | 1.98                     | 0.45              |
| 5:05:27:ALA:O      | 5:05:31:GLN:HG3    | 2.16                     | 0.45              |
| 11:I:45:ARG:HG2    | 11:I:45:ARG:HH11   | 1.81                     | 0.45              |
| 20:R:61:GLN:O      | 20:R:65:LEU:HB2    | 2.16                     | 0.45              |
| 21:S:47:GLU:OE1    | 21:S:47:GLU:N      | 2.49                     | 0.45              |
| 23:U:12:ARG:HH21   | 23:U:12:ARG:HG2    | 1.81                     | 0.45              |
| 1:A:128:G:O2'      | 1:A:129:A:H5'      | 2.16                     | 0.45              |
| 1:A:594:U:O2'      | 1:A:595:A:H5'      | 2.17                     | 0.45              |
| 1:A:686:U:H1'      | 16:N:43:TRP:HE1    | 1.82                     | 0.45              |
| 1:A:770:C:H1'      | 1:A:900:A:C2       | 2.46                     | 0.45              |
| 2:01:99:ILE:HA     | 2:01:144:ILE:O     | 2.17                     | 0.45              |
| 3:03:54:ARG:HH11   | 3:03:54:ARG:CB     | 2.30                     | 0.45              |
| 3:03:699:LEU:HG    | 3:03:799:ASN:ND2   | 2.32                     | 0.45              |
| 4:04:75:TYR:HB3    | 4:04:80:HIS:CG     | 2.52                     | 0.45              |
| 4:04:526:VAL:C     | 4:04:527:LEU:HD12  | 2.42                     | 0.45              |
| 9:G:23:GLY:HA2     | 9:G:160:LEU:HD11   | 1.99                     | 0.45              |
| 9:G:98:ASP:OD1     | 9:G:132:ALA:HB1    | 2.16                     | 0.45              |
| 10:H:68:ARG:HD2    | 10:H:68:ARG:C      | 2.42                     | 0.45              |
| 13:K:105:THR:C     | 13:K:107:LYS:H     | 2.25                     | 0.45              |
| 23:U:26:ILE:O      | 23:U:30:LYS:HG3    | 2.16                     | 0.45              |
| 24:V:18:VAL:O      | 24:V:21:ALA:HB3    | 2.16                     | 0.45              |
| 26:X:47:ARG:HH11   | 26:X:47:ARG:HG3    | 1.81                     | 0.45              |
| 1:A:136:C:H2'      | 1:A:137:U:H5''     | 1.97                     | 0.45              |
| 1:A:337:G:H2'      | 1:A:338:A:C8       | 2.52                     | 0.45              |
| 1:A:1250:A:H2'     | 1:A:1251:A:C8      | 2.52                     | 0.45              |
| 1:A:1514:G:H2'     | 1:A:1515:G:C8      | 2.52                     | 0.45              |
| 2:02:35:PHE:HA     | 2:02:38:THR:CG2    | 2.35                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:03:232:ILE:HG12 | 3:03:237:LEU:HD23 | 1.98                     | 0.45              |
| 4:04:106:GLU:O    | 4:04:280:LYS:HD3  | 2.17                     | 0.45              |
| 4:04:926:PRO:HG2  | 4:04:1248:ILE:CD1 | 2.46                     | 0.45              |
| 11:I:18:VAL:HG12  | 11:I:19:PRO:HD3   | 1.98                     | 0.45              |
| 11:I:47:LEU:H     | 11:I:56:LYS:H     | 1.65                     | 0.45              |
| 13:K:31:LEU:N     | 13:K:31:LEU:HD12  | 2.32                     | 0.45              |
| 18:P:3:ILE:HG22   | 18:P:56:ARG:HB2   | 1.97                     | 0.45              |
| 18:P:15:VAL:O     | 18:P:19:THR:HG23  | 2.16                     | 0.45              |
| 1:A:586:C:H2'     | 1:A:587:G:O4'     | 2.16                     | 0.45              |
| 1:A:1238:A:C2'    | 1:A:1239:A:H5'    | 2.46                     | 0.45              |
| 2:02:9:LEU:C      | 2:02:10:LYS:HD2   | 2.41                     | 0.45              |
| 3:03:207:THR:HG22 | 3:03:210:LEU:HD12 | 1.98                     | 0.45              |
| 3:03:421:SER:O    | 3:03:425:ILE:HG13 | 2.17                     | 0.45              |
| 3:03:551:HIS:HA   | 3:03:552:PRO:HD3  | 1.85                     | 0.45              |
| 3:03:642:SER:HB3  | 4:04:770:LEU:HD23 | 1.99                     | 0.45              |
| 3:03:1184:THR:HA  | 3:03:1185:PRO:HD3 | 1.87                     | 0.45              |
| 4:04:337:ARG:HD2  | 4:04:337:ARG:N    | 2.26                     | 0.45              |
| 4:04:1219:ASP:O   | 4:04:1223:LEU:HB3 | 2.17                     | 0.45              |
| 7:E:104:TRP:O     | 7:E:108:ARG:HG3   | 2.16                     | 0.45              |
| 9:G:13:ARG:CZ     | 9:G:37:PRO:HB2    | 2.46                     | 0.45              |
| 9:G:196:GLU:N     | 9:G:196:GLU:OE1   | 2.49                     | 0.45              |
| 14:L:53:LEU:HD13  | 14:L:96:GLU:O     | 2.17                     | 0.45              |
| 1:A:107:G:O6      | 25:W:6:ALA:HB1    | 2.16                     | 0.45              |
| 1:A:173:U:H3      | 1:A:198:G:H21     | 1.65                     | 0.45              |
| 1:A:1270:G:H2'    | 1:A:1271:A:H8     | 1.80                     | 0.45              |
| 2:02:64:VAL:HG23  | 2:02:71:LYS:HD3   | 1.99                     | 0.45              |
| 3:03:75:LEU:N     | 3:03:75:LEU:HD22  | 2.31                     | 0.45              |
| 3:03:75:LEU:HD11  | 3:03:127:ILE:HD11 | 1.98                     | 0.45              |
| 3:03:273:HIS:O    | 3:03:277:LEU:HG   | 2.17                     | 0.45              |
| 3:03:903:ARG:NH2  | 3:03:908:GLU:HG3  | 2.32                     | 0.45              |
| 4:04:769:VAL:HG12 | 4:04:773:PHE:CE2  | 2.52                     | 0.45              |
| 4:04:848:VAL:HB   | 4:04:858:VAL:HG12 | 1.98                     | 0.45              |
| 7:E:25:PRO:HB2    | 7:E:28:LYS:CB     | 2.22                     | 0.45              |
| 10:H:159:SER:HB3  | 10:H:162:GLU:CB   | 2.47                     | 0.45              |
| 19:Q:23:ARG:HH11  | 19:Q:23:ARG:HG3   | 1.82                     | 0.45              |
| 24:V:10:ILE:HG21  | 24:V:40:PHE:CE1   | 2.51                     | 0.45              |
| 25:W:27:MET:HE2   | 25:W:28:ARG:HH11  | 1.82                     | 0.45              |
| 1:A:242:G:C2'     | 1:A:243:A:H5'     | 2.47                     | 0.45              |
| 1:A:917:G:H2'     | 1:A:918:A:H8      | 1.82                     | 0.45              |
| 2:02:17:GLU:OE1   | 2:02:25:LYS:HD3   | 2.15                     | 0.45              |
| 2:02:192:VAL:O    | 2:02:192:VAL:HG12 | 2.16                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:03:637:ARG:HA   | 3:03:641:GLU:O     | 2.17                     | 0.45              |
| 3:03:810:TYR:C    | 3:03:811:ASN:HD22  | 2.25                     | 0.45              |
| 4:04:45:ASN:HB2   | 4:04:48:THR:O      | 2.17                     | 0.45              |
| 4:04:287:ALA:HB1  | 4:04:288:PRO:HD2   | 1.99                     | 0.45              |
| 4:04:490:ILE:HD12 | 4:04:490:ILE:C     | 2.42                     | 0.45              |
| 4:04:968:ASN:ND2  | 4:04:974:VAL:HG13  | 2.31                     | 0.45              |
| 4:04:1010:GLN:CD  | 4:04:1010:GLN:N    | 2.74                     | 0.45              |
| 10:H:9:GLU:OE1    | 10:H:9:GLU:N       | 2.50                     | 0.45              |
| 18:P:22:TYR:HB3   | 18:P:65:GLU:HG2    | 1.99                     | 0.45              |
| 1:A:219:U:C2'     | 1:A:220:G:H5''     | 2.47                     | 0.44              |
| 2:01:140:ILE:O    | 2:01:140:ILE:HG13  | 2.17                     | 0.44              |
| 2:02:51:MET:H     | 2:02:151:GLY:HA2   | 1.81                     | 0.44              |
| 3:03:451:ARG:HG3  | 3:03:451:ARG:HH11  | 1.82                     | 0.44              |
| 3:03:1023:HIS:O   | 3:03:1027:LYS:HG2  | 2.18                     | 0.44              |
| 4:04:378:LYS:HB2  | 4:04:379:PRO:HD3   | 1.97                     | 0.44              |
| 4:04:620:PHE:O    | 4:04:624:ILE:HG13  | 2.17                     | 0.44              |
| 4:04:1151:LYS:O   | 4:04:1153:PRO:HD3  | 2.17                     | 0.44              |
| 7:E:74:ARG:HH21   | 7:E:77:SER:HB3     | 1.82                     | 0.44              |
| 12:J:70:PRO:HG3   | 12:J:102:TRP:HZ3   | 1.82                     | 0.44              |
| 17:O:43:LYS:HG3   | 17:O:44:PRO:CD     | 2.41                     | 0.44              |
| 1:A:7:A:O2'       | 10:H:125:LYS:HB2   | 2.17                     | 0.44              |
| 1:A:932:C:OP2     | 12:J:2:ARG:HB3     | 2.17                     | 0.44              |
| 3:03:26:TYR:CE2   | 3:03:32:LEU:HD13   | 2.50                     | 0.44              |
| 3:03:636:CYS:HB2  | 3:03:645:PHE:CD2   | 2.52                     | 0.44              |
| 4:04:122:SER:OG   | 4:04:125:GLY:HA3   | 2.18                     | 0.44              |
| 4:04:1350:ASN:HB2 | 4:04:1357:ILE:HG22 | 1.98                     | 0.44              |
| 7:E:24:ASN:HA     | 7:E:25:PRO:HD2     | 1.61                     | 0.44              |
| 7:E:34:ALA:O      | 7:E:40:ILE:HG13    | 2.17                     | 0.44              |
| 8:F:41:TYR:CE2    | 8:F:89:VAL:HG11    | 2.51                     | 0.44              |
| 8:F:86:LEU:O      | 8:F:90:VAL:HG23    | 2.16                     | 0.44              |
| 8:F:156:LEU:HD12  | 8:F:156:LEU:O      | 2.17                     | 0.44              |
| 16:N:21:HIS:HA    | 16:N:84:MET:O      | 2.17                     | 0.44              |
| 19:Q:12:ARG:O     | 19:Q:16:ALA:HB2    | 2.18                     | 0.44              |
| 22:T:44:HIS:HB2   | 22:T:69:THR:O      | 2.17                     | 0.44              |
| 1:A:200:G:H2'     | 1:A:201:G:H8       | 1.81                     | 0.44              |
| 1:A:744:C:H2'     | 1:A:745:G:C8       | 2.53                     | 0.44              |
| 1:A:1073:U:OP1    | 10:H:61:LYS:HG3    | 2.16                     | 0.44              |
| 2:01:125:LYS:NZ   | 2:01:128:HIS:HB2   | 2.32                     | 0.44              |
| 2:02:83:LEU:CB    | 4:04:528:THR:HB    | 2.40                     | 0.44              |
| 4:04:85:CYS:H     | 4:04:90:VAL:H      | 1.62                     | 0.44              |
| 4:04:894:VAL:HG12 | 4:04:895:CYS:N     | 2.32                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:F:42:LEU:HD22   | 8:F:54:ILE:HD13    | 1.99                     | 0.44              |
| 10:H:10:LEU:HD11  | 10:H:67:ARG:NH2    | 2.32                     | 0.44              |
| 12:J:89:GLU:CD    | 12:J:89:GLU:H      | 2.24                     | 0.44              |
| 13:K:100:ILE:HD12 | 13:K:111:THR:CG2   | 2.47                     | 0.44              |
| 14:L:25:GLY:C     | 14:L:26:LYS:HD2    | 2.42                     | 0.44              |
| 18:P:18:LEU:HD21  | 18:P:55:LEU:HD13   | 1.97                     | 0.44              |
| 1:A:309:A:H2'     | 1:A:310:G:C8       | 2.52                     | 0.44              |
| 1:A:1239:A:H5''   | 1:A:1240:U:C5      | 2.51                     | 0.44              |
| 2:01:79:LEU:HD13  | 2:01:79:LEU:O      | 2.17                     | 0.44              |
| 2:01:224:LEU:HD13 | 2:02:228:LEU:CD1   | 2.47                     | 0.44              |
| 3:03:828:PHE:CE2  | 3:03:1234:LYS:HD2  | 2.52                     | 0.44              |
| 4:04:98:ARG:O     | 4:04:98:ARG:HG2    | 2.17                     | 0.44              |
| 4:04:293:ARG:HA   | 4:04:296:LYS:HG3   | 2.00                     | 0.44              |
| 4:04:510:LEU:HD13 | 4:04:628:GLY:HA2   | 1.98                     | 0.44              |
| 4:04:757:THR:HA   | 4:04:758:PRO:HD3   | 1.79                     | 0.44              |
| 4:04:1323:ALA:CA  | 4:04:1331:VAL:HG21 | 2.47                     | 0.44              |
| 7:E:35:ARG:HG3    | 7:E:35:ARG:NH1     | 2.31                     | 0.44              |
| 8:F:37:LYS:HA     | 8:F:40:GLN:HE21    | 1.83                     | 0.44              |
| 14:L:121:ARG:HG3  | 14:L:121:ARG:HH11  | 1.82                     | 0.44              |
| 21:S:14:ARG:HH11  | 21:S:14:ARG:HG3    | 1.82                     | 0.44              |
| 1:A:244:U:H3      | 1:A:893:C:H42      | 1.66                     | 0.44              |
| 1:A:358:U:H2'     | 1:A:359:G:H8       | 1.82                     | 0.44              |
| 1:A:404:G:H1      | 1:A:499:A:H62      | 1.65                     | 0.44              |
| 1:A:668:G:H21     | 20:R:45:HIS:CE1    | 2.35                     | 0.44              |
| 1:A:692:U:H2'     | 1:A:694:A:OP2      | 2.17                     | 0.44              |
| 1:A:903:G:H2'     | 1:A:904:U:C6       | 2.53                     | 0.44              |
| 1:A:1066:C:O2'    | 1:A:1067:A:H5'     | 2.16                     | 0.44              |
| 3:03:347:ILE:O    | 3:03:351:LEU:HG    | 2.18                     | 0.44              |
| 3:03:673:HIS:HB3  | 3:03:1109:ILE:HG23 | 1.99                     | 0.44              |
| 3:03:952:GLN:HB2  | 3:03:1036:ILE:HD13 | 1.98                     | 0.44              |
| 4:04:109:SER:OG   | 4:04:296:LYS:HA    | 2.17                     | 0.44              |
| 4:04:193:ASP:OD2  | 4:04:196:GLN:HG2   | 2.17                     | 0.44              |
| 4:04:250:ARG:HD3  | 4:04:250:ARG:N     | 2.32                     | 0.44              |
| 4:04:328:ALA:HA   | 4:04:331:ILE:HG13  | 1.98                     | 0.44              |
| 4:04:956:GLY:HA2  | 4:04:986:ASP:HA    | 1.98                     | 0.44              |
| 4:04:1123:ARG:O   | 4:04:1125:PRO:HD3  | 2.18                     | 0.44              |
| 4:04:1261:LEU:C   | 4:04:1261:LEU:HD12 | 2.43                     | 0.44              |
| 7:E:38:VAL:O      | 7:E:39:HIS:CB      | 2.66                     | 0.44              |
| 8:F:126:ARG:HD3   | 8:F:126:ARG:N      | 2.32                     | 0.44              |
| 12:J:65:LEU:HD21  | 12:J:96:ASN:HD22   | 1.83                     | 0.44              |
| 15:M:10:LEU:HB2   | 15:M:72:ARG:HB2    | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:P:44:ILE:HG13   | 18:P:47:LEU:HD12   | 2.00                     | 0.44              |
| 24:V:55:GLN:HG3    | 24:V:56:HIS:N      | 2.33                     | 0.44              |
| 1:A:192:A:O2'      | 25:W:55:PRO:HG3    | 2.18                     | 0.44              |
| 1:A:1071:C:H2'     | 1:A:1072:G:H8      | 1.81                     | 0.44              |
| 2:02:100:LEU:N     | 2:02:100:LEU:HD12  | 2.32                     | 0.44              |
| 3:03:183:TRP:HB2   | 3:03:199:ASP:HA    | 2.00                     | 0.44              |
| 3:03:448:LEU:HA    | 3:03:451:ARG:HB2   | 1.99                     | 0.44              |
| 3:03:522:SER:HA    | 3:03:525:THR:HG22  | 1.99                     | 0.44              |
| 3:03:618:GLN:HG3   | 3:03:620:ASN:H     | 1.82                     | 0.44              |
| 3:03:834:GLN:O     | 3:03:1053:TYR:HA   | 2.17                     | 0.44              |
| 3:03:1141:LEU:HD12 | 3:03:1141:LEU:C    | 2.43                     | 0.44              |
| 3:03:1238:LEU:HB2  | 3:03:1241:ASP:OD2  | 2.18                     | 0.44              |
| 4:04:47:ARG:HA     | 4:04:47:ARG:NE     | 2.32                     | 0.44              |
| 4:04:1249:ASN:OD1  | 4:04:1251:LYS:HG3  | 2.18                     | 0.44              |
| 7:E:57:LEU:CD1     | 7:E:217:VAL:HG13   | 2.47                     | 0.44              |
| 8:F:12:GLY:HA3     | 19:Q:96:LYS:HG3    | 1.99                     | 0.44              |
| 8:F:129:PHE:HD1    | 8:F:129:PHE:H      | 1.65                     | 0.44              |
| 9:G:118:SER:C      | 9:G:120:LYS:H      | 2.26                     | 0.44              |
| 9:G:190:LEU:HD12   | 9:G:192:ALA:N      | 2.29                     | 0.44              |
| 16:N:72:ALA:H      | 16:N:74:LYS:NZ     | 2.14                     | 0.44              |
| 18:P:95:PRO:HA     | 18:P:108:ARG:HG2   | 2.00                     | 0.44              |
| 21:S:25:ARG:HD3    | 21:S:25:ARG:H      | 1.82                     | 0.44              |
| 1:A:171:A:O2'      | 1:A:172:A:H5'      | 2.17                     | 0.44              |
| 1:A:631:C:H3'      | 1:A:632:U:H5'      | 2.00                     | 0.44              |
| 2:01:89:ALA:CB     | 2:01:208:ASN:HD22  | 2.28                     | 0.44              |
| 2:02:224:LEU:HD23  | 2:02:224:LEU:O     | 2.17                     | 0.44              |
| 3:03:616:ILE:N     | 3:03:616:ILE:CD1   | 2.79                     | 0.44              |
| 3:03:974:ARG:NE    | 3:03:974:ARG:HA    | 2.32                     | 0.44              |
| 3:03:1119:MET:HG3  | 3:03:1204:LEU:HD11 | 2.00                     | 0.44              |
| 3:03:1304:MET:O    | 3:03:1308:ILE:HG12 | 2.18                     | 0.44              |
| 4:04:230:SER:OG    | 4:04:232:ASN:ND2   | 2.51                     | 0.44              |
| 4:04:422:LEU:HD11  | 4:04:484:MET:HE2   | 1.99                     | 0.44              |
| 4:04:615:LYS:HG2   | 5:05:5:THR:OG1     | 2.18                     | 0.44              |
| 4:04:997:VAL:HA    | 4:04:998:PRO:HD3   | 1.88                     | 0.44              |
| 4:04:1346:GLY:O    | 4:04:1350:ASN:ND2  | 2.51                     | 0.44              |
| 7:E:188:ASP:OD1    | 7:E:188:ASP:N      | 2.51                     | 0.44              |
| 16:N:60:PHE:O      | 16:N:64:VAL:HG23   | 2.18                     | 0.44              |
| 17:O:3:VAL:HA      | 17:O:6:LEU:HD12    | 1.99                     | 0.44              |
| 18:P:32:ILE:HG13   | 18:P:59:VAL:HG12   | 1.99                     | 0.44              |
| 18:P:78:ARG:HH21   | 24:V:64:GLU:HB3    | 1.83                     | 0.44              |
| 19:Q:61:ASN:HB3    | 19:Q:72:PHE:CZ     | 2.53                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:X:55:ARG:O      | 26:X:59:LYS:HG2    | 2.17                     | 0.44              |
| 1:A:352:C:H4'      | 1:A:354:G:OP1      | 2.17                     | 0.44              |
| 1:A:372:C:H41      | 1:A:387:U:H2'      | 1.83                     | 0.44              |
| 1:A:521:G:OP1      | 17:O:69:GLU:HG3    | 2.18                     | 0.44              |
| 1:A:831:A:H2'      | 1:A:832:G:H5''     | 2.00                     | 0.44              |
| 1:A:1119:C:H5'     | 14:L:84:ARG:HH22   | 1.82                     | 0.44              |
| 1:A:1238:A:H2'     | 1:A:1239:A:H5'     | 2.00                     | 0.44              |
| 2:02:31:LEU:HD22   | 2:02:31:LEU:N      | 2.33                     | 0.44              |
| 3:03:951:MET:O     | 3:03:951:MET:HE3   | 2.17                     | 0.44              |
| 4:04:242:LEU:HA    | 4:04:243:PRO:HD3   | 1.78                     | 0.44              |
| 4:04:614:LEU:O     | 4:04:618:VAL:HG23  | 2.18                     | 0.44              |
| 4:04:697:MET:O     | 4:04:701:LEU:HD23  | 2.17                     | 0.44              |
| 4:04:1046:ILE:HG22 | 4:04:1061:VAL:HA   | 1.99                     | 0.44              |
| 4:04:1286:LYS:O    | 4:04:1290:ARG:HB2  | 2.17                     | 0.44              |
| 7:E:31:ILE:O       | 7:E:32:PHE:CB      | 2.66                     | 0.44              |
| 11:I:47:LEU:HD21   | 11:I:57:ALA:HB3    | 2.00                     | 0.44              |
| 12:J:13:PRO:HB3    | 12:J:20:GLU:HG2    | 2.00                     | 0.44              |
| 12:J:134:VAL:O     | 12:J:138:GLU:HG2   | 2.17                     | 0.44              |
| 22:T:11:VAL:HG23   | 22:T:56:ASP:O      | 2.17                     | 0.44              |
| 25:W:27:MET:SD     | 25:W:66:ILE:HG13   | 2.58                     | 0.44              |
| 2:02:50:SER:HA     | 2:02:151:GLY:HA3   | 2.00                     | 0.44              |
| 3:03:552:PRO:HB3   | 4:04:770:LEU:HD11  | 2.00                     | 0.44              |
| 3:03:1305:TYR:O    | 3:03:1309:VAL:HG13 | 2.18                     | 0.44              |
| 4:04:285:LEU:N     | 4:04:285:LEU:HD12  | 2.33                     | 0.44              |
| 4:04:844:THR:HG21  | 4:04:858:VAL:HG11  | 2.00                     | 0.44              |
| 5:05:10:VAL:O      | 5:05:14:GLY:HA2    | 2.18                     | 0.44              |
| 7:E:9:MET:SD       | 7:E:10:LEU:N       | 2.91                     | 0.44              |
| 10:H:131:ASN:HB2   | 10:H:134:ASN:HD22  | 1.82                     | 0.44              |
| 13:K:5:PRO:HB2     | 13:K:32:LYS:CE     | 2.48                     | 0.44              |
| 13:K:104:SER:HB2   | 13:K:125:ILE:HD11  | 1.99                     | 0.44              |
| 16:N:12:ARG:NE     | 16:N:12:ARG:HA     | 2.33                     | 0.44              |
| 17:O:109:ARG:HB2   | 17:O:118:VAL:HG21  | 1.99                     | 0.44              |
| 1:A:548:G:O2'      | 1:A:549:C:H5'      | 2.18                     | 0.43              |
| 3:03:33:ASP:HA     | 3:03:36:GLN:HB2    | 1.99                     | 0.43              |
| 3:03:1289:GLU:HA   | 3:03:1293:VAL:HB   | 2.00                     | 0.43              |
| 4:04:62:PHE:HD1    | 4:04:101:ARG:HB3   | 1.82                     | 0.43              |
| 4:04:332:LYS:C     | 4:04:332:LYS:HD3   | 2.43                     | 0.43              |
| 4:04:894:VAL:HG22  | 4:04:1258:ARG:NH1  | 2.33                     | 0.43              |
| 7:E:80:VAL:HA      | 7:E:214:LEU:HD21   | 2.00                     | 0.43              |
| 7:E:104:TRP:CZ2    | 7:E:108:ARG:HD2    | 2.53                     | 0.43              |
| 9:G:58:GLN:OE1     | 9:G:61:ARG:HD3     | 2.18                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:G:68:GLU:OE1     | 9:G:68:GLU:C       | 2.61                     | 0.43              |
| 11:I:9:MET:HE3     | 11:I:86:ARG:HB2    | 1.99                     | 0.43              |
| 11:I:18:VAL:O      | 11:I:22:ILE:HG13   | 2.18                     | 0.43              |
| 11:I:25:TYR:O      | 11:I:29:ILE:HG13   | 2.17                     | 0.43              |
| 15:M:6:ILE:O       | 15:M:75:ASP:HA     | 2.18                     | 0.43              |
| 21:S:11:ALA:HB3    | 21:S:14:ARG:HB2    | 1.99                     | 0.43              |
| 22:T:47:ASP:HB3    | 22:T:74:LEU:HD21   | 1.99                     | 0.43              |
| 25:W:80:ALA:O      | 25:W:84:LYS:HG3    | 2.18                     | 0.43              |
| 26:X:17:ARG:HG2    | 26:X:17:ARG:HH11   | 1.83                     | 0.43              |
| 1:A:156:C:O2'      | 1:A:157:U:H5'      | 2.18                     | 0.43              |
| 1:A:253:A:H61      | 1:A:273:U:H3       | 1.64                     | 0.43              |
| 1:A:337:G:H2'      | 1:A:338:A:H8       | 1.82                     | 0.43              |
| 1:A:654:G:N2       | 1:A:755:G:H5'      | 2.33                     | 0.43              |
| 3:03:974:ARG:O     | 3:03:978:VAL:HG23  | 2.18                     | 0.43              |
| 3:03:1271:GLY:O    | 3:03:1274:GLU:HB2  | 2.17                     | 0.43              |
| 4:04:755:ILE:HG22  | 4:04:757:THR:H     | 1.83                     | 0.43              |
| 4:04:1041:ILE:N    | 4:04:1041:ILE:CD1  | 2.81                     | 0.43              |
| 4:04:1323:ALA:HB1  | 4:04:1328:THR:HG23 | 2.00                     | 0.43              |
| 7:E:162:PHE:HA     | 7:E:184:PHE:O      | 2.17                     | 0.43              |
| 9:G:43:ARG:NH1     | 9:G:43:ARG:HB3     | 2.33                     | 0.43              |
| 9:G:150:LYS:HA     | 9:G:154:VAL:HB     | 1.99                     | 0.43              |
| 11:I:48:ALA:HB1    | 23:U:69:PRO:HB3    | 1.99                     | 0.43              |
| 12:J:125:ASP:HB3   | 12:J:130:LYS:O     | 2.18                     | 0.43              |
| 14:L:9:GLY:HA3     | 14:L:16:ALA:HB3    | 1.99                     | 0.43              |
| 17:O:86:VAL:HG23   | 17:O:88:ASP:H      | 1.82                     | 0.43              |
| 1:A:302:G:H2'      | 1:A:303:A:H8       | 1.82                     | 0.43              |
| 1:A:1082:A:H2'     | 1:A:1083:U:O4'     | 2.19                     | 0.43              |
| 1:A:1123:U:H2'     | 1:A:1124:G:C8      | 2.53                     | 0.43              |
| 1:A:1128:C:H2'     | 1:A:1129:C:C6      | 2.53                     | 0.43              |
| 1:A:1155:A:H2'     | 1:A:1156:G:O4'     | 2.17                     | 0.43              |
| 1:A:1204:A:O2'     | 1:A:1205:U:H5'     | 2.18                     | 0.43              |
| 1:A:1293:C:H2'     | 1:A:1294:G:C8      | 2.53                     | 0.43              |
| 1:A:1371:G:OP2     | 14:L:12:LYS:HE2    | 2.18                     | 0.43              |
| 2:01:55:ALA:C      | 2:01:146:VAL:HG13  | 2.42                     | 0.43              |
| 2:01:219:ARG:O     | 2:01:223:ILE:HG13  | 2.19                     | 0.43              |
| 2:02:182:ARG:HG3   | 2:02:182:ARG:NH1   | 2.34                     | 0.43              |
| 3:03:693:LEU:HG    | 3:03:829:THR:O     | 2.18                     | 0.43              |
| 3:03:742:TYR:C     | 3:03:744:GLY:H     | 2.25                     | 0.43              |
| 4:04:1090:ILE:HD12 | 4:04:1095:MET:HB2  | 2.00                     | 0.43              |
| 4:04:1183:SER:OG   | 4:04:1185:PRO:HD2  | 2.18                     | 0.43              |
| 5:05:15:ASN:C      | 5:05:17:PHE:H      | 2.25                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:E:9:MET:C       | 7:E:11:LYS:H       | 2.25                     | 0.43              |
| 13:K:31:LEU:O     | 13:K:35:ILE:HG13   | 2.18                     | 0.43              |
| 13:K:94:VAL:HB    | 13:K:99:GLY:C      | 2.43                     | 0.43              |
| 1:A:118:U:C2'     | 1:A:119:A:H5'      | 2.48                     | 0.43              |
| 1:A:545:C:H5'     | 9:G:61:ARG:HH12    | 1.83                     | 0.43              |
| 2:01:171:LEU:C    | 2:01:172:LEU:HD12  | 2.43                     | 0.43              |
| 4:04:56:LEU:N     | 4:04:56:LEU:HD12   | 2.33                     | 0.43              |
| 4:04:320:ASN:HD22 | 4:04:321:LYS:N     | 2.15                     | 0.43              |
| 4:04:368:LEU:HA   | 4:04:369:PRO:HD3   | 1.85                     | 0.43              |
| 4:04:767:LEU:HD23 | 4:04:767:LEU:H     | 1.83                     | 0.43              |
| 4:04:1275:LEU:C   | 4:04:1275:LEU:HD12 | 2.44                     | 0.43              |
| 7:E:56:GLU:OE2    | 7:E:60:ILE:HG23    | 2.18                     | 0.43              |
| 7:E:68:LEU:HD23   | 7:E:161:LEU:HD11   | 2.00                     | 0.43              |
| 12:J:20:GLU:O     | 12:J:23:ALA:HB3    | 2.18                     | 0.43              |
| 12:J:58:LEU:C     | 12:J:58:LEU:HD23   | 2.43                     | 0.43              |
| 25:W:34:VAL:CG1   | 25:W:78:LEU:HD11   | 2.48                     | 0.43              |
| 1:A:730:G:H2'     | 1:A:731:G:O4'      | 2.18                     | 0.43              |
| 1:A:1306:A:H2'    | 1:A:1307:U:C6      | 2.53                     | 0.43              |
| 3:03:817:LEU:HD13 | 3:03:817:LEU:C     | 2.42                     | 0.43              |
| 4:04:431:ARG:HD2  | 4:04:493:PRO:HG3   | 2.01                     | 0.43              |
| 4:04:431:ARG:HG2  | 4:04:431:ARG:HH11  | 1.84                     | 0.43              |
| 4:04:555:TYR:CD2  | 4:04:585:LYS:HB3   | 2.54                     | 0.43              |
| 7:E:27:MET:SD     | 7:E:193:PRO:HD3    | 2.59                     | 0.43              |
| 7:E:27:MET:HE3    | 7:E:27:MET:HB3     | 1.73                     | 0.43              |
| 8:F:91:ALA:HA     | 8:F:96:VAL:O       | 2.18                     | 0.43              |
| 8:F:206:ILE:OXT   | 8:F:206:ILE:HG12   | 2.19                     | 0.43              |
| 9:G:36:ALA:HA     | 9:G:37:PRO:HD2     | 1.94                     | 0.43              |
| 10:H:82:HIS:HB3   | 13:K:98:LEU:HD22   | 1.99                     | 0.43              |
| 13:K:6:ILE:O      | 13:K:10:LEU:HG     | 2.18                     | 0.43              |
| 14:L:49:GLN:C     | 14:L:51:LEU:H      | 2.25                     | 0.43              |
| 23:U:28:THR:HA    | 23:U:31:ASN:ND2    | 2.33                     | 0.43              |
| 26:X:10:GLU:N     | 26:X:11:PRO:HD2    | 2.33                     | 0.43              |
| 1:A:211:G:H3'     | 1:A:211:G:N3       | 2.33                     | 0.43              |
| 1:A:1100:C:P      | 26:X:67:ARG:HD2    | 2.59                     | 0.43              |
| 3:03:663:VAL:O    | 3:03:667:LEU:HG    | 2.18                     | 0.43              |
| 3:03:1086:PRO:HD2 | 3:03:1094:VAL:CG1  | 2.48                     | 0.43              |
| 3:03:1299:ASN:O   | 3:03:1303:LYS:HG2  | 2.18                     | 0.43              |
| 4:04:78:LEU:HD12  | 4:04:78:LEU:N      | 2.34                     | 0.43              |
| 4:04:94:GLN:HB2   | 4:04:97:VAL:CG2    | 2.35                     | 0.43              |
| 4:04:184:ALA:O    | 4:04:187:ALA:HB3   | 2.18                     | 0.43              |
| 4:04:447:ILE:HD13 | 4:04:468:VAL:CG1   | 2.49                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:04:569:LEU:HD12  | 4:04:569:LEU:N    | 2.34                     | 0.43              |
| 4:04:850:LYS:C     | 4:04:852:GLY:N    | 2.72                     | 0.43              |
| 7:E:18:HIS:HA      | 7:E:40:ILE:CG2    | 2.47                     | 0.43              |
| 15:M:66:GLU:HG2    | 19:Q:96:LYS:O     | 2.19                     | 0.43              |
| 16:N:17:ASP:HA     | 16:N:80:ASN:O     | 2.18                     | 0.43              |
| 16:N:80:ASN:HA     | 16:N:105:ARG:O    | 2.17                     | 0.43              |
| 23:U:48:ARG:H      | 23:U:48:ARG:HD2   | 1.83                     | 0.43              |
| 24:V:48:ILE:O      | 24:V:48:ILE:HG13  | 2.19                     | 0.43              |
| 1:A:3:A:H2         | 1:A:628:G:H21     | 1.66                     | 0.43              |
| 1:A:9:G:O2'        | 1:A:10:A:H5'      | 2.19                     | 0.43              |
| 3:03:104:ILE:N     | 3:03:104:ILE:CD1  | 2.82                     | 0.43              |
| 3:03:777:VAL:HG11  | 3:03:783:LEU:HD11 | 2.00                     | 0.43              |
| 3:03:817:LEU:HD13  | 3:03:818:VAL:N    | 2.34                     | 0.43              |
| 3:03:1012:GLU:O    | 3:03:1016:GLU:HG3 | 2.19                     | 0.43              |
| 3:03:1255:THR:CG2  | 3:03:1256:GLN:H   | 2.23                     | 0.43              |
| 4:04:56:LEU:HD12   | 4:04:56:LEU:H     | 1.83                     | 0.43              |
| 4:04:374:LEU:O     | 4:04:378:LYS:HG3  | 2.19                     | 0.43              |
| 4:04:378:LYS:HB3   | 4:04:382:TYR:CE2  | 2.54                     | 0.43              |
| 4:04:550:VAL:O     | 4:04:569:LEU:HA   | 2.19                     | 0.43              |
| 4:04:600:ALA:HA    | 4:04:603:LYS:HZ2  | 1.81                     | 0.43              |
| 4:04:690:ASN:HD21  | 4:04:738:ARG:HD3  | 1.83                     | 0.43              |
| 4:04:1183:SER:C    | 4:04:1185:PRO:HD2 | 2.44                     | 0.43              |
| 4:04:1265:THR:HG23 | 4:04:1305:ASP:HB2 | 2.00                     | 0.43              |
| 7:E:18:HIS:HA      | 7:E:40:ILE:CB     | 2.49                     | 0.43              |
| 9:G:184:LYS:CD     | 9:G:185:PRO:HD2   | 2.49                     | 0.43              |
| 10:H:20:VAL:HG23   | 10:H:31:SER:HB3   | 2.01                     | 0.43              |
| 11:I:47:LEU:HD21   | 11:I:57:ALA:HB2   | 2.01                     | 0.43              |
| 13:K:116:ARG:CB    | 13:K:116:ARG:HH11 | 2.31                     | 0.43              |
| 16:N:22:ILE:HG12   | 16:N:31:VAL:HG13  | 2.00                     | 0.43              |
| 1:A:10:A:H2'       | 1:A:11:G:H8       | 1.84                     | 0.43              |
| 1:A:920:U:H2'      | 1:A:921:U:C5      | 2.54                     | 0.43              |
| 2:01:66:HIS:C      | 2:01:68:TYR:H     | 2.27                     | 0.43              |
| 2:02:82:LEU:HA     | 2:02:85:LEU:HD12  | 2.00                     | 0.43              |
| 3:03:54:ARG:O      | 3:03:57:PHE:O     | 2.36                     | 0.43              |
| 4:04:308:ASP:C     | 4:04:310:GLY:N    | 2.76                     | 0.43              |
| 4:04:884:SER:OG    | 4:04:886:VAL:HG12 | 2.18                     | 0.43              |
| 9:G:151:GLN:C      | 9:G:153:ARG:H     | 2.27                     | 0.43              |
| 11:I:11:HIS:HB2    | 11:I:14:GLN:NE2   | 2.34                     | 0.43              |
| 20:R:10:ILE:HG23   | 20:R:14:PHE:HE2   | 1.83                     | 0.43              |
| 2:01:65:LEU:HD22   | 2:01:65:LEU:N     | 2.34                     | 0.43              |
| 2:02:61:ILE:HG12   | 2:02:171:LEU:HD12 | 2.01                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:03:139:ASN:H    | 3:03:143:ARG:NH2   | 2.15                     | 0.43              |
| 3:03:339:ASN:HD21 | 3:03:343:HIS:HB2   | 1.83                     | 0.43              |
| 3:03:644:LEU:HD22 | 3:03:644:LEU:N     | 2.34                     | 0.43              |
| 3:03:1059:ARG:HG3 | 3:03:1059:ARG:NH1  | 2.33                     | 0.43              |
| 3:03:1063:GLY:H   | 3:03:1076:ILE:CG2  | 2.25                     | 0.43              |
| 4:04:26:SER:O     | 4:04:29:MET:HB2    | 2.18                     | 0.43              |
| 4:04:29:MET:O     | 4:04:32:SER:HB2    | 2.19                     | 0.43              |
| 4:04:63:GLY:HA3   | 4:04:64:PRO:HD3    | 1.73                     | 0.43              |
| 4:04:111:THR:HB   | 4:04:239:LEU:HB3   | 2.00                     | 0.43              |
| 4:04:133:ARG:NH2  | 4:04:136:GLU:HB3   | 2.34                     | 0.43              |
| 4:04:958:ILE:HG23 | 4:04:982:LEU:HD12  | 2.01                     | 0.43              |
| 4:04:1089:LEU:N   | 4:04:1089:LEU:HD12 | 2.34                     | 0.43              |
| 5:05:27:ALA:CA    | 5:05:30:MET:HE3    | 2.39                     | 0.43              |
| 7:E:120:GLN:CB    | 7:E:137:ARG:HH22   | 2.31                     | 0.43              |
| 10:H:95:MET:HG2   | 10:H:124:ALA:HB2   | 2.00                     | 0.43              |
| 12:J:47:GLU:OE2   | 12:J:57:GLU:HG2    | 2.19                     | 0.43              |
| 12:J:90:VAL:HG13  | 12:J:95:ARG:HE     | 1.84                     | 0.43              |
| 13:K:49:LYS:O     | 13:K:58:LEU:HD12   | 2.19                     | 0.43              |
| 19:Q:5:MET:CG     | 19:Q:62:ARG:NH1    | 2.81                     | 0.43              |
| 1:A:104:G:OP2     | 25:W:11:ILE:HD12   | 2.19                     | 0.43              |
| 1:A:880:C:H5''    | 17:O:8:ARG:HH12    | 1.84                     | 0.43              |
| 2:01:167:PRO:HG2  | 2:01:170:ARG:NE    | 2.33                     | 0.43              |
| 3:03:424:ASP:O    | 3:03:428:VAL:HG23  | 2.19                     | 0.43              |
| 3:03:615:VAL:C    | 3:03:616:ILE:HD12  | 2.43                     | 0.43              |
| 3:03:801:ARG:HG2  | 3:03:1094:VAL:HA   | 2.01                     | 0.43              |
| 4:04:492:SER:HB2  | 4:04:499:ILE:HD13  | 2.01                     | 0.43              |
| 7:E:61:ALA:HB3    | 7:E:224:GLY:HA3    | 2.00                     | 0.43              |
| 7:E:133:GLU:O     | 7:E:137:ARG:HG2    | 2.19                     | 0.43              |
| 8:F:16:PRO:HG2    | 8:F:53:ARG:HH22    | 1.84                     | 0.43              |
| 8:F:56:ILE:HG23   | 8:F:63:ILE:HD11    | 2.00                     | 0.43              |
| 10:H:131:ASN:HD22 | 10:H:133:ILE:HD13  | 1.83                     | 0.43              |
| 12:J:49:LEU:HB3   | 12:J:120:ALA:HA    | 2.00                     | 0.43              |
| 17:O:3:VAL:O      | 17:O:6:LEU:HB2     | 2.19                     | 0.43              |
| 18:P:32:ILE:HG23  | 18:P:58:GLU:CG     | 2.49                     | 0.43              |
| 25:W:27:MET:N     | 25:W:56:ILE:HG21   | 2.34                     | 0.43              |
| 1:A:730:G:H2'     | 1:A:731:G:H5'      | 2.01                     | 0.42              |
| 1:A:911:U:H2'     | 1:A:912:C:C6       | 2.53                     | 0.42              |
| 1:A:1313:U:OP2    | 24:V:4:LEU:HB2     | 2.19                     | 0.42              |
| 1:A:1328:C:OP1    | 18:P:27:THR:HG21   | 2.19                     | 0.42              |
| 2:01:208:ASN:HD21 | 2:01:210:THR:CG2   | 2.32                     | 0.42              |
| 3:03:448:LEU:HD12 | 3:03:608:ALA:HB2   | 2.01                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:03:578:TYR:HD2   | 3:03:659:GLN:HA   | 1.84                     | 0.42              |
| 3:03:603:ILE:O     | 3:03:603:ILE:HG13 | 2.18                     | 0.42              |
| 3:03:690:VAL:HG11  | 3:03:1234:LYS:HB3 | 2.01                     | 0.42              |
| 3:03:732:ILE:CG1   | 3:03:753:LEU:HD11 | 2.45                     | 0.42              |
| 3:03:1082:ILE:HG22 | 3:03:1082:ILE:O   | 2.19                     | 0.42              |
| 4:04:70:CYS:HB2    | 4:04:75:TYR:HB2   | 2.00                     | 0.42              |
| 4:04:293:ARG:HA    | 4:04:296:LYS:HD2  | 2.01                     | 0.42              |
| 4:04:420:PRO:HG3   | 4:04:481:ARG:HH21 | 1.84                     | 0.42              |
| 4:04:468:VAL:HG23  | 4:04:468:VAL:O    | 2.19                     | 0.42              |
| 4:04:849:LEU:H     | 4:04:849:LEU:CD2  | 2.27                     | 0.42              |
| 4:04:984:LEU:HB3   | 4:04:993:GLU:H    | 1.84                     | 0.42              |
| 6:B:139:UNK:O      | 6:B:141:UNK:N     | 2.51                     | 0.42              |
| 7:E:91:PHE:N       | 7:E:91:PHE:CD1    | 2.87                     | 0.42              |
| 8:F:7:ASN:O        | 8:F:11:LEU:HG     | 2.19                     | 0.42              |
| 17:O:26:CYS:O      | 17:O:27:PRO:C     | 2.62                     | 0.42              |
| 21:S:12:LYS:O      | 21:S:13:LYS:HB2   | 2.19                     | 0.42              |
| 22:T:12:VAL:HG13   | 22:T:13:SER:N     | 2.34                     | 0.42              |
| 22:T:65:PRO:HA     | 22:T:71:SER:HA    | 2.01                     | 0.42              |
| 23:U:43:ARG:HG2    | 23:U:43:ARG:HH11  | 1.84                     | 0.42              |
| 1:A:323:U:H2'      | 1:A:324:G:O4'     | 2.19                     | 0.42              |
| 1:A:723:U:C2       | 1:A:855:U:H4'     | 2.54                     | 0.42              |
| 2:01:108:GLY:HA2   | 2:01:109:PRO:HD3  | 1.88                     | 0.42              |
| 2:02:148:ARG:HH11  | 2:02:148:ARG:HG3  | 1.85                     | 0.42              |
| 3:03:28:LEU:CD1    | 3:03:527:LYS:HZ1  | 2.32                     | 0.42              |
| 3:03:1150:ASP:C    | 3:03:1152:GLY:H   | 2.22                     | 0.42              |
| 4:04:147:ILE:HA    | 4:04:188:LEU:HD21 | 2.00                     | 0.42              |
| 4:04:190:LYS:NZ    | 4:04:190:LYS:HB3  | 2.34                     | 0.42              |
| 4:04:195:GLU:HA    | 4:04:198:CYS:CB   | 2.46                     | 0.42              |
| 4:04:268:LEU:HD11  | 4:04:325:LYS:HB2  | 2.00                     | 0.42              |
| 4:04:478:LEU:HD23  | 4:04:478:LEU:O    | 2.19                     | 0.42              |
| 4:04:870:ASP:O     | 4:04:874:GLU:HG2  | 2.19                     | 0.42              |
| 4:04:1220:ILE:O    | 4:04:1224:ARG:HB3 | 2.20                     | 0.42              |
| 5:05:27:ALA:HB1    | 5:05:46:THR:OG1   | 2.19                     | 0.42              |
| 7:E:76:ALA:HB1     | 7:E:210:VAL:HG11  | 2.00                     | 0.42              |
| 9:G:30:LYS:O       | 9:G:32:LYS:N      | 2.49                     | 0.42              |
| 11:I:86:ARG:HD3    | 23:U:64:TYR:O     | 2.18                     | 0.42              |
| 20:R:21:THR:OG1    | 20:R:30:LEU:HD22  | 2.18                     | 0.42              |
| 23:U:62:ALA:HB3    | 23:U:68:LEU:HD12  | 2.00                     | 0.42              |
| 1:A:211:G:C2'      | 1:A:212:G:H5'     | 2.49                     | 0.42              |
| 1:A:440:C:H2'      | 1:A:441:A:C5'     | 2.47                     | 0.42              |
| 1:A:546:A:OP2      | 9:G:67:LEU:HD22   | 2.18                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:867:G:H21      | 1:A:873:A:H2       | 1.66                     | 0.42              |
| 1:A:1351:U:H2'     | 1:A:1352:C:C6      | 2.54                     | 0.42              |
| 2:01:224:LEU:O     | 2:01:228:LEU:HG    | 2.19                     | 0.42              |
| 2:02:39:LEU:HD23   | 2:02:39:LEU:C      | 2.44                     | 0.42              |
| 3:03:194:LEU:HD11  | 3:03:432:LEU:HD23  | 2.02                     | 0.42              |
| 3:03:364:VAL:HG13  | 3:03:376:PRO:CG    | 2.46                     | 0.42              |
| 3:03:398:SER:C     | 3:03:400:VAL:N     | 2.76                     | 0.42              |
| 3:03:854:ILE:O     | 3:03:854:ILE:HG23  | 2.19                     | 0.42              |
| 3:03:1014:LEU:HD12 | 3:03:1014:LEU:N    | 2.35                     | 0.42              |
| 3:03:1233:LEU:C    | 3:03:1233:LEU:HD13 | 2.44                     | 0.42              |
| 4:04:250:ARG:HH11  | 4:04:250:ARG:HG3   | 1.84                     | 0.42              |
| 4:04:583:VAL:HA    | 4:04:620:PHE:CE1   | 2.54                     | 0.42              |
| 4:04:661:VAL:CG1   | 4:04:685:ILE:HD11  | 2.49                     | 0.42              |
| 4:04:863:LEU:HD22  | 4:04:908:ILE:HD11  | 2.02                     | 0.42              |
| 4:04:896:ALA:HA    | 4:04:909:ILE:HG22  | 2.00                     | 0.42              |
| 4:04:1068:THR:O    | 4:04:1072:LYS:HG3  | 2.19                     | 0.42              |
| 4:04:1327:GLU:O    | 4:04:1331:VAL:HG23 | 2.19                     | 0.42              |
| 7:E:148:LEU:N      | 7:E:148:LEU:HD12   | 2.34                     | 0.42              |
| 7:E:157:LEU:HD12   | 7:E:157:LEU:C      | 2.44                     | 0.42              |
| 8:F:115:VAL:O      | 8:F:119:ILE:HG13   | 2.20                     | 0.42              |
| 13:K:76:ARG:HH11   | 13:K:76:ARG:HG3    | 1.84                     | 0.42              |
| 16:N:12:ARG:O      | 16:N:13:LYS:HB2    | 2.19                     | 0.42              |
| 18:P:96:VAL:HG13   | 18:P:108:ARG:HH21  | 1.84                     | 0.42              |
| 19:Q:44:VAL:HA     | 19:Q:47:LEU:HB3    | 2.00                     | 0.42              |
| 22:T:25:GLU:HB3    | 22:T:38:LYS:HB3    | 2.00                     | 0.42              |
| 22:T:58:VAL:HG21   | 22:T:74:LEU:HD22   | 2.01                     | 0.42              |
| 1:A:406:G:H2'      | 1:A:407:U:C6       | 2.54                     | 0.42              |
| 2:02:143:ARG:HG2   | 2:02:143:ARG:HH11  | 1.85                     | 0.42              |
| 3:03:232:ILE:HG12  | 3:03:237:LEU:CD2   | 2.49                     | 0.42              |
| 3:03:671:LEU:C     | 3:03:673:HIS:N     | 2.78                     | 0.42              |
| 3:03:782:VAL:C     | 3:03:783:LEU:HD22  | 2.44                     | 0.42              |
| 3:03:1268:GLN:HB2  | 4:04:467:ALA:CB    | 2.49                     | 0.42              |
| 4:04:506:VAL:HG13  | 4:04:507:VAL:HG13  | 2.01                     | 0.42              |
| 4:04:740:LEU:O     | 4:04:764:ARG:HB2   | 2.19                     | 0.42              |
| 4:04:843:VAL:O     | 4:04:882:VAL:HG13  | 2.20                     | 0.42              |
| 4:04:1357:ILE:C    | 4:04:1359:ALA:H    | 2.27                     | 0.42              |
| 9:G:127:ARG:O      | 9:G:129:VAL:HG23   | 2.20                     | 0.42              |
| 14:L:74:GLN:O      | 14:L:78:ILE:HG13   | 2.18                     | 0.42              |
| 15:M:15:HIS:HA     | 15:M:18:ILE:HG22   | 2.01                     | 0.42              |
| 18:P:73:SER:O      | 18:P:77:LYS:HG3    | 2.19                     | 0.42              |
| 21:S:28:ARG:HG2    | 21:S:29:ASN:OD1    | 2.19                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:03:862:LEU:HD23  | 3:03:865:LEU:HD12 | 2.02                     | 0.42              |
| 4:04:144:TYR:HA    | 4:04:180:MET:HB3  | 2.00                     | 0.42              |
| 4:04:360:TYR:O     | 4:04:626:TYR:OH   | 2.37                     | 0.42              |
| 4:04:609:TYR:CE1   | 4:04:614:LEU:HB2  | 2.48                     | 0.42              |
| 12:J:137:ARG:O     | 12:J:137:ARG:HD2  | 2.19                     | 0.42              |
| 1:A:774:G:C2'      | 1:A:775:G:H5'     | 2.49                     | 0.42              |
| 1:A:1099:G:H2'     | 1:A:1100:C:O4'    | 2.20                     | 0.42              |
| 2:01:27:THR:HA     | 2:01:201:LEU:O    | 2.20                     | 0.42              |
| 2:01:40:GLY:O      | 2:01:44:ARG:HG3   | 2.19                     | 0.42              |
| 2:02:196:THR:O     | 2:02:198:LEU:HD22 | 2.20                     | 0.42              |
| 3:03:1258:PRO:HB3  | 4:04:346:ARG:NH1  | 2.26                     | 0.42              |
| 3:03:1328:LYS:HZ2  | 4:04:245:LEU:HA   | 1.83                     | 0.42              |
| 4:04:215:LYS:O     | 4:04:218:THR:HG22 | 2.20                     | 0.42              |
| 4:04:1177:ILE:HB   | 4:04:1186:TYR:O   | 2.19                     | 0.42              |
| 4:04:1307:LEU:HD12 | 4:04:1307:LEU:N   | 2.34                     | 0.42              |
| 5:05:27:ALA:O      | 5:05:30:MET:HB2   | 2.20                     | 0.42              |
| 7:E:108:ARG:HA     | 7:E:111:ILE:CG1   | 2.49                     | 0.42              |
| 9:G:171:GLU:HB2    | 9:G:180:THR:HB    | 2.00                     | 0.42              |
| 12:J:129:ASN:C     | 12:J:134:VAL:HG11 | 2.45                     | 0.42              |
| 13:K:7:ALA:HB2     | 13:K:76:ARG:HD2   | 2.01                     | 0.42              |
| 16:N:15:VAL:HG11   | 16:N:41:LEU:HD11  | 2.01                     | 0.42              |
| 25:W:28:ARG:HH11   | 25:W:28:ARG:HG3   | 1.85                     | 0.42              |
| 1:A:106:C:H2'      | 1:A:107:G:O4'     | 2.18                     | 0.42              |
| 1:A:427:U:H5''     | 1:A:428:G:H2'     | 2.02                     | 0.42              |
| 2:01:14:VAL:HG22   | 2:01:15:ASP:N     | 2.33                     | 0.42              |
| 2:01:166:ARG:C     | 2:01:166:ARG:HD3  | 2.44                     | 0.42              |
| 3:03:339:ASN:ND2   | 3:03:343:HIS:HB2  | 2.33                     | 0.42              |
| 3:03:681:MET:HE2   | 3:03:1073:LYS:HZ1 | 1.84                     | 0.42              |
| 4:04:335:GLN:HG2   | 4:04:340:GLN:O    | 2.20                     | 0.42              |
| 4:04:682:VAL:O     | 4:04:683:ILE:C    | 2.63                     | 0.42              |
| 4:04:801:VAL:O     | 4:04:805:GLN:HG3  | 2.19                     | 0.42              |
| 9:G:144:ILE:HD12   | 9:G:177:MET:HB2   | 2.00                     | 0.42              |
| 19:Q:45:LEU:O      | 24:V:12:LEU:HD13  | 2.20                     | 0.42              |
| 19:Q:59:GLN:OE1    | 19:Q:59:GLN:HA    | 2.19                     | 0.42              |
| 21:S:78:VAL:HG13   | 21:S:80:LYS:H     | 1.85                     | 0.42              |
| 1:A:219:U:H3'      | 1:A:220:G:H5''    | 2.02                     | 0.42              |
| 1:A:505:G:H2'      | 1:A:506:G:C8      | 2.55                     | 0.42              |
| 1:A:672:U:H2'      | 1:A:673:A:H8      | 1.85                     | 0.42              |
| 1:A:831:A:C2'      | 1:A:832:G:H5''    | 2.49                     | 0.42              |
| 1:A:981:U:C5'      | 19:Q:62:ARG:HH22  | 2.33                     | 0.42              |
| 2:02:178:SER:C     | 2:02:180:VAL:H    | 2.28                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:03:689:ALA:HB2  | 3:03:796:LEU:HD23 | 2.01                     | 0.42              |
| 3:03:1022:LYS:O   | 3:03:1025:PHE:HB3 | 2.20                     | 0.42              |
| 4:04:197:GLU:O    | 4:04:201:LEU:HG   | 2.20                     | 0.42              |
| 4:04:279:LEU:O    | 4:04:283:LEU:HG   | 2.20                     | 0.42              |
| 4:04:681:LYS:O    | 4:04:684:ASP:HB2  | 2.20                     | 0.42              |
| 4:04:857:LEU:HD22 | 4:04:875:ASN:OD1  | 2.20                     | 0.42              |
| 4:04:901:ARG:HG3  | 4:04:901:ARG:NH1  | 2.35                     | 0.42              |
| 14:L:7:GLY:N      | 14:L:85:ALA:HB2   | 2.35                     | 0.42              |
| 18:P:18:LEU:O     | 18:P:24:VAL:HG13  | 2.20                     | 0.42              |
| 24:V:30:LEU:H     | 24:V:30:LEU:CD1   | 2.33                     | 0.42              |
| 26:X:16:LEU:HA    | 26:X:18:ARG:NH1   | 2.33                     | 0.42              |
| 26:X:17:ARG:HG2   | 26:X:17:ARG:NH1   | 2.34                     | 0.42              |
| 1:A:454:G:H2'     | 1:A:455:G:C8      | 2.55                     | 0.42              |
| 1:A:952:U:H4'     | 1:A:964:A:H61     | 1.85                     | 0.42              |
| 1:A:1516:G:H2'    | 1:A:1518:A:OP2    | 2.19                     | 0.42              |
| 3:03:426:ILE:O    | 3:03:430:LYS:HG3  | 2.20                     | 0.42              |
| 3:03:575:LEU:HG   | 3:03:576:SER:N    | 2.32                     | 0.42              |
| 3:03:1257:GLN:HA  | 3:03:1258:PRO:HD3 | 1.89                     | 0.42              |
| 3:03:1294:LYS:HD3 | 3:03:1295:SER:HB2 | 2.01                     | 0.42              |
| 4:04:356:THR:CG2  | 4:04:448:GLN:HG2  | 2.50                     | 0.42              |
| 4:04:410:ASP:HA   | 4:04:413:ASP:OD2  | 2.20                     | 0.42              |
| 4:04:515:ARG:HH11 | 4:04:515:ARG:HG2  | 1.85                     | 0.42              |
| 4:04:649:LYS:O    | 4:04:653:ILE:HG13 | 2.20                     | 0.42              |
| 4:04:850:LYS:O    | 4:04:851:PRO:C    | 2.63                     | 0.42              |
| 7:E:23:TRP:CE3    | 7:E:189:THR:HB    | 2.43                     | 0.42              |
| 17:O:3:VAL:O      | 17:O:7:VAL:HG23   | 2.20                     | 0.42              |
| 1:A:176:C:C5'     | 25:W:19:HIS:NE2   | 2.83                     | 0.42              |
| 1:A:358:U:H2'     | 1:A:359:G:C8      | 2.54                     | 0.42              |
| 1:A:663:A:H5'     | 1:A:836:G:OP1     | 2.20                     | 0.42              |
| 2:01:106:GLY:HA2  | 2:01:136:GLU:HA   | 2.02                     | 0.42              |
| 2:02:148:ARG:C    | 2:02:148:ARG:HD3  | 2.45                     | 0.42              |
| 3:03:696:ASP:O    | 3:03:795:ALA:HB1  | 2.20                     | 0.42              |
| 3:03:1107:MET:HG2 | 4:04:740:LEU:HB2  | 2.02                     | 0.42              |
| 3:03:1335:ILE:N   | 3:03:1335:ILE:CD1 | 2.79                     | 0.42              |
| 4:04:203:GLU:O    | 4:04:207:GLU:HG2  | 2.19                     | 0.42              |
| 4:04:352:ARG:HH12 | 4:04:465:GLN:HG2  | 1.85                     | 0.42              |
| 4:04:363:LEU:HD23 | 4:04:618:VAL:HG13 | 2.02                     | 0.42              |
| 4:04:812:ASP:C    | 4:04:895:CYS:HB2  | 2.45                     | 0.42              |
| 4:04:901:ARG:HG3  | 4:04:901:ARG:HH11 | 1.85                     | 0.42              |
| 4:04:1076:PRO:O   | 4:04:1100:PHE:HA  | 2.20                     | 0.42              |
| 6:B:208:UNK:HA    | 6:B:216:UNK:O     | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:E:120:GLN:HB2   | 7:E:137:ARG:HH22  | 1.85                     | 0.42              |
| 8:F:40:GLN:O      | 8:F:44:LYS:HG2    | 2.20                     | 0.42              |
| 8:F:55:VAL:HG22   | 8:F:66:THR:O      | 2.19                     | 0.42              |
| 16:N:97:ARG:HH11  | 16:N:97:ARG:HG3   | 1.84                     | 0.42              |
| 19:Q:65:GLN:HG3   | 19:Q:66:THR:HG23  | 2.02                     | 0.42              |
| 22:T:10:ARG:HG3   | 22:T:10:ARG:NH1   | 2.35                     | 0.42              |
| 22:T:27:PHE:CZ    | 22:T:38:LYS:HE2   | 2.54                     | 0.42              |
| 26:X:10:GLU:H     | 26:X:11:PRO:HD2   | 1.85                     | 0.42              |
| 1:A:701:U:H5''    | 1:A:703:G:H1'     | 2.02                     | 0.41              |
| 1:A:779:C:O2'     | 1:A:780:A:H5'     | 2.20                     | 0.41              |
| 2:01:39:LEU:HD11  | 2:02:227:GLN:HB3  | 2.01                     | 0.41              |
| 2:02:182:ARG:C    | 2:02:183:ILE:HD12 | 2.45                     | 0.41              |
| 3:03:178:PRO:HA   | 3:03:397:LEU:HD21 | 2.02                     | 0.41              |
| 3:03:540:ARG:HB3  | 3:03:571:LEU:HD11 | 2.02                     | 0.41              |
| 3:03:875:ALA:H    | 3:03:928:VAL:HG23 | 1.84                     | 0.41              |
| 4:04:320:ASN:ND2  | 4:04:321:LYS:H    | 2.16                     | 0.41              |
| 4:04:543:SER:O    | 4:04:574:VAL:HG21 | 2.20                     | 0.41              |
| 4:04:620:PHE:CE2  | 4:04:624:ILE:HD11 | 2.55                     | 0.41              |
| 8:F:59:PRO:HG2    | 8:F:62:SER:OG     | 2.20                     | 0.41              |
| 11:I:9:MET:O      | 11:I:84:VAL:HA    | 2.20                     | 0.41              |
| 12:J:12:LEU:HD12  | 12:J:12:LEU:N     | 2.35                     | 0.41              |
| 16:N:12:ARG:C     | 16:N:14:GLN:H     | 2.28                     | 0.41              |
| 1:A:412:A:H3'     | 1:A:413:G:C5'     | 2.50                     | 0.41              |
| 1:A:1148:U:O2'    | 14:L:15:ALA:HB1   | 2.20                     | 0.41              |
| 4:04:116:PHE:CE1  | 4:04:1333:THR:HA  | 2.44                     | 0.41              |
| 4:04:141:PHE:HB3  | 4:04:180:MET:CE   | 2.49                     | 0.41              |
| 4:04:181:GLY:O    | 4:04:185:ILE:HG12 | 2.19                     | 0.41              |
| 4:04:394:ILE:O    | 4:04:398:LYS:HG3  | 2.21                     | 0.41              |
| 4:04:478:LEU:HD22 | 5:05:20:VAL:HG22  | 2.01                     | 0.41              |
| 4:04:1158:GLU:HA  | 4:04:1223:LEU:CD2 | 2.50                     | 0.41              |
| 5:05:44:ASP:HB3   | 5:05:48:VAL:HB    | 2.02                     | 0.41              |
| 9:G:158:LEU:HD23  | 9:G:158:LEU:C     | 2.45                     | 0.41              |
| 10:H:44:ARG:HE    | 10:H:70:MET:CB    | 2.29                     | 0.41              |
| 26:X:12:PHE:CD1   | 26:X:12:PHE:N     | 2.87                     | 0.41              |
| 1:A:177:G:OP2     | 1:A:195:A:H5''    | 2.21                     | 0.41              |
| 1:A:273:U:H2'     | 1:A:274:A:H5'     | 2.01                     | 0.41              |
| 1:A:395:C:O2'     | 1:A:396:C:H5'     | 2.20                     | 0.41              |
| 1:A:639:G:O2'     | 1:A:640:A:H5'     | 2.19                     | 0.41              |
| 1:A:1134:G:H2'    | 1:A:1135:U:O4'    | 2.20                     | 0.41              |
| 1:A:1175:G:H2'    | 1:A:1176:A:H8     | 1.85                     | 0.41              |
| 1:A:1204:A:H2'    | 1:A:1205:U:O4'    | 2.20                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:01:118:ASP:HB3  | 2:01:121:VAL:HG23  | 2.02                     | 0.41              |
| 3:03:816:ILE:O    | 3:03:1076:ILE:HD12 | 2.20                     | 0.41              |
| 4:04:520:ALA:HB3  | 4:04:523:GLU:OE1   | 2.20                     | 0.41              |
| 4:04:624:ILE:O    | 4:04:628:GLY:N     | 2.51                     | 0.41              |
| 4:04:833:GLU:OE1  | 4:04:1242:ARG:NH2  | 2.53                     | 0.41              |
| 4:04:982:LEU:HD21 | 4:04:1017:VAL:HG21 | 2.01                     | 0.41              |
| 7:E:21:ARG:HA     | 7:E:38:VAL:O       | 2.20                     | 0.41              |
| 7:E:26:LYS:C      | 7:E:28:LYS:N       | 2.78                     | 0.41              |
| 8:F:42:LEU:HD23   | 8:F:42:LEU:C       | 2.45                     | 0.41              |
| 9:G:43:ARG:HB3    | 9:G:43:ARG:CZ      | 2.50                     | 0.41              |
| 11:I:85:ILE:HG13  | 11:I:86:ARG:N      | 2.35                     | 0.41              |
| 13:K:46:GLU:HG3   | 13:K:47:ASP:OD2    | 2.20                     | 0.41              |
| 16:N:30:ILE:HG13  | 16:N:45:THR:HG22   | 2.01                     | 0.41              |
| 25:W:23:ARG:HB3   | 25:W:60:GLN:HE22   | 1.85                     | 0.41              |
| 1:A:35:G:H4'      | 17:O:117:GLY:CA    | 2.50                     | 0.41              |
| 1:A:273:U:C2'     | 1:A:274:A:H5'      | 2.50                     | 0.41              |
| 1:A:1144:G:O2'    | 1:A:1145:A:H5'     | 2.20                     | 0.41              |
| 1:A:1259:C:H2'    | 1:A:1260:G:H4'     | 2.02                     | 0.41              |
| 2:01:19:VAL:HG13  | 2:01:20:SER:N      | 2.35                     | 0.41              |
| 2:02:79:LEU:O     | 2:02:83:LEU:HD13   | 2.20                     | 0.41              |
| 3:03:678:ARG:CZ   | 3:03:1072:ASN:HA   | 2.50                     | 0.41              |
| 3:03:1214:ASP:HA  | 3:03:1221:PHE:CZ   | 2.56                     | 0.41              |
| 4:04:278:ARG:O    | 4:04:282:LEU:HG    | 2.20                     | 0.41              |
| 4:04:478:LEU:HD11 | 5:05:51:LEU:HD21   | 2.03                     | 0.41              |
| 4:04:661:VAL:HG11 | 4:04:686:TRP:HE1   | 1.85                     | 0.41              |
| 4:04:1047:THR:CG2 | 4:04:1049:GLN:HE21 | 2.32                     | 0.41              |
| 4:04:1287:ILE:HA  | 4:04:1290:ARG:HB3  | 2.01                     | 0.41              |
| 7:E:31:ILE:O      | 7:E:33:GLY:N       | 2.53                     | 0.41              |
| 7:E:89:GLN:H      | 7:E:89:GLN:HE21    | 1.64                     | 0.41              |
| 7:E:101:LEU:CD2   | 7:E:176:ALA:HA     | 2.51                     | 0.41              |
| 8:F:173:PRO:HB2   | 8:F:176:THR:HB     | 2.02                     | 0.41              |
| 11:I:7:VAL:HG22   | 11:I:61:LEU:HG     | 2.03                     | 0.41              |
| 15:M:88:MET:C     | 15:M:90:LEU:H      | 2.29                     | 0.41              |
| 18:P:12:LYS:HB3   | 18:P:16:ILE:HB     | 2.01                     | 0.41              |
| 18:P:72:ILE:HG13  | 18:P:73:SER:N      | 2.35                     | 0.41              |
| 20:R:63:ARG:NE    | 20:R:63:ARG:HA     | 2.35                     | 0.41              |
| 25:W:28:ARG:O     | 25:W:32:LYS:HG2    | 2.21                     | 0.41              |
| 1:A:669:G:OP1     | 1:A:807:A:H5''     | 2.21                     | 0.41              |
| 1:A:686:U:H2'     | 1:A:687:A:C8       | 2.55                     | 0.41              |
| 1:A:993:G:H2'     | 1:A:993:G:N3       | 2.35                     | 0.41              |
| 1:A:1293:C:H2'    | 1:A:1294:G:H8      | 1.84                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:02:12:ARG:O     | 2:02:13:LEU:C     | 2.62                     | 0.41              |
| 3:03:216:THR:HG22 | 3:03:217:THR:N    | 2.35                     | 0.41              |
| 3:03:501:ALA:O    | 3:03:504:GLU:HB3  | 2.21                     | 0.41              |
| 3:03:851:THR:CB   | 3:03:885:GLY:HA3  | 2.50                     | 0.41              |
| 4:04:390:LEU:N    | 4:04:390:LEU:HD12 | 2.35                     | 0.41              |
| 4:04:417:ARG:HG2  | 4:04:417:ARG:NH1  | 2.33                     | 0.41              |
| 4:04:1232:TYR:O   | 4:04:1235:ASN:HB2 | 2.21                     | 0.41              |
| 7:E:43:LEU:HB3    | 7:E:44:GLU:H      | 1.54                     | 0.41              |
| 7:E:108:ARG:HA    | 7:E:111:ILE:HG12  | 2.02                     | 0.41              |
| 9:G:99:ASN:O      | 9:G:102:TYR:HB3   | 2.20                     | 0.41              |
| 11:I:29:ILE:HD11  | 11:I:62:MET:HE2   | 2.02                     | 0.41              |
| 13:K:101:ALA:HB3  | 13:K:112:ASP:HB3  | 2.03                     | 0.41              |
| 14:L:8:THR:O      | 14:L:81:GLY:HA2   | 2.20                     | 0.41              |
| 15:M:66:GLU:OE1   | 19:Q:98:ALA:HA    | 2.21                     | 0.41              |
| 18:P:12:LYS:O     | 18:P:43:LYS:HA    | 2.21                     | 0.41              |
| 1:A:50:A:C4'      | 1:A:51:A:H5'      | 2.50                     | 0.41              |
| 1:A:104:G:H3'     | 25:W:8:LYS:HD2    | 2.02                     | 0.41              |
| 1:A:113:G:H1'     | 1:A:354:G:C5'     | 2.50                     | 0.41              |
| 1:A:185:U:H2'     | 1:A:186:C:C6      | 2.55                     | 0.41              |
| 1:A:366:A:H2      | 1:A:394:G:H1      | 1.69                     | 0.41              |
| 1:A:803:G:O2'     | 1:A:804:U:H5'     | 2.20                     | 0.41              |
| 1:A:1175:G:H2'    | 1:A:1176:A:C8     | 2.56                     | 0.41              |
| 1:A:1348:U:O2'    | 1:A:1349:A:H5'    | 2.20                     | 0.41              |
| 1:A:1353:G:H2'    | 1:A:1354:U:C6     | 2.56                     | 0.41              |
| 2:02:31:LEU:HD12  | 2:02:35:PHE:HB3   | 2.01                     | 0.41              |
| 3:03:184:LEU:HD12 | 3:03:184:LEU:HA   | 1.72                     | 0.41              |
| 4:04:86:GLU:H     | 4:04:86:GLU:CD    | 2.28                     | 0.41              |
| 4:04:119:SER:O    | 4:04:120:LEU:C    | 2.64                     | 0.41              |
| 4:04:328:ALA:C    | 4:04:330:MET:N    | 2.68                     | 0.41              |
| 4:04:552:ILE:H    | 4:04:552:ILE:HG13 | 1.57                     | 0.41              |
| 4:04:615:LYS:HB2  | 4:04:616:PRO:HD3  | 2.02                     | 0.41              |
| 4:04:668:PHE:C    | 4:04:670:SER:H    | 2.28                     | 0.41              |
| 4:04:749:LYS:HE2  | 4:04:751:ASP:OD2  | 2.20                     | 0.41              |
| 4:04:959:LYS:C    | 4:04:959:LYS:HD3  | 2.45                     | 0.41              |
| 4:04:1319:PHE:H   | 4:04:1319:PHE:HD1 | 1.68                     | 0.41              |
| 8:F:139:ASN:O     | 8:F:143:LEU:HB2   | 2.20                     | 0.41              |
| 11:I:18:VAL:CG1   | 11:I:19:PRO:HD3   | 2.51                     | 0.41              |
| 14:L:121:ARG:HG3  | 14:L:121:ARG:NH1  | 2.35                     | 0.41              |
| 16:N:43:TRP:HE3   | 16:N:45:THR:HG23  | 1.86                     | 0.41              |
| 16:N:84:MET:HB3   | 16:N:112:VAL:HG22 | 2.01                     | 0.41              |
| 17:O:31:GLY:HA3   | 17:O:54:VAL:HG13  | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:P:43:LYS:O      | 18:P:47:LEU:HG     | 2.20                     | 0.41              |
| 18:P:48:SER:HB2    | 18:P:51:GLN:HG3    | 2.03                     | 0.41              |
| 19:Q:40:ARG:HH11   | 19:Q:40:ARG:HG3    | 1.86                     | 0.41              |
| 24:V:13:HIS:HE1    | 24:V:34:SER:HB2    | 1.86                     | 0.41              |
| 25:W:16:ALA:HB1    | 25:W:20:ASN:ND2    | 2.35                     | 0.41              |
| 1:A:104:G:OP2      | 25:W:8:LYS:HG3     | 2.20                     | 0.41              |
| 1:A:227:G:O2'      | 1:A:228:A:H5'      | 2.20                     | 0.41              |
| 1:A:521:G:O2'      | 1:A:536:C:H4'      | 2.20                     | 0.41              |
| 1:A:872:A:H2'      | 1:A:872:A:N3       | 2.36                     | 0.41              |
| 3:03:57:PHE:HB2    | 3:03:70:TYR:HB2    | 2.03                     | 0.41              |
| 3:03:119:GLU:HG3   | 3:03:489:PRO:HD2   | 2.02                     | 0.41              |
| 3:03:287:VAL:O     | 3:03:287:VAL:HG23  | 2.20                     | 0.41              |
| 3:03:451:ARG:HG3   | 3:03:451:ARG:NH1   | 2.36                     | 0.41              |
| 4:04:97:VAL:HG12   | 4:04:97:VAL:O      | 2.20                     | 0.41              |
| 4:04:483:LEU:HG    | 4:04:484:MET:HG3   | 2.03                     | 0.41              |
| 4:04:586:GLY:HA3   | 4:04:612:LEU:HD13  | 2.01                     | 0.41              |
| 4:04:1322:ALA:C    | 4:04:1331:VAL:HG21 | 2.46                     | 0.41              |
| 8:F:149:LYS:HE2    | 8:F:168:ARG:HD3    | 2.03                     | 0.41              |
| 11:I:54:LEU:HD12   | 11:I:54:LEU:O      | 2.20                     | 0.41              |
| 15:M:9:ARG:HA      | 15:M:73:LEU:HD23   | 2.02                     | 0.41              |
| 19:Q:12:ARG:NH1    | 19:Q:12:ARG:HG3    | 2.36                     | 0.41              |
| 1:A:826:C:H2'      | 1:A:827:U:H6       | 1.85                     | 0.41              |
| 1:A:1005:A:H2'     | 1:A:1006:G:O4'     | 2.21                     | 0.41              |
| 1:A:1342:C:H2'     | 1:A:1343:G:C8      | 2.55                     | 0.41              |
| 2:01:56:VAL:HG11   | 2:01:85:LEU:HB3    | 2.02                     | 0.41              |
| 2:02:211:ILE:HD11  | 2:02:215:GLU:HB3   | 2.02                     | 0.41              |
| 3:03:72:SER:OG     | 3:03:73:TYR:N      | 2.52                     | 0.41              |
| 3:03:498:ILE:N     | 3:03:498:ILE:CD1   | 2.83                     | 0.41              |
| 3:03:686:GLN:C     | 3:03:688:GLN:H     | 2.29                     | 0.41              |
| 3:03:1032:LYS:HA   | 3:03:1035:LYS:HE2  | 2.03                     | 0.41              |
| 3:03:1294:LYS:HE2  | 4:04:348:ASP:H     | 1.86                     | 0.41              |
| 4:04:108:ALA:CB    | 4:04:283:LEU:HD11  | 2.46                     | 0.41              |
| 4:04:339:ARG:O     | 4:04:344:GLY:HA3   | 2.20                     | 0.41              |
| 4:04:474:LEU:H     | 4:04:474:LEU:HD22  | 1.86                     | 0.41              |
| 4:04:596:LEU:HD13  | 4:04:596:LEU:C     | 2.45                     | 0.41              |
| 4:04:1227:HIS:HA   | 4:04:1230:THR:CG2  | 2.49                     | 0.41              |
| 4:04:1320:ILE:HD12 | 4:04:1349:GLU:CG   | 2.49                     | 0.41              |
| 9:G:158:LEU:HD23   | 9:G:158:LEU:O      | 2.21                     | 0.41              |
| 1:A:26:A:H61       | 1:A:558:G:H1'      | 1.85                     | 0.41              |
| 1:A:516:U:O4       | 1:A:533:A:N7       | 2.54                     | 0.41              |
| 1:A:658:C:C1'      | 20:R:21:THR:HG21   | 2.51                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:736:C:H2'      | 1:A:737:C:C6       | 2.56                     | 0.41              |
| 1:A:739:C:H2'      | 1:A:740:U:O4'      | 2.21                     | 0.41              |
| 1:A:1068:G:H5'     | 1:A:1388:C:H5'     | 2.03                     | 0.41              |
| 1:A:1078:U:H2'     | 1:A:1079:G:H5'     | 2.02                     | 0.41              |
| 1:A:1237:C:OP1     | 1:A:1238:A:H1'     | 2.21                     | 0.41              |
| 2:02:104:LYS:HD3   | 2:02:114:ASP:OD2   | 2.20                     | 0.41              |
| 3:03:189:ASP:C     | 3:03:191:LYS:H     | 2.28                     | 0.41              |
| 3:03:678:ARG:NH2   | 3:03:1106:ARG:HH11 | 2.18                     | 0.41              |
| 3:03:678:ARG:HD2   | 3:03:1071:GLY:C    | 2.46                     | 0.41              |
| 3:03:771:VAL:HG21  | 3:03:783:LEU:HD13  | 2.03                     | 0.41              |
| 3:03:926:GLY:HA3   | 3:03:1054:LEU:HB3  | 2.03                     | 0.41              |
| 3:03:1130:ALA:O    | 3:03:1134:GLN:HG3  | 2.21                     | 0.41              |
| 4:04:77:ARG:HA     | 4:04:77:ARG:HD2    | 1.92                     | 0.41              |
| 4:04:116:PHE:CD1   | 4:04:123:ARG:HG3   | 2.56                     | 0.41              |
| 4:04:154:LEU:HD23  | 4:04:158:GLN:HE21  | 1.85                     | 0.41              |
| 4:04:221:ILE:HG23  | 4:04:222:LYS:N     | 2.35                     | 0.41              |
| 4:04:226:ALA:O     | 4:04:229:GLN:HB3   | 2.20                     | 0.41              |
| 4:04:502:PRO:HG2   | 4:04:601:ILE:HD13  | 2.02                     | 0.41              |
| 4:04:746:LEU:HB3   | 4:04:754:ILE:HD11  | 2.03                     | 0.41              |
| 4:04:841:GLY:O     | 4:04:900:GLY:HA3   | 2.20                     | 0.41              |
| 4:04:1010:GLN:CD   | 4:04:1010:GLN:H    | 2.28                     | 0.41              |
| 4:04:1047:THR:HG23 | 4:04:1049:GLN:HG3  | 2.02                     | 0.41              |
| 4:04:1095:MET:HA   | 4:04:1096:PRO:HD3  | 1.82                     | 0.41              |
| 7:E:44:GLU:O       | 7:E:48:PRO:HD2     | 2.20                     | 0.41              |
| 8:F:55:VAL:CG2     | 8:F:66:THR:HB      | 2.50                     | 0.41              |
| 9:G:3:TYR:HE2      | 9:G:6:PRO:HG2      | 1.86                     | 0.41              |
| 9:G:44:LYS:HA      | 9:G:45:PRO:HD3     | 1.83                     | 0.41              |
| 9:G:169:TRP:CD1    | 9:G:170:LEU:HG     | 2.55                     | 0.41              |
| 14:L:48:ARG:HG3    | 14:L:48:ARG:HH11   | 1.86                     | 0.41              |
| 14:L:83:THR:O      | 14:L:94:ARG:NH1    | 2.54                     | 0.41              |
| 14:L:109:GLN:HG2   | 14:L:110:VAL:N     | 2.34                     | 0.41              |
| 14:L:112:ARG:HD3   | 14:L:113:LYS:O     | 2.21                     | 0.41              |
| 15:M:83:THR:O      | 15:M:87:LEU:HG     | 2.21                     | 0.41              |
| 18:P:85:TYR:O      | 18:P:89:ARG:HG2    | 2.21                     | 0.41              |
| 22:T:46:HIS:HB2    | 22:T:70:LYS:HD3    | 2.03                     | 0.41              |
| 23:U:48:ARG:HD3    | 23:U:51:TYR:CE2    | 2.56                     | 0.41              |
| 26:X:34:ARG:HH11   | 26:X:34:ARG:HG3    | 1.86                     | 0.41              |
| 1:A:962:C:O2'      | 1:A:963:G:H5'      | 2.21                     | 0.41              |
| 2:02:100:LEU:HD21  | 2:02:121:VAL:CG1   | 2.50                     | 0.41              |
| 2:02:182:ARG:HE    | 2:02:184:ALA:HB2   | 1.86                     | 0.41              |
| 3:03:257:ALA:HB3   | 3:03:262:TYR:CE2   | 2.56                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:03:528:ARG:HH21  | 3:03:663:VAL:HG13  | 1.86                     | 0.41              |
| 3:03:617:ALA:HB2   | 3:03:650:VAL:CG1   | 2.51                     | 0.41              |
| 3:03:886:LYS:CB    | 3:03:917:SER:HA    | 2.49                     | 0.41              |
| 3:03:1119:MET:HG3  | 3:03:1204:LEU:CD1  | 2.50                     | 0.41              |
| 3:03:1230:MET:HE2  | 3:03:1232:MET:CE   | 2.51                     | 0.41              |
| 3:03:1253:LEU:HD13 | 3:03:1253:LEU:C    | 2.46                     | 0.41              |
| 4:04:38:VAL:HB     | 4:04:105:ILE:HD11  | 2.03                     | 0.41              |
| 4:04:110:PRO:HD2   | 4:04:296:LYS:HE3   | 2.01                     | 0.41              |
| 4:04:278:ARG:HG3   | 4:04:281:ARG:NH2   | 2.35                     | 0.41              |
| 4:04:480:ALA:HA    | 4:04:484:MET:HB2   | 2.02                     | 0.41              |
| 4:04:603:LYS:O     | 4:04:607:THR:HG23  | 2.21                     | 0.41              |
| 4:04:1039:ASP:OD1  | 4:04:1074:LEU:HD13 | 2.21                     | 0.41              |
| 4:04:1242:ARG:HA   | 4:04:1242:ARG:HD3  | 1.85                     | 0.41              |
| 4:04:1268:ASN:HB3  | 4:04:1301:THR:H    | 1.86                     | 0.41              |
| 7:E:21:ARG:NH1     | 7:E:21:ARG:HB2     | 2.35                     | 0.41              |
| 7:E:45:LYS:HD3     | 7:E:45:LYS:HA      | 1.89                     | 0.41              |
| 9:G:131:ILE:HG22   | 9:G:133:SER:H      | 1.86                     | 0.41              |
| 12:J:4:ARG:HD2     | 12:J:6:ILE:HD11    | 2.03                     | 0.41              |
| 12:J:31:VAL:HG22   | 12:J:32:ASP:OD2    | 2.21                     | 0.41              |
| 12:J:110:ARG:HG2   | 12:J:110:ARG:HH11  | 1.85                     | 0.41              |
| 14:L:26:LYS:HD2    | 14:L:26:LYS:N      | 2.36                     | 0.41              |
| 21:S:39:PHE:CD2    | 21:S:41:PRO:HD3    | 2.56                     | 0.41              |
| 26:X:35:ARG:N      | 26:X:35:ARG:HD2    | 2.36                     | 0.41              |
| 1:A:1014:A:H2'     | 1:A:1015:G:O4'     | 2.21                     | 0.40              |
| 1:A:1233:G:OP1     | 14:L:124:PRO:HB3   | 2.20                     | 0.40              |
| 1:A:1255:G:H2'     | 1:A:1279:G:N2      | 2.36                     | 0.40              |
| 3:03:502:VAL:HG22  | 3:03:506:PHE:HD2   | 1.87                     | 0.40              |
| 4:04:165:TYR:CE1   | 4:04:178:ALA:HB3   | 2.56                     | 0.40              |
| 4:04:579:LEU:HA    | 4:04:582:ILE:HD12  | 2.03                     | 0.40              |
| 4:04:641:ILE:HA    | 4:04:644:MET:HE3   | 2.02                     | 0.40              |
| 4:04:1189:MET:N    | 4:04:1189:MET:SD   | 2.94                     | 0.40              |
| 9:G:124:VAL:HB     | 9:G:142:VAL:HG23   | 2.03                     | 0.40              |
| 10:H:97:PRO:HG2    | 10:H:98:ALA:H      | 1.85                     | 0.40              |
| 11:I:86:ARG:HH11   | 11:I:86:ARG:HG2    | 1.85                     | 0.40              |
| 13:K:45:ILE:HG12   | 13:K:60:LEU:HD22   | 2.03                     | 0.40              |
| 14:L:20:ILE:HD11   | 14:L:82:ILE:HA     | 2.02                     | 0.40              |
| 14:L:60:LEU:HD12   | 14:L:60:LEU:C      | 2.45                     | 0.40              |
| 1:A:419:C:H2'      | 1:A:420:U:O4'      | 2.22                     | 0.40              |
| 2:01:28:LEU:HD21   | 2:02:231:PHE:HE2   | 1.85                     | 0.40              |
| 2:01:74:VAL:HG22   | 2:01:75:GLN:N      | 2.36                     | 0.40              |
| 2:01:195:ARG:HE    | 2:01:195:ARG:HA    | 1.86                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:03:406:ASN:HA    | 3:03:409:LEU:HD12 | 2.03                     | 0.40              |
| 3:03:487:LEU:HD23  | 3:03:487:LEU:H    | 1.86                     | 0.40              |
| 4:04:201:LEU:O     | 4:04:217:LEU:HD21 | 2.20                     | 0.40              |
| 4:04:797:THR:O     | 4:04:801:VAL:HG13 | 2.21                     | 0.40              |
| 6:B:4:SER:HA       | 6:B:7:GLN:OE1     | 2.22                     | 0.40              |
| 9:G:82:LYS:HZ3     | 9:G:82:LYS:HB2    | 1.86                     | 0.40              |
| 11:I:29:ILE:HD11   | 11:I:62:MET:SD    | 2.61                     | 0.40              |
| 20:R:35:ILE:HG22   | 20:R:39:GLN:HE21  | 1.85                     | 0.40              |
| 22:T:58:VAL:HG23   | 22:T:76:ARG:O     | 2.21                     | 0.40              |
| 25:W:84:LYS:HB2    | 25:W:84:LYS:NZ    | 2.37                     | 0.40              |
| 1:A:71:A:H3'       | 1:A:72:A:C5'      | 2.48                     | 0.40              |
| 1:A:560:A:H4'      | 1:A:561:U:H5'     | 2.03                     | 0.40              |
| 2:01:90:VAL:HG21   | 2:01:121:VAL:HG13 | 2.03                     | 0.40              |
| 2:01:192:VAL:HG11  | 2:01:195:ARG:HB3  | 2.02                     | 0.40              |
| 3:03:318:SER:C     | 3:03:320:ASP:H    | 2.29                     | 0.40              |
| 3:03:528:ARG:HH11  | 3:03:575:LEU:HB3  | 1.87                     | 0.40              |
| 3:03:1087:TYR:CE1  | 3:03:1213:TYR:HB2 | 2.56                     | 0.40              |
| 3:03:1094:VAL:HG22 | 3:03:1095:ASP:N   | 2.35                     | 0.40              |
| 4:04:37:GLU:HA     | 4:04:104:HIS:O    | 2.21                     | 0.40              |
| 4:04:514:THR:HB    | 4:04:576:ARG:HG2  | 2.04                     | 0.40              |
| 4:04:665:GLN:HA    | 4:04:665:GLN:OE1  | 2.22                     | 0.40              |
| 4:04:717:VAL:O     | 4:04:718:SER:C    | 2.63                     | 0.40              |
| 4:04:726:ALA:HA    | 4:04:732:GLY:O    | 2.21                     | 0.40              |
| 4:04:1357:ILE:HG13 | 4:04:1359:ALA:H   | 1.86                     | 0.40              |
| 6:B:115:UNK:HA     | 6:B:119:UNK:O     | 2.20                     | 0.40              |
| 6:B:171:UNK:O      | 6:B:175:UNK:N     | 2.54                     | 0.40              |
| 14:L:53:LEU:HD12   | 14:L:97:LEU:HD12  | 2.03                     | 0.40              |
| 20:R:31:LEU:O      | 20:R:35:ILE:HG12  | 2.22                     | 0.40              |
| 22:T:30:HIS:HA     | 22:T:31:PRO:HD3   | 1.89                     | 0.40              |
| 25:W:35:TYR:CE1    | 25:W:78:LEU:HD13  | 2.56                     | 0.40              |
| 25:W:57:VAL:O      | 25:W:61:ALA:HB2   | 2.21                     | 0.40              |
| 1:A:606:G:O5'      | 1:A:607:A:H5'     | 2.21                     | 0.40              |
| 1:A:748:G:O2'      | 1:A:749:A:H5'     | 2.21                     | 0.40              |
| 1:A:1372:U:H2'     | 1:A:1373:G:O4'    | 2.21                     | 0.40              |
| 3:03:159:SER:HA    | 3:03:172:TYR:HA   | 2.03                     | 0.40              |
| 3:03:697:LYS:H     | 3:03:697:LYS:CD   | 2.28                     | 0.40              |
| 3:03:1239:VAL:HG23 | 3:03:1240:ASP:N   | 2.36                     | 0.40              |
| 3:03:1252:SER:HB3  | 3:03:1255:THR:O   | 2.22                     | 0.40              |
| 4:04:431:ARG:HD3   | 4:04:431:ARG:C    | 2.47                     | 0.40              |
| 4:04:672:LEU:N     | 4:04:672:LEU:HD12 | 2.37                     | 0.40              |
| 4:04:1038:THR:O    | 4:04:1040:MET:HG3 | 2.21                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:04:1206:ARG:HG3 | 4:04:1206:ARG:O    | 2.21                     | 0.40              |
| 7:E:21:ARG:HB2    | 7:E:21:ARG:HH11    | 1.87                     | 0.40              |
| 7:E:23:TRP:CH2    | 7:E:25:PRO:HB3     | 2.52                     | 0.40              |
| 7:E:209:ALA:HB1   | 7:E:213:TYR:CD2    | 2.57                     | 0.40              |
| 11:I:71:ILE:HA    | 11:I:74:LEU:HB3    | 2.04                     | 0.40              |
| 26:X:42:THR:C     | 26:X:46:LYS:HZ3    | 2.30                     | 0.40              |
| 1:A:252:U:O2      | 1:A:253:A:C8       | 2.75                     | 0.40              |
| 1:A:893:C:H2'     | 1:A:894:G:H8       | 1.87                     | 0.40              |
| 1:A:1513:A:H2'    | 1:A:1514:G:H8      | 1.85                     | 0.40              |
| 2:02:100:LEU:HD21 | 2:02:121:VAL:CG2   | 2.49                     | 0.40              |
| 3:03:272:ARG:O    | 3:03:276:GLN:HG3   | 2.22                     | 0.40              |
| 3:03:595:THR:O    | 3:03:596:ASP:C     | 2.64                     | 0.40              |
| 3:03:710:VAL:HA   | 3:03:715:THR:HG21  | 2.03                     | 0.40              |
| 4:04:58:CYS:SG    | 4:04:61:ILE:HG13   | 2.61                     | 0.40              |
| 4:04:399:LYS:HA   | 4:04:402:GLU:CB    | 2.52                     | 0.40              |
| 4:04:851:PRO:HG3  | 4:04:876:SER:HB2   | 2.02                     | 0.40              |
| 4:04:861:ASN:OD1  | 4:04:861:ASN:O     | 2.39                     | 0.40              |
| 4:04:1231:ARG:HA  | 4:04:1234:VAL:HG22 | 2.03                     | 0.40              |
| 7:E:26:LYS:O      | 7:E:28:LYS:N       | 2.54                     | 0.40              |
| 11:I:38:ARG:HA    | 11:I:38:ARG:NE     | 2.37                     | 0.40              |
| 13:K:45:ILE:CD1   | 13:K:60:LEU:HB3    | 2.52                     | 0.40              |
| 13:K:76:ARG:HG3   | 13:K:76:ARG:NH1    | 2.37                     | 0.40              |
| 14:L:29:ILE:HA    | 14:L:64:ILE:O      | 2.22                     | 0.40              |
| 16:N:124:LYS:C    | 16:N:124:LYS:HD3   | 2.47                     | 0.40              |
| 23:U:30:LYS:HA    | 23:U:33:ILE:CG1    | 2.50                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2   | 01    | 225/229 (98%) | 192 (85%) | 30 (13%) | 3 (1%)   | 9           | 42 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 2   | 02    | 225/229 (98%)   | 176 (78%)  | 36 (16%)  | 13 (6%)  | 1           | 14  |
| 3   | 03    | 1323/1340 (99%) | 1076 (81%) | 209 (16%) | 38 (3%)  | 3           | 23  |
| 4   | 04    | 1339/1369 (98%) | 1128 (84%) | 167 (12%) | 44 (3%)  | 3           | 21  |
| 5   | 05    | 57/59 (97%)     | 46 (81%)   | 9 (16%)   | 2 (4%)   | 3           | 20  |
| 6   | B     | 6/153 (4%)      | 6 (100%)   | 0         | 0        | 100         | 100 |
| 7   | E     | 216/218 (99%)   | 159 (74%)  | 31 (14%)  | 26 (12%) | 0           | 4   |
| 8   | F     | 204/206 (99%)   | 185 (91%)  | 17 (8%)   | 2 (1%)   | 12          | 49  |
| 9   | G     | 203/205 (99%)   | 166 (82%)  | 32 (16%)  | 5 (2%)   | 4           | 26  |
| 10  | H     | 155/157 (99%)   | 123 (79%)  | 28 (18%)  | 4 (3%)   | 4           | 25  |
| 11  | I     | 98/100 (98%)    | 82 (84%)   | 14 (14%)  | 2 (2%)   | 6           | 31  |
| 12  | J     | 149/151 (99%)   | 133 (89%)  | 14 (9%)   | 2 (1%)   | 9           | 42  |
| 13  | K     | 127/129 (98%)   | 105 (83%)  | 20 (16%)  | 2 (2%)   | 7           | 38  |
| 14  | L     | 125/127 (98%)   | 98 (78%)   | 25 (20%)  | 2 (2%)   | 7           | 38  |
| 15  | M     | 96/98 (98%)     | 72 (75%)   | 19 (20%)  | 5 (5%)   | 1           | 15  |
| 16  | N     | 114/116 (98%)   | 87 (76%)   | 20 (18%)  | 7 (6%)   | 1           | 13  |
| 17  | O     | 121/123 (98%)   | 92 (76%)   | 23 (19%)  | 6 (5%)   | 1           | 16  |
| 18  | P     | 112/114 (98%)   | 95 (85%)   | 14 (12%)  | 3 (3%)   | 4           | 25  |
| 19  | Q     | 98/100 (98%)    | 79 (81%)   | 14 (14%)  | 5 (5%)   | 1           | 15  |
| 20  | R     | 86/88 (98%)     | 77 (90%)   | 9 (10%)   | 0        | 100         | 100 |
| 21  | S     | 80/82 (98%)     | 66 (82%)   | 12 (15%)  | 2 (2%)   | 4           | 26  |
| 22  | T     | 78/80 (98%)     | 63 (81%)   | 13 (17%)  | 2 (3%)   | 4           | 25  |
| 23  | U     | 63/65 (97%)     | 51 (81%)   | 8 (13%)   | 4 (6%)   | 1           | 13  |
| 24  | V     | 77/79 (98%)     | 63 (82%)   | 13 (17%)  | 1 (1%)   | 9           | 42  |
| 25  | W     | 83/85 (98%)     | 66 (80%)   | 16 (19%)  | 1 (1%)   | 10          | 44  |
| 26  | X     | 63/65 (97%)     | 47 (75%)   | 12 (19%)  | 4 (6%)   | 1           | 13  |
| All | All   | 5523/5767 (96%) | 4533 (82%) | 805 (15%) | 185 (3%) | 5           | 21  |

All (185) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 02    | 20  | SER  |
| 2   | 02    | 136 | GLU  |
| 2   | 02    | 137 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 03    | 398  | SER  |
| 3   | 03    | 625  | GLU  |
| 3   | 03    | 672  | GLU  |
| 3   | 03    | 674  | ASP  |
| 3   | 03    | 842  | ASP  |
| 3   | 03    | 1321 | GLU  |
| 4   | 04    | 122  | SER  |
| 4   | 04    | 345  | LYS  |
| 4   | 04    | 357  | VAL  |
| 4   | 04    | 503  | SER  |
| 4   | 04    | 1167 | LYS  |
| 4   | 04    | 1343 | GLU  |
| 7   | E     | 14   | VAL  |
| 7   | E     | 25   | PRO  |
| 7   | E     | 39   | HIS  |
| 7   | E     | 40   | ILE  |
| 7   | E     | 44   | GLU  |
| 7   | E     | 189  | THR  |
| 9   | G     | 31   | CYS  |
| 16  | N     | 126  | ARG  |
| 17  | O     | 27   | PRO  |
| 18  | P     | 26   | LYS  |
| 23  | U     | 20   | GLU  |
| 2   | 01    | 168  | ILE  |
| 3   | 03    | 16   | GLY  |
| 3   | 03    | 47   | TYR  |
| 3   | 03    | 63   | SER  |
| 3   | 03    | 491  | ASP  |
| 3   | 03    | 566  | GLY  |
| 3   | 03    | 655  | VAL  |
| 3   | 03    | 673  | HIS  |
| 3   | 03    | 917  | SER  |
| 3   | 03    | 1224 | PRO  |
| 4   | 04    | 89   | GLY  |
| 4   | 04    | 175  | GLU  |
| 4   | 04    | 318  | GLY  |
| 4   | 04    | 332  | LYS  |
| 4   | 04    | 860  | ARG  |
| 4   | 04    | 1084 | GLN  |
| 4   | 04    | 1341 | ARG  |
| 7   | E     | 37   | LYS  |
| 7   | E     | 43   | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | E     | 76   | ALA  |
| 7   | E     | 89   | GLN  |
| 7   | E     | 101  | LEU  |
| 8   | F     | 126  | ARG  |
| 9   | G     | 26   | ALA  |
| 9   | G     | 47   | LEU  |
| 10  | H     | 11   | GLN  |
| 15  | M     | 53   | ILE  |
| 16  | N     | 87   | GLY  |
| 16  | N     | 119  | GLY  |
| 17  | O     | 23   | LEU  |
| 18  | P     | 98   | GLY  |
| 22  | T     | 19   | SER  |
| 23  | U     | 49   | ALA  |
| 26  | X     | 38   | TYR  |
| 2   | 01    | 67   | GLU  |
| 2   | 02    | 13   | LEU  |
| 2   | 02    | 63   | GLY  |
| 3   | 03    | 596  | ASP  |
| 3   | 03    | 746  | ALA  |
| 3   | 03    | 1157 | GLN  |
| 4   | 04    | 49   | PHE  |
| 4   | 04    | 108  | ALA  |
| 4   | 04    | 264  | ASP  |
| 4   | 04    | 307  | LEU  |
| 4   | 04    | 343  | LEU  |
| 4   | 04    | 417  | ARG  |
| 4   | 04    | 523  | GLU  |
| 4   | 04    | 596  | LEU  |
| 4   | 04    | 840  | LEU  |
| 4   | 04    | 1170 | LYS  |
| 7   | E     | 18   | HIS  |
| 7   | E     | 27   | MET  |
| 7   | E     | 45   | LYS  |
| 7   | E     | 64   | LYS  |
| 7   | E     | 152  | LYS  |
| 7   | E     | 213  | TYR  |
| 10  | H     | 110  | MET  |
| 11  | I     | 53   | LYS  |
| 13  | K     | 47   | ASP  |
| 14  | L     | 107  | ALA  |
| 15  | M     | 43   | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 15  | M     | 56   | HIS  |
| 15  | M     | 75   | ASP  |
| 16  | N     | 14   | GLN  |
| 17  | O     | 108  | ASP  |
| 19  | Q     | 31   | SER  |
| 19  | Q     | 61   | ASN  |
| 21  | S     | 28   | ARG  |
| 2   | 02    | 130  | ILE  |
| 3   | 03    | 342  | ASP  |
| 3   | 03    | 841  | ARG  |
| 3   | 03    | 851  | THR  |
| 3   | 03    | 879  | GLY  |
| 3   | 03    | 1270 | PHE  |
| 4   | 04    | 256  | ASP  |
| 4   | 04    | 903  | LEU  |
| 4   | 04    | 1250 | ASP  |
| 4   | 04    | 1275 | LEU  |
| 4   | 04    | 1334 | GLU  |
| 5   | 05    | 16   | ARG  |
| 7   | E     | 77   | SER  |
| 7   | E     | 88   | ASP  |
| 10  | H     | 23   | THR  |
| 14  | L     | 124  | PRO  |
| 15  | M     | 92   | LEU  |
| 16  | N     | 91   | GLY  |
| 16  | N     | 93   | GLU  |
| 17  | O     | 35   | ARG  |
| 23  | U     | 19   | GLN  |
| 23  | U     | 44   | ILE  |
| 26  | X     | 25   | LYS  |
| 2   | 02    | 52   | PRO  |
| 3   | 03    | 1062 | PRO  |
| 3   | 03    | 1151 | LEU  |
| 3   | 03    | 1249 | GLY  |
| 4   | 04    | 595  | ALA  |
| 4   | 04    | 761  | ALA  |
| 4   | 04    | 826  | ILE  |
| 4   | 04    | 1294 | ALA  |
| 4   | 04    | 1332 | LEU  |
| 7   | E     | 11   | LYS  |
| 7   | E     | 29   | PRO  |
| 9   | G     | 45   | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | H     | 77   | ASN  |
| 11  | I     | 33   | GLU  |
| 12  | J     | 57   | GLU  |
| 12  | J     | 149  | ALA  |
| 13  | K     | 53   | ASP  |
| 17  | O     | 41   | PRO  |
| 19  | Q     | 65   | GLN  |
| 25  | W     | 65   | LEU  |
| 2   | 02    | 72   | GLU  |
| 2   | 02    | 138  | ALA  |
| 2   | 02    | 169  | GLY  |
| 2   | 02    | 209  | GLY  |
| 3   | 03    | 545  | PHE  |
| 3   | 03    | 840  | SER  |
| 3   | 03    | 853  | ASP  |
| 3   | 03    | 1320 | PRO  |
| 4   | 04    | 251  | PRO  |
| 4   | 04    | 734  | ALA  |
| 7   | E     | 21   | ARG  |
| 7   | E     | 47   | VAL  |
| 19  | Q     | 21   | ALA  |
| 22  | T     | 50   | ASN  |
| 26  | X     | 10   | GLU  |
| 3   | 03    | 1317 | PRO  |
| 4   | 04    | 815  | GLY  |
| 5   | 05    | 4    | VAL  |
| 3   | 03    | 21   | VAL  |
| 4   | 04    | 998  | PRO  |
| 4   | 04    | 1000 | GLY  |
| 16  | N     | 38   | GLY  |
| 17  | O     | 62   | VAL  |
| 18  | P     | 23   | GLY  |
| 2   | 02    | 166  | ARG  |
| 3   | 03    | 110  | PRO  |
| 3   | 03    | 329  | GLY  |
| 3   | 03    | 355  | PRO  |
| 4   | 04    | 451  | PRO  |
| 4   | 04    | 825  | VAL  |
| 7   | E     | 193  | PRO  |
| 8   | F     | 144  | GLY  |
| 9   | G     | 24   | VAL  |
| 24  | V     | 75   | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 01    | 179  | PRO  |
| 2   | 02    | 167  | PRO  |
| 3   | 03    | 302  | ILE  |
| 3   | 03    | 564  | PRO  |
| 3   | 03    | 1155 | VAL  |
| 4   | 04    | 333  | GLY  |
| 4   | 04    | 1171 | GLY  |
| 7   | E     | 33   | GLY  |
| 7   | E     | 98   | GLY  |
| 21  | S     | 36   | VAL  |
| 4   | 04    | 92   | VAL  |
| 4   | 04    | 258  | GLY  |
| 26  | X     | 11   | PRO  |
| 19  | Q     | 56   | 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 |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 2   | 01    | 194/197 (98%)   | 193 (100%) | 1 (0%)   | 81          | 83  |
| 2   | 02    | 194/197 (98%)   | 189 (97%)  | 5 (3%)   | 40          | 62  |
| 3   | 03    | 1098/1155 (95%) | 1086 (99%) | 12 (1%)  | 65          | 76  |
| 4   | 04    | 1103/1141 (97%) | 1090 (99%) | 13 (1%)  | 63          | 75  |
| 5   | 05    | 49/49 (100%)    | 49 (100%)  | 0        | 100         | 100 |
| 6   | B     | 6/7 (86%)       | 6 (100%)   | 0        | 100         | 100 |
| 7   | E     | 180/180 (100%)  | 171 (95%)  | 9 (5%)   | 22          | 43  |
| 8   | F     | 170/170 (100%)  | 169 (99%)  | 1 (1%)   | 78          | 83  |
| 9   | G     | 172/172 (100%)  | 166 (96%)  | 6 (4%)   | 32          | 53  |
| 10  | H     | 119/119 (100%)  | 118 (99%)  | 1 (1%)   | 73          | 80  |
| 11  | I     | 87/87 (100%)    | 86 (99%)   | 1 (1%)   | 65          | 76  |
| 12  | J     | 124/124 (100%)  | 122 (98%)  | 2 (2%)   | 55          | 70  |
| 13  | K     | 104/104 (100%)  | 103 (99%)  | 1 (1%)   | 68          | 78  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 14  | L     | 105/105 (100%)  | 105 (100%) | 0        | 100         | 100 |
| 15  | M     | 86/86 (100%)    | 84 (98%)   | 2 (2%)   | 44          | 64  |
| 16  | N     | 89/89 (100%)    | 89 (100%)  | 0        | 100         | 100 |
| 17  | O     | 103/103 (100%)  | 102 (99%)  | 1 (1%)   | 68          | 78  |
| 18  | P     | 92/92 (100%)    | 91 (99%)   | 1 (1%)   | 65          | 76  |
| 19  | Q     | 83/83 (100%)    | 83 (100%)  | 0        | 100         | 100 |
| 20  | R     | 76/76 (100%)    | 75 (99%)   | 1 (1%)   | 61          | 74  |
| 21  | S     | 65/65 (100%)    | 63 (97%)   | 2 (3%)   | 35          | 56  |
| 22  | T     | 74/74 (100%)    | 73 (99%)   | 1 (1%)   | 59          | 72  |
| 23  | U     | 56/56 (100%)    | 56 (100%)  | 0        | 100         | 100 |
| 24  | V     | 70/70 (100%)    | 70 (100%)  | 0        | 100         | 100 |
| 25  | W     | 65/65 (100%)    | 62 (95%)   | 3 (5%)   | 24          | 45  |
| 26  | X     | 55/55 (100%)    | 52 (94%)   | 3 (6%)   | 19          | 41  |
| All | All   | 4619/4721 (98%) | 4553 (99%) | 66 (1%)  | 57          | 72  |

All (66) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 01    | 71   | LYS  |
| 2   | 02    | 13   | LEU  |
| 2   | 02    | 14   | VAL  |
| 2   | 02    | 102  | LEU  |
| 2   | 02    | 133  | LEU  |
| 2   | 02    | 172  | LEU  |
| 3   | 03    | 498  | ILE  |
| 3   | 03    | 616  | ILE  |
| 3   | 03    | 791  | LEU  |
| 3   | 03    | 850  | ILE  |
| 3   | 03    | 1082 | ILE  |
| 3   | 03    | 1111 | GLN  |
| 3   | 03    | 1170 | MET  |
| 3   | 03    | 1172 | LEU  |
| 3   | 03    | 1224 | PRO  |
| 3   | 03    | 1233 | LEU  |
| 3   | 03    | 1235 | LEU  |
| 3   | 03    | 1335 | ILE  |
| 4   | 04    | 53   | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | 04    | 217  | LEU  |
| 4   | 04    | 239  | LEU  |
| 4   | 04    | 250  | ARG  |
| 4   | 04    | 290  | ILE  |
| 4   | 04    | 331  | ILE  |
| 4   | 04    | 431  | ARG  |
| 4   | 04    | 514  | THR  |
| 4   | 04    | 552  | ILE  |
| 4   | 04    | 596  | LEU  |
| 4   | 04    | 704  | GLU  |
| 4   | 04    | 1126 | GLN  |
| 4   | 04    | 1332 | LEU  |
| 7   | E     | 14   | VAL  |
| 7   | E     | 19   | GLN  |
| 7   | E     | 20   | THR  |
| 7   | E     | 21   | ARG  |
| 7   | E     | 35   | ARG  |
| 7   | E     | 42   | ASN  |
| 7   | E     | 43   | LEU  |
| 7   | E     | 89   | GLN  |
| 7   | E     | 186  | ILE  |
| 8   | F     | 163  | ARG  |
| 9   | G     | 29   | THR  |
| 9   | G     | 68   | GLU  |
| 9   | G     | 80   | ARG  |
| 9   | G     | 82   | LYS  |
| 9   | G     | 149  | LYS  |
| 9   | G     | 196  | GLU  |
| 10  | H     | 131  | ASN  |
| 11  | I     | 14   | GLN  |
| 12  | J     | 9    | ARG  |
| 12  | J     | 24   | LYS  |
| 13  | K     | 107  | LYS  |
| 15  | M     | 43   | PRO  |
| 15  | M     | 48   | ARG  |
| 17  | O     | 27   | PRO  |
| 18  | P     | 16   | ILE  |
| 20  | R     | 9    | LYS  |
| 21  | S     | 5    | ARG  |
| 21  | S     | 25   | ARG  |
| 22  | T     | 70   | LYS  |
| 25  | W     | 8    | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | W     | 65  | LEU  |
| 25  | W     | 68  | LYS  |
| 26  | X     | 17  | ARG  |
| 26  | X     | 34  | ARG  |
| 26  | X     | 38  | TYR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 01    | 84   | ASN  |
| 2   | 01    | 128  | HIS  |
| 2   | 01    | 208  | ASN  |
| 2   | 02    | 37   | HIS  |
| 2   | 02    | 75   | GLN  |
| 2   | 02    | 103  | ASN  |
| 2   | 02    | 137  | ASN  |
| 3   | 03    | 31   | GLN  |
| 3   | 03    | 86   | GLN  |
| 3   | 03    | 133  | ASN  |
| 3   | 03    | 139  | ASN  |
| 3   | 03    | 214  | ASN  |
| 3   | 03    | 258  | ASN  |
| 3   | 03    | 327  | GLN  |
| 3   | 03    | 406  | ASN  |
| 3   | 03    | 437  | ASN  |
| 3   | 03    | 450  | ASN  |
| 3   | 03    | 494  | ASN  |
| 3   | 03    | 519  | ASN  |
| 3   | 03    | 554  | HIS  |
| 3   | 03    | 580  | GLN  |
| 3   | 03    | 620  | ASN  |
| 3   | 03    | 761  | GLN  |
| 3   | 03    | 834  | GLN  |
| 3   | 03    | 1070 | HIS  |
| 3   | 03    | 1080 | ASN  |
| 3   | 03    | 1090 | ASN  |
| 3   | 03    | 1099 | ASN  |
| 3   | 03    | 1111 | GLN  |
| 3   | 03    | 1175 | ASN  |
| 3   | 03    | 1220 | GLN  |
| 3   | 03    | 1237 | HIS  |
| 3   | 03    | 1314 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 03    | 1324 | ASN  |
| 4   | 04    | 113  | HIS  |
| 4   | 04    | 158  | GLN  |
| 4   | 04    | 164  | GLN  |
| 4   | 04    | 186  | GLN  |
| 4   | 04    | 200  | GLN  |
| 4   | 04    | 232  | ASN  |
| 4   | 04    | 300  | GLN  |
| 4   | 04    | 320  | ASN  |
| 4   | 04    | 435  | GLN  |
| 4   | 04    | 450  | HIS  |
| 4   | 04    | 465  | GLN  |
| 4   | 04    | 469  | HIS  |
| 4   | 04    | 488  | ASN  |
| 4   | 04    | 489  | ASN  |
| 4   | 04    | 504  | GLN  |
| 4   | 04    | 669  | GLN  |
| 4   | 04    | 716  | GLN  |
| 4   | 04    | 792  | ASN  |
| 4   | 04    | 861  | ASN  |
| 4   | 04    | 875  | ASN  |
| 4   | 04    | 907  | HIS  |
| 4   | 04    | 929  | GLN  |
| 4   | 04    | 954  | ASN  |
| 4   | 04    | 1023 | HIS  |
| 4   | 04    | 1049 | GLN  |
| 4   | 04    | 1197 | ASN  |
| 4   | 04    | 1218 | HIS  |
| 4   | 04    | 1235 | ASN  |
| 4   | 04    | 1244 | GLN  |
| 4   | 04    | 1259 | GLN  |
| 4   | 04    | 1326 | GLN  |
| 4   | 04    | 1350 | ASN  |
| 5   | 05    | 15   | ASN  |
| 7   | E     | 42   | ASN  |
| 7   | E     | 89   | GLN  |
| 7   | E     | 103  | ASN  |
| 7   | E     | 177  | ASN  |
| 8   | F     | 24   | ASN  |
| 8   | F     | 40   | GLN  |
| 8   | F     | 139  | ASN  |
| 8   | F     | 184  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | G     | 39  | GLN  |
| 9   | G     | 73  | ASN  |
| 9   | G     | 84  | ASN  |
| 9   | G     | 88  | ASN  |
| 9   | G     | 99  | ASN  |
| 9   | G     | 115 | GLN  |
| 9   | G     | 125 | ASN  |
| 9   | G     | 163 | GLN  |
| 10  | H     | 76  | ASN  |
| 10  | H     | 77  | ASN  |
| 10  | H     | 81  | GLN  |
| 10  | H     | 96  | GLN  |
| 10  | H     | 131 | ASN  |
| 10  | H     | 134 | ASN  |
| 10  | H     | 145 | ASN  |
| 12  | J     | 8   | GLN  |
| 12  | J     | 27  | ASN  |
| 12  | J     | 121 | ASN  |
| 13  | K     | 15  | ASN  |
| 13  | K     | 20  | ASN  |
| 13  | K     | 37  | ASN  |
| 14  | L     | 30  | ASN  |
| 14  | L     | 74  | GLN  |
| 15  | M     | 58  | ASN  |
| 15  | M     | 99  | GLN  |
| 16  | N     | 21  | HIS  |
| 16  | N     | 28  | ASN  |
| 16  | N     | 118 | ASN  |
| 17  | O     | 28  | GLN  |
| 17  | O     | 72  | ASN  |
| 17  | O     | 74  | GLN  |
| 19  | Q     | 34  | ASN  |
| 19  | Q     | 65  | GLN  |
| 19  | Q     | 70  | HIS  |
| 20  | R     | 34  | GLN  |
| 20  | R     | 36  | ASN  |
| 20  | R     | 39  | GLN  |
| 20  | R     | 50  | HIS  |
| 20  | R     | 79  | GLN  |
| 21  | S     | 18  | GLN  |
| 21  | S     | 26  | ASN  |
| 21  | S     | 40  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | T     | 30  | HIS  |
| 22  | T     | 50  | ASN  |
| 23  | U     | 31  | ASN  |
| 24  | V     | 13  | HIS  |
| 25  | W     | 2   | ASN  |
| 25  | W     | 12  | GLN  |
| 25  | W     | 20  | ASN  |
| 25  | W     | 54  | GLN  |
| 25  | W     | 74  | HIS  |
| 25  | W     | 81  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1441/1539 (93%) | 164 (11%)         | 2 (0%)          |

All (164) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | G    |
| 1   | A     | 31  | G    |
| 1   | A     | 32  | A    |
| 1   | A     | 39  | G    |
| 1   | A     | 40  | C    |
| 1   | A     | 48  | C    |
| 1   | A     | 51  | A    |
| 1   | A     | 60  | A    |
| 1   | A     | 61  | G    |
| 1   | A     | 66  | A    |
| 1   | A     | 68  | G    |
| 1   | A     | 70  | U    |
| 1   | A     | 71  | A    |
| 1   | A     | 72  | A    |
| 1   | A     | 83  | C    |
| 1   | A     | 85  | U    |
| 1   | A     | 86  | G    |
| 1   | A     | 89  | U    |
| 1   | A     | 90  | C    |
| 1   | A     | 94  | G    |
| 1   | A     | 95  | C    |
| 1   | A     | 137 | U    |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 144 | G    |
| 1   | A     | 174 | A    |
| 1   | A     | 180 | U    |
| 1   | A     | 183 | C    |
| 1   | A     | 184 | G    |
| 1   | A     | 185 | U    |
| 1   | A     | 209 | U    |
| 1   | A     | 210 | C    |
| 1   | A     | 220 | G    |
| 1   | A     | 245 | U    |
| 1   | A     | 247 | G    |
| 1   | A     | 251 | G    |
| 1   | A     | 266 | G    |
| 1   | A     | 267 | C    |
| 1   | A     | 280 | C    |
| 1   | A     | 281 | G    |
| 1   | A     | 289 | G    |
| 1   | A     | 306 | A    |
| 1   | A     | 328 | C    |
| 1   | A     | 344 | A    |
| 1   | A     | 345 | C    |
| 1   | A     | 352 | C    |
| 1   | A     | 372 | C    |
| 1   | A     | 377 | G    |
| 1   | A     | 388 | G    |
| 1   | A     | 397 | A    |
| 1   | A     | 398 | U    |
| 1   | A     | 406 | G    |
| 1   | A     | 413 | G    |
| 1   | A     | 414 | A    |
| 1   | A     | 423 | G    |
| 1   | A     | 427 | U    |
| 1   | A     | 429 | U    |
| 1   | A     | 441 | A    |
| 1   | A     | 448 | A    |
| 1   | A     | 467 | U    |
| 1   | A     | 468 | A    |
| 1   | A     | 479 | U    |
| 1   | A     | 480 | U    |
| 1   | A     | 486 | U    |
| 1   | A     | 487 | A    |
| 1   | A     | 495 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 497 | G    |
| 1   | A     | 500 | G    |
| 1   | A     | 509 | A    |
| 1   | A     | 513 | C    |
| 1   | A     | 518 | C    |
| 1   | A     | 524 | G    |
| 1   | A     | 530 | G    |
| 1   | A     | 531 | U    |
| 1   | A     | 532 | A    |
| 1   | A     | 533 | A    |
| 1   | A     | 534 | U    |
| 1   | A     | 535 | A    |
| 1   | A     | 536 | C    |
| 1   | A     | 547 | A    |
| 1   | A     | 559 | A    |
| 1   | A     | 560 | A    |
| 1   | A     | 561 | U    |
| 1   | A     | 572 | A    |
| 1   | A     | 573 | A    |
| 1   | A     | 575 | G    |
| 1   | A     | 576 | C    |
| 1   | A     | 577 | G    |
| 1   | A     | 615 | G    |
| 1   | A     | 633 | G    |
| 1   | A     | 642 | A    |
| 1   | A     | 665 | A    |
| 1   | A     | 703 | G    |
| 1   | A     | 723 | U    |
| 1   | A     | 724 | G    |
| 1   | A     | 755 | G    |
| 1   | A     | 777 | A    |
| 1   | A     | 817 | C    |
| 1   | A     | 818 | G    |
| 1   | A     | 819 | A    |
| 1   | A     | 821 | G    |
| 1   | A     | 828 | U    |
| 1   | A     | 832 | G    |
| 1   | A     | 843 | U    |
| 1   | A     | 846 | G    |
| 1   | A     | 871 | U    |
| 1   | A     | 873 | A    |
| 1   | A     | 902 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 926  | G    |
| 1   | A     | 934  | C    |
| 1   | A     | 935  | A    |
| 1   | A     | 945  | G    |
| 1   | A     | 960  | U    |
| 1   | A     | 961  | U    |
| 1   | A     | 966  | G    |
| 1   | A     | 969  | A    |
| 1   | A     | 975  | A    |
| 1   | A     | 977  | A    |
| 1   | A     | 982  | U    |
| 1   | A     | 984  | C    |
| 1   | A     | 992  | U    |
| 1   | A     | 993  | G    |
| 1   | A     | 994  | A    |
| 1   | A     | 1004 | A    |
| 1   | A     | 1031 | C    |
| 1   | A     | 1033 | G    |
| 1   | A     | 1055 | A    |
| 1   | A     | 1068 | G    |
| 1   | A     | 1094 | G    |
| 1   | A     | 1101 | A    |
| 1   | A     | 1118 | U    |
| 1   | A     | 1137 | C    |
| 1   | A     | 1138 | G    |
| 1   | A     | 1139 | G    |
| 1   | A     | 1159 | U    |
| 1   | A     | 1168 | U    |
| 1   | A     | 1182 | G    |
| 1   | A     | 1184 | G    |
| 1   | A     | 1196 | A    |
| 1   | A     | 1213 | A    |
| 1   | A     | 1215 | G    |
| 1   | A     | 1225 | A    |
| 1   | A     | 1226 | C    |
| 1   | A     | 1238 | A    |
| 1   | A     | 1240 | U    |
| 1   | A     | 1241 | G    |
| 1   | A     | 1258 | G    |
| 1   | A     | 1260 | G    |
| 1   | A     | 1261 | A    |
| 1   | A     | 1275 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1280 | A    |
| 1   | A     | 1282 | C    |
| 1   | A     | 1287 | A    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1317 | C    |
| 1   | A     | 1347 | G    |
| 1   | A     | 1364 | U    |
| 1   | A     | 1394 | A    |
| 1   | A     | 1395 | C    |
| 1   | A     | 1398 | A    |
| 1   | A     | 1498 | U    |
| 1   | A     | 1503 | A    |
| 1   | A     | 1506 | U    |
| 1   | A     | 1517 | G    |
| 1   | A     | 1529 | G    |
| 1   | A     | 1530 | G    |

All (2) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 69  | G    |
| 1   | A     | 343 | U    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 6   | B     | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | B     | 10:GLU    | C      | 107:UNK   | N      | 53.99        |
| 1     | B     | 179:UNK   | C      | 191:UNK   | N      | 19.24        |

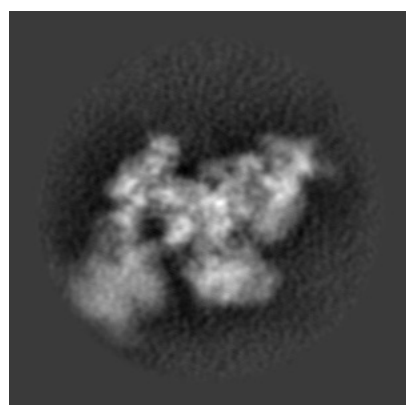
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7015. These allow visual inspection of the internal detail of the map and identification of artifacts.

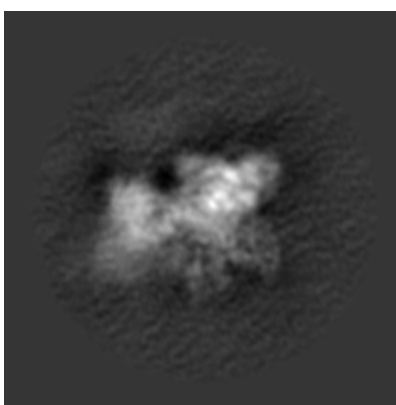
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

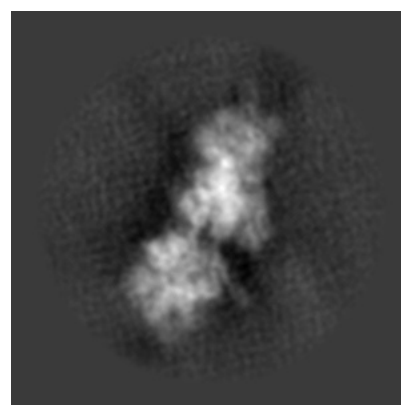
#### 6.1.1 Primary map



X



Y

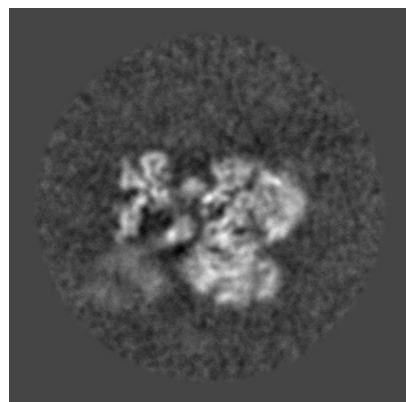


Z

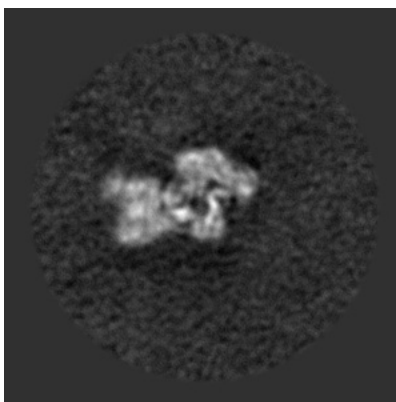
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

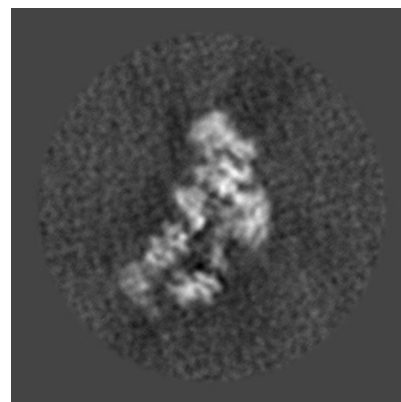
#### 6.2.1 Primary map



X Index: 140



Y Index: 140

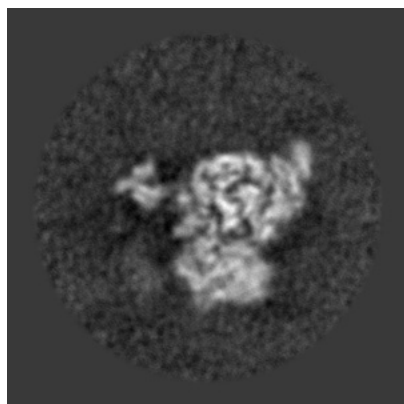


Z Index: 140

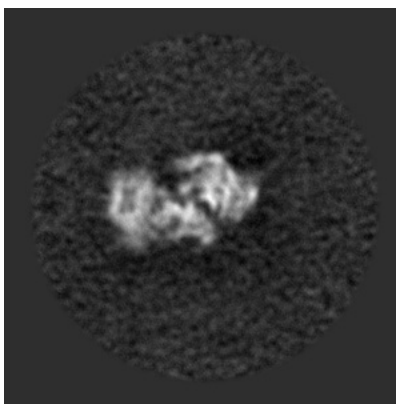
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

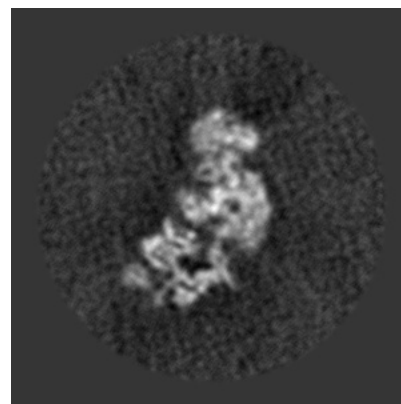
### 6.3.1 Primary map



X Index: 149



Y Index: 150

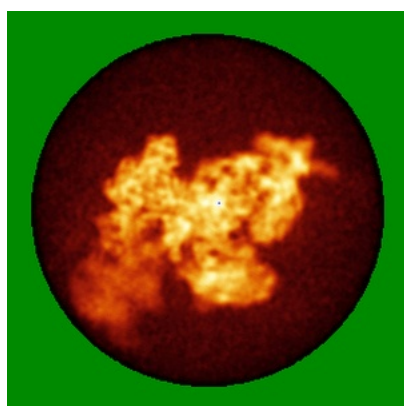


Z Index: 146

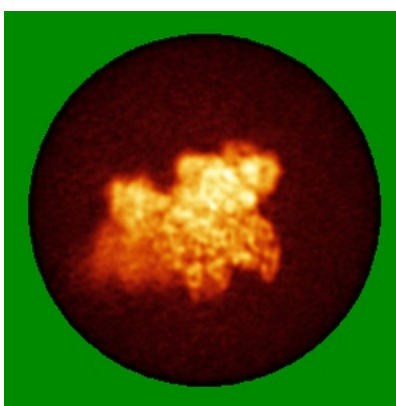
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

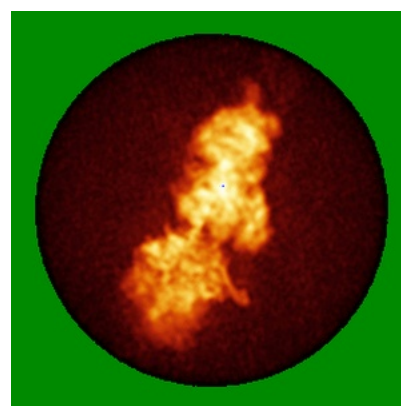
### 6.4.1 Primary map



X



Y

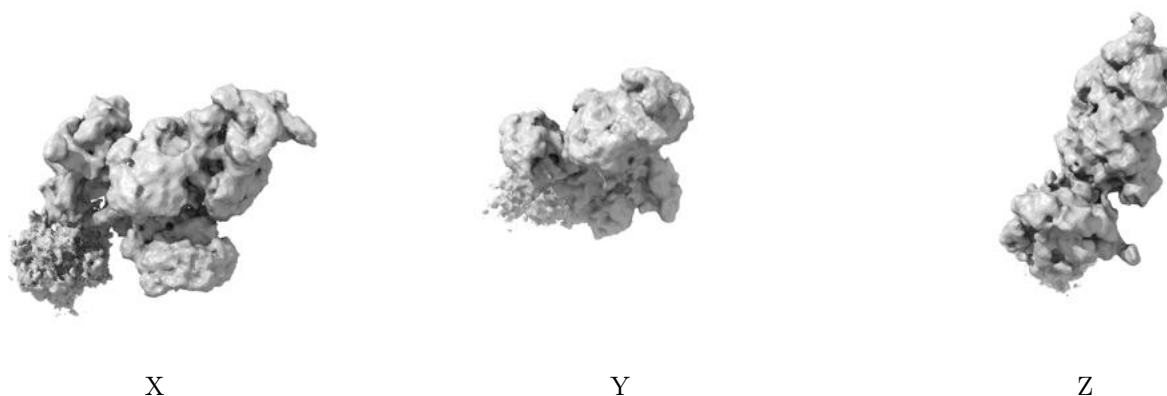


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

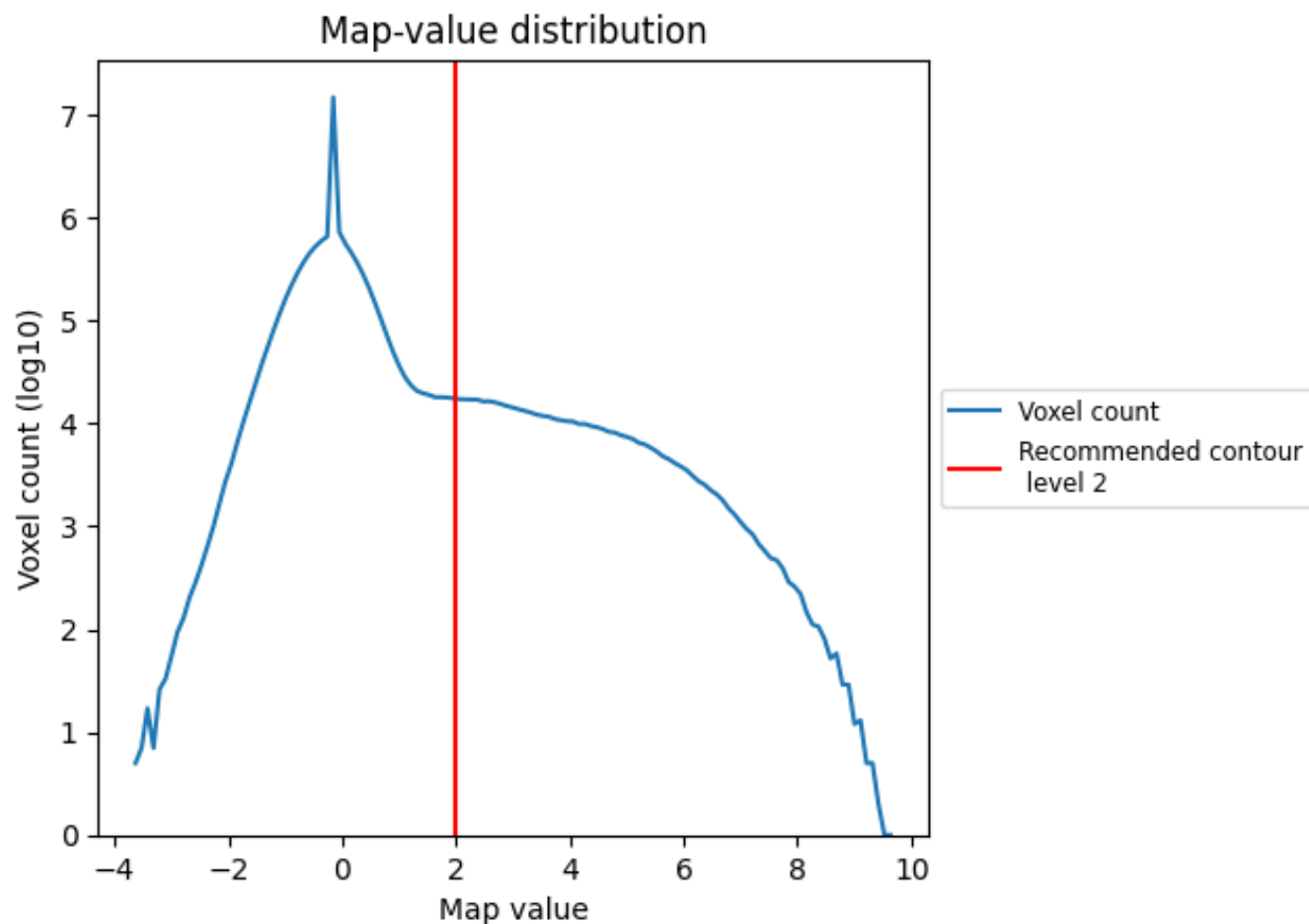
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

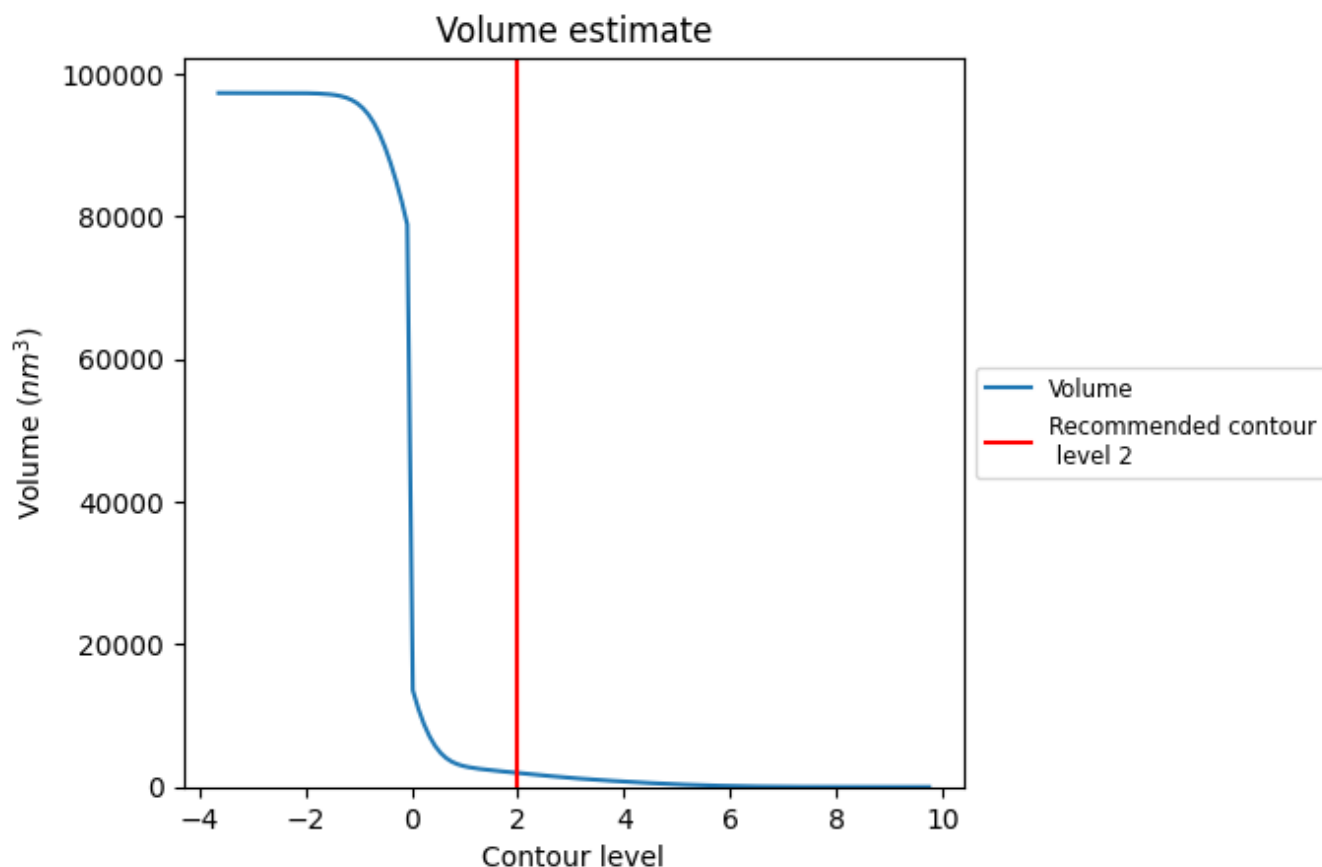
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

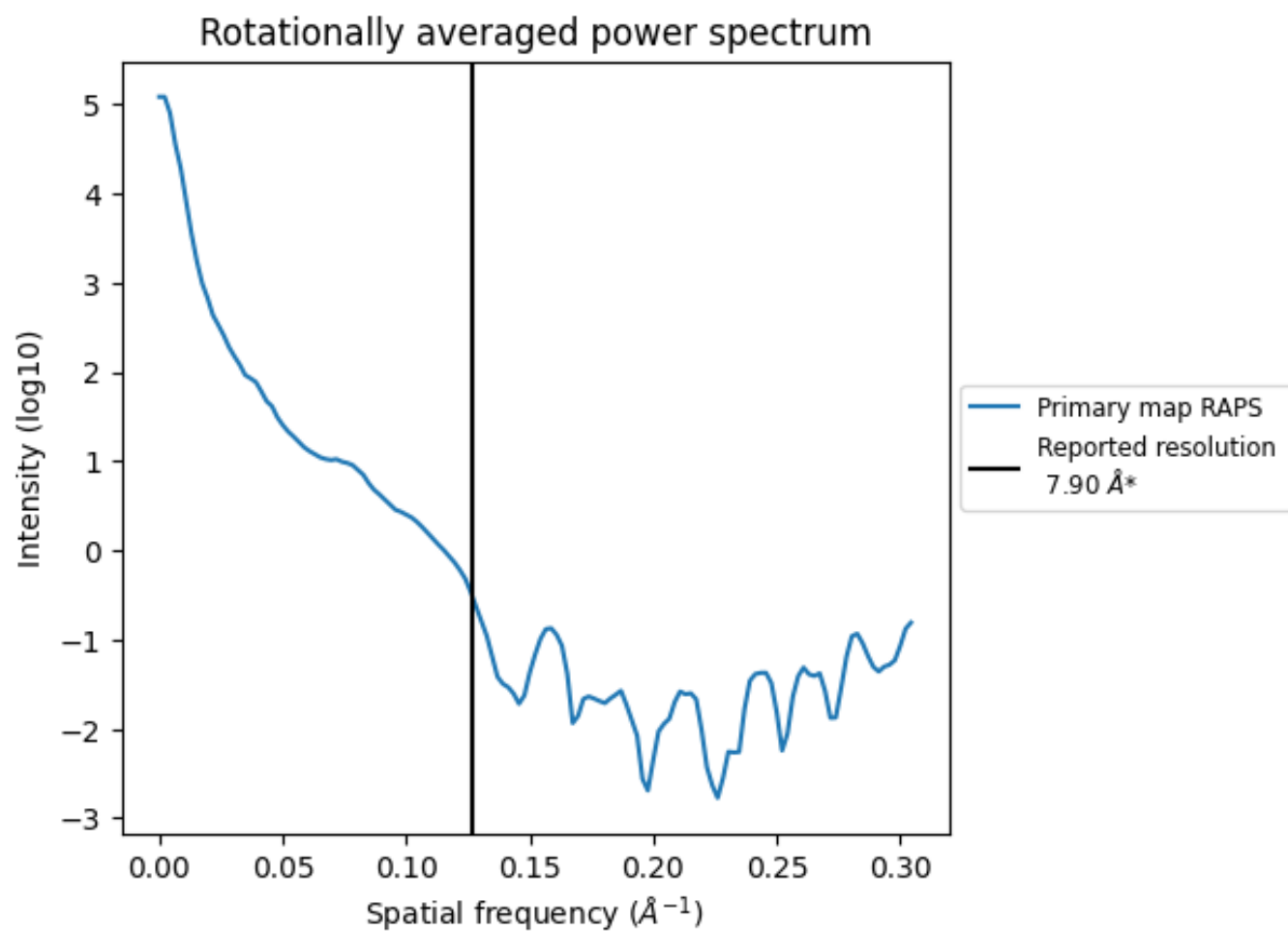
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1962 nm<sup>3</sup>; this corresponds to an approximate mass of 1773 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.127 Å<sup>-1</sup>

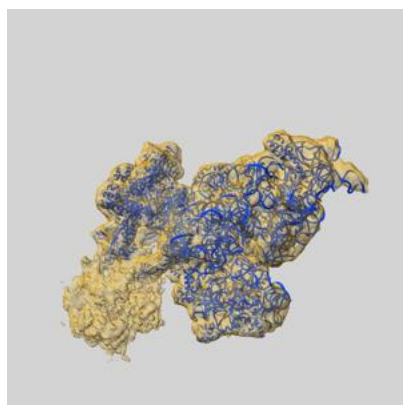
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

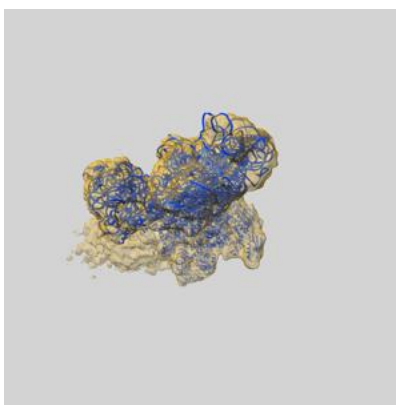
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7015 and PDB model 6AWC. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

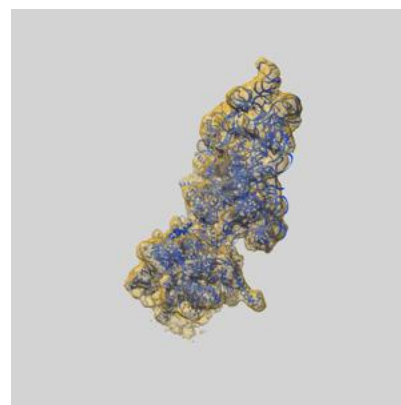
### 9.1 Map-model overlay [i](#)



X



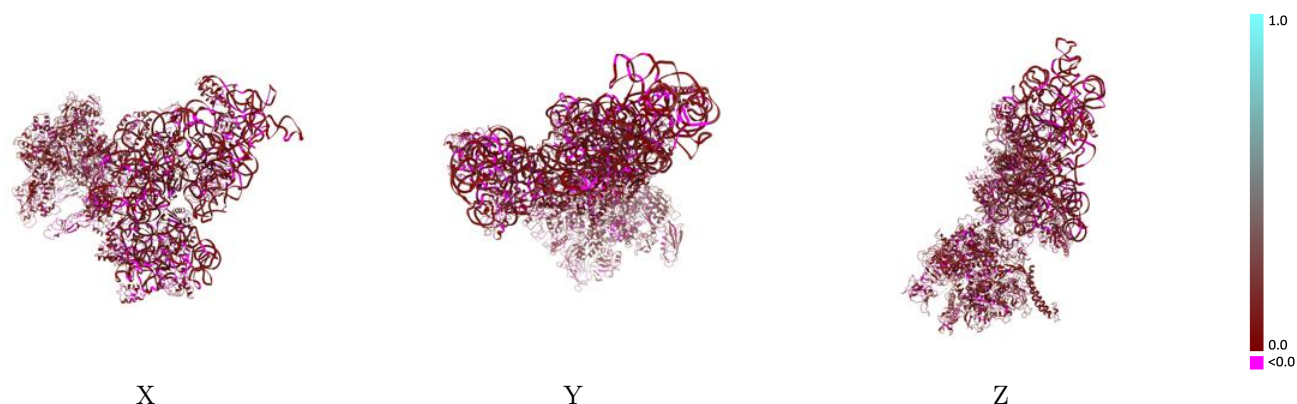
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



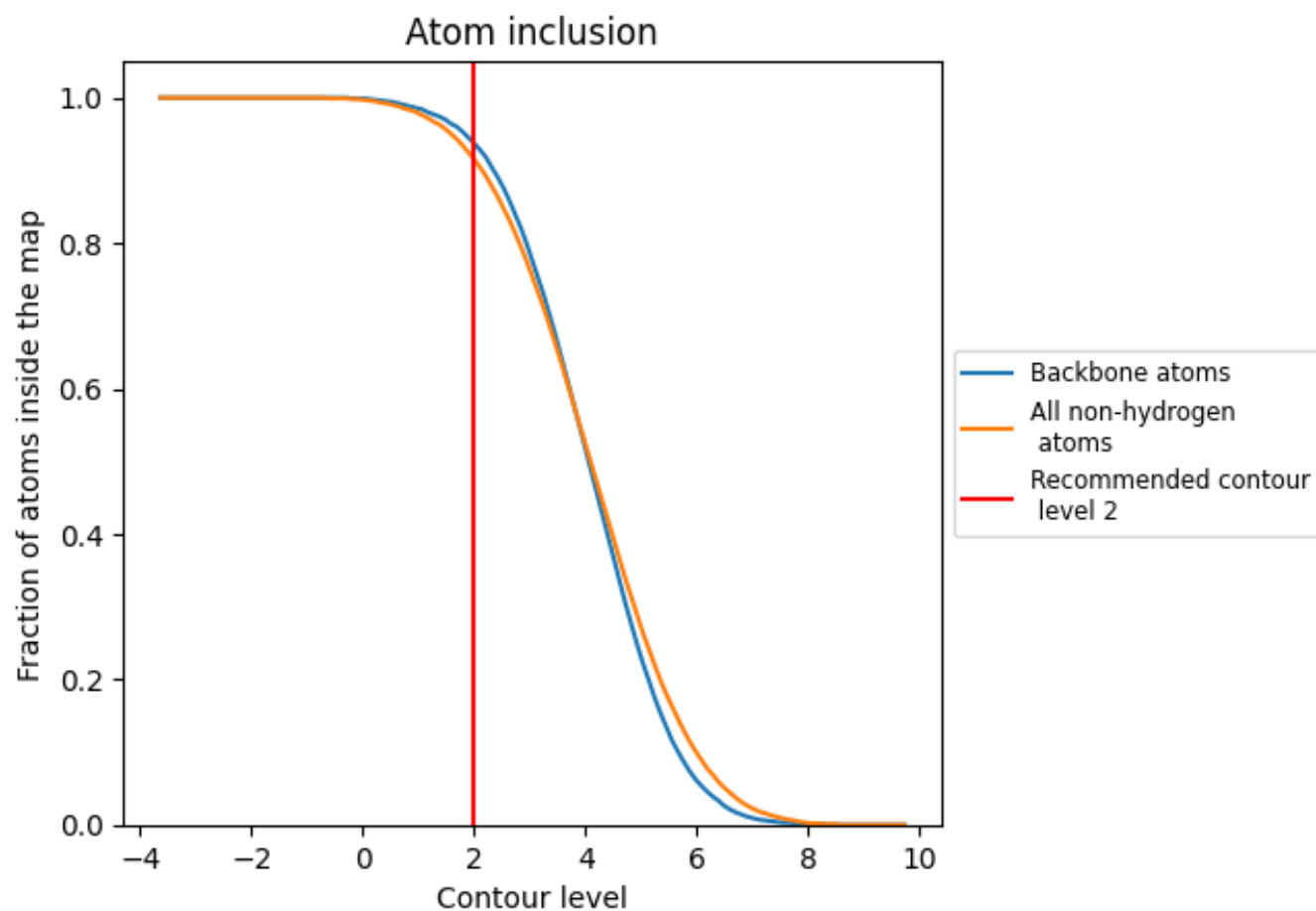
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9160   |  0.0950   |
| 01    |  0.9410   |  0.1410   |
| 02    |  0.9460   |  0.1200   |
| 03    |  0.9060   |  0.1110   |
| 04    |  0.9140   |  0.1210   |
| 05    |  0.2890   |  0.0470   |
| A     |  0.9260   |  0.0890   |
| B     |  0.8900   |  0.0700   |
| E     |  0.9680   |  0.1250   |
| F     |  0.8560   |  0.0970   |
| G     |  0.9270   |  0.0660   |
| H     |  0.9180   |  0.1200   |
| I     |  0.8470   |  0.1130   |
| J     |  0.8500   |  0.0660   |
| K     |  0.9290  |  0.0960  |
| L     |  0.8980 |  0.0530 |
| M     |  0.8910 |  0.0440 |
| N     |  0.9720 |  0.0530 |
| O     |  0.8790 |  0.0640 |
| P     |  0.9270 |  0.0590 |
| Q     |  0.9700 |  0.0330 |
| R     |  0.9350 |  0.0940 |
| S     |  0.9430 |  0.0640 |
| T     |  0.9590 |  0.0860 |
| U     |  0.9110 |  0.0610 |
| V     |  0.9320 |  0.0380 |
| W     |  0.9680 |  0.0750 |
| X     |  0.8820 |  0.1080 |

