



# Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 04:01 AM EDT

PDB ID : 8SCB / pdb\_00008scb  
EMDB ID : EMD-40344  
Title : Terminating ribosome with SRI-41315  
Authors : Yip, M.C.J.; Coelho, J.P.L.; Oltion, K.; Tauton, J.; Shao, S.  
Deposited on : 2023-04-05  
Resolution : 2.50 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  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

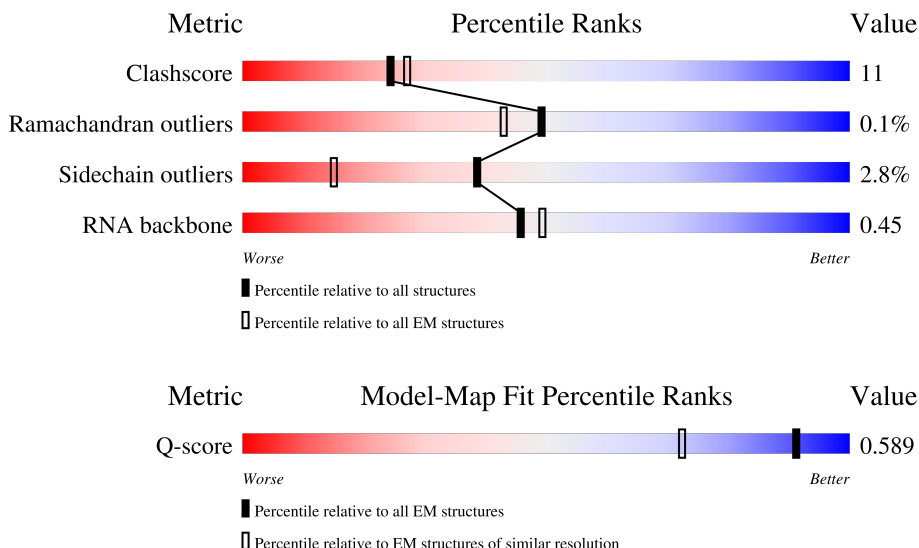
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.50 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                       | 7115 ( 2.00 - 3.00 )                                     |

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     | 257    |                  |
| 2   | B     | 403    |                  |
| 3   | C     | 413    |                  |

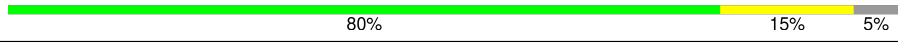
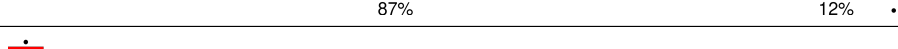
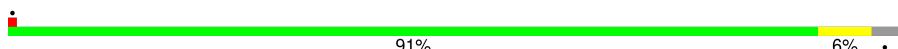
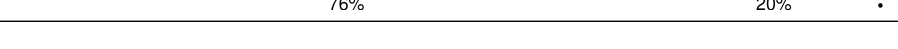
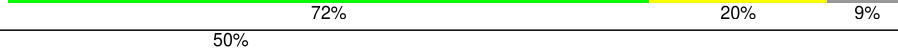
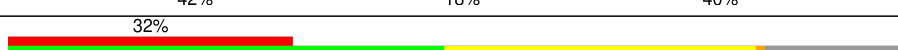
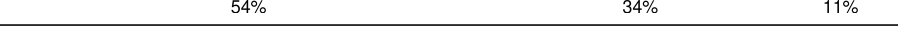
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | D     | 297    |    |
| 5   | E     | 291    |    |
| 6   | F     | 247    |    |
| 7   | G     | 319    |    |
| 8   | H     | 192    |    |
| 9   | I     | 214    |    |
| 10  | J     | 178    |    |
| 11  | L     | 211    |    |
| 12  | M     | 218    |    |
| 13  | N     | 204    |    |
| 14  | O     | 203    |    |
| 15  | P     | 184    |   |
| 16  | Q     | 188    |  |
| 17  | R     | 196    |  |
| 18  | S     | 176    |  |
| 19  | T     | 160    |  |
| 20  | U     | 128    |  |
| 21  | V     | 140    |  |
| 22  | W     | 157    |  |
| 23  | X     | 156    |  |
| 24  | Y     | 145    |  |
| 25  | Z     | 136    |  |
| 26  | a     | 148    |  |
| 27  | b     | 245    |  |
| 28  | c     | 115    |  |

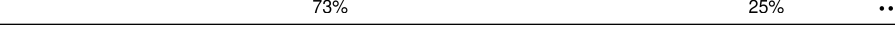
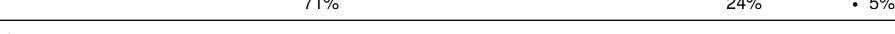
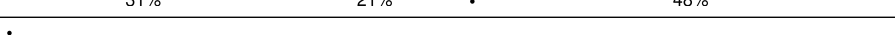
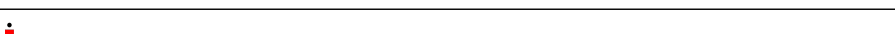
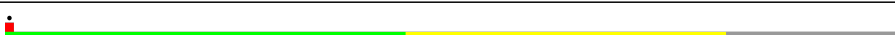
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | d     | 125    |    |
| 30  | e     | 135    |    |
| 31  | f     | 110    |    |
| 32  | g     | 117    |    |
| 33  | h     | 123    |    |
| 34  | i     | 105    |    |
| 35  | j     | 97     |    |
| 36  | k     | 70     |    |
| 37  | l     | 51     |    |
| 38  | m     | 93     |   |
| 39  | n     | 25     |  |
| 40  | o     | 106    |  |
| 41  | p     | 92     |  |
| 42  | r     | 137    |  |
| 43  | s     | 318    |  |
| 44  | t     | 165    |  |
| 45  | 1     | 130    |  |
| 46  | 2     | 76     |  |
| 47  | 3     | 75     |  |
| 48  | 5     | 3543   |  |
| 49  | 7     | 120    |  |
| 50  | 8     | 156    |  |
| 51  | 9     | 1869   |  |
| 52  | AA    | 295    |  |
| 53  | BB    | 264    |  |

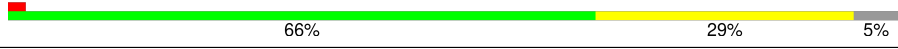
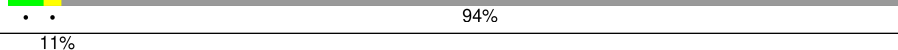
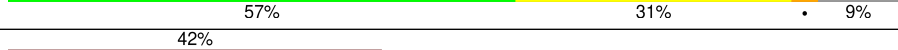
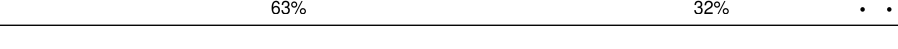
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 54  | CC    | 293    |    |
| 55  | DD    | 243    |    |
| 56  | EE    | 263    |    |
| 57  | FF    | 204    |    |
| 58  | GG    | 249    |    |
| 59  | HH    | 194    |    |
| 60  | II    | 208    |    |
| 61  | JJ    | 194    |    |
| 62  | KK    | 165    |    |
| 63  | LL    | 158    |    |
| 64  | MM    | 132    |    |
| 65  | NN    | 151    |  |
| 66  | OO    | 168    |  |
| 67  | PP    | 145    |  |
| 68  | QQ    | 146    |  |
| 69  | RR    | 135    |  |
| 70  | SS    | 152    |  |
| 71  | TT    | 145    |  |
| 72  | UU    | 119    |  |
| 73  | VV    | 83     |  |
| 74  | WW    | 130    |  |
| 75  | XX    | 143    |  |
| 76  | YY    | 130    |  |
| 77  | ZZ    | 125    |  |
| 78  | aa    | 115    |  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 79  | bb    | 84     |  |
| 80  | cc    | 69     |  |
| 81  | dd    | 56     |  |
| 82  | ee    | 133    |  |
| 83  | ff    | 156    |  |
| 84  | gg    | 317    |  |
| 85  | hh    | 197    |  |
| 86  | ii    | 459    |  |
| 87  | jj    | 599    |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 90  | ZVM  | ii    | 501 | X         | -        | -       | -                |
| 91  | SF4  | jj    | 601 | -         | -        | X       | -                |

## 2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 222478 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 244      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1868  | 1171 | 382 | 309 | 6 |         |       |

- Molecule 2 is a protein called Ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 394      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3148  | 2007 | 591 | 537 | 13 |         |       |

- Molecule 3 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 362      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2883  | 1812 | 577 | 480 | 14 |         |       |

- Molecule 4 is a protein called Ribosomal\_L18\_c domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | D     | 289      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2361  | 1495 | 431 | 421 | 14 |         |       |

- Molecule 5 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | E     | 215      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1726  | 1110 | 327 | 286 | 3 |         |       |

- Molecule 6 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | F     | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1875  | 1205 | 358 | 303 | 9 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| F     | 61      | ARG      | GLY    | conflict | UNP G1TUB1 |
| F     | 93      | ARG      | GLY    | conflict | UNP G1TUB1 |
| F     | 131     | MET      | VAL    | conflict | UNP G1TUB1 |
| F     | 153     | ILE      | VAL    | conflict | UNP G1TUB1 |

- Molecule 7 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | G     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1768  | 1127 | 341 | 296 | 4 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| G     | 191     | GLY      | CYS    | conflict | UNP G1STW0 |

- Molecule 8 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1516  | 954 | 284 | 272 | 6 |         |       |

- Molecule 9 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | I     | 204      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1655  | 1051 | 319 | 272 | 13 |         |       |

- Molecule 10 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | J     | 167      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1336  | 846 | 249 | 235 | 6 |         |       |

- Molecule 11 is a protein called eL13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | L     | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1702  | 1065 | 354 | 279 | 4 |         |       |

- Molecule 12 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | M     | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1137  | 727 | 221 | 182 | 7 |         |       |

- Molecule 13 is a protein called Ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | N     | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |

- Molecule 14 is a protein called uL13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | O     | 198      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1621  | 1046 | 317 | 253 | 5 |         |       |

- Molecule 15 is a protein called uL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | P     | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1242  | 777 | 241 | 215 | 9 |         |       |

- Molecule 16 is a protein called Ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | Q     | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1515  | 946 | 315 | 250 | 4 |         |       |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Q     | 4       | ASP      | ASN    | conflict | UNP G1TFE0 |
| Q     | 14      | ARG      | TRP    | conflict | UNP G1TFE0 |
| Q     | 53      | MET      | LEU    | conflict | UNP G1TFE0 |
| Q     | 58      | ARG      | TRP    | conflict | UNP G1TFE0 |
| Q     | 75      | ARG      | GLN    | conflict | UNP G1TFE0 |
| Q     | 80      | ALA      | PRO    | conflict | UNP G1TFE0 |
| Q     | 86      | VAL      | ILE    | conflict | UNP G1TFE0 |
| Q     | 104     | ARG      | HIS    | conflict | UNP G1TFE0 |
| Q     | 110     | ARG      | CYS    | conflict | UNP G1TFE0 |
| Q     | 137     | VAL      | GLY    | conflict | UNP G1TFE0 |
| Q     | 157     | GLY      | ARG    | conflict | UNP G1TFE0 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Q     | 181     | ARG      | TRP    | conflict | UNP G1TFE0 |

- Molecule 17 is a protein called Ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | R     | 179      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1502  | 930 | 327 | 236 | 9 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| R     | 38      | ARG      | CYS    | conflict | UNP G1TJR3 |
| R     | 64      | ARG      | GLN    | conflict | UNP G1TJR3 |
| R     | 94      | THR      | LYS    | conflict | UNP G1TJR3 |

- Molecule 18 is a protein called eL20.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 18  | S     | 176      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1462  | 930 | 285 | 236 | 11 |         |       |

- Molecule 19 is a protein called eL21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | T     | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1298  | 823 | 252 | 217 | 6 |         |       |

- Molecule 20 is a protein called eL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | U     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 800   | 514 | 139 | 145 | 2 |         |       |

There are 11 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| U     | 18      | LEU      | VAL    | conflict | UNP G1TSG1 |
| U     | 32      | GLY      | ARG    | conflict | UNP G1TSG1 |
| U     | 36      | ALA      | GLU    | conflict | UNP G1TSG1 |
| U     | 39      | PHE      | SER    | conflict | UNP G1TSG1 |
| U     | 54      | GLY      | ARG    | conflict | UNP G1TSG1 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| U     | 60      | VAL      | ALA    | conflict | UNP G1TSG1 |
| U     | 62      | SER      | THR    | conflict | UNP G1TSG1 |
| U     | 63      | LEU      | ILE    | conflict | UNP G1TSG1 |
| U     | 97      | ARG      | HIS    | conflict | UNP G1TSG1 |
| U     | 106     | THR      | SER    | conflict | UNP G1TSG1 |
| U     | 126     | GLU      | ASP    | conflict | UNP G1TSG1 |

- Molecule 21 is a protein called Ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | V     | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 973   | 615 | 183 | 170 | 5 |         |       |

- Molecule 22 is a protein called 60S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 22  | W     | 63       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 528   | 337 | 103 | 85 | 3 |         |       |

- Molecule 23 is a protein called eL23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | X     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 949   | 606 | 178 | 164 | 1 |         |       |

- Molecule 24 is a protein called uL24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | Y     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 700 | 226 | 186 | 3 |         |       |

- Molecule 25 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | Z     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1107  | 714 | 208 | 182 | 3 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | a     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 734 | 239 | 185 | 4 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 27  | b     | 75       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 609   | 378 | 130 | 98 | 3 |         |       |

- Molecule 28 is a protein called eL30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | c     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 732   | 464 | 130 | 132 | 6 |         |       |

- Molecule 29 is a protein called eL31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | d     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 833   | 530 | 163 | 138 | 2 |         |       |

- Molecule 30 is a protein called eL32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | e     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 667 | 216 | 165 | 5 |         |       |

- Molecule 31 is a protein called eL33.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | f     | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 143 | 4 |         |       |

- Molecule 32 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | g     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 906   | 566 | 187 | 147 | 6 |         |       |

- Molecule 33 is a protein called eL35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | h     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1013  | 640 | 204 | 168 | 1 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | i     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 830   | 520 | 176 | 129 | 5 |         |       |

- Molecule 35 is a protein called Ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | j     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 434 | 155 | 111 | 5 |         |       |

- Molecule 36 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 36  | k     | 68       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 559   | 360 | 101 | 97 | 1 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| k     | 24      | LYS      | ASN    | conflict | UNP G1U001 |

- Molecule 37 is a protein called eL39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 37  | l     | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 438   | 280 | 95 | 62 | 1 |         |       |

- Molecule 38 is a protein called Ubiquitin A-52 residue ribosomal protein fusion product 1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 38  | m     | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 421   | 260 | 89 | 66 | 6 |         |       |

- Molecule 39 is a protein called eL41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 39  | n     | 23       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 222   | 134 | 61 | 25 | 2 |         |       |

- Molecule 40 is a protein called eL42.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | o     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 842   | 528 | 172 | 136 | 6 |         |       |

- Molecule 41 is a protein called eL43.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | p     | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 136 | 120 | 7 |         |       |

- Molecule 42 is a protein called eL28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | r     | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1001  | 621 | 206 | 168 | 6 |         |       |

- Molecule 43 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | s     | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1461  | 931 | 255 | 266 | 9 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | t     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1059  | 662 | 195 | 199 | 3 |         |       |

- Molecule 45 is a protein called NC.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 45  | 1     | 15       | Total | C  | N  | O  | S | 0       | 0     |
|     |       |          | 125   | 82 | 20 | 22 | 1 |         |       |

- Molecule 46 is a RNA chain called P\_tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 46  | 2     | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1616  | 723 | 291 | 527 | 75 |         |       |

- Molecule 47 is a RNA chain called E\_tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 47  | 3     | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1593  | 712 | 281 | 526 | 74 |         |       |

- Molecule 48 is a RNA chain called 28S\_rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 48  | 5     | 3530     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 75735 | 33780 | 13869 | 24556 | 3530 |         |       |

- Molecule 49 is a RNA chain called 5S\_rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 49  | 7     | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2558  | 1141 | 456 | 842 | 119 |         |       |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference   |
|-------|---------|----------|--------|----------|-------------|
| 7     | 2       | U        | N      | conflict | GB X06789.1 |
| 7     | 36      | C        | N      | conflict | GB X06789.1 |
| 7     | 102     | U        | N      | conflict | GB X06789.1 |
| 7     | 112     | U        | N      | conflict | GB X06789.1 |
| 7     | 114     | U        | N      | conflict | GB X06789.1 |
| 7     | 119     | U        | C      | conflict | GB X06789.1 |
| 7     | 120     | U        | N      | conflict | GB X06789.1 |

- Molecule 50 is a RNA chain called 5.8S\_rRNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 50  | 8     | 156      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3315  | 1481 | 585 | 1094 | 155 |         |       |

- Molecule 51 is a RNA chain called 18S\_rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 51  | 9     | 1692     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 36134 | 16163 | 6486 | 11794 | 1691 |         |       |

- Molecule 52 is a protein called uS2 (SA).

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 52  | AA    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1624  | 1035 | 287 | 294 | 8 |         |       |

- Molecule 53 is a protein called eS1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 53  | BB    | 212      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1722  | 1093 | 308 | 307 | 14 |         |       |

- Molecule 54 is a protein called uS5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 54  | CC    | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1674  | 1085 | 286 | 294 | 9 |         |       |

- Molecule 55 is a protein called Ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 55  | DD    | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1723  | 1098 | 311 | 307 | 7 |         |       |

- Molecule 56 is a protein called eS4 (S4 X isoform).

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 56  | EE    | 259      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2059  | 1316 | 383 | 352 | 8 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| EE    | 25      | GLY      | SER    | conflict | UNP G1TK17 |
| EE    | 51      | ARG      | LYS    | conflict | UNP G1TK17 |
| EE    | 78      | THR      | ALA    | conflict | UNP G1TK17 |
| EE    | 156     | VAL      | MET    | conflict | UNP G1TK17 |

- Molecule 57 is a protein called uS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | FF    | 181      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1441  | 902 | 273 | 259 | 7 |         |       |

- Molecule 58 is a protein called eS6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 58  | GG    | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1923  | 1200 | 387 | 329 | 7 |         |       |

- Molecule 59 is a protein called eS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | HH    | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1425  | 912 | 258 | 254 | 1 |         |       |

- Molecule 60 is a protein called eS8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 60  | II    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1686  | 1058 | 332 | 291 | 5 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| II    | 47      | ARG      | GLY    | conflict | UNP G1TJW1 |

- Molecule 61 is a protein called uS4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | JJ    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1525  | 969 | 306 | 248 | 2 |         |       |

- Molecule 62 is a protein called S10\_ plectin domain-containing protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | KK    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 729   | 479 | 127 | 118 | 5 |         |       |

- Molecule 63 is a protein called uS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | LL    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1123  | 717 | 210 | 190 | 6 |         |       |

- Molecule 64 is a protein called eS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | MM    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 939   | 588 | 166 | 176 | 9 |         |       |

- Molecule 65 is a protein called uS15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | NN    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 773 | 229 | 205 | 1 |         |       |

- Molecule 66 is a protein called uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | OO    | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 957   | 585 | 189 | 177 | 6 |         |       |

- Molecule 67 is a protein called uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | PP    | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 968   | 615 | 181 | 165 | 7 |         |       |

- Molecule 68 is a protein called uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | QQ    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1117  | 710 | 211 | 193 | 3 |         |       |

- Molecule 69 is a protein called eS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | RR    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 962   | 604 | 179 | 176 | 3 |         |       |

- Molecule 70 is a protein called uS13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | SS    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 731 | 234 | 196 | 1 |         |       |

- Molecule 71 is a protein called eS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | TT    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1075  | 674 | 206 | 192 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| TT    | 119     | GLY      | TRP    | conflict | UNP G1TN62 |

- Molecule 72 is a protein called uS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | UU    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 807   | 507 | 153 | 143 | 4 |         |       |

- Molecule 73 is a protein called eS21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73  | VV    | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 617   | 380 | 114 | 118 | 5 |         |       |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| VV    | 3       | ASN      | SER    | conflict | UNP G1TM82 |
| VV    | 4       | ASP      | ASN    | conflict | UNP G1TM82 |
| VV    | 33      | GLN      | PRO    | conflict | UNP G1TM82 |
| VV    | 50      | PHE      | SER    | conflict | UNP G1TM82 |
| VV    | 75      | ALA      | SER    | conflict | UNP G1TM82 |
| VV    | 76      | ASP      | HIS    | conflict | UNP G1TM82 |
| VV    | 81      | LYS      | GLN    | conflict | UNP G1TM82 |

- Molecule 74 is a protein called uS8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | WW    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 75 is a protein called uS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | XX    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1098  | 693 | 219 | 183 | 3 |         |       |

- Molecule 76 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | YY    | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1006  | 637 | 197 | 167 | 5 |         |       |

- Molecule 77 is a protein called eS25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | ZZ    | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 574   | 368 | 104 | 101 | 1 |         |       |

- Molecule 78 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78  | aa    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 781   | 486 | 161 | 129 | 5 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| aa    | 28      | ARG      | CYS    | conflict | UNP G1TFE8 |
| aa    | 56      | ALA      | VAL    | conflict | UNP G1TFE8 |
| aa    | 109     | ARG      | PRO    | conflict | UNP G1TFE8 |

- Molecule 79 is a protein called eS27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 79  | bb    | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 628   | 395 | 117 | 110 | 6 |         |       |

- Molecule 80 is a protein called eS28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 80  | cc    | 61       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 479   | 292 | 95 | 90 | 2 |         |       |

- Molecule 81 is a protein called uS14.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 81  | dd    | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 445   | 278 | 90 | 72 | 5 |         |       |

- Molecule 82 is a protein called eS30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 82  | ee    | 47       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 380   | 231 | 86 | 62 | 1 |         |       |

- Molecule 83 is a protein called eS31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 83  | ff    | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 527   | 336 | 99 | 86 | 6 |         |       |

- Molecule 84 is a protein called Receptor for Activated C Kinase 1 (RACK1).

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 84  | gg    | 304      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2371  | 1496 | 414 | 449 | 12 |         |       |

- Molecule 85 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 85  | hh    | 11       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 236   | 106 | 44 | 75 | 11 |         |       |

- Molecule 86 is a protein called Eukaryotic peptide chain release factor subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 86  | ii    | 416      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3280  | 2087 | 559 | 623 | 11 |         |       |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| ii    | -21     | MET      | -      | expression tag | UNP P62495 |
| ii    | -20     | ARG      | -      | expression tag | UNP P62495 |
| ii    | -19     | GLY      | -      | expression tag | UNP P62495 |
| ii    | -18     | SER      | -      | expression tag | UNP P62495 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| ii    | -17     | HIS      | -      | expression tag | UNP P62495 |
| ii    | -16     | HIS      | -      | expression tag | UNP P62495 |
| ii    | -15     | HIS      | -      | expression tag | UNP P62495 |
| ii    | -14     | HIS      | -      | expression tag | UNP P62495 |
| ii    | -13     | HIS      | -      | expression tag | UNP P62495 |
| ii    | -12     | HIS      | -      | expression tag | UNP P62495 |
| ii    | -11     | GLY      | -      | expression tag | UNP P62495 |
| ii    | -10     | MET      | -      | expression tag | UNP P62495 |
| ii    | -9      | ALA      | -      | expression tag | UNP P62495 |
| ii    | -8      | SER      | -      | expression tag | UNP P62495 |
| ii    | -7      | GLU      | -      | expression tag | UNP P62495 |
| ii    | -6      | ASN      | -      | expression tag | UNP P62495 |
| ii    | -5      | LEU      | -      | expression tag | UNP P62495 |
| ii    | -4      | TYR      | -      | expression tag | UNP P62495 |
| ii    | -3      | PHE      | -      | expression tag | UNP P62495 |
| ii    | -2      | GLN      | -      | expression tag | UNP P62495 |
| ii    | -1      | GLY      | -      | expression tag | UNP P62495 |
| ii    | 0       | SER      | -      | expression tag | UNP P62495 |
| ii    | 183     | ALA      | GLY    | conflict       | UNP P62495 |
| ii    | 184     | ALA      | GLY    | conflict       | UNP P62495 |

- Molecule 87 is a protein called ATP binding cassette subfamily E member 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 87  | jj    | 578      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4558  | 2914 | 780 | 835 | 29 |         |       |

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 88  | A     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 88  | I     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 88  | N     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 88  | P     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 88  | V     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 88  | a     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms        |           | AltConf |
|-----|-------|----------|--------------|-----------|---------|
| 88  | e     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 88  | f     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 88  | g     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 88  | o     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 88  | 2     | 2        | Total<br>2   | Mg<br>2   | 0       |
| 88  | 5     | 221      | Total<br>221 | Mg<br>221 | 0       |
| 88  | 7     | 6        | Total<br>6   | Mg<br>6   | 0       |
| 88  | 8     | 2        | Total<br>2   | Mg<br>2   | 0       |
| 88  | 9     | 64       | Total<br>64  | Mg<br>64  | 0       |
| 88  | EE    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 88  | LL    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 88  | OO    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 88  | XX    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 88  | hh    | 1        | Total<br>1   | Mg<br>1   | 0       |

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

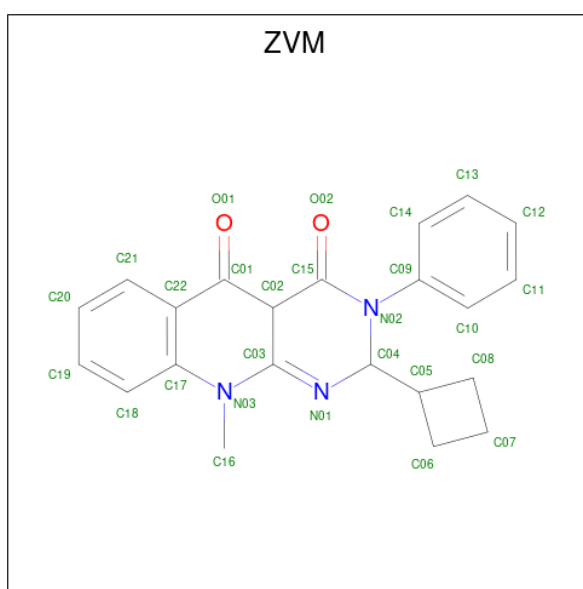
| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 89  | g     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 89  | j     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 89  | m     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 89  | o     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 89  | p     | 1        | Total<br>1 | Zn<br>1 | 0       |

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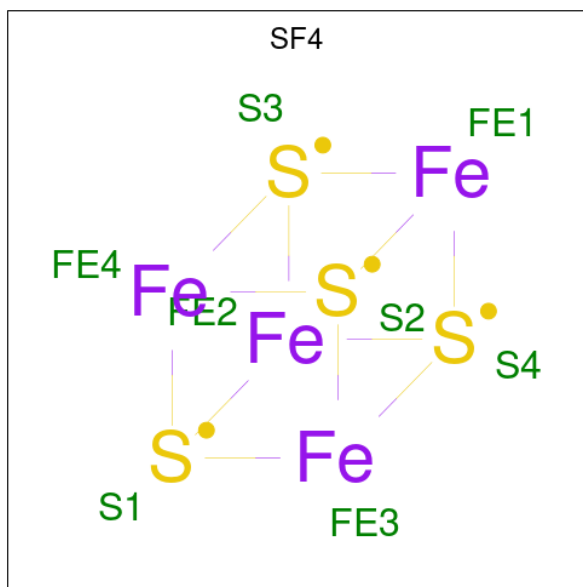
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 89  | aa    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 89  | dd    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 89  | ff    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 90 is (2S,4aS)-2-cyclobutyl-10-methyl-3-phenyl-2,10-dihydropyrimido[4,5-b]quinoline-4,5(3H,4aH)-dione (CCD ID: ZVM) (formula: C<sub>22</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 90  | ii    | 1        | Total | C  | N | O | 0       |
|     |       |          | 27    | 22 | 3 | 2 |         |

- Molecule 91 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 91  | jj    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 91  | jj    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 92 is water.

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 92  | A     | 6        | Total | O | 0       |
|     |       |          | 6     | 6 |         |
| 92  | B     | 2        | Total | O | 0       |
|     |       |          | 2     | 2 |         |
| 92  | C     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 92  | F     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 92  | I     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 92  | L     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 92  | N     | 4        | Total | O | 0       |
|     |       |          | 4     | 4 |         |
| 92  | Q     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 92  | R     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 92  | V     | 2        | Total | O | 0       |
|     |       |          | 2     | 2 |         |

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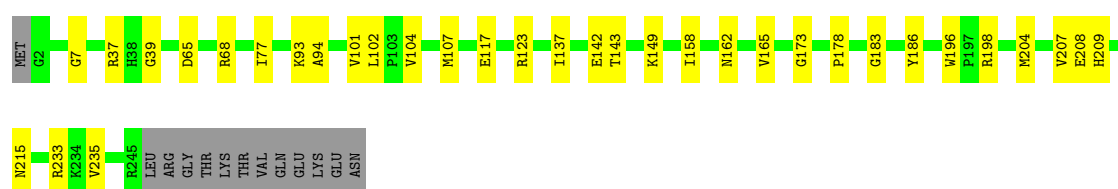
| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 92  | X     | 2        | Total<br>2   | O<br>2   | 0       |
| 92  | a     | 5        | Total<br>5   | O<br>5   | 0       |
| 92  | e     | 5        | Total<br>5   | O<br>5   | 0       |
| 92  | j     | 1        | Total<br>1   | O<br>1   | 0       |
| 92  | o     | 2        | Total<br>2   | O<br>2   | 0       |
| 92  | 5     | 723      | Total<br>723 | O<br>723 | 0       |
| 92  | 7     | 13       | Total<br>13  | O<br>13  | 0       |
| 92  | 8     | 8        | Total<br>8   | O<br>8   | 0       |
| 92  | 9     | 173      | Total<br>173 | O<br>173 | 0       |
| 92  | II    | 1        | Total<br>1   | O<br>1   | 0       |
| 92  | OO    | 1        | Total<br>1   | O<br>1   | 0       |
| 92  | XX    | 1        | Total<br>1   | O<br>1   | 0       |
| 92  | aa    | 1        | Total<br>1   | O<br>1   | 0       |
| 92  | ii    | 2        | Total<br>2   | O<br>2   | 0       |

### 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.

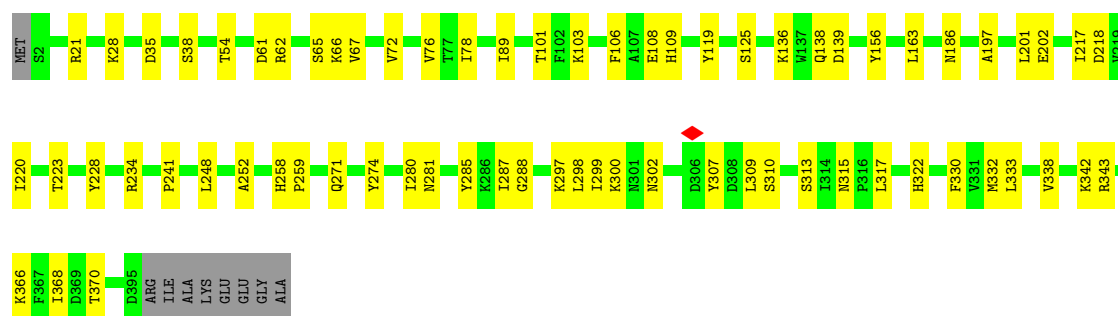
#### • Molecule 1: Ribosomal protein L8

Chain A: 



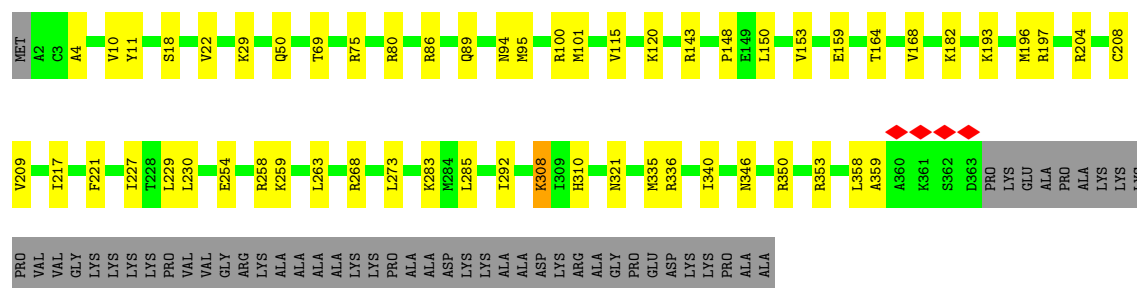
#### • Molecule 2: Ribosomal protein L3

Chain B: 

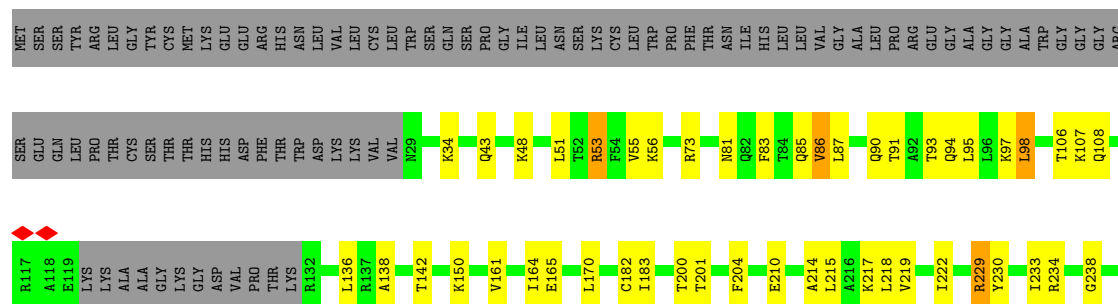
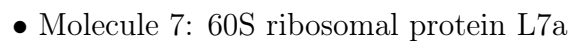
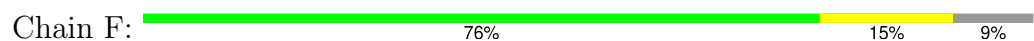
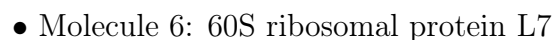
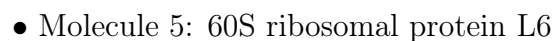


#### • Molecule 3: 60S ribosomal protein L4

Chain C: 



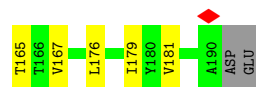
Chain D:  75% 21% ..





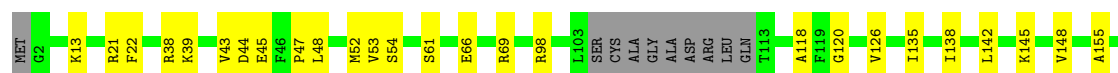
• Molecule 8: 60S ribosomal protein L9

Chain H: 80% 19%



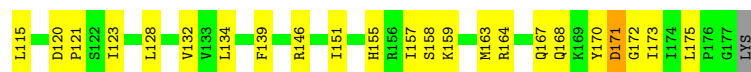
• Molecule 9: 60S ribosomal protein L10

Chain I: 79% 16% 5%



• Molecule 10: 60S ribosomal protein L11

Chain J: 67% 26% 6%



• Molecule 11: eL13

Chain L: 87% 12%



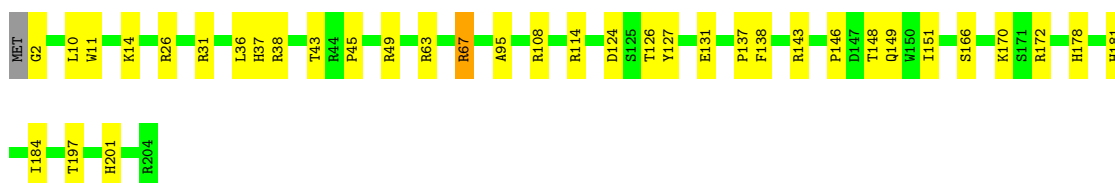
• Molecule 12: 60S ribosomal protein L14

Chain M: 53% 10% 37%



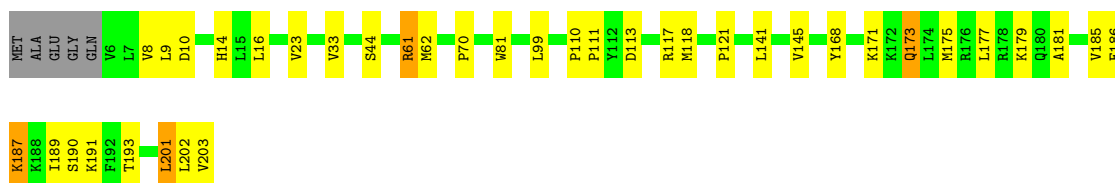
- Molecule 13: Ribosomal protein L15

Chain N:  82% 17%



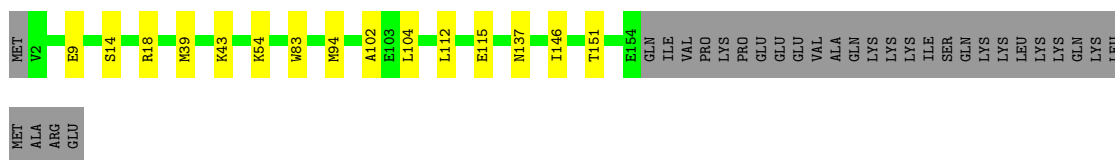
- Molecule 14: uL13

Chain O:  79% 17% .



- Molecule 15: uL22

Chain P:  75% 8% 17%



- Molecule 16: Ribosomal protein L18

Chain Q:  87% 12% •



- Molecule 17: Ribosomal protein L19

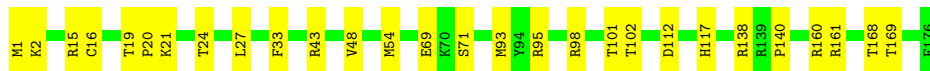
Chain R:  5% 82% 10% 9%



LYS

- Molecule 18: eL20

Chain S: 84% 16%



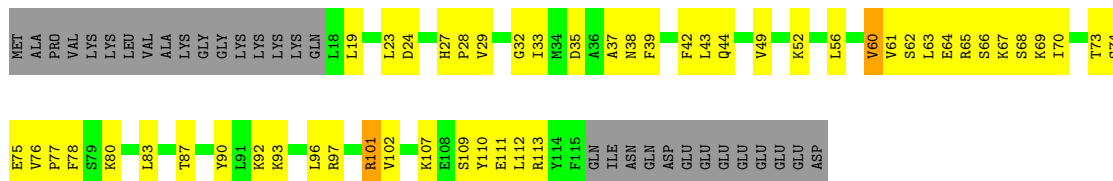
- Molecule 19: eL21

Chain T: 89% 10%



- Molecule 20: eL22

Chain U: 37% 38% 23%



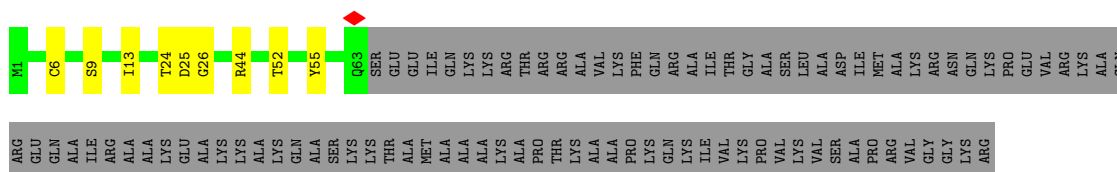
- Molecule 21: Ribosomal protein L23

Chain V: 86% 6% 7%



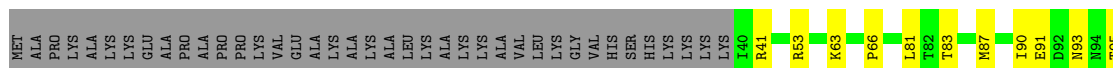
- Molecule 22: 60S ribosomal protein L24

Chain W: 34% 6% 60%



- Molecule 23: eL23

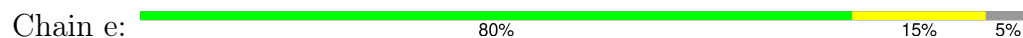
Chain X: 63% 12% 26%



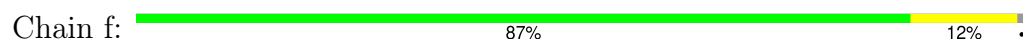




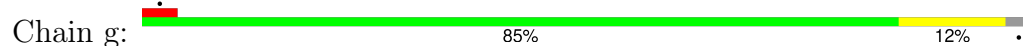
- Molecule 30: eL32



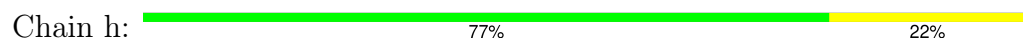
- Molecule 31: eL33



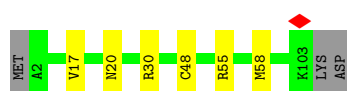
- Molecule 32: 60S ribosomal protein L34



- Molecule 33: eL35



- Molecule 34: 60S ribosomal protein L36



- Molecule 35: Ribosomal protein L37





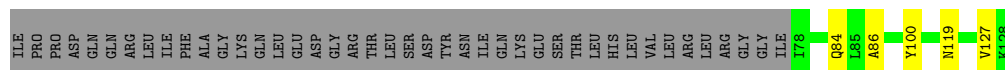
- Molecule 36: 60S ribosomal protein L38



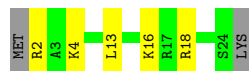
- Molecule 37: eL39



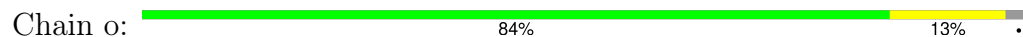
- Molecule 38: Ubiquitin A-52 residue ribosomal protein fusion product 1



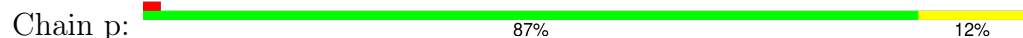
- Molecule 39: eL41



- Molecule 40: eL42

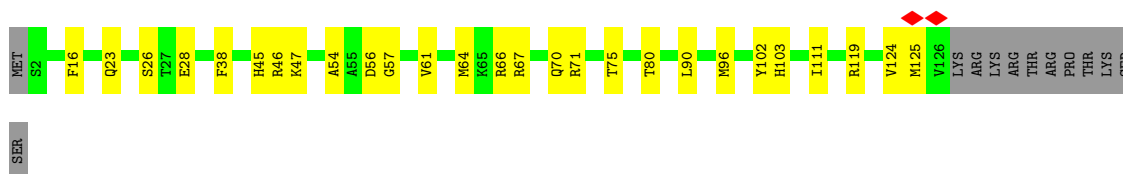


- Molecule 41: eL43

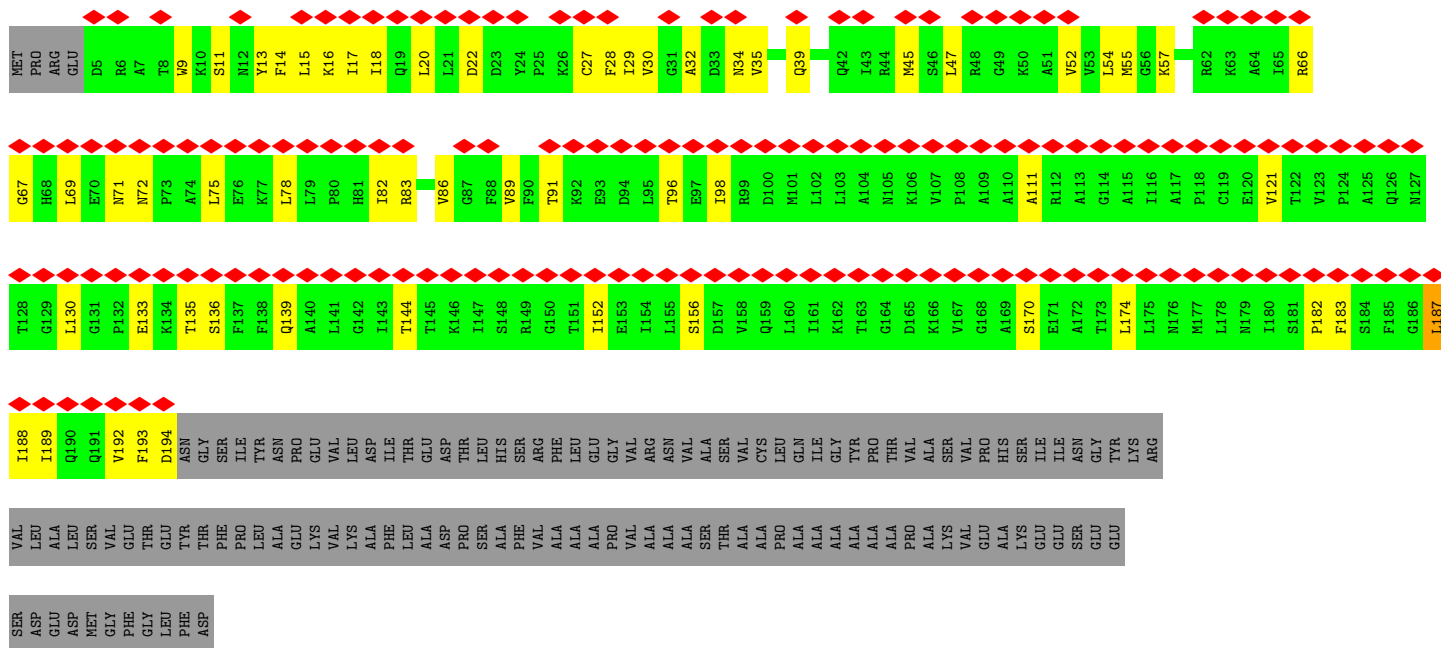
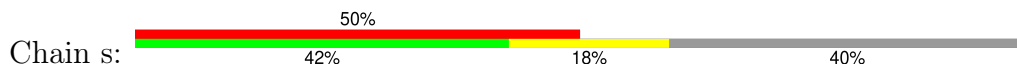


- Molecule 42: eL28

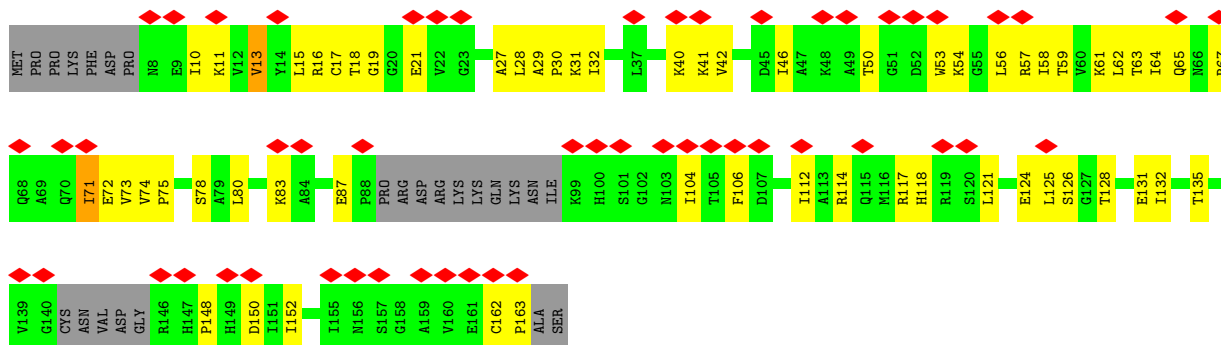




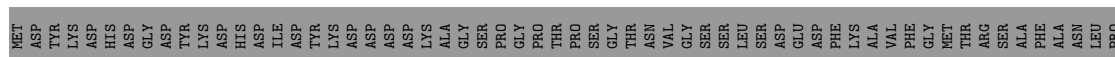
• Molecule 43: 60S acidic ribosomal protein P0

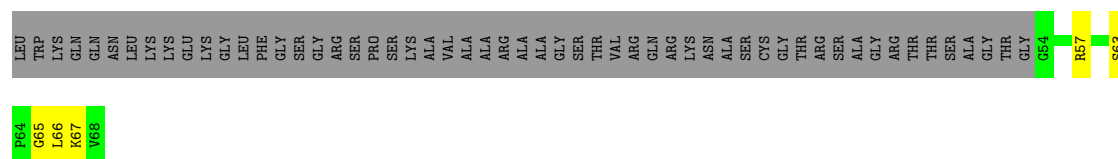


• Molecule 44: 60S ribosomal protein L12

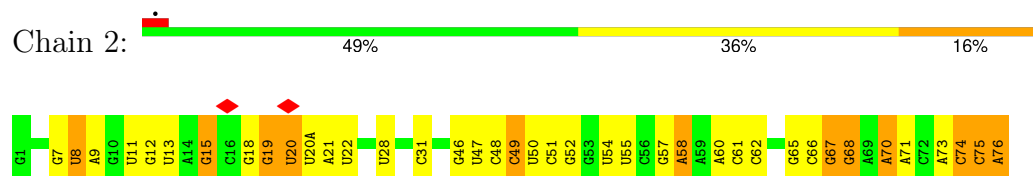


• Molecule 45: NC

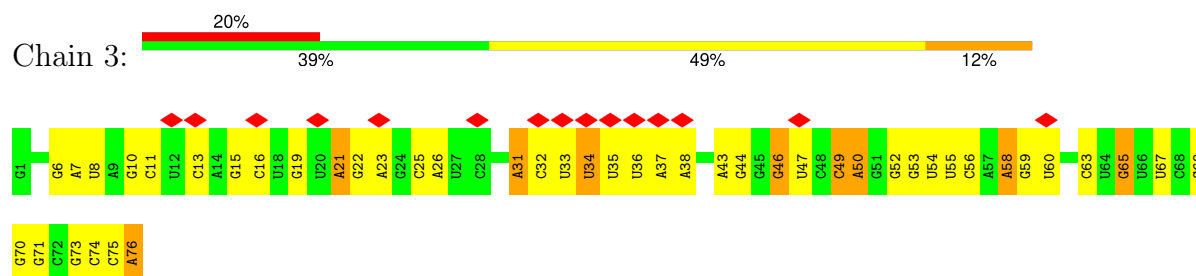




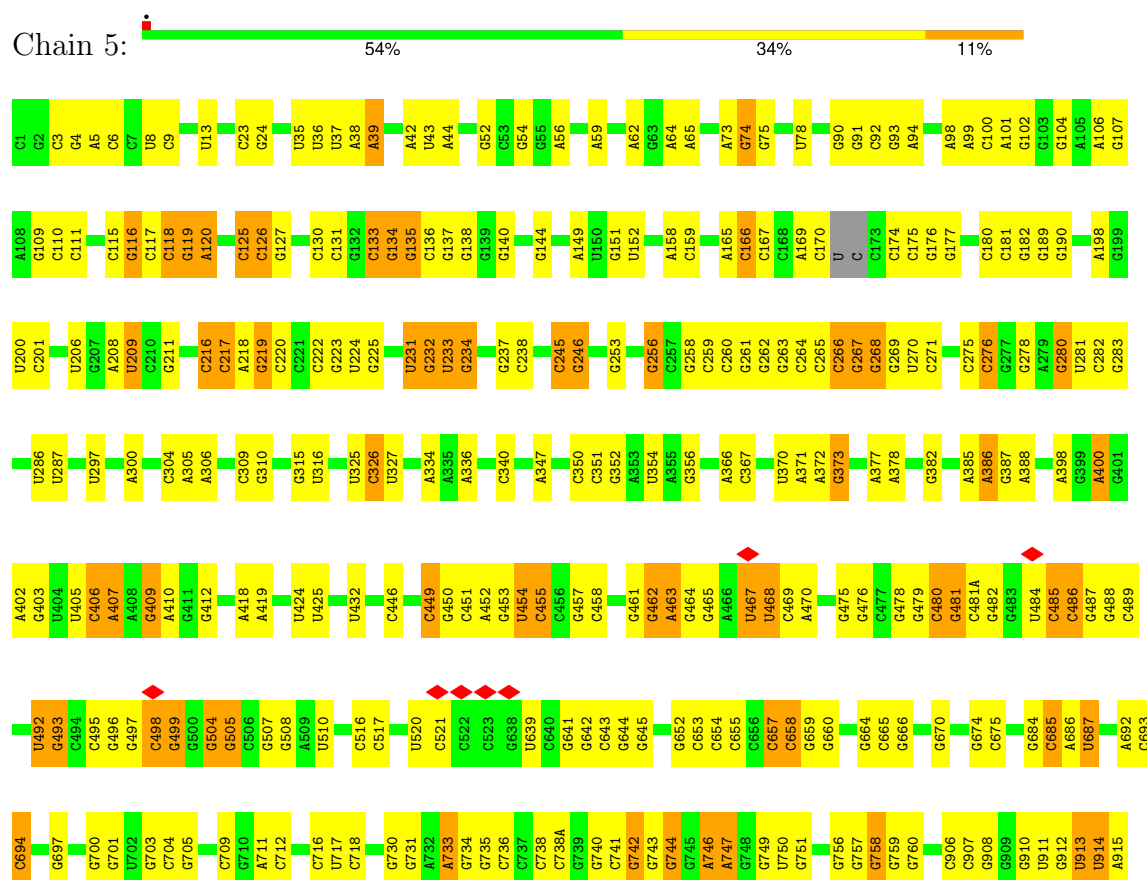
• Molecule 46: P\_tRNA



• Molecule 47: E\_tRNA

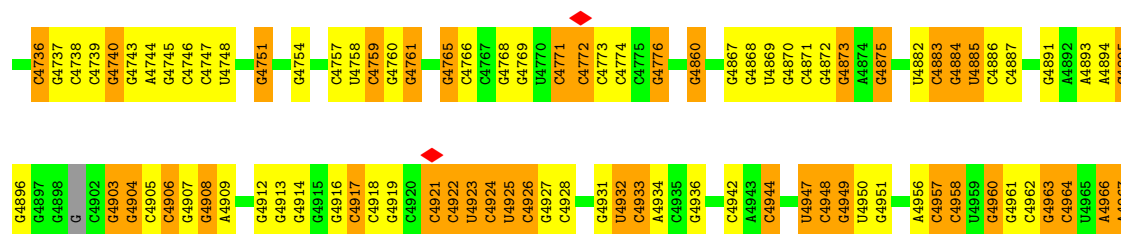


• Molecule 48: 28S\_rRNA



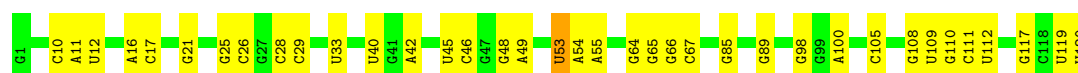
|       |       |       |       |       |       |       |       |       |        |        |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|--------|-------|-------|
| C2441 | G2314 | U2080 | A1998 | C1928 | U1834 | G1758 | G1633 | G1517 | G1432  | A1337  | C     | C916  |
| C2446 | G2327 | C2083 | A1999 | A1929 | G1835 | G1759 | A1634 | G1522 | G1433  | G1338  | G     | A917  |
| C2447 | G2328 | U2084 | G2000 | U1930 | G1836 | G1760 | A1635 | G1523 | G1434  | A1433  | U     | G918  |
| G2450 | U2329 | G2089 | G2001 | A1932 | A1837 | G1761 | A1638 | A1524 | G1437  | C1340  | C     | C922B |
| A2453 | A2332 | U2090 | G2002 | C1938 | G1840 | G1762 | G1641 | G1532 | U      | A1345  | C     | C924  |
| G2457 | G2333 | C2091 | G2003 | A1939 | C1841 | G1764 | G1645 | A1533 | U1440  | C1346  | C     | G925  |
| C2458 | G2336 | G2092 | G2004 | G1940 | G1842 | A1765 | A1646 | A1534 | C1441  | G1353  | C     | A929  |
| C2459 | C2337 | G2093 | G2005 | A1941 | G1846 | A1766 | G1654 | C1535 | C1442  | C1272  | C1271 | G930  |
| A2460 | G2348 | C2094 | U2008 | A1942 | A1847 | A1767 | G1654 | U1536 | A1443  | G1355  | G1273 | G931  |
| G2461 | G2349 | A2095 | A2009 | A1943 | G1855 | C1768 | C1661 | G1543 | G1444  | G1358  | A1274 | G932  |
| C2462 | U2350 | A2097 | C2011 | G1948 | C1856 | G1769 | C1662 | G1546 | U1445  | G1359  | G1275 | G933  |
| G2465 | C2351 | G2098 | U2015 | U1949 | C1857 | A1770 | C1663 | C1547 | C1446  | G1360  | G1276 | A943  |
| G2466 | U2352 | C2099 | C2016 | G1952 | A1858 | U1771 | G1666 | A1546 | C1449  | G1361  | G1277 | U945  |
| G2470 | U2353 | G2100 | A2017 | G1956 | C1859 | C1772 | C1667 | G1548 | G1450  | G1362  | C1278 | G959  |
| G2475 | G2360 | C2102 | C2018 | A1957 | U1861 | U1773 | A1669 | A1554 | G1451  | U1364  | G1279 | A960  |
| G2480 | A2363 | A2103 | C2019 | U1957 | G1862 | A1775 | U1672 | A1564 | G1453  | A1366  | G1280 | G961  |
| G2481 | G2370 | A2104 | G2020 | U1958 | G1865 | C1777 | U1673 | A1565 | G1455  | G1369  | G1281 | A964  |
| G2486 | A2376 | A2105 | G2021 | U1959 | U1866 | C1778 | C1676 | A1566 | C1456  | G1370  | G1282 | G965  |
| G2487 | G2380 | G2106 | A2024 | A1960 | A1867 | U1781 | U1677 | C1567 | G1457  | A1371  | G1283 | A966  |
| C2488 | A2381 | A2107 | G2025 | G1961 | U1868 | U1782 | U1683 | U1578 | C1461  | G1377  | G1284 | G967  |
| C2489 | G2382 | C2108 | A2026 | C1962 | G1869 | U1786 | A1684 | C1579 | G1466  | C1378  | U1285 | U945  |
| U2490 | G2383 | G2109 | G2027 | C1963 | C1870 | A1787 | G1685 | G1586 | G1467  | C1379  | G1286 | G959  |
| C2491 | G2389 | C2110 | C2028 | U1964 | A1871 | A1788 | G1686 | G1587 | C1468  | U1381  | G1287 | A964  |
| C2492 | G2394 | A2111 | A2029 | G1966 | G1877 | C1789 | U1687 | G1588 | C1469  | U1387  | G1288 | G965  |
| U2494 | A2395 | C2112 | C2030 | A1967 | U1878 | C1790 | G1688 | C1589 | C1472  | A1387  | G1289 | A966  |
| G2495 | G2399 | G2113 | U2032 | G1968 | C1879 | U1792 | U1689 | C1590 | C1473  | A1391  | G1290 | G967  |
| C2501 | G2407 | C2114 | A2033 | A1970 | U1882 | A1802 | C1694 | U1591 | G1474  | A1392  | G1291 | G968  |
| C2502 | U2408 | G2274 | G2046 | G1971 | G1890 | G1803 | U1695 | U1596 | G1475  | G1393  | G1292 | G969  |
| C2503 | U2409 | G2275 | A2047 | U1972 | A1891 | A1804 | C1696 | G1599 | G1476  | G1394  | G1293 | G970  |
| C2504 | C2277 | G2276 | G2048 | G1973 | A1892 | A1805 | U1726 | G1600 | C1477  | A1303  | G1294 | U971  |
| C2505 | G2278 | C2277 | U2054 | G1974 | G1895 | G1806 | U1731 | A1601 | C1478  | A1307  | G1295 | G971A |
| C2506 | U2412 | A2279 | G2055 | G1975 | A1896 | C1807 | G1732 | U1602 | C1479  | A1308  | G1296 | C972  |
| U2507 | G2413 | G2279 | G2056 | G1976 | A1897 | C1808 | G1733 | U1603 | C1480  | C1309  | G1297 | C973  |
| U2508 | G2414 | C2289 | G2062 | U1981 | G1898 | C1809 | G1734 | C1604 | C1481  | G1404  | G1298 | G978  |
| A2511 | G2422 | C2292 | C2063 | U1982 | U1906 | G1810 | U1735 | G1605 | G1482  | C1313  | G1299 | G981  |
| A2512 | A2423 | U2293 | G2064 | C1983 | G1915 | G1811 | G1736 | U1609 | G1483  | G1406  | G1299 | U982  |
| A2513 | G2424 | G2299 | G2065 | G1984 | U1918 | C1812 | G1741 | C1610 | G1484  | G1406A | G1299 | C983  |
| G2516 | U2425 | A2300 | C2066 | G1985 | G1919 | U1813 | A1742 | C1611 | C1411A | U1317  | G1299 | G1066 |
| A2517 | U2426 | G2301 | C2067 | A1986 | C1920 | U1814 | A1743 | G1612 | C1411B | G1316  | G1299 | G1067 |
| G2518 | G2427 | C2302 | U2068 | U1987 | G1921 | G1815 | U1744 | A1613 | C1411C | U1317  | G1299 | G1068 |
| U2519 | G2433 | U2304 | A2069 | C1988 | G1922 | G1816 | G1750 | G1624 | G1502  | U1320  | G1299 | G1069 |
| C2520 | G2438 | U2305 | U2070 | C1989 | G1923 | C1817 | G1753 | G1625 | G1503  | A1322  | G1299 | G1070 |
| G2521 | A2438 | G2306 | A2071 | G1990 | G1924 | G1818 | U1754 | G1626 | G1504  | A1326  | G1299 | C1071 |
| G2522 | G     | G2307 | U2072 | C1991 | G1925 | G1819 | C1755 | G1629 | G1510  | G1327  | G1299 | G1072 |
| G2528 | G     | A2313 | G2079 | U1997 | U1927 | A1825 | U1757 | A1630 | U1511  | G1328  | G1299 | G1073 |
|       |       |       |       |       |       | C1828 |       | A1632 | U1514  | A1420  | G     | G1076 |
|       |       |       |       |       |       | G1833 |       |       |        | A1333  |       | C1077 |
|       |       |       |       |       |       |       |       |       |        | A1333  |       | A1078 |
|       |       |       |       |       |       |       |       |       |        | A1333  |       | C1079 |

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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| C4592 | C4508 | U4419 | U4229 | U4120 | U3838 | G3740 | U3640 | A2833 | G2735 | U2639 | A2529 |
| C4596 | A4511 | U4420 | U4232 | G4121 | G3839 | G3743 | U3641 | C2834 | G2740 | G2640 | U2530 |
| U4597 | U4512 | A4421 | A4233 | G4122 | C3841 | G3744 | U3644 | A2835 | U2740 | A2641 | U2538 |
| A4605 | A4513 | U4423 | A4233 | A4127 | U3851 | U3745 | A3646 | U2837 | A2743 | C2539 | C2540 |
| G4606 | C4519 | G4427 | G4236 | A4128 | U3852 | A3748 | G3654 | G2842 | A2744 | G2647 |       |
| G4618 | G4520 | A4426 | A4244 | G4129 | U3853 | C3749 | G3654 | U2843 | A2745 | G2652 | U2543 |
| U4619 | C4429 | U4426 | G4245 | G4130 | U3856 | G3750 | G3654 | U2844 | G2750 | G2653 | A2544 |
| U4620 | U4521 | G4430 | U4340 | G4131 | A3856 | G3751 | U3657 | G2855 | G2751 | G2658 | U2545 |
| U4621 | U4522 | U4431 | A4248 | C4132 | A3856 | C3752 | U3657 | G2856 | G2752 | G2658 | U2546 |
| A4622 | C4523 | C4432 | C4133 | C4133 | A3860 | G3753 | A3662 | G2856 | G2753 | G2662 | C2547 |
| C4623 | C4524 | C4432 | C4134 | C4134 | A3861 | G3753 | A3662 | G2856 | G2754 | G2663 |       |
| C4624 | C4525 | C4432 | C4252 | G4135 | A3862 | G3759 | G3664 | G2861 |       |       | G2550 |
| C4625 | U4530 | G4439 | A4253 | G4136 | A3863 | A3759 | G3664 | G2862 | G2758 | U2666 | A2551 |
| A4626 | U4531 | G4440 | G4254 | C4148 | C3864 | C3761 | C3667 | G2869 | G2759 | C2667 | C2552 |
| U4627 | U4532 | U4442 | A4254 | C4149 | A3865 | U3762 | C3667 | U2869 | G2760 | G2668 | U2553 |
| U4628 | C4536 | C4443 | A4257 | G4152 | C3866 | A3763 | G3672 | A2871 | G2763 | C2670 | U2554 |
|       | C4537 | C4444 | C4258 | C4153 | A3867 | U3764 | C3673 | C2872 | A2764 | G2673 | C2555 |
| G4631 | C4538 | C4447 | C4259 | G4154 | G3868 | C3771 | G3684 | G2876 | A2765 | G2674 | C2556 |
| U4632 | U4539 | G4448 | C4261 | C4155 | C3869 | U3772 | C3685 | A2877 | G2766 | G2675 | G2557 |
| U4633 | U4543 | A4449 | C4262 | C4158 | A3871 | A3774 | G3686 | G2877 | C2768 |       | G2558 |
| A4635 | A4544 | U4450 | C4263 | G4161 | A3872 | A3775 | U3688 | A2882 | U2769 | G2686 | C2562 |
| U4636 | G4545 | U4452 | U4265 | C4162 | A3876 | G3776 | G3689 | U2886 | A2783 | U2687 | C2563 |
| G4637 | A4546 | C4456 | G4267 | U4163 | C3877 | G3777 | A3692 | U2887 | G2787 | C2688 | A2564 |
| C4653 | C4547 | U4457 | A4268 | A4170 | C3878 | C3782 | U3694 | C2890 | U2788 | C2689 | A2565 |
| C4654 | A4548 | C4458 | A4271 | G4173 | G3881 | A3785 | U3695 | G2898 | A2789 | G2690 | C2566 |
| C4655 | C4549 | U4459 | C4272 | U4174 | C3887 | U3786 | C3701 | U2900 | U2790 | U2691 | G2567 |
| A4656 | U4551 | U4460 | A4273 | C4181 | G3888 | G3787 | C3706 | C3598 | C2791 | G2694 | C2568 |
|       | U4552 | A4464 | U4275 | C4182 | G3889 | C3788 | C3707 | A3599 | G2792 | A2695 | C2569 |
| G4663 | C4553 | U4471 | A4281 | G4183 | C3893 | G3792 | C3708 | C3602 | G2793 | A2696 | U2570 |
| C4670 | A4559 | U4472 | G4291 | C4184 | A3894 | U3793 | U3709 | G3603 | G2796 | A2697 | C2571 |
| C4671 | C4560 | G4475 | A4292 | U4188 | G3895 | A3807 | G3710 | A3604 | C2797 | G2700 | C2583 |
| A4672 | U4564 | U4476 | U4293 | U4189 | C3896 | C3808 | A3711 | G3626 | G2703 |       | G2584 |
| G4676 | G4567 | G4477 | U4296 | U4190 | C3897 | C3809 | A3712 | G3627 | G2706 | C2587 | C2588 |
| U4682 | C4570 | U4478 | U4296 | C4191 | G3898 | G3810 | A3713 | A3605 | G2707 | C2589 | C2590 |
| A4691 | U4571 | A4487 | U4299 | U4194 | G3900 | G3811 | U3715 | G3619 | U2708 | A2601 |       |
| G4694 | C4573 | U4488 | U4302 | G4195 | A3901 | C3812 | C3716 | G3615 | C2709 | G2602 | C2603 |
| U4699 | U4574 | G4489 | C4303 | G4196 | A3902 | A3813 | A3717 | G3616 | G2710 | C2604 |       |
| A4700 | C4575 | U4491 | A4304 | G4197 | G3904 | G3815 | A3718 | G3617 | G2711 | G2711 |       |
|       | U4579 | U4492 | G4305 | C4198 | A3905 | A3816 | G3720 | G3618 | C2716 | C2716 | A2611 |
| C4582 | U4582 | U4493 | U4306 | A4203 | A3906 | A3817 | A3724 | G3619 | G2717 | G2717 | C2616 |
| C4583 | C4584 | G4494 | C4314 | U4208 | G3907 | U3818 | A3724 | A3624 | U2718 | G2617 | G2617 |
| U4585 | U4585 | U4498 | C4314 | U4208 | A3908 | G3819 | A3732 | G3625 | G2721 | U2626 | U2626 |
| G4718 | C4586 | U4500 | G4322 | U4111 | C3909 | U3822 | A3732 | G3626 | C2824 | C2627 | C2627 |
| C4720 | U4587 | C4504 | A4324 | U4112 | C3911 | G3823 | U3734 | G3627 | A2725 | U2628 | U2628 |
| A4724 | U4588 | C4505 | A4325 | U4113 | U3912 | A3824 | U3735 | A3635 | U2826 | G2726 | U2632 |
|       | A4589 | C4506 | G4326 | C4114 | U3915 | A3825 | A3736 | G3636 | G2827 | C2727 | U2632 |
|       | U4590 | U4227 | U4327 | G4115 | U3915 | A3830 | G3738 | U3637 | U2828 | C2733 | U2637 |
|       | U4591 | C4228 | G4228 | U4117 | U3920 | A3830 | G3739 | U3639 | U2829 | U2734 | C2638 |
|       |       |       |       | C4119 |       |       |       |       |       |       |       |



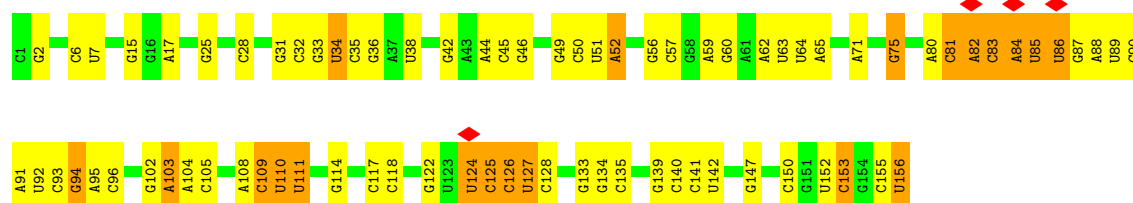
• Molecule 49: 5S\_rRNA

Chain 7: 69% 30%



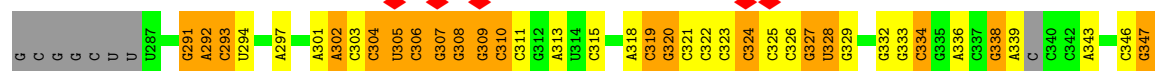
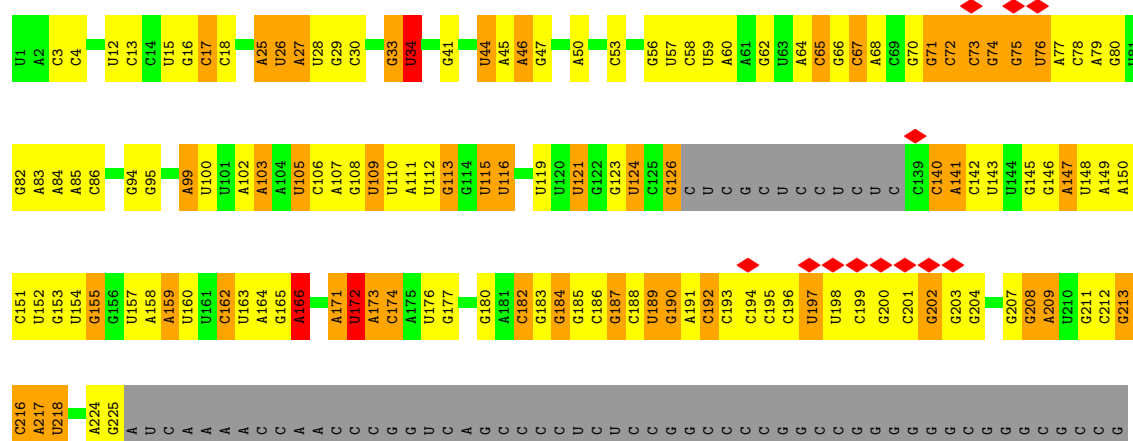
• Molecule 50: 5.8S\_rRNA

Chain 8: 49% 38% 13%

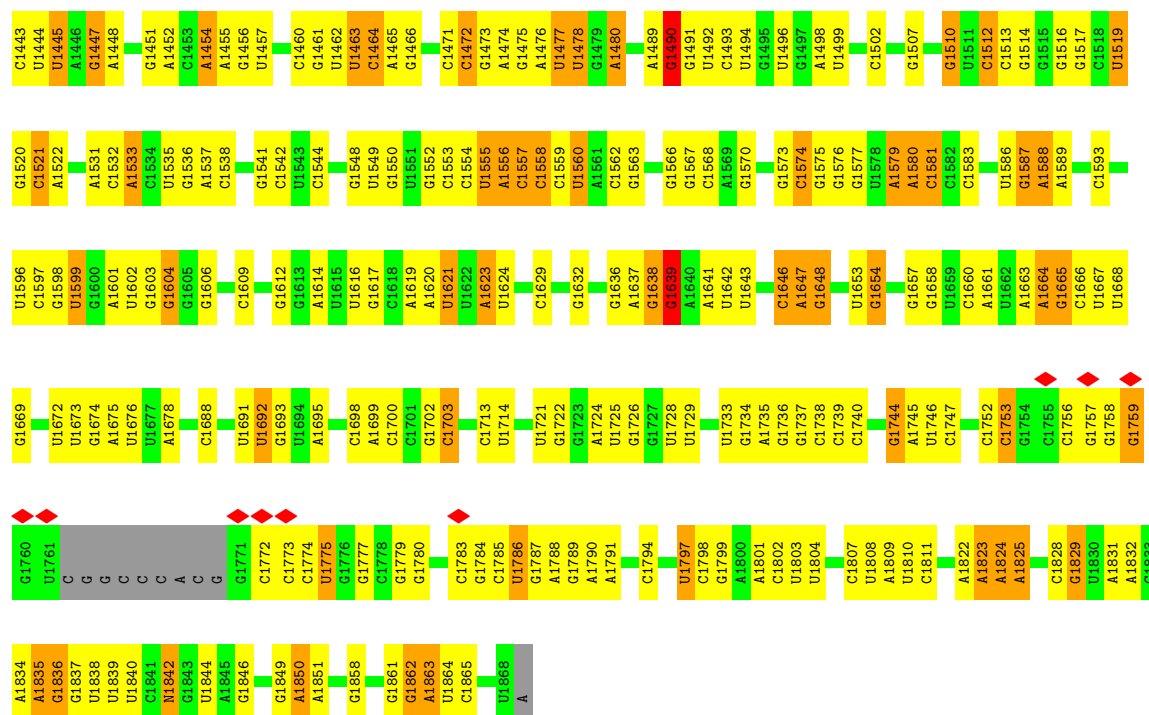


• Molecule 51: 18S\_rRNA

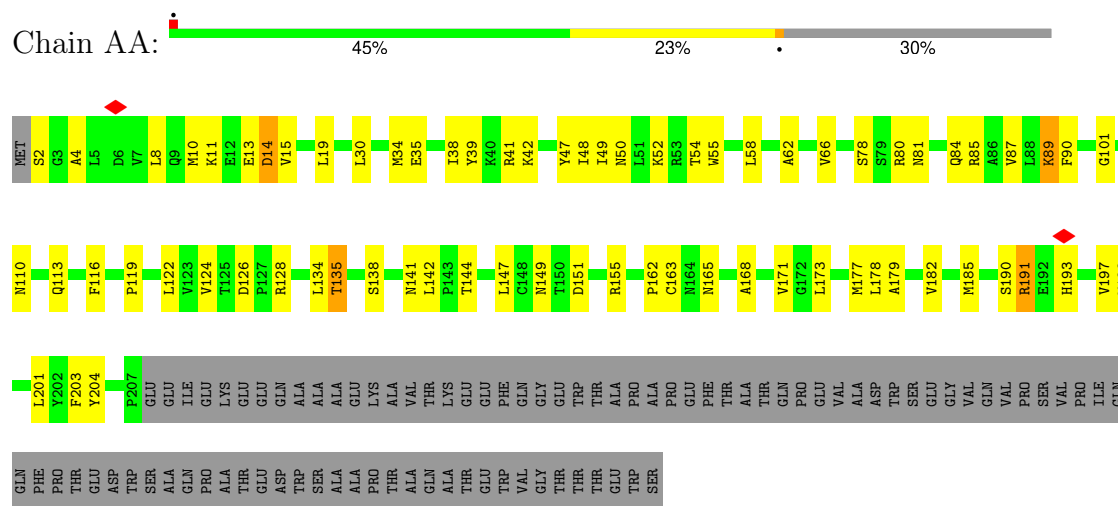
Chain 9: 39% 35% 16% 9%



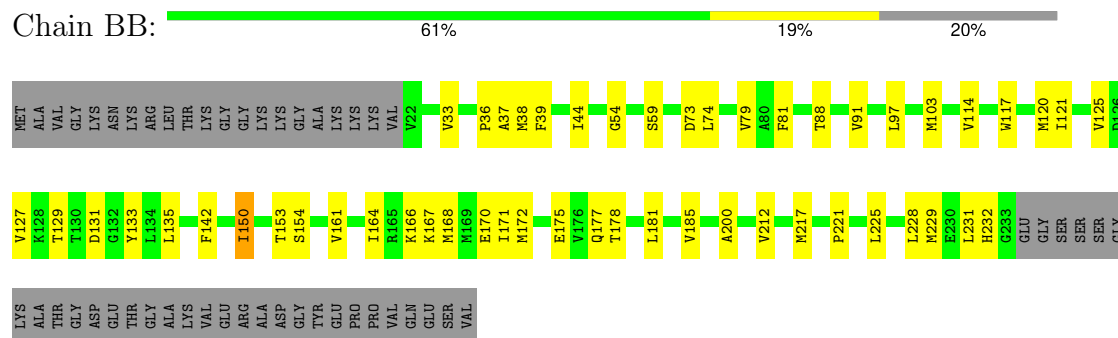




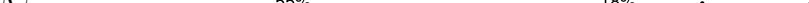
### • Molecule 52: uS2 (SA)

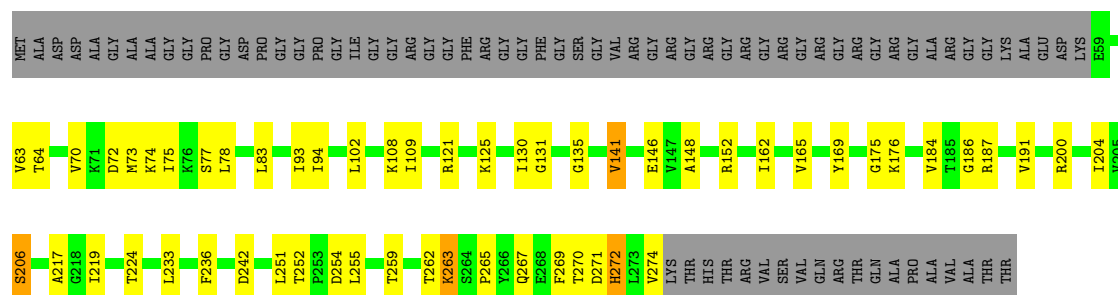


### • Molecule 53: eS1

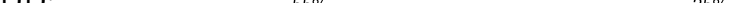


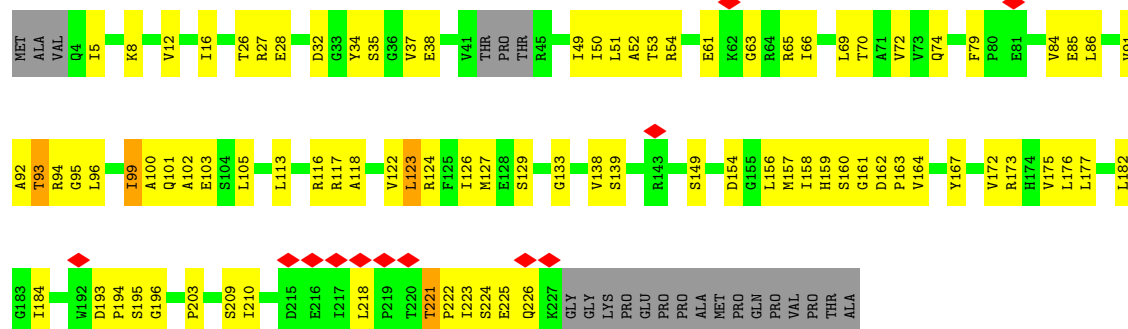
- Molecule 54: uS5

Chain CC:  55% 18% 26%



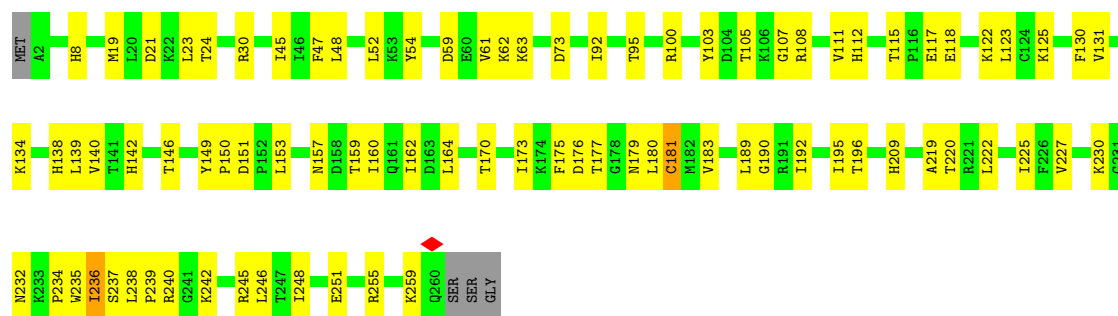
- Molecule 55: Ribosomal protein S3

Chain DD: 



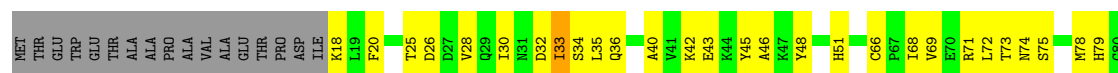
- Molecule 56: eS4 (S4 X isoform)

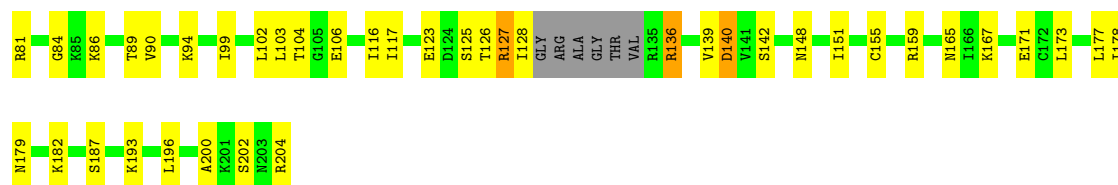
Chain EE: 67% 31% ..



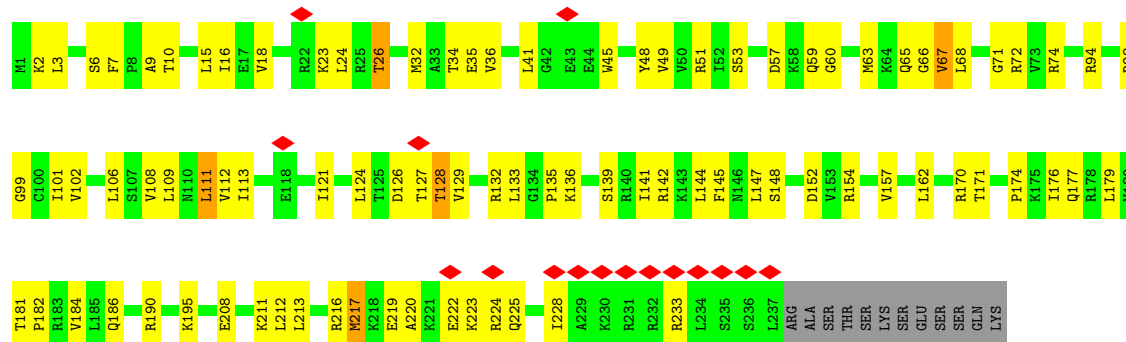
- Molecule 57: uS7

Chain FF: 

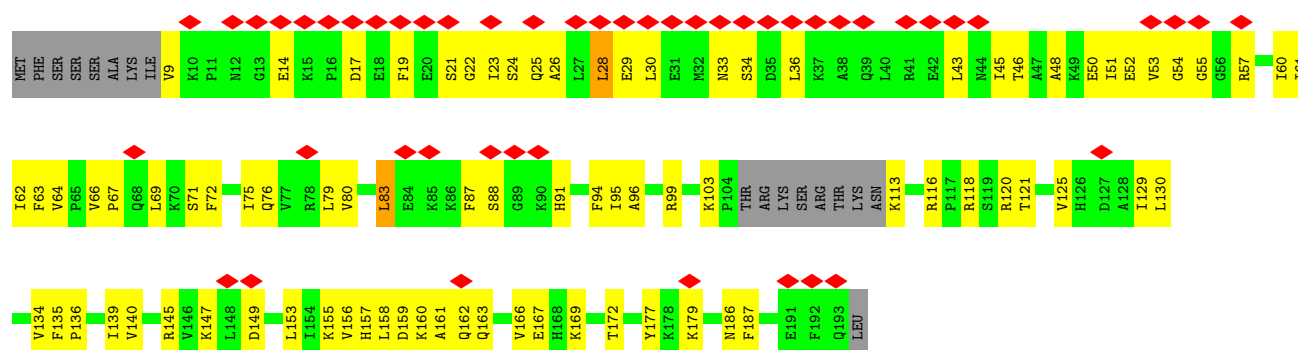




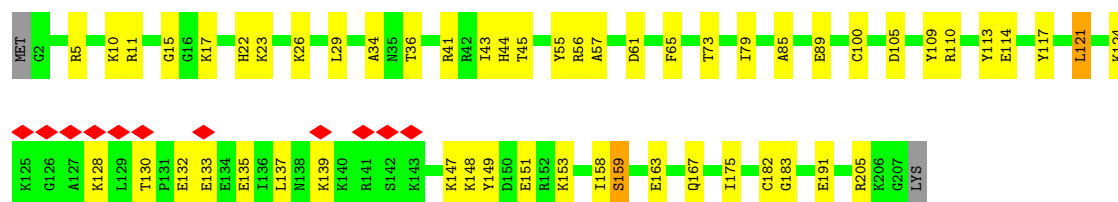
• Molecule 58: eS6



• Molecule 59: eS7

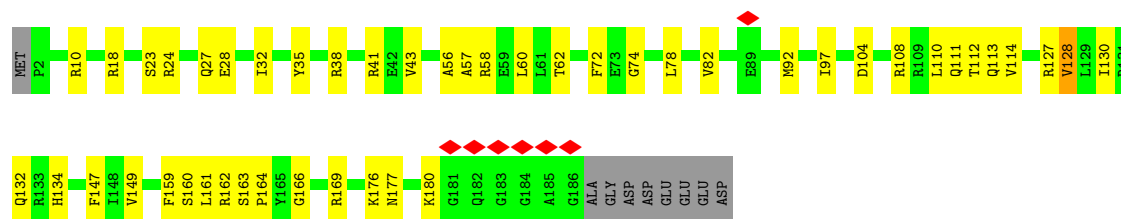


• Molecule 60: eS8

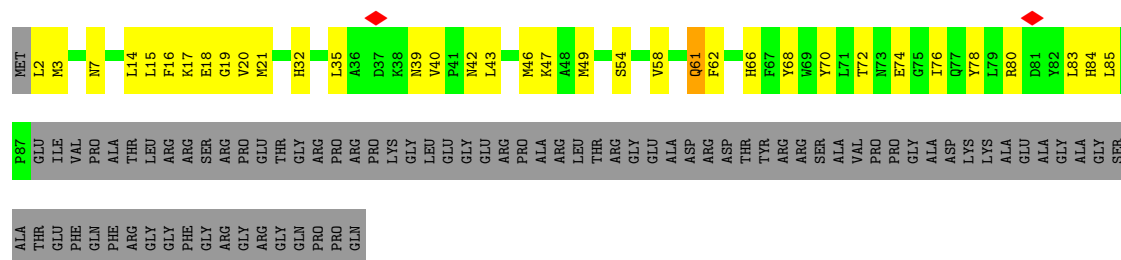
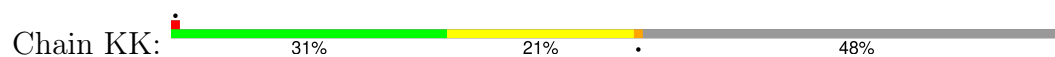


• Molecule 61: uS4





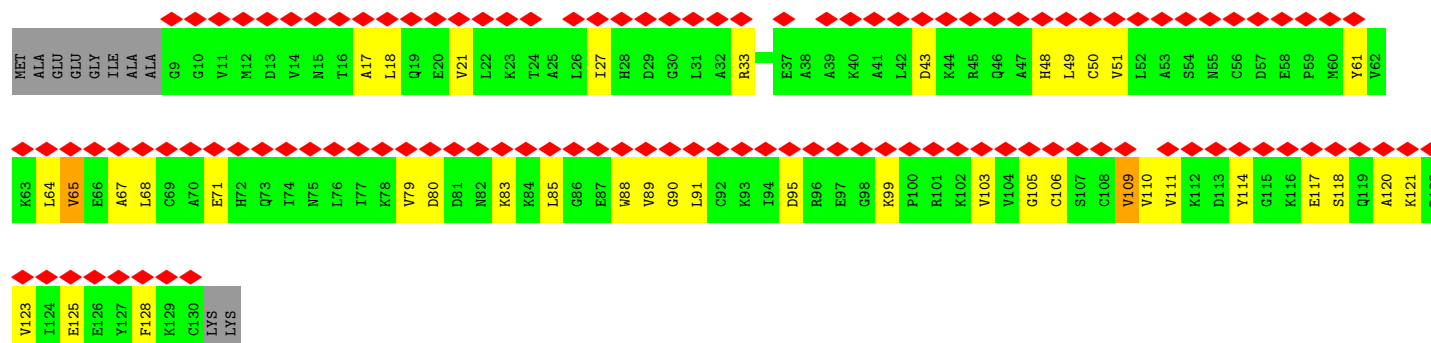
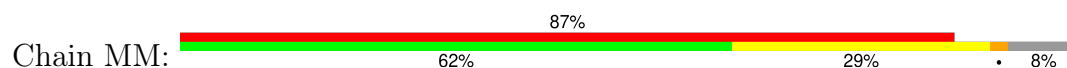
- Molecule 62: S10\_pectin domain-containing protein



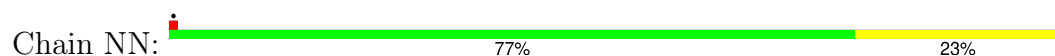
- Molecule 63: uS17

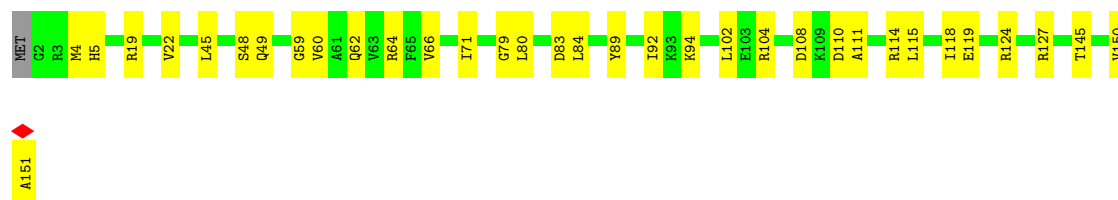


- Molecule 64: eS12

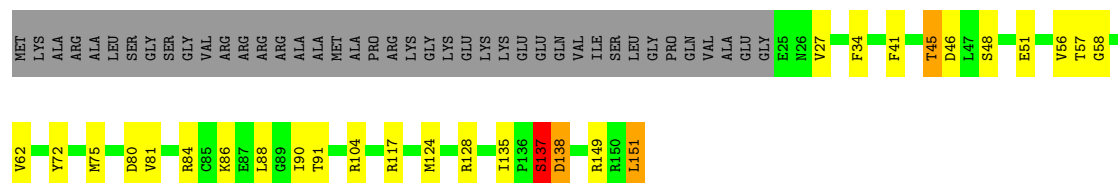


- Molecule 65: uS15

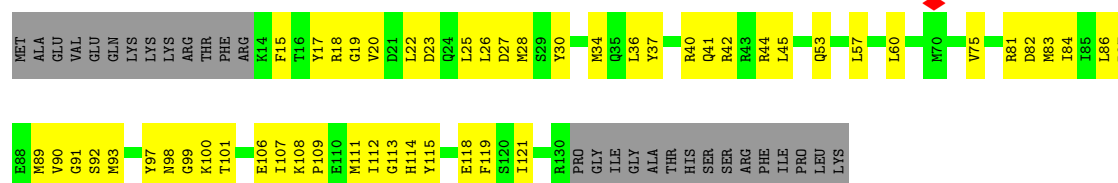




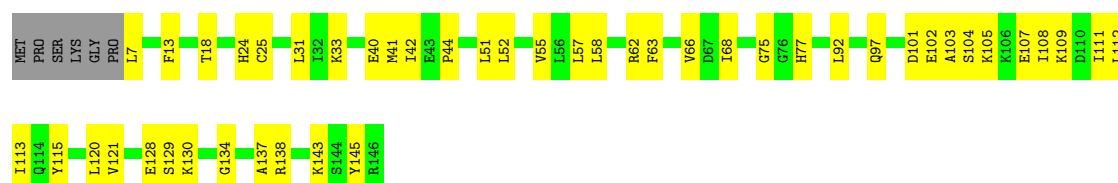
- Molecule 66: uS11



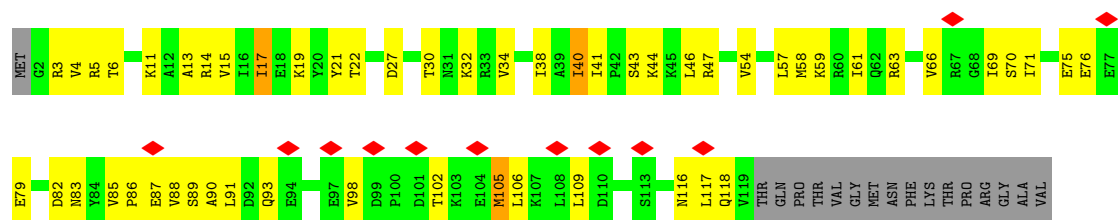
- Molecule 67: uS19



- Molecule 68: uS9

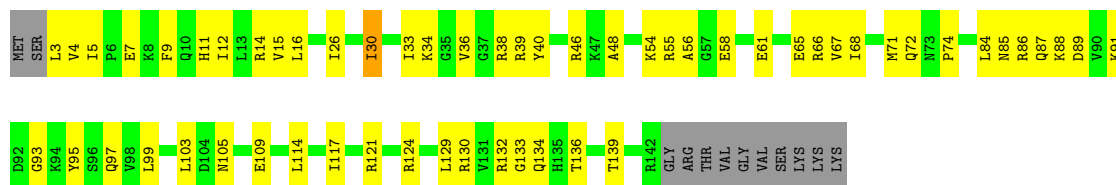


- Molecule 69: eS17



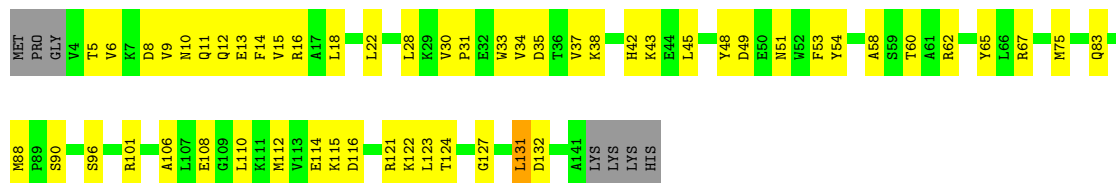
- Molecule 70: uS13

Chain SS:  55% 37% 8%



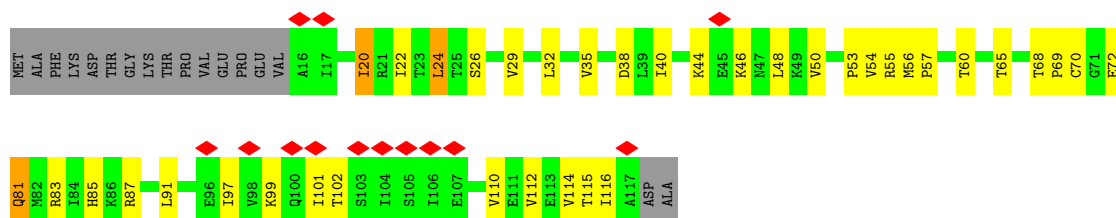
• Molecule 71: eS19

Chain TT:  58% 37% 5%



• Molecule 72: uS10

Chain UU:  11% 54% 29% 14%



• Molecule 73: eS21

Chain VV:  81% 17% 2%



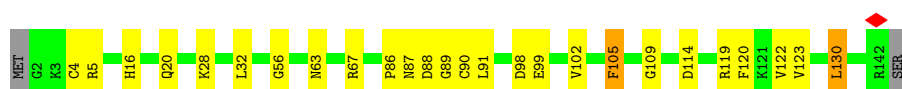
• Molecule 74: uS8

Chain WW:  82% 16% 2%



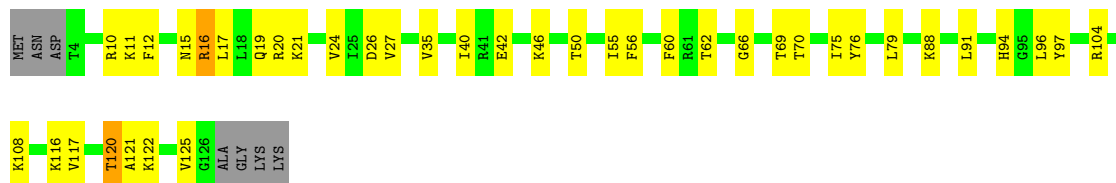
• Molecule 75: uS12

Chain XX:  80% 17% 3%

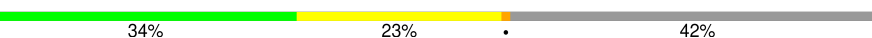


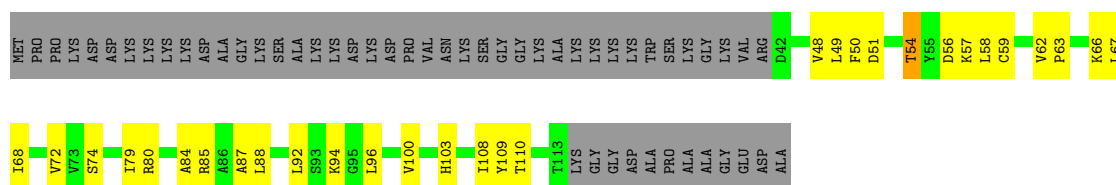
- Molecule 76: 40S ribosomal protein S24

Chain YY:  64% 29% 5%



- Molecule 77: eS25

Chain ZZ:  34% 23% 42%



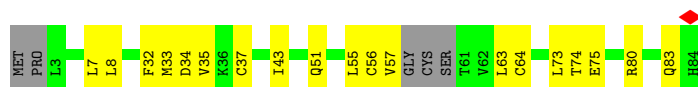
- Molecule 78: 40S ribosomal protein S26

Chain aa:  74% 10% 15%



- Molecule 79: eS27

Chain bb:  71% 23% 6%



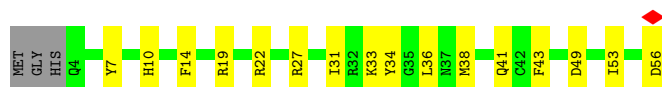
- Molecule 80: eS28

Chain cc:  49% 35% 12%



- Molecule 81: uS14

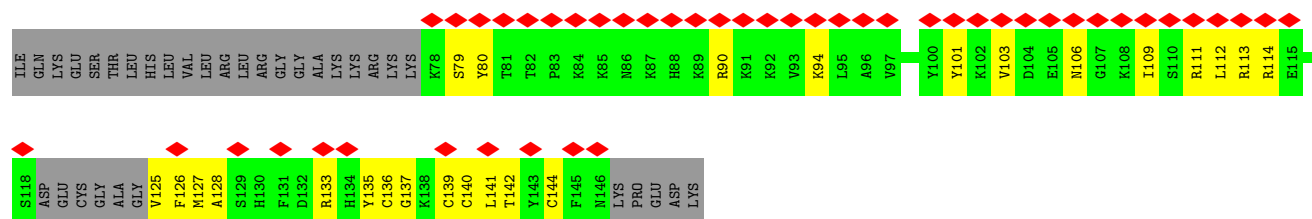
Chain dd:  66% 29% 5%



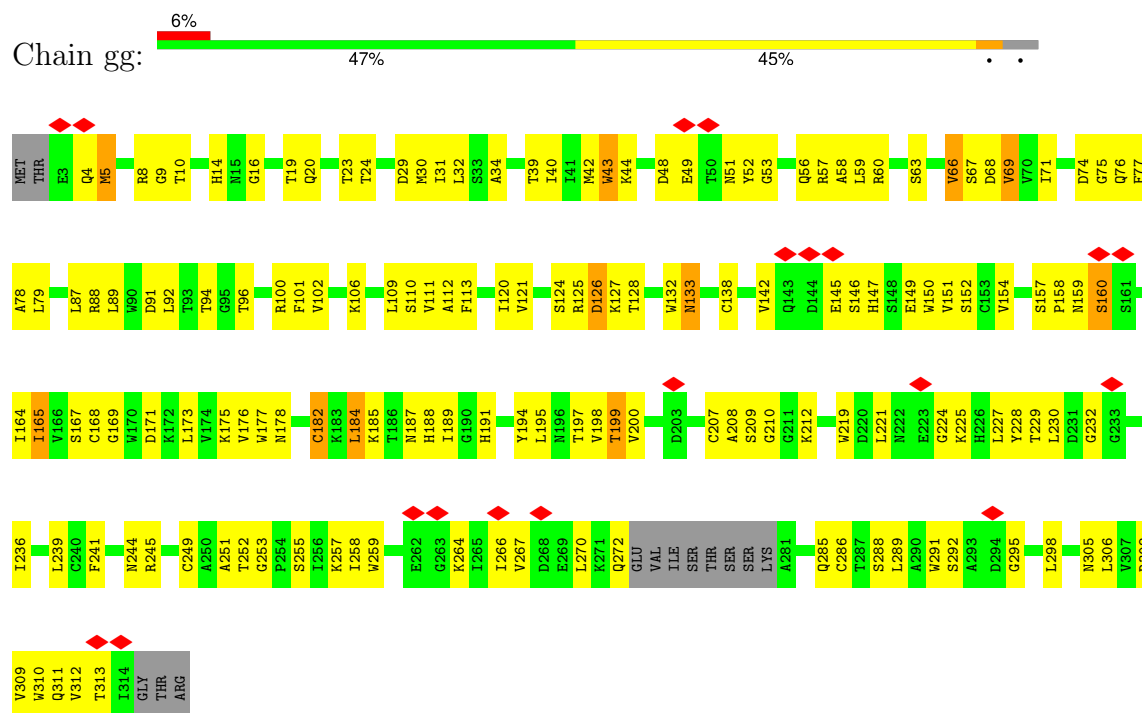
- Molecule 82: eS30



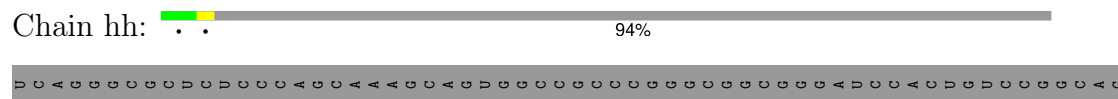
- Molecule 83: eS31



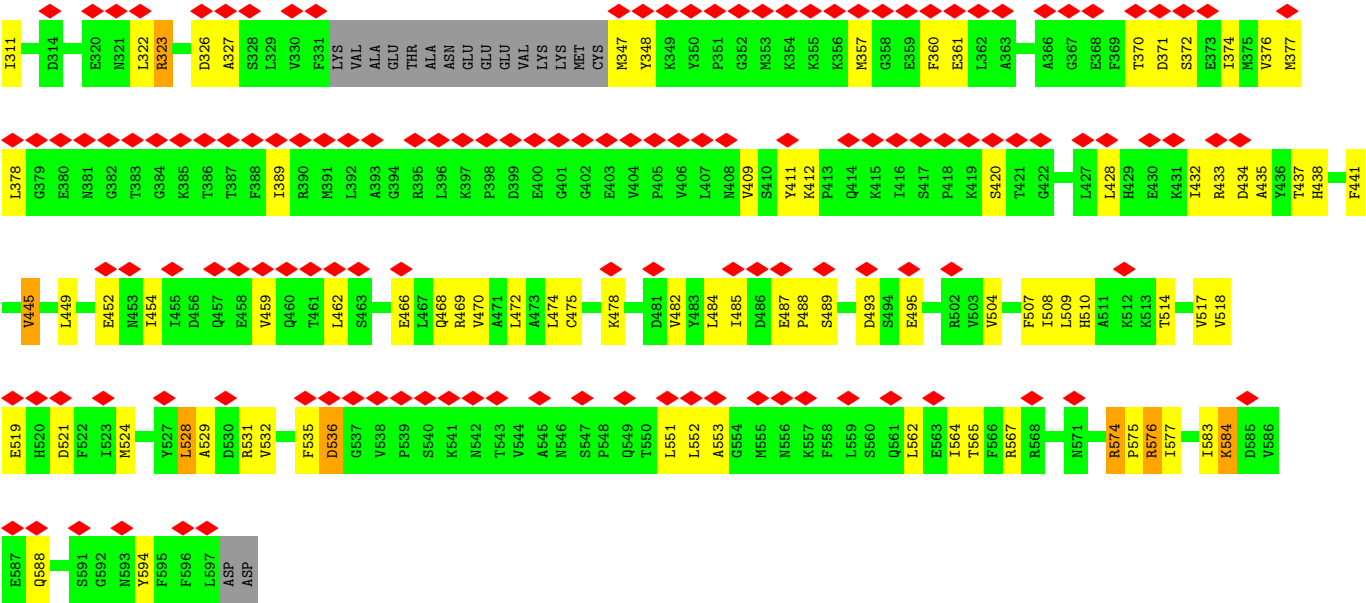
- Molecule 84: Receptor for Activated C Kinase 1 (RACK1)



- Molecule 85: mRNA







## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 90190                                   | 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 ( $e^-/\text{\AA}^2$ ) | 53.8                                    | Depositor |
| Minimum defocus (nm)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.050                                   | Depositor |
| Minimum map value                    | -0.013                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.002                                   | Depositor |
| Recommended contour level            | 0.005                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 396.0, 396.0, 396.0                     | wwPDB     |
| Map dimensions                       | 480, 480, 480                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.825, 0.825, 0.825                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, PSU, B9B, ZN, OMU, SF4, OMG, 4AC, A2M, OMC, B8N, ZVM, UY1, UR3, 5MC, G7M, 2MG, 6MZ, 1MA, MG

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

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 1   | A     | 0.33         | 0/1906  | 0.44        | 0/2556        |
| 2   | B     | 0.32         | 0/3216  | 0.46        | 0/4311        |
| 3   | C     | 0.33         | 0/2937  | 0.46        | 0/3946        |
| 4   | D     | 0.30         | 0/2407  | 0.44        | 0/3224        |
| 5   | E     | 0.28         | 0/1760  | 0.43        | 0/2362        |
| 6   | F     | 0.32         | 0/1911  | 0.43        | 0/2549        |
| 7   | G     | 0.30         | 0/1799  | 0.47        | 0/2424        |
| 8   | H     | 0.29         | 0/1535  | 0.42        | 0/2063        |
| 9   | I     | 0.29         | 0/1693  | 0.40        | 0/2260        |
| 10  | J     | 0.27         | 0/1359  | 0.46        | 0/1817        |
| 11  | L     | 0.30         | 0/1733  | 0.44        | 0/2316        |
| 12  | M     | 0.28         | 0/1158  | 0.37        | 0/1547        |
| 13  | N     | 0.35         | 0/1746  | 0.46        | 0/2338        |
| 14  | O     | 0.31         | 0/1653  | 0.48        | 0/2210        |
| 15  | P     | 0.33         | 0/1268  | 0.44        | 0/1700        |
| 16  | Q     | 0.34         | 0/1539  | 0.45        | 0/2054        |
| 17  | R     | 0.28         | 0/1518  | 0.41        | 0/2005        |
| 18  | S     | 0.32         | 0/1501  | 0.43        | 0/2012        |
| 19  | T     | 0.30         | 0/1326  | 0.41        | 0/1770        |
| 20  | U     | 0.29         | 0/814   | 0.53        | 0/1092        |
| 21  | V     | 0.30         | 0/987   | 0.43        | 0/1324        |
| 22  | W     | 0.32         | 0/541   | 0.41        | 0/720         |
| 23  | X     | 0.29         | 0/966   | 0.42        | 0/1301        |
| 24  | Y     | 0.29         | 0/1132  | 0.42        | 0/1504        |
| 25  | Z     | 0.39         | 0/1130  | 0.55        | 1/1507 (0.1%) |
| 26  | a     | 0.34         | 0/1191  | 0.44        | 0/1590        |
| 27  | b     | 0.33         | 0/619   | 0.48        | 0/818         |
| 28  | c     | 0.29         | 0/742   | 0.44        | 0/995         |
| 29  | d     | 0.29         | 0/846   | 0.42        | 0/1136        |
| 30  | e     | 0.34         | 0/1071  | 0.44        | 0/1429        |
| 31  | f     | 0.35         | 0/895   | 0.47        | 0/1198        |

| Mol | Chain | Bond lengths |                | Bond angles |               |
|-----|-------|--------------|----------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5       |
| 32  | g     | 0.29         | 0/916          | 0.39        | 0/1220        |
| 33  | h     | 0.29         | 0/1021         | 0.43        | 0/1348        |
| 34  | i     | 0.26         | 0/841          | 0.38        | 0/1112        |
| 35  | j     | 0.36         | 0/720          | 0.51        | 0/952         |
| 36  | k     | 0.41         | 0/565          | 0.62        | 0/750         |
| 37  | l     | 0.32         | 0/450          | 0.47        | 0/597         |
| 38  | m     | 0.30         | 0/427          | 0.39        | 0/564         |
| 39  | n     | 0.34         | 0/223          | 0.46        | 0/284         |
| 40  | o     | 0.30         | 0/855          | 0.41        | 0/1128        |
| 41  | p     | 0.31         | 0/718          | 0.46        | 0/953         |
| 42  | r     | 0.33         | 0/1017         | 0.43        | 0/1364        |
| 43  | s     | 0.23         | 0/1483         | 0.41        | 0/2000        |
| 44  | t     | 0.22         | 0/1071         | 0.48        | 0/1444        |
| 45  | 1     | 0.26         | 0/129          | 0.40        | 0/173         |
| 46  | 2     | 0.27         | 0/1805         | 0.43        | 0/2809        |
| 47  | 3     | 0.23         | 0/1777         | 0.45        | 0/2763        |
| 48  | 5     | 0.41         | 4/82331 (0.0%) | 0.46        | 0/128398      |
| 49  | 7     | 0.37         | 0/2858         | 0.40        | 0/4455        |
| 50  | 8     | 0.40         | 0/3675         | 0.43        | 0/5725        |
| 51  | 9     | 0.35         | 6/38943 (0.0%) | 0.46        | 0/60686       |
| 52  | AA    | 0.29         | 0/1661         | 0.44        | 0/2259        |
| 53  | BB    | 0.28         | 0/1749         | 0.45        | 1/2340 (0.0%) |
| 54  | CC    | 0.28         | 0/1710         | 0.43        | 0/2312        |
| 55  | DD    | 0.26         | 0/1749         | 0.45        | 0/2350        |
| 56  | EE    | 0.27         | 0/2101         | 0.48        | 0/2828        |
| 57  | FF    | 0.26         | 0/1461         | 0.43        | 0/1961        |
| 58  | GG    | 0.29         | 0/1946         | 0.49        | 0/2590        |
| 59  | HH    | 0.25         | 0/1447         | 0.49        | 0/1939        |
| 60  | II    | 0.27         | 0/1715         | 0.45        | 0/2287        |
| 61  | JJ    | 0.26         | 0/1550         | 0.43        | 0/2069        |
| 62  | KK    | 0.31         | 0/752          | 0.54        | 0/1014        |
| 63  | LL    | 0.29         | 0/1143         | 0.43        | 0/1529        |
| 64  | MM    | 0.23         | 0/949          | 0.44        | 0/1274        |
| 65  | NN    | 0.26         | 0/1232         | 0.41        | 0/1656        |
| 66  | OO    | 0.36         | 0/969          | 0.61        | 1/1298 (0.1%) |
| 67  | PP    | 0.25         | 0/986          | 0.47        | 0/1316        |
| 68  | QQ    | 0.27         | 0/1134         | 0.45        | 0/1517        |
| 69  | RR    | 0.26         | 0/973          | 0.45        | 0/1304        |
| 70  | SS    | 0.25         | 0/1180         | 0.40        | 0/1581        |
| 71  | TT    | 0.25         | 0/1093         | 0.42        | 0/1466        |
| 72  | UU    | 0.25         | 0/817          | 0.44        | 0/1097        |
| 73  | VV    | 0.27         | 0/623          | 0.42        | 0/833         |
| 74  | WW    | 0.29         | 0/1051         | 0.45        | 0/1406        |

| Mol | Chain | Bond lengths |                  | Bond angles |                 |
|-----|-------|--------------|------------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5         |
| 75  | XX    | 0.28         | 0/1116           | 0.42        | 0/1490          |
| 76  | YY    | 0.25         | 0/1023           | 0.44        | 0/1359          |
| 77  | ZZ    | 0.25         | 0/580            | 0.41        | 0/780           |
| 78  | aa    | 0.28         | 0/794            | 0.46        | 0/1065          |
| 79  | bb    | 0.26         | 0/640            | 0.45        | 0/856           |
| 80  | cc    | 0.26         | 0/481            | 0.48        | 0/643           |
| 81  | dd    | 0.27         | 0/455            | 0.48        | 0/603           |
| 82  | ee    | 0.25         | 0/381            | 0.41        | 0/498           |
| 83  | ff    | 0.22         | 0/538            | 0.43        | 0/713           |
| 84  | gg    | 0.24         | 0/2427           | 0.48        | 0/3303          |
| 85  | hh    | 0.33         | 0/264            | 0.47        | 0/409           |
| 86  | ii    | 0.26         | 0/3333           | 0.47        | 0/4483          |
| 87  | jj    | 0.22         | 0/4644           | 0.42        | 0/6272          |
| All | All   | 0.35         | 10/233391 (0.0%) | 0.45        | 3/341503 (0.0%) |

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 |
|-----|-------|---------------------|---------------------|
| 57  | FF    | 0                   | 1                   |
| 63  | LL    | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (10) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 48  | 5     | 3785 | A2M  | O3'-P | 6.06 | 1.62        | 1.56     |
| 48  | 5     | 2787 | A2M  | O3'-P | 5.54 | 1.61        | 1.56     |
| 51  | 9     | 1442 | OMU  | O3'-P | 5.30 | 1.61        | 1.56     |
| 51  | 9     | 668  | A2M  | O3'-P | 5.13 | 1.61        | 1.56     |
| 51  | 9     | 1031 | A2M  | O3'-P | 5.12 | 1.61        | 1.56     |
| 51  | 9     | 27   | A2M  | O3'-P | 5.08 | 1.61        | 1.56     |
| 51  | 9     | 484  | A2M  | O3'-P | 5.07 | 1.61        | 1.56     |
| 51  | 9     | 1678 | A2M  | O3'-P | 5.04 | 1.61        | 1.56     |
| 48  | 5     | 3825 | A2M  | O3'-P | 5.04 | 1.61        | 1.56     |
| 48  | 5     | 3760 | A2M  | O3'-P | 5.03 | 1.61        | 1.56     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 66  | OO    | 137 | SER  | N-CA-C | -6.03 | 103.66      | 111.02   |
| 25  | Z     | 26  | VAL  | N-CA-C | -5.90 | 107.06      | 112.96   |
| 53  | BB    | 150 | ILE  | N-CA-C | -5.35 | 107.21      | 111.81   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 57  | FF    | 136 | ARG  | Sidechain |
| 63  | LL    | 118 | ARG  | Sidechain |

## 5.2 Too-close contacts [i](#)

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     | 1868  | 0        | 1959     | 26      | 0            |
| 2   | B     | 3148  | 0        | 3267     | 48      | 0            |
| 3   | C     | 2883  | 0        | 3053     | 41      | 0            |
| 4   | D     | 2361  | 0        | 2395     | 53      | 0            |
| 5   | E     | 1726  | 0        | 1869     | 29      | 0            |
| 6   | F     | 1875  | 0        | 1995     | 26      | 0            |
| 7   | G     | 1768  | 0        | 1891     | 42      | 0            |
| 8   | H     | 1516  | 0        | 1597     | 24      | 0            |
| 9   | I     | 1655  | 0        | 1704     | 24      | 0            |
| 10  | J     | 1336  | 0        | 1375     | 28      | 0            |
| 11  | L     | 1702  | 0        | 1820     | 25      | 0            |
| 12  | M     | 1137  | 0        | 1211     | 18      | 0            |
| 13  | N     | 1701  | 0        | 1749     | 31      | 0            |
| 14  | O     | 1621  | 0        | 1770     | 35      | 0            |
| 15  | P     | 1242  | 0        | 1274     | 12      | 0            |
| 16  | Q     | 1515  | 0        | 1634     | 23      | 0            |
| 17  | R     | 1502  | 0        | 1659     | 13      | 0            |
| 18  | S     | 1462  | 0        | 1508     | 19      | 0            |
| 19  | T     | 1298  | 0        | 1366     | 17      | 0            |
| 20  | U     | 800   | 0        | 825      | 37      | 0            |
| 21  | V     | 973   | 0        | 1034     | 7       | 0            |
| 22  | W     | 528   | 0        | 541      | 7       | 0            |
| 23  | X     | 949   | 0        | 1016     | 12      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24  | Y     | 1115  | 0        | 1205     | 14      | 0            |
| 25  | Z     | 1107  | 0        | 1182     | 26      | 0            |
| 26  | a     | 1162  | 0        | 1209     | 31      | 0            |
| 27  | b     | 609   | 0        | 650      | 11      | 0            |
| 28  | c     | 732   | 0        | 767      | 11      | 0            |
| 29  | d     | 833   | 0        | 891      | 14      | 0            |
| 30  | e     | 1053  | 0        | 1147     | 15      | 0            |
| 31  | f     | 876   | 0        | 912      | 10      | 0            |
| 32  | g     | 906   | 0        | 998      | 10      | 0            |
| 33  | h     | 1013  | 0        | 1147     | 20      | 0            |
| 34  | i     | 830   | 0        | 916      | 4       | 0            |
| 35  | j     | 705   | 0        | 737      | 13      | 0            |
| 36  | k     | 559   | 0        | 624      | 15      | 0            |
| 37  | l     | 438   | 0        | 469      | 10      | 0            |
| 38  | m     | 421   | 0        | 454      | 4       | 0            |
| 39  | n     | 222   | 0        | 264      | 4       | 0            |
| 40  | o     | 842   | 0        | 912      | 8       | 0            |
| 41  | p     | 708   | 0        | 756      | 7       | 0            |
| 42  | r     | 1001  | 0        | 1060     | 21      | 0            |
| 43  | s     | 1461  | 0        | 1524     | 55      | 0            |
| 44  | t     | 1059  | 0        | 1106     | 51      | 0            |
| 45  | 1     | 125   | 0        | 117      | 5       | 0            |
| 46  | 2     | 1616  | 0        | 823      | 30      | 0            |
| 47  | 3     | 1593  | 0        | 811      | 35      | 0            |
| 48  | 5     | 75735 | 0        | 38351    | 1073    | 0            |
| 49  | 7     | 2558  | 0        | 1296     | 19      | 0            |
| 50  | 8     | 3315  | 0        | 1685     | 66      | 0            |
| 51  | 9     | 36134 | 0        | 18306    | 822     | 0            |
| 52  | AA    | 1624  | 0        | 1634     | 57      | 0            |
| 53  | BB    | 1722  | 0        | 1794     | 40      | 0            |
| 54  | CC    | 1674  | 0        | 1759     | 37      | 0            |
| 55  | DD    | 1723  | 0        | 1815     | 81      | 0            |
| 56  | EE    | 2059  | 0        | 2164     | 65      | 0            |
| 57  | FF    | 1441  | 0        | 1493     | 60      | 0            |
| 58  | GG    | 1923  | 0        | 2089     | 87      | 0            |
| 59  | HH    | 1425  | 0        | 1504     | 74      | 0            |
| 60  | II    | 1686  | 0        | 1772     | 47      | 0            |
| 61  | JJ    | 1525  | 0        | 1640     | 35      | 0            |
| 62  | KK    | 729   | 0        | 742      | 34      | 0            |
| 63  | LL    | 1123  | 0        | 1186     | 20      | 0            |
| 64  | MM    | 939   | 0        | 967      | 41      | 0            |
| 65  | NN    | 1208  | 0        | 1294     | 27      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 66  | OO    | 957   | 0        | 982      | 36      | 0            |
| 67  | PP    | 968   | 0        | 1016     | 43      | 0            |
| 68  | QQ    | 1117  | 0        | 1185     | 44      | 0            |
| 69  | RR    | 962   | 0        | 1013     | 57      | 0            |
| 70  | SS    | 1162  | 0        | 1221     | 51      | 0            |
| 71  | TT    | 1075  | 0        | 1103     | 45      | 0            |
| 72  | UU    | 807   | 0        | 874      | 32      | 0            |
| 73  | VV    | 617   | 0        | 622      | 11      | 0            |
| 74  | WW    | 1034  | 0        | 1080     | 19      | 0            |
| 75  | XX    | 1098  | 0        | 1167     | 24      | 0            |
| 76  | YY    | 1006  | 0        | 1078     | 34      | 0            |
| 77  | ZZ    | 574   | 0        | 627      | 27      | 0            |
| 78  | aa    | 781   | 0        | 828      | 10      | 0            |
| 79  | bb    | 628   | 0        | 650      | 17      | 0            |
| 80  | cc    | 479   | 0        | 507      | 25      | 0            |
| 81  | dd    | 445   | 0        | 438      | 16      | 0            |
| 82  | ee    | 380   | 0        | 417      | 14      | 0            |
| 83  | ff    | 527   | 0        | 543      | 30      | 0            |
| 84  | gg    | 2371  | 0        | 2324     | 137     | 0            |
| 85  | hh    | 236   | 0        | 119      | 0       | 0            |
| 86  | ii    | 3280  | 0        | 3326     | 118     | 0            |
| 87  | jj    | 4558  | 0        | 4679     | 172     | 0            |
| 88  | 2     | 2     | 0        | 0        | 0       | 0            |
| 88  | 5     | 221   | 0        | 0        | 0       | 0            |
| 88  | 7     | 6     | 0        | 0        | 0       | 0            |
| 88  | 8     | 2     | 0        | 0        | 0       | 0            |
| 88  | 9     | 64    | 0        | 0        | 0       | 0            |
| 88  | A     | 2     | 0        | 0        | 0       | 0            |
| 88  | EE    | 1     | 0        | 0        | 0       | 0            |
| 88  | I     | 2     | 0        | 0        | 0       | 0            |
| 88  | LL    | 1     | 0        | 0        | 0       | 0            |
| 88  | N     | 1     | 0        | 0        | 0       | 0            |
| 88  | OO    | 1     | 0        | 0        | 0       | 0            |
| 88  | P     | 1     | 0        | 0        | 0       | 0            |
| 88  | V     | 1     | 0        | 0        | 0       | 0            |
| 88  | XX    | 1     | 0        | 0        | 0       | 0            |
| 88  | a     | 1     | 0        | 0        | 0       | 0            |
| 88  | e     | 1     | 0        | 0        | 0       | 0            |
| 88  | f     | 1     | 0        | 0        | 0       | 0            |
| 88  | g     | 1     | 0        | 0        | 0       | 0            |
| 88  | hh    | 1     | 0        | 0        | 0       | 0            |
| 88  | o     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 89  | aa    | 1      | 0        | 0        | 0       | 0            |
| 89  | dd    | 1      | 0        | 0        | 0       | 0            |
| 89  | ff    | 1      | 0        | 0        | 0       | 0            |
| 89  | g     | 1      | 0        | 0        | 0       | 0            |
| 89  | j     | 1      | 0        | 0        | 0       | 0            |
| 89  | m     | 1      | 0        | 0        | 0       | 0            |
| 89  | o     | 1      | 0        | 0        | 0       | 0            |
| 89  | p     | 1      | 0        | 0        | 0       | 0            |
| 90  | ii    | 27     | 0        | 0        | 0       | 0            |
| 91  | jj    | 16     | 0        | 0        | 4       | 0            |
| 92  | 5     | 723    | 0        | 0        | 30      | 0            |
| 92  | 7     | 13     | 0        | 0        | 3       | 0            |
| 92  | 8     | 8      | 0        | 0        | 0       | 0            |
| 92  | 9     | 173    | 0        | 0        | 12      | 0            |
| 92  | A     | 6      | 0        | 0        | 0       | 0            |
| 92  | B     | 2      | 0        | 0        | 0       | 0            |
| 92  | C     | 1      | 0        | 0        | 0       | 0            |
| 92  | F     | 1      | 0        | 0        | 0       | 0            |
| 92  | I     | 1      | 0        | 0        | 0       | 0            |
| 92  | II    | 1      | 0        | 0        | 0       | 0            |
| 92  | L     | 1      | 0        | 0        | 0       | 0            |
| 92  | N     | 4      | 0        | 0        | 0       | 0            |
| 92  | OO    | 1      | 0        | 0        | 0       | 0            |
| 92  | Q     | 1      | 0        | 0        | 0       | 0            |
| 92  | R     | 1      | 0        | 0        | 0       | 0            |
| 92  | V     | 2      | 0        | 0        | 0       | 0            |
| 92  | X     | 2      | 0        | 0        | 0       | 0            |
| 92  | XX    | 1      | 0        | 0        | 0       | 0            |
| 92  | a     | 5      | 0        | 0        | 0       | 0            |
| 92  | aa    | 1      | 0        | 0        | 0       | 0            |
| 92  | e     | 5      | 0        | 0        | 0       | 0            |
| 92  | ii    | 2      | 0        | 0        | 1       | 0            |
| 92  | j     | 1      | 0        | 0        | 0       | 0            |
| 92  | o     | 2      | 0        | 0        | 0       | 0            |
| All | All   | 222478 | 0        | 166483   | 4092    | 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 11.

All (4092) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:2638:G:N2     | 48:5:2697:A:N1     | 1.92                     | 1.18              |
| 48:5:461:G:N2      | 48:5:694:C:O2      | 1.82                     | 1.13              |
| 5:E:96:THR:HG22    | 5:E:109:VAL:HG22   | 1.33                     | 1.07              |
| 48:5:973:G:N2      | 48:5:1282:G:N7     | 2.03                     | 1.07              |
| 69:RR:105:MET:HE2  | 69:RR:109:LEU:HD11 | 1.36                     | 1.05              |
| 51:9:197:U:O2      | 51:9:202:G:O6      | 1.74                     | 1.04              |
| 43:s:20:LEU:HD22   | 43:s:52:VAL:HG11   | 1.39                     | 1.03              |
| 51:9:1109:C:O2'    | 51:9:1110:G:O5'    | 1.75                     | 1.02              |
| 69:RR:41:ILE:HG23  | 69:RR:46:LEU:HD23  | 1.41                     | 1.02              |
| 48:5:1072:C:O2'    | 48:5:1073:G:O5'    | 1.77                     | 1.01              |
| 48:5:1235:G:O2'    | 48:5:1236:C:OP2    | 1.78                     | 1.00              |
| 51:9:1418:C:O2'    | 51:9:1421:A:OP2    | 1.80                     | 0.99              |
| 48:5:1981:G:O2'    | 86:ii:314:MET:O    | 1.81                     | 0.98              |
| 48:5:1999:A:O2'    | 48:5:2000:G:O4'    | 1.81                     | 0.98              |
| 48:5:4903:G:N2     | 48:5:4918:C:O2     | 1.97                     | 0.98              |
| 46:2:18:G:O2'      | 46:2:57:G:N2       | 1.97                     | 0.97              |
| 48:5:4633:G:O2'    | 48:5:4635:A:OP2    | 1.81                     | 0.97              |
| 51:9:1396:A:O2'    | 51:9:1398:G:N7     | 1.99                     | 0.96              |
| 86:ii:330:ARG:O    | 86:ii:371:SER:OG   | 1.82                     | 0.96              |
| 48:5:2797:C:OP1    | 92:5:5401:HOH:O    | 1.83                     | 0.96              |
| 48:5:1992:U:O2'    | 48:5:2002:A:OP1    | 1.83                     | 0.96              |
| 51:9:1085:C:OP2    | 92:9:2001:HOH:O    | 1.84                     | 0.96              |
| 48:5:3692:A:H62    | 48:5:3823:G:H21    | 0.99                     | 0.95              |
| 50:8:110:U:O2'     | 50:8:111:U:O4'     | 1.84                     | 0.95              |
| 48:5:913:U:O2'     | 48:5:914:U:OP2     | 1.83                     | 0.95              |
| 51:9:1480:A:O2'    | 81:dd:56:ASP:OD1   | 1.83                     | 0.95              |
| 51:9:1109:C:O2'    | 51:9:1110:G:O4'    | 1.81                     | 0.95              |
| 58:GG:102:VAL:HG21 | 58:GG:109:LEU:HD21 | 1.46                     | 0.95              |
| 58:GG:157:VAL:HG11 | 58:GG:176:ILE:HD11 | 1.47                     | 0.95              |
| 43:s:22:ASP:OD1    | 43:s:66:ARG:NH2    | 1.98                     | 0.95              |
| 51:9:73:C:O2'      | 51:9:74:G:N3       | 2.01                     | 0.94              |
| 50:8:109:C:O2'     | 50:8:110:U:OP2     | 1.86                     | 0.94              |
| 51:9:417:C:O2'     | 51:9:418:A:OP1     | 1.83                     | 0.94              |
| 51:9:1441:U:O2     | 51:9:1443:C:N4     | 1.99                     | 0.94              |
| 65:NN:60:VAL:HG13  | 65:NN:66:VAL:HG21  | 1.47                     | 0.94              |
| 48:5:922(B):C:O2'  | 48:5:923:C:OP1     | 1.86                     | 0.93              |
| 68:QQ:42:ILE:HD11  | 68:QQ:51:LEU:HD11  | 1.48                     | 0.93              |
| 4:D:253:TYR:OH     | 49:7:117:G:OP1     | 1.86                     | 0.93              |
| 59:HH:17:ASP:OD2   | 59:HH:22:GLY:N     | 2.02                     | 0.92              |
| 32:g:76:ARG:NH2    | 48:5:2583:C:OP2    | 2.02                     | 0.92              |
| 51:9:1757:G:O6     | 51:9:1775:U:O2     | 1.89                     | 0.91              |
| 86:ii:326:LEU:HD21 | 86:ii:409:ILE:HD11 | 1.52                     | 0.91              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:9:208:G:O2'    | 51:9:209:A:O5'     | 1.87                     | 0.91              |
| 48:5:1956:A:O2'   | 48:5:1957:U:OP1    | 1.88                     | 0.90              |
| 51:9:607:U:O2'    | 51:9:608:C:OP1     | 1.89                     | 0.90              |
| 51:9:1663:A:O2'   | 51:9:1664:A:OP2    | 1.89                     | 0.90              |
| 51:9:1512:C:O2'   | 81:dd:7:TYR:O      | 1.87                     | 0.90              |
| 55:DD:103:GLU:OE2 | 55:DD:173:ARG:NE   | 2.05                     | 0.90              |
| 58:GG:18:VAL:HG11 | 58:GG:24:LEU:HD21  | 1.51                     | 0.90              |
| 49:7:21:G:N7      | 92:7:301:HOH:O     | 2.05                     | 0.90              |
| 48:5:2104:A:O2'   | 48:5:2105:A:O5'    | 1.88                     | 0.90              |
| 51:9:1298:G:O2'   | 51:9:1299:A:O5'    | 1.89                     | 0.89              |
| 51:9:1068:G:O6    | 92:9:2002:HOH:O    | 1.89                     | 0.89              |
| 48:5:4136:G:N2    | 48:5:4148:C:O2     | 2.05                     | 0.89              |
| 51:9:1395:C:O2'   | 51:9:1396:A:OP1    | 1.89                     | 0.89              |
| 51:9:103:A:OP2    | 51:9:356:C:N4      | 2.06                     | 0.88              |
| 59:HH:52:GLU:N    | 59:HH:52:GLU:OE1   | 2.07                     | 0.88              |
| 31:f:58:VAL:O     | 48:5:4944:C:N4     | 2.07                     | 0.88              |
| 48:5:1076:C:O2    | 48:5:1235:G:N2     | 2.07                     | 0.88              |
| 48:5:1990:A:O2'   | 48:5:1991:A:OP1    | 1.92                     | 0.87              |
| 76:YY:122:LYS:O   | 76:YY:125:VAL:HG22 | 1.73                     | 0.87              |
| 48:5:1481:C:O2'   | 48:5:1482:G:O5'    | 1.91                     | 0.87              |
| 86:ii:189:ARG:NH2 | 92:ii:601:HOH:O    | 2.06                     | 0.87              |
| 48:5:3717:A:OP2   | 48:5:3735:G:N2     | 2.07                     | 0.87              |
| 48:5:3751:G:H21   | 48:5:3775:A:H8     | 1.19                     | 0.86              |
| 51:9:1456:G:OP1   | 69:RR:59:LYS:NZ    | 2.08                     | 0.86              |
| 76:YY:26:ASP:OD1  | 76:YY:70:THR:OG1   | 1.92                     | 0.86              |
| 86:ii:217:ASP:OD1 | 86:ii:245:ARG:NH1  | 2.08                     | 0.86              |
| 4:D:286:SER:OG    | 48:5:1179:U:O2     | 1.93                     | 0.86              |
| 48:5:245:C:O2'    | 48:5:246:G:OP2     | 1.92                     | 0.86              |
| 70:SS:15:VAL:HG12 | 70:SS:68:ILE:HD11  | 1.57                     | 0.86              |
| 48:5:480:C:O2'    | 48:5:481:G:OP1     | 1.92                     | 0.86              |
| 48:5:1233:G:O2'   | 48:5:1234:G:OP2    | 1.92                     | 0.86              |
| 56:EE:21:ASP:OD2  | 56:EE:24:THR:OG1   | 1.92                     | 0.85              |
| 87:jj:62:ILE:HD11 | 87:jj:72:ILE:HG12  | 1.56                     | 0.85              |
| 48:5:5047:C:O2'   | 48:5:5050:C:OP2    | 1.94                     | 0.85              |
| 51:9:1061:U:OP1   | 92:9:2003:HOH:O    | 1.93                     | 0.85              |
| 77:ZZ:56:ASP:OD1  | 77:ZZ:57:LYS:N     | 2.09                     | 0.85              |
| 48:5:4927:G:OP2   | 48:5:4928:C:N4     | 2.09                     | 0.85              |
| 47:3:54:U:O4      | 47:3:58:A:N7       | 2.09                     | 0.85              |
| 68:QQ:101:ASP:OD1 | 68:QQ:103:ALA:N    | 2.09                     | 0.85              |
| 51:9:71:G:O2'     | 51:9:72:C:OP1      | 1.94                     | 0.85              |
| 37:l:21:ARG:NH1   | 50:8:52:A:OP1      | 2.10                     | 0.85              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:1890:G:N2     | 48:5:1939:A:H61    | 1.75                     | 0.85              |
| 87:jj:432:ILE:O    | 87:jj:432:ILE:HD12 | 1.76                     | 0.85              |
| 48:5:3759:A:OP2    | 92:5:5402:HOH:O    | 1.94                     | 0.85              |
| 48:5:4415:A:N6     | 48:5:4427:G:O2'    | 2.09                     | 0.85              |
| 51:9:1231:C:OP2    | 70:SS:139:THR:OG1  | 1.94                     | 0.85              |
| 65:NN:19:ARG:NH2   | 79:bb:83:GLN:OE1   | 2.10                     | 0.84              |
| 80:cc:44:ARG:NH2   | 80:cc:60:GLU:O     | 2.09                     | 0.84              |
| 4:D:212:MET:HE1    | 4:D:233:PRO:HG2    | 1.59                     | 0.84              |
| 51:9:1432:U:O2'    | 51:9:1433:C:OP1    | 1.94                     | 0.84              |
| 24:Y:88:GLU:OE1    | 24:Y:88:GLU:N      | 2.09                     | 0.84              |
| 51:9:1408:U:O2'    | 51:9:1409:A:O5'    | 1.95                     | 0.84              |
| 48:5:3692:A:H62    | 48:5:3823:G:N2     | 1.74                     | 0.84              |
| 50:8:122:G:H21     | 50:8:128:C:H41     | 1.19                     | 0.84              |
| 1:A:142:GLU:O      | 1:A:143:THR:OG1    | 1.94                     | 0.83              |
| 48:5:1998:A:N3     | 48:5:2019:C:O2'    | 2.10                     | 0.83              |
| 55:DD:226:GLN:NE2  | 84:gg:224:GLY:O    | 2.12                     | 0.83              |
| 51:9:100:U:OP2     | 92:9:2004:HOH:O    | 1.96                     | 0.83              |
| 48:5:3672:G:O2'    | 48:5:3673:C:OP1    | 1.95                     | 0.83              |
| 51:9:1616:U:O2'    | 51:9:1661:A:O2'    | 1.95                     | 0.82              |
| 55:DD:167:TYR:OH   | 55:DD:193:ASP:OD1  | 1.97                     | 0.82              |
| 60:II:114:GLU:OE2  | 60:II:128:LYS:NZ   | 2.12                     | 0.82              |
| 77:ZZ:74:SER:OG    | 77:ZZ:79:ILE:O     | 1.97                     | 0.82              |
| 48:5:1455:G:O2'    | 48:5:1456:C:OP1    | 1.96                     | 0.82              |
| 25:Z:30:ASP:O      | 25:Z:39:SER:OG     | 1.96                     | 0.82              |
| 48:5:1982:G:O2'    | 48:5:1983:A:OP1    | 1.96                     | 0.82              |
| 54:CC:255:LEU:HD23 | 73:VV:1:MET:HE2    | 1.59                     | 0.82              |
| 51:9:1303:C:OP2    | 83:ff:90:ARG:NH2   | 2.13                     | 0.82              |
| 51:9:306:C:O4'     | 60:II:41:ARG:NH2   | 2.13                     | 0.82              |
| 59:HH:139:ILE:HD12 | 59:HH:139:ILE:O    | 1.79                     | 0.82              |
| 48:5:4487:A:N7     | 92:5:5415:HOH:O    | 2.13                     | 0.81              |
| 48:5:1077:C:N4     | 48:5:1233:G:O6     | 2.11                     | 0.81              |
| 51:9:537:C:N3      | 51:9:547:G:N2      | 2.27                     | 0.81              |
| 55:DD:158:ILE:HD12 | 55:DD:164:VAL:HG12 | 1.61                     | 0.81              |
| 51:9:1521:C:OP2    | 70:SS:136:THR:OG1  | 1.99                     | 0.81              |
| 13:N:124:ASP:OD1   | 48:5:3937:C:O2'    | 1.97                     | 0.81              |
| 48:5:1444:G:N2     | 48:5:2110:G:O6     | 2.13                     | 0.81              |
| 53:BB:125:VAL:HG12 | 53:BB:172:MET:HE3  | 1.63                     | 0.81              |
| 87:jj:389:ILE:HD13 | 87:jj:484:LEU:HD23 | 1.61                     | 0.81              |
| 51:9:95:G:O6       | 92:9:2006:HOH:O    | 1.98                     | 0.81              |
| 10:J:113:ILE:HD12  | 70:SS:14:ARG:HD3   | 1.63                     | 0.80              |
| 48:5:3603:G:O2'    | 48:5:3604:A:OP1    | 1.99                     | 0.80              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:3:70:G:HO2'     | 48:5:3740:G:HO2'   | 1.21                     | 0.80              |
| 48:5:738(A):C:O2'  | 48:5:740:G:OP2     | 1.98                     | 0.80              |
| 50:8:110:U:HO2'    | 50:8:111:U:C4'     | 1.92                     | 0.80              |
| 71:TT:60:THR:HG23  | 71:TT:75:MET:HE2   | 1.63                     | 0.80              |
| 51:9:1560:U:O2'    | 51:9:1583:C:O2'    | 1.88                     | 0.80              |
| 56:EE:195:ILE:O    | 56:EE:196:THR:OG1  | 1.99                     | 0.80              |
| 55:DD:28:GLU:OE1   | 55:DD:65:ARG:NH2   | 2.16                     | 0.79              |
| 51:9:1091:C:HO2'   | 74:WW:2:VAL:N      | 1.80                     | 0.79              |
| 9:I:66:GLU:OE1     | 9:I:69:ARG:NH2     | 2.15                     | 0.79              |
| 51:9:488:U:O2'     | 51:9:489:A:OP1     | 1.99                     | 0.79              |
| 52:AA:50:ASN:HA    | 69:RR:105:MET:HE1  | 1.64                     | 0.79              |
| 68:QQ:130:LYS:NZ   | 68:QQ:134:GLY:O    | 2.15                     | 0.79              |
| 20:U:111:GLU:OE2   | 20:U:113:ARG:NE    | 2.15                     | 0.79              |
| 48:5:1611:C:OP1    | 92:5:5404:HOH:O    | 2.01                     | 0.79              |
| 48:5:2457:G:H21    | 48:5:3672:G:N2     | 1.81                     | 0.79              |
| 43:s:9:TRP:NE1     | 48:5:1999:A:OP1    | 2.16                     | 0.79              |
| 57:FF:74:ASN:OD1   | 57:FF:86:LYS:NZ    | 2.14                     | 0.79              |
| 51:9:44:U:O4       | 51:9:485:A:N6      | 2.16                     | 0.79              |
| 51:9:1249:C:O2'    | 68:QQ:143:LYS:NZ   | 2.15                     | 0.79              |
| 9:I:162:ARG:NH2    | 48:5:2033:A:OP1    | 2.16                     | 0.79              |
| 48:5:4572:U:O2'    | 48:5:4573:G:O4'    | 2.01                     | 0.78              |
| 51:9:71:G:O6       | 58:GG:170:ARG:NH1  | 2.17                     | 0.78              |
| 48:5:1991:A:O2'    | 48:5:1992:U:O4'    | 2.00                     | 0.78              |
| 75:XX:98:ASP:OD1   | 75:XX:99:GLU:N     | 2.15                     | 0.78              |
| 86:ii:24:LEU:HD21  | 86:ii:112:ILE:HD12 | 1.64                     | 0.78              |
| 48:5:3860:A:H61    | 48:5:4560:C:H5     | 1.31                     | 0.78              |
| 51:9:1291:A:HO2'   | 83:ff:135:TYR:HH   | 1.11                     | 0.78              |
| 86:ii:24:LEU:HD21  | 86:ii:112:ILE:CD1  | 2.13                     | 0.78              |
| 48:5:1629:G:OP1    | 92:5:5403:HOH:O    | 2.00                     | 0.78              |
| 51:9:872:A:O2'     | 51:9:873:G:O5'     | 2.00                     | 0.78              |
| 87:jj:165:LYS:NZ   | 87:jj:234:LYS:O    | 2.16                     | 0.78              |
| 87:jj:168:ILE:HG22 | 87:jj:239:MET:HB2  | 1.65                     | 0.78              |
| 13:N:2:GLY:N       | 48:5:116:G:OP2     | 2.17                     | 0.78              |
| 52:AA:90:PHE:CD2   | 52:AA:179:ALA:HB2  | 2.19                     | 0.78              |
| 4:D:43:LYS:O       | 4:D:46:THR:HG22    | 1.82                     | 0.78              |
| 48:5:3637:U:OP2    | 92:5:5405:HOH:O    | 2.02                     | 0.78              |
| 51:9:1192:U:OP2    | 75:XX:119:ARG:NH2  | 2.17                     | 0.78              |
| 48:5:3897:G:OP2    | 92:5:5406:HOH:O    | 2.02                     | 0.78              |
| 78:aa:3:LYS:NZ     | 78:aa:8:ASN:OD1    | 2.17                     | 0.78              |
| 4:D:75:VAL:O       | 4:D:112:ARG:NH1    | 2.16                     | 0.77              |
| 48:5:2092:G:O2'    | 48:5:2262:G:O6     | 2.03                     | 0.77              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:2638:G:H1     | 48:5:2697:A:H61    | 1.33                     | 0.77              |
| 66:OO:86:LYS:HD2   | 66:OO:124:MET:HE3  | 1.66                     | 0.77              |
| 55:DD:66:ILE:HD11  | 55:DD:86:LEU:O     | 1.85                     | 0.77              |
| 57:FF:73:THR:O     | 57:FF:89:THR:HG21  | 1.84                     | 0.77              |
| 87:jj:377:MET:HA   | 87:jj:377:MET:HE3  | 1.65                     | 0.77              |
| 71:TT:22:LEU:HD22  | 71:TT:28:LEU:HD13  | 1.67                     | 0.77              |
| 7:G:95:LEU:HD13    | 7:G:218:LEU:HD13   | 1.66                     | 0.77              |
| 51:9:197:U:O2      | 51:9:202:G:C6      | 2.38                     | 0.77              |
| 72:UU:24:LEU:CD1   | 72:UU:112:VAL:HG13 | 2.15                     | 0.77              |
| 76:YY:27:VAL:HG11  | 76:YY:35:VAL:HG21  | 1.66                     | 0.77              |
| 51:9:165:G:N2      | 51:9:165:G:OP2     | 2.16                     | 0.76              |
| 48:5:467:U:N3      | 48:5:685:C:N3      | 2.34                     | 0.76              |
| 69:RR:105:MET:HE2  | 69:RR:109:LEU:CD1  | 2.15                     | 0.76              |
| 48:5:2553:A:H2     | 48:5:2765:A:H62    | 1.34                     | 0.76              |
| 51:9:399:C:N3      | 63:LL:104:LYS:NZ   | 2.33                     | 0.76              |
| 66:OO:124:MET:HE2  | 66:OO:124:MET:HA   | 1.65                     | 0.76              |
| 67:PP:89:MET:O     | 67:PP:107:ILE:HD11 | 1.85                     | 0.76              |
| 4:D:284:LYS:O      | 4:D:288:LEU:HD22   | 1.85                     | 0.76              |
| 84:gg:288:SER:O    | 84:gg:289:LEU:HD23 | 1.84                     | 0.76              |
| 51:9:1407:U:H2'    | 51:9:1408:U:C5     | 2.20                     | 0.76              |
| 58:GG:7:PHE:CE1    | 58:GG:9:ALA:HB3    | 2.21                     | 0.76              |
| 26:a:77:LYS:CE     | 48:5:1502:G:H22    | 1.99                     | 0.76              |
| 48:5:2100:G:O2'    | 48:5:2101:A:OP2    | 2.03                     | 0.76              |
| 51:9:1560:U:HO2'   | 51:9:1583:C:HO2'   | 0.98                     | 0.76              |
| 59:HH:66:VAL:HG22  | 59:HH:96:ALA:HB1   | 1.67                     | 0.76              |
| 80:cc:14:VAL:HG22  | 80:cc:30:VAL:HG21  | 1.67                     | 0.76              |
| 25:Z:24:VAL:HG21   | 25:Z:87:VAL:HG22   | 1.68                     | 0.76              |
| 44:t:114:ARG:NH2   | 44:t:126:SER:OG    | 2.19                     | 0.76              |
| 87:jj:552:LEU:HD12 | 87:jj:553:ALA:H    | 1.50                     | 0.76              |
| 31:f:106:TYR:O     | 31:f:108:SER:N     | 2.19                     | 0.75              |
| 70:SS:58:GLU:OE2   | 77:ZZ:49:LEU:HD11  | 1.86                     | 0.75              |
| 5:E:209:VAL:HG22   | 5:E:259:GLN:HB3    | 1.69                     | 0.75              |
| 48:5:115:C:O2'     | 48:5:276:C:OP1     | 2.03                     | 0.75              |
| 48:5:1449:C:O2     | 48:5:2105:A:O2'    | 2.03                     | 0.75              |
| 51:9:1292:C:N4     | 51:9:1307:U:O2     | 2.19                     | 0.75              |
| 51:9:1491:G:OP2    | 92:9:2007:HOH:O    | 2.05                     | 0.75              |
| 51:9:33:G:H2'      | 51:9:34:PSU:H5''   | 1.67                     | 0.75              |
| 51:9:217:A:O2'     | 51:9:218:PSU:H5''  | 1.87                     | 0.75              |
| 87:jj:374:ILE:HG21 | 87:jj:528:LEU:HG   | 1.69                     | 0.75              |
| 48:5:1322:1MA:OP1  | 92:5:5407:HOH:O    | 2.05                     | 0.75              |
| 51:9:1407:U:O2     | 51:9:1407:U:O2'    | 2.00                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:E:185:ASN:ND2    | 5:E:274:LEU:O      | 2.20                     | 0.75              |
| 87:jj:454:ILE:HD13 | 87:jj:466:GLU:HB3  | 1.67                     | 0.75              |
| 48:5:2457:G:H21    | 48:5:3672:G:H21    | 1.35                     | 0.74              |
| 48:5:2465:C:H1'    | 48:5:3672:G:H22    | 1.49                     | 0.74              |
| 84:gg:5:MET:SD     | 84:gg:270:LEU:HD11 | 2.27                     | 0.74              |
| 51:9:872:A:HO2'    | 51:9:873:G:C5'     | 1.99                     | 0.74              |
| 86:ii:160:THR:HG23 | 86:ii:169:LEU:HD11 | 1.68                     | 0.74              |
| 58:GG:126:ASP:OD1  | 58:GG:127:THR:HG23 | 1.87                     | 0.74              |
| 7:G:73:ARG:NE      | 48:5:4076:G:OP1    | 2.21                     | 0.74              |
| 48:5:3692:A:N6     | 48:5:3823:G:H21    | 1.81                     | 0.74              |
| 24:Y:126:ARG:NH2   | 48:5:198:A:OP2     | 2.19                     | 0.74              |
| 51:9:160:U:O2'     | 51:9:162:C:OP2     | 2.06                     | 0.74              |
| 7:G:98:LEU:HD13    | 7:G:218:LEU:HD12   | 1.69                     | 0.74              |
| 87:jj:237:ILE:HG22 | 87:jj:239:MET:HE2  | 1.69                     | 0.74              |
| 59:HH:30:LEU:O     | 59:HH:36:LEU:HD23  | 1.88                     | 0.74              |
| 64:MM:48:HIS:O     | 64:MM:49:LEU:HD12  | 1.88                     | 0.74              |
| 5:E:58:ARG:NH1     | 5:E:58:ARG:O       | 2.19                     | 0.74              |
| 51:9:291:G:N2      | 51:9:293:C:OP2     | 2.12                     | 0.74              |
| 51:9:688:U:OP2     | 59:HH:116:ARG:NH2  | 2.19                     | 0.74              |
| 87:jj:244:SER:O    | 87:jj:252:ARG:NH2  | 2.21                     | 0.74              |
| 26:a:2:PRO:HG2     | 26:a:5:LEU:HD12    | 1.70                     | 0.74              |
| 51:9:535:G:O6      | 51:9:547:G:N1      | 2.20                     | 0.74              |
| 80:cc:13:ARG:HH22  | 80:cc:35:MET:HE3   | 1.50                     | 0.74              |
| 33:h:7:ARG:NH1     | 50:8:86:U:O4'      | 2.21                     | 0.73              |
| 87:jj:260:ARG:O    | 87:jj:263:ILE:HG22 | 1.88                     | 0.73              |
| 48:5:1072:C:N4     | 48:5:1239:C:H42    | 1.86                     | 0.73              |
| 52:AA:66:VAL:HG21  | 52:AA:185:MET:HB3  | 1.71                     | 0.73              |
| 55:DD:138:VAL:HG12 | 55:DD:184:ILE:HD12 | 1.69                     | 0.73              |
| 8:H:134:CYS:SG     | 8:H:144:LEU:HD13   | 2.27                     | 0.73              |
| 42:r:26:SER:OG     | 42:r:28:GLU:OE1    | 2.05                     | 0.73              |
| 48:5:2351:OMC:HM22 | 48:5:2352:U:H5'    | 1.70                     | 0.73              |
| 25:Z:74:VAL:HG23   | 25:Z:101:PHE:CE2   | 2.23                     | 0.73              |
| 48:5:4189:U:O4     | 92:5:5408:HOH:O    | 2.06                     | 0.73              |
| 66:OO:84:ARG:CZ    | 66:OO:88:LEU:HD21  | 2.19                     | 0.73              |
| 48:5:451:C:OP2     | 48:5:1294:A:N6     | 2.20                     | 0.73              |
| 48:5:1072:C:H42    | 48:5:1239:C:H42    | 1.33                     | 0.73              |
| 48:5:1369:C:OP2    | 48:5:1370:G:O2'    | 2.00                     | 0.73              |
| 84:gg:272:GLN:OE1  | 84:gg:272:GLN:N    | 2.22                     | 0.73              |
| 3:C:10:VAL:O       | 3:C:18:SER:OG      | 2.04                     | 0.73              |
| 84:gg:176:VAL:O    | 84:gg:185:LYS:N    | 2.22                     | 0.73              |
| 51:9:197:U:C2      | 51:9:202:G:O6      | 2.41                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:1617:G:N1     | 51:9:1620:A:OP2    | 2.22                     | 0.72              |
| 87:jj:495:GLU:OE1  | 87:jj:495:GLU:N    | 2.21                     | 0.72              |
| 24:Y:74:TYR:OH     | 50:8:75:OMG:OP2    | 2.06                     | 0.72              |
| 51:9:860:G:H21     | 74:WW:107:SER:HB3  | 1.53                     | 0.72              |
| 53:BB:228:LEU:HD23 | 53:BB:229:MET:CE   | 2.20                     | 0.72              |
| 84:gg:39:THR:HG22  | 84:gg:60:ARG:HD2   | 1.70                     | 0.72              |
| 9:I:184:MET:HB2    | 9:I:190:LEU:HD12   | 1.72                     | 0.72              |
| 51:9:654:A:N7      | 92:9:2010:HOH:O    | 2.21                     | 0.72              |
| 48:5:2647:A:H62    | 48:5:2686:G:H8     | 1.36                     | 0.72              |
| 9:I:13:LYS:NZ      | 48:5:1867:A:OP1    | 2.21                     | 0.72              |
| 48:5:2819:U:OP2    | 92:5:5411:HOH:O    | 2.08                     | 0.72              |
| 51:9:935:G:O2'     | 65:NN:108:ASP:OD1  | 2.07                     | 0.72              |
| 51:9:1785:C:O2'    | 51:9:1786:U:O5'    | 2.07                     | 0.72              |
| 58:GG:126:ASP:O    | 58:GG:127:THR:OG1  | 2.06                     | 0.72              |
| 84:gg:79:LEU:HD21  | 84:gg:120:ILE:HG21 | 1.70                     | 0.72              |
| 87:jj:284:ASP:N    | 87:jj:284:ASP:OD1  | 2.23                     | 0.72              |
| 59:HH:134:VAL:HG23 | 59:HH:134:VAL:O    | 1.90                     | 0.71              |
| 10:J:22:LEU:HD13   | 10:J:43:LEU:HD23   | 1.71                     | 0.71              |
| 48:5:267:G:O2'     | 48:5:268:G:OP1     | 2.06                     | 0.71              |
| 51:9:1612:G:OP1    | 67:PP:18:ARG:NH2   | 2.22                     | 0.71              |
| 72:UU:48:LEU:HD22  | 72:UU:101:ILE:HD11 | 1.70                     | 0.71              |
| 6:F:65:ARG:CZ      | 48:5:1210:C:H42    | 2.02                     | 0.71              |
| 51:9:1348:G:H1     | 51:9:1381:G:H22    | 1.37                     | 0.71              |
| 48:5:746:A:O2'     | 48:5:747:A:OP2     | 2.04                     | 0.71              |
| 51:9:840:C:O2'     | 51:9:841:G:O5'     | 2.08                     | 0.71              |
| 67:PP:37:TYR:O     | 67:PP:42:ARG:NH2   | 2.23                     | 0.71              |
| 51:9:688:U:O2'     | 51:9:689:U:OP2     | 2.09                     | 0.71              |
| 51:9:1316:C:O2'    | 51:9:1317:C:OP2    | 2.06                     | 0.71              |
| 58:GG:181:THR:HG22 | 58:GG:182:PRO:HD2  | 1.73                     | 0.71              |
| 1:A:93:LYS:NZ      | 48:5:4115:G:OP1    | 2.23                     | 0.71              |
| 2:B:223:THR:HG22   | 2:B:338:VAL:HG23   | 1.72                     | 0.71              |
| 43:s:34:ASN:ND2    | 48:5:1969:G:OP1    | 2.23                     | 0.71              |
| 48:5:1481:C:O2'    | 48:5:1482:G:O4'    | 2.08                     | 0.71              |
| 57:FF:43:GLU:OE1   | 57:FF:43:GLU:N     | 2.23                     | 0.71              |
| 59:HH:25:GLN:O     | 59:HH:29:GLU:OE1   | 2.09                     | 0.71              |
| 61:JJ:177:ASN:OD1  | 61:JJ:180:LYS:NZ   | 2.23                     | 0.71              |
| 1:A:123:ARG:NH1    | 48:5:4083:U:OP1    | 2.24                     | 0.71              |
| 48:5:4921:C:O2'    | 48:5:4922:C:OP2    | 2.09                     | 0.71              |
| 51:9:1102:G:H22    | 51:9:1130:G:N2     | 1.89                     | 0.71              |
| 87:jj:371:ASP:O    | 87:jj:372:SER:OG   | 2.07                     | 0.71              |
| 87:jj:588:GLN:NE2  | 87:jj:594:TYR:O    | 2.23                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:G:85:GLN:OE1     | 7:G:229:ARG:NH1    | 2.24                     | 0.71              |
| 48:5:1904:G:O6     | 92:5:5409:HOH:O    | 2.06                     | 0.71              |
| 62:KK:16:PHE:CE1   | 62:KK:76:ILE:HG23  | 2.26                     | 0.71              |
| 51:9:488:U:H3'     | 51:9:489:A:H5'     | 1.71                     | 0.70              |
| 67:PP:19:GLY:N     | 70:SS:91:LYS:O     | 2.24                     | 0.70              |
| 50:8:85:U:O2'      | 50:8:87:G:OP1      | 2.05                     | 0.70              |
| 51:9:33:G:C2'      | 51:9:34:PSU:H5''   | 2.20                     | 0.70              |
| 64:MM:64:LEU:HD22  | 83:ff:103:VAL:HG23 | 1.71                     | 0.70              |
| 48:5:981:C:H42     | 48:5:1274:A:H61    | 1.38                     | 0.70              |
| 51:9:213:G:O2'     | 51:9:214:U:OP1     | 2.08                     | 0.70              |
| 25:Z:95:VAL:HG12   | 25:Z:110:ALA:HA    | 1.73                     | 0.70              |
| 51:9:525:A:O2'     | 82:ee:31:ARG:NH2   | 2.23                     | 0.70              |
| 64:MM:64:LEU:CD2   | 83:ff:103:VAL:HG23 | 2.21                     | 0.70              |
| 71:TT:108:GLU:OE2  | 71:TT:115:LYS:NZ   | 2.24                     | 0.70              |
| 84:gg:4:GLN:O      | 84:gg:313:THR:N    | 2.23                     | 0.70              |
| 87:jj:347:MET:SD   | 87:jj:348:TYR:N    | 2.64                     | 0.70              |
| 13:N:148:THR:O     | 13:N:151:ILE:HG22  | 1.91                     | 0.70              |
| 67:PP:17:TYR:HB3   | 67:PP:25:LEU:HD11  | 1.74                     | 0.70              |
| 87:jj:322:LEU:HD13 | 87:jj:323:ARG:N    | 2.07                     | 0.70              |
| 51:9:1616:U:HO2'   | 51:9:1661:A:HO2'   | 1.37                     | 0.70              |
| 4:D:107:ARG:NH1    | 4:D:169:GLY:O      | 2.24                     | 0.70              |
| 72:UU:48:LEU:HD21  | 72:UU:97:ILE:CG2   | 2.22                     | 0.70              |
| 76:YY:10:ARG:NH1   | 76:YY:26:ASP:OD2   | 2.24                     | 0.70              |
| 49:7:65:G:N7       | 92:7:303:HOH:O     | 2.25                     | 0.69              |
| 76:YY:55:ILE:HD12  | 76:YY:75:ILE:HD12  | 1.72                     | 0.69              |
| 51:9:1570:G:O2'    | 51:9:1614:A:O2'    | 2.09                     | 0.69              |
| 48:5:3786:U:OP1    | 48:5:4550:G:O2'    | 2.10                     | 0.69              |
| 51:9:64:A:H2       | 51:9:83:A:H62      | 1.38                     | 0.69              |
| 79:bb:35:VAL:HG11  | 79:bb:73:LEU:HD11  | 1.75                     | 0.69              |
| 84:gg:9:GLY:O      | 84:gg:309:VAL:HG12 | 1.92                     | 0.69              |
| 87:jj:409:VAL:HG22 | 87:jj:482:VAL:CG2  | 2.22                     | 0.69              |
| 87:jj:519:GLU:OE2  | 87:jj:521:ASP:N    | 2.25                     | 0.69              |
| 2:B:302:ASN:ND2    | 2:B:370:THR:OG1    | 2.26                     | 0.69              |
| 32:g:29:ARG:NH2    | 48:5:2522:G:OP2    | 2.26                     | 0.69              |
| 43:s:144:THR:OG1   | 43:s:156:SER:OG    | 2.11                     | 0.69              |
| 48:5:4627:U:OP2    | 92:5:5412:HOH:O    | 2.11                     | 0.69              |
| 51:9:583:A:OP1     | 61:JJ:162:ARG:NH2  | 2.26                     | 0.69              |
| 51:9:835:C:O2'     | 51:9:838:G:OP2     | 2.07                     | 0.69              |
| 51:9:1394:G:O2'    | 51:9:1395:C:OP1    | 2.11                     | 0.69              |
| 48:5:52:G:N7       | 92:5:5437:HOH:O    | 2.24                     | 0.69              |
| 51:9:1752:C:H2'    | 51:9:1753:C:O4'    | 1.93                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:AA:19:LEU:HD11  | 69:RR:106:LEU:HD11 | 1.74                     | 0.69              |
| 58:GG:74:ARG:NH2   | 58:GG:94:ARG:O     | 2.26                     | 0.69              |
| 87:jj:218:SER:OG   | 87:jj:221:GLU:OE1  | 2.09                     | 0.69              |
| 44:t:50:THR:HG21   | 44:t:72:GLU:HG2    | 1.75                     | 0.69              |
| 51:9:1744:G:O2'    | 51:9:1745:A:OP2    | 2.10                     | 0.69              |
| 53:BB:38:MET:HE2   | 53:BB:231:LEU:HD11 | 1.75                     | 0.69              |
| 53:BB:97:LEU:HD12  | 53:BB:232:HIS:CD2  | 2.28                     | 0.69              |
| 57:FF:171:GLU:OE2  | 77:ZZ:72:VAL:HG23  | 1.92                     | 0.69              |
| 62:KK:15:LEU:O     | 62:KK:18:GLU:O     | 2.11                     | 0.69              |
| 21:V:99:GLU:OE1    | 22:W:24:THR:HG22   | 1.92                     | 0.68              |
| 40:o:2:VAL:N       | 40:o:90:HIS:O      | 2.26                     | 0.68              |
| 74:WW:26:LEU:HB2   | 79:bb:7:LEU:HD23   | 1.76                     | 0.68              |
| 75:XX:109:GLY:O    | 75:XX:119:ARG:NE   | 2.26                     | 0.68              |
| 4:D:208:MET:CB     | 4:D:233:PRO:HG3    | 2.23                     | 0.68              |
| 48:5:4635:A:H2     | 48:5:4663:G:H21    | 1.41                     | 0.68              |
| 62:KK:15:LEU:O     | 62:KK:19:GLY:HA2   | 1.93                     | 0.68              |
| 86:ii:407:GLY:HA2  | 87:jj:34:MET:HE2   | 1.74                     | 0.68              |
| 51:9:292:A:OP2     | 63:LL:42:LEU:HD21  | 1.94                     | 0.68              |
| 51:9:1598:G:O2'    | 51:9:1599:U:OP2    | 2.11                     | 0.68              |
| 3:C:335:MET:HE1    | 48:5:943:A:N3      | 2.08                     | 0.68              |
| 20:U:76:VAL:HG13   | 20:U:77:PRO:HD2    | 1.76                     | 0.68              |
| 48:5:4743:G:O2'    | 48:5:4744:A:O4'    | 2.10                     | 0.68              |
| 51:9:65:C:C2       | 58:GG:133:LEU:HD22 | 2.28                     | 0.68              |
| 67:PP:81:ARG:NH1   | 67:PP:97:TYR:O     | 2.26                     | 0.68              |
| 71:TT:30:VAL:HG12  | 71:TT:34:VAL:HG21  | 1.74                     | 0.68              |
| 87:jj:466:GLU:OE1  | 87:jj:469:ARG:NH1  | 2.27                     | 0.68              |
| 2:B:217:ILE:HD11   | 2:B:333:LEU:HD21   | 1.76                     | 0.68              |
| 7:G:34:LYS:NZ      | 48:5:4129:G:O2'    | 2.22                     | 0.68              |
| 67:PP:17:TYR:CB    | 67:PP:25:LEU:HD11  | 2.24                     | 0.68              |
| 48:5:1413:C:O2'    | 48:5:1414:C:O5'    | 2.08                     | 0.68              |
| 51:9:1507:G:HO2'   | 83:ff:80:TYR:HH    | 0.84                     | 0.68              |
| 7:G:161:VAL:O      | 7:G:161:VAL:HG12   | 1.94                     | 0.68              |
| 48:5:4244:A:O2'    | 48:5:4268:A:OP1    | 2.12                     | 0.68              |
| 55:DD:177:LEU:HD12 | 55:DD:182:LEU:HD12 | 1.75                     | 0.68              |
| 8:H:12:ILE:HG12    | 8:H:18:ILE:HD12    | 1.76                     | 0.68              |
| 17:R:88:ARG:O      | 48:5:2725:A:N6     | 2.26                     | 0.68              |
| 47:3:58:A:O2'      | 47:3:60:U:OP2      | 2.05                     | 0.68              |
| 83:ff:103:VAL:HG13 | 83:ff:106:ASN:O    | 1.94                     | 0.68              |
| 84:gg:270:LEU:HD22 | 84:gg:310:TRP:CZ3  | 2.28                     | 0.68              |
| 56:EE:95:THR:HG22  | 76:YY:16:ARG:HG2   | 1.74                     | 0.67              |
| 79:bb:63:LEU:O     | 79:bb:64:CYS:SG    | 2.53                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 87:jj:235:ALA:HB3  | 87:jj:238:PHE:CE1  | 2.28                     | 0.67              |
| 48:5:2562:G:N1     | 48:5:2565:A:OP2    | 2.27                     | 0.67              |
| 52:AA:34:MET:HE2   | 52:AA:149:ASN:O    | 1.94                     | 0.67              |
| 87:jj:152:LEU:HD22 | 87:jj:156:PHE:CE2  | 2.28                     | 0.67              |
| 12:M:96:GLU:OE2    | 12:M:100:ARG:NH2   | 2.28                     | 0.67              |
| 13:N:67:ARG:NH1    | 48:5:2458:C:OP1    | 2.27                     | 0.67              |
| 44:t:41:LYS:HE3    | 86:ii:343:ILE:HD11 | 1.76                     | 0.67              |
| 51:9:1490:OMG:HM22 | 51:9:1491:G:O4'    | 1.95                     | 0.67              |
| 55:DD:93:THR:HG23  | 55:DD:93:THR:O     | 1.94                     | 0.67              |
| 58:GG:157:VAL:CG1  | 58:GG:176:ILE:HD11 | 2.24                     | 0.67              |
| 2:B:322:HIS:O      | 2:B:342:LYS:NZ     | 2.19                     | 0.67              |
| 12:M:11:ARG:NH1    | 12:M:61:ILE:HD11   | 2.09                     | 0.67              |
| 30:e:117:GLN:O     | 42:r:119:ARG:NH2   | 2.27                     | 0.67              |
| 50:8:122:G:N2      | 50:8:128:C:H41     | 1.92                     | 0.67              |
| 51:9:1566:G:N7     | 71:TT:101:ARG:NH2  | 2.42                     | 0.67              |
| 55:DD:70:THR:HG22  | 55:DD:86:LEU:HD13  | 1.77                     | 0.67              |
| 84:gg:292:SER:O    | 84:gg:295:GLY:N    | 2.26                     | 0.67              |
| 48:5:261:G:H2'     | 48:5:262:G:O4'     | 1.93                     | 0.67              |
| 2:B:370:THR:O      | 2:B:370:THR:HG22   | 1.94                     | 0.67              |
| 4:D:208:MET:HB2    | 4:D:233:PRO:HG3    | 1.76                     | 0.67              |
| 48:5:2758:G:O2'    | 48:5:2765:A:N3     | 2.25                     | 0.67              |
| 51:9:218:PSU:O2'   | 51:9:305:U:N3      | 2.28                     | 0.67              |
| 51:9:846:G:C5      | 56:EE:19:MET:HE3   | 2.29                     | 0.67              |
| 86:ii:287:ILE:HD11 | 86:ii:392:VAL:HB   | 1.77                     | 0.67              |
| 51:9:551:U:N3      | 51:9:552:G:O6      | 2.25                     | 0.67              |
| 63:LL:14:PRO:O     | 63:LL:15:THR:OG1   | 2.11                     | 0.67              |
| 86:ii:287:ILE:HD13 | 86:ii:399:GLY:HA2  | 1.77                     | 0.67              |
| 7:G:161:VAL:HG13   | 7:G:200:THR:HG22   | 1.77                     | 0.67              |
| 48:5:2811:G:N1     | 48:5:2814:C:OP2    | 2.23                     | 0.67              |
| 87:jj:114:ILE:HG22 | 87:jj:114:ILE:O    | 1.94                     | 0.67              |
| 48:5:5068:G:N2     | 48:5:5069:U:O4     | 2.19                     | 0.67              |
| 29:d:36:VAL:HG21   | 29:d:44:ARG:HG2    | 1.76                     | 0.67              |
| 48:5:4903:G:N1     | 48:5:4918:C:N3     | 2.39                     | 0.67              |
| 53:BB:225:LEU:HD23 | 53:BB:229:MET:HE3  | 1.76                     | 0.67              |
| 71:TT:30:VAL:CG1   | 71:TT:34:VAL:HG21  | 2.24                     | 0.67              |
| 48:5:4682:U:OP2    | 92:5:5413:HOH:O    | 2.12                     | 0.66              |
| 7:G:182:CYS:HB3    | 7:G:222:ILE:HD12   | 1.78                     | 0.66              |
| 17:R:151:ARG:NH1   | 63:LL:119:ASP:OD2  | 2.28                     | 0.66              |
| 51:9:834:C:H2'     | 51:9:835:C:O4'     | 1.96                     | 0.66              |
| 51:9:1160:U:OP2    | 75:XX:4:CYS:O      | 2.13                     | 0.66              |
| 55:DD:51:LEU:HG    | 55:DD:91:VAL:HG22  | 1.76                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:L:135:LYS:N     | 11:L:138:ASP:OD2   | 2.29                     | 0.66              |
| 43:s:139:GLN:OE1   | 87:jj:433:ARG:NH2  | 2.28                     | 0.66              |
| 54:CC:191:VAL:HG11 | 54:CC:236:PHE:HA   | 1.78                     | 0.66              |
| 58:GG:6:SER:OG     | 58:GG:112:VAL:HG12 | 1.95                     | 0.66              |
| 8:H:37:ASP:OD1     | 8:H:39:ASN:OD1     | 2.13                     | 0.66              |
| 51:9:1403:C:N4     | 51:9:1436:C:OP2    | 2.29                     | 0.66              |
| 47:3:54:U:H3       | 47:3:58:A:H62      | 1.44                     | 0.66              |
| 55:DD:8:LYS:O      | 55:DD:12:VAL:HG23  | 1.94                     | 0.66              |
| 46:2:18:G:OP2      | 46:2:60:A:O2'      | 2.13                     | 0.66              |
| 84:gg:288:SER:C    | 84:gg:289:LEU:HD23 | 2.21                     | 0.66              |
| 86:ii:326:LEU:HD21 | 86:ii:409:ILE:CD1  | 2.25                     | 0.66              |
| 48:5:3865:A:OP2    | 92:5:5416:HOH:O    | 2.13                     | 0.66              |
| 69:RR:106:LEU:HD23 | 69:RR:109:LEU:HD12 | 1.78                     | 0.66              |
| 43:s:20:LEU:HD22   | 43:s:52:VAL:CG1    | 2.21                     | 0.66              |
| 70:SS:30:ILE:CG2   | 70:SS:36:VAL:HG11  | 2.26                     | 0.66              |
| 42:r:124:VAL:HG13  | 42:r:125:MET:H     | 1.61                     | 0.65              |
| 51:9:217:A:H2      | 51:9:309:G:H22     | 1.43                     | 0.65              |
| 72:UU:26:SER:HB3   | 72:UU:110:VAL:HG22 | 1.78                     | 0.65              |
| 6:F:52:LYS:NZ      | 6:F:188:ASP:OD2    | 2.18                     | 0.65              |
| 43:s:91:THR:HG21   | 43:s:98:ILE:HD11   | 1.78                     | 0.65              |
| 59:HH:158:LEU:HD11 | 59:HH:187:PHE:HD2  | 1.61                     | 0.65              |
| 60:II:36:THR:OG1   | 60:II:57:ALA:O     | 2.07                     | 0.65              |
| 46:2:74:C:OP1      | 48:5:4548:A:O2'    | 2.13                     | 0.65              |
| 48:5:4719:G:H4'    | 48:5:4720:C:OP1    | 1.95                     | 0.65              |
| 56:EE:21:ASP:OD1   | 56:EE:23:LEU:N     | 2.30                     | 0.65              |
| 56:EE:54:TYR:O     | 76:YY:15:ASN:ND2   | 2.30                     | 0.65              |
| 56:EE:176:ASP:OD1  | 56:EE:177:THR:N    | 2.29                     | 0.65              |
| 4:D:150:LEU:HD12   | 10:J:146:ARG:HG3   | 1.79                     | 0.65              |
| 20:U:92:LYS:NZ     | 48:5:2627:C:OP1    | 2.30                     | 0.65              |
| 24:Y:38:LEU:HD22   | 24:Y:42:TYR:HE2    | 1.61                     | 0.65              |
| 48:5:1480:C:C2'    | 48:5:1483:C:H42    | 2.09                     | 0.65              |
| 48:5:2047:A:C8     | 48:5:2047:A:OP2    | 2.50                     | 0.65              |
| 48:5:2459:G:OP1    | 92:5:5414:HOH:O    | 2.13                     | 0.65              |
| 48:5:4743:G:O2'    | 48:5:4744:A:O5'    | 2.14                     | 0.65              |
| 51:9:208:G:HO2'    | 51:9:209:A:P       | 2.20                     | 0.65              |
| 70:SS:15:VAL:CG1   | 70:SS:68:ILE:HD11  | 2.27                     | 0.65              |
| 48:5:1976:G:N2     | 48:5:1991:A:N7     | 2.45                     | 0.65              |
| 51:9:1419:C:O2     | 51:9:1429:G:N2     | 2.30                     | 0.65              |
| 69:RR:117:LEU:HD23 | 69:RR:118:GLN:N    | 2.11                     | 0.65              |
| 84:gg:253:GLY:O    | 84:gg:286:CYS:N    | 2.29                     | 0.65              |
| 29:d:33:ILE:HG22   | 29:d:44:ARG:HG3    | 1.78                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:DD:53:THR:HG22  | 55:DD:91:VAL:HB    | 1.78                     | 0.65              |
| 59:HH:155:LYS:NZ   | 74:WW:51:GLU:OE2   | 2.23                     | 0.65              |
| 24:Y:102:SER:OG    | 24:Y:103:LYS:NZ    | 2.30                     | 0.65              |
| 29:d:20:VAL:HG12   | 29:d:20:VAL:O      | 1.97                     | 0.65              |
| 76:YY:40:ILE:HD13  | 76:YY:60:PHE:CE2   | 2.32                     | 0.65              |
| 87:jj:552:LEU:HD12 | 87:jj:553:ALA:N    | 2.11                     | 0.65              |
| 48:5:1077:C:N3     | 48:5:1233:G:N1     | 2.40                     | 0.65              |
| 84:gg:173:LEU:HD23 | 84:gg:189:ILE:HG12 | 1.78                     | 0.65              |
| 84:gg:236:ILE:HG21 | 84:gg:239:LEU:HD21 | 1.79                     | 0.65              |
| 86:ii:188:LEU:O    | 86:ii:192:ARG:HG3  | 1.96                     | 0.65              |
| 86:ii:310:LYS:NZ   | 86:ii:314:MET:SD   | 2.70                     | 0.65              |
| 5:E:64:MET:HE2     | 5:E:64:MET:HA      | 1.78                     | 0.64              |
| 55:DD:210:ILE:HG21 | 69:RR:19:LYS:HZ3   | 1.62                     | 0.64              |
| 80:cc:13:ARG:NH2   | 80:cc:35:MET:HE3   | 2.12                     | 0.64              |
| 83:ff:112:LEU:HD12 | 83:ff:113:ARG:HH12 | 1.61                     | 0.64              |
| 87:jj:378:LEU:HD11 | 87:jj:532:VAL:HG11 | 1.78                     | 0.64              |
| 48:5:1991:A:O2'    | 48:5:1992:U:O5'    | 2.14                     | 0.64              |
| 52:AA:178:LEU:O    | 52:AA:182:VAL:HG23 | 1.97                     | 0.64              |
| 86:ii:146:PHE:CD1  | 86:ii:275:LEU:HD22 | 2.32                     | 0.64              |
| 36:k:7:GLU:N       | 36:k:7:GLU:OE1     | 2.30                     | 0.64              |
| 51:9:985:G:H4'     | 66:OO:138:ASP:CG   | 2.22                     | 0.64              |
| 51:9:1542:C:OP1    | 71:TT:62:ARG:NH1   | 2.28                     | 0.64              |
| 55:DD:32:ASP:O     | 55:DD:34:TYR:N     | 2.29                     | 0.64              |
| 61:JJ:58:ARG:O     | 61:JJ:62:THR:HG23  | 1.97                     | 0.64              |
| 48:5:3888:G:O2'    | 48:5:3889:G:OP1    | 2.15                     | 0.64              |
| 62:KK:39:ASN:OD1   | 62:KK:39:ASN:O     | 2.15                     | 0.64              |
| 51:9:691:G:N2      | 51:9:692:G:N7      | 2.45                     | 0.64              |
| 51:9:190:G:O2'     | 51:9:209:A:N6      | 2.29                     | 0.64              |
| 59:HH:153:LEU:HD21 | 59:HH:186:ASN:OD1  | 1.98                     | 0.64              |
| 68:QQ:63:PHE:CE2   | 68:QQ:92:LEU:HD22  | 2.33                     | 0.64              |
| 84:gg:145:GLU:O    | 84:gg:175:LYS:NZ   | 2.30                     | 0.64              |
| 4:D:209:ARG:HA     | 4:D:212:MET:HE2    | 1.80                     | 0.64              |
| 16:Q:122:THR:OG1   | 16:Q:124:ASP:OD1   | 2.14                     | 0.64              |
| 35:j:49:TRP:O      | 48:5:1646:A:O2'    | 2.12                     | 0.64              |
| 48:5:4378:A:O2'    | 48:5:4379:A:H2'    | 1.98                     | 0.64              |
| 84:gg:48:ASP:N     | 84:gg:51:ASN:O     | 2.31                     | 0.64              |
| 84:gg:270:LEU:HD13 | 84:gg:310:TRP:CD2  | 2.33                     | 0.64              |
| 48:5:37:U:OP1      | 92:5:5417:HOH:O    | 2.14                     | 0.64              |
| 51:9:1354:G:N2     | 51:9:1357:A:OP2    | 2.30                     | 0.64              |
| 57:FF:20:PHE:CE2   | 57:FF:69:VAL:HG21  | 2.33                     | 0.64              |
| 1:A:37:ARG:NH2     | 48:5:4088:C:OP1    | 2.26                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:O:173:GLN:OE1   | 14:O:177:LEU:HD12  | 1.98                     | 0.64              |
| 51:9:1281:G:O2'    | 51:9:1282:A:OP1    | 2.10                     | 0.64              |
| 11:L:158:ARG:NH2   | 48:5:1378:C:C5     | 2.66                     | 0.64              |
| 72:UU:48:LEU:CD2   | 72:UU:101:ILE:HD11 | 2.28                     | 0.64              |
| 48:5:2489:C:O2'    | 48:5:2491:C:N4     | 2.31                     | 0.63              |
| 53:BB:225:LEU:CD2  | 53:BB:229:MET:HE3  | 2.28                     | 0.63              |
| 48:5:749:G:O2'     | 48:5:750:U:OP2     | 2.16                     | 0.63              |
| 51:9:1429:G:H2'    | 51:9:1430:C:O4'    | 1.97                     | 0.63              |
| 51:9:1461:G:O2'    | 51:9:1464:C:N4     | 2.31                     | 0.63              |
| 54:CC:94:ILE:HG21  | 54:CC:162:ILE:HD12 | 1.80                     | 0.63              |
| 33:h:35:LYS:HA     | 33:h:44:LEU:HD11   | 1.80                     | 0.63              |
| 48:5:3654:G:O2'    | 48:5:3693:U:OP1    | 2.15                     | 0.63              |
| 48:5:4944:C:OP1    | 48:5:4944:C:H4'    | 1.97                     | 0.63              |
| 51:9:75:G:O2'      | 51:9:76:U:H3'      | 1.97                     | 0.63              |
| 51:9:1351:G:O2'    | 51:9:1378:A:N1     | 2.31                     | 0.63              |
| 55:DD:93:THR:OG1   | 55:DD:96:LEU:HD12  | 1.98                     | 0.63              |
| 66:OO:117:ARG:NH1  | 78:aa:48:ALA:O     | 2.30                     | 0.63              |
| 87:jj:235:ALA:HB3  | 87:jj:238:PHE:HE1  | 1.64                     | 0.63              |
| 48:5:978:G:N2      | 48:5:1277:G:H22    | 1.96                     | 0.63              |
| 48:5:4098:A:H61    | 48:5:4110:C:H42    | 1.46                     | 0.63              |
| 48:5:4635:A:H8     | 48:5:5048:A:H61    | 1.46                     | 0.63              |
| 70:SS:55:ARG:HD2   | 77:ZZ:48:VAL:HG22  | 1.80                     | 0.63              |
| 84:gg:249:CYS:SG   | 84:gg:291:TRP:NE1  | 2.71                     | 0.63              |
| 19:T:70:HIS:NE2    | 48:5:4327:C:OP1    | 2.31                     | 0.63              |
| 58:GG:157:VAL:HG11 | 58:GG:176:ILE:CD1  | 2.25                     | 0.63              |
| 64:MM:85:LEU:HD22  | 64:MM:106:CYS:O    | 1.98                     | 0.63              |
| 67:PP:93:MET:HE2   | 67:PP:106:GLU:HB2  | 1.80                     | 0.63              |
| 3:C:95:MET:HG3     | 48:5:2351:OMC:HM23 | 1.78                     | 0.63              |
| 10:J:105:PHE:HE1   | 10:J:134:LEU:HD11  | 1.63                     | 0.63              |
| 48:5:406:C:O2'     | 48:5:407:A:OP1     | 2.14                     | 0.63              |
| 59:HH:95:ILE:HD12  | 59:HH:129:ILE:HG23 | 1.81                     | 0.63              |
| 63:LL:111:VAL:HG12 | 63:LL:140:PHE:HB2  | 1.80                     | 0.63              |
| 84:gg:8:ARG:HA     | 84:gg:8:ARG:HE     | 1.64                     | 0.63              |
| 84:gg:270:LEU:HD22 | 84:gg:310:TRP:CE3  | 2.34                     | 0.63              |
| 46:2:54:U:H2'      | 46:2:55:U:O4'      | 1.99                     | 0.63              |
| 51:9:176:U:H2'     | 51:9:177:G:O4'     | 1.98                     | 0.63              |
| 80:cc:26:GLN:OE1   | 80:cc:26:GLN:N     | 2.31                     | 0.63              |
| 32:g:45:ALA:HB3    | 32:g:82:MET:HE2    | 1.81                     | 0.63              |
| 63:LL:65:ASN:O     | 63:LL:132:ARG:NH1  | 2.32                     | 0.63              |
| 72:UU:26:SER:CB    | 72:UU:110:VAL:HG22 | 2.28                     | 0.63              |
| 84:gg:198:VAL:HA   | 84:gg:209:SER:HA   | 1.80                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 87:jj:271:VAL:HG11 | 87:jj:282:LEU:HD21 | 1.81                     | 0.63              |
| 44:t:21:GLU:HG2    | 44:t:56:LEU:HD12   | 1.81                     | 0.62              |
| 51:9:495:U:H2'     | 51:9:496:C:O4'     | 1.99                     | 0.62              |
| 67:PP:60:LEU:HD12  | 67:PP:92:SER:OG    | 1.99                     | 0.62              |
| 86:ii:374:LEU:O    | 86:ii:374:LEU:HD23 | 1.99                     | 0.62              |
| 4:D:166:ALA:HB1    | 4:D:171:LEU:HD12   | 1.81                     | 0.62              |
| 7:G:86:VAL:HG13    | 7:G:183:ILE:HG22   | 1.81                     | 0.62              |
| 20:U:23:LEU:HD21   | 20:U:87:THR:OG1    | 1.99                     | 0.62              |
| 51:9:1406:G:N2     | 51:9:1442:OMU:O4   | 2.32                     | 0.62              |
| 51:9:1490:OMG:N2   | 72:UU:72:GLU:OE1   | 2.32                     | 0.62              |
| 52:AA:34:MET:HE2   | 52:AA:149:ASN:C    | 2.24                     | 0.62              |
| 3:C:254:GLU:OE2    | 3:C:258:ARG:NH1    | 2.30                     | 0.62              |
| 47:3:43:A:H2'      | 47:3:44:G:C8       | 2.33                     | 0.62              |
| 52:AA:119:PRO:O    | 52:AA:142:LEU:HD13 | 1.99                     | 0.62              |
| 72:UU:48:LEU:HD21  | 72:UU:97:ILE:HG22  | 1.82                     | 0.62              |
| 74:WW:86:LEU:HD21  | 74:WW:104:LEU:HD11 | 1.80                     | 0.62              |
| 48:5:3689:G:O2'    | 48:5:3818:UY1:OP2  | 2.17                     | 0.62              |
| 51:9:1347:PSU:H2'  | 51:9:1348:G:C8     | 2.34                     | 0.62              |
| 56:EE:248:ILE:HD12 | 61:JJ:72:PHE:CD2   | 2.33                     | 0.62              |
| 84:gg:23:THR:HG22  | 84:gg:24:THR:H     | 1.65                     | 0.62              |
| 18:S:169:THR:HG21  | 48:5:4875:G:C5     | 2.34                     | 0.62              |
| 30:e:21:ILE:HD11   | 30:e:53:ILE:HD11   | 1.81                     | 0.62              |
| 51:9:1740:C:OP1    | 60:II:44:HIS:ND1   | 2.30                     | 0.62              |
| 62:KK:72:THR:O     | 62:KK:76:ILE:HG13  | 1.99                     | 0.62              |
| 84:gg:199:THR:OG1  | 84:gg:200:VAL:N    | 2.32                     | 0.62              |
| 48:5:1477:C:O2'    | 48:5:1478:C:OP1    | 2.18                     | 0.62              |
| 51:9:1664:A:O2'    | 51:9:1666:C:N4     | 2.33                     | 0.62              |
| 62:KK:16:PHE:HE1   | 62:KK:76:ILE:HG23  | 1.63                     | 0.62              |
| 69:RR:90:ALA:O     | 69:RR:93:GLN:NE2   | 2.32                     | 0.62              |
| 74:WW:50:PHE:HB3   | 74:WW:63:VAL:HG13  | 1.82                     | 0.62              |
| 86:ii:308:THR:O    | 86:ii:312:LEU:HD12 | 1.99                     | 0.62              |
| 48:5:914:U:O2'     | 48:5:915:A:O4'     | 2.18                     | 0.62              |
| 48:5:3899:OMG:OP2  | 92:5:5418:HOH:O    | 2.16                     | 0.62              |
| 48:5:4605:A:H2'    | 48:5:4606:G:O4'    | 2.00                     | 0.62              |
| 51:9:846:G:C4      | 56:EE:19:MET:HE3   | 2.34                     | 0.62              |
| 35:j:26:ALA:O      | 35:j:34:CYS:O      | 2.18                     | 0.62              |
| 48:5:734:G:H1      | 48:5:929:A:H62     | 1.47                     | 0.62              |
| 50:8:83:C:H4'      | 50:8:85:U:O2       | 2.00                     | 0.62              |
| 58:GG:102:VAL:HG23 | 58:GG:106:LEU:CD1  | 2.29                     | 0.62              |
| 87:jj:128:LYS:NZ   | 87:jj:138:PRO:O    | 2.32                     | 0.62              |
| 69:RR:11:LYS:O     | 69:RR:15:VAL:HG23  | 2.00                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:2409:U:H5     | 48:5:2783:A:N1     | 1.97                     | 0.62              |
| 56:EE:19:MET:SD    | 56:EE:108:ARG:HD2  | 2.40                     | 0.62              |
| 57:FF:99:ILE:HG22  | 57:FF:103:LEU:HD12 | 1.82                     | 0.62              |
| 6:F:25:ALA:O       | 6:F:29:ILE:HD13    | 1.99                     | 0.61              |
| 51:9:1589:A:N3     | 51:9:1653:U:O2'    | 2.29                     | 0.61              |
| 67:PP:100:LYS:HG3  | 67:PP:101:THR:HG23 | 1.82                     | 0.61              |
| 72:UU:40:ILE:HG23  | 72:UU:50:VAL:HG11  | 1.81                     | 0.61              |
| 83:ff:127:MET:HE2  | 83:ff:136:CYS:N    | 2.16                     | 0.61              |
| 84:gg:79:LEU:HD21  | 84:gg:120:ILE:CG2  | 2.30                     | 0.61              |
| 12:M:119:ARG:NE    | 14:O:193:THR:OG1   | 2.32                     | 0.61              |
| 49:7:98:G:O6       | 92:7:302:HOH:O     | 2.12                     | 0.61              |
| 84:gg:191:HIS:CG   | 84:gg:195:LEU:HD21 | 2.34                     | 0.61              |
| 3:C:193:LYS:HD2    | 3:C:196:MET:HE2    | 1.82                     | 0.61              |
| 4:D:3:PHE:HD2      | 48:5:1753:G:H21    | 1.49                     | 0.61              |
| 36:k:23:VAL:HG23   | 36:k:64:LEU:HG     | 1.81                     | 0.61              |
| 51:9:3:C:O2        | 61:JJ:18:ARG:NH2   | 2.29                     | 0.61              |
| 51:9:586:G:OP1     | 61:JJ:176:LYS:NZ   | 2.31                     | 0.61              |
| 51:9:1350:U:O2'    | 52:AA:110:ASN:OD1  | 2.09                     | 0.61              |
| 58:GG:102:VAL:HG21 | 58:GG:109:LEU:CD2  | 2.26                     | 0.61              |
| 60:II:149:TYR:O    | 60:II:153:LYS:HG2  | 2.00                     | 0.61              |
| 48:5:1979:A:H2'    | 48:5:1980:U:C1'    | 2.30                     | 0.61              |
| 51:9:833:C:O2'     | 51:9:834:C:O5'     | 2.16                     | 0.61              |
| 51:9:1348:G:H22    | 51:9:1381:G:N2     | 1.98                     | 0.61              |
| 68:QQ:128:GLU:CD   | 68:QQ:137:ALA:HB1  | 2.25                     | 0.61              |
| 61:JJ:108:ARG:O    | 61:JJ:149:VAL:HG22 | 2.00                     | 0.61              |
| 70:SS:30:ILE:HD11  | 70:SS:67:VAL:HG11  | 1.82                     | 0.61              |
| 81:dd:31:ILE:HB    | 81:dd:36:LEU:HD23  | 1.83                     | 0.61              |
| 84:gg:207:CYS:HB2  | 84:gg:221:LEU:HD11 | 1.82                     | 0.61              |
| 87:jj:428:LEU:HD23 | 87:jj:474:LEU:HD23 | 1.82                     | 0.61              |
| 1:A:137:ILE:HD11   | 1:A:149:LYS:HB2    | 1.82                     | 0.61              |
| 48:5:711:A:H2'     | 48:5:712:C:C6      | 2.36                     | 0.61              |
| 51:9:488:U:O2      | 51:9:488:U:H2'     | 2.01                     | 0.61              |
| 51:9:1588:A:H2'    | 51:9:1589:A:C8     | 2.36                     | 0.61              |
| 53:BB:73:ASP:OD1   | 66:OO:128:ARG:NE   | 2.29                     | 0.61              |
| 8:H:43:VAL:HG21    | 8:H:73:ILE:HD13    | 1.83                     | 0.61              |
| 16:Q:150:ARG:NH1   | 48:5:1498:G:OP1    | 2.29                     | 0.61              |
| 48:5:2502:A:O2'    | 48:5:2503:G:OP1    | 2.09                     | 0.61              |
| 51:9:333:G:H2'     | 51:9:334:C:O4'     | 2.00                     | 0.61              |
| 51:9:1745:A:H1'    | 58:GG:66:GLY:HA2   | 1.82                     | 0.61              |
| 67:PP:107:ILE:HA   | 67:PP:111:MET:SD   | 2.40                     | 0.61              |
| 87:jj:529:ALA:HB3  | 87:jj:551:LEU:HD11 | 1.83                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:L:125:VAL:HG22  | 33:h:123:ALA:HB3   | 1.82                     | 0.61              |
| 42:r:80:THR:HG21   | 42:r:96:MET:HE1    | 1.83                     | 0.61              |
| 51:9:1348:G:H22    | 51:9:1381:G:H22    | 1.47                     | 0.61              |
| 53:BB:114:VAL:HG22 | 53:BB:120:MET:CE   | 2.31                     | 0.61              |
| 76:YY:55:ILE:CD1   | 76:YY:75:ILE:HD12  | 2.30                     | 0.61              |
| 13:N:45:PRO:O      | 13:N:49:ARG:HG3    | 2.01                     | 0.61              |
| 54:CC:102:LEU:HD22 | 54:CC:130:ILE:HG12 | 1.83                     | 0.61              |
| 48:5:758:G:H2'     | 48:5:759:G:O4'     | 2.01                     | 0.60              |
| 48:5:2568:C:N4     | 48:5:2569:G:O6     | 2.32                     | 0.60              |
| 55:DD:177:LEU:CD1  | 55:DD:182:LEU:HD12 | 2.30                     | 0.60              |
| 63:LL:42:LEU:HD13  | 63:LL:72:ILE:HD11  | 1.83                     | 0.60              |
| 86:ii:347:THR:OG1  | 86:ii:350:GLN:OE1  | 2.13                     | 0.60              |
| 87:jj:240:PHE:HB2  | 87:jj:271:VAL:HG12 | 1.82                     | 0.60              |
| 13:N:108:ARG:NH2   | 48:5:54:G:O2'      | 2.32                     | 0.60              |
| 18:S:24:THR:O      | 18:S:24:THR:HG22   | 1.99                     | 0.60              |
| 58:GG:7:PHE:HB2    | 58:GG:113:ILE:HD12 | 1.83                     | 0.60              |
| 48:5:1234:G:O2'    | 48:5:1235:G:OP2    | 2.17                     | 0.60              |
| 48:5:1377:G:H21    | 48:5:1380:G:H5'    | 1.65                     | 0.60              |
| 56:EE:112:HIS:NE2  | 56:EE:237:SER:OG   | 2.34                     | 0.60              |
| 58:GG:145:PHE:HB2  | 58:GG:147:LEU:HD11 | 1.83                     | 0.60              |
| 87:jj:223:GLN:HE21 | 87:jj:247:LEU:HD21 | 1.66                     | 0.60              |
| 7:G:83:PHE:HA      | 7:G:183:ILE:HD13   | 1.82                     | 0.60              |
| 7:G:254:GLU:OE1    | 7:G:255:LYS:N      | 2.34                     | 0.60              |
| 45:1:63:SER:O      | 45:1:66:LEU:HD13   | 2.01                     | 0.60              |
| 49:7:111:C:H2'     | 49:7:112:U:O4'     | 2.01                     | 0.60              |
| 51:9:1466:G:C5'    | 69:RR:4:VAL:HG22   | 2.30                     | 0.60              |
| 86:ii:145:LYS:O    | 86:ii:222:ALA:N    | 2.32                     | 0.60              |
| 22:W:44:ARG:NE     | 48:5:3615:G:N3     | 2.46                     | 0.60              |
| 48:5:1235:G:HO2'   | 48:5:1236:C:P      | 2.21                     | 0.60              |
| 76:YY:55:ILE:O     | 76:YY:94:HIS:NE2   | 2.31                     | 0.60              |
| 48:5:4407:G:N7     | 92:5:5458:HOH:O    | 2.31                     | 0.60              |
| 51:9:94:G:N7       | 92:9:2019:HOH:O    | 2.31                     | 0.60              |
| 52:AA:62:ALA:O     | 52:AA:66:VAL:HG23  | 2.02                     | 0.60              |
| 59:HH:169:LYS:O    | 59:HH:172:THR:OG1  | 2.16                     | 0.60              |
| 48:5:263:G:H2'     | 48:5:264:C:O4'     | 2.02                     | 0.60              |
| 48:5:1432:G:O2'    | 48:5:1451:G:N2     | 2.33                     | 0.60              |
| 54:CC:146:GLU:OE1  | 55:DD:116:ARG:NH1  | 2.35                     | 0.60              |
| 58:GG:66:GLY:O     | 58:GG:68:LEU:HD12  | 2.02                     | 0.60              |
| 48:5:4739:C:N4     | 48:5:4740:G:O6     | 2.34                     | 0.60              |
| 51:9:1535:U:O4     | 57:FF:159:ARG:NH1  | 2.33                     | 0.60              |
| 53:BB:120:MET:HE2  | 53:BB:142:PHE:CE2  | 2.37                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 72:UU:44:LYS:HE2   | 72:UU:44:LYS:HA    | 1.82                     | 0.60              |
| 84:gg:305:ASN:O    | 84:gg:306:LEU:HD12 | 2.02                     | 0.60              |
| 47:3:6:G:H2'       | 47:3:7:A:C8        | 2.36                     | 0.60              |
| 48:5:3641:U:H5     | 48:5:3646:A:N7     | 1.99                     | 0.60              |
| 87:jj:59:GLY:HA2   | 87:jj:62:ILE:HD13  | 1.84                     | 0.60              |
| 13:N:67:ARG:NH2    | 48:5:3673:C:OP2    | 2.34                     | 0.60              |
| 48:5:470:A:N6      | 48:5:684:G:O2'     | 2.34                     | 0.60              |
| 48:5:1238:A:O2'    | 48:5:1239:C:OP1    | 2.18                     | 0.60              |
| 60:II:57:ALA:HB2   | 60:II:183:GLY:HA2  | 1.84                     | 0.60              |
| 80:cc:20:ARG:CD    | 80:cc:28:THR:HG22  | 2.32                     | 0.60              |
| 84:gg:40:ILE:HD11  | 84:gg:66:VAL:HG21  | 1.84                     | 0.60              |
| 84:gg:198:VAL:O    | 84:gg:198:VAL:HG12 | 2.01                     | 0.60              |
| 86:ii:372:MET:HE3  | 86:ii:376:GLU:OE2  | 2.02                     | 0.60              |
| 87:jj:428:LEU:O    | 87:jj:432:ILE:O    | 2.20                     | 0.60              |
| 51:9:695:C:N4      | 51:9:735:C:H42     | 2.00                     | 0.59              |
| 51:9:862:A:O2'     | 51:9:863:PSU:H5''  | 2.02                     | 0.59              |
| 56:EE:115:THR:OG1  | 56:EE:117:GLU:O    | 2.18                     | 0.59              |
| 86:ii:34:MET:HE1   | 86:ii:100:ILE:HG22 | 1.82                     | 0.59              |
| 87:jj:485:ILE:HB   | 87:jj:517:VAL:HG22 | 1.84                     | 0.59              |
| 25:Z:136:PHE:OXT   | 48:5:4122:G:O2'    | 2.20                     | 0.59              |
| 51:9:932:G:O2'     | 51:9:934:G:OP2     | 2.10                     | 0.59              |
| 68:QQ:31:LEU:HD11  | 68:QQ:33:LYS:HD3   | 1.84                     | 0.59              |
| 75:XX:89:GLY:HA2   | 82:ee:9:VAL:HG12   | 1.82                     | 0.59              |
| 86:ii:77:SER:OG    | 86:ii:111:ASN:OD1  | 2.19                     | 0.59              |
| 87:jj:169:LYS:HB2  | 87:jj:230:VAL:HG21 | 1.84                     | 0.59              |
| 1:A:207:VAL:HG13   | 1:A:208:GLU:HG3    | 1.83                     | 0.59              |
| 29:d:87:ARG:NH2    | 29:d:122:VAL:HG11  | 2.17                     | 0.59              |
| 47:3:70:G:O2'      | 48:5:3740:G:O2'    | 1.98                     | 0.59              |
| 51:9:1306:U:H3'    | 51:9:1307:U:H5''   | 1.84                     | 0.59              |
| 53:BB:114:VAL:HG22 | 53:BB:120:MET:HE1  | 1.84                     | 0.59              |
| 51:9:1466:G:OP2    | 69:RR:5:ARG:NH1    | 2.35                     | 0.59              |
| 57:FF:71:ARG:NH2   | 57:FF:148:ASN:OD1  | 2.34                     | 0.59              |
| 57:FF:142:SER:HB2  | 80:cc:50:VAL:HG12  | 1.84                     | 0.59              |
| 42:r:66:ARG:NH1    | 42:r:75:THR:O      | 2.32                     | 0.59              |
| 67:PP:26:LEU:HD12  | 67:PP:26:LEU:O     | 2.02                     | 0.59              |
| 87:jj:371:ASP:HA   | 87:jj:514:THR:HG22 | 1.83                     | 0.59              |
| 44:t:28:LEU:HD23   | 44:t:28:LEU:C      | 2.28                     | 0.59              |
| 48:5:1547:A:O2'    | 48:5:2814:C:O2     | 2.18                     | 0.59              |
| 51:9:546:G:H2'     | 51:9:547:G:O4'     | 2.02                     | 0.59              |
| 51:9:1109:C:HO2'   | 51:9:1110:G:C1'    | 2.13                     | 0.59              |
| 51:9:1298:G:O2'    | 51:9:1299:A:O4'    | 2.20                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:1408:U:O2'    | 51:9:1409:A:C5'    | 2.51                     | 0.59              |
| 61:JJ:163:SER:O    | 61:JJ:166:GLY:N    | 2.34                     | 0.59              |
| 67:PP:87:PRO:HA    | 67:PP:112:ILE:HD11 | 1.83                     | 0.59              |
| 86:ii:219:VAL:HG11 | 86:ii:249:LYS:HG3  | 1.83                     | 0.59              |
| 51:9:1261:C:O2     | 81:dd:10:HIS:NE2   | 2.35                     | 0.59              |
| 52:AA:190:SER:O    | 52:AA:191:ARG:HB3  | 2.02                     | 0.59              |
| 9:I:38:ARG:NH1     | 9:I:45:GLU:OE2     | 2.34                     | 0.59              |
| 35:j:36:LYS:NZ     | 48:5:372:A:OP1     | 2.33                     | 0.59              |
| 36:k:15:ALA:O      | 36:k:64:LEU:HD22   | 2.03                     | 0.59              |
| 43:s:13:TYR:CE1    | 43:s:54:LEU:HD21   | 2.38                     | 0.59              |
| 51:9:1295:A:H2'    | 51:9:1296:U:O4'    | 2.02                     | 0.59              |
| 26:a:39:HIS:O      | 26:a:40:HIS:ND1    | 2.35                     | 0.59              |
| 48:5:2501:C:H2'    | 48:5:2502:A:O4'    | 2.02                     | 0.59              |
| 48:5:2639:U:H2'    | 48:5:2694:G:H1     | 1.68                     | 0.59              |
| 52:AA:42:LYS:HD2   | 52:AA:48:ILE:HD11  | 1.83                     | 0.59              |
| 20:U:97:ARG:NH1    | 48:5:2626:U:O4     | 2.35                     | 0.59              |
| 51:9:1139:C:H5     | 51:9:1149:A:H62    | 1.49                     | 0.59              |
| 57:FF:32:ASP:O     | 57:FF:34:SER:N     | 2.36                     | 0.59              |
| 44:t:18:THR:OG1    | 44:t:59:THR:O      | 2.18                     | 0.58              |
| 47:3:75:C:O2'      | 47:3:76:A:H4'      | 2.03                     | 0.58              |
| 48:5:165:A:H2'     | 48:5:166:C:O4'     | 2.02                     | 0.58              |
| 54:CC:255:LEU:HD23 | 73:VV:1:MET:CE     | 2.29                     | 0.58              |
| 58:GG:181:THR:CG2  | 58:GG:182:PRO:HD2  | 2.33                     | 0.58              |
| 68:QQ:105:LYS:C    | 68:QQ:105:LYS:HD3  | 2.28                     | 0.58              |
| 42:r:38:PHE:O      | 42:r:45:HIS:NE2    | 2.29                     | 0.58              |
| 43:s:45:MET:HA     | 43:s:45:MET:HE3    | 1.86                     | 0.58              |
| 51:9:323:C:H3'     | 51:9:324:C:H5''    | 1.85                     | 0.58              |
| 51:9:563:G:O2'     | 51:9:564:A:O5'     | 2.19                     | 0.58              |
| 55:DD:210:ILE:N    | 55:DD:210:ILE:HD12 | 2.19                     | 0.58              |
| 59:HH:79:LEU:HD23  | 59:HH:83:LEU:HD13  | 1.84                     | 0.58              |
| 69:RR:14:ARG:HG2   | 69:RR:69:ILE:HD11  | 1.84                     | 0.58              |
| 86:ii:305:VAL:HG13 | 86:ii:306:GLU:N    | 2.19                     | 0.58              |
| 48:5:1098:G:N3     | 48:5:1198:G:N2     | 2.52                     | 0.58              |
| 57:FF:35:LEU:HD12  | 57:FF:117:ILE:HG12 | 1.85                     | 0.58              |
| 58:GG:102:VAL:HG23 | 58:GG:106:LEU:HD11 | 1.85                     | 0.58              |
| 69:RR:40:ILE:O     | 69:RR:40:ILE:HG13  | 2.04                     | 0.58              |
| 27:b:44:ARG:NH2    | 48:5:1466:G:OP2    | 2.35                     | 0.58              |
| 28:c:99:PRO:HG3    | 28:c:105:ILE:HD12  | 1.84                     | 0.58              |
| 39:n:18:ARG:NH2    | 51:9:1183:A:OP2    | 2.37                     | 0.58              |
| 43:s:29:ILE:HD11   | 43:s:78:LEU:HD13   | 1.85                     | 0.58              |
| 52:AA:85:ARG:NH2   | 69:RR:82:ASP:O     | 2.37                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 54:CC:146:GLU:OE1 | 55:DD:116:ARG:HD2  | 2.04                     | 0.58              |
| 70:SS:36:VAL:HG22 | 70:SS:40:TYR:CD2   | 2.38                     | 0.58              |
| 87:jj:78:ASN:OD1  | 87:jj:79:LEU:N     | 2.36                     | 0.58              |
| 87:jj:79:LEU:O    | 87:jj:82:GLU:N     | 2.33                     | 0.58              |
| 3:C:196:MET:HE3   | 48:5:352:G:C5      | 2.39                     | 0.58              |
| 4:D:261:VAL:HG21  | 49:7:119:U:C2      | 2.38                     | 0.58              |
| 51:9:465:A:OP1    | 87:jj:584:LYS:NZ   | 2.36                     | 0.58              |
| 87:jj:221:GLU:OE1 | 87:jj:221:GLU:N    | 2.37                     | 0.58              |
| 7:G:136:LEU:HD21  | 7:G:204:PHE:CD2    | 2.39                     | 0.58              |
| 48:5:1198:G:H2'   | 48:5:1199:G:C1'    | 2.34                     | 0.58              |
| 48:5:1475:G:O2'   | 48:5:1476:C:O4'    | 2.10                     | 0.58              |
| 51:9:986:G:C8     | 66:OO:137:SER:O    | 2.56                     | 0.58              |
| 60:II:100:CYS:SG  | 60:II:175:ILE:HD12 | 2.43                     | 0.58              |
| 75:XX:123:VAL:C   | 75:XX:130:LEU:HD12 | 2.29                     | 0.58              |
| 23:X:95:THR:HG22  | 23:X:139:ARG:HA    | 1.85                     | 0.58              |
| 48:5:1320:U:O2'   | 48:5:1891:A:N1     | 2.34                     | 0.58              |
| 67:PP:30:TYR:O    | 67:PP:34:MET:HG3   | 2.03                     | 0.58              |
| 86:ii:34:MET:HE1  | 86:ii:100:ILE:CG2  | 2.33                     | 0.58              |
| 4:D:278:ASP:OD2   | 48:5:1185:G:O2'    | 2.22                     | 0.58              |
| 11:L:7:GLY:O      | 26:a:49:HIS:NE2    | 2.37                     | 0.58              |
| 26:a:77:LYS:HE2   | 48:5:1502:G:H22    | 1.69                     | 0.58              |
| 53:BB:225:LEU:O   | 53:BB:229:MET:HG2  | 2.04                     | 0.58              |
| 84:gg:32:LEU:HB3  | 84:gg:71:ILE:HD11  | 1.85                     | 0.58              |
| 86:ii:317:VAL:O   | 86:ii:317:VAL:HG13 | 2.02                     | 0.58              |
| 3:C:4:ALA:O       | 3:C:29:LYS:NZ      | 2.32                     | 0.58              |
| 48:5:1978:C:N4    | 48:5:1979:A:C2     | 2.72                     | 0.58              |
| 48:5:2564:G:O2'   | 48:5:2565:A:O4'    | 2.17                     | 0.58              |
| 48:5:2795:A:OP1   | 92:5:5423:HOH:O    | 2.17                     | 0.58              |
| 48:5:3603:G:HO2'  | 48:5:3604:A:P      | 2.25                     | 0.58              |
| 48:5:4348:A:O2'   | 48:5:4350:C:OP2    | 2.22                     | 0.58              |
| 51:9:77:A:O2'     | 58:GG:174:PRO:O    | 2.15                     | 0.58              |
| 67:PP:41:GLN:HG3  | 67:PP:84:ILE:HD12  | 1.85                     | 0.58              |
| 25:Z:74:VAL:HG23  | 25:Z:101:PHE:HE2   | 1.69                     | 0.57              |
| 48:5:4208:U:OP1   | 48:5:4334:U:O2'    | 2.21                     | 0.57              |
| 51:9:25:A:O2'     | 51:9:26:U:O5'      | 2.22                     | 0.57              |
| 51:9:420:G:O2'    | 51:9:660:C:N3      | 2.33                     | 0.57              |
| 51:9:1240:A:H8    | 51:9:1267:C:HO2'   | 1.52                     | 0.57              |
| 61:JJ:110:LEU:O   | 61:JJ:114:VAL:HG23 | 2.03                     | 0.57              |
| 84:gg:178:ASN:O   | 84:gg:182:CYS:N    | 2.32                     | 0.57              |
| 48:5:4444:C:OP1   | 92:5:5424:HOH:O    | 2.17                     | 0.57              |
| 51:9:308:G:N3     | 60:II:45:THR:HG22  | 2.18                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:RR:27:ASP:OD2   | 69:RR:30:THR:OG1   | 2.09                     | 0.57              |
| 84:gg:210:GLY:HA3  | 84:gg:239:LEU:HD11 | 1.86                     | 0.57              |
| 25:Z:97:ASN:OD1    | 25:Z:100:VAL:HG13  | 2.05                     | 0.57              |
| 51:9:147:A:H2'     | 51:9:148:U:C6      | 2.39                     | 0.57              |
| 53:BB:39:PHE:CE2   | 53:BB:74:LEU:HD13  | 2.39                     | 0.57              |
| 55:DD:138:VAL:HG12 | 55:DD:184:ILE:CD1  | 2.33                     | 0.57              |
| 58:GG:7:PHE:CZ     | 58:GG:9:ALA:HB3    | 2.38                     | 0.57              |
| 84:gg:74:ASP:HB3   | 84:gg:76:GLN:HG2   | 1.86                     | 0.57              |
| 7:G:106:THR:HG22   | 7:G:107:LYS:H      | 1.69                     | 0.57              |
| 48:5:130:C:H2'     | 48:5:131:C:O4'     | 2.04                     | 0.57              |
| 48:5:504:G:O2'     | 48:5:505:G:OP1     | 2.21                     | 0.57              |
| 48:5:1098:G:N1     | 48:5:1196:G:O6     | 2.36                     | 0.57              |
| 48:5:4393:G:O4'    | 48:5:4447:5MC:HM53 | 2.05                     | 0.57              |
| 48:5:5016:A:H2     | 48:5:5033:G:H21    | 1.44                     | 0.57              |
| 51:9:1391:OMC:HM23 | 81:dd:56:ASP:HB2   | 1.87                     | 0.57              |
| 56:EE:117:GLU:OE2  | 56:EE:118:GLU:N    | 2.35                     | 0.57              |
| 67:PP:22:LEU:O     | 67:PP:25:LEU:N     | 2.37                     | 0.57              |
| 70:SS:5:ILE:N      | 77:ZZ:50:PHE:O     | 2.36                     | 0.57              |
| 80:cc:52:GLU:OE1   | 80:cc:52:GLU:N     | 2.33                     | 0.57              |
| 48:5:158:A:N1      | 48:5:276:C:O2'     | 2.32                     | 0.57              |
| 48:5:4118:U:O2'    | 48:5:4119:C:OP2    | 2.21                     | 0.57              |
| 51:9:562:U:H2'     | 51:9:563:G:C8      | 2.40                     | 0.57              |
| 86:ii:100:ILE:HD11 | 86:ii:108:LYS:HD3  | 1.86                     | 0.57              |
| 48:5:485:C:O2'     | 48:5:486:C:O5'     | 2.22                     | 0.57              |
| 48:5:930:G:O2'     | 48:5:931:C:P       | 2.63                     | 0.57              |
| 51:9:942:G:H2'     | 51:9:943:U:C6      | 2.40                     | 0.57              |
| 51:9:1018:U:H5''   | 65:NN:71:ILE:HD12  | 1.87                     | 0.57              |
| 67:PP:37:TYR:OH    | 67:PP:86:LEU:HD23  | 2.05                     | 0.57              |
| 75:XX:91:LEU:HB3   | 82:ee:9:VAL:HG11   | 1.87                     | 0.57              |
| 86:ii:169:LEU:HB2  | 86:ii:212:LEU:HD13 | 1.86                     | 0.57              |
| 42:r:66:ARG:O      | 48:5:479:G:OP1     | 2.21                     | 0.57              |
| 48:5:1380:G:H4'    | 48:5:1381:U:O2     | 2.05                     | 0.57              |
| 48:5:4635:A:H3'    | 48:5:4636:U:H4'    | 1.85                     | 0.57              |
| 52:AA:168:ALA:HB1  | 52:AA:204:TYR:HB3  | 1.85                     | 0.57              |
| 11:L:36:ARG:NH1    | 48:5:1364:U:OP2    | 2.37                     | 0.57              |
| 51:9:57:U:OP1      | 51:9:504:G:O2'     | 2.20                     | 0.57              |
| 51:9:1394:G:HO2'   | 51:9:1395:C:P      | 2.27                     | 0.57              |
| 52:AA:11:LYS:O     | 52:AA:15:VAL:HG13  | 2.05                     | 0.57              |
| 71:TT:13:GLU:OE2   | 71:TT:16:ARG:NH1   | 2.38                     | 0.57              |
| 25:Z:102:ARG:HG2   | 25:Z:102:ARG:HH11  | 1.70                     | 0.57              |
| 51:9:561:A:H2'     | 51:9:562:U:O4'     | 2.05                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:1373:C:O2'    | 51:9:1465:A:O2'    | 2.07                     | 0.57              |
| 60:II:61:ASP:OD1   | 60:II:61:ASP:N     | 2.38                     | 0.57              |
| 61:JJ:113:GLN:OE1  | 61:JJ:113:GLN:HA   | 2.04                     | 0.57              |
| 31:f:106:TYR:HB2   | 31:f:107:PRO:HD3   | 1.85                     | 0.57              |
| 44:t:128:THR:O     | 44:t:132:ILE:HG13  | 2.05                     | 0.57              |
| 48:5:4136:G:N1     | 48:5:4148:C:N3     | 2.44                     | 0.57              |
| 51:9:686:PSU:O4    | 59:HH:118:ARG:NH2  | 2.38                     | 0.57              |
| 51:9:1536:G:H2'    | 51:9:1537:A:C8     | 2.39                     | 0.57              |
| 70:SS:84:LEU:HD12  | 70:SS:95:TYR:HB3   | 1.86                     | 0.57              |
| 84:gg:52:TYR:CZ    | 84:gg:309:VAL:HG21 | 2.39                     | 0.57              |
| 7:G:161:VAL:O      | 7:G:161:VAL:CG1    | 2.53                     | 0.56              |
| 16:Q:49:LYS:HG2    | 16:Q:53:MET:HE3    | 1.87                     | 0.56              |
| 48:5:1980:U:O2'    | 48:5:1982:G:H3'    | 2.05                     | 0.56              |
| 51:9:147:A:O2'     | 51:9:148:U:O5'     | 2.22                     | 0.56              |
| 51:9:691:G:C2      | 51:9:692:G:N7      | 2.72                     | 0.56              |
| 53:BB:129:THR:OG1  | 53:BB:131:ASP:O    | 2.18                     | 0.56              |
| 57:FF:20:PHE:HE1   | 57:FF:94:LYS:HZ1   | 1.53                     | 0.56              |
| 77:ZZ:92:LEU:HD22  | 77:ZZ:109:TYR:HE1  | 1.70                     | 0.56              |
| 84:gg:76:GLN:O     | 84:gg:77:PHE:C     | 2.48                     | 0.56              |
| 5:E:209:VAL:HG23   | 5:E:263:LYS:HE3    | 1.87                     | 0.56              |
| 14:O:110:PRO:HA    | 14:O:113:ASP:OD1   | 2.05                     | 0.56              |
| 20:U:33:ILE:HG22   | 20:U:96:LEU:HD21   | 1.87                     | 0.56              |
| 48:5:497:G:O2'     | 48:5:499:G:O4'     | 2.23                     | 0.56              |
| 48:5:964:A:H2'     | 48:5:965:G:O4'     | 2.04                     | 0.56              |
| 51:9:1452:A:OP2    | 69:RR:32:LYS:NZ    | 2.36                     | 0.56              |
| 51:9:1797:U:H2'    | 51:9:1798:C:C6     | 2.40                     | 0.56              |
| 87:jj:62:ILE:HD11  | 87:jj:72:ILE:CG1   | 2.32                     | 0.56              |
| 4:D:265:ARG:NE     | 4:D:267:ASN:O      | 2.39                     | 0.56              |
| 44:t:42:VAL:O      | 44:t:46:ILE:HD12   | 2.05                     | 0.56              |
| 48:5:692:A:H2'     | 48:5:693:C:C6      | 2.41                     | 0.56              |
| 51:9:308:G:C2      | 60:II:45:THR:HG22  | 2.41                     | 0.56              |
| 51:9:466:G:O2'     | 58:GG:72:ARG:NH2   | 2.38                     | 0.56              |
| 51:9:1427:C:N4     | 51:9:1428:G:O6     | 2.38                     | 0.56              |
| 54:CC:70:VAL:HG21  | 54:CC:93:ILE:HG23  | 1.87                     | 0.56              |
| 55:DD:113:LEU:HD23 | 55:DD:118:ALA:HB2  | 1.87                     | 0.56              |
| 59:HH:69:LEU:HD12  | 59:HH:96:ALA:HB2   | 1.88                     | 0.56              |
| 68:QQ:41:MET:SD    | 71:TT:10:ASN:N     | 2.79                     | 0.56              |
| 70:SS:86:ARG:NE    | 70:SS:89:ASP:OD1   | 2.34                     | 0.56              |
| 84:gg:14:HIS:O     | 84:gg:305:ASN:HB3  | 2.05                     | 0.56              |
| 84:gg:24:THR:HB    | 84:gg:71:ILE:HG21  | 1.86                     | 0.56              |
| 12:M:31:ILE:O      | 18:S:98:ARG:NE     | 2.33                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:1866:U:H2'    | 48:5:1867:A:O4'    | 2.06                     | 0.56              |
| 51:9:1447:G:OP1    | 72:UU:87:ARG:NH2   | 2.35                     | 0.56              |
| 56:EE:47:PHE:CE2   | 56:EE:52:LEU:HD11  | 2.41                     | 0.56              |
| 56:EE:95:THR:HG22  | 76:YY:16:ARG:CG    | 2.35                     | 0.56              |
| 58:GG:152:ASP:OD2  | 58:GG:154:ARG:NH2  | 2.38                     | 0.56              |
| 15:P:39:MET:HE2    | 15:P:43:LYS:HZ2    | 1.69                     | 0.56              |
| 40:o:56:PHE:N      | 47:3:76:A:OP1      | 2.36                     | 0.56              |
| 48:5:261:G:C2'     | 48:5:262:G:O4'     | 2.52                     | 0.56              |
| 48:5:1072:C:HO2'   | 48:5:1073:G:P      | 2.24                     | 0.56              |
| 48:5:1073:G:H1     | 48:5:1238:A:H2     | 1.49                     | 0.56              |
| 48:5:1764:G:O2'    | 48:5:1767:A:N6     | 2.38                     | 0.56              |
| 51:9:1430:C:O2     | 51:9:1431:G:N7     | 2.39                     | 0.56              |
| 53:BB:117:TRP:O    | 53:BB:153:THR:O    | 2.24                     | 0.56              |
| 53:BB:228:LEU:HD23 | 53:BB:229:MET:HE1  | 1.88                     | 0.56              |
| 42:r:125:MET:HA    | 42:r:125:MET:HE3   | 1.87                     | 0.56              |
| 43:s:28:PHE:CE2    | 43:s:98:ILE:HG21   | 2.41                     | 0.56              |
| 48:5:1100:U:N3     | 48:5:1168:G:N7     | 2.54                     | 0.56              |
| 48:5:2259:G:H3'    | 48:5:2260:C:H5'    | 1.88                     | 0.56              |
| 48:5:4111:U:H2'    | 48:5:4112:C:C6     | 2.41                     | 0.56              |
| 51:9:873:G:O2'     | 51:9:874:G:OP1     | 2.17                     | 0.56              |
| 51:9:1308:U:O2'    | 83:ff:128:ALA:HB1  | 2.05                     | 0.56              |
| 59:HH:43:LEU:HD21  | 59:HH:71:SER:OG    | 2.05                     | 0.56              |
| 10:J:92:TYR:O      | 10:J:172:GLY:O     | 2.23                     | 0.56              |
| 36:k:57:LYS:HA     | 36:k:60:LEU:HD12   | 1.88                     | 0.56              |
| 48:5:4574:U:H3'    | 48:5:4575:G:H5''   | 1.88                     | 0.56              |
| 51:9:940:U:H2'     | 51:9:941:C:C6      | 2.41                     | 0.56              |
| 52:AA:10:MET:HE2   | 52:AA:55:TRP:HB2   | 1.86                     | 0.56              |
| 55:DD:12:VAL:HG21  | 81:dd:34:TYR:HB3   | 1.87                     | 0.56              |
| 84:gg:197:THR:O    | 84:gg:239:LEU:HD12 | 2.05                     | 0.56              |
| 84:gg:232:GLY:O    | 84:gg:257:LYS:NZ   | 2.39                     | 0.56              |
| 3:C:196:MET:HE3    | 48:5:352:G:C6      | 2.40                     | 0.56              |
| 19:T:32:ARG:HG2    | 19:T:32:ARG:HH11   | 1.69                     | 0.56              |
| 46:2:19:G:OP1      | 46:2:60:A:N6       | 2.33                     | 0.56              |
| 48:5:4131:G:H2'    | 48:5:4132:C:C6     | 2.40                     | 0.56              |
| 48:5:4751:G:H1     | 48:5:4948:C:H5     | 1.54                     | 0.56              |
| 48:5:4771:C:HO2'   | 48:5:4772:C:H6     | 1.53                     | 0.56              |
| 51:9:1596:U:H2'    | 51:9:1597:C:O4'    | 2.06                     | 0.56              |
| 64:MM:83:LYS:HG2   | 64:MM:103:VAL:HG12 | 1.87                     | 0.56              |
| 72:UU:60:THR:HG23  | 72:UU:60:THR:O     | 2.05                     | 0.56              |
| 47:3:25:C:H2'      | 47:3:26:A:O4'      | 2.06                     | 0.56              |
| 48:5:1477:C:HO2'   | 48:5:1478:C:P      | 2.29                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:CC:176:LYS:O    | 54:CC:200:ARG:NH2  | 2.39                     | 0.56              |
| 62:KK:43:LEU:C     | 62:KK:43:LEU:HD13  | 2.31                     | 0.56              |
| 72:UU:48:LEU:HD21  | 72:UU:97:ILE:HG21  | 1.87                     | 0.56              |
| 86:ii:251:LEU:HD11 | 86:ii:274:VAL:HG13 | 1.88                     | 0.56              |
| 87:jj:411:TYR:CD1  | 87:jj:484:LEU:HD12 | 2.40                     | 0.56              |
| 48:5:1802:A:O2'    | 48:5:1837:A:OP1    | 2.14                     | 0.56              |
| 51:9:913:A:H1'     | 59:HH:66:VAL:HB    | 1.88                     | 0.56              |
| 52:AA:10:MET:SD    | 52:AA:15:VAL:HG12  | 2.46                     | 0.56              |
| 59:HH:14:GLU:OE1   | 59:HH:14:GLU:N     | 2.37                     | 0.56              |
| 1:A:65:ASP:OD2     | 1:A:68:ARG:HG2     | 2.07                     | 0.55              |
| 7:G:136:LEU:HD21   | 7:G:204:PHE:CE2    | 2.41                     | 0.55              |
| 56:EE:153:LEU:HD11 | 58:GG:216:ARG:HH11 | 1.71                     | 0.55              |
| 69:RR:17:ILE:HD11  | 69:RR:54:VAL:HG13  | 1.88                     | 0.55              |
| 86:ii:96:TYR:OH    | 86:ii:132:HIS:O    | 2.22                     | 0.55              |
| 45:1:65:GLY:O      | 48:5:3908:A:N6     | 2.38                     | 0.55              |
| 60:II:113:TYR:CD2  | 60:II:121:LEU:HD22 | 2.42                     | 0.55              |
| 61:JJ:113:GLN:HG3  | 61:JJ:149:VAL:HG21 | 1.87                     | 0.55              |
| 76:YY:27:VAL:HG11  | 76:YY:35:VAL:CG2   | 2.36                     | 0.55              |
| 87:jj:123:LEU:O    | 87:jj:155:TYR:OH   | 2.25                     | 0.55              |
| 14:O:175:MET:HE1   | 14:O:179:LYS:CE    | 2.36                     | 0.55              |
| 34:i:30:ARG:NH1    | 48:5:327:U:O2'     | 2.39                     | 0.55              |
| 51:9:190:G:OP1     | 60:II:149:TYR:OH   | 2.24                     | 0.55              |
| 51:9:319:C:N4      | 58:GG:186:GLN:OE1  | 2.39                     | 0.55              |
| 51:9:1623:A:H5''   | 70:SS:133:GLY:HA3  | 1.87                     | 0.55              |
| 56:EE:125:LYS:O    | 56:EE:142:HIS:N    | 2.40                     | 0.55              |
| 57:FF:125:SER:HB2  | 57:FF:136:ARG:NH2  | 2.21                     | 0.55              |
| 64:MM:21:VAL:HG23  | 64:MM:121:LYS:CD   | 2.37                     | 0.55              |
| 84:gg:124:SER:OG   | 84:gg:125:ARG:N    | 2.39                     | 0.55              |
| 35:j:82:THR:HB     | 50:8:94:G:H21      | 1.70                     | 0.55              |
| 43:s:121:VAL:HG21  | 43:s:183:PHE:CE1   | 2.41                     | 0.55              |
| 48:5:407:A:O2'     | 48:5:410:A:OP1     | 2.18                     | 0.55              |
| 48:5:1755:C:O2'    | 48:5:1757:U:OP2    | 2.20                     | 0.55              |
| 51:9:213:G:HO2'    | 51:9:214:U:P       | 2.30                     | 0.55              |
| 51:9:1801:A:H2'    | 51:9:1802:C:C6     | 2.41                     | 0.55              |
| 54:CC:252:THR:HG22 | 74:WW:99:PHE:CE1   | 2.42                     | 0.55              |
| 84:gg:10:THR:HB    | 84:gg:306:LEU:HD23 | 1.88                     | 0.55              |
| 87:jj:106:LEU:HD23 | 87:jj:106:LEU:C    | 2.30                     | 0.55              |
| 2:B:35:ASP:HB3     | 2:B:186:ASN:CG     | 2.32                     | 0.55              |
| 47:3:37:A:C5       | 47:3:38:A:C8       | 2.95                     | 0.55              |
| 48:5:930:G:O2'     | 48:5:931:C:OP1     | 2.22                     | 0.55              |
| 48:5:2759:G:O2'    | 48:5:2760:G:O4'    | 2.24                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:203:G:P       | 60:II:147:LYS:NZ   | 2.80                     | 0.55              |
| 51:9:1084:A:OP1    | 51:9:1858:G:O2'    | 2.25                     | 0.55              |
| 51:9:1126:G:OP1    | 52:AA:41:ARG:NH1   | 2.39                     | 0.55              |
| 58:GG:98:ARG:NH1   | 58:GG:101:ILE:O    | 2.38                     | 0.55              |
| 58:GG:145:PHE:HB3  | 58:GG:147:LEU:HD21 | 1.88                     | 0.55              |
| 77:ZZ:56:ASP:OD1   | 77:ZZ:56:ASP:C     | 2.50                     | 0.55              |
| 23:X:93:ASN:O      | 23:X:95:THR:HG23   | 2.07                     | 0.55              |
| 24:Y:111:LEU:HD12  | 24:Y:116:LYS:HG3   | 1.89                     | 0.55              |
| 48:5:3773:U:O2'    | 48:5:3775:A:C2     | 2.58                     | 0.55              |
| 51:9:629:A:O2'     | 51:9:631:U:OP1     | 2.24                     | 0.55              |
| 51:9:687:C:O3'     | 59:HH:121:THR:HG23 | 2.07                     | 0.55              |
| 51:9:955:A:N1      | 51:9:968:U:O2'     | 2.37                     | 0.55              |
| 51:9:1408:U:HO2'   | 51:9:1409:A:C5'    | 2.16                     | 0.55              |
| 51:9:1563:G:OP1    | 71:TT:121:ARG:NE   | 2.37                     | 0.55              |
| 56:EE:45:ILE:HA    | 56:EE:61:VAL:HG21  | 1.89                     | 0.55              |
| 59:HH:50:GLU:HA    | 59:HH:60:ILE:HD13  | 1.87                     | 0.55              |
| 60:II:34:ALA:HB2   | 60:II:56:ARG:HD3   | 1.88                     | 0.55              |
| 75:XX:122:VAL:HG12 | 75:XX:130:LEU:HD11 | 1.87                     | 0.55              |
| 10:J:105:PHE:CE1   | 10:J:134:LEU:HD11  | 2.41                     | 0.55              |
| 23:X:63:LYS:HZ1    | 23:X:66:PRO:HA     | 1.72                     | 0.55              |
| 25:Z:115:LYS:NZ    | 25:Z:119:GLU:OE2   | 2.40                     | 0.55              |
| 35:j:59:THR:O      | 50:8:42:G:OP1      | 2.24                     | 0.55              |
| 48:5:1199:G:O2'    | 48:5:1200:G:O5'    | 2.25                     | 0.55              |
| 51:9:464:A:OP1     | 87:jj:576:ARG:NH1  | 2.38                     | 0.55              |
| 51:9:1416:C:H2'    | 51:9:1417:C:C2     | 2.41                     | 0.55              |
| 56:EE:103:TYR:CD1  | 56:EE:189:LEU:HD21 | 2.41                     | 0.55              |
| 75:XX:63:ASN:ND2   | 75:XX:114:ASP:OD2  | 2.38                     | 0.55              |
| 8:H:111:LEU:HD11   | 8:H:125:ARG:HG2    | 1.89                     | 0.55              |
| 16:Q:83:VAL:O      | 16:Q:83:VAL:HG12   | 2.07                     | 0.55              |
| 33:h:110:LYS:NZ    | 48:5:111:C:OP1     | 2.39                     | 0.55              |
| 48:5:1978:C:HO2'   | 48:5:1979:A:P      | 2.30                     | 0.55              |
| 48:5:2093:G:H4'    | 48:5:2094:C:H5'    | 1.89                     | 0.55              |
| 48:5:4992:G:H2'    | 48:5:4993:G:C8     | 2.42                     | 0.55              |
| 51:9:1757:G:C6     | 51:9:1775:U:O2     | 2.59                     | 0.55              |
| 84:gg:120:ILE:HD12 | 84:gg:133:ASN:O    | 2.07                     | 0.55              |
| 86:ii:389:LEU:HD21 | 86:ii:391:ILE:HD11 | 1.88                     | 0.55              |
| 7:G:93:THR:HG22    | 7:G:97:LYS:HZ2     | 1.72                     | 0.55              |
| 8:H:140:GLN:OE1    | 8:H:140:GLN:HA     | 2.07                     | 0.55              |
| 56:EE:105:THR:HG21 | 56:EE:245:ARG:H    | 1.71                     | 0.55              |
| 7:G:142:THR:HG23   | 48:5:151:G:O6      | 2.07                     | 0.55              |
| 15:P:104:LEU:HD23  | 48:5:400:A2M:CM'   | 2.37                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:e:48:ARG:NH2    | 48:5:2279:A:O2'    | 2.39                     | 0.55              |
| 48:5:1414:C:C4     | 48:5:1415:G:N7     | 2.75                     | 0.55              |
| 51:9:1255:G:OP1    | 51:9:1256:G:O2'    | 2.17                     | 0.55              |
| 53:BB:131:ASP:O    | 53:BB:133:TYR:N    | 2.39                     | 0.55              |
| 60:II:22:HIS:ND1   | 60:II:23:LYS:O     | 2.38                     | 0.55              |
| 65:NN:79:GLY:O     | 65:NN:80:LEU:HD23  | 2.06                     | 0.55              |
| 84:gg:94:THR:HG23  | 84:gg:96:THR:HG22  | 1.89                     | 0.55              |
| 87:jj:61:CYS:SG    | 87:jj:62:ILE:HD12  | 2.47                     | 0.55              |
| 33:h:60:VAL:O      | 33:h:64:THR:HG22   | 2.07                     | 0.54              |
| 48:5:1484:G:H2'    | 48:5:1484:G:N3     | 2.22                     | 0.54              |
| 48:5:1996:C:H3'    | 48:5:1997:U:H5''   | 1.89                     | 0.54              |
| 48:5:4382:G:O2'    | 48:5:4544:A:N1     | 2.37                     | 0.54              |
| 51:9:71:G:O2'      | 51:9:71:G:N3       | 2.41                     | 0.54              |
| 51:9:1636:G:H2'    | 51:9:1636:G:N3     | 2.22                     | 0.54              |
| 51:9:1663:A:HO2'   | 51:9:1664:A:P      | 2.24                     | 0.54              |
| 51:9:1757:G:O6     | 51:9:1775:U:C2     | 2.59                     | 0.54              |
| 52:AA:42:LYS:CD    | 52:AA:48:ILE:HD11  | 2.37                     | 0.54              |
| 55:DD:209:SER:O    | 69:RR:40:ILE:HG22  | 2.06                     | 0.54              |
| 66:OO:117:ARG:HD3  | 80:cc:62:GLU:OE1   | 2.06                     | 0.54              |
| 84:gg:16:GLY:N     | 84:gg:305:ASN:OD1  | 2.40                     | 0.54              |
| 86:ii:251:LEU:HD23 | 86:ii:275:LEU:HD23 | 1.88                     | 0.54              |
| 87:jj:428:LEU:HD23 | 87:jj:474:LEU:CD2  | 2.38                     | 0.54              |
| 3:C:292:ILE:HG23   | 16:Q:128:LEU:CD1   | 2.38                     | 0.54              |
| 5:E:94:THR:OG1     | 48:5:2258:C:O2     | 2.24                     | 0.54              |
| 28:c:81:LEU:HD21   | 28:c:94:LEU:CD2    | 2.37                     | 0.54              |
| 33:h:24:LEU:HD22   | 33:h:53:SER:OG     | 2.07                     | 0.54              |
| 48:5:1982:G:HO2'   | 48:5:1983:A:P      | 2.29                     | 0.54              |
| 48:5:2046:G:O2'    | 48:5:2047:A:OP2    | 2.14                     | 0.54              |
| 48:5:5001:U:H2'    | 48:5:5002:U:O4'    | 2.06                     | 0.54              |
| 51:9:65:C:OP1      | 58:GG:136:LYS:NZ   | 2.39                     | 0.54              |
| 51:9:77:A:H1'      | 58:GG:176:ILE:HD13 | 1.88                     | 0.54              |
| 51:9:654:A:N6      | 92:9:2021:HOH:O    | 2.32                     | 0.54              |
| 51:9:877:C:C4      | 51:9:879:C:OP1     | 2.60                     | 0.54              |
| 51:9:1834:A:N3     | 51:9:1834:A:O2'    | 2.35                     | 0.54              |
| 68:QQ:112:LEU:HB2  | 68:QQ:120:LEU:HD11 | 1.88                     | 0.54              |
| 30:e:17:THR:HG21   | 48:5:1301:C:O2     | 2.07                     | 0.54              |
| 48:5:2024:G:O2'    | 48:5:2025:A:OP2    | 2.19                     | 0.54              |
| 51:9:531:A:H3'     | 51:9:532:C:H5''    | 1.89                     | 0.54              |
| 51:9:563:G:O2'     | 51:9:564:A:P       | 2.65                     | 0.54              |
| 64:MM:21:VAL:HG23  | 64:MM:121:LYS:HD3  | 1.88                     | 0.54              |
| 11:L:128:PRO:HD2   | 11:L:144:LEU:HD11  | 1.89                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:d:22:THR:HG23   | 29:d:122:VAL:HB    | 1.88                     | 0.54              |
| 48:5:2259:G:H5'    | 48:5:2260:C:OP2    | 2.07                     | 0.54              |
| 48:5:3807:A:N7     | 92:5:5462:HOH:O    | 2.33                     | 0.54              |
| 51:9:203:G:H2'     | 51:9:204:G:O4'     | 2.07                     | 0.54              |
| 69:RR:105:MET:CE   | 69:RR:109:LEU:HD11 | 2.24                     | 0.54              |
| 6:F:28:LYS:HE2     | 6:F:32:LEU:HD11    | 1.90                     | 0.54              |
| 10:J:170:TYR:O     | 10:J:171:ASP:OD2   | 2.26                     | 0.54              |
| 15:P:54:LYS:HA     | 15:P:83:TRP:CD1    | 2.42                     | 0.54              |
| 37:l:2:SER:N       | 48:5:2407:G:O6     | 2.40                     | 0.54              |
| 48:5:1307:A:H2'    | 48:5:1308:C:C6     | 2.43                     | 0.54              |
| 48:5:2394:G:O6     | 92:5:5422:HOH:O    | 2.17                     | 0.54              |
| 48:5:2415:U:H2'    | 48:5:2416:G:O4'    | 2.07                     | 0.54              |
| 48:5:3910:C:H2'    | 48:5:3911:C:C6     | 2.42                     | 0.54              |
| 51:9:216:C:OP1     | 56:EE:134:LYS:HE3  | 2.08                     | 0.54              |
| 51:9:376:A:H2'     | 51:9:377:G:O4'     | 2.07                     | 0.54              |
| 51:9:1059:G:C6     | 51:9:1060:A:N1     | 2.75                     | 0.54              |
| 51:9:1228:A:H2'    | 51:9:1229:G:C8     | 2.43                     | 0.54              |
| 51:9:1439:A:H2'    | 51:9:1440:C:C6     | 2.42                     | 0.54              |
| 51:9:1646:C:O2'    | 51:9:1647:A:OP2    | 2.22                     | 0.54              |
| 56:EE:180:LEU:HD11 | 56:EE:192:ILE:HG22 | 1.90                     | 0.54              |
| 70:SS:48:ALA:O     | 70:SS:66:ARG:NH2   | 2.41                     | 0.54              |
| 84:gg:8:ARG:N      | 84:gg:309:VAL:O    | 2.38                     | 0.54              |
| 87:jj:377:MET:HE2  | 87:jj:535:PHE:CZ   | 2.42                     | 0.54              |
| 48:5:1890:G:N2     | 48:5:1938:C:N4     | 2.55                     | 0.54              |
| 51:9:928:G:H1      | 51:9:1013:U:H3     | 1.56                     | 0.54              |
| 56:EE:180:LEU:HD11 | 56:EE:192:ILE:CG2  | 2.38                     | 0.54              |
| 58:GG:57:ASP:OD1   | 58:GG:59:GLN:N     | 2.32                     | 0.54              |
| 69:RR:38:ILE:C     | 69:RR:38:ILE:HD12  | 2.33                     | 0.54              |
| 84:gg:68:ASP:HB3   | 84:gg:111:VAL:HG22 | 1.90                     | 0.54              |
| 87:jj:435:ALA:HB1  | 87:jj:441:PHE:CG   | 2.42                     | 0.54              |
| 16:Q:61:LEU:HD23   | 16:Q:66:MET:HE2    | 1.90                     | 0.54              |
| 16:Q:134:ARG:NH2   | 48:5:1449:C:OP1    | 2.40                     | 0.54              |
| 48:5:261:G:O2'     | 48:5:262:G:O4'     | 2.26                     | 0.54              |
| 48:5:1804:A:O4'    | 48:5:1806:G:C8     | 2.61                     | 0.54              |
| 51:9:929:G:H2'     | 51:9:930:C:O4'     | 2.07                     | 0.54              |
| 51:9:1223:A:OP1    | 57:FF:79:HIS:N     | 2.39                     | 0.54              |
| 55:DD:52:ALA:O     | 55:DD:91:VAL:HG23  | 2.08                     | 0.54              |
| 55:DD:158:ILE:HD12 | 55:DD:164:VAL:CG1  | 2.36                     | 0.54              |
| 59:HH:140:VAL:HG11 | 59:HH:159:ASP:OD1  | 2.08                     | 0.54              |
| 80:cc:25:GLY:N     | 80:cc:26:GLN:OE1   | 2.41                     | 0.54              |
| 43:s:17:ILE:HG22   | 43:s:54:LEU:CD2    | 2.37                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:4065:G:O3'    | 48:5:4066:U:O4'    | 2.26                     | 0.54              |
| 52:AA:203:PHE:CE2  | 69:RR:91:LEU:HD13  | 2.42                     | 0.54              |
| 54:CC:270:THR:O    | 54:CC:274:VAL:HG23 | 2.07                     | 0.54              |
| 59:HH:139:ILE:HG22 | 59:HH:156:VAL:CG1  | 2.38                     | 0.54              |
| 87:jj:459:VAL:HA   | 87:jj:462:LEU:HD13 | 1.89                     | 0.54              |
| 4:D:76:CYS:SG      | 4:D:112:ARG:NH2    | 2.81                     | 0.54              |
| 33:h:3:LYS:NZ      | 50:8:80:A:O2'      | 2.39                     | 0.54              |
| 36:k:15:ALA:CB     | 36:k:61:PRO:HG2    | 2.38                     | 0.54              |
| 48:5:966:A:H62     | 48:5:2096:G:H2'    | 1.73                     | 0.54              |
| 48:5:1979:A:H2'    | 48:5:1980:U:O4'    | 2.07                     | 0.54              |
| 48:5:4894:A:O2'    | 48:5:4895:C:OP1    | 2.24                     | 0.54              |
| 51:9:1409:A:H4'    | 68:QQ:24:HIS:NE2   | 2.23                     | 0.54              |
| 55:DD:38:GLU:O     | 55:DD:49:ILE:HD12  | 2.08                     | 0.54              |
| 59:HH:51:ILE:HG23  | 59:HH:179:LYS:HD3  | 1.89                     | 0.54              |
| 87:jj:86:ARG:O     | 87:jj:130:ASN:ND2  | 2.39                     | 0.54              |
| 3:C:358:LEU:C      | 3:C:358:LEU:HD23   | 2.33                     | 0.54              |
| 6:F:107:VAL:HG13   | 6:F:131:MET:HE2    | 1.90                     | 0.54              |
| 7:G:93:THR:HG22    | 7:G:97:LYS:NZ      | 2.23                     | 0.54              |
| 9:I:21:ARG:NH2     | 48:5:1789:C:OP1    | 2.40                     | 0.54              |
| 9:I:39:LYS:NZ      | 48:5:1750:G:OP1    | 2.30                     | 0.54              |
| 14:O:168:TYR:OH    | 48:5:4768:G:OP1    | 2.23                     | 0.54              |
| 14:O:189:ILE:O     | 14:O:190:SER:OG    | 2.24                     | 0.54              |
| 48:5:2639:U:O2'    | 48:5:2640:G:O5'    | 2.26                     | 0.54              |
| 51:9:123:G:H3'     | 51:9:124:U:H5''    | 1.90                     | 0.54              |
| 51:9:862:A:C2'     | 51:9:863:PSU:H5''  | 2.37                     | 0.54              |
| 51:9:1541:G:N3     | 71:TT:12:GLN:NE2   | 2.56                     | 0.54              |
| 60:II:148:LYS:O    | 60:II:151:GLU:HG3  | 2.08                     | 0.54              |
| 83:ff:136:CYS:CB   | 83:ff:139:CYS:SG   | 2.95                     | 0.54              |
| 87:jj:41:VAL:HG22  | 87:jj:48:ALA:HA    | 1.90                     | 0.54              |
| 14:O:181:ALA:O     | 14:O:185:VAL:HG22  | 2.08                     | 0.53              |
| 51:9:799:U:H2'     | 51:9:800:U:C6      | 2.43                     | 0.53              |
| 56:EE:100:ARG:NH2  | 56:EE:118:GLU:O    | 2.41                     | 0.53              |
| 87:jj:217:LEU:HD12 | 87:jj:221:GLU:HB3  | 1.90                     | 0.53              |
| 5:E:48:ARG:O       | 5:E:67:ARG:NH2     | 2.40                     | 0.53              |
| 5:E:184:LEU:O      | 48:5:4883:C:N4     | 2.41                     | 0.53              |
| 6:F:40:MET:HE2     | 6:F:40:MET:N       | 2.24                     | 0.53              |
| 9:I:179:ASP:OD1    | 9:I:180:GLU:N      | 2.40                     | 0.53              |
| 13:N:126:THR:HG23  | 13:N:127:TYR:CD2   | 2.43                     | 0.53              |
| 33:h:121:VAL:HG12  | 33:h:122:LYS:N     | 2.23                     | 0.53              |
| 51:9:17:C:O2'      | 51:9:1194:A:N1     | 2.37                     | 0.53              |
| 51:9:1629:C:OP1    | 70:SS:39:ARG:NE    | 2.38                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:AA:135:THR:O    | 52:AA:138:SER:OG   | 2.25                     | 0.53              |
| 54:CC:206:SER:HB2  | 54:CC:224:THR:HG21 | 1.90                     | 0.53              |
| 59:HH:25:GLN:O     | 59:HH:28:LEU:HB2   | 2.08                     | 0.53              |
| 69:RR:17:ILE:HG21  | 69:RR:69:ILE:HD13  | 1.90                     | 0.53              |
| 3:C:164:THR:O      | 3:C:168:VAL:HG23   | 2.08                     | 0.53              |
| 4:D:208:MET:HB3    | 4:D:233:PRO:HG3    | 1.90                     | 0.53              |
| 15:P:104:LEU:HD23  | 48:5:400:A2M:HM'3  | 1.90                     | 0.53              |
| 43:s:83:ARG:O      | 43:s:86:VAL:HG23   | 2.08                     | 0.53              |
| 48:5:1455:G:HO2'   | 48:5:1456:C:P      | 2.29                     | 0.53              |
| 48:5:1755:C:H42    | 48:5:1775:A:H61    | 1.57                     | 0.53              |
| 48:5:1890:G:N2     | 48:5:1939:A:N6     | 2.51                     | 0.53              |
| 48:5:1990:A:HO2'   | 48:5:1991:A:P      | 2.25                     | 0.53              |
| 48:5:4927:G:H2'    | 48:5:4928:C:O2     | 2.08                     | 0.53              |
| 58:GG:41:LEU:O     | 58:GG:41:LEU:HD13  | 2.09                     | 0.53              |
| 87:jj:129:PRO:O    | 87:jj:143:ILE:HD11 | 2.08                     | 0.53              |
| 87:jj:326:ASP:OD1  | 87:jj:327:ALA:N    | 2.41                     | 0.53              |
| 3:C:143:ARG:NH1    | 48:5:2300:A:N7     | 2.56                     | 0.53              |
| 29:d:46:LEU:HD22   | 29:d:72:VAL:HG11   | 1.90                     | 0.53              |
| 44:t:15:LEU:C      | 44:t:15:LEU:HD12   | 2.33                     | 0.53              |
| 48:5:2544:G:C8     | 50:8:126:C:O4'     | 2.62                     | 0.53              |
| 57:FF:20:PHE:HE2   | 57:FF:69:VAL:HG21  | 1.73                     | 0.53              |
| 58:GG:171:THR:HG23 | 58:GG:171:THR:O    | 2.09                     | 0.53              |
| 87:jj:111:THR:HG23 | 87:jj:495:GLU:OE2  | 2.08                     | 0.53              |
| 87:jj:245:SER:O    | 87:jj:247:LEU:HD23 | 2.08                     | 0.53              |
| 30:e:86:GLU:OE2    | 30:e:118:LEU:HD11  | 2.09                     | 0.53              |
| 43:s:66:ARG:NH1    | 43:s:69:LEU:HD23   | 2.24                     | 0.53              |
| 48:5:206:U:O2'     | 48:5:208:A:N7      | 2.32                     | 0.53              |
| 51:9:1284:A:O2'    | 64:MM:105:GLY:O    | 2.25                     | 0.53              |
| 57:FF:127:ARG:O    | 57:FF:128:ILE:HG23 | 2.08                     | 0.53              |
| 59:HH:147:LYS:HD3  | 74:WW:49:GLU:OE2   | 2.09                     | 0.53              |
| 84:gg:197:THR:HG21 | 84:gg:239:LEU:H    | 1.74                     | 0.53              |
| 87:jj:120:LEU:HD22 | 87:jj:239:MET:HG2  | 1.90                     | 0.53              |
| 87:jj:168:ILE:HG22 | 87:jj:239:MET:CB   | 2.35                     | 0.53              |
| 2:B:139:ASP:OD1    | 2:B:139:ASP:N      | 2.41                     | 0.53              |
| 4:D:15:ARG:HD2     | 48:5:1743:A:O4'    | 2.09                     | 0.53              |
| 25:Z:24:VAL:HG21   | 25:Z:87:VAL:CG2    | 2.37                     | 0.53              |
| 47:3:10:G:N2       | 47:3:26:A:H1'      | 2.23                     | 0.53              |
| 48:5:4162:C:O2     | 48:5:4162:C:O5'    | 2.27                     | 0.53              |
| 48:5:4904:G:C2     | 48:5:4918:C:C2     | 2.97                     | 0.53              |
| 51:9:75:G:HO2'     | 51:9:76:U:H3'      | 1.72                     | 0.53              |
| 51:9:141:A:H61     | 51:9:177:G:H21     | 1.57                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:196:C:H3'     | 51:9:197:U:C6      | 2.44                     | 0.53              |
| 51:9:643:A:OP1     | 61:JJ:41:ARG:NH2   | 2.38                     | 0.53              |
| 87:jj:165:LYS:HZ3  | 87:jj:235:ALA:HB2  | 1.73                     | 0.53              |
| 26:a:132:ARG:HA    | 26:a:135:GLU:OE1   | 2.09                     | 0.53              |
| 51:9:53:C:O2'      | 51:9:507:G:N7      | 2.24                     | 0.53              |
| 51:9:108:G:C2'     | 51:9:109:PSU:H5''  | 2.39                     | 0.53              |
| 51:9:1493:C:OP1    | 51:9:1494:U:O2'    | 2.26                     | 0.53              |
| 58:GG:220:ALA:HB3  | 58:GG:224:ARG:HH21 | 1.74                     | 0.53              |
| 70:SS:16:LEU:HD11  | 70:SS:72:GLN:HE21  | 1.73                     | 0.53              |
| 84:gg:199:THR:HG21 | 84:gg:239:LEU:O    | 2.08                     | 0.53              |
| 87:jj:65:CYS:HB2   | 87:jj:70:LEU:HD12  | 1.90                     | 0.53              |
| 12:M:11:ARG:CZ     | 12:M:61:ILE:HD11   | 2.39                     | 0.53              |
| 48:5:1662:C:H2'    | 48:5:1663:C:C6     | 2.44                     | 0.53              |
| 48:5:4459:U:H2'    | 48:5:4460:U:C6     | 2.44                     | 0.53              |
| 51:9:872:A:O2'     | 51:9:873:G:P       | 2.67                     | 0.53              |
| 51:9:1102:G:H1     | 51:9:1130:G:H1     | 1.57                     | 0.53              |
| 51:9:1118:C:O2'    | 79:bb:75:GLU:OE2   | 2.20                     | 0.53              |
| 55:DD:113:LEU:CD2  | 55:DD:118:ALA:HB2  | 2.38                     | 0.53              |
| 57:FF:32:ASP:C     | 57:FF:34:SER:H     | 2.17                     | 0.53              |
| 64:MM:50:CYS:HB2   | 64:MM:110:VAL:HG22 | 1.91                     | 0.53              |
| 80:cc:42:ILE:HD11  | 80:cc:64:GLU:HB2   | 1.91                     | 0.53              |
| 87:jj:14:ASP:O     | 87:jj:17:LYS:NZ    | 2.35                     | 0.53              |
| 13:N:43:THR:OG1    | 13:N:131:GLU:OE2   | 2.25                     | 0.53              |
| 25:Z:58:GLY:O      | 25:Z:62:ILE:HG12   | 2.09                     | 0.53              |
| 44:t:15:LEU:CA     | 44:t:62:LEU:HD12   | 2.39                     | 0.53              |
| 48:5:4872:G:H4'    | 48:5:4873:G:H5'    | 1.90                     | 0.53              |
| 51:9:962:A:N1      | 51:9:1055:A:O2'    | 2.41                     | 0.53              |
| 55:DD:172:VAL:O    | 55:DD:173:ARG:NH1  | 2.42                     | 0.53              |
| 61:JJ:128:VAL:HG13 | 61:JJ:132:GLN:OE1  | 2.08                     | 0.53              |
| 87:jj:449:LEU:HD11 | 87:jj:472:LEU:HD12 | 1.90                     | 0.53              |
| 8:H:106:GLN:HG2    | 8:H:111:LEU:HD12   | 1.91                     | 0.53              |
| 12:M:85:LYS:O      | 12:M:89:THR:HG23   | 2.09                     | 0.53              |
| 51:9:1315:U:OP1    | 62:KK:2:LEU:HD22   | 2.09                     | 0.53              |
| 51:9:1429:G:H2'    | 51:9:1430:C:C1'    | 2.39                     | 0.53              |
| 70:SS:46:ARG:HG2   | 71:TT:35:ASP:HB2   | 1.91                     | 0.53              |
| 71:TT:6:VAL:HG23   | 71:TT:14:PHE:CZ    | 2.44                     | 0.53              |
| 72:UU:24:LEU:HD12  | 72:UU:112:VAL:HG22 | 1.91                     | 0.53              |
| 81:dd:38:MET:SD    | 81:dd:43:PHE:HA    | 2.49                     | 0.53              |
| 86:ii:287:ILE:HD13 | 86:ii:399:GLY:CA   | 2.38                     | 0.53              |
| 1:A:198:ARG:NH2    | 48:5:3687:A:OP2    | 2.42                     | 0.52              |
| 48:5:1452:A:H2'    | 48:5:1453:G:O4'    | 2.09                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:2567:G:H2'    | 48:5:2568:C:O4'    | 2.09                     | 0.52              |
| 48:5:4635:A:H8     | 48:5:5048:A:N6     | 2.08                     | 0.52              |
| 51:9:305:U:H6      | 60:II:182:CYS:O    | 1.91                     | 0.52              |
| 51:9:1451:G:N7     | 69:RR:44:LYS:NZ    | 2.49                     | 0.52              |
| 52:AA:14:ASP:OD1   | 52:AA:14:ASP:N     | 2.40                     | 0.52              |
| 84:gg:127:LYS:HD2  | 84:gg:149:GLU:O    | 2.09                     | 0.52              |
| 87:jj:377:MET:HB2  | 87:jj:518:VAL:HG22 | 1.90                     | 0.52              |
| 6:F:49:ILE:HD11    | 6:F:184:ILE:HD12   | 1.90                     | 0.52              |
| 6:F:59:GLU:HG2     | 6:F:63:MET:HE2     | 1.92                     | 0.52              |
| 6:F:85:GLU:OE2     | 19:T:136:ARG:NH2   | 2.43                     | 0.52              |
| 48:5:4584:A:H1'    | 48:5:4719:G:C2     | 2.45                     | 0.52              |
| 48:5:4967:A:H2'    | 48:5:4968:A:C8     | 2.44                     | 0.52              |
| 48:5:5016:A:C2     | 48:5:5033:G:N2     | 2.65                     | 0.52              |
| 51:9:1007:C:O2'    | 65:NN:104:ARG:NH1  | 2.41                     | 0.52              |
| 54:CC:263:LYS:HG2  | 54:CC:267:GLN:NE2  | 2.24                     | 0.52              |
| 62:KK:21:MET:HE2   | 62:KK:32:HIS:CE1   | 2.44                     | 0.52              |
| 72:UU:68:THR:HG23  | 72:UU:70:CYS:O     | 2.09                     | 0.52              |
| 84:gg:42:MET:HE2   | 84:gg:57:ARG:HB2   | 1.92                     | 0.52              |
| 16:Q:13:VAL:O      | 16:Q:13:VAL:HG12   | 2.08                     | 0.52              |
| 18:S:15:ARG:HB3    | 18:S:27:LEU:HD23   | 1.91                     | 0.52              |
| 43:s:135:THR:HG22  | 43:s:152:ILE:HD13  | 1.90                     | 0.52              |
| 46:2:8:U:O2'       | 46:2:21:A:N1       | 2.41                     | 0.52              |
| 46:2:15:G:N2       | 46:2:48:C:O2       | 2.33                     | 0.52              |
| 48:5:1087:A:H2'    | 48:5:1088:C:C6     | 2.45                     | 0.52              |
| 48:5:1214:C:H3'    | 48:5:1215:C:C5'    | 2.39                     | 0.52              |
| 48:5:1990:A:H2'    | 48:5:1990:A:N3     | 2.23                     | 0.52              |
| 48:5:4260:U:H2'    | 48:5:4261:C:C6     | 2.44                     | 0.52              |
| 48:5:4963:G:H2'    | 48:5:4964:C:O5'    | 2.08                     | 0.52              |
| 51:9:71:G:H1       | 51:9:74:G:H22      | 1.57                     | 0.52              |
| 51:9:837:A:N1      | 51:9:840:C:C2      | 2.77                     | 0.52              |
| 54:CC:262:THR:HG22 | 54:CC:263:LYS:N    | 2.24                     | 0.52              |
| 56:EE:48:LEU:HA    | 56:EE:52:LEU:HD12  | 1.91                     | 0.52              |
| 79:bb:35:VAL:HG11  | 79:bb:73:LEU:CD1   | 2.39                     | 0.52              |
| 87:jj:281:TYR:CD1  | 87:jj:281:TYR:C    | 2.87                     | 0.52              |
| 87:jj:564:ILE:HG23 | 87:jj:577:ILE:CD1  | 2.39                     | 0.52              |
| 32:g:62:LYS:NZ     | 48:5:2516:G:O2'    | 2.42                     | 0.52              |
| 33:h:116:LEU:HD13  | 33:h:117:ARG:O     | 2.09                     | 0.52              |
| 44:t:148:PRO:O     | 44:t:150:ASP:N     | 2.42                     | 0.52              |
| 48:5:1199:G:N3     | 48:5:1200:G:N7     | 2.57                     | 0.52              |
| 48:5:1999:A:H2'    | 48:5:2000:G:C4     | 2.44                     | 0.52              |
| 51:9:1598:G:N7     | 77:ZZ:85:ARG:NH2   | 2.55                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:QQ:57:LEU:HD23  | 68:QQ:112:LEU:HD23 | 1.91                     | 0.52              |
| 84:gg:152:SER:OG   | 84:gg:195:LEU:O    | 2.22                     | 0.52              |
| 87:jj:441:PHE:CE1  | 87:jj:445:VAL:HG21 | 2.43                     | 0.52              |
| 46:2:75:C:H2'      | 46:2:76:A:O4'      | 2.10                     | 0.52              |
| 51:9:488:U:H3'     | 51:9:489:A:C5'     | 2.39                     | 0.52              |
| 52:AA:52:LYS:HB2   | 69:RR:109:LEU:HD22 | 1.92                     | 0.52              |
| 54:CC:252:THR:OG1  | 54:CC:254:ASP:OD1  | 2.25                     | 0.52              |
| 55:DD:139:SER:OG   | 55:DD:149:SER:OG   | 2.06                     | 0.52              |
| 57:FF:79:HIS:O     | 57:FF:81:ARG:N     | 2.43                     | 0.52              |
| 59:HH:145:ARG:NE   | 74:WW:51:GLU:HG3   | 2.25                     | 0.52              |
| 70:SS:34:LYS:HG2   | 70:SS:103:LEU:HD23 | 1.91                     | 0.52              |
| 2:B:67:VAL:HG21    | 2:B:72:VAL:CG1     | 2.40                     | 0.52              |
| 44:t:13:VAL:HG23   | 44:t:64:ILE:HD12   | 1.91                     | 0.52              |
| 48:5:2095:A:H2'    | 48:5:2096:G:C8     | 2.44                     | 0.52              |
| 51:9:928:G:H2'     | 51:9:929:G:C8      | 2.45                     | 0.52              |
| 53:BB:135:LEU:HD23 | 53:BB:217:MET:SD   | 2.49                     | 0.52              |
| 58:GG:48:TYR:OH    | 58:GG:121:ILE:HG12 | 2.09                     | 0.52              |
| 59:HH:53:VAL:HG12  | 59:HH:54:GLY:N     | 2.25                     | 0.52              |
| 59:HH:76:GLN:HG2   | 59:HH:135:PHE:CD2  | 2.44                     | 0.52              |
| 68:QQ:63:PHE:CZ    | 68:QQ:92:LEU:HD22  | 2.44                     | 0.52              |
| 76:YY:117:VAL:HG21 | 76:YY:125:VAL:HG11 | 1.92                     | 0.52              |
| 86:ii:319:ILE:HG22 | 86:ii:321:ILE:HD13 | 1.92                     | 0.52              |
| 13:N:184:ILE:O     | 48:5:78:U:OP1      | 2.27                     | 0.52              |
| 48:5:1976:G:C6     | 48:5:2002:A:O2'    | 2.62                     | 0.52              |
| 48:5:2814:C:O2     | 48:5:2814:C:H2'    | 2.10                     | 0.52              |
| 48:5:3783:A:O5'    | 48:5:3784:A:H5''   | 2.09                     | 0.52              |
| 48:5:3786:U:O2     | 48:5:3814:U:H4'    | 2.09                     | 0.52              |
| 48:5:4591:U:H2'    | 48:5:4592:C:C6     | 2.45                     | 0.52              |
| 48:5:4884:G:O2'    | 48:5:4885:U:P      | 2.68                     | 0.52              |
| 48:5:5057:C:H2'    | 48:5:5058:A:C8     | 2.44                     | 0.52              |
| 51:9:491:C:O2'     | 51:9:493:A:N7      | 2.37                     | 0.52              |
| 3:C:335:MET:HE2    | 6:F:57:HIS:CG      | 2.45                     | 0.52              |
| 11:L:39:ARG:NH2    | 48:5:1362:G:OP1    | 2.38                     | 0.52              |
| 21:V:48:ARG:HD2    | 48:5:4621:C:OP1    | 2.10                     | 0.52              |
| 48:5:480:C:HO2'    | 48:5:481:G:P       | 2.25                     | 0.52              |
| 48:5:3867:A2M:HM'3 | 48:5:3880:G:N2     | 2.24                     | 0.52              |
| 51:9:303:C:H2'     | 51:9:304:C:O4'     | 2.09                     | 0.52              |
| 51:9:1658:G:OP2    | 51:9:1660:C:N4     | 2.36                     | 0.52              |
| 55:DD:193:ASP:CB   | 55:DD:194:PRO:HD3  | 2.40                     | 0.52              |
| 59:HH:43:LEU:HD12  | 59:HH:75:ILE:HD11  | 1.92                     | 0.52              |
| 66:OO:58:GLY:O     | 66:OO:62:VAL:HG22  | 2.09                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 67:PP:111:MET:HE2  | 67:PP:119:PHE:CD1  | 2.45                     | 0.52              |
| 84:gg:32:LEU:CB    | 84:gg:71:ILE:HD11  | 2.40                     | 0.52              |
| 87:jj:56:ILE:N     | 91:jj:601:SF4:S3   | 2.74                     | 0.52              |
| 48:5:643:C:H2'     | 48:5:644:G:C8      | 2.45                     | 0.52              |
| 51:9:546:G:C2'     | 51:9:547:G:O4'     | 2.58                     | 0.52              |
| 56:EE:107:GLY:HA3  | 56:EE:189:LEU:HD22 | 1.92                     | 0.52              |
| 59:HH:17:ASP:OD1   | 59:HH:19:PHE:N     | 2.42                     | 0.52              |
| 63:LL:20:LYS:O     | 63:LL:21:LYS:CB    | 2.57                     | 0.52              |
| 2:B:78:ILE:N       | 2:B:78:ILE:HD12    | 2.24                     | 0.52              |
| 3:C:89:GLN:O       | 48:5:2353:U:OP1    | 2.28                     | 0.52              |
| 30:e:57:ASN:OD1    | 48:5:1899:G:O2'    | 2.24                     | 0.52              |
| 48:5:1358:G:O2'    | 48:5:1360:G:O6     | 2.20                     | 0.52              |
| 48:5:1755:C:H42    | 48:5:1775:A:N6     | 2.06                     | 0.52              |
| 48:5:2055:G:H4'    | 48:5:2056:G:OP2    | 2.10                     | 0.52              |
| 51:9:1227:G:C2     | 51:9:1228:A:C8     | 2.98                     | 0.52              |
| 51:9:1344:A:H4'    | 51:9:1345:G:OP1    | 2.10                     | 0.52              |
| 76:YY:56:PHE:CZ    | 76:YY:91:LEU:HD23  | 2.45                     | 0.52              |
| 87:jj:377:MET:HG3  | 87:jj:518:VAL:HG22 | 1.91                     | 0.52              |
| 7:G:56:LYS:HA      | 48:5:4085:A:C8     | 2.45                     | 0.51              |
| 7:G:108:GLN:OE1    | 7:G:108:GLN:N      | 2.38                     | 0.51              |
| 42:r:64:MET:HE3    | 42:r:102:TYR:CD2   | 2.45                     | 0.51              |
| 48:5:23:C:H2'      | 48:5:24:G:O4'      | 2.10                     | 0.51              |
| 48:5:99:A:H2'      | 48:5:100:C:O2      | 2.10                     | 0.51              |
| 48:5:496:G:H2'     | 48:5:497:G:O4'     | 2.10                     | 0.51              |
| 48:5:1996:C:H42    | 48:5:2000:G:H22    | 1.58                     | 0.51              |
| 48:5:2706:G:O2'    | 48:5:2709:C:N4     | 2.43                     | 0.51              |
| 48:5:3701:OMC:N4   | 48:5:3745:U:H2'    | 2.26                     | 0.51              |
| 50:8:81:C:H5'      | 50:8:82:A:O5'      | 2.10                     | 0.51              |
| 51:9:507:G:O2'     | 51:9:508:A:OP1     | 2.24                     | 0.51              |
| 51:9:1444:U:O2'    | 51:9:1445:PSU:H5'' | 2.09                     | 0.51              |
| 51:9:1477:U:O2'    | 51:9:1478:U:P      | 2.67                     | 0.51              |
| 57:FF:32:ASP:C     | 57:FF:34:SER:N     | 2.67                     | 0.51              |
| 83:ff:114:ARG:O    | 83:ff:127:MET:HG3  | 2.11                     | 0.51              |
| 84:gg:244:ASN:OD1  | 84:gg:245:ARG:N    | 2.43                     | 0.51              |
| 86:ii:188:LEU:HD21 | 86:ii:192:ARG:NH2  | 2.25                     | 0.51              |
| 87:jj:164:LEU:HD22 | 87:jj:236:ASP:CB   | 2.40                     | 0.51              |
| 87:jj:472:LEU:HD13 | 87:jj:472:LEU:C    | 2.34                     | 0.51              |
| 2:B:252:ALA:HB1    | 48:5:4524:G:N3     | 2.24                     | 0.51              |
| 3:C:80:ARG:NH2     | 48:5:1645:C:OP1    | 2.42                     | 0.51              |
| 37:l:44:TRP:CE3    | 48:5:2409:U:O2     | 2.63                     | 0.51              |
| 48:5:1957:U:O2'    | 48:5:1958:A:O5'    | 2.28                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:3625:G:O2'    | 48:5:3626:G:P      | 2.68                     | 0.51              |
| 54:CC:102:LEU:HD23 | 54:CC:131:GLY:C    | 2.35                     | 0.51              |
| 59:HH:33:ASN:OD1   | 59:HH:34:SER:N     | 2.43                     | 0.51              |
| 65:NN:45:LEU:HD23  | 65:NN:49:GLN:HB3   | 1.92                     | 0.51              |
| 86:ii:332:VAL:O    | 86:ii:332:VAL:HG13 | 2.09                     | 0.51              |
| 87:jj:133:LYS:HD2  | 87:jj:136:ASP:O    | 2.10                     | 0.51              |
| 8:H:106:GLN:CG     | 8:H:111:LEU:HD12   | 2.41                     | 0.51              |
| 24:Y:92:GLY:O      | 24:Y:93:THR:OG1    | 2.28                     | 0.51              |
| 48:5:2490:U:H2'    | 48:5:2491:C:C2     | 2.46                     | 0.51              |
| 51:9:688:U:OP1     | 59:HH:103:LYS:HD2  | 2.10                     | 0.51              |
| 51:9:1411:G:H8     | 51:9:1411:G:O5'    | 1.94                     | 0.51              |
| 84:gg:178:ASN:O    | 84:gg:178:ASN:OD1  | 2.29                     | 0.51              |
| 87:jj:470:VAL:O    | 87:jj:474:LEU:HG   | 2.10                     | 0.51              |
| 26:a:2:PRO:CG      | 26:a:5:LEU:HD12    | 2.39                     | 0.51              |
| 26:a:100:ILE:N     | 26:a:100:ILE:HD12  | 2.26                     | 0.51              |
| 35:j:39:TYR:C      | 35:j:39:TYR:CD1    | 2.87                     | 0.51              |
| 44:t:28:LEU:HD23   | 44:t:29:ALA:N      | 2.26                     | 0.51              |
| 44:t:50:THR:HG21   | 44:t:72:GLU:CG     | 2.41                     | 0.51              |
| 48:5:266:C:OP1     | 48:5:266:C:O4'     | 2.28                     | 0.51              |
| 48:5:4152:G:H2'    | 48:5:4153:C:O4'    | 2.10                     | 0.51              |
| 51:9:306:C:O2      | 51:9:307:G:N2      | 2.39                     | 0.51              |
| 51:9:1310:U:OP1    | 83:ff:126:PHE:N    | 2.43                     | 0.51              |
| 51:9:1404:U:O2     | 51:9:1580:A:H5'    | 2.11                     | 0.51              |
| 51:9:1550:G:O2'    | 51:9:1558:C:O2     | 2.27                     | 0.51              |
| 51:9:1809:A:H2'    | 51:9:1810:U:C6     | 2.46                     | 0.51              |
| 71:TT:11:GLN:O     | 71:TT:15:VAL:HG23  | 2.10                     | 0.51              |
| 2:B:223:THR:HA     | 2:B:338:VAL:HG22   | 1.92                     | 0.51              |
| 10:J:167:GLN:HA    | 10:J:172:GLY:CA    | 2.41                     | 0.51              |
| 11:L:128:PRO:CD    | 11:L:144:LEU:HD11  | 2.40                     | 0.51              |
| 42:r:70:GLN:O      | 42:r:71:ARG:HG2    | 2.09                     | 0.51              |
| 48:5:2504:C:O2     | 48:5:2505:C:C4     | 2.63                     | 0.51              |
| 48:5:3706:C:H2'    | 48:5:3707:U:O4'    | 2.10                     | 0.51              |
| 48:5:4397:A:OP1    | 92:5:5425:HOH:O    | 2.19                     | 0.51              |
| 48:5:5006:U:H4'    | 48:5:5007:A:H5'    | 1.92                     | 0.51              |
| 51:9:857:U:H2'     | 51:9:858:A:C8      | 2.45                     | 0.51              |
| 51:9:1406:G:O3'    | 51:9:1407:U:H4'    | 2.11                     | 0.51              |
| 57:FF:102:LEU:HD21 | 77:ZZ:100:VAL:HG21 | 1.91                     | 0.51              |
| 64:MM:18:LEU:HD23  | 64:MM:18:LEU:C     | 2.35                     | 0.51              |
| 68:QQ:109:LYS:HG2  | 68:QQ:120:LEU:HD13 | 1.93                     | 0.51              |
| 73:VV:39:VAL:HG12  | 73:VV:45:ARG:O     | 2.09                     | 0.51              |
| 87:jj:263:ILE:HG23 | 87:jj:263:ILE:O    | 2.09                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:I:118:ALA:O      | 48:5:1865:G:H5'    | 2.10                     | 0.51              |
| 15:P:39:MET:HE2    | 15:P:43:LYS:NZ     | 2.26                     | 0.51              |
| 25:Z:53:VAL:HB     | 25:Z:62:ILE:HD12   | 1.92                     | 0.51              |
| 48:5:106:A:H2'     | 48:5:107:G:O4'     | 2.11                     | 0.51              |
| 48:5:1905:U:OP1    | 92:5:5426:HOH:O    | 2.19                     | 0.51              |
| 48:5:1931:C:O2'    | 48:5:1932:A:O5'    | 2.26                     | 0.51              |
| 48:5:2002:A:N3     | 48:5:2002:A:H2'    | 2.26                     | 0.51              |
| 48:5:2040:A:H4'    | 48:5:2041:A:O5'    | 2.10                     | 0.51              |
| 48:5:2100:G:OP2    | 48:5:2100:G:H4'    | 2.11                     | 0.51              |
| 51:9:13:C:H4'      | 51:9:1355:C:O2     | 2.10                     | 0.51              |
| 51:9:327:G:H1'     | 51:9:328:U:OP2     | 2.10                     | 0.51              |
| 51:9:526:A:OP1     | 82:ee:35:ARG:NH1   | 2.43                     | 0.51              |
| 51:9:833:C:O2'     | 51:9:834:C:O4'     | 2.28                     | 0.51              |
| 55:DD:127:MET:HE1  | 55:DD:133:GLY:HA2  | 1.91                     | 0.51              |
| 59:HH:136:PRO:HB2  | 59:HH:166:VAL:HG23 | 1.92                     | 0.51              |
| 62:KK:76:ILE:O     | 62:KK:80:ARG:HG2   | 2.11                     | 0.51              |
| 87:jj:377:MET:CB   | 87:jj:518:VAL:HG22 | 2.41                     | 0.51              |
| 8:H:165:THR:HG21   | 8:H:179:ILE:HG13   | 1.93                     | 0.51              |
| 14:O:23:VAL:HG13   | 14:O:33:VAL:HG11   | 1.93                     | 0.51              |
| 28:c:48:LEU:HD21   | 28:c:60:ILE:HG21   | 1.91                     | 0.51              |
| 48:5:2065:G:H2'    | 48:5:2066:C:O4'    | 2.10                     | 0.51              |
| 48:5:4395:U:OP2    | 92:5:5428:HOH:O    | 2.20                     | 0.51              |
| 51:9:1039:C:H2'    | 51:9:1040:G:H5''   | 1.93                     | 0.51              |
| 53:BB:154:SER:O    | 53:BB:154:SER:OG   | 2.27                     | 0.51              |
| 59:HH:158:LEU:HD11 | 59:HH:187:PHE:CD2  | 2.44                     | 0.51              |
| 62:KK:78:TYR:CD1   | 62:KK:78:TYR:C     | 2.88                     | 0.51              |
| 68:QQ:25:CYS:SG    | 68:QQ:66:VAL:HG11  | 2.50                     | 0.51              |
| 86:ii:135:ALA:O    | 86:ii:139:LEU:HD13 | 2.10                     | 0.51              |
| 87:jj:281:TYR:HB2  | 87:jj:577:ILE:HG21 | 1.92                     | 0.51              |
| 4:D:56:THR:HG22    | 4:D:57:ASN:H       | 1.75                     | 0.51              |
| 12:M:136:LEU:HD13  | 12:M:136:LEU:C     | 2.36                     | 0.51              |
| 48:5:1072:C:O2'    | 48:5:1073:G:P      | 2.67                     | 0.51              |
| 48:5:1197:C:H2'    | 48:5:1198:G:C8     | 2.45                     | 0.51              |
| 48:5:4508:C:N3     | 48:5:4512:U:H5     | 2.09                     | 0.51              |
| 51:9:71:G:O2'      | 51:9:72:C:P        | 2.69                     | 0.51              |
| 51:9:140:C:O2'     | 51:9:141:A:OP1     | 2.27                     | 0.51              |
| 51:9:690:G:H3'     | 51:9:691:G:H8      | 1.74                     | 0.51              |
| 58:GG:102:VAL:HG13 | 58:GG:102:VAL:O    | 2.10                     | 0.51              |
| 1:A:215:ASN:ND2    | 48:5:4546:A:N7     | 2.57                     | 0.51              |
| 32:g:56:VAL:HG13   | 32:g:72:LYS:HA     | 1.92                     | 0.51              |
| 37:l:2:SER:O       | 37:l:3:SER:HB3     | 2.11                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:m:100:TYR:O     | 48:5:4472:G:O2'    | 2.26                     | 0.51              |
| 48:5:1980:U:H2'    | 48:5:1982:G:H5'    | 1.92                     | 0.51              |
| 48:5:4906:C:H2'    | 48:5:4906:C:O2     | 2.11                     | 0.51              |
| 51:9:985:G:H5'     | 66:OO:138:ASP:OD2  | 2.11                     | 0.51              |
| 51:9:1418:C:H4'    | 51:9:1419:C:OP1    | 2.11                     | 0.51              |
| 51:9:1746:U:H2'    | 51:9:1747:C:O4'    | 2.10                     | 0.51              |
| 58:GG:142:ARG:HA   | 58:GG:147:LEU:HD12 | 1.92                     | 0.51              |
| 20:U:23:LEU:HD21   | 20:U:87:THR:HG1    | 1.76                     | 0.51              |
| 20:U:38:ASN:OD1    | 20:U:38:ASN:N      | 2.41                     | 0.51              |
| 20:U:93:LYS:HE3    | 20:U:93:LYS:HA     | 1.92                     | 0.51              |
| 44:t:62:LEU:HB2    | 44:t:75:PRO:CD     | 2.41                     | 0.51              |
| 51:9:465:A:H4'     | 51:9:466:G:O5'     | 2.11                     | 0.51              |
| 51:9:1102:G:N2     | 51:9:1130:G:N2     | 2.56                     | 0.51              |
| 51:9:1531:A:H2'    | 51:9:1532:C:C6     | 2.45                     | 0.51              |
| 53:BB:178:THR:O    | 53:BB:178:THR:CG2  | 2.59                     | 0.51              |
| 55:DD:50:ILE:H     | 55:DD:50:ILE:HD12  | 1.75                     | 0.51              |
| 58:GG:176:ILE:HG22 | 58:GG:179:LEU:HD23 | 1.93                     | 0.51              |
| 59:HH:139:ILE:HG22 | 59:HH:156:VAL:HG11 | 1.93                     | 0.51              |
| 71:TT:28:LEU:HA    | 71:TT:110:LEU:HD11 | 1.92                     | 0.51              |
| 87:jj:188:LEU:HD23 | 87:jj:197:GLN:OE1  | 2.11                     | 0.51              |
| 18:S:93:MET:HG2    | 48:5:1952:G:H4'    | 1.92                     | 0.50              |
| 27:b:69:ALA:O      | 27:b:73:LYS:HG3    | 2.11                     | 0.50              |
| 35:j:9:GLY:HA3     | 48:5:2800:G:H1'    | 1.93                     | 0.50              |
| 48:5:922(B):C:C2'  | 48:5:923:C:OP1     | 2.59                     | 0.50              |
| 48:5:1957:U:HO2'   | 48:5:1958:A:P      | 2.32                     | 0.50              |
| 48:5:2503:G:H2'    | 48:5:2504:C:C1'    | 2.41                     | 0.50              |
| 48:5:2528:G:H2'    | 48:5:2529:A:O4'    | 2.10                     | 0.50              |
| 50:8:122:G:H21     | 50:8:128:C:N4      | 1.97                     | 0.50              |
| 51:9:1019:C:H2'    | 51:9:1020:A:O4'    | 2.11                     | 0.50              |
| 51:9:1130:G:H2'    | 51:9:1131:G:H5''   | 1.92                     | 0.50              |
| 51:9:1744:G:HO2'   | 51:9:1745:A:P      | 2.33                     | 0.50              |
| 57:FF:116:ILE:HD11 | 57:FF:151:ILE:HD11 | 1.93                     | 0.50              |
| 58:GG:224:ARG:O    | 58:GG:228:ILE:HD12 | 2.11                     | 0.50              |
| 68:QQ:42:ILE:CD1   | 68:QQ:51:LEU:HD11  | 2.31                     | 0.50              |
| 72:UU:24:LEU:HD11  | 72:UU:112:VAL:HG13 | 1.89                     | 0.50              |
| 74:WW:94:LEU:HD11  | 74:WW:102:ILE:HG23 | 1.93                     | 0.50              |
| 76:YY:117:VAL:HG21 | 76:YY:125:VAL:CG1  | 2.41                     | 0.50              |
| 87:jj:292:VAL:HG23 | 87:jj:292:VAL:O    | 2.10                     | 0.50              |
| 25:Z:57:MET:HB2    | 25:Z:62:ILE:HD11   | 1.93                     | 0.50              |
| 35:j:44:LYS:NZ     | 48:5:23:C:OP1      | 2.43                     | 0.50              |
| 43:s:30:VAL:HG12   | 43:s:189:ILE:HD12  | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:s:67:GLY:N      | 43:s:75:LEU:HD12   | 2.27                     | 0.50              |
| 48:5:258:G:O2'     | 48:5:259:C:H5'     | 2.11                     | 0.50              |
| 54:CC:78:LEU:HD23  | 54:CC:78:LEU:H     | 1.75                     | 0.50              |
| 57:FF:40:ALA:HB1   | 57:FF:45:TYR:CG    | 2.46                     | 0.50              |
| 59:HH:118:ARG:C    | 59:HH:121:THR:HG1  | 2.19                     | 0.50              |
| 63:LL:76:VAL:HG22  | 63:LL:125:ILE:HD13 | 1.92                     | 0.50              |
| 64:MM:21:VAL:CG2   | 64:MM:121:LYS:HD3  | 2.41                     | 0.50              |
| 86:ii:332:VAL:O    | 86:ii:332:VAL:CG1  | 2.60                     | 0.50              |
| 87:jj:564:ILE:HG23 | 87:jj:577:ILE:HD11 | 1.92                     | 0.50              |
| 2:B:223:THR:HA     | 2:B:338:VAL:CG2    | 2.42                     | 0.50              |
| 25:Z:91:LEU:HD22   | 25:Z:96:VAL:HG21   | 1.93                     | 0.50              |
| 40:o:99:ARG:NH1    | 40:o:102:GLN:OE1   | 2.44                     | 0.50              |
| 43:s:121:VAL:HG22  | 43:s:182:PRO:HB2   | 1.93                     | 0.50              |
| 48:5:267:G:O2'     | 48:5:268:G:P       | 2.69                     | 0.50              |
| 48:5:1316:OMG:HM22 | 48:5:1317:U:H5'    | 1.93                     | 0.50              |
| 48:5:3736:A:H2'    | 48:5:3737:A:C8     | 2.46                     | 0.50              |
| 48:5:4963:G:C2'    | 48:5:4964:C:O5'    | 2.59                     | 0.50              |
| 51:9:532:C:C2'     | 51:9:533:A:O5'     | 2.60                     | 0.50              |
| 51:9:640:A:H2'     | 51:9:641:A:C8      | 2.46                     | 0.50              |
| 51:9:1287:A:H2'    | 51:9:1288:U:H5''   | 1.91                     | 0.50              |
| 51:9:1441:U:H1'    | 51:9:1442:OMU:H5   | 1.92                     | 0.50              |
| 54:CC:186:GLY:HA2  | 54:CC:242:ASP:OD2  | 2.11                     | 0.50              |
| 55:DD:113:LEU:HD21 | 55:DD:117:ARG:HG2  | 1.92                     | 0.50              |
| 64:MM:71:GLU:HG2   | 83:ff:109:ILE:HD12 | 1.93                     | 0.50              |
| 76:YY:35:VAL:HG23  | 76:YY:40:ILE:HD11  | 1.93                     | 0.50              |
| 78:aa:32:LYS:O     | 78:aa:37:LYS:NZ    | 2.40                     | 0.50              |
| 84:gg:51:ASN:C     | 84:gg:51:ASN:OD1   | 2.55                     | 0.50              |
| 84:gg:133:ASN:OD1  | 84:gg:133:ASN:N    | 2.44                     | 0.50              |
| 14:O:190:SER:HA    | 14:O:193:THR:HB    | 1.93                     | 0.50              |
| 16:Q:14:ARG:NH2    | 48:5:2083:C:OP1    | 2.44                     | 0.50              |
| 30:e:98:GLU:OE1    | 30:e:123:THR:OG1   | 2.29                     | 0.50              |
| 48:5:4990:C:OP2    | 48:5:4990:C:H4'    | 2.12                     | 0.50              |
| 51:9:1088:U:H4'    | 51:9:1089:G:OP2    | 2.10                     | 0.50              |
| 51:9:1395:C:HO2'   | 51:9:1396:A:P      | 2.26                     | 0.50              |
| 51:9:1660:C:O5'    | 51:9:1660:C:O2     | 2.29                     | 0.50              |
| 56:EE:73:ASP:OD2   | 56:EE:122:LYS:NZ   | 2.35                     | 0.50              |
| 56:EE:195:ILE:C    | 56:EE:196:THR:HG1  | 2.10                     | 0.50              |
| 71:TT:123:LEU:HD22 | 71:TT:127:GLY:HA3  | 1.94                     | 0.50              |
| 72:UU:81:GLN:OE1   | 72:UU:83:ARG:NE    | 2.41                     | 0.50              |
| 87:jj:484:LEU:HD13 | 87:jj:484:LEU:C    | 2.36                     | 0.50              |
| 18:S:19:THR:HB     | 18:S:20:PRO:HD2    | 1.94                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:1218:G:H2'    | 48:5:1219:G:O4'    | 2.12                     | 0.50              |
| 48:5:1445:U:H2'    | 48:5:1446:C:C6     | 2.45                     | 0.50              |
| 51:9:1037:G:OP2    | 92:9:2008:HOH:O    | 2.20                     | 0.50              |
| 51:9:1324:G:H21    | 51:9:1510:G:C5'    | 2.24                     | 0.50              |
| 75:XX:122:VAL:HG12 | 75:XX:130:LEU:CD1  | 2.41                     | 0.50              |
| 86:ii:81:ARG:NE    | 86:ii:113:ASP:OD1  | 2.45                     | 0.50              |
| 87:jj:258:THR:O    | 87:jj:262:LEU:HG   | 2.11                     | 0.50              |
| 8:H:56:ARG:NE      | 8:H:58:ASP:OD2     | 2.45                     | 0.50              |
| 10:J:164:ARG:HG3   | 10:J:168:GLN:OE1   | 2.12                     | 0.50              |
| 27:b:53:GLY:O      | 27:b:57:MET:HG3    | 2.12                     | 0.50              |
| 29:d:63:ARG:HD3    | 29:d:103:TYR:CD1   | 2.47                     | 0.50              |
| 33:h:7:ARG:NH1     | 50:8:86:U:C2       | 2.80                     | 0.50              |
| 48:5:269:G:H2'     | 48:5:270:U:C6      | 2.47                     | 0.50              |
| 48:5:366:A:H2'     | 48:5:367:C:O4'     | 2.12                     | 0.50              |
| 48:5:492:U:O2'     | 48:5:493:G:OP1     | 2.21                     | 0.50              |
| 48:5:1982:G:O2'    | 48:5:1983:A:P      | 2.69                     | 0.50              |
| 48:5:2092:G:N3     | 48:5:2093:G:N2     | 2.59                     | 0.50              |
| 48:5:2465:C:H1'    | 48:5:3672:G:N2     | 2.23                     | 0.50              |
| 51:9:196:C:H3'     | 51:9:197:U:H6      | 1.77                     | 0.50              |
| 51:9:1823:A:N6     | 51:9:1824:A:C6     | 2.80                     | 0.50              |
| 58:GG:113:ILE:HD11 | 58:GG:124:LEU:HD23 | 1.94                     | 0.50              |
| 67:PP:87:PRO:HA    | 67:PP:90:VAL:HG23  | 1.94                     | 0.50              |
| 70:SS:114:LEU:HD13 | 70:SS:121:ARG:HG2  | 1.93                     | 0.50              |
| 2:B:285:TYR:HB2    | 2:B:332:MET:HG2    | 1.94                     | 0.50              |
| 3:C:336:ARG:O      | 3:C:340:ILE:HD12   | 2.12                     | 0.50              |
| 18:S:1:MET:HE1     | 18:S:33:PHE:O      | 2.12                     | 0.50              |
| 38:m:127:VAL:HG13  | 38:m:127:VAL:O     | 2.12                     | 0.50              |
| 48:5:978:G:H22     | 48:5:1277:G:H1     | 1.58                     | 0.50              |
| 48:5:1397:A:N1     | 48:5:1498:G:O2'    | 2.42                     | 0.50              |
| 51:9:108:G:H2'     | 51:9:109:PSU:H5''  | 1.93                     | 0.50              |
| 51:9:838:G:H4'     | 51:9:839:C:H3'     | 1.93                     | 0.50              |
| 51:9:1700:C:C2     | 51:9:1834:A:N6     | 2.79                     | 0.50              |
| 86:ii:152:ASP:OD1  | 86:ii:154:SER:N    | 2.36                     | 0.50              |
| 2:B:21:ARG:NH2     | 48:5:4981:G:O6     | 2.44                     | 0.50              |
| 13:N:172:ARG:NH1   | 48:5:62:A:OP1      | 2.44                     | 0.50              |
| 28:c:37:MET:SD     | 28:c:97:ILE:HD11   | 2.52                     | 0.50              |
| 39:n:2:ARG:NE      | 51:9:1842:4AC:OP2  | 2.39                     | 0.50              |
| 48:5:2412:A:H2'    | 48:5:2413:U:C6     | 2.47                     | 0.50              |
| 57:FF:25:THR:O     | 57:FF:28:VAL:HG12  | 2.12                     | 0.50              |
| 62:KK:83:LEU:HB3   | 62:KK:85:LEU:HD23  | 1.93                     | 0.50              |
| 67:PP:111:MET:HE2  | 67:PP:119:PHE:CE1  | 2.47                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:RR:21:TYR:CE1   | 69:RR:61:ILE:HG21  | 2.47                     | 0.50              |
| 86:ii:289:ARG:HD3  | 86:ii:412:ILE:HD13 | 1.92                     | 0.50              |
| 1:A:142:GLU:C      | 1:A:143:THR:HG1    | 2.08                     | 0.50              |
| 2:B:228:TYR:O      | 48:5:2835:A:O2'    | 2.28                     | 0.50              |
| 7:G:90:GLN:NE2     | 7:G:94:GLN:OE1     | 2.45                     | 0.50              |
| 10:J:57:VAL:HG11   | 10:J:60:PHE:CD2    | 2.46                     | 0.50              |
| 12:M:97:ALA:HB2    | 14:O:203:VAL:HB    | 1.93                     | 0.50              |
| 14:O:201:LEU:HD22  | 14:O:201:LEU:N     | 2.27                     | 0.50              |
| 48:5:2588:C:OP1    | 48:5:2768:C:O2'    | 2.26                     | 0.50              |
| 48:5:5003:U:H2'    | 48:5:5004:C:C6     | 2.47                     | 0.50              |
| 51:9:157:U:H5''    | 87:jj:583:ILE:HD11 | 1.94                     | 0.50              |
| 56:EE:111:VAL:HG23 | 56:EE:111:VAL:O    | 2.12                     | 0.50              |
| 60:II:11:ARG:CZ    | 60:II:17:LYS:HE3   | 2.42                     | 0.50              |
| 62:KK:74:GLU:OE1   | 62:KK:74:GLU:N     | 2.40                     | 0.50              |
| 87:jj:111:THR:HG22 | 87:jj:112:ASN:H    | 1.76                     | 0.50              |
| 44:t:112:ILE:H     | 44:t:112:ILE:HD12  | 1.76                     | 0.49              |
| 51:9:1288:U:O2'    | 51:9:1289:U:OP2    | 2.28                     | 0.49              |
| 51:9:1466:G:H5'    | 69:RR:4:VAL:HG22   | 1.93                     | 0.49              |
| 64:MM:89:VAL:HG22  | 64:MM:109:VAL:HG21 | 1.92                     | 0.49              |
| 68:QQ:107:GLU:O    | 68:QQ:111:ILE:HD13 | 2.11                     | 0.49              |
| 69:RR:98:VAL:O     | 69:RR:118:GLN:HA   | 2.12                     | 0.49              |
| 84:gg:112:ALA:HB3  | 84:gg:121:VAL:HG23 | 1.92                     | 0.49              |
| 86:ii:318:GLU:C    | 86:ii:319:ILE:HD13 | 2.36                     | 0.49              |
| 12:M:46:ARG:NH1    | 48:5:937:U:OP1     | 2.45                     | 0.49              |
| 43:s:187:LEU:HD23  | 43:s:187:LEU:H     | 1.76                     | 0.49              |
| 47:3:76:A:C8       | 48:5:4341:C:N4     | 2.73                     | 0.49              |
| 54:CC:63:VAL:O     | 54:CC:64:THR:HB    | 2.11                     | 0.49              |
| 58:GG:18:VAL:CG1   | 58:GG:24:LEU:HD21  | 2.35                     | 0.49              |
| 69:RR:17:ILE:HG21  | 69:RR:61:ILE:HD11  | 1.93                     | 0.49              |
| 81:dd:19:ARG:O     | 81:dd:27:ARG:NH1   | 2.45                     | 0.49              |
| 84:gg:91:ASP:HB3   | 84:gg:94:THR:HG22  | 1.94                     | 0.49              |
| 84:gg:109:LEU:HD13 | 84:gg:152:SER:HA   | 1.94                     | 0.49              |
| 87:jj:434:ASP:OD1  | 87:jj:435:ALA:N    | 2.45                     | 0.49              |
| 87:jj:531:ARG:HG2  | 87:jj:531:ARG:HH11 | 1.76                     | 0.49              |
| 4:D:56:THR:HG21    | 49:7:26:C:OP1      | 2.12                     | 0.49              |
| 9:I:203:ARG:NH1    | 49:7:105:C:OP2     | 2.46                     | 0.49              |
| 11:L:59:VAL:HB     | 48:5:74:G:H5'      | 1.94                     | 0.49              |
| 14:O:61:ARG:NH1    | 48:5:4587:G:OP1    | 2.40                     | 0.49              |
| 14:O:81:TRP:CZ2    | 14:O:99:LEU:HD21   | 2.47                     | 0.49              |
| 33:h:103:LYS:O     | 33:h:108:GLN:NE2   | 2.45                     | 0.49              |
| 36:k:16:ARG:CD     | 36:k:61:PRO:HG3    | 2.41                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:s:29:ILE:CD1   | 43:s:78:LEU:HD13   | 2.42                     | 0.49              |
| 47:3:21:A:N6      | 47:3:46:G:O2'      | 2.46                     | 0.49              |
| 48:5:2750:G:H2'   | 48:5:2751:G:O4'    | 2.13                     | 0.49              |
| 48:5:3773:U:C2'   | 48:5:3775:A:C2     | 2.96                     | 0.49              |
| 48:5:3773:U:C2'   | 48:5:3775:A:H2     | 2.26                     | 0.49              |
| 48:5:3792:OMG:H2' | 48:5:3793:U:C6     | 2.47                     | 0.49              |
| 48:5:3810:C:O2'   | 48:5:3811:G:P      | 2.70                     | 0.49              |
| 51:9:899:U:H2'    | 51:9:900:C:O4'     | 2.12                     | 0.49              |
| 51:9:1432:U:O2'   | 51:9:1433:C:P      | 2.70                     | 0.49              |
| 51:9:1661:A:C8    | 81:dd:14:PHE:CD1   | 3.00                     | 0.49              |
| 51:9:1693:G:N2    | 51:9:1834:A:C8     | 2.81                     | 0.49              |
| 59:HH:17:ASP:OD2  | 59:HH:21:SER:OG    | 2.20                     | 0.49              |
| 84:gg:177:TRP:HA  | 84:gg:184:LEU:HA   | 1.94                     | 0.49              |
| 87:jj:377:MET:CG  | 87:jj:518:VAL:HG22 | 2.42                     | 0.49              |
| 20:U:113:ARG:NH1  | 48:5:2703:G:OP1    | 2.46                     | 0.49              |
| 29:d:114:PHE:HA   | 29:d:117:LEU:HD12  | 1.94                     | 0.49              |
| 31:f:52:LYS:NZ    | 48:5:4751:G:N7     | 2.57                     | 0.49              |
| 48:5:3603:G:H2'   | 48:5:3604:A:C8     | 2.47                     | 0.49              |
| 48:5:4119:C:C4'   | 48:5:4120:U:OP1    | 2.60                     | 0.49              |
| 48:5:4331:G:O2'   | 48:5:4332:C:OP1    | 2.26                     | 0.49              |
| 51:9:1421:A:H3'   | 51:9:1422:G:C8     | 2.47                     | 0.49              |
| 51:9:1779:G:H2'   | 51:9:1780:G:C8     | 2.48                     | 0.49              |
| 58:GG:147:LEU:O   | 58:GG:148:SER:C    | 2.56                     | 0.49              |
| 59:HH:55:GLY:HA3  | 59:HH:57:ARG:HH11  | 1.78                     | 0.49              |
| 62:KK:21:MET:HE1  | 62:KK:35:LEU:CD1   | 2.42                     | 0.49              |
| 64:MM:18:LEU:HD22 | 64:MM:88:TRP:CZ3   | 2.48                     | 0.49              |
| 72:UU:24:LEU:HB3  | 72:UU:32:LEU:HD11  | 1.95                     | 0.49              |
| 76:YY:15:ASN:O    | 76:YY:19:GLN:N     | 2.45                     | 0.49              |
| 84:gg:19:THR:OG1  | 84:gg:66:VAL:O     | 2.21                     | 0.49              |
| 84:gg:24:THR:HG22 | 84:gg:30:MET:CE    | 2.43                     | 0.49              |
| 10:J:128:LEU:N    | 10:J:128:LEU:HD23  | 2.28                     | 0.49              |
| 14:O:9:LEU:HD23   | 14:O:118:MET:HB2   | 1.93                     | 0.49              |
| 36:k:10:ASP:O     | 36:k:14:THR:OG1    | 2.30                     | 0.49              |
| 48:5:467:U:O4'    | 48:5:467:U:OP2     | 2.30                     | 0.49              |
| 48:5:4440:G:OP2   | 86:ii:189:ARG:HD2  | 2.12                     | 0.49              |
| 48:5:4966:A:H2'   | 48:5:4967:A:O4'    | 2.11                     | 0.49              |
| 51:9:799:U:O2'    | 51:9:800:U:O5'     | 2.23                     | 0.49              |
| 51:9:925:G:N2     | 65:NN:48:SER:OG    | 2.45                     | 0.49              |
| 51:9:1562:C:C2    | 51:9:1563:G:C8     | 3.00                     | 0.49              |
| 51:9:1617:G:C2    | 51:9:1620:A:C2     | 3.01                     | 0.49              |
| 55:DD:93:THR:O    | 55:DD:93:THR:CG2   | 2.61                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:DD:162:ASP:N    | 55:DD:163:PRO:CD   | 2.75                     | 0.49              |
| 59:HH:46:THR:HG22  | 59:HH:63:PHE:C     | 2.37                     | 0.49              |
| 65:NN:94:LYS:HG2   | 65:NN:118:ILE:HD13 | 1.94                     | 0.49              |
| 68:QQ:113:ILE:HG12 | 68:QQ:120:LEU:HD12 | 1.93                     | 0.49              |
| 69:RR:82:ASP:OD1   | 69:RR:83:ASN:N     | 2.45                     | 0.49              |
| 75:XX:56:GLY:N     | 82:ee:6:LEU:HD21   | 2.28                     | 0.49              |
| 2:B:223:THR:HG22   | 2:B:338:VAL:CG2    | 2.39                     | 0.49              |
| 47:3:73:G:O2'      | 47:3:74:C:H5'      | 2.12                     | 0.49              |
| 48:5:5:A:H2'       | 48:5:6:C:O4'       | 2.12                     | 0.49              |
| 48:5:914:U:H1'     | 48:5:915:A:C5      | 2.47                     | 0.49              |
| 48:5:2627:C:O4'    | 48:5:2627:C:O2     | 2.30                     | 0.49              |
| 48:5:4583:C:O2     | 48:5:4719:G:O6     | 2.31                     | 0.49              |
| 51:9:115:U:H2'     | 51:9:116:OMU:C6    | 2.43                     | 0.49              |
| 51:9:1124:C:H5''   | 53:BB:150:ILE:HG12 | 1.95                     | 0.49              |
| 51:9:1407:U:O2'    | 51:9:1408:U:H5'    | 2.12                     | 0.49              |
| 51:9:1606:G:N2     | 51:9:1632:G:H1'    | 2.28                     | 0.49              |
| 53:BB:167:LYS:HE2  | 53:BB:200:ALA:HB1  | 1.94                     | 0.49              |
| 64:MM:99:LYS:HG3   | 64:MM:99:LYS:O     | 2.13                     | 0.49              |
| 68:QQ:40:GLU:OE1   | 68:QQ:40:GLU:HA    | 2.13                     | 0.49              |
| 69:RR:98:VAL:HG13  | 69:RR:102:THR:HB   | 1.94                     | 0.49              |
| 83:ff:136:CYS:SG   | 83:ff:137:GLY:N    | 2.85                     | 0.49              |
| 5:E:97:LYS:HD3     | 48:5:687:U:O2'     | 2.12                     | 0.49              |
| 14:O:186:GLU:O     | 14:O:187:LYS:HB2   | 2.11                     | 0.49              |
| 21:V:129:TRP:CB    | 21:V:132:ILE:HD12  | 2.43                     | 0.49              |
| 48:5:1440:U:H2'    | 48:5:1441:C:O5'    | 2.13                     | 0.49              |
| 48:5:2104:A:O2'    | 48:5:2105:A:O4'    | 2.27                     | 0.49              |
| 48:5:4395:U:H6     | 48:5:4395:U:H5'    | 1.77                     | 0.49              |
| 50:8:124:U:O5'     | 50:8:124:U:H6      | 1.96                     | 0.49              |
| 51:9:147:A:HO2'    | 51:9:148:U:C5'     | 2.25                     | 0.49              |
| 51:9:1533:A:H2     | 51:9:1536:G:N3     | 2.11                     | 0.49              |
| 55:DD:27:ARG:O     | 62:KK:61:GLN:NE2   | 2.46                     | 0.49              |
| 63:LL:55:TYR:OH    | 63:LL:116:CYS:HB3  | 2.13                     | 0.49              |
| 86:ii:170:HIS:HB2  | 86:ii:212:LEU:HD11 | 1.95                     | 0.49              |
| 11:L:170:THR:HG22  | 11:L:171:GLU:N     | 2.28                     | 0.49              |
| 26:a:132:ARG:NH2   | 48:5:1468:C:OP1    | 2.43                     | 0.49              |
| 48:5:978:G:H22     | 48:5:1277:G:H22    | 1.61                     | 0.49              |
| 48:5:1077:C:H4'    | 48:5:1215:C:H5     | 1.76                     | 0.49              |
| 48:5:1755:C:C2     | 48:5:1757:U:C5     | 3.00                     | 0.49              |
| 48:5:2089:G:H1'    | 48:5:2090:U:OP2    | 2.12                     | 0.49              |
| 50:8:110:U:HO2'    | 50:8:111:U:C1'     | 2.13                     | 0.49              |
| 50:8:141:C:H2'     | 50:8:142:U:C6      | 2.48                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:9:151:C:OP1    | 76:YY:120:THR:OG1  | 2.28                     | 0.49              |
| 51:9:184:G:C4     | 51:9:185:G:C8      | 3.01                     | 0.49              |
| 51:9:216:C:O2     | 51:9:216:C:O4'     | 2.31                     | 0.49              |
| 51:9:687:C:H4'    | 59:HH:121:THR:HG21 | 1.94                     | 0.49              |
| 51:9:1313:A:OP1   | 64:MM:33:ARG:NH1   | 2.42                     | 0.49              |
| 51:9:1538:C:O2    | 71:TT:48:TYR:OH    | 2.25                     | 0.49              |
| 52:AA:30:LEU:HD22 | 52:AA:47:TYR:HE2   | 1.78                     | 0.49              |
| 59:HH:118:ARG:O   | 59:HH:121:THR:OG1  | 2.30                     | 0.49              |
| 64:MM:49:LEU:O    | 64:MM:111:VAL:HG12 | 2.12                     | 0.49              |
| 76:YY:56:PHE:HZ   | 76:YY:91:LEU:HD23  | 1.78                     | 0.49              |
| 86:ii:166:ARG:NH1 | 86:ii:265:ASN:OD1  | 2.41                     | 0.49              |
| 3:C:321:ASN:OD1   | 48:5:1280:C:O2'    | 2.30                     | 0.49              |
| 4:D:204:VAL:O     | 4:D:208:MET:HG3    | 2.13                     | 0.49              |
| 7:G:215:LEU:O     | 7:G:219:VAL:HG13   | 2.11                     | 0.49              |
| 27:b:52:LYS:O     | 48:5:1813:U:C5'    | 2.61                     | 0.49              |
| 36:k:60:LEU:HD23  | 36:k:61:PRO:HD2    | 1.94                     | 0.49              |
| 43:s:29:ILE:CD1   | 43:s:78:LEU:HD22   | 2.43                     | 0.49              |
| 48:5:1771:U:H2'   | 48:5:1772:C:C1'    | 2.43                     | 0.49              |
| 51:9:301:A:H2'    | 51:9:302:A:O4'     | 2.13                     | 0.49              |
| 51:9:736:C:H2'    | 51:9:737:G:C8      | 2.48                     | 0.49              |
| 51:9:1790:A:H2'   | 51:9:1791:A:O4'    | 2.13                     | 0.49              |
| 70:SS:26:ILE:HD13 | 70:SS:56:ALA:HA    | 1.93                     | 0.49              |
| 73:VV:67:ASP:O    | 73:VV:71:ARG:HG3   | 2.13                     | 0.49              |
| 4:D:232:THR:O     | 4:D:233:PRO:C      | 2.56                     | 0.49              |
| 43:s:32:ALA:HB1   | 43:s:35:VAL:HG11   | 1.95                     | 0.49              |
| 43:s:170:SER:O    | 43:s:174:LEU:HG    | 2.12                     | 0.49              |
| 44:t:15:LEU:HA    | 44:t:62:LEU:HD12   | 1.95                     | 0.49              |
| 46:2:18:G:HO2'    | 46:2:57:G:H22      | 1.52                     | 0.49              |
| 46:2:74:C:C5'     | 48:5:4548:A:H2'    | 2.43                     | 0.49              |
| 48:5:169:A:C6     | 48:5:267:G:C6      | 3.01                     | 0.49              |
| 48:5:449:C:H4'    | 48:5:449:C:OP1     | 2.12                     | 0.49              |
| 48:5:978:G:N2     | 48:5:1277:G:H1     | 2.11                     | 0.49              |
| 48:5:1586:G:O2'   | 48:5:1587:G:H5'    | 2.13                     | 0.49              |
| 48:5:1693:U:H2'   | 48:5:1694:C:O4'    | 2.13                     | 0.49              |
| 48:5:3598:C:H2'   | 48:5:3599:A:C8     | 2.47                     | 0.49              |
| 48:5:4072:C:H2'   | 48:5:4073:A:O4'    | 2.13                     | 0.49              |
| 48:5:4448:G:H4'   | 48:5:4449:A:OP2    | 2.12                     | 0.49              |
| 48:5:4932:U:H2'   | 48:5:4933:C:O5'    | 2.13                     | 0.49              |
| 51:9:50:A:N1      | 51:9:488:U:C5      | 2.81                     | 0.49              |
| 51:9:1617:G:H4'   | 81:dd:14:PHE:CE2   | 2.48                     | 0.49              |
| 51:9:1786:U:H2'   | 51:9:1787:G:H8     | 1.78                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:AA:197:VAL:HG12 | 52:AA:198:MET:H    | 1.78                     | 0.49              |
| 53:BB:164:ILE:O    | 53:BB:168:MET:HG3  | 2.13                     | 0.49              |
| 57:FF:28:VAL:O     | 57:FF:42:LYS:NZ    | 2.35                     | 0.49              |
| 63:LL:88:ILE:HG21  | 63:LL:126:VAL:HG21 | 1.94                     | 0.49              |
| 70:SS:7:GLU:OE1    | 70:SS:7:GLU:N      | 2.46                     | 0.49              |
| 84:gg:121:VAL:HG11 | 84:gg:165:ILE:HD13 | 1.94                     | 0.49              |
| 84:gg:184:LEU:HD12 | 84:gg:184:LEU:O    | 2.12                     | 0.49              |
| 2:B:61:ASP:O       | 2:B:61:ASP:OD2     | 2.31                     | 0.48              |
| 8:H:92:MET:HE3     | 8:H:181:VAL:HG23   | 1.94                     | 0.48              |
| 43:s:30:VAL:O      | 43:s:86:VAL:HA     | 2.13                     | 0.48              |
| 43:s:189:ILE:HG23  | 43:s:189:ILE:O     | 2.12                     | 0.48              |
| 44:t:28:LEU:HD22   | 44:t:40:LYS:HD3    | 1.95                     | 0.48              |
| 46:2:28:U:OP2      | 86:ii:50:LYS:NZ    | 2.46                     | 0.48              |
| 48:5:658:C:OP1     | 48:5:658:C:H4'     | 2.13                     | 0.48              |
| 51:9:914:U:O2      | 51:9:914:U:O4'     | 2.31                     | 0.48              |
| 51:9:1394:G:O2'    | 51:9:1395:C:P      | 2.71                     | 0.48              |
| 51:9:1435:C:O3'    | 51:9:1436:C:O4'    | 2.31                     | 0.48              |
| 51:9:1665:G:C8     | 71:TT:88:MET:HE3   | 2.48                     | 0.48              |
| 52:AA:30:LEU:HD21  | 52:AA:35:GLU:HG3   | 1.94                     | 0.48              |
| 55:DD:72:VAL:HG13  | 62:KK:20:VAL:HG21  | 1.94                     | 0.48              |
| 59:HH:30:LEU:C     | 59:HH:36:LEU:HD23  | 2.36                     | 0.48              |
| 83:ff:111:ARG:NE   | 83:ff:113:ARG:O    | 2.46                     | 0.48              |
| 86:ii:179:LYS:O    | 86:ii:180:HIS:CG   | 2.66                     | 0.48              |
| 87:jj:116:LYS:HD2  | 87:jj:116:LYS:C    | 2.38                     | 0.48              |
| 7:G:55:VAL:HG21    | 23:X:41:ARG:CD     | 2.43                     | 0.48              |
| 7:G:138:ALA:O      | 7:G:201:THR:O      | 2.31                     | 0.48              |
| 14:O:141:LEU:O     | 14:O:145:VAL:HG22  | 2.13                     | 0.48              |
| 16:Q:108:ARG:NH2   | 48:5:1355:G:OP1    | 2.45                     | 0.48              |
| 36:k:15:ALA:HB3    | 36:k:61:PRO:HG2    | 1.94                     | 0.48              |
| 48:5:507:G:O2'     | 48:5:508:G:H5'     | 2.13                     | 0.48              |
| 48:5:1238:A:HO2'   | 48:5:1239:C:P      | 2.35                     | 0.48              |
| 48:5:1381:U:O2     | 48:5:1381:U:O4'    | 2.31                     | 0.48              |
| 48:5:2695:A:H1'    | 48:5:2696:A:OP2    | 2.13                     | 0.48              |
| 48:5:4128:A:H2'    | 48:5:4129:G:O4'    | 2.12                     | 0.48              |
| 48:5:4302:U:H3'    | 48:5:4303:C:O2     | 2.12                     | 0.48              |
| 48:5:4525:C:OP1    | 92:5:5427:HOH:O    | 2.19                     | 0.48              |
| 51:9:310:C:H2'     | 51:9:311:C:C6      | 2.48                     | 0.48              |
| 51:9:852:G:H3'     | 51:9:853:C:O2      | 2.14                     | 0.48              |
| 51:9:996:A:H2'     | 51:9:997:A:C8      | 2.48                     | 0.48              |
| 51:9:1406:G:C4     | 51:9:1407:U:H1'    | 2.48                     | 0.48              |
| 56:EE:123:LEU:HD12 | 56:EE:236:ILE:HG12 | 1.95                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 77:ZZ:66:LYS:O    | 77:ZZ:110:THR:OG1  | 2.26                     | 0.48              |
| 80:cc:46:VAL:HG11 | 80:cc:50:VAL:HG11  | 1.94                     | 0.48              |
| 84:gg:10:THR:HG22 | 84:gg:308:ARG:CG   | 2.43                     | 0.48              |
| 84:gg:229:THR:OG1 | 84:gg:230:LEU:N    | 2.46                     | 0.48              |
| 84:gg:245:ARG:NH2 | 84:gg:312:VAL:HG11 | 2.28                     | 0.48              |
| 86:ii:52:LEU:HD12 | 86:ii:82:LEU:HD12  | 1.95                     | 0.48              |
| 2:B:297:LYS:HG3   | 2:B:299:ILE:HG23   | 1.95                     | 0.48              |
| 3:C:193:LYS:CD    | 3:C:196:MET:HE2    | 2.43                     | 0.48              |
| 48:5:743:G:H2'    | 48:5:744:G:O4'     | 2.13                     | 0.48              |
| 48:5:3603:G:O2'   | 48:5:3604:A:P      | 2.70                     | 0.48              |
| 48:5:4274:A:H2'   | 48:5:4275:G:C8     | 2.48                     | 0.48              |
| 51:9:112:U:OP1    | 51:9:292:A:N1      | 2.46                     | 0.48              |
| 51:9:927:C:H1'    | 79:bb:51:GLN:OE1   | 2.13                     | 0.48              |
| 51:9:1401:A:H2'   | 51:9:1402:A:C8     | 2.49                     | 0.48              |
| 51:9:1646:C:OP1   | 68:QQ:138:ARG:NH1  | 2.42                     | 0.48              |
| 84:gg:74:ASP:HB3  | 84:gg:76:GLN:CG    | 2.42                     | 0.48              |
| 1:A:117:GLU:HB2   | 1:A:162:ASN:HB2    | 1.95                     | 0.48              |
| 36:k:16:ARG:HD3   | 36:k:61:PRO:HG3    | 1.94                     | 0.48              |
| 48:5:749:G:HO2'   | 48:5:750:U:P       | 2.36                     | 0.48              |
| 48:5:1214:C:O2    | 48:5:1214:C:O4'    | 2.32                     | 0.48              |
| 51:9:661:U:OP2    | 51:9:662:G:O2'     | 2.31                     | 0.48              |
| 51:9:1310:U:H4'   | 83:ff:137:GLY:HA3  | 1.95                     | 0.48              |
| 70:SS:55:ARG:CD   | 77:ZZ:48:VAL:HG22  | 2.42                     | 0.48              |
| 74:WW:51:GLU:OE1  | 79:bb:8:LEU:CD1    | 2.61                     | 0.48              |
| 86:ii:356:HIS:CG  | 86:ii:356:HIS:O    | 2.66                     | 0.48              |
| 4:D:234:ASP:O     | 4:D:235:MET:CB     | 2.61                     | 0.48              |
| 15:P:9:GLU:CD     | 15:P:9:GLU:N       | 2.71                     | 0.48              |
| 20:U:60:VAL:O     | 20:U:74:SER:HA     | 2.14                     | 0.48              |
| 32:g:37:LYS:NZ    | 48:5:2516:G:OP2    | 2.40                     | 0.48              |
| 35:j:9:GLY:HA2    | 48:5:2792:C:O2     | 2.13                     | 0.48              |
| 38:m:119:ASN:C    | 38:m:119:ASN:OD1   | 2.56                     | 0.48              |
| 48:5:405:U:O2'    | 48:5:407:A:N7      | 2.41                     | 0.48              |
| 48:5:504:G:HO2'   | 48:5:505:G:P       | 2.35                     | 0.48              |
| 48:5:1198:G:H2'   | 48:5:1199:G:N9     | 2.28                     | 0.48              |
| 48:5:1345:A:H2'   | 48:5:1346:C:C6     | 2.48                     | 0.48              |
| 48:5:1599:G:H21   | 48:5:1601:A:C4'    | 2.26                     | 0.48              |
| 48:5:2504:C:O2'   | 48:5:2505:C:O2     | 2.22                     | 0.48              |
| 51:9:368:U:C2'    | 51:9:369:C:OP2     | 2.62                     | 0.48              |
| 51:9:544:G:H2'    | 51:9:545:A:C8      | 2.48                     | 0.48              |
| 51:9:1120:U:H2'   | 51:9:1121:G:C8     | 2.48                     | 0.48              |
| 51:9:1199:A:H2'   | 51:9:1200:A:O4'    | 2.14                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:1415:C:H2'    | 51:9:1416:C:C6     | 2.49                     | 0.48              |
| 51:9:1434:C:O3'    | 51:9:1435:C:O4'    | 2.31                     | 0.48              |
| 56:EE:8:HIS:O      | 56:EE:30:ARG:NH1   | 2.47                     | 0.48              |
| 70:SS:36:VAL:HG22  | 70:SS:40:TYR:CE2   | 2.48                     | 0.48              |
| 84:gg:87:LEU:HB2   | 84:gg:101:PHE:HB2  | 1.95                     | 0.48              |
| 19:T:87:LYS:NZ     | 48:5:4305:G:H22    | 2.12                     | 0.48              |
| 19:T:144:ASN:ND2   | 19:T:144:ASN:O     | 2.46                     | 0.48              |
| 27:b:18:ARG:NH1    | 48:5:1669:A:OP1    | 2.36                     | 0.48              |
| 43:s:14:PHE:HA     | 43:s:17:ILE:HG12   | 1.95                     | 0.48              |
| 43:s:29:ILE:HD12   | 43:s:78:LEU:HD22   | 1.95                     | 0.48              |
| 47:3:37:A:H2'      | 47:3:38:A:H5'      | 1.96                     | 0.48              |
| 48:5:911:U:H2'     | 48:5:912:G:O4'     | 2.13                     | 0.48              |
| 48:5:2045:G:O6     | 48:5:3870:C:O2'    | 2.32                     | 0.48              |
| 48:5:2862:G:N3     | 48:5:3624:A:H2'    | 2.28                     | 0.48              |
| 48:5:3718:A2M:H8   | 48:5:3718:A2M:O5'  | 2.13                     | 0.48              |
| 51:9:115:U:O2'     | 51:9:381:C:O2      | 2.21                     | 0.48              |
| 51:9:1265:A:C2'    | 51:9:1265:A:N3     | 2.76                     | 0.48              |
| 54:CC:272:HIS:ND1  | 54:CC:272:HIS:O    | 2.47                     | 0.48              |
| 84:gg:16:GLY:CA    | 84:gg:305:ASN:OD1  | 2.61                     | 0.48              |
| 8:H:103:VAL:HG11   | 8:H:144:LEU:HD21   | 1.95                     | 0.48              |
| 26:a:94:LYS:O      | 26:a:95:THR:HG23   | 2.13                     | 0.48              |
| 42:r:90:LEU:HG     | 42:r:111:ILE:HG23  | 1.96                     | 0.48              |
| 44:t:19:GLY:HA2    | 44:t:58:ILE:HA     | 1.96                     | 0.48              |
| 48:5:709:C:H1'     | 48:5:4942:C:H5     | 1.79                     | 0.48              |
| 48:5:1767:A:H3'    | 48:5:1769:G:N7     | 2.29                     | 0.48              |
| 48:5:1810:G:H2'    | 48:5:1811:G:O4'    | 2.13                     | 0.48              |
| 48:5:1981:G:H5''   | 48:5:1982:G:H4'    | 1.94                     | 0.48              |
| 48:5:2673:G:H5''   | 48:5:2675:G:O4'    | 2.14                     | 0.48              |
| 48:5:3923:A:H2'    | 48:5:3924:C:C6     | 2.48                     | 0.48              |
| 48:5:4548:A:N1     | 86:ii:181:GLY:O    | 2.47                     | 0.48              |
| 48:5:4583:C:O2'    | 48:5:4718:G:N2     | 2.40                     | 0.48              |
| 51:9:66:G:H2'      | 51:9:67:C:H4'      | 1.94                     | 0.48              |
| 51:9:484:A2M:H8    | 51:9:484:A2M:O5'   | 2.13                     | 0.48              |
| 51:9:880:G:C8      | 51:9:907:G:N1      | 2.82                     | 0.48              |
| 51:9:1130:G:O5'    | 51:9:1130:G:H8     | 1.95                     | 0.48              |
| 52:AA:30:LEU:HD11  | 52:AA:35:GLU:HA    | 1.95                     | 0.48              |
| 56:EE:123:LEU:HD11 | 56:EE:235:TRP:HB2  | 1.96                     | 0.48              |
| 57:FF:75:SER:O     | 57:FF:78:MET:HE3   | 2.13                     | 0.48              |
| 63:LL:48:LYS:NZ    | 63:LL:52:GLU:OE1   | 2.47                     | 0.48              |
| 70:SS:3:LEU:HD23   | 70:SS:4:VAL:N      | 2.29                     | 0.48              |
| 87:jj:529:ALA:O    | 87:jj:551:LEU:HD21 | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:R:151:ARG:HH21 | 63:LL:118:ARG:NH1 | 2.10                     | 0.48              |
| 26:a:103:VAL:CG1  | 26:a:108:TYR:HB2  | 2.44                     | 0.48              |
| 48:5:1096:C:O2'   | 48:5:1097:C:O5'   | 2.28                     | 0.48              |
| 48:5:1098:G:C2    | 48:5:1198:G:N1    | 2.82                     | 0.48              |
| 48:5:1378:C:H4'   | 48:5:1379:C:H5'   | 1.96                     | 0.48              |
| 48:5:1444:G:H2'   | 48:5:1445:U:H6    | 1.79                     | 0.48              |
| 48:5:1959:U:OP1   | 48:5:1960:A:O2'   | 2.28                     | 0.48              |
| 48:5:2640:G:H2'   | 48:5:2641:A:C8    | 2.49                     | 0.48              |
| 48:5:4559:A:O3'   | 48:5:4560:C:O2    | 2.32                     | 0.48              |
| 51:9:84:A:N3      | 51:9:150:A:O2'    | 2.42                     | 0.48              |
| 51:9:171:A:H5''   | 58:GG:177:GLN:OE1 | 2.13                     | 0.48              |
| 51:9:546:G:O2'    | 51:9:547:G:O4'    | 2.30                     | 0.48              |
| 51:9:697:G:N3     | 51:9:697:G:H2'    | 2.28                     | 0.48              |
| 51:9:886:A:H3'    | 51:9:887:U:H5''   | 1.95                     | 0.48              |
| 51:9:1025:U:H2'   | 51:9:1026:C:O4'   | 2.14                     | 0.48              |
| 51:9:1190:A:H2'   | 51:9:1191:C:O4'   | 2.12                     | 0.48              |
| 51:9:1348:G:N2    | 51:9:1381:G:H22   | 2.10                     | 0.48              |
| 51:9:1744:G:H8    | 51:9:1744:G:OP2   | 1.97                     | 0.48              |
| 51:9:1788:A:H2'   | 51:9:1789:G:O4'   | 2.13                     | 0.48              |
| 53:BB:59:SER:HA   | 53:BB:91:VAL:HG21 | 1.95                     | 0.48              |
| 55:DD:35:SER:O    | 55:DD:99:ILE:HD11 | 2.14                     | 0.48              |
| 66:OO:84:ARG:O    | 66:OO:88:LEU:HD23 | 2.13                     | 0.48              |
| 71:TT:116:ASP:OD1 | 71:TT:116:ASP:C   | 2.57                     | 0.48              |
| 87:jj:357:MET:HE2 | 87:jj:357:MET:HA  | 1.96                     | 0.48              |
| 2:B:54:THR:HG22   | 2:B:78:ILE:HD11   | 1.95                     | 0.48              |
| 9:I:22:PHE:CZ     | 48:5:1788:A:H2'   | 2.48                     | 0.48              |
| 14:O:175:MET:HE1  | 14:O:179:LYS:NZ   | 2.29                     | 0.48              |
| 14:O:185:VAL:O    | 14:O:187:LYS:O    | 2.31                     | 0.48              |
| 27:b:38:LYS:NZ    | 48:5:1816:C:O3'   | 2.47                     | 0.48              |
| 48:5:504:G:O2'    | 48:5:505:G:P      | 2.71                     | 0.48              |
| 48:5:2276:A:H2'   | 48:5:2277:C:O4'   | 2.13                     | 0.48              |
| 48:5:2726:G:H2'   | 48:5:2727:C:C6    | 2.49                     | 0.48              |
| 50:8:102:G:OP2    | 50:8:104:A:O2'    | 2.29                     | 0.48              |
| 51:9:642:U:OP2    | 82:ee:34:ARG:NH2  | 2.42                     | 0.48              |
| 51:9:1520:G:H5''  | 51:9:1521:C:OP2   | 2.14                     | 0.48              |
| 51:9:1667:U:H2'   | 51:9:1668:U:C6    | 2.49                     | 0.48              |
| 67:PP:17:TYR:HB2  | 67:PP:25:LEU:HD11 | 1.96                     | 0.48              |
| 68:QQ:44:PRO:HD3  | 68:QQ:77:HIS:HB3  | 1.95                     | 0.48              |
| 18:S:1:MET:HG2    | 18:S:2:LYS:N      | 2.29                     | 0.48              |
| 42:r:124:VAL:HG13 | 42:r:125:MET:N    | 2.28                     | 0.48              |
| 43:s:78:LEU:HD11  | 43:s:193:PHE:HB3  | 1.95                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:2:74:C:H5'      | 48:5:4548:A:H2'    | 1.95                     | 0.48              |
| 47:3:52:G:H2'      | 47:3:53:G:O4'      | 2.13                     | 0.48              |
| 48:5:1308:C:H2'    | 48:5:1309:C:C6     | 2.49                     | 0.48              |
| 48:5:1444:G:C2     | 48:5:1445:U:C5     | 3.02                     | 0.48              |
| 48:5:2550:G:O2'    | 48:5:2587:A:N1     | 2.43                     | 0.48              |
| 48:5:2639:U:O2'    | 48:5:2640:G:P      | 2.72                     | 0.48              |
| 48:5:4625:C:O2'    | 48:5:4626:A:H5'    | 2.14                     | 0.48              |
| 48:5:4932:U:C2'    | 48:5:4933:C:O5'    | 2.62                     | 0.48              |
| 50:8:126:C:H1'     | 50:8:127:U:C6      | 2.49                     | 0.48              |
| 51:9:16:G:H2'      | 51:9:17:C:C6       | 2.49                     | 0.48              |
| 51:9:29:G:H2'      | 51:9:30:C:C6       | 2.49                     | 0.48              |
| 51:9:684:G:OP1     | 92:9:2009:HOH:O    | 2.20                     | 0.48              |
| 51:9:1409:A:C8     | 51:9:1410:C:O4'    | 2.67                     | 0.48              |
| 51:9:1533:A:C8     | 51:9:1604:G:H1'    | 2.49                     | 0.48              |
| 55:DD:12:VAL:HG21  | 81:dd:34:TYR:CB    | 2.43                     | 0.48              |
| 58:GG:135:PRO:HB2  | 58:GG:141:ILE:HD12 | 1.96                     | 0.48              |
| 87:jj:111:THR:HG22 | 87:jj:112:ASN:N    | 2.29                     | 0.48              |
| 2:B:101:THR:HG21   | 48:5:4724:A:H1'    | 1.96                     | 0.47              |
| 7:G:81:ASN:CG      | 7:G:238:GLY:HA3    | 2.39                     | 0.47              |
| 48:5:1455:G:O2'    | 48:5:1456:C:P      | 2.72                     | 0.47              |
| 48:5:1870:C:H2'    | 48:5:1871:A2M:H8   | 1.96                     | 0.47              |
| 48:5:1920:C:H3'    | 48:5:1921:C:H5''   | 1.96                     | 0.47              |
| 48:5:4305:G:H2'    | 48:5:4305:G:N3     | 2.29                     | 0.47              |
| 51:9:1507:G:C2     | 83:ff:80:TYR:CG    | 3.02                     | 0.47              |
| 51:9:1673:U:O2'    | 57:FF:84:GLY:O     | 2.27                     | 0.47              |
| 54:CC:217:ALA:HB3  | 54:CC:219:ILE:HD12 | 1.94                     | 0.47              |
| 55:DD:52:ALA:C     | 55:DD:91:VAL:HG23  | 2.39                     | 0.47              |
| 55:DD:122:VAL:HG22 | 55:DD:126:ILE:HD12 | 1.95                     | 0.47              |
| 58:GG:41:LEU:HD12  | 58:GG:45:TRP:CE3   | 2.48                     | 0.47              |
| 61:JJ:28:GLU:OE1   | 61:JJ:43:VAL:HG11  | 2.14                     | 0.47              |
| 67:PP:22:LEU:O     | 67:PP:23:ASP:C     | 2.57                     | 0.47              |
| 84:gg:187:ASN:O    | 84:gg:188:HIS:ND1  | 2.46                     | 0.47              |
| 86:ii:128:ASP:OD1  | 86:ii:129:ASN:N    | 2.42                     | 0.47              |
| 86:ii:202:VAL:HG13 | 86:ii:236:LEU:HD12 | 1.96                     | 0.47              |
| 1:A:142:GLU:OE1    | 1:A:142:GLU:N      | 2.47                     | 0.47              |
| 16:Q:89:ASP:O      | 16:Q:112:ARG:NH2   | 2.47                     | 0.47              |
| 33:h:53:SER:O      | 33:h:57:VAL:HG23   | 2.14                     | 0.47              |
| 48:5:1981:G:C5'    | 48:5:1982:G:H4'    | 2.44                     | 0.47              |
| 48:5:2487:G:H8     | 48:5:2487:G:O5'    | 1.97                     | 0.47              |
| 48:5:2501:C:C2'    | 48:5:2502:A:O4'    | 2.62                     | 0.47              |
| 50:8:91:A:H2'      | 50:8:92:U:O4'      | 2.14                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:9:28:U:H2'     | 51:9:29:G:H8       | 1.79                     | 0.47              |
| 51:9:183:G:C2     | 51:9:184:G:C8      | 3.02                     | 0.47              |
| 51:9:213:G:O2'    | 51:9:214:U:P       | 2.72                     | 0.47              |
| 51:9:547:G:O2'    | 51:9:548:C:H5''    | 2.14                     | 0.47              |
| 51:9:1055:A:N1    | 51:9:1063:C:N4     | 2.59                     | 0.47              |
| 51:9:1302:G:O6    | 51:9:1307:U:C2     | 2.67                     | 0.47              |
| 51:9:1474:A:H5''  | 68:QQ:121:VAL:HG13 | 1.97                     | 0.47              |
| 57:FF:33:ILE:O    | 57:FF:33:ILE:CG2   | 2.62                     | 0.47              |
| 58:GG:71:GLY:O    | 58:GG:98:ARG:HD2   | 2.15                     | 0.47              |
| 59:HH:76:GLN:O    | 59:HH:80:VAL:HG12  | 2.14                     | 0.47              |
| 63:LL:20:LYS:O    | 63:LL:21:LYS:HB3   | 2.15                     | 0.47              |
| 74:WW:28:ARG:HB3  | 74:WW:29:PRO:CD    | 2.44                     | 0.47              |
| 84:gg:236:ILE:CG2 | 84:gg:239:LEU:HD21 | 2.43                     | 0.47              |
| 86:ii:142:ASP:C   | 86:ii:142:ASP:OD1  | 2.57                     | 0.47              |
| 1:A:158:ILE:HB    | 1:A:162:ASN:HD21   | 1.80                     | 0.47              |
| 2:B:258:HIS:HA    | 2:B:259:PRO:C      | 2.39                     | 0.47              |
| 5:E:164:ARG:O     | 5:E:185:ASN:OD1    | 2.31                     | 0.47              |
| 26:a:29:PRO:O     | 48:5:39:A:N7       | 2.47                     | 0.47              |
| 40:o:37:GLY:HA3   | 48:5:4342:C:O3'    | 2.14                     | 0.47              |
| 46:2:18:G:H4'     | 46:2:60:A:C2       | 2.48                     | 0.47              |
| 48:5:978:G:H1     | 48:5:1277:G:H1     | 1.62                     | 0.47              |
| 48:5:1214:C:H3'   | 48:5:1215:C:H5''   | 1.96                     | 0.47              |
| 48:5:1920:C:O2'   | 48:5:1922:G:O5'    | 2.31                     | 0.47              |
| 48:5:2843:U:O2'   | 48:5:4632:U:OP1    | 2.25                     | 0.47              |
| 48:5:3866:C:H2'   | 48:5:3867:A2M:O4'  | 2.14                     | 0.47              |
| 48:5:4121:G:H4'   | 48:5:4122:G:OP2    | 2.14                     | 0.47              |
| 48:5:4962:C:C4    | 48:5:4963:G:N7     | 2.82                     | 0.47              |
| 51:9:12:U:H2'     | 51:9:13:C:C6       | 2.49                     | 0.47              |
| 51:9:301:A:N3     | 60:II:73:THR:HG21  | 2.30                     | 0.47              |
| 51:9:876:C:H2'    | 51:9:878:G:H1'     | 1.96                     | 0.47              |
| 51:9:1533:A:C2    | 51:9:1536:G:N3     | 2.82                     | 0.47              |
| 53:BB:33:VAL:HG12 | 53:BB:44:ILE:HD12  | 1.96                     | 0.47              |
| 56:EE:181:CYS:SG  | 56:EE:225:ILE:HD12 | 2.55                     | 0.47              |
| 57:FF:33:ILE:O    | 57:FF:33:ILE:HG22  | 2.14                     | 0.47              |
| 57:FF:72:LEU:HD12 | 57:FF:155:CYS:SG   | 2.54                     | 0.47              |
| 58:GG:127:THR:O   | 58:GG:128:THR:O    | 2.31                     | 0.47              |
| 65:NN:84:LEU:HD21 | 65:NN:89:TYR:HD1   | 1.79                     | 0.47              |
| 86:ii:22:LYS:HG3  | 86:ii:23:SER:N     | 2.28                     | 0.47              |
| 87:jj:191:LYS:HD2 | 87:jj:229:VAL:HG13 | 1.96                     | 0.47              |
| 2:B:103:LYS:NZ    | 48:5:4725:C:OP1    | 2.33                     | 0.47              |
| 4:D:67:ALA:HA     | 4:D:72:ASP:HB3     | 1.96                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:U:39:PHE:CZ     | 20:U:43:LEU:HD11   | 2.49                     | 0.47              |
| 26:a:117:LEU:HD23  | 26:a:140:VAL:HG21  | 1.95                     | 0.47              |
| 43:s:35:VAL:HG23   | 43:s:39:GLN:OE1    | 2.14                     | 0.47              |
| 44:t:16:ARG:HH21   | 44:t:18:THR:HG22   | 1.80                     | 0.47              |
| 48:5:1066:G:H2'    | 48:5:1067:G:O4'    | 2.14                     | 0.47              |
| 50:8:6:C:H2'       | 50:8:7:U:C6        | 2.49                     | 0.47              |
| 50:8:155:C:H2'     | 50:8:156:U:O4'     | 2.14                     | 0.47              |
| 51:9:551:U:H2'     | 51:9:552:G:C8      | 2.49                     | 0.47              |
| 51:9:581:U:H4'     | 76:YY:66:GLY:HA2   | 1.96                     | 0.47              |
| 51:9:1117:C:O2     | 51:9:1117:C:O4'    | 2.32                     | 0.47              |
| 51:9:1344:A:N1     | 51:9:1385:G:O2'    | 2.41                     | 0.47              |
| 53:BB:178:THR:O    | 53:BB:178:THR:HG22 | 2.15                     | 0.47              |
| 64:MM:43:ASP:OD1   | 83:ff:101:TYR:OH   | 2.27                     | 0.47              |
| 65:NN:92:ILE:HG22  | 65:NN:150:VAL:HG11 | 1.97                     | 0.47              |
| 68:QQ:143:LYS:HD3  | 68:QQ:145:TYR:CZ   | 2.50                     | 0.47              |
| 84:gg:219:TRP:C    | 84:gg:227:LEU:HD12 | 2.39                     | 0.47              |
| 86:ii:312:LEU:HD21 | 86:ii:320:LEU:HD22 | 1.96                     | 0.47              |
| 87:jj:531:ARG:HG2  | 87:jj:531:ARG:NH1  | 2.30                     | 0.47              |
| 12:M:29:ASP:OD1    | 12:M:30:VAL:N      | 2.47                     | 0.47              |
| 26:a:35:ALA:HB2    | 48:5:38:A:H5''     | 1.96                     | 0.47              |
| 36:k:32:VAL:HG21   | 36:k:53:ALA:CB     | 2.44                     | 0.47              |
| 44:t:73:VAL:HG12   | 44:t:74:VAL:N      | 2.30                     | 0.47              |
| 48:5:750:U:H2'     | 48:5:751:G:O4'     | 2.14                     | 0.47              |
| 48:5:1195:G:C6     | 48:5:1196:G:N7     | 2.82                     | 0.47              |
| 48:5:1296:G:HO2'   | 48:5:1297:U:H6     | 1.57                     | 0.47              |
| 48:5:1339:U:H2'    | 48:5:1340:OMC:C6   | 2.49                     | 0.47              |
| 48:5:1846:G:H2'    | 48:5:1847:C:C6     | 2.49                     | 0.47              |
| 48:5:2504:C:H2'    | 48:5:2505:C:C2     | 2.49                     | 0.47              |
| 48:5:4263:C:H2'    | 48:5:4264:G:O4'    | 2.14                     | 0.47              |
| 51:9:217:A:C2'     | 51:9:218:PSU:H5''  | 2.45                     | 0.47              |
| 51:9:319:C:C2'     | 51:9:320:G:OP1     | 2.62                     | 0.47              |
| 51:9:1675:A:O2'    | 57:FF:74:ASN:HB3   | 2.15                     | 0.47              |
| 64:MM:125:GLU:HA   | 64:MM:128:PHE:CD2  | 2.50                     | 0.47              |
| 71:TT:114:GLU:HG3  | 71:TT:122:LYS:HG3  | 1.95                     | 0.47              |
| 77:ZZ:68:ILE:HD12  | 77:ZZ:110:THR:HA   | 1.96                     | 0.47              |
| 86:ii:251:LEU:HD12 | 86:ii:251:LEU:O    | 2.14                     | 0.47              |
| 87:jj:155:TYR:CE2  | 87:jj:159:ILE:HD11 | 2.50                     | 0.47              |
| 87:jj:305:VAL:HG13 | 87:jj:306:ARG:N    | 2.30                     | 0.47              |
| 6:F:240:ASN:O      | 6:F:244:ARG:HG2    | 2.14                     | 0.47              |
| 45:1:67:LYS:HD3    | 48:5:4452:U:H1'    | 1.97                     | 0.47              |
| 48:5:485:C:O2'     | 48:5:486:C:P       | 2.72                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:1076:C:O2'    | 48:5:1077:C:H5'    | 2.14                     | 0.47              |
| 48:5:1535:C:H2'    | 48:5:1536:U:O4'    | 2.15                     | 0.47              |
| 48:5:1992:U:H4'    | 48:5:1993:C:O4'    | 2.15                     | 0.47              |
| 51:9:70:G:N1       | 58:GG:170:ARG:NH1  | 2.63                     | 0.47              |
| 51:9:146:G:HO2'    | 51:9:147:A:C5'     | 2.28                     | 0.47              |
| 51:9:688:U:H1'     | 51:9:689:U:C5      | 2.48                     | 0.47              |
| 51:9:984:C:O2'     | 66:OO:138:ASP:OD2  | 2.29                     | 0.47              |
| 51:9:1281:G:C6     | 51:9:1282:A:H1'    | 2.49                     | 0.47              |
| 52:AA:2:SER:N      | 52:AA:8:LEU:HD12   | 2.30                     | 0.47              |
| 55:DD:210:ILE:HG21 | 69:RR:19:LYS:NZ    | 2.28                     | 0.47              |
| 58:GG:144:LEU:HD22 | 58:GG:145:PHE:CE1  | 2.49                     | 0.47              |
| 59:HH:147:LYS:HA   | 74:WW:49:GLU:OE2   | 2.13                     | 0.47              |
| 84:gg:48:ASP:O     | 84:gg:49:GLU:C     | 2.58                     | 0.47              |
| 84:gg:75:GLY:O     | 84:gg:76:GLN:NE2   | 2.47                     | 0.47              |
| 87:jj:273:GLU:OE2  | 87:jj:275:ASP:HB3  | 2.14                     | 0.47              |
| 13:N:114:ARG:HD3   | 13:N:151:ILE:O     | 2.15                     | 0.47              |
| 21:V:41:SER:CB     | 48:5:4507:A:O2'    | 2.63                     | 0.47              |
| 25:Z:57:MET:CB     | 25:Z:62:ILE:HD11   | 2.45                     | 0.47              |
| 47:3:33:U:C3'      | 47:3:34:U:H2'      | 2.45                     | 0.47              |
| 48:5:233:U:H2'     | 48:5:234:G:C8      | 2.50                     | 0.47              |
| 48:5:377:A:H2'     | 48:5:378:A:O4'     | 2.15                     | 0.47              |
| 48:5:1371:A:N1     | 50:8:28:C:O2'      | 2.44                     | 0.47              |
| 48:5:1633:G:H5'    | 48:5:1634:A:OP1    | 2.15                     | 0.47              |
| 48:5:1956:A:O2'    | 48:5:1957:U:P      | 2.72                     | 0.47              |
| 48:5:2090:U:H4'    | 48:5:2091:C:OP2    | 2.14                     | 0.47              |
| 48:5:2494:U:O3'    | 48:5:2495:U:O4'    | 2.33                     | 0.47              |
| 48:5:3707:U:H2'    | 48:5:3708:C:C6     | 2.50                     | 0.47              |
| 48:5:4119:C:O2     | 48:5:4120:U:N3     | 2.48                     | 0.47              |
| 48:5:4758:U:O2     | 48:5:4758:U:O4'    | 2.33                     | 0.47              |
| 51:9:15:U:H2'      | 51:9:16:G:O4'      | 2.14                     | 0.47              |
| 51:9:201:C:H2'     | 51:9:202:G:H5'     | 1.97                     | 0.47              |
| 51:9:867:G:C2      | 51:9:868:G:C6      | 3.03                     | 0.47              |
| 51:9:1553:C:H2'    | 51:9:1554:C:O4'    | 2.14                     | 0.47              |
| 51:9:1653:U:H2'    | 51:9:1654:G:C8     | 2.49                     | 0.47              |
| 51:9:1842:4AC:O7   | 51:9:1842:4AC:H5   | 2.14                     | 0.47              |
| 52:AA:89:LYS:HD3   | 52:AA:201:LEU:HG   | 1.97                     | 0.47              |
| 52:AA:197:VAL:HG12 | 52:AA:198:MET:N    | 2.30                     | 0.47              |
| 57:FF:51:HIS:HB2   | 57:FF:90:VAL:HG21  | 1.95                     | 0.47              |
| 57:FF:139:VAL:HG12 | 57:FF:140:ASP:O    | 2.15                     | 0.47              |
| 61:JJ:24:ARG:O     | 61:JJ:28:GLU:HG2   | 2.14                     | 0.47              |
| 64:MM:89:VAL:CG2   | 64:MM:109:VAL:HG21 | 2.45                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 64:MM:114:TYR:HA   | 64:MM:121:LYS:HZ2  | 1.79                     | 0.47              |
| 69:RR:41:ILE:HG21  | 69:RR:47:ARG:HB3   | 1.97                     | 0.47              |
| 70:SS:54:LYS:NZ    | 70:SS:58:GLU:OE1   | 2.47                     | 0.47              |
| 70:SS:84:LEU:N     | 70:SS:84:LEU:HD23  | 2.30                     | 0.47              |
| 70:SS:89:ASP:O     | 70:SS:93:GLY:N     | 2.45                     | 0.47              |
| 71:TT:18:LEU:HD23  | 71:TT:58:ALA:HA    | 1.95                     | 0.47              |
| 78:aa:45:VAL:O     | 78:aa:45:VAL:CG1   | 2.62                     | 0.47              |
| 86:ii:326:LEU:HD11 | 86:ii:409:ILE:CG1  | 2.45                     | 0.47              |
| 86:ii:347:THR:HB   | 86:ii:348:PRO:CD   | 2.45                     | 0.47              |
| 87:jj:164:LEU:HD22 | 87:jj:236:ASP:HB3  | 1.96                     | 0.47              |
| 4:D:7:VAL:HG13     | 4:D:8:LYS:N        | 2.29                     | 0.47              |
| 11:L:21:ARG:O      | 13:N:197:THR:HG23  | 2.15                     | 0.47              |
| 26:a:39:HIS:O      | 26:a:40:HIS:CG     | 2.68                     | 0.47              |
| 27:b:49:HIS:NE2    | 48:5:1815:G:O6     | 2.34                     | 0.47              |
| 40:o:75:PRO:O      | 40:o:76:ASN:HB2    | 2.15                     | 0.47              |
| 46:2:20(A):U:O2'   | 46:2:21:A:H5''     | 2.14                     | 0.47              |
| 48:5:1591:U:OP2    | 48:5:2856:C:O2'    | 2.28                     | 0.47              |
| 48:5:4537:C:H2'    | 48:5:4538:G:C8     | 2.50                     | 0.47              |
| 51:9:82:G:O2'      | 51:9:83:A:O5'      | 2.33                     | 0.47              |
| 51:9:319:C:H2'     | 51:9:320:G:OP1     | 2.15                     | 0.47              |
| 51:9:463:C:OP2     | 87:jj:306:ARG:NH2  | 2.48                     | 0.47              |
| 51:9:551:U:H2'     | 51:9:552:G:N7      | 2.29                     | 0.47              |
| 51:9:587:A:HO2'    | 51:9:588:G:N2      | 2.13                     | 0.47              |
| 51:9:1094:C:OP1    | 74:WW:28:ARG:NH2   | 2.48                     | 0.47              |
| 51:9:1265:A:H4'    | 51:9:1327:G:OP1    | 2.14                     | 0.47              |
| 51:9:1348:G:H1     | 51:9:1381:G:N2     | 2.11                     | 0.47              |
| 52:AA:80:ARG:HH22  | 52:AA:126:ASP:CB   | 2.28                     | 0.47              |
| 56:EE:107:GLY:CA   | 56:EE:189:LEU:HD22 | 2.45                     | 0.47              |
| 68:QQ:57:LEU:HD21  | 68:QQ:115:TYR:CB   | 2.45                     | 0.47              |
| 69:RR:66:VAL:HG11  | 69:RR:69:ILE:HD12  | 1.97                     | 0.47              |
| 78:aa:36:ILE:HD12  | 78:aa:36:ILE:N     | 2.29                     | 0.47              |
| 86:ii:394:ASP:HB3  | 86:ii:400:SER:HA   | 1.95                     | 0.47              |
| 86:ii:416:ARG:O    | 86:ii:417:VAL:HG23 | 2.15                     | 0.47              |
| 87:jj:106:LEU:CD2  | 87:jj:108:LEU:HD23 | 2.44                     | 0.47              |
| 9:I:48:LEU:HD11    | 9:I:145:LYS:HG3    | 1.95                     | 0.47              |
| 9:I:52:MET:HE1     | 9:I:155:ALA:HB3    | 1.96                     | 0.47              |
| 20:U:76:VAL:CG1    | 20:U:77:PRO:HD2    | 2.44                     | 0.47              |
| 22:W:44:ARG:HD3    | 48:5:3615:G:H21    | 1.80                     | 0.47              |
| 48:5:35:U:H2'      | 48:5:36:U:H5'      | 1.96                     | 0.47              |
| 48:5:1548:G:O2'    | 48:5:2812:A:N3     | 2.46                     | 0.47              |
| 48:5:2486:G:C6     | 48:5:2493:G:O6     | 2.68                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:833:C:O2'     | 51:9:834:C:C6      | 2.68                     | 0.47              |
| 51:9:1374:C:H2'    | 51:9:1375:G:O4'    | 2.15                     | 0.47              |
| 51:9:1406:G:N3     | 51:9:1407:U:H1'    | 2.30                     | 0.47              |
| 51:9:1834:A:H2     | 51:9:1837:G:H22    | 1.63                     | 0.47              |
| 55:DD:161:GLY:O    | 55:DD:164:VAL:HG22 | 2.15                     | 0.47              |
| 59:HH:161:ALA:O    | 59:HH:162:GLN:HB2  | 2.15                     | 0.47              |
| 79:bb:55:LEU:HD22  | 79:bb:55:LEU:N     | 2.30                     | 0.47              |
| 7:G:170:LEU:CD2    | 7:G:201:THR:HG21   | 2.45                     | 0.47              |
| 8:H:115:ARG:HE     | 8:H:123:ILE:HD13   | 1.80                     | 0.47              |
| 48:5:516:C:O2'     | 48:5:517:C:H5'     | 2.15                     | 0.47              |
| 48:5:1776:A:H3'    | 48:5:1777:C:H6     | 1.79                     | 0.47              |
| 48:5:1998:A:O2'    | 48:5:1999:A:O5'    | 2.33                     | 0.47              |
| 48:5:3604:A:H2'    | 48:5:3605:C:C6     | 2.50                     | 0.47              |
| 48:5:3880:G:H2'    | 48:5:3881:G:C8     | 2.50                     | 0.47              |
| 48:5:4420:PSU:O2   | 48:5:4475:G:N2     | 2.48                     | 0.47              |
| 51:9:153:G:C2'     | 51:9:154:U:O5'     | 2.63                     | 0.47              |
| 51:9:598:G:O2'     | 51:9:605:A:N1      | 2.37                     | 0.47              |
| 51:9:886:A:C5      | 51:9:901:G:C2      | 3.03                     | 0.47              |
| 51:9:926:A:H61     | 51:9:1015:U:H3     | 1.63                     | 0.47              |
| 51:9:1401:A:O3'    | 51:9:1402:A:O4'    | 2.33                     | 0.47              |
| 51:9:1698:C:H4'    | 51:9:1699:A:OP2    | 2.14                     | 0.47              |
| 51:9:1835:A:O2'    | 51:9:1836:G:P      | 2.73                     | 0.47              |
| 55:DD:102:ALA:HB1  | 55:DD:173:ARG:HG3  | 1.96                     | 0.47              |
| 57:FF:103:LEU:HD11 | 77:ZZ:67:LEU:HD22  | 1.97                     | 0.47              |
| 60:II:132:GLU:O    | 60:II:133:GLU:C    | 2.56                     | 0.47              |
| 65:NN:102:LEU:HD11 | 65:NN:111:ALA:C    | 2.40                     | 0.47              |
| 66:OO:41:PHE:HA    | 66:OO:57:THR:HG22  | 1.97                     | 0.47              |
| 83:ff:133:ARG:HD2  | 83:ff:142:THR:CG2  | 2.44                     | 0.47              |
| 84:gg:158:PRO:O    | 84:gg:160:SER:N    | 2.47                     | 0.47              |
| 84:gg:191:HIS:CD2  | 84:gg:195:LEU:HD11 | 2.50                     | 0.47              |
| 86:ii:35:ILE:HD12  | 86:ii:74:ALA:CB    | 2.45                     | 0.47              |
| 3:C:94:ASN:HA      | 3:C:100:ARG:O      | 2.15                     | 0.46              |
| 10:J:83:LEU:HD12   | 10:J:83:LEU:O      | 2.14                     | 0.46              |
| 25:Z:10:VAL:HG11   | 25:Z:129:TRP:HZ3   | 1.80                     | 0.46              |
| 36:k:12:LEU:HD11   | 36:k:59:SER:O      | 2.15                     | 0.46              |
| 48:5:652:G:H2'     | 48:5:653:C:C6      | 2.50                     | 0.46              |
| 48:5:978:G:H22     | 48:5:1277:G:N2     | 2.13                     | 0.46              |
| 48:5:5015:G:O2'    | 48:5:5034:A:N6     | 2.46                     | 0.46              |
| 51:9:1016:U:O2     | 51:9:1016:U:H2'    | 2.14                     | 0.46              |
| 51:9:1304:U:OP1    | 83:ff:90:ARG:N     | 2.48                     | 0.46              |
| 51:9:1420:G:H2'    | 51:9:1421:A:C8     | 2.50                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:9:1435:C:H2'   | 51:9:1436:C:C2     | 2.50                     | 0.46              |
| 52:AA:58:LEU:HD22 | 52:AA:178:LEU:HD13 | 1.97                     | 0.46              |
| 58:GG:67:VAL:HG11 | 58:GG:99:GLY:HA2   | 1.97                     | 0.46              |
| 87:jj:55:CYS:HA   | 91:jj:601:SF4:S3   | 2.55                     | 0.46              |
| 87:jj:274:HIS:CG  | 87:jj:493:ASP:HA   | 2.49                     | 0.46              |
| 9:I:138:ILE:HG21  | 9:I:148:VAL:HG12   | 1.97                     | 0.46              |
| 20:U:78:PHE:CE2   | 20:U:83:LEU:HD21   | 2.50                     | 0.46              |
| 23:X:90:ILE:HD11  | 23:X:155:ILE:HD11  | 1.97                     | 0.46              |
| 44:t:74:VAL:O     | 44:t:74:VAL:HG12   | 2.15                     | 0.46              |
| 48:5:174:C:H2'    | 48:5:175:C:O4'     | 2.15                     | 0.46              |
| 48:5:1986:U:H3'   | 48:5:1987:C:H5'    | 1.96                     | 0.46              |
| 48:5:2708:U:O2'   | 48:5:2709:C:O4'    | 2.33                     | 0.46              |
| 48:5:4273:A:H2'   | 48:5:4274:A:C8     | 2.50                     | 0.46              |
| 48:5:4947:U:O2'   | 48:5:4948:C:OP1    | 2.32                     | 0.46              |
| 51:9:26:U:H2'     | 51:9:27:A2M:H8     | 1.98                     | 0.46              |
| 51:9:1118:C:O2    | 51:9:1118:C:O4'    | 2.33                     | 0.46              |
| 51:9:1646:C:C2'   | 51:9:1647:A:OP2    | 2.63                     | 0.46              |
| 52:AA:122:LEU:HB3 | 52:AA:144:THR:HG22 | 1.97                     | 0.46              |
| 58:GG:225:GLN:HA  | 58:GG:228:ILE:CD1  | 2.45                     | 0.46              |
| 59:HH:9:VAL:HG23  | 59:HH:9:VAL:O      | 2.16                     | 0.46              |
| 62:KK:62:PHE:O    | 62:KK:66:HIS:O     | 2.34                     | 0.46              |
| 69:RR:75:GLU:O    | 69:RR:79:GLU:HG2   | 2.14                     | 0.46              |
| 72:UU:20:ILE:HG22 | 72:UU:91:LEU:HB2   | 1.97                     | 0.46              |
| 84:gg:34:ALA:HB2  | 84:gg:40:ILE:HG12  | 1.96                     | 0.46              |
| 4:D:163:LEU:HD13  | 4:D:173:ILE:HG21   | 1.97                     | 0.46              |
| 8:H:1:MET:HE3     | 18:S:140:PRO:HB2   | 1.97                     | 0.46              |
| 15:P:115:GLU:OE1  | 15:P:151:THR:OG1   | 2.33                     | 0.46              |
| 47:3:35:U:H2'     | 47:3:36:U:C5'      | 2.45                     | 0.46              |
| 48:5:1991:A:O2'   | 48:5:1992:U:C6     | 2.69                     | 0.46              |
| 48:5:2505:C:O2    | 48:5:2505:C:O4'    | 2.33                     | 0.46              |
| 48:5:4719:G:C4'   | 48:5:4720:C:OP1    | 2.64                     | 0.46              |
| 48:5:4922:C:H3'   | 48:5:4923:U:C6     | 2.50                     | 0.46              |
| 48:5:4925:U:C4'   | 48:5:4926:C:OP2    | 2.63                     | 0.46              |
| 50:8:92:U:H2'     | 50:8:93:C:O4'      | 2.15                     | 0.46              |
| 51:9:191:A:C2'    | 51:9:192:C:OP1     | 2.62                     | 0.46              |
| 51:9:846:G:C6     | 56:EE:19:MET:HE3   | 2.51                     | 0.46              |
| 51:9:1398:G:H1'   | 84:gg:63:SER:OG    | 2.15                     | 0.46              |
| 51:9:1417:C:H2'   | 51:9:1419:C:H5''   | 1.97                     | 0.46              |
| 54:CC:75:ILE:HD11 | 54:CC:265:PRO:CB   | 2.46                     | 0.46              |
| 59:HH:69:LEU:CD1  | 59:HH:96:ALA:HB2   | 2.46                     | 0.46              |
| 61:JJ:57:ALA:HB2  | 61:JJ:97:ILE:HG21  | 1.97                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 61:JJ:82:VAL:HG11  | 61:JJ:92:MET:HG3  | 1.96                     | 0.46              |
| 72:UU:20:ILE:HD12  | 72:UU:116:ILE:HA  | 1.96                     | 0.46              |
| 86:ii:56:PHE:HE1   | 86:ii:72:LEU:O    | 1.97                     | 0.46              |
| 86:ii:414:ARG:HG3  | 86:ii:415:TYR:CD1 | 2.50                     | 0.46              |
| 87:jj:435:ALA:O    | 87:jj:441:PHE:CD2 | 2.68                     | 0.46              |
| 2:B:218:ASP:OD1    | 2:B:280:ILE:HA    | 2.15                     | 0.46              |
| 6:F:114:ARG:NH1    | 16:Q:4:ASP:O      | 2.42                     | 0.46              |
| 18:S:95:ARG:NH2    | 18:S:112:ASP:OD2  | 2.48                     | 0.46              |
| 22:W:6:CYS:HA      | 22:W:13:ILE:HD11  | 1.97                     | 0.46              |
| 42:r:66:ARG:O      | 42:r:67:ARG:HB3   | 2.15                     | 0.46              |
| 43:s:69:LEU:HG     | 43:s:71:ASN:HB2   | 1.97                     | 0.46              |
| 48:5:1604:G:H2'    | 48:5:1605:G:C8    | 2.50                     | 0.46              |
| 48:5:1978:C:O2'    | 48:5:1979:A:OP1   | 2.33                     | 0.46              |
| 48:5:2258:C:C2'    | 48:5:2259:G:OP1   | 2.63                     | 0.46              |
| 48:5:2570:U:H2'    | 48:5:2571:C:C6    | 2.50                     | 0.46              |
| 48:5:4305:G:N3     | 48:5:4305:G:C2'   | 2.79                     | 0.46              |
| 48:5:4699:U:H1'    | 48:5:4700:A:H5''  | 1.98                     | 0.46              |
| 51:9:107:A:H2'     | 51:9:108:G:C8     | 2.50                     | 0.46              |
| 51:9:146:G:O2'     | 51:9:147:A:O5'    | 2.30                     | 0.46              |
| 51:9:147:A:O2'     | 51:9:148:U:C5'    | 2.64                     | 0.46              |
| 51:9:455:A:H2'     | 51:9:456:C:C6     | 2.51                     | 0.46              |
| 51:9:524:U:OP2     | 82:ee:31:ARG:NH1  | 2.48                     | 0.46              |
| 51:9:925:G:H1      | 51:9:1017:U:H3    | 1.63                     | 0.46              |
| 51:9:1408:U:H1'    | 51:9:1409:A:C8    | 2.51                     | 0.46              |
| 51:9:1646:C:O2'    | 51:9:1647:A:P     | 2.74                     | 0.46              |
| 51:9:1798:C:H2'    | 51:9:1799:G:O4'   | 2.16                     | 0.46              |
| 53:BB:166:LYS:O    | 53:BB:170:GLU:HG2 | 2.15                     | 0.46              |
| 56:EE:195:ILE:O    | 56:EE:209:HIS:O   | 2.33                     | 0.46              |
| 65:NN:59:GLY:HA2   | 79:bb:32:PHE:CE1  | 2.51                     | 0.46              |
| 71:TT:28:LEU:O     | 71:TT:106:ALA:HB1 | 2.15                     | 0.46              |
| 86:ii:346:LEU:HD23 | 86:ii:351:GLU:HA  | 1.96                     | 0.46              |
| 2:B:300:LYS:HE3    | 2:B:300:LYS:O     | 2.14                     | 0.46              |
| 15:P:18:ARG:C      | 15:P:94:MET:HE2   | 2.40                     | 0.46              |
| 24:Y:65:GLN:HA     | 24:Y:65:GLN:OE1   | 2.16                     | 0.46              |
| 35:j:31:LYS:NZ     | 48:5:1532:G:OP2   | 2.37                     | 0.46              |
| 47:3:59:G:H2'      | 47:3:59:G:N3      | 2.30                     | 0.46              |
| 48:5:100:C:H2'     | 48:5:101:A:O4'    | 2.14                     | 0.46              |
| 48:5:717:U:H2'     | 48:5:718:C:C6     | 2.51                     | 0.46              |
| 51:9:305:U:C6      | 60:II:55:TYR:CD2  | 3.03                     | 0.46              |
| 51:9:618:C:H41     | 75:XX:67:ARG:NH2  | 2.14                     | 0.46              |
| 51:9:853:C:O2      | 51:9:853:C:O4'    | 2.34                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:1609:C:OP2    | 70:SS:134:GLN:NE2  | 2.46                     | 0.46              |
| 55:DD:218:LEU:O    | 55:DD:218:LEU:HD23 | 2.15                     | 0.46              |
| 68:QQ:52:LEU:O     | 68:QQ:55:VAL:HG22  | 2.16                     | 0.46              |
| 71:TT:28:LEU:HD22  | 71:TT:54:TYR:HD1   | 1.81                     | 0.46              |
| 79:bb:80:ARG:CZ    | 79:bb:80:ARG:HA    | 2.46                     | 0.46              |
| 84:gg:20:GLN:HB3   | 84:gg:69:VAL:HG12  | 1.97                     | 0.46              |
| 86:ii:389:LEU:HD21 | 86:ii:391:ILE:CD1  | 2.44                     | 0.46              |
| 87:jj:83:THR:HG23  | 87:jj:83:THR:O     | 2.16                     | 0.46              |
| 87:jj:564:ILE:HG22 | 87:jj:565:THR:N    | 2.31                     | 0.46              |
| 5:E:209:VAL:HG21   | 5:E:260:ILE:HD13   | 1.98                     | 0.46              |
| 17:R:151:ARG:NH2   | 63:LL:118:ARG:NH1  | 2.64                     | 0.46              |
| 19:T:105:PHE:CD1   | 48:5:1802:A:H4'    | 2.51                     | 0.46              |
| 31:f:47:CYS:SG     | 31:f:74:VAL:HG23   | 2.56                     | 0.46              |
| 48:5:1477:C:O2'    | 48:5:1478:C:P      | 2.74                     | 0.46              |
| 48:5:1695:U:H2'    | 48:5:1696:C:O4'    | 2.15                     | 0.46              |
| 48:5:4948:C:O2     | 48:5:4949:G:H2'    | 2.16                     | 0.46              |
| 50:8:83:C:H4'      | 50:8:85:U:C2       | 2.50                     | 0.46              |
| 51:9:140:C:HO2'    | 51:9:141:A:P       | 2.38                     | 0.46              |
| 51:9:981:A:H2'     | 51:9:982:G:C8      | 2.50                     | 0.46              |
| 51:9:1746:U:H4'    | 58:GG:65:GLN:NE2   | 2.31                     | 0.46              |
| 64:MM:114:TYR:HA   | 64:MM:121:LYS:NZ   | 2.31                     | 0.46              |
| 65:NN:60:VAL:HG13  | 65:NN:66:VAL:CG2   | 2.32                     | 0.46              |
| 66:OO:149:ARG:CZ   | 66:OO:151:LEU:HD13 | 2.45                     | 0.46              |
| 67:PP:28:MET:CE    | 67:PP:36:LEU:HD11  | 2.46                     | 0.46              |
| 68:QQ:105:LYS:C    | 68:QQ:105:LYS:CD   | 2.88                     | 0.46              |
| 77:ZZ:58:LEU:HD11  | 77:ZZ:87:ALA:HB1   | 1.96                     | 0.46              |
| 86:ii:286:LEU:HD11 | 86:ii:321:ILE:HD12 | 1.97                     | 0.46              |
| 4:D:208:MET:HE2    | 4:D:233:PRO:HD3    | 1.97                     | 0.46              |
| 6:F:92:ILE:HG21    | 6:F:246:MET:HE1    | 1.96                     | 0.46              |
| 18:S:93:MET:HE1    | 18:S:117:HIS:CE1   | 2.51                     | 0.46              |
| 20:U:24:ASP:OD1    | 20:U:69:LYS:HD3    | 2.16                     | 0.46              |
| 48:5:700:G:O2'     | 48:5:701:G:H5'     | 2.16                     | 0.46              |
| 48:5:1976:G:N2     | 48:5:1991:A:C8     | 2.84                     | 0.46              |
| 48:5:1993:C:H5     | 48:5:2002:A:OP1    | 1.98                     | 0.46              |
| 48:5:4739:C:C2     | 48:5:4961:G:N2     | 2.84                     | 0.46              |
| 49:7:16:A:H2'      | 49:7:17:C:C6       | 2.50                     | 0.46              |
| 50:8:152:U:H2'     | 50:8:153:C:O4'     | 2.16                     | 0.46              |
| 51:9:154:U:O3'     | 58:GG:15:LEU:HD22  | 2.14                     | 0.46              |
| 51:9:429:C:O2'     | 51:9:811:A:N1      | 2.44                     | 0.46              |
| 51:9:526:A:H2'     | 51:9:527:C:O4'     | 2.15                     | 0.46              |
| 51:9:535:G:O6      | 51:9:547:G:C2      | 2.68                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:589:G:O6      | 51:9:591:U:H2'     | 2.16                     | 0.46              |
| 51:9:816:A:H2'     | 51:9:817:G:H5'     | 1.98                     | 0.46              |
| 51:9:952:G:H2'     | 51:9:953:C:C6      | 2.51                     | 0.46              |
| 51:9:1345:G:OP1    | 51:9:1688:C:O2'    | 2.33                     | 0.46              |
| 52:AA:197:VAL:HG13 | 52:AA:201:LEU:HD22 | 1.98                     | 0.46              |
| 55:DD:176:LEU:HD13 | 55:DD:177:LEU:N    | 2.31                     | 0.46              |
| 59:HH:61:ILE:HG13  | 59:HH:63:PHE:CE1   | 2.51                     | 0.46              |
| 84:gg:168:CYS:SG   | 84:gg:198:VAL:HG23 | 2.56                     | 0.46              |
| 84:gg:251:ALA:HB2  | 84:gg:289:LEU:HD21 | 1.98                     | 0.46              |
| 86:ii:91:ASN:HA    | 86:ii:119:PRO:HA   | 1.97                     | 0.46              |
| 8:H:71:ARG:HD3     | 48:5:4691:A:H4'    | 1.97                     | 0.46              |
| 9:I:47:PRO:HG2     | 9:I:142:LEU:CD1    | 2.46                     | 0.46              |
| 9:I:180:GLU:O      | 9:I:184:MET:HG3    | 2.16                     | 0.46              |
| 9:I:184:MET:CB     | 9:I:190:LEU:HD12   | 2.44                     | 0.46              |
| 19:T:39:ILE:N      | 19:T:39:ILE:HD13   | 2.31                     | 0.46              |
| 19:T:105:PHE:O     | 19:T:109:VAL:HG23  | 2.15                     | 0.46              |
| 20:U:44:GLN:HG3    | 20:U:56:LEU:HD21   | 1.97                     | 0.46              |
| 20:U:61:VAL:HG22   | 20:U:74:SER:OG     | 2.15                     | 0.46              |
| 20:U:62:SER:OG     | 20:U:73:THR:CG2    | 2.64                     | 0.46              |
| 23:X:150:ALA:HB1   | 23:X:155:ILE:HG13  | 1.97                     | 0.46              |
| 24:Y:37:GLU:OE2    | 24:Y:37:GLU:HA     | 2.16                     | 0.46              |
| 28:c:98:ASP:C      | 28:c:98:ASP:OD1    | 2.59                     | 0.46              |
| 33:h:35:LYS:NZ     | 50:8:49:G:O3'      | 2.49                     | 0.46              |
| 41:p:58:GLY:O      | 48:5:2652:G:N1     | 2.38                     | 0.46              |
| 42:r:47:LYS:O      | 42:r:103:HIS:CD2   | 2.69                     | 0.46              |
| 43:s:57:LYS:HA     | 48:5:2020:U:O3'    | 2.15                     | 0.46              |
| 44:t:27:ALA:O      | 44:t:31:LYS:HG3    | 2.16                     | 0.46              |
| 48:5:8:U:H2'       | 48:5:9:C:O4'       | 2.16                     | 0.46              |
| 48:5:746:A:O2'     | 48:5:747:A:H8      | 1.99                     | 0.46              |
| 48:5:2461:G:H2'    | 48:5:2462:C:C6     | 2.51                     | 0.46              |
| 48:5:2545:U:H3'    | 48:5:2546:G:C5'    | 2.46                     | 0.46              |
| 48:5:3625:G:O2'    | 48:5:3626:G:OP1    | 2.34                     | 0.46              |
| 48:5:4390:A:H2'    | 48:5:4391:G:O4'    | 2.16                     | 0.46              |
| 48:5:5052:C:H2'    | 48:5:5053:U:O4'    | 2.15                     | 0.46              |
| 51:9:292:A:OP2     | 63:LL:42:LEU:HD11  | 2.16                     | 0.46              |
| 51:9:1220:A:H2'    | 51:9:1221:G:O4'    | 2.15                     | 0.46              |
| 51:9:1307:U:N3     | 51:9:1308:U:O2     | 2.49                     | 0.46              |
| 51:9:1425:G:H3'    | 51:9:1426:U:C5     | 2.51                     | 0.46              |
| 51:9:1647:A:H1'    | 51:9:1648:G:OP2    | 2.16                     | 0.46              |
| 53:BB:103:MET:HE1  | 53:BB:212:VAL:O    | 2.16                     | 0.46              |
| 53:BB:121:ILE:HG23 | 53:BB:161:VAL:HG13 | 1.97                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 68:QQ:97:GLN:HG3  | 68:QQ:105:LYS:HG3  | 1.98                     | 0.46              |
| 68:QQ:104:SER:HA  | 68:QQ:107:GLU:HG3  | 1.96                     | 0.46              |
| 70:SS:36:VAL:HG23 | 70:SS:99:LEU:HD22  | 1.96                     | 0.46              |
| 1:A:101:VAL:HG22  | 1:A:165:VAL:HG22   | 1.97                     | 0.46              |
| 2:B:302:ASN:OD1   | 2:B:368:ILE:HG21   | 2.15                     | 0.46              |
| 3:C:346:ASN:O     | 3:C:350:ARG:HG3    | 2.16                     | 0.46              |
| 10:J:155:HIS:HB2  | 49:7:55:A:H4'      | 1.97                     | 0.46              |
| 43:s:15:LEU:HA    | 43:s:18:ILE:HG22   | 1.98                     | 0.46              |
| 44:t:41:LYS:CE    | 86:ii:343:ILE:HD11 | 2.45                     | 0.46              |
| 48:5:176:G:C6     | 48:5:261:G:C2      | 3.03                     | 0.46              |
| 48:5:1298:C:H2'   | 48:5:1299:G:C8     | 2.51                     | 0.46              |
| 48:5:1588:U:H2'   | 48:5:1589:C:C6     | 2.50                     | 0.46              |
| 48:5:1736:A:H2'   | 48:5:1737:A:O4'    | 2.16                     | 0.46              |
| 48:5:1817:U:C4    | 48:5:1818:G:C6     | 3.04                     | 0.46              |
| 48:5:4266:G:N3    | 48:5:4266:G:H2'    | 2.31                     | 0.46              |
| 51:9:17:C:H2'     | 51:9:18:C:C6       | 2.51                     | 0.46              |
| 51:9:113:G:N2     | 51:9:293:C:O5'     | 2.49                     | 0.46              |
| 51:9:346:C:H2'    | 51:9:347:G:O4'     | 2.16                     | 0.46              |
| 51:9:1243:U:H2'   | 51:9:1244:PSU:O4'  | 2.16                     | 0.46              |
| 51:9:1277:C:O4'   | 62:KK:54:SER:OG    | 2.33                     | 0.46              |
| 51:9:1407:U:O2    | 51:9:1407:U:C2'    | 2.62                     | 0.46              |
| 51:9:1745:A:C2    | 51:9:1789:G:N2     | 2.80                     | 0.46              |
| 56:EE:239:PRO:O   | 56:EE:240:ARG:C    | 2.59                     | 0.46              |
| 59:HH:51:ILE:HD12 | 59:HH:61:ILE:HD13  | 1.98                     | 0.46              |
| 65:NN:4:MET:O     | 65:NN:5:HIS:HB2    | 2.14                     | 0.46              |
| 1:A:94:ALA:O      | 1:A:102:LEU:HD21   | 2.16                     | 0.46              |
| 5:E:108:ARG:NH1   | 48:5:469:C:N3      | 2.58                     | 0.46              |
| 7:G:51:LEU:HD11   | 48:5:4086:G:C4     | 2.51                     | 0.46              |
| 11:L:165:LYS:O    | 26:a:100:ILE:HD13  | 2.16                     | 0.46              |
| 17:R:120:TYR:CD1  | 17:R:120:TYR:C     | 2.93                     | 0.46              |
| 30:e:76:LYS:NZ    | 30:e:98:GLU:OE2    | 2.48                     | 0.46              |
| 44:t:46:ILE:O     | 44:t:50:THR:HG23   | 2.16                     | 0.46              |
| 48:5:106:A:H1'    | 48:5:336:A:N3      | 2.31                     | 0.46              |
| 48:5:211:G:H1'    | 48:5:233:U:O4      | 2.16                     | 0.46              |
| 48:5:388:A:O2'    | 48:5:402:A:N1      | 2.39                     | 0.46              |
| 48:5:914:U:HO2'   | 48:5:915:A:C1'     | 2.27                     | 0.46              |
| 48:5:1672:U:H2'   | 48:5:1673:U:C6     | 2.51                     | 0.46              |
| 48:5:4459:U:H2'   | 48:5:4460:U:O4'    | 2.16                     | 0.46              |
| 51:9:617:G:OP1    | 82:ee:9:VAL:HG13   | 2.16                     | 0.46              |
| 51:9:919:A:O2'    | 51:9:1020:A:N6     | 2.48                     | 0.46              |
| 51:9:919:A:OP2    | 65:NN:64:ARG:NH1   | 2.38                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:1366:G:H2'    | 51:9:1367:PSU:O4'  | 2.16                     | 0.46              |
| 51:9:1675:A:N3     | 51:9:1675:A:O4'    | 2.47                     | 0.46              |
| 71:TT:5:THR:OG1    | 71:TT:6:VAL:N      | 2.48                     | 0.46              |
| 79:bb:74:THR:HG22  | 79:bb:75:GLU:N     | 2.31                     | 0.46              |
| 87:jj:468:GLN:NE2  | 87:jj:487:GLU:O    | 2.41                     | 0.46              |
| 3:C:263:LEU:HG     | 3:C:273:LEU:HD12   | 1.98                     | 0.45              |
| 4:D:43:LYS:HB3     | 4:D:46:THR:CG2     | 2.45                     | 0.45              |
| 17:R:178:GLN:O     | 17:R:181:LYS:HD2   | 2.16                     | 0.45              |
| 44:t:50:THR:HA     | 44:t:53:TRP:CE2    | 2.50                     | 0.45              |
| 48:5:125:C:O2'     | 48:5:126:C:O5'     | 2.25                     | 0.45              |
| 48:5:1734:G:N2     | 48:5:1735:U:O4     | 2.40                     | 0.45              |
| 48:5:4893:A:H2'    | 48:5:4894:A:O4'    | 2.16                     | 0.45              |
| 48:5:4962:C:H2'    | 48:5:4963:G:O4'    | 2.15                     | 0.45              |
| 51:9:1559:C:H2'    | 51:9:1560:U:O4'    | 2.15                     | 0.45              |
| 51:9:1620:A:N3     | 51:9:1620:A:H2'    | 2.30                     | 0.45              |
| 51:9:1621:U:O4     | 67:PP:82:ASP:HB3   | 2.17                     | 0.45              |
| 57:FF:204:ARG:HD3  | 80:cc:60:GLU:HG3   | 1.98                     | 0.45              |
| 59:HH:160:LYS:HA   | 59:HH:163:GLN:HB2  | 1.98                     | 0.45              |
| 64:MM:85:LEU:HD23  | 64:MM:85:LEU:C     | 2.40                     | 0.45              |
| 66:OO:128:ARG:HG2  | 66:OO:128:ARG:HH11 | 1.80                     | 0.45              |
| 84:gg:154:VAL:HG12 | 84:gg:167:SER:CB   | 2.45                     | 0.45              |
| 87:jj:79:LEU:O     | 87:jj:80:GLU:C     | 2.58                     | 0.45              |
| 18:S:1:MET:HE3     | 18:S:43:ARG:HG3    | 1.97                     | 0.45              |
| 30:e:4:LEU:O       | 30:e:121:ARG:NH1   | 2.46                     | 0.45              |
| 44:t:135:THR:HB    | 48:5:1993:C:O2     | 2.16                     | 0.45              |
| 48:5:3:C:H2'       | 48:5:4:G:O4'       | 2.15                     | 0.45              |
| 48:5:37:U:H2'      | 48:5:38:A:O4'      | 2.16                     | 0.45              |
| 48:5:1328:G:O2'    | 48:5:2349:A:OP1    | 2.33                     | 0.45              |
| 48:5:1433:A:H2'    | 48:5:1434:G:O4'    | 2.16                     | 0.45              |
| 48:5:1759:G:C6     | 48:5:1760:G:N7     | 2.85                     | 0.45              |
| 48:5:1979:A:H2'    | 48:5:1980:U:H1'    | 1.99                     | 0.45              |
| 48:5:2627:C:O2     | 48:5:2627:C:O5'    | 2.34                     | 0.45              |
| 51:9:309:G:OP2     | 51:9:309:G:O3'     | 2.34                     | 0.45              |
| 51:9:1822:A:H2'    | 51:9:1823:A:O4'    | 2.17                     | 0.45              |
| 56:EE:255:ARG:O    | 56:EE:259:LYS:HG2  | 2.17                     | 0.45              |
| 59:HH:19:PHE:O     | 59:HH:48:ALA:HB3   | 2.16                     | 0.45              |
| 62:KK:84:HIS:C     | 62:KK:85:LEU:HD22  | 2.41                     | 0.45              |
| 67:PP:44:ARG:NH1   | 67:PP:82:ASP:O     | 2.42                     | 0.45              |
| 83:ff:136:CYS:HB3  | 83:ff:141:LEU:N    | 2.31                     | 0.45              |
| 84:gg:173:LEU:HD23 | 84:gg:189:ILE:CG1  | 2.45                     | 0.45              |
| 6:F:198:LYS:HE3    | 6:F:198:LYS:H      | 1.80                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:G:55:VAL:HG21    | 23:X:41:ARG:HD3    | 1.98                     | 0.45              |
| 16:Q:156:PRO:O     | 26:a:50:PRO:HD3    | 2.17                     | 0.45              |
| 25:Z:61:LYS:O      | 25:Z:65:ARG:HG2    | 2.17                     | 0.45              |
| 26:a:75:LEU:HD11   | 26:a:133:ALA:HA    | 1.98                     | 0.45              |
| 43:s:91:THR:HG21   | 43:s:98:ILE:CD1    | 2.46                     | 0.45              |
| 44:t:135:THR:OG1   | 48:5:1973:G:N2     | 2.49                     | 0.45              |
| 48:5:419:A:N6      | 50:8:15:G:H1'      | 2.31                     | 0.45              |
| 48:5:2899:C:C2     | 48:5:2900:U:C5     | 3.04                     | 0.45              |
| 48:5:5061:A:H3'    | 48:5:5062:G:H5'    | 1.98                     | 0.45              |
| 51:9:85:A:N3       | 51:9:149:A:H2      | 2.15                     | 0.45              |
| 51:9:203:G:O2'     | 51:9:204:G:H5'     | 2.17                     | 0.45              |
| 51:9:301:A:N3      | 60:II:73:THR:CG2   | 2.80                     | 0.45              |
| 51:9:555:A:H5''    | 51:9:556:U:OP2     | 2.17                     | 0.45              |
| 51:9:887:U:O2      | 51:9:887:U:O4'     | 2.33                     | 0.45              |
| 51:9:1059:G:H2'    | 51:9:1060:A:H5'    | 1.97                     | 0.45              |
| 51:9:1664:A:HO2'   | 51:9:1666:C:H41    | 1.64                     | 0.45              |
| 53:BB:39:PHE:CD2   | 53:BB:74:LEU:HD13  | 2.51                     | 0.45              |
| 60:II:41:ARG:HD3   | 60:II:43:ILE:HD12  | 1.99                     | 0.45              |
| 70:SS:38:ARG:CG    | 71:TT:45:LEU:HD21  | 2.47                     | 0.45              |
| 72:UU:46:LYS:HB3   | 72:UU:48:LEU:HD13  | 1.98                     | 0.45              |
| 75:XX:28:LYS:CE    | 75:XX:32:LEU:HD13  | 2.46                     | 0.45              |
| 83:ff:136:CYS:HB3  | 83:ff:141:LEU:H    | 1.82                     | 0.45              |
| 3:C:86:ARG:HG3     | 3:C:86:ARG:O       | 2.16                     | 0.45              |
| 5:E:185:ASN:HD21   | 5:E:274:LEU:C      | 2.24                     | 0.45              |
| 10:J:94:LEU:O      | 10:J:175:LEU:N     | 2.41                     | 0.45              |
| 25:Z:46:ILE:HG23   | 25:Z:68:ILE:HG23   | 1.97                     | 0.45              |
| 47:3:76:A:N6       | 48:5:4371:G:N7     | 2.64                     | 0.45              |
| 48:5:233:U:H5      | 48:5:2304:U:O2'    | 1.99                     | 0.45              |
| 48:5:1413:C:H2'    | 48:5:1414:C:C6     | 2.51                     | 0.45              |
| 48:5:1817:U:O2'    | 48:5:1818:G:H5'    | 2.16                     | 0.45              |
| 48:5:2543:A:H4'    | 50:8:127:U:O2      | 2.17                     | 0.45              |
| 51:9:964:A:H1'     | 51:9:1054:G:O2'    | 2.17                     | 0.45              |
| 51:9:1303:C:O2     | 51:9:1303:C:O4'    | 2.34                     | 0.45              |
| 51:9:1314:U:H5'    | 51:9:1315:U:OP2    | 2.16                     | 0.45              |
| 51:9:1733:U:H2'    | 51:9:1734:G:O4'    | 2.16                     | 0.45              |
| 55:DD:37:VAL:O     | 55:DD:37:VAL:HG13  | 2.15                     | 0.45              |
| 59:HH:130:LEU:HD11 | 59:HH:156:VAL:HG21 | 1.98                     | 0.45              |
| 65:NN:4:MET:HE2    | 65:NN:124:ARG:NH2  | 2.31                     | 0.45              |
| 68:QQ:57:LEU:HD23  | 68:QQ:112:LEU:CD2  | 2.46                     | 0.45              |
| 68:QQ:58:LEU:HD22  | 68:QQ:108:ILE:HG22 | 1.98                     | 0.45              |
| 77:ZZ:58:LEU:HD23  | 77:ZZ:59:CYS:N     | 2.32                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 86:ii:52:LEU:CD1  | 86:ii:78:VAL:HG12 | 2.46                     | 0.45              |
| 1:A:204:MET:HE2   | 48:5:1631:A:N1    | 2.31                     | 0.45              |
| 5:E:199:ALA:HB3   | 31:f:110:ILE:OXT  | 2.15                     | 0.45              |
| 6:F:112:ARG:HD2   | 48:5:1840:G:H5''  | 1.99                     | 0.45              |
| 8:H:44:GLU:OE2    | 12:M:2:VAL:N      | 2.50                     | 0.45              |
| 44:t:11:LYS:HA    | 44:t:65:GLN:O     | 2.17                     | 0.45              |
| 48:5:137:G:O2'    | 48:5:138:G:H5'    | 2.16                     | 0.45              |
| 48:5:488:G:H2'    | 48:5:489:C:C6     | 2.52                     | 0.45              |
| 48:5:1178:G:H2'   | 48:5:1179:U:H5'   | 1.99                     | 0.45              |
| 48:5:2028:C:H2'   | 48:5:2029:A:O4'   | 2.17                     | 0.45              |
| 48:5:2379:A:H2'   | 48:5:2380:G:O4'   | 2.17                     | 0.45              |
| 48:5:2601:A:N6    | 48:5:2744:A:OP2   | 2.44                     | 0.45              |
| 48:5:4653:C:H2'   | 48:5:4654:C:C6    | 2.52                     | 0.45              |
| 51:9:333:G:OP2    | 58:GG:190:ARG:NH2 | 2.32                     | 0.45              |
| 51:9:1287:A:C2    | 51:9:1313:A:C4    | 3.05                     | 0.45              |
| 51:9:1401:A:O2'   | 72:UU:53:PRO:O    | 2.28                     | 0.45              |
| 53:BB:168:MET:O   | 53:BB:172:MET:HG3 | 2.15                     | 0.45              |
| 53:BB:171:ILE:O   | 53:BB:175:GLU:HG2 | 2.16                     | 0.45              |
| 63:LL:91:ASP:OD1  | 63:LL:104:LYS:NZ  | 2.42                     | 0.45              |
| 67:PP:98:ASN:OD1  | 67:PP:121:ILE:O   | 2.34                     | 0.45              |
| 76:YY:24:VAL:HG13 | 76:YY:70:THR:HG23 | 1.98                     | 0.45              |
| 79:bb:37:CYS:HB2  | 79:bb:63:LEU:HD11 | 1.98                     | 0.45              |
| 87:jj:106:LEU:HG  | 87:jj:285:PHE:CE2 | 2.51                     | 0.45              |
| 87:jj:187:ILE:O   | 87:jj:191:LYS:HG2 | 2.17                     | 0.45              |
| 1:A:7:GLY:O       | 48:5:3667:C:H4'   | 2.17                     | 0.45              |
| 2:B:370:THR:O     | 2:B:370:THR:CG2   | 2.64                     | 0.45              |
| 4:D:186:GLU:O     | 4:D:187:SER:HB3   | 2.16                     | 0.45              |
| 9:I:184:MET:HE2   | 9:I:190:LEU:HG    | 1.99                     | 0.45              |
| 14:O:110:PRO:O    | 14:O:113:ASP:OD1  | 2.34                     | 0.45              |
| 43:s:9:TRP:HE1    | 48:5:1999:A:P     | 2.40                     | 0.45              |
| 48:5:2538:U:H2'   | 48:5:2539:C:C6    | 2.51                     | 0.45              |
| 48:5:4419:U:OP1   | 48:5:4421:C:N4    | 2.47                     | 0.45              |
| 48:5:4765:G:O6    | 48:5:4869:U:H5    | 1.98                     | 0.45              |
| 48:5:4924:C:H2'   | 48:5:4925:U:O4'   | 2.17                     | 0.45              |
| 51:9:643:A:OP2    | 61:JJ:38:ARG:NH2  | 2.44                     | 0.45              |
| 51:9:1133:A:H4'   | 78:aa:13:LYS:HD3  | 1.98                     | 0.45              |
| 51:9:1810:U:O2'   | 51:9:1811:C:H5'   | 2.16                     | 0.45              |
| 52:AA:30:LEU:HD22 | 52:AA:47:TYR:CE2  | 2.52                     | 0.45              |
| 60:II:158:ILE:HB  | 60:II:163:GLU:OE2 | 2.17                     | 0.45              |
| 66:OO:56:VAL:HG21 | 66:OO:80:ASP:CG   | 2.41                     | 0.45              |
| 66:OO:56:VAL:HG12 | 66:OO:57:THR:N    | 2.31                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:QQ:40:GLU:OE1   | 68:QQ:40:GLU:CA    | 2.64                     | 0.45              |
| 84:gg:146:SER:O    | 84:gg:147:HIS:CD2  | 2.70                     | 0.45              |
| 84:gg:197:THR:HG21 | 84:gg:239:LEU:N    | 2.31                     | 0.45              |
| 86:ii:24:LEU:HD21  | 86:ii:112:ILE:HD13 | 1.96                     | 0.45              |
| 1:A:209:HIS:CE1    | 1:A:235:VAL:HG21   | 2.52                     | 0.45              |
| 5:E:286:PRO:HB2    | 31:f:41:PHE:CZ     | 2.52                     | 0.45              |
| 7:G:165:GLU:OE1    | 13:N:26:ARG:NH2    | 2.46                     | 0.45              |
| 17:R:10:LEU:O      | 17:R:14:VAL:HG23   | 2.17                     | 0.45              |
| 20:U:66:SER:OG     | 20:U:67:LYS:N      | 2.46                     | 0.45              |
| 28:c:18:LEU:O      | 28:c:22:MET:HG2    | 2.16                     | 0.45              |
| 40:o:38:LYS:HA     | 47:3:75:C:N4       | 2.31                     | 0.45              |
| 48:5:418:A:C2      | 50:8:17:A:H1'      | 2.51                     | 0.45              |
| 48:5:462:G:H2'     | 48:5:463:A:N9      | 2.32                     | 0.45              |
| 48:5:978:G:N2      | 48:5:1278:C:C2     | 2.85                     | 0.45              |
| 48:5:1420:A:H4'    | 48:5:1421:G:C5'    | 2.47                     | 0.45              |
| 48:5:5004:C:H2'    | 48:5:5005:G:O4'    | 2.17                     | 0.45              |
| 51:9:224:A:H2'     | 51:9:225:G:C8      | 2.52                     | 0.45              |
| 51:9:379:C:O2      | 60:II:5:ARG:NE     | 2.44                     | 0.45              |
| 51:9:1491:G:H2'    | 51:9:1492:U:C6     | 2.52                     | 0.45              |
| 51:9:1536:G:H2'    | 51:9:1537:A:H8     | 1.82                     | 0.45              |
| 51:9:1587:G:N3     | 51:9:1587:G:H2'    | 2.32                     | 0.45              |
| 51:9:1839:U:H2'    | 51:9:1840:U:C6     | 2.52                     | 0.45              |
| 61:JJ:104:ASP:OD1  | 61:JJ:104:ASP:N    | 2.49                     | 0.45              |
| 76:YY:20:ARG:HB3   | 76:YY:76:TYR:CD1   | 2.52                     | 0.45              |
| 87:jj:504:VAL:CG2  | 87:jj:528:LEU:HD13 | 2.47                     | 0.45              |
| 1:A:173:GLY:O      | 41:p:69:TRP:NE1    | 2.49                     | 0.45              |
| 2:B:156:TYR:OH     | 48:5:4909:A:OP2    | 2.28                     | 0.45              |
| 25:Z:123:LYS:O     | 25:Z:124:THR:OG1   | 2.27                     | 0.45              |
| 27:b:69:ALA:O      | 27:b:72:ILE:HG22   | 2.16                     | 0.45              |
| 33:h:75:GLY:HA2    | 48:5:133:C:O2      | 2.17                     | 0.45              |
| 44:t:73:VAL:HG12   | 44:t:74:VAL:H      | 1.82                     | 0.45              |
| 48:5:125:C:O2'     | 48:5:126:C:P       | 2.74                     | 0.45              |
| 48:5:325:U:H2'     | 48:5:326:C:C6      | 2.52                     | 0.45              |
| 48:5:2552:G:O2'    | 48:5:2766:A:N6     | 2.44                     | 0.45              |
| 48:5:2733:C:H2'    | 48:5:2734:U:O4'    | 2.16                     | 0.45              |
| 50:8:126:C:O2      | 50:8:127:U:C4      | 2.69                     | 0.45              |
| 51:9:113:G:C2      | 51:9:292:A:H1'     | 2.52                     | 0.45              |
| 51:9:126:G:O5'     | 58:GG:195:LYS:HD2  | 2.16                     | 0.45              |
| 51:9:203:G:P       | 60:II:147:LYS:HZ1  | 2.39                     | 0.45              |
| 51:9:734:C:C4      | 51:9:735:C:C5      | 3.05                     | 0.45              |
| 51:9:835:C:O2      | 51:9:837:A:H4'     | 2.16                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:876:C:H5'     | 51:9:877:C:P       | 2.57                     | 0.45              |
| 51:9:1386:A:OP2    | 55:DD:160:SER:OG   | 2.34                     | 0.45              |
| 54:CC:83:LEU:HD11  | 73:VV:15:ARG:HG3   | 1.99                     | 0.45              |
| 55:DD:51:LEU:HD11  | 55:DD:91:VAL:HA    | 1.99                     | 0.45              |
| 58:GG:10:THR:O     | 58:GG:129:VAL:HB   | 2.17                     | 0.45              |
| 64:MM:51:VAL:HB    | 64:MM:109:VAL:HG12 | 1.98                     | 0.45              |
| 66:OO:27:VAL:HG12  | 66:OO:90:ILE:HD13  | 1.99                     | 0.45              |
| 86:ii:326:LEU:HD11 | 86:ii:409:ILE:HG13 | 1.98                     | 0.45              |
| 3:C:268:ARG:NH1    | 48:5:655:C:OP2     | 2.49                     | 0.45              |
| 4:D:41:LYS:HB2     | 19:T:68:THR:O      | 2.17                     | 0.45              |
| 25:Z:100:VAL:HG12  | 25:Z:106:LEU:HB3   | 1.99                     | 0.45              |
| 48:5:93:G:H2'      | 48:5:94:A:C8       | 2.51                     | 0.45              |
| 48:5:733:A:H2'     | 48:5:734:G:O4'     | 2.16                     | 0.45              |
| 48:5:1238:A:O2'    | 48:5:1239:C:P      | 2.75                     | 0.45              |
| 48:5:2273:G:H2'    | 48:5:2274:C:C6     | 2.52                     | 0.45              |
| 48:5:2555:G:H2'    | 48:5:2556:G:O4'    | 2.17                     | 0.45              |
| 48:5:4349:C:H3'    | 48:5:4350:C:H5'    | 1.98                     | 0.45              |
| 48:5:4394:A:H4'    | 48:5:4395:U:OP2    | 2.17                     | 0.45              |
| 48:5:4922:C:OP2    | 48:5:4922:C:C6     | 2.70                     | 0.45              |
| 51:9:158:A:H2'     | 51:9:159:A2M:O4'   | 2.17                     | 0.45              |
| 51:9:338:G:H2'     | 51:9:339:A:N7      | 2.32                     | 0.45              |
| 51:9:599:A:H2'     | 51:9:606:G:N2      | 2.31                     | 0.45              |
| 51:9:953:C:H2'     | 51:9:954:U:O4'     | 2.16                     | 0.45              |
| 51:9:1139:C:O2     | 51:9:1139:C:O4'    | 2.32                     | 0.45              |
| 51:9:1298:G:O2'    | 51:9:1299:A:H8     | 1.99                     | 0.45              |
| 51:9:1372:U:O2'    | 69:RR:6:THR:HG22   | 2.17                     | 0.45              |
| 51:9:1380:C:H2'    | 51:9:1381:G:O4'    | 2.17                     | 0.45              |
| 51:9:1516:G:H2'    | 51:9:1517:G:O4'    | 2.16                     | 0.45              |
| 52:AA:84:GLN:O     | 52:AA:87:VAL:HG22  | 2.17                     | 0.45              |
| 57:FF:18:LYS:HD2   | 57:FF:48:TYR:CZ    | 2.52                     | 0.45              |
| 69:RR:82:ASP:OD1   | 69:RR:82:ASP:C     | 2.59                     | 0.45              |
| 70:SS:124:ARG:NE   | 70:SS:130:ARG:O    | 2.48                     | 0.45              |
| 84:gg:154:VAL:HG12 | 84:gg:167:SER:HB2  | 1.99                     | 0.45              |
| 84:gg:252:THR:O    | 84:gg:255:SER:O    | 2.34                     | 0.45              |
| 86:ii:177:PRO:HG2  | 86:ii:197:LYS:HG3  | 1.99                     | 0.45              |
| 5:E:195:LYS:O      | 31:f:106:TYR:O     | 2.34                     | 0.45              |
| 48:5:495:C:H2'     | 48:5:496:G:C8      | 2.52                     | 0.45              |
| 48:5:2699:C:O2'    | 48:5:2700:G:H5'    | 2.16                     | 0.45              |
| 51:9:320:G:OP1     | 51:9:320:G:C4'     | 2.65                     | 0.45              |
| 51:9:1013:U:OP1    | 51:9:1129:G:O2'    | 2.35                     | 0.45              |
| 51:9:1407:U:H2'    | 51:9:1408:U:C6     | 2.52                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:1577:G:O2'    | 51:9:1579:A:N3     | 2.42                     | 0.45              |
| 53:BB:37:ALA:O     | 53:BB:38:MET:C     | 2.60                     | 0.45              |
| 58:GG:16:ILE:HG22  | 58:GG:18:VAL:HG23  | 1.99                     | 0.45              |
| 59:HH:51:ILE:CD1   | 59:HH:61:ILE:HD13  | 2.47                     | 0.45              |
| 67:PP:119:PHE:CE1  | 70:SS:117:ILE:HG22 | 2.51                     | 0.45              |
| 68:QQ:128:GLU:HG2  | 68:QQ:129:SER:N    | 2.32                     | 0.45              |
| 76:YY:12:PHE:CZ    | 76:YY:21:LYS:HB3   | 2.51                     | 0.45              |
| 86:ii:161:LEU:HG   | 86:ii:162:GLN:O    | 2.17                     | 0.45              |
| 87:jj:41:VAL:O     | 87:jj:42:THR:HG23  | 2.17                     | 0.45              |
| 4:D:234:ASP:O      | 4:D:235:MET:HB3    | 2.17                     | 0.44              |
| 5:E:94:THR:HG22    | 5:E:111:LYS:HA     | 1.99                     | 0.44              |
| 9:I:43:VAL:HG13    | 9:I:44:ASP:N       | 2.32                     | 0.44              |
| 48:5:118:C:H3'     | 48:5:119:G:C5'     | 2.46                     | 0.44              |
| 48:5:222:C:H2'     | 48:5:223:G:O4'     | 2.17                     | 0.44              |
| 48:5:2390:G:H22    | 48:5:2825:A:H2     | 1.64                     | 0.44              |
| 48:5:2480:G:C2     | 48:5:2481:G:C8     | 3.05                     | 0.44              |
| 50:8:56:G:H2'      | 50:8:57:C:O4'      | 2.17                     | 0.44              |
| 51:9:186:C:H2'     | 51:9:187:G:C8      | 2.52                     | 0.44              |
| 51:9:371:A:OP2     | 60:II:10:LYS:HB2   | 2.16                     | 0.44              |
| 51:9:532:C:H2'     | 51:9:533:A:O5'     | 2.18                     | 0.44              |
| 51:9:674:C:H2'     | 51:9:675:U:C6      | 2.52                     | 0.44              |
| 51:9:841:G:N7      | 76:YY:12:PHE:N     | 2.65                     | 0.44              |
| 52:AA:128:ARG:NH2  | 52:AA:151:ASP:O    | 2.50                     | 0.44              |
| 52:AA:141:ASN:ND2  | 73:VV:31:SER:O     | 2.40                     | 0.44              |
| 58:GG:132:ARG:O    | 58:GG:133:LEU:HD23 | 2.18                     | 0.44              |
| 58:GG:219:GLU:O    | 58:GG:223:LYS:HE2  | 2.17                     | 0.44              |
| 59:HH:14:GLU:O     | 59:HH:14:GLU:CD    | 2.60                     | 0.44              |
| 61:JJ:32:ILE:O     | 61:JJ:35:TYR:O     | 2.35                     | 0.44              |
| 80:cc:28:THR:O     | 80:cc:30:VAL:HG13  | 2.16                     | 0.44              |
| 84:gg:30:MET:HA    | 84:gg:43:TRP:O     | 2.17                     | 0.44              |
| 84:gg:195:LEU:HD13 | 84:gg:195:LEU:HA   | 1.86                     | 0.44              |
| 84:gg:241:PHE:N    | 84:gg:241:PHE:CD1  | 2.85                     | 0.44              |
| 86:ii:33:SER:HB3   | 86:ii:70:SER:HB3   | 1.99                     | 0.44              |
| 86:ii:389:LEU:HD23 | 86:ii:389:LEU:O    | 2.17                     | 0.44              |
| 87:jj:372:SER:HA   | 87:jj:508:ILE:HG22 | 1.98                     | 0.44              |
| 2:B:297:LYS:C      | 2:B:298:LEU:HD23   | 2.42                     | 0.44              |
| 29:d:68:LEU:CD2    | 29:d:106:VAL:HG12  | 2.47                     | 0.44              |
| 43:s:27:CYS:HA     | 43:s:89:VAL:O      | 2.17                     | 0.44              |
| 48:5:475:G:H2'     | 48:5:476:G:O4'     | 2.16                     | 0.44              |
| 48:5:692:A:H2'     | 48:5:693:C:H6      | 1.82                     | 0.44              |
| 48:5:1480:C:H2'    | 48:5:1483:C:H42    | 1.79                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:1685:G:H2'    | 48:5:1686:C:C6     | 2.52                     | 0.44              |
| 48:5:3861:A:H2'    | 48:5:3862:A:C8     | 2.51                     | 0.44              |
| 48:5:4418:G:H2'    | 48:5:4475:G:N2     | 2.32                     | 0.44              |
| 48:5:4476:C:O2'    | 48:5:4478:G:OP2    | 2.31                     | 0.44              |
| 48:5:4886:C:H2'    | 48:5:4887:C:C6     | 2.52                     | 0.44              |
| 51:9:305:U:C2      | 60:II:55:TYR:CE2   | 3.05                     | 0.44              |
| 51:9:816:A:C2'     | 51:9:817:G:H5'     | 2.47                     | 0.44              |
| 51:9:876:C:H2'     | 51:9:878:G:C1'     | 2.47                     | 0.44              |
| 51:9:926:A:H2'     | 51:9:927:C:O4'     | 2.17                     | 0.44              |
| 51:9:1109:C:O2'    | 51:9:1110:G:P      | 2.75                     | 0.44              |
| 51:9:1144:A:H2'    | 51:9:1145:A:C8     | 2.53                     | 0.44              |
| 51:9:1364:U:O2     | 51:9:1364:U:O4'    | 2.35                     | 0.44              |
| 59:HH:64:VAL:HG22  | 59:HH:95:ILE:O     | 2.16                     | 0.44              |
| 60:II:133:GLU:O    | 60:II:137:LEU:HG   | 2.17                     | 0.44              |
| 84:gg:23:THR:HG23  | 84:gg:31:ILE:HD13  | 2.00                     | 0.44              |
| 84:gg:198:VAL:HG13 | 84:gg:209:SER:HB2  | 1.99                     | 0.44              |
| 86:ii:337:GLY:C    | 86:ii:338:THR:HG23 | 2.42                     | 0.44              |
| 87:jj:437:THR:O    | 87:jj:438:HIS:C    | 2.59                     | 0.44              |
| 2:B:248:LEU:HD12   | 2:B:248:LEU:C      | 2.42                     | 0.44              |
| 5:E:157:THR:HG23   | 5:E:158:GLY:N      | 2.31                     | 0.44              |
| 8:H:62:GLY:HA2     | 8:H:66:GLU:OE1     | 2.17                     | 0.44              |
| 10:J:24:ILE:HD12   | 10:J:40:LEU:HG     | 2.00                     | 0.44              |
| 14:O:10:ASP:O      | 14:O:14:HIS:CE1    | 2.70                     | 0.44              |
| 26:a:25:HIS:ND1    | 48:5:1338:G:N7     | 2.64                     | 0.44              |
| 30:e:78:LEU:HD11   | 30:e:100:ALA:HA    | 1.98                     | 0.44              |
| 44:t:114:ARG:CZ    | 44:t:118:HIS:NE2   | 2.80                     | 0.44              |
| 48:5:102:G:HO2'    | 48:5:1381:U:HO2'   | 1.61                     | 0.44              |
| 48:5:286:U:H2'     | 48:5:287:U:C6      | 2.52                     | 0.44              |
| 48:5:462:G:N2      | 48:5:694:C:H1'     | 2.33                     | 0.44              |
| 48:5:1217:G:O2'    | 48:5:1218:G:H5'    | 2.18                     | 0.44              |
| 48:5:1967:A:C2     | 48:5:2021:G:C5     | 3.05                     | 0.44              |
| 48:5:1972:G:C6     | 48:5:1995:G:C6     | 3.05                     | 0.44              |
| 48:5:1993:C:N3     | 48:5:2002:A:C6     | 2.85                     | 0.44              |
| 48:5:2104:A:O2'    | 48:5:2105:A:P      | 2.76                     | 0.44              |
| 48:5:3673:C:O5'    | 48:5:3673:C:O2     | 2.35                     | 0.44              |
| 48:5:4738:C:H2'    | 48:5:4739:C:C6     | 2.53                     | 0.44              |
| 51:9:185:G:H2'     | 51:9:186:C:C6      | 2.53                     | 0.44              |
| 51:9:559:G:O2'     | 51:9:560:A:O4'     | 2.36                     | 0.44              |
| 51:9:730:C:N3      | 51:9:731:G:C8      | 2.85                     | 0.44              |
| 51:9:821:G:C6      | 61:JJ:147:PHE:CZ   | 3.05                     | 0.44              |
| 51:9:943:U:O2'     | 66:OO:135:ILE:O    | 2.36                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:9:1109:C:H2'    | 51:9:1110:G:C8    | 2.53                     | 0.44              |
| 51:9:1240:A:C8     | 51:9:1267:C:O2'   | 2.68                     | 0.44              |
| 51:9:1259:A:N6     | 51:9:1519:U:H5''  | 2.32                     | 0.44              |
| 51:9:1298:G:HO2'   | 51:9:1299:A:H8    | 1.64                     | 0.44              |
| 51:9:1593:C:OP1    | 77:ZZ:103:HIS:NE2 | 2.40                     | 0.44              |
| 51:9:1598:G:HO2'   | 51:9:1599:U:P     | 2.40                     | 0.44              |
| 51:9:1803:U:H2'    | 51:9:1804:U:O4'   | 2.17                     | 0.44              |
| 55:DD:28:GLU:HA    | 62:KK:61:GLN:NE2  | 2.33                     | 0.44              |
| 56:EE:59:ASP:OD1   | 56:EE:62:LYS:NZ   | 2.32                     | 0.44              |
| 63:LL:109:MET:HE1  | 63:LL:140:PHE:CE1 | 2.53                     | 0.44              |
| 64:MM:17:ALA:O     | 64:MM:21:VAL:HG12 | 2.17                     | 0.44              |
| 64:MM:49:LEU:HD21  | 64:MM:128:PHE:CE2 | 2.52                     | 0.44              |
| 68:QQ:13:PHE:CD1   | 68:QQ:13:PHE:C    | 2.95                     | 0.44              |
| 70:SS:105:ASN:O    | 70:SS:109:GLU:HG3 | 2.17                     | 0.44              |
| 75:XX:98:ASP:OD1   | 75:XX:98:ASP:C    | 2.59                     | 0.44              |
| 86:ii:161:LEU:HD23 | 86:ii:275:LEU:CD1 | 2.48                     | 0.44              |
| 86:ii:335:CYS:HB2  | 86:ii:366:HIS:CE1 | 2.52                     | 0.44              |
| 87:jj:80:GLU:O     | 87:jj:83:THR:HG22 | 2.18                     | 0.44              |
| 1:A:198:ARG:NH1    | 48:5:3688:U:OP2   | 2.50                     | 0.44              |
| 3:C:209:VAL:HB     | 3:C:229:LEU:HD13  | 1.99                     | 0.44              |
| 12:M:74:ARG:NH2    | 48:5:736:C:OP1    | 2.43                     | 0.44              |
| 15:P:83:TRP:O      | 48:5:3856:A:H5''  | 2.16                     | 0.44              |
| 16:Q:49:LYS:CG     | 16:Q:53:MET:HE3   | 2.47                     | 0.44              |
| 19:T:126:VAL:HG12  | 19:T:127:GLN:N    | 2.33                     | 0.44              |
| 20:U:67:LYS:HD2    | 20:U:68:SER:N     | 2.32                     | 0.44              |
| 26:a:100:ILE:HG13  | 26:a:123:ILE:HB   | 1.98                     | 0.44              |
| 32:g:66:ARG:NH2    | 48:5:2517:A:O2'   | 2.50                     | 0.44              |
| 43:s:121:VAL:HG22  | 43:s:182:PRO:CB   | 2.48                     | 0.44              |
| 48:5:693:C:H2'     | 48:5:694:C:C6     | 2.52                     | 0.44              |
| 48:5:1234:G:O2'    | 48:5:1235:G:P     | 2.74                     | 0.44              |
| 48:5:1786:A:H2'    | 48:5:1789:C:C5    | 2.53                     | 0.44              |
| 48:5:2292:C:H2'    | 48:5:2293:U:C6    | 2.52                     | 0.44              |
| 48:5:2494:U:H2'    | 48:5:2495:U:N1    | 2.32                     | 0.44              |
| 48:5:4173:G:H2'    | 48:5:4174:U:C6    | 2.52                     | 0.44              |
| 48:5:4322:G:O2'    | 48:5:4324:A:N7    | 2.42                     | 0.44              |
| 48:5:4344:U:H2'    | 48:5:4345:C:C6    | 2.52                     | 0.44              |
| 48:5:4916:G:H2'    | 48:5:4917:C:C5'   | 2.47                     | 0.44              |
| 51:9:906:U:N3      | 51:9:907:G:N7     | 2.66                     | 0.44              |
| 51:9:1440:C:H2'    | 51:9:1441:U:C6    | 2.51                     | 0.44              |
| 59:HH:43:LEU:HD11  | 59:HH:72:PHE:HA   | 2.00                     | 0.44              |
| 66:OO:151:LEU:HD23 | 66:OO:151:LEU:C   | 2.42                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 70:SS:30:ILE:HG23  | 70:SS:36:VAL:HG11  | 2.00                     | 0.44              |
| 86:ii:305:VAL:CG1  | 86:ii:306:GLU:N    | 2.81                     | 0.44              |
| 87:jj:191:LYS:CD   | 87:jj:229:VAL:HG13 | 2.47                     | 0.44              |
| 87:jj:594:TYR:N    | 87:jj:594:TYR:CD1  | 2.84                     | 0.44              |
| 2:B:307:TYR:CD2    | 2:B:366:LYS:HA     | 2.53                     | 0.44              |
| 7:G:34:LYS:O       | 48:5:4128:A:N3     | 2.51                     | 0.44              |
| 12:M:34:ASN:ND2    | 48:5:1925:G:OP1    | 2.46                     | 0.44              |
| 29:d:30:HIS:NE2    | 48:5:4637:OMG:OP1  | 2.42                     | 0.44              |
| 32:g:75:SER:OG     | 48:5:2584:G:O6     | 2.34                     | 0.44              |
| 35:j:79:ARG:HE     | 50:8:94:G:H5'      | 1.81                     | 0.44              |
| 39:n:13:LEU:HD12   | 39:n:16:LYS:HE2    | 2.00                     | 0.44              |
| 44:t:162:CYS:HB2   | 44:t:163:PRO:HD3   | 1.99                     | 0.44              |
| 46:2:70:A:N6       | 46:2:71:A:N6       | 2.66                     | 0.44              |
| 48:5:216:C:O2'     | 48:5:217:C:O2'     | 2.31                     | 0.44              |
| 48:5:373:OMG:HM21  | 48:5:1645:C:H4'    | 1.99                     | 0.44              |
| 48:5:741:C:H2'     | 48:5:742:G:O4'     | 2.17                     | 0.44              |
| 48:5:1078:A:C2     | 48:5:1233:G:C6     | 3.06                     | 0.44              |
| 48:5:1201:U:H2'    | 48:5:1202:C:O4'    | 2.18                     | 0.44              |
| 48:5:1979:A:C2     | 48:5:1988:G:O6     | 2.71                     | 0.44              |
| 48:5:2027:U:O2'    | 48:5:2028:C:H5'    | 2.18                     | 0.44              |
| 48:5:2370:A:N1     | 48:5:2390:G:O2'    | 2.45                     | 0.44              |
| 48:5:3871:A:H2'    | 48:5:3872:A:C8     | 2.52                     | 0.44              |
| 48:5:4194:U:H5     | 48:5:4198:G:OP2    | 2.00                     | 0.44              |
| 48:5:4572:U:HO2'   | 48:5:4573:G:H8     | 1.60                     | 0.44              |
| 51:9:64:A:OP1      | 58:GG:177:GLN:NE2  | 2.44                     | 0.44              |
| 51:9:126:G:C5'     | 58:GG:195:LYS:HD2  | 2.48                     | 0.44              |
| 51:9:297:A:H5'     | 56:EE:131:VAL:O    | 2.18                     | 0.44              |
| 51:9:897:U:N3      | 51:9:898:U:C6      | 2.86                     | 0.44              |
| 51:9:1406:G:C3'    | 51:9:1407:U:H4'    | 2.47                     | 0.44              |
| 51:9:1456:G:H2'    | 51:9:1457:U:C6     | 2.52                     | 0.44              |
| 51:9:1724:A:H2'    | 51:9:1725:U:C6     | 2.52                     | 0.44              |
| 56:EE:179:ASN:OD1  | 56:EE:230:LYS:HA   | 2.18                     | 0.44              |
| 58:GG:225:GLN:HA   | 58:GG:228:ILE:HD12 | 2.00                     | 0.44              |
| 60:II:79:ILE:HD11  | 60:II:105:ASP:CA   | 2.47                     | 0.44              |
| 60:II:113:TYR:CD1  | 60:II:117:TYR:HD2  | 2.35                     | 0.44              |
| 73:VV:1:MET:O      | 73:VV:9:VAL:HG22   | 2.17                     | 0.44              |
| 84:gg:251:ALA:HB1  | 84:gg:286:CYS:SG   | 2.57                     | 0.44              |
| 86:ii:334:HIS:CG   | 86:ii:369:ILE:HD13 | 2.53                     | 0.44              |
| 87:jj:168:ILE:HG22 | 87:jj:239:MET:SD   | 2.57                     | 0.44              |
| 5:E:245:ILE:HG22   | 5:E:246:THR:N      | 2.32                     | 0.44              |
| 14:O:191:LYS:HE2   | 14:O:191:LYS:N     | 2.33                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:S:160:ARG:O    | 18:S:161:ARG:HB2   | 2.17                     | 0.44              |
| 19:T:87:LYS:CD    | 48:5:4305:G:H22    | 2.31                     | 0.44              |
| 23:X:106:LYS:NZ   | 48:5:2438:A:OP1    | 2.43                     | 0.44              |
| 44:t:50:THR:HA    | 44:t:53:TRP:CZ2    | 2.52                     | 0.44              |
| 44:t:54:LYS:O     | 44:t:54:LYS:NZ     | 2.41                     | 0.44              |
| 44:t:87:GLU:HG3   | 44:t:104:ILE:HD12  | 1.99                     | 0.44              |
| 47:3:54:U:H2'     | 47:3:55:U:O4'      | 2.17                     | 0.44              |
| 48:5:644:G:H8     | 48:5:644:G:O5'     | 2.01                     | 0.44              |
| 48:5:2005:G:C2    | 48:5:2015:U:H1'    | 2.53                     | 0.44              |
| 48:5:2611:A:OP1   | 48:5:2688:G:O2'    | 2.32                     | 0.44              |
| 48:5:4188:U:H2'   | 48:5:4189:U:C6     | 2.52                     | 0.44              |
| 49:7:53:U:H4'     | 49:7:54:A:OP1      | 2.17                     | 0.44              |
| 51:9:458:A:H2'    | 51:9:459:C:O4'     | 2.17                     | 0.44              |
| 51:9:839:C:O2     | 51:9:839:C:H2'     | 2.17                     | 0.44              |
| 51:9:1354:G:H2'   | 51:9:1356:G:N7     | 2.33                     | 0.44              |
| 51:9:1406:G:H2'   | 51:9:1407:U:C4'    | 2.48                     | 0.44              |
| 51:9:1620:A:H1'   | 51:9:1624:U:OP2    | 2.18                     | 0.44              |
| 52:AA:10:MET:HE2  | 52:AA:55:TRP:CB    | 2.48                     | 0.44              |
| 55:DD:94:ARG:O    | 55:DD:101:GLN:NE2  | 2.50                     | 0.44              |
| 57:FF:20:PHE:CZ   | 57:FF:69:VAL:HG21  | 2.53                     | 0.44              |
| 64:MM:95:ASP:N    | 64:MM:95:ASP:OD1   | 2.51                     | 0.44              |
| 65:NN:62:GLN:O    | 65:NN:66:VAL:HG23  | 2.18                     | 0.44              |
| 67:PP:92:SER:HB3  | 67:PP:107:ILE:HG12 | 2.00                     | 0.44              |
| 70:SS:40:TYR:CD1  | 70:SS:97:GLN:OE1   | 2.70                     | 0.44              |
| 77:ZZ:68:ILE:HB   | 77:ZZ:109:TYR:HB2  | 2.00                     | 0.44              |
| 86:ii:407:GLY:HA2 | 87:jj:34:MET:CE    | 2.44                     | 0.44              |
| 13:N:31:ARG:NH1   | 48:5:4078:C:OP1    | 2.44                     | 0.44              |
| 19:T:35:LYS:NZ    | 48:5:1824:G:OP1    | 2.51                     | 0.44              |
| 20:U:75:GLU:OE1   | 20:U:75:GLU:N      | 2.44                     | 0.44              |
| 36:k:49:ASP:HB2   | 36:k:52:LYS:HD3    | 1.99                     | 0.44              |
| 43:s:55:MET:C     | 43:s:55:MET:SD     | 3.00                     | 0.44              |
| 48:5:468:U:O2'    | 48:5:469:C:C5      | 2.69                     | 0.44              |
| 48:5:966:A:H2'    | 48:5:966:A:N3      | 2.32                     | 0.44              |
| 48:5:1411:C:H2'   | 48:5:1411(A):G:C8  | 2.53                     | 0.44              |
| 48:5:1967:A:C2    | 48:5:2021:G:C4     | 3.06                     | 0.44              |
| 49:7:45:U:H2'     | 49:7:46:C:O4'      | 2.17                     | 0.44              |
| 51:9:73:C:O3'     | 51:9:74:G:O4'      | 2.36                     | 0.44              |
| 51:9:189:U:H3'    | 51:9:190:G:C8      | 2.53                     | 0.44              |
| 51:9:689:U:C5     | 51:9:690:G:N2      | 2.86                     | 0.44              |
| 51:9:1466:G:H5''  | 69:RR:4:VAL:HG22   | 2.00                     | 0.44              |
| 54:CC:169:TYR:OH  | 54:CC:175:GLY:O    | 2.20                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:FF:25:THR:HG21  | 57:FF:46:ALA:HB1   | 1.99                     | 0.44              |
| 57:FF:51:HIS:ND1   | 57:FF:51:HIS:C     | 2.76                     | 0.44              |
| 60:II:132:GLU:O    | 60:II:135:GLU:N    | 2.51                     | 0.44              |
| 66:OO:56:VAL:HG21  | 66:OO:80:ASP:OD2   | 2.18                     | 0.44              |
| 69:RR:17:ILE:HG13  | 69:RR:58:MET:HE2   | 2.00                     | 0.44              |
| 84:gg:58:ALA:C     | 84:gg:59:LEU:HD12  | 2.42                     | 0.44              |
| 84:gg:149:GLU:O    | 84:gg:150:TRP:CD1  | 2.70                     | 0.44              |
| 84:gg:258:ILE:O    | 84:gg:267:VAL:HB   | 2.18                     | 0.44              |
| 86:ii:21:ILE:HG23  | 86:ii:133:THR:HB   | 2.00                     | 0.44              |
| 87:jj:285:PHE:CE1  | 87:jj:302:PRO:HB3  | 2.52                     | 0.44              |
| 1:A:183:GLY:HA2    | 48:5:1613:A:H5''   | 2.00                     | 0.44              |
| 2:B:76:VAL:HG21    | 2:B:332:MET:HE2    | 2.00                     | 0.44              |
| 3:C:100:ARG:HG2    | 3:C:101:MET:O      | 2.17                     | 0.44              |
| 3:C:208:CYS:SG     | 3:C:230:LEU:HD12   | 2.57                     | 0.44              |
| 3:C:350:ARG:HG2    | 3:C:353:ARG:NH2    | 2.33                     | 0.44              |
| 7:G:254:GLU:OE1    | 7:G:254:GLU:C      | 2.61                     | 0.44              |
| 30:e:86:GLU:OE2    | 30:e:86:GLU:HA     | 2.18                     | 0.44              |
| 40:o:73:VAL:O      | 40:o:78:ARG:NH2    | 2.51                     | 0.44              |
| 48:5:180:C:H2'     | 48:5:181:C:C6      | 2.53                     | 0.44              |
| 48:5:1411(C):C:O5' | 48:5:1411(C):C:H6  | 2.01                     | 0.44              |
| 48:5:1767:A:H2'    | 48:5:1769:G:C8     | 2.52                     | 0.44              |
| 48:5:1977:C:C4     | 48:5:1978:C:N4     | 2.85                     | 0.44              |
| 51:9:197:U:O2'     | 51:9:198:U:H5'     | 2.18                     | 0.44              |
| 51:9:309:G:O2'     | 51:9:310:C:H5'     | 2.18                     | 0.44              |
| 51:9:872:A:H2'     | 51:9:872:A:N3      | 2.33                     | 0.44              |
| 51:9:1221:G:O2'    | 51:9:1676:U:O2     | 2.35                     | 0.44              |
| 51:9:1305:C:H2'    | 51:9:1306:U:C6     | 2.53                     | 0.44              |
| 51:9:1408:U:H3'    | 51:9:1408:U:OP2    | 2.18                     | 0.44              |
| 55:DD:95:GLY:HA3   | 55:DD:129:SER:OG   | 2.17                     | 0.44              |
| 60:II:26:LYS:O     | 60:II:29:LEU:HD23  | 2.17                     | 0.44              |
| 60:II:113:TYR:CE1  | 60:II:117:TYR:CD2  | 3.06                     | 0.44              |
| 69:RR:87:GLU:O     | 69:RR:88:VAL:HG23  | 2.18                     | 0.44              |
| 70:SS:33:ILE:HD13  | 70:SS:71:MET:CE    | 2.48                     | 0.44              |
| 87:jj:106:LEU:HD21 | 87:jj:287:CYS:SG   | 2.58                     | 0.44              |
| 87:jj:108:LEU:HB2  | 87:jj:272:VAL:HG22 | 2.00                     | 0.44              |
| 3:C:358:LEU:HD23   | 3:C:359:ALA:N      | 2.32                     | 0.44              |
| 4:D:187:SER:OG     | 4:D:188:LYS:N      | 2.51                     | 0.44              |
| 7:G:210:GLU:OE1    | 7:G:210:GLU:N      | 2.48                     | 0.44              |
| 14:O:110:PRO:C     | 14:O:113:ASP:OD1   | 2.61                     | 0.44              |
| 16:Q:156:PRO:O     | 26:a:47:LYS:O      | 2.36                     | 0.44              |
| 48:5:219:G:OP2     | 48:5:219:G:O4'     | 2.36                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:5:1194:G:N3     | 48:5:1195:G:H1'   | 2.33                     | 0.44              |
| 48:5:1477:C:H2'    | 48:5:1478:C:H6    | 1.82                     | 0.44              |
| 48:5:1921:C:H4'    | 48:5:1922:G:OP2   | 2.18                     | 0.44              |
| 48:5:2519:U:H1'    | 48:5:2520:C:C6    | 2.53                     | 0.44              |
| 48:5:4960:G:H2'    | 48:5:4961:G:C8    | 2.53                     | 0.44              |
| 51:9:441:C:H4'     | 51:9:1737:G:O2'   | 2.17                     | 0.44              |
| 51:9:808:A:H5''    | 56:EE:219:ALA:O   | 2.16                     | 0.44              |
| 51:9:833:C:O2'     | 51:9:834:C:P      | 2.76                     | 0.44              |
| 51:9:889:U:O5'     | 51:9:889:U:H6     | 2.01                     | 0.44              |
| 51:9:1274:G:H5'    | 51:9:1274:G:N3    | 2.32                     | 0.44              |
| 51:9:1402:A:H1'    | 72:UU:54:VAL:HG22 | 1.99                     | 0.44              |
| 51:9:1828:C:H2'    | 51:9:1829:G:O4'   | 2.18                     | 0.44              |
| 52:AA:203:PHE:HE2  | 69:RR:91:LEU:HD13 | 1.83                     | 0.44              |
| 61:JJ:56:ALA:O     | 61:JJ:60:LEU:HG   | 2.18                     | 0.44              |
| 64:MM:110:VAL:HG12 | 64:MM:111:VAL:N   | 2.33                     | 0.44              |
| 70:SS:61:GLU:O     | 70:SS:65:GLU:HG2  | 2.18                     | 0.44              |
| 5:E:205:ASP:C      | 5:E:205:ASP:OD1   | 2.60                     | 0.43              |
| 7:G:214:ALA:HA     | 7:G:217:LYS:NZ    | 2.33                     | 0.43              |
| 13:N:114:ARG:HD3   | 13:N:151:ILE:HG13 | 2.00                     | 0.43              |
| 23:X:117:TYR:O     | 23:X:119:ILE:HG23 | 2.17                     | 0.43              |
| 25:Z:116:VAL:O     | 25:Z:120:GLU:HG2  | 2.17                     | 0.43              |
| 26:a:76:ASP:OD1    | 26:a:76:ASP:C     | 2.61                     | 0.43              |
| 35:j:65:ARG:O      | 35:j:69:ILE:HD12  | 2.18                     | 0.43              |
| 41:p:26:VAL:O      | 41:p:30:GLU:HG2   | 2.17                     | 0.43              |
| 42:r:16:PHE:CG     | 42:r:28:GLU:HB3   | 2.52                     | 0.43              |
| 48:5:309:C:H5''    | 48:5:310:G:O4'    | 2.18                     | 0.43              |
| 48:5:734:G:C2      | 48:5:735:G:C8     | 3.06                     | 0.43              |
| 48:5:1291:G:O2'    | 48:5:1292:C:O5'   | 2.30                     | 0.43              |
| 48:5:2637:U:O2'    | 48:5:2718:U:O2'   | 2.24                     | 0.43              |
| 48:5:3732:A:H2'    | 48:5:3733:A:C8    | 2.53                     | 0.43              |
| 48:5:3810:C:C2     | 86:ii:258:TYR:HE1 | 2.36                     | 0.43              |
| 48:5:3911:C:H2'    | 48:5:3912:U:C6    | 2.53                     | 0.43              |
| 48:5:4094:G:C2     | 48:5:4115:G:N2    | 2.86                     | 0.43              |
| 48:5:4476:C:O2     | 48:5:4476:C:O4'   | 2.34                     | 0.43              |
| 48:5:4584:A:H2'    | 48:5:4585:U:O4'   | 2.18                     | 0.43              |
| 49:7:12:U:OP2      | 49:7:67:C:O2'     | 2.33                     | 0.43              |
| 51:9:201:C:C4      | 51:9:202:G:H1'    | 2.53                     | 0.43              |
| 51:9:1395:C:O2'    | 51:9:1396:A:P     | 2.75                     | 0.43              |
| 51:9:1597:C:H4'    | 51:9:1603:G:C6    | 2.53                     | 0.43              |
| 51:9:1713:C:H2'    | 51:9:1714:U:C6    | 2.53                     | 0.43              |
| 52:AA:39:TYR:CE2   | 69:RR:105:MET:HB3 | 2.53                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:AA:78:SER:O     | 52:AA:101:GLY:N    | 2.40                     | 0.43              |
| 57:FF:123:GLU:HG2  | 57:FF:200:ALA:HB1  | 2.00                     | 0.43              |
| 58:GG:222:GLU:O    | 58:GG:225:GLN:HG2  | 2.18                     | 0.43              |
| 60:II:113:TYR:CE1  | 60:II:158:ILE:HD11 | 2.53                     | 0.43              |
| 66:OO:27:VAL:CG1   | 66:OO:90:ILE:HD13  | 2.48                     | 0.43              |
| 84:gg:29:ASP:N     | 84:gg:29:ASP:OD1   | 2.51                     | 0.43              |
| 84:gg:51:ASN:OD1   | 84:gg:53:GLY:N     | 2.51                     | 0.43              |
| 86:ii:35:ILE:HD12  | 86:ii:74:ALA:HB3   | 2.00                     | 0.43              |
| 86:ii:343:ILE:H    | 86:ii:343:ILE:HD12 | 1.83                     | 0.43              |
| 87:jj:484:LEU:HD13 | 87:jj:485:ILE:N    | 2.33                     | 0.43              |
| 2:B:119:TYR:HE1    | 48:5:4967:A:H5'    | 1.83                     | 0.43              |
| 2:B:252:ALA:HB1    | 48:5:4524:G:C2     | 2.53                     | 0.43              |
| 4:D:188:LYS:O      | 4:D:189:GLU:CB     | 2.66                     | 0.43              |
| 10:J:120:ASP:HB3   | 10:J:123:ILE:HB    | 1.99                     | 0.43              |
| 10:J:159:LYS:O     | 10:J:163:MET:HG3   | 2.17                     | 0.43              |
| 13:N:138:PHE:HA    | 13:N:143:ARG:HD2   | 2.00                     | 0.43              |
| 14:O:8:VAL:HG12    | 14:O:117:ARG:HG3   | 2.00                     | 0.43              |
| 30:e:127:ALA:O     | 48:5:2327:G:OP1    | 2.37                     | 0.43              |
| 43:s:17:ILE:HG13   | 43:s:18:ILE:N      | 2.32                     | 0.43              |
| 44:t:104:ILE:O     | 44:t:106:PHE:CE1   | 2.71                     | 0.43              |
| 46:2:18:G:H21      | 46:2:58:A:H5'      | 1.82                     | 0.43              |
| 48:5:657:C:H5'     | 48:5:658:C:OP2     | 2.19                     | 0.43              |
| 48:5:700:G:H2'     | 48:5:701:G:O5'     | 2.18                     | 0.43              |
| 48:5:906:C:H2'     | 48:5:907:C:O4'     | 2.18                     | 0.43              |
| 48:5:930:G:HO2'    | 48:5:931:C:P       | 2.36                     | 0.43              |
| 48:5:1363:C:H2'    | 48:5:1364:U:O4'    | 2.19                     | 0.43              |
| 48:5:1404:G:N2     | 48:5:1414:C:C2     | 2.86                     | 0.43              |
| 48:5:3902:A:OP1    | 48:5:4450:U:H4'    | 2.17                     | 0.43              |
| 51:9:172:OMU:OP1   | 51:9:315:C:O2'     | 2.31                     | 0.43              |
| 51:9:318:A:H2      | 51:9:332:G:H22     | 1.66                     | 0.43              |
| 51:9:588:G:H1'     | 51:9:589:G:H5''    | 1.99                     | 0.43              |
| 51:9:898:U:H2'     | 51:9:898:U:O2      | 2.17                     | 0.43              |
| 51:9:1535:U:O4     | 57:FF:159:ARG:HG3  | 2.17                     | 0.43              |
| 51:9:1641:A:H2'    | 51:9:1642:U:O4'    | 2.18                     | 0.43              |
| 52:AA:124:VAL:HG21 | 52:AA:134:LEU:HD11 | 1.99                     | 0.43              |
| 56:EE:92:ILE:CG2   | 76:YY:17:LEU:HD21  | 2.48                     | 0.43              |
| 56:EE:177:THR:HG23 | 56:EE:196:THR:HA   | 2.01                     | 0.43              |
| 57:FF:25:THR:HG21  | 57:FF:46:ALA:CB    | 2.48                     | 0.43              |
| 57:FF:99:ILE:HG23  | 77:ZZ:67:LEU:HD13  | 2.01                     | 0.43              |
| 57:FF:99:ILE:HG13  | 77:ZZ:108:ILE:HD11 | 1.98                     | 0.43              |
| 61:JJ:110:LEU:HD12 | 61:JJ:114:VAL:HG23 | 1.99                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:OO:46:ASP:OD1   | 66:OO:46:ASP:N     | 2.50                     | 0.43              |
| 69:RR:34:VAL:O     | 69:RR:38:ILE:HG13  | 2.17                     | 0.43              |
| 84:gg:16:GLY:O     | 84:gg:305:ASN:HA   | 2.18                     | 0.43              |
| 87:jj:249:VAL:O    | 87:jj:252:ARG:HG2  | 2.18                     | 0.43              |
| 87:jj:432:ILE:HD12 | 87:jj:432:ILE:C    | 2.39                     | 0.43              |
| 6:F:150:ASN:HD21   | 48:5:943:A:H62     | 1.65                     | 0.43              |
| 16:Q:177:ALA:O     | 16:Q:178:ARG:C     | 2.61                     | 0.43              |
| 28:c:35:LEU:O      | 28:c:39:ARG:HG3    | 2.19                     | 0.43              |
| 30:e:81:ASN:HA     | 30:e:111:ILE:HD11  | 2.00                     | 0.43              |
| 42:r:54:ALA:HA     | 42:r:61:VAL:HG23   | 2.00                     | 0.43              |
| 43:s:16:LYS:O      | 43:s:20:LEU:HG     | 2.19                     | 0.43              |
| 44:t:117:ARG:O     | 44:t:121:LEU:HD12  | 2.18                     | 0.43              |
| 46:2:19:G:H3'      | 46:2:20:U:C5'      | 2.48                     | 0.43              |
| 48:5:457:G:C6      | 48:5:458:C:C4      | 3.07                     | 0.43              |
| 48:5:924:C:O2'     | 48:5:925:C:OP1     | 2.34                     | 0.43              |
| 48:5:970:G:H2'     | 48:5:971:U:O4'     | 2.18                     | 0.43              |
| 48:5:1380:G:N2     | 48:5:1381:U:O4     | 2.43                     | 0.43              |
| 48:5:1890:G:N2     | 48:5:1938:C:H42    | 2.16                     | 0.43              |
| 48:5:3662:A:H5'    | 48:5:3664:G:O4'    | 2.19                     | 0.43              |
| 48:5:4596:C:C4     | 48:5:4597:U:C4     | 3.06                     | 0.43              |
| 51:9:293:C:OP1     | 63:LL:39:ASN:O     | 2.35                     | 0.43              |
| 51:9:309:G:C2      | 51:9:310:C:C5      | 3.05                     | 0.43              |
| 51:9:546:G:C6      | 51:9:547:G:C2      | 3.05                     | 0.43              |
| 51:9:1170:A:H4'    | 51:9:1171:G:OP1    | 2.18                     | 0.43              |
| 51:9:1435:C:H2'    | 51:9:1436:C:N1     | 2.33                     | 0.43              |
| 51:9:1862:G:H4'    | 51:9:1863:A:OP1    | 2.17                     | 0.43              |
| 54:CC:251:LEU:HA   | 73:VV:23:ILE:HD11  | 2.00                     | 0.43              |
| 58:GG:108:VAL:HG12 | 58:GG:109:LEU:N    | 2.32                     | 0.43              |
| 64:MM:117:GLU:O    | 64:MM:118:SER:OG   | 2.20                     | 0.43              |
| 67:PP:15:PHE:CD2   | 67:PP:109:PRO:HB2  | 2.53                     | 0.43              |
| 71:TT:114:GLU:HG2  | 71:TT:124:THR:HG23 | 1.99                     | 0.43              |
| 86:ii:306:GLU:HG2  | 86:ii:307:ASP:N    | 2.34                     | 0.43              |
| 4:D:35:ARG:HG2     | 48:5:4326:G:O2'    | 2.18                     | 0.43              |
| 4:D:71:GLY:O       | 4:D:73:MET:HE3     | 2.18                     | 0.43              |
| 6:F:156:ARG:HG3    | 6:F:247:ASN:OD1    | 2.18                     | 0.43              |
| 8:H:45:LEU:HD22    | 8:H:57:VAL:HG22    | 1.99                     | 0.43              |
| 11:L:125:VAL:CG2   | 33:h:123:ALA:HB3   | 2.48                     | 0.43              |
| 11:L:201:GLU:OE1   | 11:L:202:ALA:N     | 2.51                     | 0.43              |
| 14:O:186:GLU:O     | 14:O:187:LYS:CB    | 2.65                     | 0.43              |
| 16:Q:178:ARG:HA    | 16:Q:184:ARG:O     | 2.18                     | 0.43              |
| 23:X:154:GLY:O     | 33:h:37:THR:HG21   | 2.18                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:c:84:ALA:HA    | 65:NN:151:ALA:O    | 2.18                     | 0.43              |
| 44:t:64:ILE:HG23  | 44:t:71:ILE:HB     | 2.00                     | 0.43              |
| 46:2:66:C:H2'     | 46:2:67:G:C8       | 2.52                     | 0.43              |
| 47:3:32:C:H5'     | 57:FF:136:ARG:NH1  | 2.32                     | 0.43              |
| 48:5:189:G:C2     | 48:5:190:G:C8      | 3.07                     | 0.43              |
| 48:5:1297:U:H2'   | 48:5:1298:C:H6     | 1.84                     | 0.43              |
| 48:5:1770:A:N1    | 48:5:1771:U:C4     | 2.87                     | 0.43              |
| 48:5:2565:A:C2'   | 48:5:2566:G:OP1    | 2.66                     | 0.43              |
| 48:5:2669:C:H2'   | 48:5:2670:C:O4'    | 2.17                     | 0.43              |
| 48:5:2844:A:O2'   | 48:5:4631:G:H4'    | 2.18                     | 0.43              |
| 48:5:4090:G:H2'   | 48:5:4091:G:O4'    | 2.18                     | 0.43              |
| 51:9:553:U:H2'    | 51:9:554:A:O4'     | 2.17                     | 0.43              |
| 51:9:587:A:O2'    | 51:9:588:G:N2      | 2.51                     | 0.43              |
| 51:9:1239:U:O2'   | 51:9:1241:A:N7     | 2.29                     | 0.43              |
| 51:9:1431:G:O5'   | 51:9:1432:U:O5'    | 2.37                     | 0.43              |
| 51:9:1477:U:H1'   | 51:9:1478:U:OP1    | 2.18                     | 0.43              |
| 51:9:1675:A:O3'   | 57:FF:74:ASN:HB3   | 2.19                     | 0.43              |
| 57:FF:173:LEU:O   | 57:FF:177:LEU:HG   | 2.19                     | 0.43              |
| 59:HH:125:VAL:O   | 59:HH:129:ILE:HG13 | 2.18                     | 0.43              |
| 72:UU:22:ILE:HD13 | 72:UU:114:VAL:HG22 | 1.99                     | 0.43              |
| 75:XX:28:LYS:HE2  | 75:XX:32:LEU:HD22  | 2.00                     | 0.43              |
| 86:ii:251:LEU:CD2 | 86:ii:275:LEU:HD23 | 2.48                     | 0.43              |
| 87:jj:204:LEU:O   | 87:jj:205:ASP:OD1  | 2.36                     | 0.43              |
| 2:B:343:ARG:NH2   | 48:5:4976:U:O2'    | 2.51                     | 0.43              |
| 4:D:185:SER:O     | 4:D:187:SER:O      | 2.36                     | 0.43              |
| 11:L:108:GLU:H    | 11:L:108:GLU:CD    | 2.25                     | 0.43              |
| 14:O:175:MET:HE3  | 14:O:175:MET:O     | 2.18                     | 0.43              |
| 26:a:8:THR:OG1    | 48:5:1339:U:OP1    | 2.30                     | 0.43              |
| 30:e:35:TRP:CE2   | 30:e:56:PRO:HD2    | 2.54                     | 0.43              |
| 33:h:29:SER:O     | 33:h:33:VAL:HG23   | 2.19                     | 0.43              |
| 36:k:11:PHE:CD1   | 36:k:11:PHE:C      | 2.97                     | 0.43              |
| 43:s:82:ILE:O     | 43:s:83:ARG:HD3    | 2.18                     | 0.43              |
| 47:3:8:U:O2       | 47:3:8:U:H3'       | 2.18                     | 0.43              |
| 47:3:33:U:O5'     | 47:3:34:U:OP2      | 2.37                     | 0.43              |
| 48:5:134:G:H1'    | 48:5:135:G:OP2     | 2.18                     | 0.43              |
| 48:5:233:U:H5'    | 48:5:234:G:OP2     | 2.17                     | 0.43              |
| 48:5:2503:G:O4'   | 48:5:4084:G:N2     | 2.51                     | 0.43              |
| 48:5:2890:C:H4'   | 48:5:5034:A:O4'    | 2.19                     | 0.43              |
| 48:5:3657:U:H5''  | 48:5:3657:U:H6     | 1.83                     | 0.43              |
| 48:5:4187:G:H2'   | 48:5:4188:U:O4'    | 2.19                     | 0.43              |
| 48:5:4412:C:H2'   | 48:5:4413:C:O2     | 2.18                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:4746:C:H2'    | 48:5:4747:C:O4'    | 2.18                     | 0.43              |
| 50:8:71:A:C2       | 50:8:88:A:H1'      | 2.53                     | 0.43              |
| 50:8:89:U:H2'      | 50:8:90:C:C6       | 2.53                     | 0.43              |
| 51:9:71:G:C2'      | 51:9:72:C:H5''     | 2.49                     | 0.43              |
| 51:9:547:G:C2      | 51:9:549:C:N4      | 2.87                     | 0.43              |
| 51:9:606:G:O4'     | 82:ee:56:ASN:HB3   | 2.18                     | 0.43              |
| 51:9:664:A:N1      | 51:9:1163:C:O2     | 2.51                     | 0.43              |
| 51:9:917:U:O4'     | 59:HH:118:ARG:HG3  | 2.19                     | 0.43              |
| 51:9:942:G:H21     | 66:OO:137:SER:HB2  | 1.82                     | 0.43              |
| 51:9:1261:C:O2     | 81:dd:10:HIS:CE1   | 2.71                     | 0.43              |
| 51:9:1672:U:OP1    | 68:QQ:18:THR:OG1   | 2.33                     | 0.43              |
| 52:AA:54:THR:HG23  | 52:AA:162:PRO:O    | 2.19                     | 0.43              |
| 55:DD:138:VAL:O    | 55:DD:138:VAL:HG23 | 2.18                     | 0.43              |
| 55:DD:156:LEU:O    | 55:DD:157:MET:HE2  | 2.19                     | 0.43              |
| 64:MM:79:VAL:HG13  | 64:MM:80:ASP:HB2   | 2.00                     | 0.43              |
| 65:NN:127:ARG:HH11 | 65:NN:127:ARG:HG2  | 1.82                     | 0.43              |
| 68:QQ:41:MET:SD    | 71:TT:9:VAL:C      | 3.01                     | 0.43              |
| 86:ii:176:LEU:HD11 | 86:ii:201:TYR:CD2  | 2.54                     | 0.43              |
| 87:jj:36:LYS:HB3   | 87:jj:54:LEU:HD21  | 2.00                     | 0.43              |
| 10:J:120:ASP:OD1   | 10:J:121:PRO:HD2   | 2.18                     | 0.43              |
| 26:a:78:LEU:HD21   | 26:a:124:VAL:HG22  | 2.00                     | 0.43              |
| 27:b:10:HIS:NE2    | 48:5:1877:G:O6     | 2.52                     | 0.43              |
| 45:1:57:ARG:HG3    | 48:5:3904:G:O3'    | 2.19                     | 0.43              |
| 48:5:90:G:OP2      | 48:5:92:C:N4       | 2.40                     | 0.43              |
| 48:5:487:G:H2'     | 48:5:488:G:O4'     | 2.19                     | 0.43              |
| 48:5:498:C:H3'     | 48:5:499:G:H4'     | 2.00                     | 0.43              |
| 48:5:1927:U:OP1    | 48:5:1949:U:O2'    | 2.33                     | 0.43              |
| 48:5:1962:A:N3     | 48:5:1962:A:H2'    | 2.33                     | 0.43              |
| 48:5:2062:C:O2'    | 48:5:2063:G:H5'    | 2.18                     | 0.43              |
| 48:5:2589:C:H2'    | 48:5:2590:G:O4'    | 2.18                     | 0.43              |
| 48:5:2898:G:H2'    | 48:5:2899:C:C6     | 2.53                     | 0.43              |
| 48:5:3909:C:O2     | 48:5:4396:A:N1     | 2.51                     | 0.43              |
| 48:5:4154:G:H2'    | 48:5:4155:C:C6     | 2.54                     | 0.43              |
| 48:5:4413:C:H5     | 48:5:4429:C:H42    | 1.66                     | 0.43              |
| 48:5:4413:C:H5     | 48:5:4429:C:N4     | 2.16                     | 0.43              |
| 48:5:4522:G:O2'    | 48:5:4525:C:OP2    | 2.37                     | 0.43              |
| 48:5:4771:C:O2'    | 48:5:4772:C:H5'    | 2.19                     | 0.43              |
| 50:8:117:C:H2'     | 50:8:118:C:O4'     | 2.18                     | 0.43              |
| 50:8:139:G:H2'     | 50:8:140:C:O4'     | 2.19                     | 0.43              |
| 50:8:140:C:H2'     | 50:8:141:C:C6      | 2.53                     | 0.43              |
| 51:9:594:A:C2      | 51:9:642:U:O2      | 2.72                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:1329:U:O2'    | 51:9:1332:A:OP2    | 2.19                     | 0.43              |
| 51:9:1728:U:H2'    | 51:9:1729:U:O4'    | 2.18                     | 0.43              |
| 51:9:1786:U:O2'    | 51:9:1787:G:H5'    | 2.18                     | 0.43              |
| 52:AA:173:LEU:HD22 | 69:RR:91:LEU:HD21  | 2.00                     | 0.43              |
| 54:CC:206:SER:CB   | 54:CC:224:THR:HG21 | 2.48                     | 0.43              |
| 55:DD:61:GLU:C     | 55:DD:63:GLY:H     | 2.26                     | 0.43              |
| 56:EE:139:LEU:HD23 | 56:EE:139:LEU:O    | 2.19                     | 0.43              |
| 59:HH:134:VAL:O    | 59:HH:134:VAL:CG2  | 2.60                     | 0.43              |
| 61:JJ:111:GLN:NE2  | 61:JJ:127:ARG:HB2  | 2.33                     | 0.43              |
| 67:PP:89:MET:C     | 67:PP:107:ILE:HD11 | 2.44                     | 0.43              |
| 69:RR:57:LEU:HD13  | 69:RR:69:ILE:HD11  | 2.01                     | 0.43              |
| 70:SS:87:GLN:O     | 70:SS:88:LYS:C     | 2.62                     | 0.43              |
| 75:XX:105:PHE:HB2  | 75:XX:119:ARG:C    | 2.43                     | 0.43              |
| 84:gg:150:TRP:O    | 84:gg:169:GLY:HA3  | 2.18                     | 0.43              |
| 86:ii:238:GLN:O    | 86:ii:238:GLN:CG   | 2.65                     | 0.43              |
| 4:D:188:LYS:O      | 4:D:189:GLU:HB2    | 2.19                     | 0.43              |
| 13:N:181:HIS:CD2   | 48:5:99:A:H4'      | 2.53                     | 0.43              |
| 18:S:16:CYS:SG     | 18:S:54:MET:HG3    | 2.58                     | 0.43              |
| 26:a:117:LEU:HD23  | 26:a:140:VAL:CG2   | 2.48                     | 0.43              |
| 48:5:1411(B):C:H2' | 48:5:1411(C):C:C6  | 2.52                     | 0.43              |
| 48:5:2638:G:H22    | 48:5:2697:A:N6     | 2.17                     | 0.43              |
| 48:5:4114:C:H2'    | 48:5:4115:G:O4'    | 2.18                     | 0.43              |
| 48:5:4491:G:O2'    | 48:5:4511:A:N1     | 2.49                     | 0.43              |
| 48:5:4504:C:H2'    | 48:5:4505:C:C6     | 2.53                     | 0.43              |
| 48:5:4957:C:H3'    | 48:5:4958:C:H5''   | 2.01                     | 0.43              |
| 50:8:31:G:H2'      | 50:8:32:C:O4'      | 2.17                     | 0.43              |
| 51:9:67:C:C2       | 58:GG:162:LEU:HD11 | 2.54                     | 0.43              |
| 51:9:529:A:H61     | 51:9:555:A:H61     | 1.65                     | 0.43              |
| 51:9:953:C:H2'     | 51:9:954:U:C6      | 2.53                     | 0.43              |
| 51:9:1240:A:H8     | 51:9:1267:C:O2'    | 2.01                     | 0.43              |
| 51:9:1328:OMG:HM23 | 51:9:1328:OMG:H1'  | 1.80                     | 0.43              |
| 51:9:1499:U:H4'    | 55:DD:176:LEU:HD23 | 2.00                     | 0.43              |
| 51:9:1513:C:OP1    | 81:dd:10:HIS:HB3   | 2.19                     | 0.43              |
| 51:9:1598:G:OP1    | 77:ZZ:80:ARG:NH1   | 2.52                     | 0.43              |
| 51:9:1692:PSU:H2'  | 51:9:1693:G:C8     | 2.53                     | 0.43              |
| 51:9:1702:G:H2'    | 51:9:1703:OMC:O4'  | 2.18                     | 0.43              |
| 52:AA:191:ARG:HG3  | 52:AA:191:ARG:O    | 2.19                     | 0.43              |
| 54:CC:187:ARG:NH1  | 54:CC:191:VAL:O    | 2.52                     | 0.43              |
| 56:EE:122:LYS:HD3  | 56:EE:164:LEU:HD21 | 2.00                     | 0.43              |
| 58:GG:181:THR:O    | 58:GG:182:PRO:C    | 2.62                     | 0.43              |
| 59:HH:57:ARG:H     | 59:HH:57:ARG:HD2   | 1.83                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 60:II:159:SER:O   | 60:II:163:GLU:HG2  | 2.18                     | 0.43              |
| 64:MM:114:TYR:HD1 | 64:MM:121:LYS:HD2  | 1.84                     | 0.43              |
| 66:OO:117:ARG:NH2 | 78:aa:48:ALA:O     | 2.51                     | 0.43              |
| 67:PP:89:MET:HB3  | 67:PP:107:ILE:HD11 | 2.00                     | 0.43              |
| 80:cc:30:VAL:HG23 | 80:cc:32:VAL:HG13  | 2.00                     | 0.43              |
| 83:ff:133:ARG:HD2 | 83:ff:142:THR:HG23 | 2.00                     | 0.43              |
| 84:gg:171:ASP:OD1 | 84:gg:173:LEU:HB2  | 2.18                     | 0.43              |
| 86:ii:162:GLN:O   | 86:ii:163:GLY:C    | 2.62                     | 0.43              |
| 2:B:108:GLU:OE1   | 2:B:109:HIS:NE2    | 2.52                     | 0.43              |
| 4:D:3:PHE:CD1     | 4:D:3:PHE:N        | 2.85                     | 0.43              |
| 5:E:150:GLY:HA3   | 5:E:204:ILE:O      | 2.18                     | 0.43              |
| 5:E:186:ARG:HD3   | 48:5:4936:G:C5     | 2.53                     | 0.43              |
| 8:H:176:LEU:HB3   | 38:m:86:ALA:HB1    | 2.01                     | 0.43              |
| 44:t:124:GLU:HG2  | 44:t:125:LEU:HG    | 2.01                     | 0.43              |
| 48:5:119:G:H3'    | 48:5:120:A:H5''    | 2.01                     | 0.43              |
| 48:5:406:C:HO2'   | 48:5:407:A:P       | 2.39                     | 0.43              |
| 48:5:1761:G:C6    | 48:5:1762:C:C2     | 3.06                     | 0.43              |
| 48:5:3944:G:O3'   | 53:BB:54:GLY:HA2   | 2.18                     | 0.43              |
| 50:8:36:G:O2'     | 50:8:103:A:N1      | 2.37                     | 0.43              |
| 51:9:488:U:O2     | 51:9:488:U:C2'     | 2.66                     | 0.43              |
| 51:9:734:C:N4     | 51:9:735:C:C5      | 2.87                     | 0.43              |
| 51:9:1164:G:O2'   | 51:9:1165:G:H5'    | 2.19                     | 0.43              |
| 51:9:1240:A:H62   | 67:PP:99:GLY:HA3   | 1.84                     | 0.43              |
| 51:9:1555:U:H6    | 51:9:1557:C:H41    | 1.66                     | 0.43              |
| 51:9:1672:U:H5''  | 68:QQ:75:GLY:HA2   | 1.99                     | 0.43              |
| 55:DD:225:GLU:O   | 55:DD:226:GLN:C    | 2.62                     | 0.43              |
| 58:GG:3:LEU:HD22  | 58:GG:111:LEU:HD11 | 2.01                     | 0.43              |
| 58:GG:108:VAL:CG1 | 58:GG:109:LEU:N    | 2.81                     | 0.43              |
| 59:HH:95:ILE:CG1  | 59:HH:96:ALA:N     | 2.80                     | 0.43              |
| 60:II:113:TYR:CE2 | 60:II:121:LEU:HB2  | 2.54                     | 0.43              |
| 64:MM:120:ALA:O   | 64:MM:123:VAL:HG22 | 2.18                     | 0.43              |
| 66:OO:91:THR:HA   | 66:OO:124:MET:HE1  | 2.00                     | 0.43              |
| 74:WW:55:ASP:O    | 74:WW:56:HIS:HB2   | 2.18                     | 0.43              |
| 84:gg:128:THR:H   | 84:gg:151:VAL:HG21 | 1.83                     | 0.43              |
| 86:ii:48:VAL:HG12 | 86:ii:82:LEU:HD11  | 2.01                     | 0.43              |
| 86:ii:136:LEU:O   | 86:ii:140:LEU:HG   | 2.18                     | 0.43              |
| 87:jj:574:ARG:HG3 | 87:jj:575:PRO:N    | 2.34                     | 0.43              |
| 3:C:22:VAL:HG22   | 3:C:258:ARG:CZ     | 2.49                     | 0.43              |
| 4:D:237:GLU:CG    | 4:D:241:LYS:HZ2    | 2.31                     | 0.43              |
| 6:F:60:TYR:HA     | 6:F:63:MET:HE3     | 2.01                     | 0.43              |
| 7:G:93:THR:O      | 7:G:97:LYS:HG2     | 2.19                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:M:98:ARG:NE     | 48:5:4872:G:O6    | 2.49                     | 0.43              |
| 20:U:23:LEU:HD11   | 20:U:83:LEU:HB3   | 2.00                     | 0.43              |
| 20:U:35:ASP:O      | 20:U:38:ASN:OD1   | 2.37                     | 0.43              |
| 30:e:76:LYS:O      | 42:r:23:GLN:NE2   | 2.50                     | 0.43              |
| 41:p:29:ILE:HG23   | 41:p:69:TRP:HB3   | 2.01                     | 0.43              |
| 44:t:10:ILE:HD11   | 44:t:67:ARG:HD2   | 2.01                     | 0.43              |
| 48:5:356:G:O2'     | 50:8:25:G:N3      | 2.52                     | 0.43              |
| 48:5:462:G:O3'     | 48:5:463:A:O4'    | 2.36                     | 0.43              |
| 48:5:1472:C:H2'    | 48:5:1473:U:H6    | 1.83                     | 0.43              |
| 48:5:2457:G:H4'    | 48:5:2470:C:N4    | 2.34                     | 0.43              |
| 48:5:3605:C:H2'    | 48:5:3606:U:O4'   | 2.19                     | 0.43              |
| 48:5:4747:C:H2'    | 48:5:4748:U:O4'   | 2.19                     | 0.43              |
| 50:8:33:G:H5''     | 50:8:34:U:OP1     | 2.19                     | 0.43              |
| 50:8:51:U:H2'      | 50:8:51:U:O2      | 2.18                     | 0.43              |
| 51:9:116:OMU:O5'   | 51:9:116:OMU:H6   | 2.18                     | 0.43              |
| 51:9:121:OMU:O5'   | 51:9:121:OMU:H6   | 2.19                     | 0.43              |
| 51:9:155:G:C6      | 51:9:164:A:C6     | 3.07                     | 0.43              |
| 51:9:464:A:H3'     | 51:9:465:A:H5'    | 2.00                     | 0.43              |
| 51:9:870:A:H5''    | 51:9:872:A:O4'    | 2.19                     | 0.43              |
| 51:9:877:C:H2'     | 51:9:879:C:OP2    | 2.19                     | 0.43              |
| 51:9:1276:A:C2     | 51:9:1277:C:H1'   | 2.54                     | 0.43              |
| 51:9:1646:C:HO2'   | 51:9:1647:A:P     | 2.41                     | 0.43              |
| 51:9:1673:U:H2'    | 51:9:1674:G:O4'   | 2.19                     | 0.43              |
| 51:9:1758:G:H2'    | 51:9:1759:G:O4'   | 2.18                     | 0.43              |
| 55:DD:70:THR:HG22  | 55:DD:86:LEU:HB2  | 2.01                     | 0.43              |
| 57:FF:140:ASP:OD2  | 80:cc:44:ARG:NH1  | 2.52                     | 0.43              |
| 61:JJ:24:ARG:O     | 61:JJ:27:GLN:HG3  | 2.19                     | 0.43              |
| 72:UU:115:THR:HG22 | 72:UU:116:ILE:N   | 2.34                     | 0.43              |
| 75:XX:88:ASP:OD1   | 82:ee:10:GLY:HA2  | 2.19                     | 0.43              |
| 77:ZZ:94:LYS:HD3   | 77:ZZ:96:LEU:HD13 | 2.00                     | 0.43              |
| 83:ff:101:TYR:HB3  | 83:ff:109:ILE:CG2 | 2.49                     | 0.43              |
| 86:ii:37:LEU:HD21  | 86:ii:39:ILE:HD11 | 2.01                     | 0.43              |
| 86:ii:309:LEU:HD21 | 86:ii:345:TYR:CZ  | 2.54                     | 0.43              |
| 87:jj:30:PRO:HD2   | 91:jj:601:SF4:S2  | 2.59                     | 0.43              |
| 87:jj:56:ILE:O     | 87:jj:56:ILE:CG2  | 2.67                     | 0.43              |
| 47:3:7:A:O2'       | 47:3:49:C:O4'     | 2.37                     | 0.43              |
| 47:3:31:A:H2'      | 47:3:32:C:C6      | 2.54                     | 0.43              |
| 48:5:1590:C:H5''   | 48:5:1591:U:O5'   | 2.19                     | 0.43              |
| 48:5:1760:G:C4     | 48:5:1761:G:C8    | 3.06                     | 0.43              |
| 48:5:2876:OMG:HM22 | 48:5:2877:G:O5'   | 2.19                     | 0.43              |
| 48:5:4524:G:OP2    | 48:5:4524:G:H4'   | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:8:84:A:N3       | 50:8:84:A:O5'      | 2.51                     | 0.43              |
| 51:9:217:A:H2      | 51:9:309:G:N2      | 2.15                     | 0.43              |
| 51:9:913:A:O3'     | 59:HH:67:PRO:HG3   | 2.19                     | 0.43              |
| 51:9:1280:G:C2     | 51:9:1281:G:C4     | 3.07                     | 0.43              |
| 51:9:1298:G:O2'    | 51:9:1299:A:P      | 2.76                     | 0.43              |
| 51:9:1834:A:H2     | 51:9:1837:G:H1     | 1.66                     | 0.43              |
| 53:BB:36:PRO:HB3   | 53:BB:231:LEU:HD23 | 2.00                     | 0.43              |
| 55:DD:65:ARG:O     | 55:DD:69:LEU:HG    | 2.19                     | 0.43              |
| 55:DD:210:ILE:HD12 | 55:DD:210:ILE:H    | 1.81                     | 0.43              |
| 56:EE:48:LEU:CD1   | 56:EE:61:VAL:HG23  | 2.49                     | 0.43              |
| 56:EE:149:TYR:N    | 56:EE:150:PRO:CD   | 2.82                     | 0.43              |
| 56:EE:189:LEU:HD23 | 56:EE:190:GLY:N    | 2.34                     | 0.43              |
| 61:JJ:163:SER:O    | 61:JJ:164:PRO:C    | 2.61                     | 0.43              |
| 67:PP:20:VAL:HG21  | 67:PP:28:MET:HE2   | 2.00                     | 0.43              |
| 67:PP:53:GLN:HB3   | 67:PP:83:MET:SD    | 2.58                     | 0.43              |
| 71:TT:33:TRP:CE3   | 71:TT:37:VAL:HG11  | 2.54                     | 0.43              |
| 75:XX:28:LYS:HE3   | 75:XX:32:LEU:HD13  | 2.00                     | 0.43              |
| 84:gg:289:LEU:HD13 | 84:gg:298:LEU:HD21 | 2.01                     | 0.43              |
| 87:jj:146:TYR:CD1  | 87:jj:146:TYR:C    | 2.97                     | 0.43              |
| 87:jj:257:ILE:HG12 | 87:jj:281:TYR:OH   | 2.19                     | 0.43              |
| 87:jj:322:LEU:HD13 | 87:jj:322:LEU:C    | 2.44                     | 0.43              |
| 2:B:288:GLY:HA3    | 2:B:330:PHE:CZ     | 2.54                     | 0.42              |
| 3:C:221:PHE:HB2    | 3:C:229:LEU:HD21   | 2.00                     | 0.42              |
| 5:E:245:ILE:HG22   | 5:E:246:THR:H      | 1.84                     | 0.42              |
| 12:M:90:ARG:NE     | 48:5:4868:G:H5''   | 2.34                     | 0.42              |
| 20:U:43:LEU:CB     | 20:U:63:LEU:HD21   | 2.48                     | 0.42              |
| 24:Y:43:ASN:OD1    | 24:Y:126:ARG:HD3   | 2.19                     | 0.42              |
| 41:p:9:GLY:C       | 48:5:1554:A:H5'    | 2.44                     | 0.42              |
| 43:s:72:ASN:OD1    | 43:s:193:PHE:HE2   | 2.01                     | 0.42              |
| 48:5:914:U:H1'     | 48:5:915:A:C4      | 2.54                     | 0.42              |
| 48:5:1440:U:C2'    | 48:5:1441:C:O5'    | 2.67                     | 0.42              |
| 48:5:1811:G:H2'    | 48:5:1812:C:C6     | 2.53                     | 0.42              |
| 48:5:1915:C:H5     | 92:5:6026:HOH:O    | 2.01                     | 0.42              |
| 48:5:2521:G:H5'    | 48:5:2640:G:H1'    | 2.01                     | 0.42              |
| 51:9:318:A:C2      | 51:9:333:G:C2      | 3.07                     | 0.42              |
| 51:9:440:G:OP1     | 51:9:1798:C:O2'    | 2.34                     | 0.42              |
| 51:9:441:C:H2'     | 51:9:442:C:C6      | 2.54                     | 0.42              |
| 51:9:1101:U:H2'    | 51:9:1102:G:C8     | 2.54                     | 0.42              |
| 52:AA:55:TRP:HZ3   | 52:AA:177:MET:SD   | 2.42                     | 0.42              |
| 52:AA:147:LEU:HB3  | 52:AA:163:CYS:SG   | 2.59                     | 0.42              |
| 54:CC:108:LYS:HD3  | 54:CC:109:ILE:N    | 2.34                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:GG:2:LYS:O      | 58:GG:108:VAL:HG13 | 2.19                     | 0.42              |
| 60:II:139:LYS:HG3  | 60:II:139:LYS:O    | 2.19                     | 0.42              |
| 61:JJ:82:VAL:HG11  | 61:JJ:92:MET:CG    | 2.49                     | 0.42              |
| 64:MM:110:VAL:CG1  | 64:MM:111:VAL:N    | 2.82                     | 0.42              |
| 66:OO:117:ARG:NH1  | 78:aa:49:ALA:HB2   | 2.34                     | 0.42              |
| 72:UU:29:VAL:HG22  | 72:UU:85:HIS:CE1   | 2.53                     | 0.42              |
| 72:UU:69:PRO:HB3   | 81:dd:41:GLN:HG2   | 2.01                     | 0.42              |
| 77:ZZ:84:ALA:O     | 77:ZZ:88:LEU:HG    | 2.18                     | 0.42              |
| 83:ff:136:CYS:HB3  | 83:ff:140:CYS:N    | 2.34                     | 0.42              |
| 84:gg:5:MET:HA     | 84:gg:311:GLN:O    | 2.18                     | 0.42              |
| 86:ii:202:VAL:HG13 | 86:ii:236:LEU:CD1  | 2.49                     | 0.42              |
| 87:jj:168:ILE:HG13 | 87:jj:168:ILE:O    | 2.18                     | 0.42              |
| 2:B:62:ARG:HG3     | 2:B:65:SER:HB3     | 2.02                     | 0.42              |
| 2:B:89:ILE:HG12    | 2:B:197:ALA:HB1    | 2.01                     | 0.42              |
| 3:C:50:GLN:OE1     | 48:5:347:A:O2'     | 2.29                     | 0.42              |
| 5:E:153:LEU:HD13   | 5:E:197:VAL:HG21   | 2.00                     | 0.42              |
| 15:P:102:ALA:CB    | 15:P:112:LEU:HD11  | 2.49                     | 0.42              |
| 17:R:32:ILE:O      | 17:R:35:ALA:HB3    | 2.17                     | 0.42              |
| 25:Z:68:ILE:HD13   | 25:Z:119:GLU:HG2   | 2.01                     | 0.42              |
| 40:o:70:LEU:HD11   | 40:o:83:LEU:HD23   | 2.02                     | 0.42              |
| 44:t:58:ILE:O      | 44:t:80:LEU:HD22   | 2.19                     | 0.42              |
| 45:1:57:ARG:CZ     | 48:5:3904:G:H4'    | 2.49                     | 0.42              |
| 48:5:125:C:H2'     | 48:5:126:C:H6      | 1.84                     | 0.42              |
| 48:5:700:G:C2'     | 48:5:701:G:O5'     | 2.67                     | 0.42              |
| 48:5:1201:U:C2'    | 48:5:1202:C:H5'    | 2.49                     | 0.42              |
| 48:5:1503:A:H4'    | 48:5:1504:G:H5'    | 2.01                     | 0.42              |
| 48:5:1759:G:C3'    | 48:5:1760:G:H5''   | 2.49                     | 0.42              |
| 48:5:2110:G:H2'    | 48:5:2111:U:H5'    | 2.00                     | 0.42              |
| 48:5:2336:G:H2'    | 48:5:2337:C:C6     | 2.54                     | 0.42              |
| 48:5:2557:G:H1     | 48:5:2570:U:H3     | 1.67                     | 0.42              |
| 48:5:4918:C:N4     | 48:5:4919:G:O6     | 2.52                     | 0.42              |
| 51:9:172:OMU:H6    | 51:9:315:C:O2'     | 2.19                     | 0.42              |
| 51:9:1068:G:N7     | 92:9:2026:HOH:O    | 2.36                     | 0.42              |
| 51:9:1279:C:H2'    | 51:9:1280:G:C1'    | 2.49                     | 0.42              |
| 51:9:1507:G:C5     | 83:ff:80:TYR:CE2   | 3.06                     | 0.42              |
| 51:9:1556:A:C2     | 51:9:1557:C:C5     | 3.07                     | 0.42              |
| 52:AA:90:PHE:CD1   | 52:AA:90:PHE:C     | 2.97                     | 0.42              |
| 53:BB:133:TYR:CE1  | 53:BB:221:PRO:HD2  | 2.54                     | 0.42              |
| 54:CC:74:LYS:HB3   | 54:CC:269:PHE:CD2  | 2.53                     | 0.42              |
| 55:DD:85:GLU:O     | 55:DD:86:LEU:HD12  | 2.19                     | 0.42              |
| 65:NN:92:ILE:HG22  | 65:NN:150:VAL:CG1  | 2.50                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 72:UU:55:ARG:HG3   | 72:UU:55:ARG:NH1   | 2.34                     | 0.42              |
| 75:XX:4:CYS:O      | 75:XX:5:ARG:HB3    | 2.18                     | 0.42              |
| 76:YY:62:THR:HB    | 76:YY:69:THR:HB    | 2.01                     | 0.42              |
| 86:ii:286:LEU:HD11 | 86:ii:321:ILE:CD1  | 2.50                     | 0.42              |
| 87:jj:182:GLY:O    | 87:jj:214:VAL:HG13 | 2.19                     | 0.42              |
| 87:jj:412:LYS:HA   | 87:jj:475:CYS:SG   | 2.59                     | 0.42              |
| 87:jj:567:ARG:NH2  | 87:jj:577:ILE:O    | 2.51                     | 0.42              |
| 1:A:39:GLY:HA2     | 1:A:93:LYS:HG3     | 2.00                     | 0.42              |
| 2:B:201:LEU:O      | 2:B:202:GLU:HB2    | 2.20                     | 0.42              |
| 8:H:5:LEU:HB2      | 8:H:60:TRP:CZ3     | 2.54                     | 0.42              |
| 13:N:14:LYS:HE2    | 48:5:280:G:H5'     | 2.01                     | 0.42              |
| 19:T:87:LYS:CE     | 48:5:4305:G:H1     | 2.32                     | 0.42              |
| 46:2:50:U:H2'      | 46:2:51:C:C6       | 2.54                     | 0.42              |
| 48:5:1332:C:H2'    | 48:5:1333:A:H8     | 1.85                     | 0.42              |
| 48:5:1786:A:O2'    | 48:5:1788:A:OP2    | 2.22                     | 0.42              |
| 48:5:4760:G:H2'    | 48:5:4761:G:O4'    | 2.19                     | 0.42              |
| 51:9:46:A:H4'      | 51:9:47:G:C5'      | 2.49                     | 0.42              |
| 51:9:50:A:N1       | 51:9:488:U:H5      | 2.17                     | 0.42              |
| 51:9:302:A:H2'     | 51:9:303:C:O4'     | 2.19                     | 0.42              |
| 51:9:305:U:C6      | 60:II:182:CYS:O    | 2.71                     | 0.42              |
| 51:9:933:G:N7      | 51:9:992:A:N1      | 2.67                     | 0.42              |
| 51:9:1336:C:H2'    | 51:9:1337:4AC:O4'  | 2.19                     | 0.42              |
| 51:9:1422:G:N1     | 51:9:1425:G:OP2    | 2.53                     | 0.42              |
| 51:9:1745:A:H2'    | 51:9:1746:U:O4'    | 2.20                     | 0.42              |
| 51:9:1810:U:H2'    | 51:9:1811:C:O4'    | 2.18                     | 0.42              |
| 52:AA:113:GLN:O    | 52:AA:116:PHE:N    | 2.52                     | 0.42              |
| 57:FF:126:THR:HB   | 57:FF:139:VAL:HG21 | 2.01                     | 0.42              |
| 59:HH:45:ILE:HD11  | 59:HH:62:ILE:HG23  | 2.01                     | 0.42              |
| 62:KK:14:LEU:HA    | 62:KK:17:LYS:HZ2   | 1.85                     | 0.42              |
| 64:MM:64:LEU:O     | 64:MM:67:ALA:HB3   | 2.18                     | 0.42              |
| 73:VV:24:ILE:O     | 73:VV:24:ILE:HG22  | 2.18                     | 0.42              |
| 86:ii:237:SER:OG   | 86:ii:238:GLN:N    | 2.51                     | 0.42              |
| 4:D:60:ILE:HB      | 4:D:80:ALA:HB2     | 2.01                     | 0.42              |
| 6:F:127:ALA:O      | 6:F:131:MET:HG3    | 2.18                     | 0.42              |
| 10:J:85:LYS:O      | 10:J:89:VAL:HG23   | 2.19                     | 0.42              |
| 10:J:89:VAL:HG21   | 10:J:115:LEU:HD23  | 2.01                     | 0.42              |
| 17:R:118:HIS:ND1   | 48:5:2663:G:OP1    | 2.52                     | 0.42              |
| 46:2:13:U:O4       | 46:2:22:U:O4       | 2.38                     | 0.42              |
| 48:5:282:C:H2'     | 48:5:283:G:O4'     | 2.19                     | 0.42              |
| 48:5:370:U:H2'     | 48:5:371:A:O4'     | 2.19                     | 0.42              |
| 48:5:1450:C:O2'    | 48:5:2104:A:H1'    | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:1578:U:H2'    | 48:5:1579:C:C6     | 2.54                     | 0.42              |
| 48:5:2030:A:H2'    | 48:5:2031:C:O4'    | 2.19                     | 0.42              |
| 48:5:2871:A:H2'    | 48:5:2872:C:O4'    | 2.20                     | 0.42              |
| 48:5:4254:G:H22    | 48:5:4257:A:H8     | 1.67                     | 0.42              |
| 48:5:4489:G:C6     | 48:5:4708:A:C5     | 3.07                     | 0.42              |
| 51:9:407:G:H5''    | 51:9:408:A:H5'     | 2.01                     | 0.42              |
| 51:9:1047:C:H2'    | 51:9:1048:G:O4'    | 2.20                     | 0.42              |
| 51:9:1280:G:C6     | 51:9:1281:G:C6     | 3.07                     | 0.42              |
| 51:9:1288:U:O4     | 51:9:1311:C:N3     | 2.52                     | 0.42              |
| 51:9:1399:C:H4'    | 84:gg:100:ARG:NH2  | 2.33                     | 0.42              |
| 54:CC:270:THR:HG23 | 54:CC:271:ASP:N    | 2.34                     | 0.42              |
| 55:DD:16:ILE:HG21  | 81:dd:22:ARG:NH1   | 2.34                     | 0.42              |
| 59:HH:91:HIS:CB    | 59:HH:172:THR:HG21 | 2.49                     | 0.42              |
| 67:PP:115:TYR:HB2  | 67:PP:118:GLU:HG3  | 2.01                     | 0.42              |
| 69:RR:85:VAL:HG22  | 69:RR:86:PRO:HD2   | 2.01                     | 0.42              |
| 71:TT:28:LEU:HB3   | 71:TT:54:TYR:HE1   | 1.84                     | 0.42              |
| 83:ff:127:MET:CE   | 83:ff:136:CYS:HB2  | 2.49                     | 0.42              |
| 86:ii:302:CYS:SG   | 86:ii:413:LEU:HD21 | 2.60                     | 0.42              |
| 86:ii:354:LYS:HD2  | 86:ii:357:PHE:CE2  | 2.55                     | 0.42              |
| 4:D:215:ASP:OD1    | 4:D:215:ASP:N      | 2.50                     | 0.42              |
| 10:J:54:ARG:NH2    | 10:J:55:TYR:OH     | 2.53                     | 0.42              |
| 10:J:103:GLY:HA3   | 10:J:157:ILE:HG22  | 2.01                     | 0.42              |
| 14:O:61:ARG:HA     | 14:O:70:PRO:HD2    | 2.01                     | 0.42              |
| 16:Q:177:ALA:O     | 26:a:51:GLY:HA2    | 2.19                     | 0.42              |
| 20:U:49:VAL:O      | 20:U:52:LYS:HG2    | 2.19                     | 0.42              |
| 44:t:57:ARG:NE     | 44:t:83:LYS:HE3    | 2.34                     | 0.42              |
| 47:3:71:G:H4'      | 48:5:3739:C:O2     | 2.19                     | 0.42              |
| 48:5:1543:G:O2'    | 48:5:2513:A:N3     | 2.51                     | 0.42              |
| 48:5:1757:U:C2     | 48:5:1758:G:C8     | 3.07                     | 0.42              |
| 48:5:1857:C:H2'    | 48:5:1858:A:C8     | 2.54                     | 0.42              |
| 48:5:1981:G:C4     | 48:5:1982:G:O4'    | 2.73                     | 0.42              |
| 48:5:2046:G:C2'    | 48:5:2047:A:OP2    | 2.66                     | 0.42              |
| 48:5:4736:C:H2'    | 48:5:4737:G:H8     | 1.85                     | 0.42              |
| 50:8:81:C:OP1      | 50:8:82:A:OP2      | 2.37                     | 0.42              |
| 51:9:145:G:H2'     | 51:9:146:G:C8      | 2.54                     | 0.42              |
| 51:9:157:U:H1'     | 58:GG:60:GLY:HA3   | 2.00                     | 0.42              |
| 51:9:328:U:H2'     | 51:9:329:G:O4'     | 2.19                     | 0.42              |
| 51:9:546:G:HO2'    | 51:9:547:G:C4'     | 2.33                     | 0.42              |
| 51:9:682:U:H5'     | 51:9:1160:U:OP1    | 2.20                     | 0.42              |
| 51:9:688:U:O2      | 51:9:688:U:P       | 2.78                     | 0.42              |
| 51:9:1279:C:H2'    | 51:9:1280:G:C8     | 2.54                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:1444:U:H2'    | 51:9:1445:PSU:O4'  | 2.20                     | 0.42              |
| 55:DD:74:GLN:HA    | 55:DD:79:PHE:HB2   | 2.01                     | 0.42              |
| 55:DD:95:GLY:O     | 55:DD:126:ILE:HG12 | 2.19                     | 0.42              |
| 56:EE:157:ASN:OD1  | 56:EE:222:LEU:HD21 | 2.20                     | 0.42              |
| 60:II:85:ALA:O     | 63:LL:8:ARG:HD2    | 2.20                     | 0.42              |
| 68:QQ:108:ILE:O    | 68:QQ:112:LEU:HG   | 2.19                     | 0.42              |
| 69:RR:40:ILE:O     | 69:RR:40:ILE:CG1   | 2.67                     | 0.42              |
| 70:SS:38:ARG:HB3   | 71:TT:45:LEU:HD21  | 2.00                     | 0.42              |
| 84:gg:252:THR:HG23 | 84:gg:255:SER:O    | 2.18                     | 0.42              |
| 86:ii:333:LEU:HB2  | 86:ii:342:LYS:HB3  | 2.00                     | 0.42              |
| 86:ii:363:GLY:O    | 86:ii:364:GLN:C    | 2.62                     | 0.42              |
| 87:jj:119:ALA:O    | 87:jj:123:LEU:HG   | 2.19                     | 0.42              |
| 87:jj:376:VAL:HG21 | 87:jj:529:ALA:HB2  | 2.02                     | 0.42              |
| 7:G:230:TYR:HA     | 7:G:233:ILE:HD12   | 2.01                     | 0.42              |
| 12:M:50:MET:HG3    | 12:M:54:CYS:SG     | 2.59                     | 0.42              |
| 14:O:121:PRO:HD3   | 18:S:168:THR:HG22  | 2.01                     | 0.42              |
| 20:U:27:HIS:N      | 20:U:28:PRO:HD2    | 2.34                     | 0.42              |
| 31:f:49:TYR:HD2    | 31:f:70:ILE:HD12   | 1.84                     | 0.42              |
| 34:i:55:ARG:HA     | 34:i:58:MET:HE3    | 2.02                     | 0.42              |
| 37:l:27:ILE:HG13   | 50:8:52:A:N6       | 2.35                     | 0.42              |
| 46:2:49:C:O2'      | 46:2:50:U:H5'      | 2.19                     | 0.42              |
| 48:5:644:G:H2'     | 48:5:645:G:C8      | 2.54                     | 0.42              |
| 48:5:1824:G:H2'    | 48:5:1825:A:O4'    | 2.19                     | 0.42              |
| 48:5:2364:OMG:OP2  | 92:5:5429:HOH:O    | 2.22                     | 0.42              |
| 48:5:2886:U:H2'    | 48:5:2887:U:C6     | 2.54                     | 0.42              |
| 48:5:3783:A:OP2    | 48:5:3808:OMC:N4   | 2.37                     | 0.42              |
| 48:5:4761:G:N2     | 48:5:4766:C:O3'    | 2.52                     | 0.42              |
| 51:9:44:U:O2       | 51:9:482:G:H1'     | 2.20                     | 0.42              |
| 51:9:501:C:O2      | 51:9:501:C:H2'     | 2.19                     | 0.42              |
| 51:9:827:A:OP1     | 61:JJ:10:ARG:HD2   | 2.19                     | 0.42              |
| 51:9:1232:PSU:H2'  | 51:9:1233:G:C8     | 2.54                     | 0.42              |
| 51:9:1520:G:N3     | 51:9:1520:G:H2'    | 2.35                     | 0.42              |
| 54:CC:148:ALA:O    | 54:CC:152:ARG:HG2  | 2.19                     | 0.42              |
| 55:DD:193:ASP:OD1  | 55:DD:203:PRO:HA   | 2.20                     | 0.42              |
| 55:DD:195:SER:OG   | 55:DD:196:GLY:N    | 2.53                     | 0.42              |
| 56:EE:159:THR:HG23 | 56:EE:173:ILE:HB   | 2.00                     | 0.42              |
| 56:EE:183:VAL:HG21 | 56:EE:220:THR:HG21 | 2.02                     | 0.42              |
| 60:II:11:ARG:NH1   | 60:II:15:GLY:O     | 2.50                     | 0.42              |
| 61:JJ:78:LEU:HD23  | 61:JJ:97:ILE:HD11  | 2.00                     | 0.42              |
| 66:OO:72:TYR:HD1   | 66:OO:75:MET:HE3   | 1.83                     | 0.42              |
| 76:YY:96:LEU:N     | 76:YY:96:LEU:HD23  | 2.34                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 77:ZZ:51:ASP:OD2   | 77:ZZ:54:THR:OG1   | 2.37                     | 0.42              |
| 79:bb:35:VAL:O     | 79:bb:43:ILE:HD12  | 2.19                     | 0.42              |
| 87:jj:420:SER:O    | 87:jj:459:VAL:HG11 | 2.20                     | 0.42              |
| 4:D:123:VAL:HG22   | 4:D:248:ARG:NH1    | 2.34                     | 0.42              |
| 10:J:96:LYS:HG2    | 10:J:163:MET:SD    | 2.60                     | 0.42              |
| 14:O:110:PRO:N     | 14:O:111:PRO:CD    | 2.83                     | 0.42              |
| 14:O:175:MET:HE1   | 14:O:179:LYS:HE2   | 2.00                     | 0.42              |
| 14:O:202:LEU:HD23  | 14:O:202:LEU:HA    | 1.90                     | 0.42              |
| 19:T:83:LYS:NZ     | 48:5:4305:G:O5'    | 2.53                     | 0.42              |
| 22:W:25:ASP:OD1    | 22:W:26:GLY:N      | 2.53                     | 0.42              |
| 28:c:65:MET:HE2    | 28:c:65:MET:HB3    | 1.97                     | 0.42              |
| 37:l:46:ARG:HH12   | 48:5:2796:G:P      | 2.42                     | 0.42              |
| 43:s:57:LYS:HD3    | 48:5:2020:U:H5''   | 2.01                     | 0.42              |
| 43:s:78:LEU:HD11   | 43:s:193:PHE:CB    | 2.49                     | 0.42              |
| 46:2:19:G:C5       | 46:2:57:G:N2       | 2.88                     | 0.42              |
| 48:5:115:C:O2      | 48:5:115:C:O4'     | 2.37                     | 0.42              |
| 48:5:120:A:H2'     | 48:5:149:A:N6      | 2.34                     | 0.42              |
| 48:5:1406(B):C:H2' | 48:5:1406(C):G:O4' | 2.19                     | 0.42              |
| 48:5:1406(C):G:C2  | 48:5:1411(A):G:C2  | 3.08                     | 0.42              |
| 48:5:1763:C:N3     | 48:5:1770:A:N1     | 2.66                     | 0.42              |
| 48:5:1857:C:H2'    | 48:5:1858:A:H8     | 1.85                     | 0.42              |
| 50:8:64:U:C2       | 50:8:65:A:C8       | 3.07                     | 0.42              |
| 51:9:103:A:C2      | 51:9:105:PSU:O2    | 2.72                     | 0.42              |
| 51:9:369:C:O2      | 51:9:369:C:O4'     | 2.36                     | 0.42              |
| 51:9:662:G:H4'     | 51:9:663:C:OP1     | 2.20                     | 0.42              |
| 51:9:963:A:H2'     | 51:9:964:A:C8      | 2.54                     | 0.42              |
| 51:9:1229:G:H2'    | 51:9:1230:C:O4'    | 2.20                     | 0.42              |
| 51:9:1280:G:N1     | 51:9:1281:G:C5     | 2.88                     | 0.42              |
| 52:AA:38:ILE:HD12  | 52:AA:38:ILE:C     | 2.45                     | 0.42              |
| 62:KK:17:LYS:NZ    | 62:KK:18:GLU:OE1   | 2.51                     | 0.42              |
| 71:TT:28:LEU:HD23  | 71:TT:53:PHE:HD2   | 1.84                     | 0.42              |
| 73:VV:39:VAL:HA    | 73:VV:45:ARG:O     | 2.19                     | 0.42              |
| 80:cc:12:ALA:HB3   | 80:cc:58:LEU:HD21  | 2.01                     | 0.42              |
| 84:gg:78:ALA:HB3   | 84:gg:92:LEU:HD11  | 2.02                     | 0.42              |
| 86:ii:372:MET:CE   | 86:ii:377:TRP:HB2  | 2.50                     | 0.42              |
| 86:ii:378:PHE:HB3  | 86:ii:389:LEU:CD1  | 2.50                     | 0.42              |
| 87:jj:478:LYS:HE3  | 87:jj:478:LYS:HB3  | 1.95                     | 0.42              |
| 2:B:223:THR:O      | 2:B:274:TYR:HA     | 2.19                     | 0.42              |
| 2:B:241:PRO:HD3    | 48:5:4456:OMC:HM21 | 2.02                     | 0.42              |
| 3:C:115:VAL:O      | 3:C:120:LYS:HE2    | 2.19                     | 0.42              |
| 6:F:91:VAL:O       | 6:F:119:GLY:HA2    | 2.20                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:L:102:ARG:HA   | 48:5:75:G:C5       | 2.54                     | 0.42              |
| 13:N:37:HIS:CE1   | 13:N:63:ARG:NH1    | 2.87                     | 0.42              |
| 22:W:55:TYR:CD1   | 22:W:55:TYR:C      | 2.97                     | 0.42              |
| 44:t:15:LEU:HD12  | 44:t:16:ARG:N      | 2.35                     | 0.42              |
| 44:t:27:ALA:C     | 44:t:30:PRO:HD2    | 2.45                     | 0.42              |
| 46:2:21:A:H2'     | 46:2:46:G:O6       | 2.20                     | 0.42              |
| 47:3:35:U:C5      | 47:3:36:U:C5       | 3.08                     | 0.42              |
| 48:5:684:G:H5''   | 48:5:685:C:OP2     | 2.20                     | 0.42              |
| 48:5:924:C:HO2'   | 48:5:925:C:P       | 2.41                     | 0.42              |
| 48:5:1211:G:C2'   | 48:5:1212:G:O5'    | 2.67                     | 0.42              |
| 48:5:1882:U:C4    | 48:5:2279:A:C2     | 3.08                     | 0.42              |
| 48:5:1929:A:H5'   | 48:5:1930:U:OP1    | 2.19                     | 0.42              |
| 48:5:1964:A:C2    | 48:5:1965:G:H1'    | 2.55                     | 0.42              |
| 48:5:1980:U:H2'   | 48:5:1982:G:C5'    | 2.50                     | 0.42              |
| 48:5:2001:G:O6    | 48:5:2003:G:N2     | 2.53                     | 0.42              |
| 48:5:3816:A:OP1   | 48:5:3818:UY1:N1   | 2.53                     | 0.42              |
| 48:5:3911:C:H4'   | 48:5:4196:OMG:HM22 | 2.01                     | 0.42              |
| 48:5:4512:U:H4'   | 48:5:4513:A:OP1    | 2.19                     | 0.42              |
| 51:9:64:A:C2      | 51:9:83:A:N7       | 2.88                     | 0.42              |
| 51:9:881:G:OP2    | 51:9:881:G:H8      | 2.02                     | 0.42              |
| 51:9:883:U:C4     | 51:9:884:C:C5      | 3.07                     | 0.42              |
| 51:9:959:G:OP1    | 66:OO:104:ARG:NH2  | 2.52                     | 0.42              |
| 51:9:1228:A:H2'   | 51:9:1229:G:H8     | 1.81                     | 0.42              |
| 51:9:1231:C:H2'   | 51:9:1232:PSU:O4'  | 2.20                     | 0.42              |
| 51:9:1426:U:H2'   | 51:9:1427:C:O4'    | 2.19                     | 0.42              |
| 51:9:1834:A:N3    | 51:9:1834:A:C2'    | 2.83                     | 0.42              |
| 55:DD:159:HIS:O   | 55:DD:164:VAL:HG11 | 2.20                     | 0.42              |
| 56:EE:180:LEU:CD1 | 56:EE:192:ILE:HG22 | 2.50                     | 0.42              |
| 57:FF:165:ASN:OD1 | 57:FF:167:LYS:N    | 2.47                     | 0.42              |
| 62:KK:58:VAL:HA   | 62:KK:70:TYR:O     | 2.19                     | 0.42              |
| 72:UU:35:VAL:HA   | 72:UU:38:ASP:OD2   | 2.20                     | 0.42              |
| 84:gg:106:LYS:HG3 | 84:gg:126:ASP:HB3  | 2.02                     | 0.42              |
| 3:C:182:LYS:NZ    | 48:5:2299:G:OP1    | 2.44                     | 0.42              |
| 4:D:160:PHE:CE2   | 4:D:179:ARG:HB3    | 2.55                     | 0.42              |
| 5:E:277:VAL:HG11  | 31:f:2:SER:HB2     | 2.02                     | 0.42              |
| 7:G:53:ARG:NH1    | 48:5:4163:U:OP2    | 2.44                     | 0.42              |
| 7:G:90:GLN:HG3    | 7:G:91:THR:N       | 2.34                     | 0.42              |
| 9:I:53:VAL:HG11   | 19:T:158:PHE:CZ    | 2.55                     | 0.42              |
| 9:I:184:MET:O     | 9:I:187:GLU:O      | 2.37                     | 0.42              |
| 11:L:39:ARG:HD2   | 48:5:1363:C:OP1    | 2.19                     | 0.42              |
| 20:U:37:ALA:HA    | 20:U:65:ARG:HD3    | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:X:81:LEU:HG     | 23:X:83:THR:HG23   | 2.02                     | 0.42              |
| 28:c:83:THR:O      | 65:NN:151:ALA:O    | 2.37                     | 0.42              |
| 42:r:80:THR:CG2    | 42:r:96:MET:HE1    | 2.49                     | 0.42              |
| 46:2:11:U:H2'      | 46:2:12:G:C8       | 2.55                     | 0.42              |
| 48:5:968:C:O2'     | 48:5:969:C:O5'     | 2.35                     | 0.42              |
| 48:5:1978:C:N4     | 48:5:1979:A:N1     | 2.67                     | 0.42              |
| 48:5:2416:G:N2     | 48:5:2427:G:N7     | 2.63                     | 0.42              |
| 48:5:2639:U:H2'    | 48:5:2694:G:N1     | 2.32                     | 0.42              |
| 48:5:4303:C:O2     | 48:5:4303:C:O5'    | 2.38                     | 0.42              |
| 48:5:4916:G:H2'    | 48:5:4917:C:O5'    | 2.20                     | 0.42              |
| 51:9:71:G:C2       | 51:9:72:C:C6       | 3.08                     | 0.42              |
| 51:9:152:U:H3      | 51:9:166:A2M:H62   | 1.67                     | 0.42              |
| 51:9:464:A:H4'     | 51:9:465:A:OP2     | 2.20                     | 0.42              |
| 51:9:878:G:C2      | 51:9:909:G:C2      | 3.07                     | 0.42              |
| 51:9:1109:C:O2'    | 51:9:1110:G:H8     | 2.02                     | 0.42              |
| 51:9:1823:A:H2'    | 51:9:1824:A:H5'    | 2.02                     | 0.42              |
| 51:9:1825:A:N6     | 86:ii:127:CYS:O    | 2.52                     | 0.42              |
| 51:9:1834:A:H2     | 51:9:1837:G:N2     | 2.17                     | 0.42              |
| 52:AA:2:SER:O      | 52:AA:4:ALA:N      | 2.52                     | 0.42              |
| 53:BB:97:LEU:HD12  | 53:BB:232:HIS:CG   | 2.55                     | 0.42              |
| 55:DD:66:ILE:O     | 55:DD:70:THR:HG23  | 2.19                     | 0.42              |
| 55:DD:223:ILE:HG22 | 55:DD:224:SER:N    | 2.35                     | 0.42              |
| 56:EE:111:VAL:O    | 56:EE:111:VAL:CG2  | 2.68                     | 0.42              |
| 59:HH:157:HIS:CD2  | 59:HH:157:HIS:N    | 2.88                     | 0.42              |
| 66:OO:80:ASP:OD1   | 66:OO:80:ASP:C     | 2.63                     | 0.42              |
| 70:SS:132:ARG:HB2  | 70:SS:134:GLN:OE1  | 2.20                     | 0.42              |
| 71:TT:14:PHE:CE2   | 71:TT:131:LEU:HD13 | 2.55                     | 0.42              |
| 75:XX:86:PRO:O     | 75:XX:87:ASN:CB    | 2.67                     | 0.42              |
| 80:cc:67:ARG:CG    | 80:cc:67:ARG:HH11  | 2.33                     | 0.42              |
| 83:ff:79:SER:O     | 83:ff:80:TYR:CD1   | 2.73                     | 0.42              |
| 84:gg:8:ARG:HB2    | 84:gg:309:VAL:HG13 | 2.01                     | 0.42              |
| 84:gg:44:LYS:HD3   | 84:gg:56:GLN:CG    | 2.49                     | 0.42              |
| 84:gg:48:ASP:O     | 84:gg:51:ASN:N     | 2.52                     | 0.42              |
| 84:gg:87:LEU:HB2   | 84:gg:101:PHE:CD1  | 2.54                     | 0.42              |
| 87:jj:507:PHE:CD2  | 87:jj:507:PHE:C    | 2.98                     | 0.42              |
| 1:A:233:ARG:HB2    | 48:5:4184:G:H5'    | 2.02                     | 0.42              |
| 4:D:205:ALA:O      | 4:D:209:ARG:HG3    | 2.20                     | 0.42              |
| 7:G:214:ALA:HA     | 7:G:217:LYS:HE3    | 2.02                     | 0.42              |
| 7:G:230:TYR:CE2    | 7:G:234:ARG:HD3    | 2.55                     | 0.42              |
| 9:I:54:SER:HB2     | 9:I:135:ILE:HD11   | 2.00                     | 0.42              |
| 14:O:62:MET:HA     | 48:5:2045:G:C6     | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:U:29:VAL:C     | 20:U:32:GLY:H     | 2.28                     | 0.42              |
| 20:U:64:GLU:O     | 20:U:70:ILE:HA    | 2.20                     | 0.42              |
| 26:a:117:LEU:HB3  | 26:a:140:VAL:HG11 | 2.01                     | 0.42              |
| 43:s:35:VAL:O     | 43:s:35:VAL:HG13  | 2.19                     | 0.42              |
| 44:t:17:CYS:SG    | 48:5:1975:G:C6    | 3.11                     | 0.42              |
| 44:t:27:ALA:O     | 44:t:31:LYS:HE2   | 2.20                     | 0.42              |
| 46:2:19:G:H3'     | 46:2:20:U:H5'     | 2.02                     | 0.42              |
| 47:3:32:C:O2'     | 47:3:33:U:H5'     | 2.20                     | 0.42              |
| 48:5:223:G:H4'    | 48:5:225:G:N7     | 2.35                     | 0.42              |
| 48:5:1208:G:O2'   | 48:5:1209:U:O5'   | 2.38                     | 0.42              |
| 48:5:1468:C:H2'   | 48:5:1469:C:C6    | 2.55                     | 0.42              |
| 48:5:1804:A:H4'   | 48:5:1805:A:O5'   | 2.20                     | 0.42              |
| 48:5:2006:U:H2'   | 48:5:2007:G:H5'   | 2.02                     | 0.42              |
| 48:5:2602:G:H2'   | 48:5:2603:C:C6    | 2.55                     | 0.42              |
| 48:5:2882:A:OP1   | 48:5:3625:G:N1    | 2.43                     | 0.42              |
| 48:5:4119:C:H4'   | 48:5:4120:U:OP1   | 2.19                     | 0.42              |
| 51:9:182:C:O4'    | 51:9:183:G:C2     | 2.73                     | 0.42              |
| 51:9:191:A:H62    | 51:9:208:G:H21    | 1.68                     | 0.42              |
| 51:9:407:G:H5''   | 51:9:408:A:C5'    | 2.50                     | 0.42              |
| 51:9:1138:C:OP1   | 52:AA:155:ARG:CZ  | 2.68                     | 0.42              |
| 51:9:1386:A:H2'   | 51:9:1387:G:O4'   | 2.18                     | 0.42              |
| 51:9:1568:C:OP1   | 71:TT:96:SER:OG   | 2.36                     | 0.42              |
| 56:EE:192:ILE:HB  | 56:EE:242:LYS:O   | 2.20                     | 0.42              |
| 64:MM:33:ARG:O    | 64:MM:33:ARG:HD2  | 2.20                     | 0.42              |
| 67:PP:111:MET:O   | 67:PP:112:ILE:C   | 2.63                     | 0.42              |
| 71:TT:42:HIS:HB2  | 71:TT:83:GLN:HA   | 2.02                     | 0.42              |
| 71:TT:51:ASN:ND2  | 71:TT:54:TYR:CD2  | 2.88                     | 0.42              |
| 76:YY:79:LEU:HD12 | 76:YY:79:LEU:O    | 2.19                     | 0.42              |
| 86:ii:335:CYS:HB3 | 86:ii:340:GLU:HB3 | 2.01                     | 0.42              |
| 4:D:261:VAL:O     | 4:D:262:LYS:C     | 2.62                     | 0.41              |
| 6:F:28:LYS:NZ     | 48:5:965:G:N7     | 2.55                     | 0.41              |
| 6:F:154:TYR:CE1   | 6:F:186:MET:HG2   | 2.55                     | 0.41              |
| 8:H:118:LEU:CD1   | 8:H:167:VAL:HG22  | 2.50                     | 0.41              |
| 9:I:61:SER:HA     | 9:I:126:VAL:HG12  | 2.01                     | 0.41              |
| 11:L:59:VAL:HB    | 48:5:74:G:C5'     | 2.50                     | 0.41              |
| 18:S:69:GLU:HG2   | 18:S:101:THR:HG22 | 2.01                     | 0.41              |
| 24:Y:89:LYS:HD2   | 24:Y:95:VAL:HG11  | 2.01                     | 0.41              |
| 33:h:85:PRO:O     | 50:8:38:U:H5      | 2.03                     | 0.41              |
| 42:r:46:ARG:NH2   | 42:r:67:ARG:HG2   | 2.35                     | 0.41              |
| 43:s:55:MET:CE    | 48:5:1998:A:O4'   | 2.68                     | 0.41              |
| 43:s:57:LYS:O     | 43:s:57:LYS:CD    | 2.69                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:119:G:H3'     | 48:5:120:A:C5'     | 2.49                     | 0.41              |
| 48:5:982:U:H3      | 48:5:1273:G:H1     | 1.68                     | 0.41              |
| 48:5:1169:G:O2'    | 48:5:1170:G:H5'    | 2.20                     | 0.41              |
| 48:5:1199:G:C4     | 48:5:1200:G:N7     | 2.88                     | 0.41              |
| 48:5:1201:U:O2'    | 48:5:1202:C:H5'    | 2.20                     | 0.41              |
| 48:5:1481:C:C2'    | 48:5:1482:G:O5'    | 2.68                     | 0.41              |
| 48:5:1567:U:H2'    | 48:5:1568:C:C6     | 2.55                     | 0.41              |
| 48:5:2046:G:H1'    | 48:5:2047:A:OP2    | 2.20                     | 0.41              |
| 48:5:2424:OMG:H2'  | 48:5:2426:U:C5     | 2.54                     | 0.41              |
| 48:5:4114:C:C2'    | 48:5:4115:G:O4'    | 2.68                     | 0.41              |
| 48:5:4776:G:C2     | 48:5:4860:G:C5     | 3.08                     | 0.41              |
| 48:5:4884:G:O2'    | 48:5:4885:U:O5'    | 2.37                     | 0.41              |
| 51:9:25:A:O2'      | 51:9:26:U:O4'      | 2.38                     | 0.41              |
| 51:9:191:A:H3'     | 51:9:192:C:H5''    | 2.01                     | 0.41              |
| 51:9:197:U:C6      | 51:9:197:U:OP2     | 2.73                     | 0.41              |
| 51:9:199:C:C2      | 51:9:200:G:C8      | 3.08                     | 0.41              |
| 51:9:1265:A:H2     | 51:9:1517:G:H22    | 1.66                     | 0.41              |
| 51:9:1306:U:H2'    | 51:9:1307:U:O5'    | 2.20                     | 0.41              |
| 51:9:1398:G:O2'    | 84:gg:88:ARG:NH2   | 2.53                     | 0.41              |
| 51:9:1419:C:O2'    | 71:TT:132:ASP:OD2  | 2.37                     | 0.41              |
| 51:9:1850:MA6:H8   | 51:9:1850:MA6:O5'  | 2.19                     | 0.41              |
| 56:EE:130:PHE:HB3  | 56:EE:138:HIS:HB2  | 2.02                     | 0.41              |
| 57:FF:99:ILE:CG1   | 77:ZZ:108:ILE:HD11 | 2.50                     | 0.41              |
| 57:FF:204:ARG:HD2  | 66:OO:72:TYR:OH    | 2.20                     | 0.41              |
| 58:GG:7:PHE:HD1    | 58:GG:10:THR:HG1   | 1.66                     | 0.41              |
| 66:OO:46:ASP:CG    | 66:OO:51:GLU:HB2   | 2.45                     | 0.41              |
| 68:QQ:58:LEU:HD21  | 68:QQ:112:LEU:HD21 | 2.02                     | 0.41              |
| 75:XX:56:GLY:CA    | 82:ee:6:LEU:HD21   | 2.50                     | 0.41              |
| 80:cc:42:ILE:CD1   | 80:cc:64:GLU:HB2   | 2.50                     | 0.41              |
| 80:cc:66:ARG:O     | 80:cc:67:ARG:HG3   | 2.20                     | 0.41              |
| 84:gg:78:ALA:O     | 84:gg:89:LEU:HD23  | 2.20                     | 0.41              |
| 84:gg:270:LEU:HD13 | 84:gg:310:TRP:CG   | 2.55                     | 0.41              |
| 87:jj:109:VAL:HB   | 87:jj:279:LEU:HD21 | 2.01                     | 0.41              |
| 87:jj:292:VAL:O    | 87:jj:292:VAL:CG2  | 2.67                     | 0.41              |
| 9:I:98:ARG:HD2     | 9:I:120:GLY:O      | 2.20                     | 0.41              |
| 10:J:15:LEU:CD2    | 10:J:157:ILE:HD13  | 2.50                     | 0.41              |
| 44:t:15:LEU:CB     | 44:t:62:LEU:HD12   | 2.50                     | 0.41              |
| 46:2:51:C:H2'      | 46:2:52:G:O4'      | 2.20                     | 0.41              |
| 48:5:245:C:O2'     | 48:5:246:G:P       | 2.76                     | 0.41              |
| 48:5:449:C:OP1     | 48:5:449:C:C4'     | 2.67                     | 0.41              |
| 48:5:1208:G:C2'    | 48:5:1209:U:O5'    | 2.68                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:1479:G:O2'    | 48:5:1480:C:H5'    | 2.19                     | 0.41              |
| 48:5:1510:G:H2'    | 48:5:1511:U:C6     | 2.55                     | 0.41              |
| 48:5:1808:C:H2'    | 48:5:1809:C:H6     | 1.84                     | 0.41              |
| 48:5:1940:G:O4'    | 48:5:1940:G:OP2    | 2.38                     | 0.41              |
| 48:5:1942:A:N3     | 48:5:4432:C:O2'    | 2.45                     | 0.41              |
| 48:5:2008:U:O2     | 48:5:2008:U:O4'    | 2.37                     | 0.41              |
| 48:5:2489:C:OP1    | 48:5:2490:U:C5     | 2.74                     | 0.41              |
| 48:5:2539:C:H2'    | 48:5:2540:C:C6     | 2.54                     | 0.41              |
| 48:5:3684:G:H2'    | 48:5:3685:C:C6     | 2.55                     | 0.41              |
| 48:5:4891:G:H1     | 48:5:4928:C:H5     | 1.67                     | 0.41              |
| 48:5:4908:G:N3     | 48:5:4913:G:O4'    | 2.53                     | 0.41              |
| 50:8:83:C:C5'      | 50:8:85:U:O2       | 2.68                     | 0.41              |
| 50:8:103:A:H3'     | 50:8:104:A:H5''    | 2.03                     | 0.41              |
| 51:9:70:G:C2       | 51:9:80:G:C6       | 3.09                     | 0.41              |
| 51:9:305:U:O2'     | 51:9:309:G:H1'     | 2.20                     | 0.41              |
| 51:9:407:G:C8      | 51:9:407:G:O5'     | 2.73                     | 0.41              |
| 51:9:1115:U:O2'    | 51:9:1116:C:N3     | 2.53                     | 0.41              |
| 51:9:1411:G:O3'    | 51:9:1412:C:H4'    | 2.19                     | 0.41              |
| 51:9:1454:A:O4'    | 69:RR:3:ARG:HD3    | 2.20                     | 0.41              |
| 51:9:1691:U:H2'    | 51:9:1692:PSU:O4'  | 2.20                     | 0.41              |
| 51:9:1693:G:N2     | 51:9:1834:A:H8     | 2.18                     | 0.41              |
| 55:DD:26:THR:HA    | 55:DD:34:TYR:CD2   | 2.55                     | 0.41              |
| 56:EE:153:LEU:HD11 | 58:GG:216:ARG:NH1  | 2.34                     | 0.41              |
| 66:OO:84:ARG:NE    | 66:OO:88:LEU:HD21  | 2.35                     | 0.41              |
| 69:RR:63:ARG:O     | 69:RR:63:ARG:HG2   | 2.18                     | 0.41              |
| 78:aa:51:ARG:O     | 78:aa:55:GLU:HG3   | 2.20                     | 0.41              |
| 80:cc:34:PHE:C     | 80:cc:36:ASP:H     | 2.28                     | 0.41              |
| 80:cc:50:VAL:O     | 80:cc:50:VAL:HG23  | 2.20                     | 0.41              |
| 84:gg:142:VAL:O    | 84:gg:142:VAL:HG23 | 2.19                     | 0.41              |
| 84:gg:228:TYR:CE2  | 84:gg:264:LYS:HG2  | 2.55                     | 0.41              |
| 86:ii:10:ARG:HD2   | 86:ii:14:ILE:HD11  | 2.01                     | 0.41              |
| 86:ii:120:ILE:HG22 | 86:ii:139:LEU:HD23 | 2.02                     | 0.41              |
| 87:jj:56:ILE:O     | 87:jj:56:ILE:HG22  | 2.19                     | 0.41              |
| 87:jj:193:GLU:OE1  | 87:jj:233:GLN:HA   | 2.21                     | 0.41              |
| 1:A:178:PRO:HG3    | 41:p:25:MET:HE3    | 2.01                     | 0.41              |
| 13:N:114:ARG:HH11  | 13:N:114:ARG:HG3   | 1.85                     | 0.41              |
| 13:N:178:HIS:HA    | 13:N:181:HIS:NE2   | 2.35                     | 0.41              |
| 25:Z:6:LYS:O       | 25:Z:25:ILE:HB     | 2.19                     | 0.41              |
| 41:p:8:VAL:O       | 41:p:11:VAL:HG22   | 2.19                     | 0.41              |
| 43:s:192:VAL:CG1   | 43:s:194:ASP:OD1   | 2.68                     | 0.41              |
| 48:5:181:C:N3      | 48:5:256:G:C2      | 2.88                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:5:258:G:H2'    | 48:5:259:C:O4'     | 2.20                     | 0.41              |
| 48:5:1332:C:H2'   | 48:5:1333:A:C8     | 2.55                     | 0.41              |
| 48:5:1546:C:H42   | 48:5:1612:G:H22    | 1.68                     | 0.41              |
| 48:5:2465:C:H2'   | 48:5:2466:G:O4'    | 2.20                     | 0.41              |
| 48:5:2488:C:H2'   | 48:5:2489:C:OP1    | 2.21                     | 0.41              |
| 48:5:3810:C:HO2'  | 48:5:3811:G:P      | 2.43                     | 0.41              |
| 48:5:3864:C:OP1   | 92:5:5430:HOH:O    | 2.22                     | 0.41              |
| 48:5:4181:U:H2'   | 48:5:4182:G:O4'    | 2.21                     | 0.41              |
| 48:5:4918:C:C4    | 48:5:4919:G:N7     | 2.88                     | 0.41              |
| 51:9:25:A:H2'     | 51:9:26:U:C6       | 2.55                     | 0.41              |
| 51:9:165:G:H21    | 51:9:165:G:P       | 2.36                     | 0.41              |
| 51:9:587:A:C2     | 51:9:592:C:C2      | 3.09                     | 0.41              |
| 51:9:637:U:H2'    | 51:9:638:C:O4'     | 2.21                     | 0.41              |
| 51:9:656:G:H5'    | 51:9:662:G:N2      | 2.35                     | 0.41              |
| 51:9:1109:C:O2'   | 51:9:1110:G:C8     | 2.73                     | 0.41              |
| 51:9:1114:U:O2'   | 51:9:1115:U:P      | 2.79                     | 0.41              |
| 51:9:1290:G:C2    | 51:9:1291:A:C8     | 3.09                     | 0.41              |
| 51:9:1298:G:O2'   | 51:9:1299:A:C5'    | 2.67                     | 0.41              |
| 51:9:1463:U:H4'   | 51:9:1464:C:O5'    | 2.21                     | 0.41              |
| 51:9:1738:C:H2'   | 51:9:1739:C:C6     | 2.55                     | 0.41              |
| 53:BB:79:VAL:HG21 | 53:BB:81:PHE:CZ    | 2.55                     | 0.41              |
| 56:EE:175:PHE:HA  | 56:EE:227:VAL:HG21 | 2.02                     | 0.41              |
| 58:GG:208:GLU:OE1 | 58:GG:211:LYS:HG2  | 2.20                     | 0.41              |
| 60:II:110:ARG:O   | 60:II:114:GLU:HG3  | 2.20                     | 0.41              |
| 65:NN:84:LEU:HD21 | 65:NN:89:TYR:CD1   | 2.55                     | 0.41              |
| 65:NN:115:LEU:O   | 65:NN:119:GLU:HG3  | 2.20                     | 0.41              |
| 67:PP:34:MET:HE2  | 67:PP:45:LEU:HB3   | 2.02                     | 0.41              |
| 68:QQ:58:LEU:O    | 68:QQ:62:ARG:HD3   | 2.20                     | 0.41              |
| 69:RR:41:ILE:HG22 | 69:RR:43:SER:H     | 1.85                     | 0.41              |
| 70:SS:36:VAL:HG22 | 70:SS:40:TYR:HD2   | 1.82                     | 0.41              |
| 79:bb:55:LEU:HD22 | 79:bb:55:LEU:H     | 1.85                     | 0.41              |
| 87:jj:107:GLY:HA2 | 87:jj:271:VAL:HG23 | 2.02                     | 0.41              |
| 87:jj:488:PRO:O   | 87:jj:524:MET:HE1  | 2.20                     | 0.41              |
| 87:jj:536:ASP:OD1 | 87:jj:536:ASP:N    | 2.52                     | 0.41              |
| 2:B:281:ASN:ND2   | 48:5:4676:G:OP1    | 2.53                     | 0.41              |
| 2:B:315:ASN:O     | 2:B:370:THR:HG23   | 2.19                     | 0.41              |
| 4:D:48:LYS:HE2    | 48:5:4325:A:O2'    | 2.21                     | 0.41              |
| 11:L:108:GLU:CD   | 11:L:108:GLU:N     | 2.78                     | 0.41              |
| 14:O:118:MET:HE1  | 18:S:169:THR:HG23  | 2.02                     | 0.41              |
| 16:Q:144:LYS:NZ   | 48:5:1461:C:OP1    | 2.37                     | 0.41              |
| 20:U:101:ARG:O    | 20:U:112:LEU:HA    | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:Y:114:ASP:O     | 24:Y:117:LYS:HG2   | 2.21                     | 0.41              |
| 37:l:31:THR:OG1    | 50:8:75:OMG:OP2    | 2.37                     | 0.41              |
| 43:s:13:TYR:O      | 43:s:17:ILE:HG23   | 2.19                     | 0.41              |
| 48:5:304:C:H2'     | 48:5:305:A:O4'     | 2.20                     | 0.41              |
| 48:5:1398:A:N6     | 48:5:1419:G:O2'    | 2.53                     | 0.41              |
| 48:5:1432:G:H1'    | 48:5:1452:A:H61    | 1.85                     | 0.41              |
| 48:5:1996:C:C4     | 48:5:1997:U:C6     | 3.08                     | 0.41              |
| 48:5:2460:A:H2'    | 48:5:2461:G:O4'    | 2.20                     | 0.41              |
| 48:5:3720:G:H22    | 48:5:3733:A:H2     | 1.67                     | 0.41              |
| 48:5:4112:C:O2'    | 48:5:4113:U:H5'    | 2.21                     | 0.41              |
| 48:5:4589:A:N1     | 48:5:4621:C:O2'    | 2.50                     | 0.41              |
| 50:8:60:G:O6       | 50:8:96:C:O2'      | 2.31                     | 0.41              |
| 51:9:71:G:C6       | 58:GG:170:ARG:NH1  | 2.88                     | 0.41              |
| 51:9:193:C:H2'     | 51:9:194:C:O4'     | 2.20                     | 0.41              |
| 51:9:417:C:O2'     | 51:9:418:A:P       | 2.77                     | 0.41              |
| 51:9:688:U:OP2     | 51:9:688:U:O2      | 2.39                     | 0.41              |
| 51:9:863:PSU:C2    | 51:9:864:A:N7      | 2.88                     | 0.41              |
| 51:9:913:A:OP2     | 59:HH:99:ARG:NH1   | 2.48                     | 0.41              |
| 51:9:1152:U:O3'    | 74:WW:19:LYS:NZ    | 2.54                     | 0.41              |
| 51:9:1208:A:O2'    | 51:9:1209:A:H5'    | 2.20                     | 0.41              |
| 51:9:1549:U:OP2    | 55:DD:8:LYS:NZ     | 2.54                     | 0.41              |
| 51:9:1587:G:O6     | 71:TT:67:ARG:HD3   | 2.20                     | 0.41              |
| 52:AA:203:PHE:CZ   | 69:RR:91:LEU:HD13  | 2.55                     | 0.41              |
| 54:CC:204:ILE:HD11 | 54:CC:219:ILE:O    | 2.18                     | 0.41              |
| 56:EE:248:ILE:HD12 | 61:JJ:72:PHE:CE2   | 2.56                     | 0.41              |
| 61:JJ:111:GLN:HA   | 61:JJ:130:ILE:CD1  | 2.51                     | 0.41              |
| 64:MM:68:LEU:HD23  | 83:ff:109:ILE:CD1  | 2.51                     | 0.41              |
| 66:OO:149:ARG:NH2  | 66:OO:151:LEU:HD13 | 2.35                     | 0.41              |
| 72:UU:99:LYS:HA    | 72:UU:102:THR:HG22 | 2.02                     | 0.41              |
| 84:gg:208:ALA:HB2  | 84:gg:241:PHE:CZ   | 2.55                     | 0.41              |
| 87:jj:165:LYS:O    | 87:jj:235:ALA:HB1  | 2.20                     | 0.41              |
| 87:jj:409:VAL:HG22 | 87:jj:482:VAL:HG22 | 2.01                     | 0.41              |
| 6:F:34:LYS:N       | 6:F:34:LYS:HD3     | 2.36                     | 0.41              |
| 7:G:48:LYS:NZ      | 48:5:4086:G:O6     | 2.39                     | 0.41              |
| 8:H:106:GLN:HB2    | 8:H:111:LEU:HB3    | 2.02                     | 0.41              |
| 16:Q:14:ARG:HH22   | 48:5:2083:C:P      | 2.43                     | 0.41              |
| 18:S:48:VAL:HG12   | 19:T:151:LEU:HD12  | 2.02                     | 0.41              |
| 37:l:18:LYS:NZ     | 50:8:46:G:OP1      | 2.41                     | 0.41              |
| 42:r:47:LYS:O      | 42:r:103:HIS:NE2   | 2.53                     | 0.41              |
| 43:s:57:LYS:O      | 43:s:57:LYS:HD2    | 2.20                     | 0.41              |
| 43:s:111:ALA:HB1   | 43:s:183:PHE:HD2   | 1.85                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:s:130:LEU:HD13  | 43:s:133:GLU:HG2   | 2.03                     | 0.41              |
| 46:2:18:G:H4'      | 46:2:60:A:C6       | 2.56                     | 0.41              |
| 47:3:15:G:N2       | 47:3:59:G:C8       | 2.89                     | 0.41              |
| 48:5:206:U:H1'     | 48:5:209:U:C4      | 2.56                     | 0.41              |
| 48:5:1295:U:O2     | 48:5:1295:U:O4'    | 2.38                     | 0.41              |
| 48:5:1472:C:H2'    | 48:5:1473:U:C6     | 2.55                     | 0.41              |
| 48:5:1666:C:O2'    | 48:5:1688:G:OP1    | 2.34                     | 0.41              |
| 48:5:1879:C:O2'    | 48:5:1891:A:N3     | 2.48                     | 0.41              |
| 48:5:1977:C:O2     | 48:5:1990:A:N6     | 2.54                     | 0.41              |
| 48:5:4152:G:H8     | 48:5:4152:G:O5'    | 2.03                     | 0.41              |
| 48:5:5034:A:H2'    | 48:5:5035:U:O4'    | 2.20                     | 0.41              |
| 50:8:103:A:C8      | 50:8:104:A:C8      | 3.09                     | 0.41              |
| 51:9:103:A:H2      | 51:9:105:PSU:O2    | 2.04                     | 0.41              |
| 51:9:688:U:O2'     | 51:9:689:U:P       | 2.78                     | 0.41              |
| 51:9:1018:U:C5'    | 65:NN:71:ILE:HD12  | 2.48                     | 0.41              |
| 51:9:1050:A:H4'    | 51:9:1846:G:O2'    | 2.20                     | 0.41              |
| 51:9:1282:A:H3'    | 51:9:1283:C:H5'    | 2.02                     | 0.41              |
| 51:9:1675:A:O2'    | 57:FF:74:ASN:O     | 2.38                     | 0.41              |
| 51:9:1807:C:H2'    | 51:9:1808:U:O4'    | 2.20                     | 0.41              |
| 55:DD:91:VAL:HG12  | 55:DD:92:ALA:O     | 2.20                     | 0.41              |
| 56:EE:180:LEU:HB2  | 56:EE:232:ASN:HA   | 2.01                     | 0.41              |
| 57:FF:116:ILE:HD11 | 57:FF:151:ILE:CD1  | 2.50                     | 0.41              |
| 58:GG:35:GLU:HA    | 58:GG:51:ARG:HA    | 2.02                     | 0.41              |
| 62:KK:7:ASN:HA     | 62:KK:40:VAL:HG22  | 2.02                     | 0.41              |
| 66:OO:45:THR:HB    | 66:OO:51:GLU:O     | 2.20                     | 0.41              |
| 68:QQ:102:GLU:HB2  | 84:gg:56:GLN:O     | 2.19                     | 0.41              |
| 69:RR:21:TYR:CD2   | 69:RR:71:ILE:HG23  | 2.56                     | 0.41              |
| 75:XX:16:HIS:O     | 75:XX:20:GLN:HG2   | 2.21                     | 0.41              |
| 76:YY:104:ARG:NH2  | 76:YY:108:LYS:HE3  | 2.35                     | 0.41              |
| 84:gg:31:ILE:HD13  | 84:gg:31:ILE:HA    | 1.96                     | 0.41              |
| 84:gg:194:TYR:CZ   | 84:gg:212:LYS:HB2  | 2.55                     | 0.41              |
| 86:ii:224:LEU:HD23 | 86:ii:250:VAL:HG12 | 2.03                     | 0.41              |
| 87:jj:252:ARG:HD3  | 87:jj:278:VAL:HG21 | 2.01                     | 0.41              |
| 2:B:309:LEU:O      | 2:B:310:SER:C      | 2.64                     | 0.41              |
| 4:D:128:ASP:O      | 4:D:164:LYS:NZ     | 2.47                     | 0.41              |
| 7:G:218:LEU:O      | 7:G:222:ILE:HG12   | 2.20                     | 0.41              |
| 10:J:62:ILE:CG2    | 10:J:68:ILE:HD12   | 2.51                     | 0.41              |
| 15:P:137:ASN:HB3   | 48:5:3860:A:O2'    | 2.21                     | 0.41              |
| 24:Y:88:GLU:HA     | 24:Y:93:THR:O      | 2.21                     | 0.41              |
| 24:Y:89:LYS:NZ     | 48:5:386:A:OP2     | 2.29                     | 0.41              |
| 25:Z:92:ASP:HB3    | 25:Z:113:GLU:OE1   | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:d:39:LYS:NZ     | 48:5:2369:U:O2     | 2.53                     | 0.41              |
| 29:d:70:LYS:HE2    | 48:5:2389:A:H4'    | 2.02                     | 0.41              |
| 39:n:4:LYS:NZ      | 51:9:1844:U:O4     | 2.49                     | 0.41              |
| 44:t:64:ILE:CG2    | 44:t:71:ILE:HB     | 2.51                     | 0.41              |
| 48:5:1565:A:C5     | 48:5:1566:C:H1'    | 2.55                     | 0.41              |
| 48:5:1984:A:OP2    | 48:5:1986:U:OP1    | 2.39                     | 0.41              |
| 48:5:2016:C:H2'    | 48:5:2017:A:H8     | 1.86                     | 0.41              |
| 48:5:2616:C:O2'    | 48:5:2617:G:H5'    | 2.20                     | 0.41              |
| 48:5:2898:G:H2'    | 48:5:2899:C:H6     | 1.85                     | 0.41              |
| 48:5:3771:C:H2'    | 48:5:3772:U:O4'    | 2.20                     | 0.41              |
| 48:5:4244:A:H2'    | 48:5:4245:G:O4'    | 2.20                     | 0.41              |
| 48:5:4254:G:N3     | 48:5:4254:G:H2'    | 2.35                     | 0.41              |
| 48:5:4439:U:OP1    | 86:ii:192:ARG:HD2  | 2.20                     | 0.41              |
| 48:5:4543:G:H2'    | 48:5:4544:A:C8     | 2.56                     | 0.41              |
| 50:8:81:C:H3'      | 50:8:82:A:H4'      | 2.02                     | 0.41              |
| 51:9:106:C:H2'     | 51:9:107:A:C8      | 2.55                     | 0.41              |
| 51:9:164:A:H2'     | 51:9:165:G:N3      | 2.36                     | 0.41              |
| 51:9:194:C:C2      | 51:9:195:C:C5      | 3.08                     | 0.41              |
| 51:9:691:G:N2      | 51:9:692:G:C8      | 2.88                     | 0.41              |
| 51:9:1265:A:N3     | 51:9:1265:A:H2'    | 2.36                     | 0.41              |
| 51:9:1420:G:OP2    | 71:TT:132:ASP:HB2  | 2.21                     | 0.41              |
| 51:9:1471:C:H2'    | 51:9:1472:C:O4'    | 2.20                     | 0.41              |
| 51:9:1863:A:OP2    | 78:aa:4:LYS:NZ     | 2.48                     | 0.41              |
| 53:BB:181:LEU:O    | 53:BB:185:VAL:HG23 | 2.20                     | 0.41              |
| 54:CC:63:VAL:HG22  | 54:CC:64:THR:N     | 2.35                     | 0.41              |
| 58:GG:213:LEU:HD11 | 58:GG:217:MET:HE1  | 2.02                     | 0.41              |
| 59:HH:79:LEU:HD22  | 59:HH:94:PHE:CE2   | 2.55                     | 0.41              |
| 62:KK:84:HIS:HB3   | 64:MM:27:ILE:HG23  | 2.03                     | 0.41              |
| 70:SS:11:HIS:O     | 70:SS:12:ILE:HD13  | 2.19                     | 0.41              |
| 70:SS:40:TYR:OH    | 70:SS:74:PRO:HG3   | 2.21                     | 0.41              |
| 71:TT:65:TYR:OH    | 71:TT:132:ASP:OD1  | 2.37                     | 0.41              |
| 72:UU:56:MET:O     | 72:UU:57:PRO:C     | 2.63                     | 0.41              |
| 73:VV:4:ASP:OD1    | 73:VV:5:ALA:N      | 2.53                     | 0.41              |
| 86:ii:407:GLY:N    | 87:jj:34:MET:HE3   | 2.35                     | 0.41              |
| 87:jj:231:CYS:SG   | 87:jj:258:THR:HG22 | 2.60                     | 0.41              |
| 87:jj:250:LYS:HD2  | 87:jj:562:LEU:HD22 | 2.02                     | 0.41              |
| 2:B:106:PHE:CZ     | 2:B:163:LEU:HD13   | 2.56                     | 0.41              |
| 3:C:197:ARG:NH1    | 48:5:351:C:OP2     | 2.50                     | 0.41              |
| 5:E:214:HIS:NE2    | 5:E:252:ASP:OD2    | 2.46                     | 0.41              |
| 6:F:221:LYS:HE2    | 49:7:85:G:OP1      | 2.20                     | 0.41              |
| 11:L:55:ILE:HA     | 11:L:154:VAL:CG1   | 2.51                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:L:108:GLU:N    | 11:L:108:GLU:OE1   | 2.41                     | 0.41              |
| 13:N:38:ARG:NH2   | 50:8:142:U:OP1     | 2.46                     | 0.41              |
| 14:O:44:SER:HG    | 48:5:2054:U:H6     | 1.63                     | 0.41              |
| 17:R:79:GLY:O     | 48:5:3619:G:H4'    | 2.20                     | 0.41              |
| 29:d:23:ARG:NH2   | 48:5:5058:A:H4'    | 2.35                     | 0.41              |
| 48:5:756:G:O2'    | 48:5:757:G:H5'     | 2.20                     | 0.41              |
| 48:5:914:U:O2'    | 48:5:915:A:C5'     | 2.69                     | 0.41              |
| 48:5:1353:G:O2'   | 48:5:1503:A:N1     | 2.50                     | 0.41              |
| 48:5:2488:C:C2'   | 48:5:2489:C:OP1    | 2.68                     | 0.41              |
| 48:5:3784:A:O2'   | 48:5:3786:U:OP2    | 2.32                     | 0.41              |
| 48:5:4065:G:P     | 48:5:4065:G:H8     | 2.44                     | 0.41              |
| 48:5:4582:C:O2'   | 48:5:4583:C:H5'    | 2.20                     | 0.41              |
| 49:7:108:G:O2'    | 49:7:109:U:H5'     | 2.21                     | 0.41              |
| 51:9:103:A:C2     | 51:9:355:G:C6      | 3.09                     | 0.41              |
| 51:9:547:G:N3     | 51:9:549:C:N4      | 2.68                     | 0.41              |
| 51:9:805:U:OP2    | 74:WW:82:GLN:HG2   | 2.21                     | 0.41              |
| 51:9:1439:A:H8    | 51:9:1439:A:O5'    | 2.03                     | 0.41              |
| 52:AA:90:PHE:HD2  | 52:AA:179:ALA:HB2  | 1.77                     | 0.41              |
| 56:EE:234:PRO:CG  | 56:EE:238:LEU:HD13 | 2.51                     | 0.41              |
| 57:FF:178:ILE:O   | 57:FF:182:LYS:HG2  | 2.20                     | 0.41              |
| 58:GG:233:ARG:HD3 | 58:GG:233:ARG:HA   | 1.90                     | 0.41              |
| 60:II:65:PHE:O    | 60:II:109:TYR:OH   | 2.31                     | 0.41              |
| 64:MM:89:VAL:CG1  | 64:MM:90:GLY:N     | 2.83                     | 0.41              |
| 67:PP:57:LEU:HD21 | 67:PP:89:MET:HE2   | 2.02                     | 0.41              |
| 67:PP:90:VAL:HG12 | 67:PP:91:GLY:N     | 2.35                     | 0.41              |
| 76:YY:117:VAL:CG1 | 76:YY:121:ALA:HB3  | 2.49                     | 0.41              |
| 84:gg:132:TRP:CD1 | 84:gg:132:TRP:N    | 2.88                     | 0.41              |
| 87:jj:240:PHE:HB3 | 87:jj:243:PRO:HG3  | 2.03                     | 0.41              |
| 4:D:289:ARG:NH1   | 4:D:289:ARG:CB     | 2.84                     | 0.41              |
| 11:L:105:LYS:O    | 34:i:20:ASN:N      | 2.41                     | 0.41              |
| 11:L:170:THR:CG2  | 11:L:171:GLU:N     | 2.83                     | 0.41              |
| 12:M:123:ILE:O    | 12:M:127:VAL:HG23  | 2.20                     | 0.41              |
| 13:N:95:ALA:O     | 48:5:300:A:H5'     | 2.20                     | 0.41              |
| 16:Q:49:LYS:HG2   | 16:Q:53:MET:CE     | 2.50                     | 0.41              |
| 16:Q:177:ALA:C    | 26:a:51:GLY:HA2    | 2.46                     | 0.41              |
| 27:b:55:LYS:O     | 27:b:58:GLN:HG2    | 2.21                     | 0.41              |
| 35:j:21:ARG:NH2   | 35:j:39:TYR:HA     | 2.36                     | 0.41              |
| 46:2:67:G:C2      | 46:2:68:G:C8       | 3.08                     | 0.41              |
| 47:3:50:A:C6      | 47:3:65:G:C6       | 3.09                     | 0.41              |
| 48:5:1450:C:H2'   | 48:5:1451:G:O4'    | 2.20                     | 0.41              |
| 48:5:4773:C:H2'   | 48:5:4774:C:O4'    | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:5065:U:H2'    | 48:5:5066:U:O4'    | 2.21                     | 0.41              |
| 51:9:202:G:H5''    | 51:9:203:G:OP2     | 2.21                     | 0.41              |
| 51:9:293:C:O2      | 51:9:293:C:H2'     | 2.21                     | 0.41              |
| 51:9:385:G:O2'     | 60:II:10:LYS:NZ    | 2.54                     | 0.41              |
| 51:9:875:A:O5'     | 51:9:875:A:H8      | 2.03                     | 0.41              |
| 51:9:1477:U:OP2    | 69:RR:3:ARG:NH1    | 2.40                     | 0.41              |
| 54:CC:135:GLY:HA2  | 54:CC:165:VAL:HB   | 2.02                     | 0.41              |
| 55:DD:99:ILE:HG13  | 55:DD:100:ALA:N    | 2.36                     | 0.41              |
| 56:EE:160:ILE:HD12 | 56:EE:162:ILE:HD11 | 2.03                     | 0.41              |
| 58:GG:23:LYS:O     | 58:GG:26:THR:HG22  | 2.21                     | 0.41              |
| 58:GG:126:ASP:C    | 58:GG:127:THR:HG1  | 2.19                     | 0.41              |
| 58:GG:181:THR:O    | 58:GG:184:VAL:N    | 2.53                     | 0.41              |
| 62:KK:15:LEU:O     | 62:KK:18:GLU:C     | 2.64                     | 0.41              |
| 68:QQ:24:HIS:O     | 68:QQ:68:ILE:HA    | 2.21                     | 0.41              |
| 68:QQ:101:ASP:OD1  | 68:QQ:101:ASP:C    | 2.63                     | 0.41              |
| 87:jj:347:MET:SD   | 87:jj:347:MET:C    | 3.04                     | 0.41              |
| 2:B:217:ILE:HD11   | 2:B:333:LEU:CD2    | 2.48                     | 0.41              |
| 3:C:120:LYS:HD2    | 48:5:1374:G:OP1    | 2.20                     | 0.41              |
| 3:C:159:GLU:HA     | 3:C:217:ILE:HB     | 2.03                     | 0.41              |
| 3:C:221:PHE:CB     | 3:C:229:LEU:HD21   | 2.51                     | 0.41              |
| 3:C:283:LYS:NZ     | 16:Q:22:ASP:OD2    | 2.50                     | 0.41              |
| 6:F:36:PHE:CG      | 48:5:1272:C:H4'    | 2.56                     | 0.41              |
| 8:H:80:MET:O       | 8:H:84:VAL:HG22    | 2.20                     | 0.41              |
| 10:J:101:ASP:OD1   | 48:5:4248:A:H1'    | 2.21                     | 0.41              |
| 17:R:3:MET:HE2     | 17:R:5:ARG:NH1     | 2.36                     | 0.41              |
| 20:U:60:VAL:HG11   | 20:U:76:VAL:CG2    | 2.51                     | 0.41              |
| 21:V:41:SER:OG     | 48:5:4507:A:O2'    | 2.34                     | 0.41              |
| 22:W:9:SER:HA      | 22:W:52:THR:HG22   | 2.02                     | 0.41              |
| 25:Z:72:VAL:O      | 25:Z:72:VAL:HG23   | 2.21                     | 0.41              |
| 33:h:17:LEU:HD13   | 33:h:61:ILE:HG13   | 2.03                     | 0.41              |
| 33:h:121:VAL:CG1   | 33:h:122:LYS:N     | 2.84                     | 0.41              |
| 36:k:7:GLU:HB2     | 36:k:10:ASP:OD2    | 2.20                     | 0.41              |
| 44:t:131:GLU:HA    | 44:t:152:ILE:HG21  | 2.02                     | 0.41              |
| 47:3:76:A:C2       | 48:5:4370:OMG:H2'  | 2.56                     | 0.41              |
| 48:5:409:G:H21     | 48:5:2329:U:H4'    | 1.86                     | 0.41              |
| 48:5:658:C:N4      | 48:5:659:G:O6      | 2.54                     | 0.41              |
| 48:5:674:G:H2'     | 48:5:675:C:C6      | 2.55                     | 0.41              |
| 48:5:756:G:C6      | 48:5:908:G:C6      | 3.09                     | 0.41              |
| 48:5:1173:G:C6     | 48:5:1174:G:C6     | 3.08                     | 0.41              |
| 48:5:1195:G:C5     | 48:5:1196:G:N7     | 2.89                     | 0.41              |
| 48:5:1445:U:H3'    | 48:5:1446:C:C5     | 2.56                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:1609:U:H2'    | 48:5:1610:C:O4'    | 2.20                     | 0.41              |
| 48:5:1818:G:N3     | 48:5:1818:G:H2'    | 2.36                     | 0.41              |
| 48:5:1895:G:H2'    | 48:5:1896:A:O4'    | 2.21                     | 0.41              |
| 48:5:1981:G:H1'    | 86:ii:315:GLY:HA3  | 2.03                     | 0.41              |
| 48:5:1994:C:H2'    | 48:5:1995:G:C8     | 2.56                     | 0.41              |
| 48:5:2079:G:H2'    | 48:5:2080:U:C6     | 2.56                     | 0.41              |
| 48:5:2306:G:H1'    | 48:5:2332:A:N6     | 2.36                     | 0.41              |
| 48:5:2485:U:H2'    | 48:5:2486:G:C8     | 2.56                     | 0.41              |
| 48:5:2491:C:H2'    | 48:5:2492:C:C4'    | 2.51                     | 0.41              |
| 48:5:2517:A:N3     | 48:5:2539:C:O2'    | 2.52                     | 0.41              |
| 48:5:2545:U:OP2    | 48:5:2546:G:H5''   | 2.21                     | 0.41              |
| 48:5:2690:C:H2'    | 48:5:2691:U:O4'    | 2.21                     | 0.41              |
| 48:5:3930:U:H2'    | 48:5:3931:C:C6     | 2.56                     | 0.41              |
| 48:5:4100:C:C4     | 48:5:4101:C:N4     | 2.89                     | 0.41              |
| 48:5:4236:G:H4'    | 48:5:4328:G:O2'    | 2.21                     | 0.41              |
| 48:5:4492:U:O2'    | 48:5:4512:U:O2     | 2.27                     | 0.41              |
| 48:5:4574:U:H3'    | 48:5:4575:G:C5'    | 2.48                     | 0.41              |
| 48:5:4884:G:O2'    | 48:5:4885:U:OP1    | 2.39                     | 0.41              |
| 50:8:88:A:H2'      | 50:8:89:U:O4'      | 2.21                     | 0.41              |
| 50:8:108:A:H2'     | 50:8:109:C:O4'     | 2.20                     | 0.41              |
| 51:9:304:C:O2'     | 51:9:309:G:C6      | 2.74                     | 0.41              |
| 51:9:902:G:H2'     | 51:9:903:A:O5'     | 2.21                     | 0.41              |
| 51:9:915:G:OP1     | 59:HH:120:ARG:NH1  | 2.41                     | 0.41              |
| 51:9:931:C:H2'     | 51:9:932:G:C8      | 2.56                     | 0.41              |
| 51:9:1059:G:C5     | 51:9:1060:A:C2     | 3.09                     | 0.41              |
| 51:9:1097:G:O2'    | 51:9:1098:C:H5'    | 2.21                     | 0.41              |
| 51:9:1287:A:OP2    | 83:ff:94:LYS:HD2   | 2.21                     | 0.41              |
| 51:9:1579:A:H4'    | 51:9:1581:C:C5     | 2.55                     | 0.41              |
| 52:AA:49:ILE:HG22  | 52:AA:50:ASN:N     | 2.36                     | 0.41              |
| 53:BB:127:VAL:HG23 | 53:BB:177:GLN:HG3  | 2.03                     | 0.41              |
| 53:BB:168:MET:O    | 53:BB:172:MET:CG   | 2.68                     | 0.41              |
| 55:DD:221:THR:OG1  | 55:DD:222:PRO:HD2  | 2.19                     | 0.41              |
| 56:EE:151:ASP:OD2  | 58:GG:212:LEU:HD21 | 2.21                     | 0.41              |
| 57:FF:20:PHE:O     | 57:FF:20:PHE:HD1   | 2.03                     | 0.41              |
| 58:GG:34:THR:HG23  | 58:GG:34:THR:O     | 2.19                     | 0.41              |
| 59:HH:79:LEU:CD2   | 59:HH:83:LEU:HD13  | 2.51                     | 0.41              |
| 60:II:149:TYR:O    | 60:II:153:LYS:NZ   | 2.54                     | 0.41              |
| 62:KK:21:MET:SD    | 62:KK:49:MET:CE    | 3.09                     | 0.41              |
| 67:PP:113:GLY:C    | 67:PP:114:HIS:ND1  | 2.79                     | 0.41              |
| 69:RR:15:VAL:HG12  | 69:RR:19:LYS:NZ    | 2.35                     | 0.41              |
| 70:SS:9:PHE:CE1    | 77:ZZ:49:LEU:HD12  | 2.56                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:XX:105:PHE:HB2  | 75:XX:119:ARG:O    | 2.21                     | 0.41              |
| 79:bb:33:MET:CE    | 79:bb:73:LEU:HD21  | 2.50                     | 0.41              |
| 80:cc:28:THR:OG1   | 80:cc:50:VAL:HG22  | 2.20                     | 0.41              |
| 84:gg:8:ARG:C      | 84:gg:309:VAL:HG13 | 2.46                     | 0.41              |
| 86:ii:30:ASN:OD1   | 86:ii:30:ASN:N     | 2.53                     | 0.41              |
| 86:ii:315:GLY:O    | 86:ii:414:ARG:NH1  | 2.54                     | 0.41              |
| 86:ii:317:VAL:HG13 | 86:ii:387:ALA:HB2  | 2.03                     | 0.41              |
| 87:jj:29:CYS:HA    | 91:jj:601:SF4:S2   | 2.61                     | 0.41              |
| 87:jj:509:LEU:HD23 | 87:jj:510:HIS:HD2  | 1.86                     | 0.41              |
| 1:A:104:VAL:HA     | 1:A:107:MET:SD     | 2.61                     | 0.41              |
| 2:B:234:ARG:HD2    | 2:B:271:GLN:O      | 2.20                     | 0.41              |
| 4:D:226:TYR:OH     | 49:7:48:G:OP1      | 2.37                     | 0.41              |
| 6:F:106:LYS:O      | 6:F:110:LEU:HG     | 2.21                     | 0.41              |
| 13:N:11:TRP:O      | 13:N:14:LYS:NZ     | 2.51                     | 0.41              |
| 14:O:118:MET:SD    | 18:S:169:THR:HG22  | 2.61                     | 0.41              |
| 19:T:4:THR:OG1     | 48:5:4208:U:OP2    | 2.35                     | 0.41              |
| 28:c:81:LEU:HD21   | 28:c:94:LEU:HD23   | 2.03                     | 0.41              |
| 43:s:187:LEU:O     | 43:s:188:ILE:HG13  | 2.21                     | 0.41              |
| 47:3:35:U:H2'      | 47:3:36:U:O5'      | 2.22                     | 0.41              |
| 48:5:664:G:H2'     | 48:5:665:C:C6      | 2.56                     | 0.41              |
| 48:5:759:G:H2'     | 48:5:760:G:H5'     | 2.03                     | 0.41              |
| 48:5:1183:C:H2'    | 48:5:1184:A:C8     | 2.56                     | 0.41              |
| 48:5:1391:A:H2'    | 48:5:1392:A:O4'    | 2.21                     | 0.41              |
| 48:5:1411(B):C:H6  | 48:5:1411(B):C:O5' | 2.04                     | 0.41              |
| 48:5:1764:G:C2'    | 48:5:1767:A:H62    | 2.34                     | 0.41              |
| 48:5:1765:A:C4     | 48:5:1766:A:C8     | 3.08                     | 0.41              |
| 48:5:2744:A:H2'    | 48:5:2745:A:C8     | 2.56                     | 0.41              |
| 48:5:3662:A:O4'    | 48:5:3664:G:C8     | 2.74                     | 0.41              |
| 48:5:3792:OMG:H1'  | 48:5:3792:OMG:HM23 | 1.84                     | 0.41              |
| 48:5:3808:OMC:C5   | 48:5:3809:G:C6     | 3.09                     | 0.41              |
| 48:5:3893:C:H2'    | 48:5:3894:A:C8     | 2.56                     | 0.41              |
| 48:5:4071:U:H2'    | 48:5:4072:C:H6     | 1.86                     | 0.41              |
| 48:5:4635:A:C8     | 48:5:5048:A:N6     | 2.86                     | 0.41              |
| 51:9:879:C:H3'     | 51:9:880:G:H5''    | 2.02                     | 0.41              |
| 51:9:1265:A:H5'    | 51:9:1326:OMU:HM21 | 2.03                     | 0.41              |
| 51:9:1473:G:N2     | 51:9:1475:G:H3'    | 2.36                     | 0.41              |
| 51:9:1624:U:O2     | 51:9:1624:U:O4'    | 2.38                     | 0.41              |
| 51:9:1638:G:H5''   | 51:9:1639:G7M:OP1  | 2.21                     | 0.41              |
| 51:9:1735:A:H2'    | 51:9:1736:G:O4'    | 2.21                     | 0.41              |
| 55:DD:92:ALA:O     | 55:DD:93:THR:HG22  | 2.21                     | 0.41              |
| 56:EE:59:ASP:O     | 56:EE:63:LYS:HG2   | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:EE:246:LEU:HD22 | 56:EE:251:GLU:OE1  | 2.21                     | 0.41              |
| 58:GG:3:LEU:O      | 58:GG:15:LEU:HA    | 2.21                     | 0.41              |
| 62:KK:18:GLU:C     | 62:KK:20:VAL:H     | 2.28                     | 0.41              |
| 62:KK:43:LEU:O     | 62:KK:47:LYS:HG2   | 2.20                     | 0.41              |
| 70:SS:5:ILE:O      | 70:SS:5:ILE:HG23   | 2.21                     | 0.41              |
| 70:SS:33:ILE:HD13  | 70:SS:71:MET:HE1   | 2.02                     | 0.41              |
| 71:TT:38:LYS:NZ    | 71:TT:43:LYS:O     | 2.48                     | 0.41              |
| 72:UU:55:ARG:HG3   | 72:UU:55:ARG:HH11  | 1.85                     | 0.41              |
| 74:WW:111:MET:SD   | 74:WW:115:GLU:HG2  | 2.61                     | 0.41              |
| 76:YY:46:LYS:N     | 76:YY:46:LYS:HD3   | 2.35                     | 0.41              |
| 79:bb:56:CYS:O     | 79:bb:57:VAL:C     | 2.64                     | 0.41              |
| 82:ee:17:LEU:HD23  | 82:ee:17:LEU:N     | 2.35                     | 0.41              |
| 84:gg:132:TRP:CZ3  | 84:gg:138:CYS:HB2  | 2.56                     | 0.41              |
| 84:gg:146:SER:OG   | 84:gg:147:HIS:N    | 2.54                     | 0.41              |
| 87:jj:256:ALA:HA   | 87:jj:282:LEU:CD1  | 2.51                     | 0.41              |
| 87:jj:303:PHE:CE1  | 87:jj:311:ILE:HD13 | 2.56                     | 0.41              |
| 3:C:69:THR:CG2     | 3:C:75:ARG:HD3     | 2.51                     | 0.40              |
| 4:D:208:MET:HB3    | 4:D:208:MET:HE2    | 1.99                     | 0.40              |
| 20:U:39:PHE:CE2    | 20:U:70:ILE:HD13   | 2.55                     | 0.40              |
| 20:U:107:LYS:O     | 20:U:109:SER:N     | 2.53                     | 0.40              |
| 21:V:30:ASP:HA     | 21:V:116:ALA:O     | 2.20                     | 0.40              |
| 26:a:77:LYS:CE     | 48:5:1502:G:N2     | 2.76                     | 0.40              |
| 43:s:28:PHE:HB3    | 43:s:189:ILE:CD1   | 2.51                     | 0.40              |
| 48:5:223:G:H4'     | 48:5:225:G:C8      | 2.57                     | 0.40              |
| 48:5:454:U:H2'     | 48:5:455:C:O4'     | 2.21                     | 0.40              |
| 48:5:478:G:H2'     | 48:5:479:G:H8      | 1.85                     | 0.40              |
| 48:5:960:A:H4'     | 48:5:961:G:OP2     | 2.21                     | 0.40              |
| 48:5:1444:G:H2'    | 48:5:1445:U:C6     | 2.56                     | 0.40              |
| 48:5:1942:A:H2'    | 48:5:1943:A:C8     | 2.56                     | 0.40              |
| 48:5:2258:C:O2'    | 48:5:2259:G:P      | 2.79                     | 0.40              |
| 48:5:2364:OMG:HM23 | 48:5:2364:OMG:H1'  | 1.80                     | 0.40              |
| 48:5:2559:G:C6     | 48:5:2569:G:C6     | 3.09                     | 0.40              |
| 48:5:4114:C:O2'    | 48:5:4115:G:O4'    | 2.38                     | 0.40              |
| 48:5:4694:G:H2'    | 48:5:4694:G:N3     | 2.36                     | 0.40              |
| 50:8:110:U:C2'     | 50:8:111:U:O4'     | 2.68                     | 0.40              |
| 51:9:94:G:O2'      | 51:9:508:A:O2'     | 2.28                     | 0.40              |
| 51:9:140:C:O2'     | 51:9:141:A:P       | 2.78                     | 0.40              |
| 51:9:356:C:O2      | 51:9:356:C:H2'     | 2.20                     | 0.40              |
| 51:9:449:A:O2'     | 51:9:452:G:N7      | 2.53                     | 0.40              |
| 51:9:882:U:H6      | 51:9:882:U:O5'     | 2.03                     | 0.40              |
| 51:9:1129:G:H2'    | 51:9:1130:G:N9     | 2.36                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:1397:U:C3'    | 51:9:1398:G:C5'    | 2.99                     | 0.40              |
| 51:9:1409:A:H61    | 51:9:1439:A:H1'    | 1.86                     | 0.40              |
| 51:9:1440:C:O2'    | 51:9:1441:U:H5'    | 2.20                     | 0.40              |
| 51:9:1456:G:C4     | 51:9:1457:U:C5     | 3.09                     | 0.40              |
| 55:DD:123:LEU:HD21 | 55:DD:154:ASP:OD2  | 2.21                     | 0.40              |
| 57:FF:68:ILE:HG12  | 57:FF:116:ILE:CD1  | 2.51                     | 0.40              |
| 57:FF:104:THR:C    | 57:FF:106:GLU:H    | 2.29                     | 0.40              |
| 60:II:34:ALA:CB    | 60:II:56:ARG:HD3   | 2.51                     | 0.40              |
| 61:JJ:74:GLY:O     | 61:JJ:78:LEU:HG    | 2.20                     | 0.40              |
| 62:KK:42:ASN:ND2   | 62:KK:46:MET:SD    | 2.94                     | 0.40              |
| 67:PP:27:ASP:OD1   | 67:PP:27:ASP:C     | 2.64                     | 0.40              |
| 68:QQ:41:MET:HE1   | 71:TT:8:ASP:O      | 2.21                     | 0.40              |
| 69:RR:13:ALA:O     | 69:RR:17:ILE:HD13  | 2.21                     | 0.40              |
| 70:SS:85:ASN:OD1   | 70:SS:85:ASN:C     | 2.63                     | 0.40              |
| 71:TT:112:MET:O    | 71:TT:123:LEU:HD23 | 2.21                     | 0.40              |
| 76:YY:88:LYS:HD3   | 76:YY:97:TYR:CE1   | 2.57                     | 0.40              |
| 80:cc:16:LYS:HD3   | 80:cc:17:VAL:H     | 1.86                     | 0.40              |
| 82:ee:36:MET:HE2   | 82:ee:36:MET:HB3   | 1.93                     | 0.40              |
| 2:B:28:LYS:O       | 2:B:220:ILE:HG21   | 2.21                     | 0.40              |
| 8:H:41:ILE:HG21    | 8:H:73:ILE:HD11    | 2.03                     | 0.40              |
| 10:J:42:GLN:OE1    | 10:J:42:GLN:HA     | 2.22                     | 0.40              |
| 23:X:87:MET:O      | 23:X:91:GLU:HG2    | 2.21                     | 0.40              |
| 25:Z:88:ASP:O      | 25:Z:89:ILE:C      | 2.64                     | 0.40              |
| 27:b:69:ALA:O      | 27:b:72:ILE:CG2    | 2.69                     | 0.40              |
| 32:g:82:MET:HE3    | 32:g:82:MET:HB2    | 2.02                     | 0.40              |
| 44:t:18:THR:HG21   | 44:t:61:LYS:HE2    | 2.02                     | 0.40              |
| 48:5:231:U:C2'     | 48:5:232:G:OP1     | 2.70                     | 0.40              |
| 48:5:3896:C:O2     | 48:5:4564:A:N1     | 2.54                     | 0.40              |
| 50:8:44:A:H2'      | 50:8:45:C:O4'      | 2.21                     | 0.40              |
| 50:8:124:U:H4'     | 50:8:125:C:O5'     | 2.20                     | 0.40              |
| 50:8:133:G:O2'     | 50:8:134:G:H5'     | 2.21                     | 0.40              |
| 51:9:64:A:OP1      | 58:GG:136:LYS:NZ   | 2.51                     | 0.40              |
| 51:9:607:U:HO2'    | 51:9:608:C:P       | 2.39                     | 0.40              |
| 51:9:608:C:O4'     | 82:ee:58:ASN:ND2   | 2.54                     | 0.40              |
| 51:9:801:PSU:H5''  | 51:9:802:A:OP2     | 2.21                     | 0.40              |
| 51:9:840:C:O2      | 76:YY:12:PHE:CE1   | 2.74                     | 0.40              |
| 51:9:870:A:C4'     | 51:9:871:U:OP2     | 2.69                     | 0.40              |
| 51:9:872:A:O2'     | 51:9:873:G:C5'     | 2.63                     | 0.40              |
| 51:9:874:G:H2'     | 51:9:875:A:C8      | 2.56                     | 0.40              |
| 51:9:1201:U:H2'    | 51:9:1202:U:C6     | 2.56                     | 0.40              |
| 51:9:1287:A:C2     | 51:9:1313:A:N3     | 2.89                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:1306:U:C3'    | 51:9:1307:U:H5''   | 2.51                     | 0.40              |
| 51:9:1557:C:O2     | 51:9:1557:C:C2'    | 2.69                     | 0.40              |
| 51:9:1772:C:O2'    | 51:9:1773:C:H5'    | 2.21                     | 0.40              |
| 54:CC:252:THR:HG22 | 74:WW:99:PHE:CZ    | 2.57                     | 0.40              |
| 55:DD:27:ARG:C     | 62:KK:61:GLN:NE2   | 2.79                     | 0.40              |
| 55:DD:139:SER:O    | 55:DD:182:LEU:HD23 | 2.21                     | 0.40              |
| 57:FF:42:LYS:HB3   | 57:FF:43:GLU:OE1   | 2.22                     | 0.40              |
| 59:HH:26:ALA:HA    | 59:HH:29:GLU:OE1   | 2.21                     | 0.40              |
| 61:JJ:160:SER:O    | 61:JJ:166:GLY:HA3  | 2.21                     | 0.40              |
| 62:KK:66:HIS:O     | 62:KK:68:TYR:CE1   | 2.75                     | 0.40              |
| 64:MM:18:LEU:HA    | 64:MM:21:VAL:HG12  | 2.04                     | 0.40              |
| 64:MM:61:TYR:CE1   | 64:MM:65:VAL:HG21  | 2.56                     | 0.40              |
| 65:NN:83:ASP:OD1   | 65:NN:84:LEU:N     | 2.54                     | 0.40              |
| 66:OO:34:PHE:HB3   | 66:OO:41:PHE:HB2   | 2.02                     | 0.40              |
| 70:SS:130:ARG:HD2  | 70:SS:134:GLN:HG3  | 2.03                     | 0.40              |
| 84:gg:8:ARG:HA     | 84:gg:8:ARG:NE     | 2.33                     | 0.40              |
| 84:gg:10:THR:HG22  | 84:gg:308:ARG:HG2  | 2.03                     | 0.40              |
| 84:gg:77:PHE:CE1   | 84:gg:91:ASP:OD2   | 2.74                     | 0.40              |
| 84:gg:210:GLY:CA   | 84:gg:239:LEU:HD11 | 2.50                     | 0.40              |
| 87:jj:120:LEU:HD23 | 87:jj:120:LEU:HA   | 1.93                     | 0.40              |
| 87:jj:253:LEU:HD13 | 87:jj:564:ILE:HD11 | 2.02                     | 0.40              |
| 87:jj:360:PHE:C    | 87:jj:361:GLU:HG2  | 2.47                     | 0.40              |
| 5:E:101:GLY:O      | 5:E:102:ASP:C      | 2.64                     | 0.40              |
| 5:E:269:GLN:N      | 48:5:4931:G:OP1    | 2.44                     | 0.40              |
| 11:L:25:TRP:CZ2    | 13:N:201:HIS:CE1   | 3.09                     | 0.40              |
| 11:L:165:LYS:O     | 26:a:100:ILE:CD1   | 2.69                     | 0.40              |
| 13:N:10:LEU:HD12   | 34:i:48:CYS:SG     | 2.61                     | 0.40              |
| 13:N:114:ARG:HD2   | 13:N:137:PRO:HG3   | 2.03                     | 0.40              |
| 13:N:146:PRO:HA    | 13:N:149:GLN:HG2   | 2.03                     | 0.40              |
| 13:N:166:SER:O     | 13:N:170:LYS:HG2   | 2.21                     | 0.40              |
| 14:O:171:LYS:NZ    | 48:5:4759:C:OP2    | 2.53                     | 0.40              |
| 17:R:28:GLU:OE1    | 17:R:28:GLU:HA     | 2.22                     | 0.40              |
| 20:U:19:LEU:HD11   | 20:U:77:PRO:HA     | 2.03                     | 0.40              |
| 20:U:42:PHE:CG     | 20:U:90:TYR:HD2    | 2.39                     | 0.40              |
| 32:g:26:PRO:HG3    | 48:5:2639:U:H1'    | 2.03                     | 0.40              |
| 37:l:26:TRP:CE3    | 37:l:27:ILE:HD13   | 2.57                     | 0.40              |
| 48:5:126:C:H2'     | 48:5:127:G:C8      | 2.55                     | 0.40              |
| 48:5:216:C:O3'     | 48:5:217:C:H2'     | 2.21                     | 0.40              |
| 48:5:424:U:H2'     | 48:5:425:U:C6      | 2.55                     | 0.40              |
| 48:5:520:U:O4      | 48:5:641:G:O6      | 2.39                     | 0.40              |
| 48:5:1834:U:O2     | 48:5:1834:U:O4'    | 2.39                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:1905:U:H2'    | 48:5:1906:U:O4'    | 2.21                     | 0.40              |
| 48:5:1987:C:P      | 48:5:1988:G:OP2    | 2.80                     | 0.40              |
| 48:5:2414:G:O2'    | 48:5:2415:U:H5'    | 2.21                     | 0.40              |
| 48:5:3907:G:O4'    | 48:5:4449:A:C5     | 2.74                     | 0.40              |
| 48:5:4232:U:H4'    | 48:5:4233:A:O5'    | 2.20                     | 0.40              |
| 48:5:5053:U:H3'    | 48:5:5054:C:O4'    | 2.21                     | 0.40              |
| 49:7:28:C:H2'      | 49:7:29:C:H5'      | 2.03                     | 0.40              |
| 50:8:49:G:H2'      | 50:8:50:C:O4'      | 2.22                     | 0.40              |
| 51:9:173:A:H2'     | 51:9:174:OMC:O4'   | 2.22                     | 0.40              |
| 51:9:488:U:O2'     | 51:9:489:A:P       | 2.79                     | 0.40              |
| 51:9:886:A:H3'     | 51:9:887:U:C5'     | 2.51                     | 0.40              |
| 51:9:1288:U:O4     | 51:9:1312:G:N2     | 2.53                     | 0.40              |
| 51:9:1420:G:OP1    | 51:9:1420:G:C8     | 2.74                     | 0.40              |
| 51:9:1573:G:H2'    | 51:9:1574:C:O4'    | 2.21                     | 0.40              |
| 51:9:1601:A:H4'    | 51:9:1602:U:C6     | 2.57                     | 0.40              |
| 51:9:1621:U:OP1    | 67:PP:40:ARG:HG2   | 2.22                     | 0.40              |
| 57:FF:128:ILE:HG21 | 80:cc:68:LEU:HD12  | 2.04                     | 0.40              |
| 59:HH:87:PHE:O     | 59:HH:88:SER:C     | 2.65                     | 0.40              |
| 60:II:124:LYS:HB3  | 60:II:167:GLN:OE1  | 2.21                     | 0.40              |
| 61:JJ:169:ARG:HE   | 61:JJ:169:ARG:HB3  | 1.81                     | 0.40              |
| 62:KK:84:HIS:N     | 62:KK:84:HIS:CD2   | 2.87                     | 0.40              |
| 64:MM:89:VAL:HG12  | 64:MM:90:GLY:N     | 2.36                     | 0.40              |
| 67:PP:83:MET:HG3   | 67:PP:89:MET:HE1   | 2.03                     | 0.40              |
| 70:SS:124:ARG:NH2  | 70:SS:129:LEU:HB3  | 2.36                     | 0.40              |
| 71:TT:18:LEU:HD23  | 71:TT:58:ALA:CA    | 2.52                     | 0.40              |
| 71:TT:28:LEU:O     | 71:TT:28:LEU:HG    | 2.21                     | 0.40              |
| 75:XX:102:VAL:CG1  | 75:XX:120:PHE:HB3  | 2.52                     | 0.40              |
| 76:YY:10:ARG:NH2   | 76:YY:24:VAL:HG11  | 2.36                     | 0.40              |
| 84:gg:4:GLN:CG     | 84:gg:5:MET:N      | 2.84                     | 0.40              |
| 84:gg:48:ASP:O     | 84:gg:51:ASN:O     | 2.39                     | 0.40              |
| 84:gg:157:SER:OG   | 84:gg:164:ILE:HB   | 2.21                     | 0.40              |
| 86:ii:252:LYS:HD3  | 86:ii:274:VAL:HG21 | 2.03                     | 0.40              |
| 87:jj:452:GLU:H    | 87:jj:452:GLU:CD   | 2.29                     | 0.40              |
| 1:A:186:TYR:HB2    | 1:A:196:TRP:CZ3    | 2.56                     | 0.40              |
| 3:C:11:TYR:CZ      | 3:C:148:PRO:HB2    | 2.57                     | 0.40              |
| 3:C:308:LYS:HD3    | 3:C:310:HIS:NE2    | 2.35                     | 0.40              |
| 4:D:108:ARG:HG2    | 4:D:112:ARG:HH21   | 1.87                     | 0.40              |
| 7:G:87:LEU:HD21    | 7:G:222:ILE:HD13   | 2.03                     | 0.40              |
| 10:J:139:PHE:HA    | 10:J:151:ILE:HD11  | 2.02                     | 0.40              |
| 13:N:49:ARG:NH2    | 48:5:152:U:OP2     | 2.54                     | 0.40              |
| 15:P:94:MET:HE1    | 15:P:146:ILE:HB    | 2.04                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:R:133:LYS:HG2   | 17:R:137:ILE:HD12  | 2.02                     | 0.40              |
| 20:U:78:PHE:HE2    | 20:U:83:LEU:HD21   | 1.86                     | 0.40              |
| 20:U:80:LYS:O      | 20:U:110:TYR:HE2   | 2.05                     | 0.40              |
| 26:a:38:MET:HE2    | 26:a:53:PHE:CG     | 2.56                     | 0.40              |
| 29:d:37:GLY:O      | 29:d:41:ARG:HG3    | 2.22                     | 0.40              |
| 44:t:78:SER:HB3    | 44:t:117:ARG:HD2   | 2.02                     | 0.40              |
| 46:2:20(A):U:C3'   | 46:2:21:A:C5'      | 3.00                     | 0.40              |
| 48:5:44:A:O2'      | 48:5:94:A:N1       | 2.45                     | 0.40              |
| 48:5:134:G:H4'     | 48:5:135:G:H5'     | 2.04                     | 0.40              |
| 48:5:231:U:O2'     | 48:5:232:G:OP1     | 2.29                     | 0.40              |
| 48:5:261:G:N1      | 48:5:262:G:C2      | 2.90                     | 0.40              |
| 48:5:382:G:H4'     | 48:5:407:A:N1      | 2.35                     | 0.40              |
| 48:5:654:C:C2      | 48:5:655:C:C6      | 3.09                     | 0.40              |
| 48:5:757:G:C2      | 48:5:758:G:N7      | 2.90                     | 0.40              |
| 48:5:913:U:HO2'    | 48:5:914:U:P       | 2.36                     | 0.40              |
| 48:5:1991:A:O2'    | 48:5:1992:U:C5'    | 2.69                     | 0.40              |
| 48:5:2415:U:H2'    | 48:5:2416:G:C8     | 2.56                     | 0.40              |
| 48:5:2446:C:H2'    | 48:5:2447:U:C1'    | 2.52                     | 0.40              |
| 48:5:2666:U:O2'    | 48:5:2668:G:N7     | 2.48                     | 0.40              |
| 48:5:3604:A:H2'    | 48:5:3605:C:N1     | 2.37                     | 0.40              |
| 48:5:4471:U:H2'    | 48:5:4472:G:C8     | 2.56                     | 0.40              |
| 48:5:4538:G:H2'    | 48:5:4539:U:C6     | 2.57                     | 0.40              |
| 51:9:85:A:H2'      | 51:9:86:C:C6       | 2.57                     | 0.40              |
| 51:9:124:U:O4      | 51:9:338:G:N1      | 2.55                     | 0.40              |
| 51:9:360:A:C2      | 51:9:362:C:H2'     | 2.57                     | 0.40              |
| 51:9:690:G:C8      | 51:9:691:G:H1'     | 2.57                     | 0.40              |
| 51:9:1134:G:H2'    | 51:9:1135:C:C6     | 2.56                     | 0.40              |
| 51:9:1139:C:O2     | 51:9:1139:C:OP1    | 2.40                     | 0.40              |
| 51:9:1315:U:O5'    | 62:KK:2:LEU:HB2    | 2.22                     | 0.40              |
| 51:9:1442:OMU:H3'  | 51:9:1442:OMU:H6   | 2.04                     | 0.40              |
| 51:9:1480:A:C2'    | 81:dd:56:ASP:OD1   | 2.66                     | 0.40              |
| 51:9:1617:G:N2     | 51:9:1619:A:H3'    | 2.36                     | 0.40              |
| 54:CC:233:LEU:HD23 | 54:CC:233:LEU:C    | 2.46                     | 0.40              |
| 55:DD:105:LEU:HD22 | 55:DD:122:VAL:HG11 | 2.03                     | 0.40              |
| 58:GG:32:MET:SD    | 58:GG:63:MET:HE2   | 2.62                     | 0.40              |
| 59:HH:135:PHE:HB3  | 59:HH:136:PRO:HD3  | 2.03                     | 0.40              |
| 59:HH:149:ASP:O    | 59:HH:149:ASP:OD1  | 2.40                     | 0.40              |
| 65:NN:110:ASP:O    | 65:NN:114:ARG:HG2  | 2.20                     | 0.40              |
| 68:QQ:57:LEU:HD21  | 68:QQ:115:TYR:HB2  | 2.03                     | 0.40              |
| 84:gg:159:ASN:O    | 84:gg:160:SER:C    | 2.64                     | 0.40              |
| 84:gg:259:TRP:HD1  | 84:gg:266:ILE:HA   | 1.86                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 87:jj:62:ILE:HD12  | 87:jj:62:ILE:H     | 1.87                     | 0.40              |
| 87:jj:105:VAL:N    | 87:jj:284:ASP:OD1  | 2.54                     | 0.40              |
| 87:jj:292:VAL:HG23 | 87:jj:295:ALA:HB3  | 2.03                     | 0.40              |
| 4:D:225:GLN:HB2    | 49:7:49:A:OP1      | 2.22                     | 0.40              |
| 12:M:129:LYS:HD2   | 48:5:4894:A:OP1    | 2.22                     | 0.40              |
| 21:V:112:MET:HE2   | 21:V:112:MET:HB3   | 1.99                     | 0.40              |
| 37:l:29:MET:HE3    | 37:l:29:MET:HA     | 2.04                     | 0.40              |
| 42:r:56:ASP:OD1    | 42:r:57:GLY:N      | 2.55                     | 0.40              |
| 46:2:18:G:O4'      | 46:2:58:A:C2       | 2.75                     | 0.40              |
| 48:5:716:C:H2'     | 48:5:717:U:O4'     | 2.22                     | 0.40              |
| 48:5:969:C:H2'     | 48:5:2259:G:O6     | 2.21                     | 0.40              |
| 48:5:4116:C:H4'    | 48:5:4117:U:OP2    | 2.22                     | 0.40              |
| 48:5:4917:C:O5'    | 48:5:4917:C:H6     | 2.05                     | 0.40              |
| 49:7:11:A:N1       | 49:7:66:G:O2'      | 2.42                     | 0.40              |
| 51:9:201:C:H6      | 51:9:201:C:O5'     | 2.05                     | 0.40              |
| 51:9:905:C:O3'     | 51:9:906:U:O4'     | 2.39                     | 0.40              |
| 51:9:1060:A:O2'    | 51:9:1062:A:N7     | 2.48                     | 0.40              |
| 51:9:1447:G:C2'    | 51:9:1448:A:H5'    | 2.52                     | 0.40              |
| 52:AA:165:ASN:HA   | 52:AA:171:VAL:HG22 | 2.03                     | 0.40              |
| 54:CC:125:LYS:HE2  | 54:CC:141:VAL:HG11 | 2.02                     | 0.40              |
| 55:DD:32:ASP:HB2   | 55:DD:54:ARG:HB3   | 2.03                     | 0.40              |
| 57:FF:179:ASN:HB2  | 57:FF:187:SER:HB2  | 2.03                     | 0.40              |
| 58:GG:35:GLU:HB3   | 58:GG:49:VAL:HG12  | 2.04                     | 0.40              |
| 61:JJ:134:HIS:O    | 61:JJ:159:PHE:HA   | 2.21                     | 0.40              |
| 69:RR:105:MET:O    | 69:RR:109:LEU:HG   | 2.22                     | 0.40              |
| 71:TT:31:PRO:O     | 71:TT:34:VAL:HG23  | 2.22                     | 0.40              |
| 77:ZZ:62:VAL:N     | 77:ZZ:63:PRO:CD    | 2.85                     | 0.40              |
| 84:gg:199:THR:HG21 | 84:gg:239:LEU:C    | 2.47                     | 0.40              |
| 86:ii:332:VAL:HG12 | 86:ii:370:GLU:HG3  | 2.03                     | 0.40              |
| 86:ii:359:ASP:O    | 86:ii:360:LYS:HB2  | 2.20                     | 0.40              |
| 87:jj:82:GLU:O     | 87:jj:83:THR:C     | 2.64                     | 0.40              |
| 87:jj:216:ASP:O    | 87:jj:217:LEU:HD22 | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

entries.

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | A     | 242/257 (94%) | 226 (93%) | 16 (7%)  | 0        | 100         | 100 |
| 2   | B     | 392/403 (97%) | 376 (96%) | 16 (4%)  | 0        | 100         | 100 |
| 3   | C     | 360/413 (87%) | 348 (97%) | 12 (3%)  | 0        | 100         | 100 |
| 4   | D     | 287/297 (97%) | 270 (94%) | 16 (6%)  | 1 (0%)   | 36          | 55  |
| 5   | E     | 209/291 (72%) | 189 (90%) | 20 (10%) | 0        | 100         | 100 |
| 6   | F     | 223/247 (90%) | 218 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 7   | G     | 214/319 (67%) | 202 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 8   | H     | 188/192 (98%) | 178 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 9   | I     | 200/214 (94%) | 193 (96%) | 7 (4%)   | 0        | 100         | 100 |
| 10  | J     | 165/178 (93%) | 151 (92%) | 13 (8%)  | 1 (1%)   | 21          | 38  |
| 11  | L     | 208/211 (99%) | 202 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 12  | M     | 136/218 (62%) | 132 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 13  | N     | 201/204 (98%) | 199 (99%) | 2 (1%)   | 0        | 100         | 100 |
| 14  | O     | 196/203 (97%) | 187 (95%) | 8 (4%)   | 1 (0%)   | 24          | 43  |
| 15  | P     | 151/184 (82%) | 145 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 16  | Q     | 185/188 (98%) | 179 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 17  | R     | 177/196 (90%) | 172 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 18  | S     | 174/176 (99%) | 166 (95%) | 8 (5%)   | 0        | 100         | 100 |
| 19  | T     | 157/160 (98%) | 152 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 20  | U     | 96/128 (75%)  | 88 (92%)  | 8 (8%)   | 0        | 100         | 100 |
| 21  | V     | 128/140 (91%) | 127 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 22  | W     | 61/157 (39%)  | 60 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 23  | X     | 114/156 (73%) | 108 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 24  | Y     | 132/145 (91%) | 127 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 25  | Z     | 133/136 (98%) | 118 (89%) | 15 (11%) | 0        | 100         | 100 |
| 26  | a     | 145/148 (98%) | 136 (94%) | 8 (6%)   | 1 (1%)   | 18          | 34  |
| 27  | b     | 73/245 (30%)  | 70 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 28  | c     | 92/115 (80%)  | 87 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 29  | d     | 96/125 (77%)  | 94 (98%)  | 2 (2%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 30  | e     | 126/135 (93%) | 122 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 31  | f     | 107/110 (97%) | 102 (95%) | 5 (5%)   | 0        | 100         | 100 |
| 32  | g     | 112/117 (96%) | 110 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 33  | h     | 120/123 (98%) | 114 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 34  | i     | 100/105 (95%) | 97 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 35  | j     | 84/97 (87%)   | 82 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 36  | k     | 66/70 (94%)   | 60 (91%)  | 5 (8%)   | 1 (2%)   | 8           | 16  |
| 37  | l     | 47/51 (92%)   | 45 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 38  | m     | 49/93 (53%)   | 47 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 39  | n     | 21/25 (84%)   | 21 (100%) | 0        | 0        | 100         | 100 |
| 40  | o     | 101/106 (95%) | 95 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 41  | p     | 89/92 (97%)   | 81 (91%)  | 8 (9%)   | 0        | 100         | 100 |
| 42  | r     | 123/137 (90%) | 113 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 43  | s     | 188/318 (59%) | 163 (87%) | 25 (13%) | 0        | 100         | 100 |
| 44  | t     | 135/165 (82%) | 113 (84%) | 21 (16%) | 1 (1%)   | 18          | 34  |
| 45  | 1     | 13/130 (10%)  | 11 (85%)  | 2 (15%)  | 0        | 100         | 100 |
| 52  | AA    | 204/295 (69%) | 189 (93%) | 15 (7%)  | 0        | 100         | 100 |
| 53  | BB    | 210/264 (80%) | 200 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 54  | CC    | 214/293 (73%) | 202 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 55  | DD    | 217/243 (89%) | 196 (90%) | 21 (10%) | 0        | 100         | 100 |
| 56  | EE    | 257/263 (98%) | 231 (90%) | 26 (10%) | 0        | 100         | 100 |
| 57  | FF    | 177/204 (87%) | 163 (92%) | 13 (7%)  | 1 (1%)   | 21          | 38  |
| 58  | GG    | 235/249 (94%) | 205 (87%) | 29 (12%) | 1 (0%)   | 30          | 49  |
| 59  | HH    | 173/194 (89%) | 146 (84%) | 27 (16%) | 0        | 100         | 100 |
| 60  | II    | 204/208 (98%) | 194 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 61  | JJ    | 183/194 (94%) | 167 (91%) | 16 (9%)  | 0        | 100         | 100 |
| 62  | KK    | 84/165 (51%)  | 76 (90%)  | 8 (10%)  | 0        | 100         | 100 |
| 63  | LL    | 132/158 (84%) | 125 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 64  | MM    | 120/132 (91%) | 91 (76%)  | 29 (24%) | 0        | 100         | 100 |
| 65  | NN    | 148/151 (98%) | 144 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 66  | OO    | 125/168 (74%) | 121 (97%) | 4 (3%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 67  | PP    | 115/145 (79%)     | 106 (92%)   | 9 (8%)   | 0        | 100         | 100 |
| 68  | QQ    | 138/146 (94%)     | 128 (93%)   | 10 (7%)  | 0        | 100         | 100 |
| 69  | RR    | 116/135 (86%)     | 106 (91%)   | 10 (9%)  | 0        | 100         | 100 |
| 70  | SS    | 138/152 (91%)     | 130 (94%)   | 8 (6%)   | 0        | 100         | 100 |
| 71  | TT    | 136/145 (94%)     | 124 (91%)   | 12 (9%)  | 0        | 100         | 100 |
| 72  | UU    | 100/119 (84%)     | 89 (89%)    | 11 (11%) | 0        | 100         | 100 |
| 73  | VV    | 79/83 (95%)       | 71 (90%)    | 8 (10%)  | 0        | 100         | 100 |
| 74  | WW    | 127/130 (98%)     | 120 (94%)   | 7 (6%)   | 0        | 100         | 100 |
| 75  | XX    | 139/143 (97%)     | 130 (94%)   | 9 (6%)   | 0        | 100         | 100 |
| 76  | YY    | 121/130 (93%)     | 111 (92%)   | 10 (8%)  | 0        | 100         | 100 |
| 77  | ZZ    | 70/125 (56%)      | 64 (91%)    | 6 (9%)   | 0        | 100         | 100 |
| 78  | aa    | 96/115 (84%)      | 86 (90%)    | 10 (10%) | 0        | 100         | 100 |
| 79  | bb    | 75/84 (89%)       | 70 (93%)    | 5 (7%)   | 0        | 100         | 100 |
| 80  | cc    | 59/69 (86%)       | 54 (92%)    | 5 (8%)   | 0        | 100         | 100 |
| 81  | dd    | 51/56 (91%)       | 45 (88%)    | 6 (12%)  | 0        | 100         | 100 |
| 82  | ee    | 43/133 (32%)      | 37 (86%)    | 6 (14%)  | 0        | 100         | 100 |
| 83  | ff    | 59/156 (38%)      | 49 (83%)    | 10 (17%) | 0        | 100         | 100 |
| 84  | gg    | 300/317 (95%)     | 252 (84%)   | 48 (16%) | 0        | 100         | 100 |
| 86  | ii    | 414/459 (90%)     | 380 (92%)   | 33 (8%)  | 1 (0%)   | 43          | 63  |
| 87  | jj    | 574/599 (96%)     | 529 (92%)   | 44 (8%)  | 1 (0%)   | 43          | 63  |
| All | All   | 12249/14542 (84%) | 11407 (93%) | 832 (7%) | 10 (0%)  | 49          | 68  |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 58  | GG    | 128 | THR  |
| 57  | FF    | 33  | ILE  |
| 86  | ii    | 180 | HIS  |
| 26  | a     | 15  | VAL  |
| 10  | J     | 173 | ILE  |
| 14  | O     | 187 | LYS  |
| 4   | D     | 235 | MET  |
| 87  | jj    | 96  | ARG  |
| 36  | k     | 61  | PRO  |
| 44  | t     | 32  | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | A     | 187/199 (94%)  | 186 (100%) | 1 (0%)   | 81          | 92  |
| 2   | B     | 336/348 (97%)  | 328 (98%)  | 8 (2%)   | 43          | 70  |
| 3   | C     | 302/337 (90%)  | 295 (98%)  | 7 (2%)   | 44          | 72  |
| 4   | D     | 245/250 (98%)  | 238 (97%)  | 7 (3%)   | 37          | 65  |
| 5   | E     | 191/251 (76%)  | 183 (96%)  | 8 (4%)   | 26          | 52  |
| 6   | F     | 196/215 (91%)  | 196 (100%) | 0        | 100         | 100 |
| 7   | G     | 189/272 (70%)  | 181 (96%)  | 8 (4%)   | 26          | 52  |
| 8   | H     | 169/171 (99%)  | 168 (99%)  | 1 (1%)   | 78          | 91  |
| 9   | I     | 174/181 (96%)  | 173 (99%)  | 1 (1%)   | 78          | 91  |
| 10  | J     | 140/149 (94%)  | 134 (96%)  | 6 (4%)   | 26          | 51  |
| 11  | L     | 175/176 (99%)  | 171 (98%)  | 4 (2%)   | 44          | 72  |
| 12  | M     | 117/161 (73%)  | 116 (99%)  | 1 (1%)   | 70          | 87  |
| 13  | N     | 171/172 (99%)  | 169 (99%)  | 2 (1%)   | 63          | 83  |
| 14  | O     | 170/173 (98%)  | 166 (98%)  | 4 (2%)   | 43          | 70  |
| 15  | P     | 134/163 (82%)  | 133 (99%)  | 1 (1%)   | 76          | 89  |
| 16  | Q     | 164/165 (99%)  | 161 (98%)  | 3 (2%)   | 51          | 77  |
| 17  | R     | 158/175 (90%)  | 155 (98%)  | 3 (2%)   | 50          | 76  |
| 18  | S     | 157/157 (100%) | 153 (98%)  | 4 (2%)   | 42          | 69  |
| 19  | T     | 139/140 (99%)  | 139 (100%) | 0        | 100         | 100 |
| 20  | U     | 88/114 (77%)   | 85 (97%)   | 3 (3%)   | 32          | 60  |
| 21  | V     | 100/107 (94%)  | 99 (99%)   | 1 (1%)   | 68          | 86  |
| 22  | W     | 55/126 (44%)   | 55 (100%)  | 0        | 100         | 100 |
| 23  | X     | 104/134 (78%)  | 103 (99%)  | 1 (1%)   | 68          | 86  |
| 24  | Y     | 124/135 (92%)  | 123 (99%)  | 1 (1%)   | 73          | 88  |
| 25  | Z     | 117/118 (99%)  | 113 (97%)  | 4 (3%)   | 32          | 60  |
| 26  | a     | 119/120 (99%)  | 118 (99%)  | 1 (1%)   | 73          | 88  |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 27  | b     | 62/184 (34%)  | 62 (100%)  | 0        | 100         | 100 |
| 28  | c     | 80/98 (82%)   | 76 (95%)   | 4 (5%)   | 22          | 44  |
| 29  | d     | 91/110 (83%)  | 89 (98%)   | 2 (2%)   | 45          | 73  |
| 30  | e     | 114/121 (94%) | 114 (100%) | 0        | 100         | 100 |
| 31  | f     | 88/89 (99%)   | 87 (99%)   | 1 (1%)   | 65          | 84  |
| 32  | g     | 98/100 (98%)  | 95 (97%)   | 3 (3%)   | 35          | 62  |
| 33  | h     | 109/110 (99%) | 106 (97%)  | 3 (3%)   | 38          | 66  |
| 34  | i     | 86/89 (97%)   | 85 (99%)   | 1 (1%)   | 63          | 83  |
| 35  | j     | 73/80 (91%)   | 68 (93%)   | 5 (7%)   | 14          | 31  |
| 36  | k     | 63/65 (97%)   | 57 (90%)   | 6 (10%)  | 8           | 17  |
| 37  | l     | 46/48 (96%)   | 46 (100%)  | 0        | 100         | 100 |
| 38  | m     | 47/84 (56%)   | 46 (98%)   | 1 (2%)   | 47          | 74  |
| 39  | n     | 22/24 (92%)   | 22 (100%)  | 0        | 100         | 100 |
| 40  | o     | 91/94 (97%)   | 90 (99%)   | 1 (1%)   | 65          | 84  |
| 41  | p     | 74/75 (99%)   | 72 (97%)   | 2 (3%)   | 39          | 67  |
| 42  | r     | 109/121 (90%) | 109 (100%) | 0        | 100         | 100 |
| 43  | s     | 159/258 (62%) | 154 (97%)  | 5 (3%)   | 35          | 62  |
| 44  | t     | 115/137 (84%) | 112 (97%)  | 3 (3%)   | 40          | 68  |
| 45  | 1     | 13/102 (13%)  | 13 (100%)  | 0        | 100         | 100 |
| 52  | AA    | 172/244 (70%) | 165 (96%)  | 7 (4%)   | 27          | 53  |
| 53  | BB    | 193/231 (84%) | 192 (100%) | 1 (0%)   | 81          | 92  |
| 54  | CC    | 182/225 (81%) | 172 (94%)  | 10 (6%)  | 19          | 40  |
| 55  | DD    | 185/202 (92%) | 177 (96%)  | 8 (4%)   | 26          | 51  |
| 56  | EE    | 222/225 (99%) | 217 (98%)  | 5 (2%)   | 44          | 72  |
| 57  | FF    | 154/170 (91%) | 145 (94%)  | 9 (6%)   | 18          | 38  |
| 58  | GG    | 207/218 (95%) | 200 (97%)  | 7 (3%)   | 32          | 60  |
| 59  | HH    | 158/174 (91%) | 151 (96%)  | 7 (4%)   | 25          | 50  |
| 60  | II    | 178/180 (99%) | 172 (97%)  | 6 (3%)   | 32          | 60  |
| 61  | JJ    | 161/168 (96%) | 157 (98%)  | 4 (2%)   | 42          | 69  |
| 62  | KK    | 78/136 (57%)  | 76 (97%)   | 2 (3%)   | 40          | 68  |
| 63  | LL    | 125/142 (88%) | 121 (97%)  | 4 (3%)   | 34          | 62  |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|----------|-------------|----|
| 64  | MM    | 102/108 (94%)     | 99 (97%)    | 3 (3%)   | 37          | 65 |
| 65  | NN    | 130/131 (99%)     | 128 (98%)   | 2 (2%)   | 57          | 80 |
| 66  | OO    | 100/130 (77%)     | 94 (94%)    | 6 (6%)   | 17          | 36 |
| 67  | PP    | 106/130 (82%)     | 104 (98%)   | 2 (2%)   | 50          | 76 |
| 68  | QQ    | 116/121 (96%)     | 115 (99%)   | 1 (1%)   | 70          | 87 |
| 69  | RR    | 107/121 (88%)     | 99 (92%)    | 8 (8%)   | 12          | 26 |
| 70  | SS    | 122/132 (92%)     | 121 (99%)   | 1 (1%)   | 73          | 88 |
| 71  | TT    | 109/115 (95%)     | 106 (97%)   | 3 (3%)   | 38          | 66 |
| 72  | UU    | 93/107 (87%)      | 89 (96%)    | 4 (4%)   | 26          | 51 |
| 73  | VV    | 65/67 (97%)       | 63 (97%)    | 2 (3%)   | 35          | 62 |
| 74  | WW    | 112/113 (99%)     | 109 (97%)   | 3 (3%)   | 39          | 67 |
| 75  | XX    | 113/115 (98%)     | 110 (97%)   | 3 (3%)   | 39          | 67 |
| 76  | YY    | 107/112 (96%)     | 101 (94%)   | 6 (6%)   | 19          | 39 |
| 77  | ZZ    | 64/103 (62%)      | 63 (98%)    | 1 (2%)   | 55          | 79 |
| 78  | aa    | 85/98 (87%)       | 83 (98%)    | 2 (2%)   | 43          | 70 |
| 79  | bb    | 72/76 (95%)       | 71 (99%)    | 1 (1%)   | 59          | 81 |
| 80  | cc    | 54/62 (87%)       | 50 (93%)    | 4 (7%)   | 13          | 27 |
| 81  | dd    | 47/49 (96%)       | 44 (94%)    | 3 (6%)   | 16          | 33 |
| 82  | ee    | 39/106 (37%)      | 38 (97%)    | 1 (3%)   | 40          | 68 |
| 83  | ff    | 59/140 (42%)      | 57 (97%)    | 2 (3%)   | 32          | 60 |
| 84  | gg    | 263/275 (96%)     | 246 (94%)   | 17 (6%)  | 15          | 32 |
| 86  | ii    | 358/394 (91%)     | 336 (94%)   | 22 (6%)  | 17          | 35 |
| 87  | jj    | 508/526 (97%)     | 491 (97%)   | 17 (3%)  | 33          | 61 |
| All | All   | 10707/12344 (87%) | 10406 (97%) | 301 (3%) | 38          | 66 |

All (301) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 77  | ILE  |
| 2   | B     | 38  | SER  |
| 2   | B     | 66  | LYS  |
| 2   | B     | 125 | SER  |
| 2   | B     | 136 | LYS  |
| 2   | B     | 138 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 287 | ILE  |
| 2   | B     | 313 | SER  |
| 2   | B     | 317 | LEU  |
| 3   | C     | 150 | LEU  |
| 3   | C     | 153 | VAL  |
| 3   | C     | 204 | ARG  |
| 3   | C     | 227 | ILE  |
| 3   | C     | 259 | LYS  |
| 3   | C     | 285 | LEU  |
| 3   | C     | 308 | LYS  |
| 4   | D     | 154 | THR  |
| 4   | D     | 185 | SER  |
| 4   | D     | 224 | SER  |
| 4   | D     | 228 | LYS  |
| 4   | D     | 232 | THR  |
| 4   | D     | 235 | MET  |
| 4   | D     | 288 | LEU  |
| 5   | E     | 62  | SER  |
| 5   | E     | 66  | SER  |
| 5   | E     | 98  | PRO  |
| 5   | E     | 124 | VAL  |
| 5   | E     | 203 | LYS  |
| 5   | E     | 204 | ILE  |
| 5   | E     | 214 | HIS  |
| 5   | E     | 276 | SER  |
| 7   | G     | 43  | GLN  |
| 7   | G     | 53  | ARG  |
| 7   | G     | 86  | VAL  |
| 7   | G     | 98  | LEU  |
| 7   | G     | 150 | LYS  |
| 7   | G     | 164 | ILE  |
| 7   | G     | 229 | ARG  |
| 7   | G     | 250 | ILE  |
| 8   | H     | 94  | SER  |
| 9   | I     | 214 | SER  |
| 10  | J     | 49  | VAL  |
| 10  | J     | 52  | LYS  |
| 10  | J     | 81  | GLU  |
| 10  | J     | 132 | VAL  |
| 10  | J     | 158 | SER  |
| 10  | J     | 171 | ASP  |
| 11  | L     | 42  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | L     | 122 | SER  |
| 11  | L     | 146 | LEU  |
| 11  | L     | 208 | GLU  |
| 12  | M     | 50  | MET  |
| 13  | N     | 36  | LEU  |
| 13  | N     | 67  | ARG  |
| 14  | O     | 16  | LEU  |
| 14  | O     | 61  | ARG  |
| 14  | O     | 173 | GLN  |
| 14  | O     | 201 | LEU  |
| 15  | P     | 14  | SER  |
| 16  | Q     | 42  | THR  |
| 16  | Q     | 128 | LEU  |
| 16  | Q     | 167 | VAL  |
| 17  | R     | 13  | SER  |
| 17  | R     | 29  | THR  |
| 17  | R     | 37  | SER  |
| 18  | S     | 21  | LYS  |
| 18  | S     | 71  | SER  |
| 18  | S     | 102 | THR  |
| 18  | S     | 138 | ARG  |
| 20  | U     | 60  | VAL  |
| 20  | U     | 101 | ARG  |
| 20  | U     | 102 | VAL  |
| 21  | V     | 139 | ILE  |
| 23  | X     | 53  | ARG  |
| 24  | Y     | 46  | SER  |
| 25  | Z     | 26  | VAL  |
| 25  | Z     | 43  | VAL  |
| 25  | Z     | 60  | LYS  |
| 25  | Z     | 96  | VAL  |
| 26  | a     | 95  | THR  |
| 28  | c     | 16  | SER  |
| 28  | c     | 75  | SER  |
| 28  | c     | 92  | CYS  |
| 28  | c     | 103 | ASP  |
| 29  | d     | 46  | LEU  |
| 29  | d     | 78  | ARG  |
| 31  | f     | 69  | VAL  |
| 32  | g     | 3   | GLN  |
| 32  | g     | 68  | SER  |
| 32  | g     | 87  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | h     | 19  | LYS  |
| 33  | h     | 20  | GLN  |
| 33  | h     | 42  | SER  |
| 34  | i     | 17  | VAL  |
| 35  | j     | 10  | LYS  |
| 35  | j     | 33  | THR  |
| 35  | j     | 36  | LYS  |
| 35  | j     | 55  | ARG  |
| 35  | j     | 82  | THR  |
| 36  | k     | 8   | ILE  |
| 36  | k     | 14  | THR  |
| 36  | k     | 21  | LYS  |
| 36  | k     | 44  | THR  |
| 36  | k     | 48  | THR  |
| 36  | k     | 61  | PRO  |
| 38  | m     | 84  | GLN  |
| 40  | o     | 79  | SER  |
| 41  | p     | 45  | THR  |
| 41  | p     | 74  | THR  |
| 43  | s     | 11  | SER  |
| 43  | s     | 47  | LEU  |
| 43  | s     | 96  | THR  |
| 43  | s     | 136 | SER  |
| 43  | s     | 187 | LEU  |
| 44  | t     | 13  | VAL  |
| 44  | t     | 63  | THR  |
| 44  | t     | 71  | ILE  |
| 52  | AA    | 13  | GLU  |
| 52  | AA    | 14  | ASP  |
| 52  | AA    | 81  | ASN  |
| 52  | AA    | 89  | LYS  |
| 52  | AA    | 135 | THR  |
| 52  | AA    | 191 | ARG  |
| 52  | AA    | 193 | HIS  |
| 53  | BB    | 88  | THR  |
| 54  | CC    | 72  | ASP  |
| 54  | CC    | 73  | MET  |
| 54  | CC    | 77  | SER  |
| 54  | CC    | 121 | ARG  |
| 54  | CC    | 141 | VAL  |
| 54  | CC    | 184 | VAL  |
| 54  | CC    | 206 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | CC    | 259 | THR  |
| 54  | CC    | 263 | LYS  |
| 54  | CC    | 272 | HIS  |
| 55  | DD    | 5   | ILE  |
| 55  | DD    | 84  | VAL  |
| 55  | DD    | 93  | THR  |
| 55  | DD    | 99  | ILE  |
| 55  | DD    | 123 | LEU  |
| 55  | DD    | 124 | ARG  |
| 55  | DD    | 175 | VAL  |
| 55  | DD    | 221 | THR  |
| 56  | EE    | 140 | VAL  |
| 56  | EE    | 146 | THR  |
| 56  | EE    | 170 | THR  |
| 56  | EE    | 181 | CYS  |
| 56  | EE    | 236 | ILE  |
| 57  | FF    | 26  | ASP  |
| 57  | FF    | 30  | ILE  |
| 57  | FF    | 36  | GLN  |
| 57  | FF    | 66  | CYS  |
| 57  | FF    | 127 | ARG  |
| 57  | FF    | 140 | ASP  |
| 57  | FF    | 193 | LYS  |
| 57  | FF    | 196 | LEU  |
| 57  | FF    | 202 | SER  |
| 58  | GG    | 26  | THR  |
| 58  | GG    | 36  | VAL  |
| 58  | GG    | 53  | SER  |
| 58  | GG    | 67  | VAL  |
| 58  | GG    | 111 | LEU  |
| 58  | GG    | 139 | SER  |
| 58  | GG    | 217 | MET  |
| 59  | HH    | 23  | ILE  |
| 59  | HH    | 24  | SER  |
| 59  | HH    | 28  | LEU  |
| 59  | HH    | 83  | LEU  |
| 59  | HH    | 113 | LYS  |
| 59  | HH    | 167 | GLU  |
| 59  | HH    | 177 | TYR  |
| 60  | II    | 89  | GLU  |
| 60  | II    | 121 | LEU  |
| 60  | II    | 130 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 60  | II    | 159 | SER  |
| 60  | II    | 191 | GLU  |
| 60  | II    | 205 | ARG  |
| 61  | JJ    | 23  | SER  |
| 61  | JJ    | 112 | THR  |
| 61  | JJ    | 128 | VAL  |
| 61  | JJ    | 161 | LEU  |
| 62  | KK    | 3   | MET  |
| 62  | KK    | 61  | GLN  |
| 63  | LL    | 20  | LYS  |
| 63  | LL    | 72  | ILE  |
| 63  | LL    | 116 | CYS  |
| 63  | LL    | 118 | ARG  |
| 64  | MM    | 65  | VAL  |
| 64  | MM    | 91  | LEU  |
| 64  | MM    | 109 | VAL  |
| 65  | NN    | 22  | VAL  |
| 65  | NN    | 145 | THR  |
| 66  | OO    | 45  | THR  |
| 66  | OO    | 48  | SER  |
| 66  | OO    | 81  | VAL  |
| 66  | OO    | 137 | SER  |
| 66  | OO    | 138 | ASP  |
| 66  | OO    | 151 | LEU  |
| 67  | PP    | 75  | VAL  |
| 67  | PP    | 108 | LYS  |
| 68  | QQ    | 7   | LEU  |
| 69  | RR    | 17  | ILE  |
| 69  | RR    | 22  | THR  |
| 69  | RR    | 40  | ILE  |
| 69  | RR    | 70  | SER  |
| 69  | RR    | 76  | GLU  |
| 69  | RR    | 89  | SER  |
| 69  | RR    | 105 | MET  |
| 69  | RR    | 116 | ASN  |
| 70  | SS    | 30  | ILE  |
| 71  | TT    | 49  | ASP  |
| 71  | TT    | 90  | SER  |
| 71  | TT    | 131 | LEU  |
| 72  | UU    | 20  | ILE  |
| 72  | UU    | 24  | LEU  |
| 72  | UU    | 65  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 72  | UU    | 81  | GLN  |
| 73  | VV    | 65  | SER  |
| 73  | VV    | 69  | ILE  |
| 74  | WW    | 63  | VAL  |
| 74  | WW    | 66  | THR  |
| 74  | WW    | 121 | THR  |
| 75  | XX    | 90  | CYS  |
| 75  | XX    | 105 | PHE  |
| 75  | XX    | 130 | LEU  |
| 76  | YY    | 11  | LYS  |
| 76  | YY    | 16  | ARG  |
| 76  | YY    | 42  | GLU  |
| 76  | YY    | 50  | THR  |
| 76  | YY    | 116 | LYS  |
| 76  | YY    | 120 | THR  |
| 77  | ZZ    | 54  | THR  |
| 78  | aa    | 45  | VAL  |
| 78  | aa    | 69  | VAL  |
| 79  | bb    | 34  | ASP  |
| 80  | cc    | 9   | ILE  |
| 80  | cc    | 30  | VAL  |
| 80  | cc    | 62  | GLU  |
| 80  | cc    | 67  | ARG  |
| 81  | dd    | 33  | LYS  |
| 81  | dd    | 49  | ASP  |
| 81  | dd    | 53  | ILE  |
| 82  | ee    | 26  | LYS  |
| 83  | ff    | 125 | VAL  |
| 83  | ff    | 144 | CYS  |
| 84  | gg    | 5   | MET  |
| 84  | gg    | 43  | TRP  |
| 84  | gg    | 66  | VAL  |
| 84  | gg    | 67  | SER  |
| 84  | gg    | 69  | VAL  |
| 84  | gg    | 102 | VAL  |
| 84  | gg    | 110 | SER  |
| 84  | gg    | 113 | PHE  |
| 84  | gg    | 126 | ASP  |
| 84  | gg    | 133 | ASN  |
| 84  | gg    | 160 | SER  |
| 84  | gg    | 165 | ILE  |
| 84  | gg    | 182 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 84  | gg    | 184 | LEU  |
| 84  | gg    | 199 | THR  |
| 84  | gg    | 225 | LYS  |
| 84  | gg    | 285 | GLN  |
| 86  | ii    | 17  | ILE  |
| 86  | ii    | 30  | ASN  |
| 86  | ii    | 123 | SER  |
| 86  | ii    | 154 | SER  |
| 86  | ii    | 166 | ARG  |
| 86  | ii    | 173 | THR  |
| 86  | ii    | 177 | PRO  |
| 86  | ii    | 179 | LYS  |
| 86  | ii    | 189 | ARG  |
| 86  | ii    | 237 | SER  |
| 86  | ii    | 258 | TYR  |
| 86  | ii    | 274 | VAL  |
| 86  | ii    | 284 | LYS  |
| 86  | ii    | 322 | VAL  |
| 86  | ii    | 332 | VAL  |
| 86  | ii    | 342 | LYS  |
| 86  | ii    | 343 | ILE  |
| 86  | ii    | 367 | GLU  |
| 86  | ii    | 368 | LEU  |
| 86  | ii    | 393 | THR  |
| 86  | ii    | 394 | ASP  |
| 86  | ii    | 400 | SER  |
| 87  | jj    | 53  | THR  |
| 87  | jj    | 73  | VAL  |
| 87  | jj    | 104 | GLU  |
| 87  | jj    | 118 | THR  |
| 87  | jj    | 143 | ILE  |
| 87  | jj    | 152 | LEU  |
| 87  | jj    | 160 | LEU  |
| 87  | jj    | 284 | ASP  |
| 87  | jj    | 323 | ARG  |
| 87  | jj    | 370 | THR  |
| 87  | jj    | 445 | VAL  |
| 87  | jj    | 489 | SER  |
| 87  | jj    | 528 | LEU  |
| 87  | jj    | 536 | ASP  |
| 87  | jj    | 574 | ARG  |
| 87  | jj    | 576 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 87  | jj    | 584 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 203 | GLN  |
| 3   | C     | 38  | ASN  |
| 3   | C     | 43  | ASN  |
| 3   | C     | 61  | GLN  |
| 3   | C     | 245 | HIS  |
| 3   | C     | 329 | ASN  |
| 4   | D     | 39  | GLN  |
| 4   | D     | 45  | ASN  |
| 4   | D     | 57  | ASN  |
| 4   | D     | 138 | GLN  |
| 4   | D     | 244 | HIS  |
| 5   | E     | 185 | ASN  |
| 6   | F     | 79  | ASN  |
| 6   | F     | 238 | GLN  |
| 7   | G     | 141 | ASN  |
| 8   | H     | 8   | GLN  |
| 9   | I     | 92  | HIS  |
| 9   | I     | 100 | ASN  |
| 11  | L     | 87  | HIS  |
| 11  | L     | 175 | ASN  |
| 12  | M     | 125 | ASN  |
| 13  | N     | 8   | GLN  |
| 14  | O     | 167 | HIS  |
| 15  | P     | 21  | ASN  |
| 15  | P     | 137 | ASN  |
| 16  | Q     | 162 | HIS  |
| 16  | Q     | 188 | ASN  |
| 20  | U     | 50  | ASN  |
| 22  | W     | 17  | HIS  |
| 22  | W     | 50  | ASN  |
| 22  | W     | 59  | HIS  |
| 23  | X     | 93  | ASN  |
| 24  | Y     | 61  | HIS  |
| 24  | Y     | 72  | GLN  |
| 27  | b     | 6   | ASN  |
| 30  | e     | 23  | HIS  |
| 30  | e     | 80  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | j     | 13  | ASN  |
| 42  | r     | 103 | HIS  |
| 43  | s     | 81  | HIS  |
| 43  | s     | 176 | ASN  |
| 44  | t     | 65  | GLN  |
| 52  | AA    | 9   | GLN  |
| 52  | AA    | 70  | ASN  |
| 53  | BB    | 124 | HIS  |
| 53  | BB    | 202 | GLN  |
| 55  | DD    | 165 | ASN  |
| 55  | DD    | 207 | HIS  |
| 56  | EE    | 216 | ASN  |
| 57  | FF    | 118 | ASN  |
| 60  | II    | 52  | ASN  |
| 60  | II    | 116 | HIS  |
| 61  | JJ    | 124 | HIS  |
| 62  | KK    | 61  | GLN  |
| 63  | LL    | 11  | GLN  |
| 63  | LL    | 18  | GLN  |
| 64  | MM    | 19  | GLN  |
| 65  | NN    | 90  | HIS  |
| 68  | QQ    | 142 | GLN  |
| 70  | SS    | 97  | GLN  |
| 71  | TT    | 51  | ASN  |
| 74  | WW    | 5   | ASN  |
| 75  | XX    | 31  | HIS  |
| 78  | aa    | 43  | ASN  |
| 86  | ii    | 61  | ASN  |
| 86  | ii    | 334 | HIS  |
| 87  | jj    | 453 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 46  | 2     | 74/76 (97%)     | 20 (27%)          | 0               |
| 47  | 3     | 72/75 (96%)     | 20 (27%)          | 0               |
| 48  | 5     | 3505/3543 (98%) | 655 (18%)         | 72 (2%)         |
| 49  | 7     | 119/120 (99%)   | 11 (9%)           | 0               |
| 50  | 8     | 155/156 (99%)   | 29 (18%)          | 3 (1%)          |
| 51  | 9     | 1685/1869 (90%) | 440 (26%)         | 36 (2%)         |
| 85  | hh    | 10/197 (5%)     | 3 (30%)           | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| All | All   | 5620/6036 (93%) | 1178 (20%)        | 111 (1%)        |

All (1178) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | 2     | 7   | G    |
| 46  | 2     | 8   | U    |
| 46  | 2     | 9   | A    |
| 46  | 2     | 15  | G    |
| 46  | 2     | 19  | G    |
| 46  | 2     | 20  | U    |
| 46  | 2     | 31  | C    |
| 46  | 2     | 47  | U    |
| 46  | 2     | 49  | C    |
| 46  | 2     | 58  | A    |
| 46  | 2     | 61  | C    |
| 46  | 2     | 62  | C    |
| 46  | 2     | 65  | G    |
| 46  | 2     | 67  | G    |
| 46  | 2     | 68  | G    |
| 46  | 2     | 70  | A    |
| 46  | 2     | 73  | A    |
| 46  | 2     | 74  | C    |
| 46  | 2     | 75  | C    |
| 46  | 2     | 76  | A    |
| 47  | 3     | 11  | C    |
| 47  | 3     | 13  | C    |
| 47  | 3     | 16  | C    |
| 47  | 3     | 19  | G    |
| 47  | 3     | 21  | A    |
| 47  | 3     | 22  | G    |
| 47  | 3     | 23  | A    |
| 47  | 3     | 31  | A    |
| 47  | 3     | 34  | U    |
| 47  | 3     | 46  | G    |
| 47  | 3     | 47  | U    |
| 47  | 3     | 49  | C    |
| 47  | 3     | 50  | A    |
| 47  | 3     | 56  | C    |
| 47  | 3     | 58  | A    |
| 47  | 3     | 63  | C    |
| 47  | 3     | 65  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | 3     | 67  | U    |
| 47  | 3     | 69  | G    |
| 47  | 3     | 76  | A    |
| 48  | 5     | 13  | U    |
| 48  | 5     | 39  | A    |
| 48  | 5     | 42  | A    |
| 48  | 5     | 43  | U    |
| 48  | 5     | 56  | A    |
| 48  | 5     | 59  | A    |
| 48  | 5     | 64  | A    |
| 48  | 5     | 65  | A    |
| 48  | 5     | 73  | A    |
| 48  | 5     | 74  | G    |
| 48  | 5     | 91  | G    |
| 48  | 5     | 98  | A    |
| 48  | 5     | 104 | G    |
| 48  | 5     | 109 | G    |
| 48  | 5     | 110 | C    |
| 48  | 5     | 116 | G    |
| 48  | 5     | 117 | C    |
| 48  | 5     | 118 | C    |
| 48  | 5     | 119 | G    |
| 48  | 5     | 120 | A    |
| 48  | 5     | 126 | C    |
| 48  | 5     | 134 | G    |
| 48  | 5     | 135 | G    |
| 48  | 5     | 136 | C    |
| 48  | 5     | 140 | G    |
| 48  | 5     | 144 | G    |
| 48  | 5     | 159 | C    |
| 48  | 5     | 166 | C    |
| 48  | 5     | 167 | C    |
| 48  | 5     | 170 | C    |
| 48  | 5     | 177 | G    |
| 48  | 5     | 182 | G    |
| 48  | 5     | 200 | U    |
| 48  | 5     | 201 | C    |
| 48  | 5     | 209 | U    |
| 48  | 5     | 216 | C    |
| 48  | 5     | 218 | A    |
| 48  | 5     | 219 | G    |
| 48  | 5     | 220 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | 5     | 224 | U    |
| 48  | 5     | 232 | G    |
| 48  | 5     | 233 | U    |
| 48  | 5     | 234 | G    |
| 48  | 5     | 238 | C    |
| 48  | 5     | 246 | G    |
| 48  | 5     | 253 | G    |
| 48  | 5     | 256 | G    |
| 48  | 5     | 260 | C    |
| 48  | 5     | 265 | C    |
| 48  | 5     | 266 | C    |
| 48  | 5     | 267 | G    |
| 48  | 5     | 268 | G    |
| 48  | 5     | 271 | C    |
| 48  | 5     | 276 | C    |
| 48  | 5     | 280 | G    |
| 48  | 5     | 281 | U    |
| 48  | 5     | 297 | U    |
| 48  | 5     | 306 | A    |
| 48  | 5     | 315 | G    |
| 48  | 5     | 316 | U    |
| 48  | 5     | 326 | C    |
| 48  | 5     | 334 | A    |
| 48  | 5     | 340 | C    |
| 48  | 5     | 350 | C    |
| 48  | 5     | 354 | U    |
| 48  | 5     | 386 | A    |
| 48  | 5     | 387 | G    |
| 48  | 5     | 403 | G    |
| 48  | 5     | 407 | A    |
| 48  | 5     | 409 | G    |
| 48  | 5     | 412 | G    |
| 48  | 5     | 432 | U    |
| 48  | 5     | 446 | C    |
| 48  | 5     | 449 | C    |
| 48  | 5     | 450 | G    |
| 48  | 5     | 452 | A    |
| 48  | 5     | 453 | G    |
| 48  | 5     | 454 | U    |
| 48  | 5     | 455 | C    |
| 48  | 5     | 462 | G    |
| 48  | 5     | 463 | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 48  | 5     | 464    | G    |
| 48  | 5     | 465    | G    |
| 48  | 5     | 467    | U    |
| 48  | 5     | 468    | U    |
| 48  | 5     | 481    | G    |
| 48  | 5     | 481(A) | C    |
| 48  | 5     | 482    | G    |
| 48  | 5     | 484    | U    |
| 48  | 5     | 485    | C    |
| 48  | 5     | 486    | C    |
| 48  | 5     | 492    | U    |
| 48  | 5     | 493    | G    |
| 48  | 5     | 498    | C    |
| 48  | 5     | 499    | G    |
| 48  | 5     | 505    | G    |
| 48  | 5     | 510    | U    |
| 48  | 5     | 521    | C    |
| 48  | 5     | 639    | U    |
| 48  | 5     | 642    | G    |
| 48  | 5     | 657    | C    |
| 48  | 5     | 658    | C    |
| 48  | 5     | 660    | G    |
| 48  | 5     | 666    | G    |
| 48  | 5     | 670    | G    |
| 48  | 5     | 685    | C    |
| 48  | 5     | 686    | A    |
| 48  | 5     | 687    | U    |
| 48  | 5     | 694    | C    |
| 48  | 5     | 697    | G    |
| 48  | 5     | 703    | G    |
| 48  | 5     | 704    | C    |
| 48  | 5     | 705    | G    |
| 48  | 5     | 730    | G    |
| 48  | 5     | 731    | G    |
| 48  | 5     | 733    | A    |
| 48  | 5     | 738    | C    |
| 48  | 5     | 742    | G    |
| 48  | 5     | 744    | G    |
| 48  | 5     | 746    | A    |
| 48  | 5     | 747    | A    |
| 48  | 5     | 758    | G    |
| 48  | 5     | 910    | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 48  | 5     | 913    | U    |
| 48  | 5     | 914    | U    |
| 48  | 5     | 917    | A    |
| 48  | 5     | 918    | G    |
| 48  | 5     | 923    | C    |
| 48  | 5     | 925    | C    |
| 48  | 5     | 926    | G    |
| 48  | 5     | 929    | A    |
| 48  | 5     | 931    | C    |
| 48  | 5     | 932    | A    |
| 48  | 5     | 933    | G    |
| 48  | 5     | 934    | C    |
| 48  | 5     | 935    | A    |
| 48  | 5     | 935(A) | G    |
| 48  | 5     | 936    | C    |
| 48  | 5     | 943    | A    |
| 48  | 5     | 945    | U    |
| 48  | 5     | 959    | G    |
| 48  | 5     | 960    | A    |
| 48  | 5     | 961    | G    |
| 48  | 5     | 966    | A    |
| 48  | 5     | 967    | C    |
| 48  | 5     | 969    | C    |
| 48  | 5     | 972    | C    |
| 48  | 5     | 973    | G    |
| 48  | 5     | 983    | C    |
| 48  | 5     | 1068   | G    |
| 48  | 5     | 1070   | G    |
| 48  | 5     | 1071   | C    |
| 48  | 5     | 1072   | C    |
| 48  | 5     | 1073   | G    |
| 48  | 5     | 1079   | C    |
| 48  | 5     | 1082   | C    |
| 48  | 5     | 1094   | G    |
| 48  | 5     | 1097   | C    |
| 48  | 5     | 1169   | G    |
| 48  | 5     | 1172   | C    |
| 48  | 5     | 1174   | G    |
| 48  | 5     | 1176   | C    |
| 48  | 5     | 1179   | U    |
| 48  | 5     | 1184   | A    |
| 48  | 5     | 1195   | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 48  | 5     | 1200    | G    |
| 48  | 5     | 1209    | U    |
| 48  | 5     | 1211    | G    |
| 48  | 5     | 1212    | G    |
| 48  | 5     | 1214    | C    |
| 48  | 5     | 1215    | C    |
| 48  | 5     | 1234    | G    |
| 48  | 5     | 1235    | G    |
| 48  | 5     | 1236    | C    |
| 48  | 5     | 1237    | C    |
| 48  | 5     | 1239    | C    |
| 48  | 5     | 1272    | C    |
| 48  | 5     | 1273    | G    |
| 48  | 5     | 1275    | G    |
| 48  | 5     | 1277    | G    |
| 48  | 5     | 1280    | C    |
| 48  | 5     | 1284    | G    |
| 48  | 5     | 1285    | U    |
| 48  | 5     | 1287    | G    |
| 48  | 5     | 1292    | C    |
| 48  | 5     | 1293    | G    |
| 48  | 5     | 1294    | A    |
| 48  | 5     | 1295    | U    |
| 48  | 5     | 1296    | G    |
| 48  | 5     | 1301    | C    |
| 48  | 5     | 1303    | A    |
| 48  | 5     | 1313    | C    |
| 48  | 5     | 1326    | A2M  |
| 48  | 5     | 1337    | A    |
| 48  | 5     | 1354    | A    |
| 48  | 5     | 1358    | G    |
| 48  | 5     | 1359    | G    |
| 48  | 5     | 1371    | A    |
| 48  | 5     | 1377    | G    |
| 48  | 5     | 1387    | A    |
| 48  | 5     | 1394    | G    |
| 48  | 5     | 1397    | A    |
| 48  | 5     | 1398    | A    |
| 48  | 5     | 1406    | G    |
| 48  | 5     | 1411(A) | G    |
| 48  | 5     | 1412    | G    |
| 48  | 5     | 1414    | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 1415 | G    |
| 48  | 5     | 1420 | A    |
| 48  | 5     | 1437 | C    |
| 48  | 5     | 1441 | C    |
| 48  | 5     | 1442 | C    |
| 48  | 5     | 1443 | A    |
| 48  | 5     | 1445 | U    |
| 48  | 5     | 1446 | C    |
| 48  | 5     | 1456 | C    |
| 48  | 5     | 1457 | G    |
| 48  | 5     | 1477 | C    |
| 48  | 5     | 1478 | C    |
| 48  | 5     | 1482 | G    |
| 48  | 5     | 1483 | C    |
| 48  | 5     | 1484 | G    |
| 48  | 5     | 1489 | G    |
| 48  | 5     | 1497 | A    |
| 48  | 5     | 1498 | G    |
| 48  | 5     | 1502 | G    |
| 48  | 5     | 1514 | U    |
| 48  | 5     | 1523 | A    |
| 48  | 5     | 1534 | A2M  |
| 48  | 5     | 1535 | C    |
| 48  | 5     | 1547 | A    |
| 48  | 5     | 1564 | A    |
| 48  | 5     | 1566 | C    |
| 48  | 5     | 1578 | U    |
| 48  | 5     | 1591 | U    |
| 48  | 5     | 1596 | U    |
| 48  | 5     | 1602 | U    |
| 48  | 5     | 1612 | G    |
| 48  | 5     | 1613 | A    |
| 48  | 5     | 1624 | G    |
| 48  | 5     | 1625 | OMG  |
| 48  | 5     | 1626 | G    |
| 48  | 5     | 1631 | A    |
| 48  | 5     | 1633 | G    |
| 48  | 5     | 1634 | A    |
| 48  | 5     | 1638 | A    |
| 48  | 5     | 1641 | G    |
| 48  | 5     | 1654 | G    |
| 48  | 5     | 1661 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 1676 | C    |
| 48  | 5     | 1677 | PSU  |
| 48  | 5     | 1694 | C    |
| 48  | 5     | 1726 | U    |
| 48  | 5     | 1731 | C    |
| 48  | 5     | 1734 | G    |
| 48  | 5     | 1735 | U    |
| 48  | 5     | 1741 | G    |
| 48  | 5     | 1742 | A    |
| 48  | 5     | 1750 | G    |
| 48  | 5     | 1754 | U    |
| 48  | 5     | 1756 | U    |
| 48  | 5     | 1757 | U    |
| 48  | 5     | 1759 | G    |
| 48  | 5     | 1760 | G    |
| 48  | 5     | 1764 | G    |
| 48  | 5     | 1768 | C    |
| 48  | 5     | 1772 | C    |
| 48  | 5     | 1773 | U    |
| 48  | 5     | 1776 | A    |
| 48  | 5     | 1780 | A    |
| 48  | 5     | 1781 | PSU  |
| 48  | 5     | 1787 | A    |
| 48  | 5     | 1804 | A    |
| 48  | 5     | 1805 | A    |
| 48  | 5     | 1806 | G    |
| 48  | 5     | 1809 | C    |
| 48  | 5     | 1819 | G    |
| 48  | 5     | 1821 | G    |
| 48  | 5     | 1822 | U    |
| 48  | 5     | 1828 | C    |
| 48  | 5     | 1833 | G    |
| 48  | 5     | 1835 | G    |
| 48  | 5     | 1836 | G    |
| 48  | 5     | 1837 | A    |
| 48  | 5     | 1842 | G    |
| 48  | 5     | 1855 | G    |
| 48  | 5     | 1869 | G    |
| 48  | 5     | 1892 | A    |
| 48  | 5     | 1897 | A    |
| 48  | 5     | 1918 | U    |
| 48  | 5     | 1920 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 1921 | C    |
| 48  | 5     | 1922 | G    |
| 48  | 5     | 1930 | U    |
| 48  | 5     | 1931 | C    |
| 48  | 5     | 1932 | A    |
| 48  | 5     | 1940 | G    |
| 48  | 5     | 1948 | G    |
| 48  | 5     | 1957 | U    |
| 48  | 5     | 1958 | A    |
| 48  | 5     | 1959 | U    |
| 48  | 5     | 1960 | A    |
| 48  | 5     | 1961 | G    |
| 48  | 5     | 1963 | C    |
| 48  | 5     | 1966 | C    |
| 48  | 5     | 1967 | A    |
| 48  | 5     | 1971 | C    |
| 48  | 5     | 1972 | G    |
| 48  | 5     | 1974 | U    |
| 48  | 5     | 1975 | G    |
| 48  | 5     | 1976 | G    |
| 48  | 5     | 1978 | C    |
| 48  | 5     | 1979 | A    |
| 48  | 5     | 1980 | U    |
| 48  | 5     | 1983 | A    |
| 48  | 5     | 1984 | A    |
| 48  | 5     | 1985 | G    |
| 48  | 5     | 1987 | C    |
| 48  | 5     | 1988 | G    |
| 48  | 5     | 1990 | A    |
| 48  | 5     | 1991 | A    |
| 48  | 5     | 1992 | U    |
| 48  | 5     | 1997 | U    |
| 48  | 5     | 1998 | A    |
| 48  | 5     | 1999 | A    |
| 48  | 5     | 2001 | G    |
| 48  | 5     | 2002 | A    |
| 48  | 5     | 2003 | G    |
| 48  | 5     | 2004 | U    |
| 48  | 5     | 2009 | A    |
| 48  | 5     | 2011 | C    |
| 48  | 5     | 2025 | A    |
| 48  | 5     | 2026 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 2046 | G    |
| 48  | 5     | 2047 | A    |
| 48  | 5     | 2048 | U    |
| 48  | 5     | 2052 | G    |
| 48  | 5     | 2055 | G    |
| 48  | 5     | 2056 | G    |
| 48  | 5     | 2069 | A    |
| 48  | 5     | 2071 | A    |
| 48  | 5     | 2084 | U    |
| 48  | 5     | 2089 | G    |
| 48  | 5     | 2090 | U    |
| 48  | 5     | 2092 | G    |
| 48  | 5     | 2093 | G    |
| 48  | 5     | 2094 | C    |
| 48  | 5     | 2095 | A    |
| 48  | 5     | 2097 | A    |
| 48  | 5     | 2098 | G    |
| 48  | 5     | 2100 | G    |
| 48  | 5     | 2102 | G    |
| 48  | 5     | 2104 | A    |
| 48  | 5     | 2105 | A    |
| 48  | 5     | 2106 | G    |
| 48  | 5     | 2107 | A    |
| 48  | 5     | 2108 | G    |
| 48  | 5     | 2110 | G    |
| 48  | 5     | 2259 | G    |
| 48  | 5     | 2260 | C    |
| 48  | 5     | 2267 | U    |
| 48  | 5     | 2289 | C    |
| 48  | 5     | 2300 | A    |
| 48  | 5     | 2301 | G    |
| 48  | 5     | 2313 | A    |
| 48  | 5     | 2314 | G    |
| 48  | 5     | 2333 | G    |
| 48  | 5     | 2348 | G    |
| 48  | 5     | 2351 | OMC  |
| 48  | 5     | 2360 | A    |
| 48  | 5     | 2382 | A    |
| 48  | 5     | 2395 | A    |
| 48  | 5     | 2422 | OMC  |
| 48  | 5     | 2424 | OMG  |
| 48  | 5     | 2425 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 2433 | G    |
| 48  | 5     | 2441 | C    |
| 48  | 5     | 2450 | G    |
| 48  | 5     | 2453 | A    |
| 48  | 5     | 2475 | G    |
| 48  | 5     | 2488 | C    |
| 48  | 5     | 2489 | C    |
| 48  | 5     | 2490 | U    |
| 48  | 5     | 2491 | C    |
| 48  | 5     | 2492 | C    |
| 48  | 5     | 2494 | U    |
| 48  | 5     | 2503 | G    |
| 48  | 5     | 2504 | C    |
| 48  | 5     | 2505 | C    |
| 48  | 5     | 2506 | G    |
| 48  | 5     | 2511 | A    |
| 48  | 5     | 2513 | A    |
| 48  | 5     | 2529 | A    |
| 48  | 5     | 2530 | U    |
| 48  | 5     | 2544 | G    |
| 48  | 5     | 2545 | U    |
| 48  | 5     | 2546 | G    |
| 48  | 5     | 2547 | G    |
| 48  | 5     | 2554 | U    |
| 48  | 5     | 2564 | G    |
| 48  | 5     | 2565 | A    |
| 48  | 5     | 2566 | G    |
| 48  | 5     | 2569 | G    |
| 48  | 5     | 2570 | U    |
| 48  | 5     | 2583 | C    |
| 48  | 5     | 2587 | A    |
| 48  | 5     | 2588 | C    |
| 48  | 5     | 2611 | A    |
| 48  | 5     | 2628 | U    |
| 48  | 5     | 2638 | G    |
| 48  | 5     | 2640 | G    |
| 48  | 5     | 2653 | C    |
| 48  | 5     | 2658 | G    |
| 48  | 5     | 2662 | G    |
| 48  | 5     | 2669 | C    |
| 48  | 5     | 2673 | G    |
| 48  | 5     | 2687 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 2695 | A    |
| 48  | 5     | 2696 | A    |
| 48  | 5     | 2707 | U    |
| 48  | 5     | 2708 | U    |
| 48  | 5     | 2709 | C    |
| 48  | 5     | 2711 | G    |
| 48  | 5     | 2716 | C    |
| 48  | 5     | 2721 | G    |
| 48  | 5     | 2726 | G    |
| 48  | 5     | 2735 | G    |
| 48  | 5     | 2740 | U    |
| 48  | 5     | 2743 | A    |
| 48  | 5     | 2753 | G    |
| 48  | 5     | 2754 | G    |
| 48  | 5     | 2763 | U    |
| 48  | 5     | 2764 | A    |
| 48  | 5     | 2765 | A    |
| 48  | 5     | 2769 | U    |
| 48  | 5     | 2788 | U    |
| 48  | 5     | 2790 | U    |
| 48  | 5     | 2799 | G    |
| 48  | 5     | 2826 | U    |
| 48  | 5     | 2827 | G    |
| 48  | 5     | 2829 | U    |
| 48  | 5     | 2833 | A    |
| 48  | 5     | 2842 | G    |
| 48  | 5     | 2855 | G    |
| 48  | 5     | 2869 | U    |
| 48  | 5     | 3598 | C    |
| 48  | 5     | 3602 | C    |
| 48  | 5     | 3604 | A    |
| 48  | 5     | 3605 | C    |
| 48  | 5     | 3606 | U    |
| 48  | 5     | 3616 | U    |
| 48  | 5     | 3617 | G    |
| 48  | 5     | 3618 | C    |
| 48  | 5     | 3625 | G    |
| 48  | 5     | 3626 | G    |
| 48  | 5     | 3635 | A    |
| 48  | 5     | 3644 | U    |
| 48  | 5     | 3657 | U    |
| 48  | 5     | 3662 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 3673 | C    |
| 48  | 5     | 3688 | U    |
| 48  | 5     | 3710 | G    |
| 48  | 5     | 3712 | A    |
| 48  | 5     | 3713 | U    |
| 48  | 5     | 3714 | G    |
| 48  | 5     | 3743 | G    |
| 48  | 5     | 3748 | A    |
| 48  | 5     | 3750 | G    |
| 48  | 5     | 3753 | G    |
| 48  | 5     | 3760 | A2M  |
| 48  | 5     | 3761 | C    |
| 48  | 5     | 3773 | U    |
| 48  | 5     | 3774 | A    |
| 48  | 5     | 3776 | G    |
| 48  | 5     | 3777 | G    |
| 48  | 5     | 3783 | A    |
| 48  | 5     | 3784 | A    |
| 48  | 5     | 3786 | U    |
| 48  | 5     | 3788 | C    |
| 48  | 5     | 3810 | C    |
| 48  | 5     | 3811 | G    |
| 48  | 5     | 3812 | C    |
| 48  | 5     | 3814 | U    |
| 48  | 5     | 3817 | A    |
| 48  | 5     | 3818 | UY1  |
| 48  | 5     | 3819 | G    |
| 48  | 5     | 3822 | U    |
| 48  | 5     | 3838 | U    |
| 48  | 5     | 3839 | G    |
| 48  | 5     | 3840 | U    |
| 48  | 5     | 3876 | A    |
| 48  | 5     | 3877 | A    |
| 48  | 5     | 3878 | C    |
| 48  | 5     | 3879 | G    |
| 48  | 5     | 3889 | G    |
| 48  | 5     | 3897 | G    |
| 48  | 5     | 3901 | A    |
| 48  | 5     | 3905 | A    |
| 48  | 5     | 3906 | A    |
| 48  | 5     | 3907 | G    |
| 48  | 5     | 3915 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 3939 | G    |
| 48  | 5     | 3943 | A    |
| 48  | 5     | 3948 | C    |
| 48  | 5     | 4066 | U    |
| 48  | 5     | 4069 | U    |
| 48  | 5     | 4076 | G    |
| 48  | 5     | 4084 | G    |
| 48  | 5     | 4096 | C    |
| 48  | 5     | 4097 | G    |
| 48  | 5     | 4119 | C    |
| 48  | 5     | 4120 | U    |
| 48  | 5     | 4122 | G    |
| 48  | 5     | 4127 | A    |
| 48  | 5     | 4134 | C    |
| 48  | 5     | 4158 | C    |
| 48  | 5     | 4161 | G    |
| 48  | 5     | 4163 | U    |
| 48  | 5     | 4170 | A    |
| 48  | 5     | 4183 | G    |
| 48  | 5     | 4184 | G    |
| 48  | 5     | 4191 | G    |
| 48  | 5     | 4203 | A    |
| 48  | 5     | 4225 | G    |
| 48  | 5     | 4229 | U    |
| 48  | 5     | 4233 | A    |
| 48  | 5     | 4251 | A    |
| 48  | 5     | 4252 | C    |
| 48  | 5     | 4254 | G    |
| 48  | 5     | 4258 | C    |
| 48  | 5     | 4266 | G    |
| 48  | 5     | 4268 | A    |
| 48  | 5     | 4271 | A    |
| 48  | 5     | 4273 | A    |
| 48  | 5     | 4281 | A    |
| 48  | 5     | 4291 | G    |
| 48  | 5     | 4304 | A    |
| 48  | 5     | 4305 | G    |
| 48  | 5     | 4314 | C    |
| 48  | 5     | 4329 | G    |
| 48  | 5     | 4330 | G    |
| 48  | 5     | 4339 | A    |
| 48  | 5     | 4349 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 4364 | G    |
| 48  | 5     | 4373 | G    |
| 48  | 5     | 4376 | A    |
| 48  | 5     | 4377 | G    |
| 48  | 5     | 4378 | A    |
| 48  | 5     | 4379 | A    |
| 48  | 5     | 4380 | A    |
| 48  | 5     | 4387 | C    |
| 48  | 5     | 4391 | G    |
| 48  | 5     | 4394 | A    |
| 48  | 5     | 4395 | U    |
| 48  | 5     | 4419 | U    |
| 48  | 5     | 4421 | C    |
| 48  | 5     | 4422 | A    |
| 48  | 5     | 4430 | G    |
| 48  | 5     | 4439 | U    |
| 48  | 5     | 4440 | G    |
| 48  | 5     | 4448 | G    |
| 48  | 5     | 4449 | A    |
| 48  | 5     | 4464 | A    |
| 48  | 5     | 4475 | G    |
| 48  | 5     | 4500 | PSU  |
| 48  | 5     | 4512 | U    |
| 48  | 5     | 4513 | A    |
| 48  | 5     | 4519 | C    |
| 48  | 5     | 4524 | G    |
| 48  | 5     | 4548 | A    |
| 48  | 5     | 4549 | G    |
| 48  | 5     | 4560 | C    |
| 48  | 5     | 4567 | G    |
| 48  | 5     | 4570 | G    |
| 48  | 5     | 4573 | G    |
| 48  | 5     | 4575 | G    |
| 48  | 5     | 4590 | A    |
| 48  | 5     | 4606 | G    |
| 48  | 5     | 4636 | U    |
| 48  | 5     | 4637 | OMG  |
| 48  | 5     | 4656 | A    |
| 48  | 5     | 4670 | C    |
| 48  | 5     | 4672 | A    |
| 48  | 5     | 4677 | U    |
| 48  | 5     | 4700 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 4709 | U    |
| 48  | 5     | 4720 | C    |
| 48  | 5     | 4736 | C    |
| 48  | 5     | 4740 | G    |
| 48  | 5     | 4745 | G    |
| 48  | 5     | 4751 | G    |
| 48  | 5     | 4754 | G    |
| 48  | 5     | 4757 | C    |
| 48  | 5     | 4759 | C    |
| 48  | 5     | 4761 | G    |
| 48  | 5     | 4765 | G    |
| 48  | 5     | 4769 | G    |
| 48  | 5     | 4771 | C    |
| 48  | 5     | 4772 | C    |
| 48  | 5     | 4776 | G    |
| 48  | 5     | 4860 | G    |
| 48  | 5     | 4867 | G    |
| 48  | 5     | 4870 | G    |
| 48  | 5     | 4871 | C    |
| 48  | 5     | 4873 | G    |
| 48  | 5     | 4875 | G    |
| 48  | 5     | 4882 | U    |
| 48  | 5     | 4883 | C    |
| 48  | 5     | 4885 | U    |
| 48  | 5     | 4895 | C    |
| 48  | 5     | 4896 | G    |
| 48  | 5     | 4903 | G    |
| 48  | 5     | 4904 | G    |
| 48  | 5     | 4905 | C    |
| 48  | 5     | 4906 | C    |
| 48  | 5     | 4907 | G    |
| 48  | 5     | 4908 | G    |
| 48  | 5     | 4912 | G    |
| 48  | 5     | 4914 | G    |
| 48  | 5     | 4917 | C    |
| 48  | 5     | 4921 | C    |
| 48  | 5     | 4922 | C    |
| 48  | 5     | 4923 | U    |
| 48  | 5     | 4924 | C    |
| 48  | 5     | 4926 | C    |
| 48  | 5     | 4933 | C    |
| 48  | 5     | 4934 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 4944 | C    |
| 48  | 5     | 4948 | C    |
| 48  | 5     | 4949 | G    |
| 48  | 5     | 4950 | U    |
| 48  | 5     | 4951 | G    |
| 48  | 5     | 4956 | A    |
| 48  | 5     | 4957 | C    |
| 48  | 5     | 4958 | C    |
| 48  | 5     | 4960 | G    |
| 48  | 5     | 4963 | G    |
| 48  | 5     | 4964 | C    |
| 48  | 5     | 4966 | A    |
| 48  | 5     | 4967 | A    |
| 48  | 5     | 4976 | U    |
| 48  | 5     | 4988 | U    |
| 48  | 5     | 4989 | U    |
| 48  | 5     | 4990 | C    |
| 48  | 5     | 4993 | G    |
| 48  | 5     | 5007 | A    |
| 48  | 5     | 5014 | A    |
| 48  | 5     | 5017 | G    |
| 48  | 5     | 5041 | G    |
| 48  | 5     | 5047 | C    |
| 48  | 5     | 5050 | C    |
| 48  | 5     | 5053 | U    |
| 48  | 5     | 5054 | C    |
| 48  | 5     | 5061 | A    |
| 48  | 5     | 5062 | G    |
| 49  | 7     | 10   | C    |
| 49  | 7     | 25   | G    |
| 49  | 7     | 33   | U    |
| 49  | 7     | 40   | U    |
| 49  | 7     | 42   | A    |
| 49  | 7     | 53   | U    |
| 49  | 7     | 64   | G    |
| 49  | 7     | 89   | G    |
| 49  | 7     | 100  | A    |
| 49  | 7     | 110  | G    |
| 49  | 7     | 120  | U    |
| 50  | 8     | 2    | G    |
| 50  | 8     | 34   | U    |
| 50  | 8     | 35   | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | 8     | 52  | A    |
| 50  | 8     | 59  | A    |
| 50  | 8     | 62  | A    |
| 50  | 8     | 63  | U    |
| 50  | 8     | 81  | C    |
| 50  | 8     | 82  | A    |
| 50  | 8     | 83  | C    |
| 50  | 8     | 84  | A    |
| 50  | 8     | 85  | U    |
| 50  | 8     | 86  | U    |
| 50  | 8     | 94  | G    |
| 50  | 8     | 95  | A    |
| 50  | 8     | 103 | A    |
| 50  | 8     | 105 | C    |
| 50  | 8     | 109 | C    |
| 50  | 8     | 110 | U    |
| 50  | 8     | 111 | U    |
| 50  | 8     | 114 | G    |
| 50  | 8     | 125 | C    |
| 50  | 8     | 126 | C    |
| 50  | 8     | 127 | U    |
| 50  | 8     | 135 | C    |
| 50  | 8     | 147 | G    |
| 50  | 8     | 150 | C    |
| 50  | 8     | 153 | C    |
| 50  | 8     | 156 | U    |
| 51  | 9     | 4   | C    |
| 51  | 9     | 17  | C    |
| 51  | 9     | 25  | A    |
| 51  | 9     | 26  | U    |
| 51  | 9     | 33  | G    |
| 51  | 9     | 34  | PSU  |
| 51  | 9     | 41  | G    |
| 51  | 9     | 44  | U    |
| 51  | 9     | 45  | A    |
| 51  | 9     | 46  | A    |
| 51  | 9     | 56  | G    |
| 51  | 9     | 58  | C    |
| 51  | 9     | 59  | U    |
| 51  | 9     | 60  | A    |
| 51  | 9     | 62  | G    |
| 51  | 9     | 65  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 9     | 67  | C    |
| 51  | 9     | 68  | A    |
| 51  | 9     | 71  | G    |
| 51  | 9     | 72  | C    |
| 51  | 9     | 73  | C    |
| 51  | 9     | 74  | G    |
| 51  | 9     | 75  | G    |
| 51  | 9     | 76  | U    |
| 51  | 9     | 78  | C    |
| 51  | 9     | 79  | A    |
| 51  | 9     | 99  | A2M  |
| 51  | 9     | 103 | A    |
| 51  | 9     | 110 | U    |
| 51  | 9     | 111 | A    |
| 51  | 9     | 113 | G    |
| 51  | 9     | 115 | U    |
| 51  | 9     | 124 | U    |
| 51  | 9     | 126 | G    |
| 51  | 9     | 141 | A    |
| 51  | 9     | 142 | C    |
| 51  | 9     | 143 | U    |
| 51  | 9     | 147 | A    |
| 51  | 9     | 155 | G    |
| 51  | 9     | 162 | C    |
| 51  | 9     | 163 | U    |
| 51  | 9     | 166 | A2M  |
| 51  | 9     | 171 | A    |
| 51  | 9     | 172 | OMU  |
| 51  | 9     | 173 | A    |
| 51  | 9     | 180 | G    |
| 51  | 9     | 182 | C    |
| 51  | 9     | 184 | G    |
| 51  | 9     | 187 | G    |
| 51  | 9     | 188 | C    |
| 51  | 9     | 189 | U    |
| 51  | 9     | 190 | G    |
| 51  | 9     | 192 | C    |
| 51  | 9     | 197 | U    |
| 51  | 9     | 202 | G    |
| 51  | 9     | 207 | G    |
| 51  | 9     | 209 | A    |
| 51  | 9     | 211 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 9     | 212 | C    |
| 51  | 9     | 214 | U    |
| 51  | 9     | 215 | G    |
| 51  | 9     | 216 | C    |
| 51  | 9     | 217 | A    |
| 51  | 9     | 291 | G    |
| 51  | 9     | 292 | A    |
| 51  | 9     | 293 | C    |
| 51  | 9     | 294 | U    |
| 51  | 9     | 302 | A    |
| 51  | 9     | 304 | C    |
| 51  | 9     | 305 | U    |
| 51  | 9     | 306 | C    |
| 51  | 9     | 307 | G    |
| 51  | 9     | 308 | G    |
| 51  | 9     | 309 | G    |
| 51  | 9     | 310 | C    |
| 51  | 9     | 313 | A    |
| 51  | 9     | 319 | C    |
| 51  | 9     | 320 | G    |
| 51  | 9     | 321 | C    |
| 51  | 9     | 322 | C    |
| 51  | 9     | 324 | C    |
| 51  | 9     | 325 | C    |
| 51  | 9     | 326 | C    |
| 51  | 9     | 327 | G    |
| 51  | 9     | 328 | U    |
| 51  | 9     | 334 | C    |
| 51  | 9     | 336 | A    |
| 51  | 9     | 338 | G    |
| 51  | 9     | 343 | A    |
| 51  | 9     | 347 | G    |
| 51  | 9     | 351 | G    |
| 51  | 9     | 360 | A    |
| 51  | 9     | 362 | C    |
| 51  | 9     | 364 | A    |
| 51  | 9     | 368 | U    |
| 51  | 9     | 369 | C    |
| 51  | 9     | 370 | G    |
| 51  | 9     | 385 | G    |
| 51  | 9     | 386 | C    |
| 51  | 9     | 400 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 9     | 408 | A    |
| 51  | 9     | 409 | C    |
| 51  | 9     | 418 | A    |
| 51  | 9     | 435 | A    |
| 51  | 9     | 438 | G    |
| 51  | 9     | 448 | A    |
| 51  | 9     | 449 | A    |
| 51  | 9     | 450 | C    |
| 51  | 9     | 465 | A    |
| 51  | 9     | 466 | G    |
| 51  | 9     | 471 | G    |
| 51  | 9     | 472 | C    |
| 51  | 9     | 473 | A    |
| 51  | 9     | 474 | G    |
| 51  | 9     | 476 | A    |
| 51  | 9     | 482 | G    |
| 51  | 9     | 487 | U    |
| 51  | 9     | 489 | A    |
| 51  | 9     | 492 | C    |
| 51  | 9     | 508 | A    |
| 51  | 9     | 525 | A    |
| 51  | 9     | 532 | C    |
| 51  | 9     | 533 | A    |
| 51  | 9     | 535 | G    |
| 51  | 9     | 536 | A    |
| 51  | 9     | 537 | C    |
| 51  | 9     | 542 | U    |
| 51  | 9     | 548 | C    |
| 51  | 9     | 549 | C    |
| 51  | 9     | 550 | C    |
| 51  | 9     | 551 | U    |
| 51  | 9     | 552 | G    |
| 51  | 9     | 555 | A    |
| 51  | 9     | 556 | U    |
| 51  | 9     | 557 | U    |
| 51  | 9     | 559 | G    |
| 51  | 9     | 560 | A    |
| 51  | 9     | 564 | A    |
| 51  | 9     | 568 | C    |
| 51  | 9     | 571 | U    |
| 51  | 9     | 576 | A    |
| 51  | 9     | 580 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 9     | 583 | A    |
| 51  | 9     | 585 | C    |
| 51  | 9     | 587 | A    |
| 51  | 9     | 588 | G    |
| 51  | 9     | 589 | G    |
| 51  | 9     | 590 | A    |
| 51  | 9     | 591 | U    |
| 51  | 9     | 600 | G    |
| 51  | 9     | 605 | A    |
| 51  | 9     | 606 | G    |
| 51  | 9     | 608 | C    |
| 51  | 9     | 614 | C    |
| 51  | 9     | 617 | G    |
| 51  | 9     | 620 | G    |
| 51  | 9     | 628 | A    |
| 51  | 9     | 631 | U    |
| 51  | 9     | 632 | C    |
| 51  | 9     | 643 | A    |
| 51  | 9     | 646 | G    |
| 51  | 9     | 655 | A    |
| 51  | 9     | 660 | C    |
| 51  | 9     | 664 | A    |
| 51  | 9     | 668 | A2M  |
| 51  | 9     | 669 | A    |
| 51  | 9     | 671 | A    |
| 51  | 9     | 672 | A    |
| 51  | 9     | 673 | G    |
| 51  | 9     | 688 | U    |
| 51  | 9     | 694 | G    |
| 51  | 9     | 696 | G    |
| 51  | 9     | 698 | G    |
| 51  | 9     | 732 | U    |
| 51  | 9     | 733 | C    |
| 51  | 9     | 734 | C    |
| 51  | 9     | 735 | C    |
| 51  | 9     | 736 | C    |
| 51  | 9     | 737 | G    |
| 51  | 9     | 738 | C    |
| 51  | 9     | 800 | U    |
| 51  | 9     | 801 | PSU  |
| 51  | 9     | 810 | A    |
| 51  | 9     | 811 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 9     | 812 | A    |
| 51  | 9     | 821 | G    |
| 51  | 9     | 822 | PSU  |
| 51  | 9     | 823 | U    |
| 51  | 9     | 827 | A    |
| 51  | 9     | 830 | A    |
| 51  | 9     | 834 | C    |
| 51  | 9     | 836 | G    |
| 51  | 9     | 837 | A    |
| 51  | 9     | 838 | G    |
| 51  | 9     | 839 | C    |
| 51  | 9     | 840 | C    |
| 51  | 9     | 841 | G    |
| 51  | 9     | 844 | U    |
| 51  | 9     | 847 | A    |
| 51  | 9     | 865 | A    |
| 51  | 9     | 870 | A    |
| 51  | 9     | 871 | U    |
| 51  | 9     | 873 | G    |
| 51  | 9     | 874 | G    |
| 51  | 9     | 875 | A    |
| 51  | 9     | 877 | C    |
| 51  | 9     | 878 | G    |
| 51  | 9     | 879 | C    |
| 51  | 9     | 880 | G    |
| 51  | 9     | 881 | G    |
| 51  | 9     | 882 | U    |
| 51  | 9     | 887 | U    |
| 51  | 9     | 888 | U    |
| 51  | 9     | 890 | U    |
| 51  | 9     | 895 | G    |
| 51  | 9     | 896 | U    |
| 51  | 9     | 897 | U    |
| 51  | 9     | 898 | U    |
| 51  | 9     | 899 | U    |
| 51  | 9     | 902 | G    |
| 51  | 9     | 903 | A    |
| 51  | 9     | 906 | U    |
| 51  | 9     | 909 | G    |
| 51  | 9     | 910 | G    |
| 51  | 9     | 913 | A    |
| 51  | 9     | 914 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 9     | 917  | U    |
| 51  | 9     | 920  | A    |
| 51  | 9     | 930  | C    |
| 51  | 9     | 933  | G    |
| 51  | 9     | 934  | G    |
| 51  | 9     | 943  | U    |
| 51  | 9     | 953  | C    |
| 51  | 9     | 970  | G    |
| 51  | 9     | 971  | G    |
| 51  | 9     | 990  | A    |
| 51  | 9     | 992  | A    |
| 51  | 9     | 999  | G    |
| 51  | 9     | 1017 | U    |
| 51  | 9     | 1023 | A    |
| 51  | 9     | 1040 | G    |
| 51  | 9     | 1044 | G    |
| 51  | 9     | 1045 | PSU  |
| 51  | 9     | 1049 | A    |
| 51  | 9     | 1060 | A    |
| 51  | 9     | 1061 | U    |
| 51  | 9     | 1062 | A    |
| 51  | 9     | 1077 | A    |
| 51  | 9     | 1083 | A    |
| 51  | 9     | 1085 | C    |
| 51  | 9     | 1086 | G    |
| 51  | 9     | 1089 | G    |
| 51  | 9     | 1096 | G    |
| 51  | 9     | 1110 | G    |
| 51  | 9     | 1113 | A    |
| 51  | 9     | 1115 | U    |
| 51  | 9     | 1116 | C    |
| 51  | 9     | 1120 | U    |
| 51  | 9     | 1131 | G    |
| 51  | 9     | 1133 | A    |
| 51  | 9     | 1138 | C    |
| 51  | 9     | 1139 | C    |
| 51  | 9     | 1148 | A    |
| 51  | 9     | 1149 | A    |
| 51  | 9     | 1153 | C    |
| 51  | 9     | 1154 | U    |
| 51  | 9     | 1158 | G    |
| 51  | 9     | 1171 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 9     | 1181 | A    |
| 51  | 9     | 1195 | A    |
| 51  | 9     | 1207 | G    |
| 51  | 9     | 1208 | A    |
| 51  | 9     | 1209 | A    |
| 51  | 9     | 1210 | G    |
| 51  | 9     | 1211 | G    |
| 51  | 9     | 1215 | C    |
| 51  | 9     | 1224 | G    |
| 51  | 9     | 1242 | U    |
| 51  | 9     | 1243 | U    |
| 51  | 9     | 1251 | A    |
| 51  | 9     | 1253 | A    |
| 51  | 9     | 1256 | G    |
| 51  | 9     | 1257 | G    |
| 51  | 9     | 1265 | A    |
| 51  | 9     | 1271 | C    |
| 51  | 9     | 1274 | G    |
| 51  | 9     | 1275 | G    |
| 51  | 9     | 1280 | G    |
| 51  | 9     | 1281 | G    |
| 51  | 9     | 1282 | A    |
| 51  | 9     | 1283 | C    |
| 51  | 9     | 1284 | A    |
| 51  | 9     | 1286 | G    |
| 51  | 9     | 1288 | U    |
| 51  | 9     | 1289 | U    |
| 51  | 9     | 1291 | A    |
| 51  | 9     | 1292 | C    |
| 51  | 9     | 1293 | A    |
| 51  | 9     | 1294 | G    |
| 51  | 9     | 1298 | G    |
| 51  | 9     | 1299 | A    |
| 51  | 9     | 1301 | A    |
| 51  | 9     | 1302 | G    |
| 51  | 9     | 1303 | C    |
| 51  | 9     | 1304 | U    |
| 51  | 9     | 1307 | U    |
| 51  | 9     | 1308 | U    |
| 51  | 9     | 1310 | U    |
| 51  | 9     | 1311 | C    |
| 51  | 9     | 1313 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 9     | 1314 | U    |
| 51  | 9     | 1315 | U    |
| 51  | 9     | 1317 | C    |
| 51  | 9     | 1319 | U    |
| 51  | 9     | 1321 | G    |
| 51  | 9     | 1333 | U    |
| 51  | 9     | 1342 | U    |
| 51  | 9     | 1345 | G    |
| 51  | 9     | 1371 | U    |
| 51  | 9     | 1372 | U    |
| 51  | 9     | 1376 | A    |
| 51  | 9     | 1378 | A    |
| 51  | 9     | 1394 | G    |
| 51  | 9     | 1395 | C    |
| 51  | 9     | 1396 | A    |
| 51  | 9     | 1397 | U    |
| 51  | 9     | 1398 | G    |
| 51  | 9     | 1401 | A    |
| 51  | 9     | 1402 | A    |
| 51  | 9     | 1407 | U    |
| 51  | 9     | 1408 | U    |
| 51  | 9     | 1409 | A    |
| 51  | 9     | 1410 | C    |
| 51  | 9     | 1412 | C    |
| 51  | 9     | 1413 | G    |
| 51  | 9     | 1416 | C    |
| 51  | 9     | 1418 | C    |
| 51  | 9     | 1419 | C    |
| 51  | 9     | 1420 | G    |
| 51  | 9     | 1423 | C    |
| 51  | 9     | 1424 | G    |
| 51  | 9     | 1426 | U    |
| 51  | 9     | 1427 | C    |
| 51  | 9     | 1429 | G    |
| 51  | 9     | 1431 | G    |
| 51  | 9     | 1432 | U    |
| 51  | 9     | 1433 | C    |
| 51  | 9     | 1434 | C    |
| 51  | 9     | 1435 | C    |
| 51  | 9     | 1436 | C    |
| 51  | 9     | 1438 | A    |
| 51  | 9     | 1439 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 9     | 1440 | C    |
| 51  | 9     | 1442 | OMU  |
| 51  | 9     | 1447 | G    |
| 51  | 9     | 1454 | A    |
| 51  | 9     | 1455 | A    |
| 51  | 9     | 1460 | C    |
| 51  | 9     | 1462 | U    |
| 51  | 9     | 1463 | U    |
| 51  | 9     | 1464 | C    |
| 51  | 9     | 1472 | C    |
| 51  | 9     | 1476 | A    |
| 51  | 9     | 1477 | U    |
| 51  | 9     | 1478 | U    |
| 51  | 9     | 1480 | A    |
| 51  | 9     | 1489 | A    |
| 51  | 9     | 1490 | OMG  |
| 51  | 9     | 1496 | U    |
| 51  | 9     | 1498 | A    |
| 51  | 9     | 1502 | C    |
| 51  | 9     | 1510 | G    |
| 51  | 9     | 1512 | C    |
| 51  | 9     | 1514 | G    |
| 51  | 9     | 1519 | U    |
| 51  | 9     | 1521 | C    |
| 51  | 9     | 1522 | A    |
| 51  | 9     | 1533 | A    |
| 51  | 9     | 1544 | C    |
| 51  | 9     | 1548 | G    |
| 51  | 9     | 1552 | G    |
| 51  | 9     | 1555 | U    |
| 51  | 9     | 1556 | A    |
| 51  | 9     | 1557 | C    |
| 51  | 9     | 1558 | C    |
| 51  | 9     | 1560 | U    |
| 51  | 9     | 1567 | G    |
| 51  | 9     | 1574 | C    |
| 51  | 9     | 1575 | G    |
| 51  | 9     | 1576 | G    |
| 51  | 9     | 1579 | A    |
| 51  | 9     | 1580 | A    |
| 51  | 9     | 1581 | C    |
| 51  | 9     | 1586 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 9     | 1587 | G    |
| 51  | 9     | 1588 | A    |
| 51  | 9     | 1599 | U    |
| 51  | 9     | 1604 | G    |
| 51  | 9     | 1621 | U    |
| 51  | 9     | 1623 | A    |
| 51  | 9     | 1637 | A    |
| 51  | 9     | 1638 | G    |
| 51  | 9     | 1639 | G7M  |
| 51  | 9     | 1647 | A    |
| 51  | 9     | 1648 | G    |
| 51  | 9     | 1654 | G    |
| 51  | 9     | 1657 | G    |
| 51  | 9     | 1664 | A    |
| 51  | 9     | 1665 | G    |
| 51  | 9     | 1669 | G    |
| 51  | 9     | 1695 | A    |
| 51  | 9     | 1721 | U    |
| 51  | 9     | 1722 | G    |
| 51  | 9     | 1726 | G    |
| 51  | 9     | 1744 | G    |
| 51  | 9     | 1753 | C    |
| 51  | 9     | 1756 | C    |
| 51  | 9     | 1759 | G    |
| 51  | 9     | 1774 | C    |
| 51  | 9     | 1775 | U    |
| 51  | 9     | 1777 | G    |
| 51  | 9     | 1783 | C    |
| 51  | 9     | 1784 | G    |
| 51  | 9     | 1786 | U    |
| 51  | 9     | 1794 | C    |
| 51  | 9     | 1797 | U    |
| 51  | 9     | 1823 | A    |
| 51  | 9     | 1824 | A    |
| 51  | 9     | 1825 | A    |
| 51  | 9     | 1829 | G    |
| 51  | 9     | 1831 | A    |
| 51  | 9     | 1835 | A    |
| 51  | 9     | 1836 | G    |
| 51  | 9     | 1838 | U    |
| 51  | 9     | 1849 | G    |
| 51  | 9     | 1861 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 9     | 1862 | G    |
| 51  | 9     | 1863 | A    |
| 51  | 9     | 1864 | U    |
| 51  | 9     | 1865 | C    |
| 85  | hh    | 43   | A    |
| 85  | hh    | 46   | G    |
| 85  | hh    | 49   | U    |

All (111) RNA pucker outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 48  | 5     | 42     | A    |
| 48  | 5     | 125    | C    |
| 48  | 5     | 133    | C    |
| 48  | 5     | 134    | G    |
| 48  | 5     | 217    | C    |
| 48  | 5     | 231    | U    |
| 48  | 5     | 245    | C    |
| 48  | 5     | 265    | C    |
| 48  | 5     | 267    | G    |
| 48  | 5     | 275    | C    |
| 48  | 5     | 278    | G    |
| 48  | 5     | 385    | A    |
| 48  | 5     | 406    | C    |
| 48  | 5     | 449    | C    |
| 48  | 5     | 480    | C    |
| 48  | 5     | 485    | C    |
| 48  | 5     | 504    | G    |
| 48  | 5     | 922(B) | C    |
| 48  | 5     | 924    | C    |
| 48  | 5     | 930    | G    |
| 48  | 5     | 959    | G    |
| 48  | 5     | 1072   | C    |
| 48  | 5     | 1211   | G    |
| 48  | 5     | 1236   | C    |
| 48  | 5     | 1238   | A    |
| 48  | 5     | 1291   | G    |
| 48  | 5     | 1370   | G    |
| 48  | 5     | 1445   | U    |
| 48  | 5     | 1455   | G    |
| 48  | 5     | 1477   | C    |
| 48  | 5     | 1590   | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 1625 | OMG  |
| 48  | 5     | 1633 | G    |
| 48  | 5     | 1733 | G    |
| 48  | 5     | 1818 | G    |
| 48  | 5     | 1956 | A    |
| 48  | 5     | 1975 | G    |
| 48  | 5     | 1978 | C    |
| 48  | 5     | 1982 | G    |
| 48  | 5     | 1990 | A    |
| 48  | 5     | 1991 | A    |
| 48  | 5     | 2046 | G    |
| 48  | 5     | 2068 | C    |
| 48  | 5     | 2089 | G    |
| 48  | 5     | 2104 | A    |
| 48  | 5     | 2258 | C    |
| 48  | 5     | 2266 | C    |
| 48  | 5     | 2488 | C    |
| 48  | 5     | 2502 | A    |
| 48  | 5     | 2529 | A    |
| 48  | 5     | 2587 | A    |
| 48  | 5     | 2639 | U    |
| 48  | 5     | 2695 | A    |
| 48  | 5     | 2794 | C    |
| 48  | 5     | 3603 | G    |
| 48  | 5     | 3625 | G    |
| 48  | 5     | 3672 | G    |
| 48  | 5     | 3876 | A    |
| 48  | 5     | 3888 | G    |
| 48  | 5     | 4119 | C    |
| 48  | 5     | 4232 | U    |
| 48  | 5     | 4378 | A    |
| 48  | 5     | 4394 | A    |
| 48  | 5     | 4395 | U    |
| 48  | 5     | 4448 | G    |
| 48  | 5     | 4548 | A    |
| 48  | 5     | 4699 | U    |
| 48  | 5     | 4719 | G    |
| 48  | 5     | 4884 | G    |
| 48  | 5     | 4925 | U    |
| 48  | 5     | 4932 | U    |
| 48  | 5     | 4947 | U    |
| 50  | 8     | 81   | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 50  | 8     | 94   | G    |
| 50  | 8     | 124  | U    |
| 51  | 9     | 72   | C    |
| 51  | 9     | 102  | A    |
| 51  | 9     | 110  | U    |
| 51  | 9     | 140  | C    |
| 51  | 9     | 208  | G    |
| 51  | 9     | 213  | G    |
| 51  | 9     | 215  | G    |
| 51  | 9     | 291  | G    |
| 51  | 9     | 327  | G    |
| 51  | 9     | 369  | C    |
| 51  | 9     | 407  | G    |
| 51  | 9     | 417  | C    |
| 51  | 9     | 434  | G    |
| 51  | 9     | 465  | A    |
| 51  | 9     | 532  | C    |
| 51  | 9     | 563  | G    |
| 51  | 9     | 642  | U    |
| 51  | 9     | 840  | C    |
| 51  | 9     | 869  | A    |
| 51  | 9     | 870  | A    |
| 51  | 9     | 1137 | U    |
| 51  | 9     | 1281 | G    |
| 51  | 9     | 1394 | G    |
| 51  | 9     | 1395 | C    |
| 51  | 9     | 1408 | U    |
| 51  | 9     | 1418 | C    |
| 51  | 9     | 1432 | U    |
| 51  | 9     | 1463 | U    |
| 51  | 9     | 1477 | U    |
| 51  | 9     | 1490 | OMG  |
| 51  | 9     | 1556 | A    |
| 51  | 9     | 1637 | A    |
| 51  | 9     | 1646 | C    |
| 51  | 9     | 1647 | A    |
| 51  | 9     | 1824 | A    |
| 51  | 9     | 1835 | A    |

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

163 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|-------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |       | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 51  | 6MZ  | 9     | 1832 | 88,51 | 22,25,26     | 2.53 | 4 (18%)     | 29,36,39    | 2.22 | 10 (34%)    |
| 48  | OMG  | 5     | 4392 | 48    | 23,26,27     | 2.32 | 8 (34%)     | 32,38,41    | 2.14 | 9 (28%)     |
| 48  | OMG  | 5     | 4196 | 48,46 | 23,26,27     | 2.42 | 7 (30%)     | 32,38,41    | 2.06 | 10 (31%)    |
| 51  | OMU  | 9     | 172  | 51    | 19,22,23     | 2.85 | 7 (36%)     | 25,31,34    | 1.82 | 5 (20%)     |
| 48  | OMU  | 5     | 4227 | 48    | 19,22,23     | 2.83 | 7 (36%)     | 25,31,34    | 1.85 | 5 (20%)     |
| 48  | A2M  | 5     | 1871 | 48,88 | 22,25,26     | 3.46 | 10 (45%)    | 30,36,39    | 2.50 | 10 (33%)    |
| 48  | A2M  | 5     | 398  | 48    | 22,25,26     | 3.53 | 9 (40%)     | 30,36,39    | 2.68 | 11 (36%)    |
| 48  | PSU  | 5     | 4532 | 48    | 17,20,22     | 1.12 | 1 (5%)      | 21,28,33    | 1.76 | 3 (14%)     |
| 48  | OMG  | 5     | 4618 | 48    | 23,26,27     | 2.33 | 8 (34%)     | 32,38,41    | 2.12 | 11 (34%)    |
| 51  | A2M  | 9     | 484  | 51    | 22,25,26     | 3.50 | 9 (40%)     | 30,36,39    | 2.69 | 10 (33%)    |
| 48  | OMG  | 5     | 1522 | 48    | 23,26,27     | 2.37 | 9 (39%)     | 32,38,41    | 2.14 | 12 (37%)    |
| 48  | A2M  | 5     | 4571 | 48    | 22,25,26     | 3.60 | 10 (45%)    | 30,36,39    | 2.64 | 11 (36%)    |
| 48  | PSU  | 5     | 4420 | 48    | 17,20,22     | 1.13 | 1 (5%)      | 21,28,33    | 2.06 | 4 (19%)     |
| 51  | OMU  | 9     | 1442 | 51    | 19,22,23     | 2.84 | 6 (31%)     | 25,31,34    | 1.83 | 4 (16%)     |
| 51  | MA6  | 9     | 1850 | 51    | 23,26,27     | 1.53 | 5 (21%)     | 33,38,41    | 3.96 | 14 (42%)    |
| 51  | PSU  | 9     | 1367 | 51    | 17,20,22     | 1.15 | 1 (5%)      | 21,28,33    | 1.90 | 4 (19%)     |
| 48  | PSU  | 5     | 1683 | 48,88 | 17,20,22     | 1.23 | 1 (5%)      | 21,28,33    | 2.02 | 4 (19%)     |
| 48  | A2M  | 5     | 3830 | 48    | 22,25,26     | 3.42 | 9 (40%)     | 30,36,39    | 2.66 | 11 (36%)    |
| 48  | OMU  | 5     | 4620 | 48    | 19,22,23     | 2.83 | 7 (36%)     | 25,31,34    | 1.87 | 5 (20%)     |
| 51  | OMC  | 9     | 1391 | 51    | 19,22,23     | 2.96 | 8 (42%)     | 25,31,34    | 0.97 | 1 (4%)      |
| 48  | A2M  | 5     | 3724 | 48    | 22,25,26     | 3.54 | 9 (40%)     | 30,36,39    | 2.51 | 9 (30%)     |
| 48  | OMC  | 5     | 2861 | 48    | 19,22,23     | 2.94 | 8 (42%)     | 25,31,34    | 0.84 | 1 (4%)      |
| 48  | A2M  | 5     | 4523 | 48,88 | 22,25,26     | 3.48 | 9 (40%)     | 30,36,39    | 2.67 | 11 (36%)    |
| 51  | A2M  | 9     | 468  | 51    | 22,25,26     | 3.55 | 9 (40%)     | 30,36,39    | 2.60 | 10 (33%)    |
| 48  | OMC  | 5     | 3701 | 48,88 | 19,22,23     | 2.76 | 8 (42%)     | 25,31,34    | 1.04 | 1 (4%)      |
| 48  | 5MC  | 5     | 4447 | 48,88 | 19,22,23     | 3.54 | 8 (42%)     | 26,32,35    | 1.14 | 2 (7%)      |
| 48  | A2M  | 5     | 2363 | 48,88 | 22,25,26     | 3.53 | 10 (45%)    | 30,36,39    | 2.59 | 9 (30%)     |
| 48  | PSU  | 5     | 2632 | 48    | 17,20,22     | 1.15 | 1 (5%)      | 21,28,33    | 1.97 | 4 (19%)     |
| 48  | A2M  | 5     | 3867 | 48    | 22,25,26     | 3.46 | 9 (40%)     | 30,36,39    | 2.57 | 8 (26%)     |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 48  | PSU  | 5     | 4423 | 48    | 17,20,22     | 1.00 | 1 (5%)   | 21,28,33    | 1.98 | 4 (19%)  |
| 48  | OMG  | 5     | 4499 | 48    | 23,26,27     | 2.45 | 9 (39%)  | 32,38,41    | 2.05 | 9 (28%)  |
| 48  | OMG  | 5     | 4228 | 48    | 23,26,27     | 2.30 | 7 (30%)  | 32,38,41    | 2.08 | 10 (31%) |
| 48  | PSU  | 5     | 4552 | 48    | 17,20,22     | 1.16 | 1 (5%)   | 21,28,33    | 1.93 | 4 (19%)  |
| 51  | PSU  | 9     | 119  | 51    | 17,20,22     | 1.08 | 1 (5%)   | 21,28,33    | 2.02 | 5 (23%)  |
| 51  | A2M  | 9     | 512  | 51    | 22,25,26     | 3.50 | 9 (40%)  | 30,36,39    | 2.77 | 10 (33%) |
| 51  | 4AC  | 9     | 1337 | 51    | 21,24,25     | 3.09 | 10 (47%) | 28,34,37    | 1.03 | 1 (3%)   |
| 48  | PSU  | 5     | 1860 | 48    | 17,20,22     | 1.03 | 1 (5%)   | 21,28,33    | 1.92 | 4 (19%)  |
| 48  | PSU  | 5     | 3715 | 48    | 17,20,22     | 1.13 | 3 (17%)  | 21,28,33    | 2.10 | 6 (28%)  |
| 48  | OMG  | 5     | 4623 | 48    | 23,26,27     | 2.43 | 8 (34%)  | 32,38,41    | 2.17 | 9 (28%)  |
| 48  | OMG  | 5     | 373  | 48    | 23,26,27     | 2.41 | 7 (30%)  | 32,38,41    | 2.21 | 11 (34%) |
| 51  | PSU  | 9     | 1177 | 51    | 17,20,22     | 1.08 | 1 (5%)   | 21,28,33    | 1.77 | 4 (19%)  |
| 48  | 6MZ  | 5     | 4220 | 48    | 22,25,26     | 2.74 | 4 (18%)  | 29,36,39    | 2.17 | 9 (31%)  |
| 48  | OMC  | 5     | 4456 | 48    | 19,22,23     | 2.80 | 8 (42%)  | 25,31,34    | 0.77 | 0        |
| 51  | A2M  | 9     | 1678 | 51    | 22,25,26     | 3.45 | 9 (40%)  | 30,36,39    | 2.72 | 11 (36%) |
| 51  | PSU  | 9     | 1692 | 51    | 17,20,22     | 1.14 | 1 (5%)   | 21,28,33    | 1.78 | 3 (14%)  |
| 51  | A2M  | 9     | 1031 | 51    | 22,25,26     | 3.51 | 10 (45%) | 30,36,39    | 2.46 | 9 (30%)  |
| 48  | PSU  | 5     | 3853 | 48    | 17,20,22     | 1.21 | 1 (5%)   | 21,28,33    | 2.19 | 5 (23%)  |
| 51  | A2M  | 9     | 166  | 51    | 22,25,26     | 3.45 | 9 (40%)  | 30,36,39    | 2.57 | 10 (33%) |
| 51  | A2M  | 9     | 668  | 88,51 | 22,25,26     | 3.45 | 9 (40%)  | 30,36,39    | 2.75 | 13 (43%) |
| 51  | PSU  | 9     | 1081 | 51    | 17,20,22     | 1.14 | 1 (5%)   | 21,28,33    | 2.03 | 6 (28%)  |
| 48  | OMU  | 5     | 2837 | 48    | 19,22,23     | 2.84 | 6 (31%)  | 25,31,34    | 2.02 | 6 (24%)  |
| 48  | PSU  | 5     | 4361 | 48    | 17,20,22     | 1.11 | 1 (5%)   | 21,28,33    | 2.01 | 5 (23%)  |
| 48  | A2M  | 5     | 3785 | 48    | 22,25,26     | 3.33 | 10 (45%) | 30,36,39    | 2.71 | 10 (33%) |
| 48  | 2MG  | 5     | 1517 | 48    | 23,26,27     | 2.57 | 9 (39%)  | 33,38,41    | 2.53 | 13 (39%) |
| 48  | UY1  | 5     | 3818 | 48,88 | 19,22,23     | 4.33 | 9 (47%)  | 21,31,34    | 2.11 | 5 (23%)  |
| 51  | OMG  | 9     | 644  | 51    | 23,26,27     | 2.37 | 7 (30%)  | 32,38,41    | 1.95 | 9 (28%)  |
| 51  | A2M  | 9     | 99   | 88,51 | 22,25,26     | 3.53 | 9 (40%)  | 30,36,39    | 2.60 | 10 (33%) |
| 48  | OMG  | 5     | 4370 | 48    | 23,26,27     | 2.36 | 8 (34%)  | 32,38,41    | 2.15 | 11 (34%) |
| 48  | OMG  | 5     | 2424 | 48    | 23,26,27     | 2.35 | 8 (34%)  | 32,38,41    | 2.06 | 9 (28%)  |
| 48  | PSU  | 5     | 3764 | 48    | 17,20,22     | 1.18 | 1 (5%)   | 21,28,33    | 2.04 | 5 (23%)  |
| 48  | PSU  | 5     | 3639 | 48    | 17,20,22     | 1.16 | 1 (5%)   | 21,28,33    | 1.91 | 4 (19%)  |
| 51  | PSU  | 9     | 109  | 51    | 17,20,22     | 1.20 | 1 (5%)   | 21,28,33    | 2.02 | 4 (19%)  |
| 51  | PSU  | 9     | 1347 | 51    | 17,20,22     | 1.08 | 1 (5%)   | 21,28,33    | 2.00 | 5 (23%)  |
| 48  | PSU  | 5     | 3851 | 48    | 17,20,22     | 1.09 | 2 (11%)  | 21,28,33    | 2.06 | 4 (19%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 48  | A2M  | 5     | 3760 | 48,88 | 22,25,26     | 3.50 | 9 (40%)  | 30,36,39    | 2.67 | 11 (36%) |
| 51  | PSU  | 9     | 1004 | 51    | 17,20,22     | 1.13 | 1 (5%)   | 21,28,33    | 1.99 | 4 (19%)  |
| 51  | PSU  | 9     | 815  | 51    | 17,20,22     | 1.06 | 1 (5%)   | 21,28,33    | 2.17 | 5 (23%)  |
| 51  | PSU  | 9     | 686  | 51    | 17,20,22     | 1.02 | 2 (11%)  | 21,28,33    | 2.29 | 6 (28%)  |
| 48  | OMG  | 5     | 3899 | 48    | 23,26,27     | 2.37 | 8 (34%)  | 32,38,41    | 2.16 | 10 (31%) |
| 48  | OMU  | 5     | 4498 | 48    | 19,22,23     | 2.81 | 8 (42%)  | 25,31,34    | 1.93 | 5 (20%)  |
| 51  | PSU  | 9     | 814  | 51    | 17,20,22     | 1.08 | 1 (5%)   | 21,28,33    | 2.05 | 5 (23%)  |
| 48  | A2M  | 5     | 1524 | 48    | 22,25,26     | 3.44 | 9 (40%)  | 30,36,39    | 2.67 | 12 (40%) |
| 48  | PSU  | 5     | 3920 | 48    | 17,20,22     | 1.05 | 1 (5%)   | 21,28,33    | 2.18 | 5 (23%)  |
| 48  | PSU  | 5     | 4579 | 48    | 17,20,22     | 1.05 | 1 (5%)   | 21,28,33    | 1.89 | 4 (19%)  |
| 51  | PSU  | 9     | 1238 | 51    | 17,20,22     | 1.22 | 2 (11%)  | 21,28,33    | 2.00 | 4 (19%)  |
| 48  | OMG  | 5     | 1625 | 48,88 | 23,26,27     | 2.46 | 7 (30%)  | 32,38,41    | 2.23 | 10 (31%) |
| 48  | OMC  | 5     | 2351 | 48    | 19,22,23     | 2.74 | 8 (42%)  | 25,31,34    | 0.82 | 0        |
| 48  | OMC  | 5     | 2365 | 48    | 19,22,23     | 2.84 | 8 (42%)  | 25,31,34    | 0.67 | 0        |
| 51  | OMG  | 9     | 1328 | 51    | 23,26,27     | 2.35 | 9 (39%)  | 32,38,41    | 2.08 | 9 (28%)  |
| 48  | PSU  | 5     | 4500 | 48    | 17,20,22     | 1.11 | 3 (17%)  | 21,28,33    | 2.07 | 5 (23%)  |
| 51  | 4AC  | 9     | 1842 | 51    | 21,24,25     | 3.00 | 10 (47%) | 28,34,37    | 1.08 | 2 (7%)   |
| 51  | OMG  | 9     | 683  | 51    | 23,26,27     | 2.46 | 8 (34%)  | 32,38,41    | 2.21 | 11 (34%) |
| 51  | B8N  | 9     | 1248 | 51    | 25,29,30     | 3.40 | 8 (32%)  | 28,42,45    | 2.31 | 7 (25%)  |
| 51  | A2M  | 9     | 159  | 51    | 22,25,26     | 3.56 | 9 (40%)  | 30,36,39    | 2.53 | 10 (33%) |
| 48  | PSU  | 5     | 4628 | 48    | 17,20,22     | 1.22 | 2 (11%)  | 21,28,33    | 2.19 | 6 (28%)  |
| 51  | OMU  | 9     | 428  | 51    | 19,22,23     | 2.87 | 7 (36%)  | 25,31,34    | 1.79 | 5 (20%)  |
| 51  | G7M  | 9     | 1639 | 46,51 | 23,26,27     | 2.77 | 9 (39%)  | 34,39,42    | 1.74 | 9 (26%)  |
| 50  | OMG  | 8     | 75   | 50    | 23,26,27     | 2.35 | 8 (34%)  | 32,38,41    | 2.11 | 11 (34%) |
| 48  | PSU  | 5     | 3734 | 48    | 17,20,22     | 1.19 | 2 (11%)  | 21,28,33    | 1.93 | 5 (23%)  |
| 51  | OMC  | 9     | 1703 | 51    | 19,22,23     | 2.96 | 8 (42%)  | 25,31,34    | 0.80 | 0        |
| 48  | PSU  | 5     | 1792 | 48    | 17,20,22     | 1.03 | 1 (5%)   | 21,28,33    | 1.89 | 3 (14%)  |
| 51  | PSU  | 9     | 863  | 51    | 17,20,22     | 0.99 | 1 (5%)   | 21,28,33    | 1.93 | 3 (14%)  |
| 51  | PSU  | 9     | 1232 | 51    | 17,20,22     | 1.20 | 1 (5%)   | 21,28,33    | 1.93 | 3 (14%)  |
| 48  | OMC  | 5     | 1340 | 48    | 19,22,23     | 2.97 | 8 (42%)  | 25,31,34    | 1.01 | 2 (8%)   |
| 48  | OMG  | 5     | 1316 | 48    | 23,26,27     | 2.37 | 8 (34%)  | 32,38,41    | 2.17 | 10 (31%) |
| 48  | OMC  | 5     | 3808 | 48    | 19,22,23     | 2.74 | 8 (42%)  | 25,31,34    | 0.65 | 0        |
| 48  | OMG  | 5     | 3627 | 48    | 23,26,27     | 2.38 | 8 (34%)  | 32,38,41    | 2.11 | 11 (34%) |
| 51  | PSU  | 9     | 572  | 51    | 17,20,22     | 1.08 | 1 (5%)   | 21,28,33    | 1.95 | 4 (19%)  |
| 48  | OMC  | 5     | 3887 | 48    | 19,22,23     | 2.78 | 7 (36%)  | 25,31,34    | 0.77 | 1 (4%)   |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 51  | A2M  | 9     | 27   | 51    | 22,25,26     | 3.43 | 9 (40%)  | 30,36,39    | 2.51 | 9 (30%)  |
| 51  | PSU  | 9     | 1046 | 51    | 17,20,22     | 1.13 | 1 (5%)   | 21,28,33    | 1.92 | 5 (23%)  |
| 48  | B9B  | 5     | 237  | 48    | 25,28,29     | 1.79 | 6 (24%)  | 35,40,43    | 2.38 | 15 (42%) |
| 48  | PSU  | 5     | 3695 | 48    | 17,20,22     | 1.05 | 1 (5%)   | 21,28,33    | 1.97 | 4 (19%)  |
| 51  | PSU  | 9     | 218  | 51    | 17,20,22     | 1.13 | 1 (5%)   | 21,28,33    | 2.28 | 7 (33%)  |
| 51  | PSU  | 9     | 609  | 51    | 17,20,22     | 1.08 | 1 (5%)   | 21,28,33    | 2.01 | 4 (19%)  |
| 51  | OMC  | 9     | 174  | 51    | 19,22,23     | 2.91 | 8 (42%)  | 25,31,34    | 0.95 | 0        |
| 51  | OMC  | 9     | 517  | 51    | 19,22,23     | 2.99 | 8 (42%)  | 25,31,34    | 0.82 | 0        |
| 51  | PSU  | 9     | 1174 | 51    | 17,20,22     | 1.11 | 1 (5%)   | 21,28,33    | 2.07 | 4 (19%)  |
| 51  | OMG  | 9     | 436  | 51    | 23,26,27     | 2.46 | 6 (26%)  | 32,38,41    | 2.09 | 9 (28%)  |
| 48  | A2M  | 5     | 1534 | 48,88 | 22,25,26     | 3.56 | 9 (40%)  | 30,36,39    | 2.64 | 11 (36%) |
| 48  | PSU  | 5     | 4521 | 48,88 | 17,20,22     | 1.24 | 2 (11%)  | 21,28,33    | 2.25 | 7 (33%)  |
| 48  | A2M  | 5     | 1326 | 48    | 22,25,26     | 3.50 | 9 (40%)  | 30,36,39    | 2.55 | 8 (26%)  |
| 51  | PSU  | 9     | 1445 | 51    | 17,20,22     | 1.05 | 1 (5%)   | 21,28,33    | 1.84 | 4 (19%)  |
| 48  | PSU  | 5     | 1862 | 48    | 17,20,22     | 1.11 | 1 (5%)   | 21,28,33    | 1.99 | 5 (23%)  |
| 51  | OMU  | 9     | 116  | 51    | 19,22,23     | 2.80 | 6 (31%)  | 25,31,34    | 1.78 | 5 (20%)  |
| 48  | OMC  | 5     | 3841 | 48    | 19,22,23     | 2.82 | 8 (42%)  | 25,31,34    | 0.90 | 0        |
| 48  | OMU  | 5     | 4306 | 48    | 19,22,23     | 2.86 | 7 (36%)  | 25,31,34    | 1.85 | 4 (16%)  |
| 48  | 5MC  | 5     | 3782 | 48,88 | 19,22,23     | 3.55 | 8 (42%)  | 26,32,35    | 1.14 | 2 (7%)   |
| 48  | PSU  | 5     | 1781 | 48    | 17,20,22     | 1.13 | 2 (11%)  | 21,28,33    | 1.96 | 5 (23%)  |
| 48  | OMG  | 5     | 3792 | 48    | 23,26,27     | 2.32 | 6 (26%)  | 32,38,41    | 2.00 | 9 (28%)  |
| 48  | PSU  | 5     | 4353 | 48    | 17,20,22     | 1.12 | 2 (11%)  | 21,28,33    | 2.11 | 5 (23%)  |
| 48  | PSU  | 5     | 4403 | 48    | 17,20,22     | 1.10 | 1 (5%)   | 21,28,33    | 1.88 | 4 (19%)  |
| 48  | A2M  | 5     | 3718 | 48    | 22,25,26     | 3.55 | 10 (45%) | 30,36,39    | 2.64 | 11 (36%) |
| 51  | OMG  | 9     | 509  | 88,51 | 23,26,27     | 2.40 | 7 (30%)  | 32,38,41    | 1.99 | 9 (28%)  |
| 48  | PSU  | 5     | 1744 | 48,88 | 17,20,22     | 0.96 | 1 (5%)   | 21,28,33    | 2.01 | 4 (19%)  |
| 48  | OMC  | 5     | 2824 | 48    | 19,22,23     | 2.84 | 8 (42%)  | 25,31,34    | 0.95 | 1 (4%)   |
| 48  | A2M  | 5     | 2815 | 48    | 22,25,26     | 3.44 | 9 (40%)  | 30,36,39    | 2.57 | 9 (30%)  |
| 48  | UR3  | 5     | 4530 | 48    | 19,22,23     | 2.64 | 8 (42%)  | 26,32,35    | 1.50 | 4 (15%)  |
| 48  | PSU  | 5     | 4442 | 48    | 17,20,22     | 1.09 | 1 (5%)   | 21,28,33    | 2.09 | 5 (23%)  |
| 48  | PSU  | 5     | 1782 | 48    | 17,20,22     | 1.10 | 1 (5%)   | 21,28,33    | 2.01 | 5 (23%)  |
| 48  | PSU  | 5     | 4293 | 48    | 17,20,22     | 1.22 | 2 (11%)  | 21,28,33    | 1.88 | 4 (19%)  |
| 48  | OMG  | 5     | 4494 | 48    | 23,26,27     | 2.30 | 8 (34%)  | 32,38,41    | 2.03 | 10 (31%) |
| 51  | OMU  | 9     | 121  | 51    | 19,22,23     | 2.72 | 6 (31%)  | 25,31,34    | 1.90 | 6 (24%)  |
| 48  | OMC  | 5     | 2422 | 48,88 | 19,22,23     | 2.93 | 8 (42%)  | 25,31,34    | 0.72 | 0        |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 48  | PSU  | 5     | 4299 | 48    | 17,20,22     | 1.00 | 1 (5%)   | 21,28,33    | 1.94 | 3 (14%)  |
| 51  | OMG  | 9     | 1490 | 88,51 | 23,26,27     | 2.33 | 8 (34%)  | 32,38,41    | 2.22 | 8 (25%)  |
| 48  | PSU  | 5     | 4296 | 48    | 17,20,22     | 1.20 | 2 (11%)  | 21,28,33    | 1.96 | 3 (14%)  |
| 51  | PSU  | 9     | 649  | 51    | 17,20,22     | 1.06 | 1 (5%)   | 21,28,33    | 1.89 | 4 (19%)  |
| 48  | PSU  | 5     | 1677 | 48    | 17,20,22     | 1.25 | 2 (11%)  | 21,28,33    | 2.17 | 4 (19%)  |
| 48  | PSU  | 5     | 3762 | 48    | 17,20,22     | 1.14 | 1 (5%)   | 21,28,33    | 2.13 | 5 (23%)  |
| 48  | 1MA  | 5     | 1322 | 48,88 | 21,25,26     | 2.66 | 6 (28%)  | 30,37,40    | 2.29 | 6 (20%)  |
| 48  | PSU  | 5     | 2508 | 48    | 17,20,22     | 1.07 | 1 (5%)   | 21,28,33    | 1.92 | 4 (19%)  |
| 48  | A2M  | 5     | 3825 | 48    | 22,25,26     | 3.48 | 9 (40%)  | 30,36,39    | 2.50 | 10 (33%) |
| 48  | OMC  | 5     | 2804 | 48    | 19,22,23     | 2.79 | 8 (42%)  | 25,31,34    | 0.72 | 0        |
| 51  | PSU  | 9     | 1045 | 51    | 17,20,22     | 1.15 | 2 (11%)  | 21,28,33    | 2.14 | 5 (23%)  |
| 48  | OMG  | 5     | 2364 | 48    | 23,26,27     | 2.34 | 8 (34%)  | 32,38,41    | 2.15 | 10 (31%) |
| 51  | PSU  | 9     | 1244 | 51    | 17,20,22     | 1.17 | 1 (5%)   | 21,28,33    | 2.06 | 5 (23%)  |
| 48  | A2M  | 5     | 400  | 48    | 22,25,26     | 3.43 | 9 (40%)  | 30,36,39    | 2.51 | 9 (30%)  |
| 51  | PSU  | 9     | 105  | 51    | 17,20,22     | 1.14 | 1 (5%)   | 21,28,33    | 2.00 | 4 (19%)  |
| 51  | OMU  | 9     | 1326 | 51    | 19,22,23     | 2.81 | 7 (36%)  | 25,31,34    | 1.95 | 5 (20%)  |
| 51  | MA6  | 9     | 1851 | 51    | 23,26,27     | 1.40 | 4 (17%)  | 33,38,41    | 4.48 | 13 (39%) |
| 51  | A2M  | 9     | 1383 | 51    | 22,25,26     | 3.46 | 10 (45%) | 30,36,39    | 2.69 | 11 (36%) |
| 48  | OMG  | 5     | 4637 | 48    | 23,26,27     | 2.38 | 8 (34%)  | 32,38,41    | 2.14 | 10 (31%) |
| 48  | OMC  | 5     | 4536 | 48    | 19,22,23     | 2.77 | 8 (42%)  | 25,31,34    | 0.86 | 0        |
| 51  | PSU  | 9     | 801  | 51    | 17,20,22     | 1.25 | 2 (11%)  | 21,28,33    | 1.67 | 4 (19%)  |
| 51  | PSU  | 9     | 1643 | 51    | 17,20,22     | 1.03 | 1 (5%)   | 21,28,33    | 2.08 | 4 (19%)  |
| 48  | PSU  | 5     | 4457 | 48    | 17,20,22     | 1.15 | 1 (5%)   | 21,28,33    | 1.77 | 3 (14%)  |
| 48  | OMU  | 5     | 3925 | 48    | 19,22,23     | 2.81 | 7 (36%)  | 25,31,34    | 1.88 | 4 (16%)  |
| 48  | A2M  | 5     | 2787 | 48    | 22,25,26     | 3.42 | 9 (40%)  | 30,36,39    | 2.69 | 10 (33%) |
| 48  | OMC  | 5     | 3869 | 48    | 19,22,23     | 2.83 | 7 (36%)  | 25,31,34    | 0.76 | 0        |
| 51  | PSU  | 9     | 822  | 51    | 17,20,22     | 1.23 | 3 (17%)  | 21,28,33    | 2.24 | 6 (28%)  |
| 48  | OMG  | 5     | 2876 | 48    | 23,26,27     | 2.40 | 7 (30%)  | 32,38,41    | 2.01 | 9 (28%)  |
| 51  | PSU  | 9     | 34   | 51    | 17,20,22     | 1.16 | 1 (5%)   | 21,28,33    | 1.96 | 4 (19%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 51  | 6MZ  | 9     | 1832 | 88,51 | -       | 2/9/27/28  | 0/3/3/3 |
| 48  | OMG  | 5     | 4392 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | OMG  | 5     | 4196 | 48,46 | -       | 0/9/27/28  | 0/3/3/3 |
| 51  | OMU  | 9     | 172  | 51    | -       | 2/9/27/28  | 0/2/2/2 |
| 48  | OMU  | 5     | 4227 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | A2M  | 5     | 1871 | 48,88 | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | A2M  | 5     | 398  | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | PSU  | 5     | 4532 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | OMG  | 5     | 4618 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 51  | A2M  | 9     | 484  | 51    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | OMG  | 5     | 1522 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | A2M  | 5     | 4571 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | PSU  | 5     | 4420 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | OMU  | 9     | 1442 | 51    | -       | 2/9/27/28  | 0/2/2/2 |
| 51  | MA6  | 9     | 1850 | 51    | -       | 0/11/29/30 | 0/3/3/3 |
| 51  | PSU  | 9     | 1367 | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | PSU  | 5     | 1683 | 48,88 | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | A2M  | 5     | 3830 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | OMU  | 5     | 4620 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 51  | OMC  | 9     | 1391 | 51    | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | A2M  | 5     | 3724 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | OMC  | 5     | 2861 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | A2M  | 5     | 4523 | 48,88 | -       | 0/9/27/28  | 0/3/3/3 |
| 51  | A2M  | 9     | 468  | 51    | -       | 1/9/27/28  | 0/3/3/3 |
| 48  | OMC  | 5     | 3701 | 48,88 | -       | 4/9/27/28  | 0/2/2/2 |
| 48  | 5MC  | 5     | 4447 | 48,88 | -       | 4/7/25/26  | 0/2/2/2 |
| 48  | A2M  | 5     | 2363 | 48,88 | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | PSU  | 5     | 2632 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | A2M  | 5     | 3867 | 48    | -       | 1/9/27/28  | 0/3/3/3 |
| 48  | PSU  | 5     | 4423 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | OMG  | 5     | 4499 | 48    | -       | 1/9/27/28  | 0/3/3/3 |
| 48  | OMG  | 5     | 4228 | 48    | -       | 1/9/27/28  | 0/3/3/3 |
| 48  | PSU  | 5     | 4552 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | PSU  | 9     | 119  | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | A2M  | 9     | 512  | 51    | -       | 1/9/27/28  | 0/3/3/3 |
| 51  | 4AC  | 9     | 1337 | 51    | -       | 0/11/29/30 | 0/2/2/2 |
| 48  | PSU  | 5     | 1860 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | PSU  | 5     | 3715 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | OMG  | 5     | 4623 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | OMG  | 5     | 373  | 48    | -       | 1/9/27/28  | 0/3/3/3 |
| 51  | PSU  | 9     | 1177 | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | 6MZ  | 5     | 4220 | 48    | -       | 0/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 48  | OMC  | 5     | 4456 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 51  | A2M  | 9     | 1678 | 51    | -       | 0/9/27/28  | 0/3/3/3 |
| 51  | PSU  | 9     | 1692 | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | A2M  | 9     | 1031 | 51    | -       | 1/9/27/28  | 0/3/3/3 |
| 48  | PSU  | 5     | 3853 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | A2M  | 9     | 166  | 51    | -       | 2/9/27/28  | 0/3/3/3 |
| 51  | A2M  | 9     | 668  | 88,51 | -       | 3/9/27/28  | 0/3/3/3 |
| 51  | PSU  | 9     | 1081 | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | OMU  | 5     | 2837 | 48    | -       | 1/9/27/28  | 0/2/2/2 |
| 48  | PSU  | 5     | 4361 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | A2M  | 5     | 3785 | 48    | -       | 3/9/27/28  | 0/3/3/3 |
| 48  | 2MG  | 5     | 1517 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | UY1  | 5     | 3818 | 48,88 | -       | 3/9/27/28  | 0/2/2/2 |
| 51  | OMG  | 9     | 644  | 51    | -       | 1/9/27/28  | 0/3/3/3 |
| 51  | A2M  | 9     | 99   | 88,51 | -       | 2/9/27/28  | 0/3/3/3 |
| 48  | OMG  | 5     | 4370 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | OMG  | 5     | 2424 | 48    | -       | 3/9/27/28  | 0/3/3/3 |
| 48  | PSU  | 5     | 3764 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | PSU  | 5     | 3639 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | PSU  | 9     | 109  | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | PSU  | 9     | 1347 | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | PSU  | 5     | 3851 | 48    | -       | 1/6/24/26  | 0/2/2/2 |
| 48  | A2M  | 5     | 3760 | 48,88 | -       | 3/9/27/28  | 0/3/3/3 |
| 51  | PSU  | 9     | 1004 | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | PSU  | 9     | 815  | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | PSU  | 9     | 686  | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | OMG  | 5     | 3899 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | OMU  | 5     | 4498 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 51  | PSU  | 9     | 814  | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | A2M  | 5     | 1524 | 48    | -       | 1/9/27/28  | 0/3/3/3 |
| 48  | PSU  | 5     | 3920 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | PSU  | 5     | 4579 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | PSU  | 9     | 1238 | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | OMG  | 5     | 1625 | 48,88 | -       | 1/9/27/28  | 0/3/3/3 |
| 48  | OMC  | 5     | 2351 | 48    | -       | 1/9/27/28  | 0/2/2/2 |
| 48  | OMC  | 5     | 2365 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 51  | OMG  | 9     | 1328 | 51    | -       | 1/9/27/28  | 0/3/3/3 |
| 48  | PSU  | 5     | 4500 | 48    | -       | 2/6/24/26  | 0/2/2/2 |
| 51  | 4AC  | 9     | 1842 | 51    | -       | 0/11/29/30 | 0/2/2/2 |
| 51  | OMG  | 9     | 683  | 51    | -       | 3/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 51  | B8N  | 9     | 1248 | 51    | -       | 4/16/34/35 | 0/2/2/2 |
| 51  | A2M  | 9     | 159  | 51    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | PSU  | 5     | 4628 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | OMU  | 9     | 428  | 51    | -       | 4/9/27/28  | 0/2/2/2 |
| 51  | G7M  | 9     | 1639 | 46,51 | -       | 2/7/25/26  | 0/3/3/3 |
| 50  | OMG  | 8     | 75   | 50    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | PSU  | 5     | 3734 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | OMC  | 9     | 1703 | 51    | -       | 2/9/27/28  | 0/2/2/2 |
| 48  | PSU  | 5     | 1792 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | PSU  | 9     | 863  | 51    | -       | 2/6/24/26  | 0/2/2/2 |
| 51  | PSU  | 9     | 1232 | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | OMC  | 5     | 1340 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | OMG  | 5     | 1316 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | OMC  | 5     | 3808 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | OMG  | 5     | 3627 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 51  | PSU  | 9     | 572  | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | OMC  | 5     | 3887 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 51  | A2M  | 9     | 27   | 51    | -       | 0/9/27/28  | 0/3/3/3 |
| 51  | PSU  | 9     | 1046 | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | B9B  | 5     | 237  | 48    | -       | 2/11/29/30 | 0/3/3/3 |
| 48  | PSU  | 5     | 3695 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | PSU  | 9     | 218  | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | PSU  | 9     | 609  | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | OMC  | 9     | 174  | 51    | -       | 0/9/27/28  | 0/2/2/2 |
| 51  | OMC  | 9     | 517  | 51    | -       | 0/9/27/28  | 0/2/2/2 |
| 51  | PSU  | 9     | 1174 | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | OMG  | 9     | 436  | 51    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | A2M  | 5     | 1534 | 48,88 | -       | 2/9/27/28  | 0/3/3/3 |
| 48  | PSU  | 5     | 4521 | 48,88 | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | A2M  | 5     | 1326 | 48    | -       | 1/9/27/28  | 0/3/3/3 |
| 51  | PSU  | 9     | 1445 | 51    | -       | 1/6/24/26  | 0/2/2/2 |
| 48  | PSU  | 5     | 1862 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | OMU  | 9     | 116  | 51    | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | OMC  | 5     | 3841 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | OMU  | 5     | 4306 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | 5MC  | 5     | 3782 | 48,88 | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | PSU  | 5     | 1781 | 48    | -       | 2/6/24/26  | 0/2/2/2 |
| 48  | OMG  | 5     | 3792 | 48    | -       | 2/9/27/28  | 0/3/3/3 |
| 48  | PSU  | 5     | 4353 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | PSU  | 5     | 4403 | 48    | -       | 0/6/24/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 48  | A2M  | 5     | 3718 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 51  | OMG  | 9     | 509  | 88,51 | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | PSU  | 5     | 1744 | 48,88 | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | OMC  | 5     | 2824 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | A2M  | 5     | 2815 | 48    | -       | 2/9/27/28  | 0/3/3/3 |
| 48  | UR3  | 5     | 4530 | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | PSU  | 5     | 4442 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | PSU  | 5     | 1782 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | PSU  | 5     | 4293 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | OMG  | 5     | 4494 | 48    | -       | 1/9/27/28  | 0/3/3/3 |
| 51  | OMU  | 9     | 121  | 51    | -       | 1/9/27/28  | 0/2/2/2 |
| 48  | OMC  | 5     | 2422 | 48,88 | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | PSU  | 5     | 4299 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | OMG  | 9     | 1490 | 88,51 | -       | 2/9/27/28  | 0/3/3/3 |
| 48  | PSU  | 5     | 4296 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | PSU  | 9     | 649  | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | PSU  | 5     | 1677 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | PSU  | 5     | 3762 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | 1MA  | 5     | 1322 | 48,88 | -       | 2/7/25/26  | 0/3/3/3 |
| 48  | PSU  | 5     | 2508 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | A2M  | 5     | 3825 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | OMC  | 5     | 2804 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 51  | PSU  | 9     | 1045 | 51    | -       | 2/6/24/26  | 0/2/2/2 |
| 48  | OMG  | 5     | 2364 | 48    | -       | 3/9/27/28  | 0/3/3/3 |
| 51  | PSU  | 9     | 1244 | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | A2M  | 5     | 400  | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 51  | PSU  | 9     | 105  | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 51  | OMU  | 9     | 1326 | 51    | -       | 0/9/27/28  | 0/2/2/2 |
| 51  | MA6  | 9     | 1851 | 51    | -       | 3/11/29/30 | 0/3/3/3 |
| 51  | A2M  | 9     | 1383 | 51    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | OMG  | 5     | 4637 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | OMC  | 5     | 4536 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 51  | PSU  | 9     | 801  | 51    | -       | 2/6/24/26  | 0/2/2/2 |
| 51  | PSU  | 9     | 1643 | 51    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | PSU  | 5     | 4457 | 48    | -       | 0/6/24/26  | 0/2/2/2 |
| 48  | OMU  | 5     | 3925 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | A2M  | 5     | 2787 | 48    | -       | 3/9/27/28  | 0/3/3/3 |
| 48  | OMC  | 5     | 3869 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 51  | PSU  | 9     | 822  | 51    | -       | 2/6/24/26  | 0/2/2/2 |
| 48  | OMG  | 5     | 2876 | 48    | -       | 0/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 51  | PSU  | 9     | 34  | 51   | -       | 4/6/24/26 | 0/2/2/2 |

All (881) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 48  | 5     | 3818 | UY1  | C6-C5   | 11.34 | 1.47        | 1.35     |
| 48  | 5     | 4220 | 6MZ  | C6-N6   | 11.33 | 1.47        | 1.34     |
| 51  | 9     | 1832 | 6MZ  | C6-N6   | 10.55 | 1.46        | 1.34     |
| 48  | 5     | 3818 | UY1  | C2-N1   | 9.65  | 1.49        | 1.36     |
| 51  | 9     | 159  | A2M  | C2'-C1' | -9.32 | 1.30        | 1.53     |
| 51  | 9     | 468  | A2M  | C2'-C1' | -9.28 | 1.30        | 1.53     |
| 48  | 5     | 3782 | 5MC  | C6-C5   | 9.13  | 1.49        | 1.34     |
| 48  | 5     | 3724 | A2M  | C2'-C1' | -9.12 | 1.30        | 1.53     |
| 48  | 5     | 2363 | A2M  | C2'-C1' | -9.12 | 1.30        | 1.53     |
| 48  | 5     | 4571 | A2M  | C2'-C1' | -9.08 | 1.30        | 1.53     |
| 51  | 9     | 1031 | A2M  | C2'-C1' | -9.07 | 1.30        | 1.53     |
| 51  | 9     | 512  | A2M  | C2'-C1' | -9.06 | 1.30        | 1.53     |
| 48  | 5     | 3718 | A2M  | C2'-C1' | -9.04 | 1.30        | 1.53     |
| 48  | 5     | 1326 | A2M  | C2'-C1' | -9.00 | 1.30        | 1.53     |
| 48  | 5     | 398  | A2M  | C2'-C1' | -8.98 | 1.31        | 1.53     |
| 51  | 9     | 99   | A2M  | C2'-C1' | -8.98 | 1.31        | 1.53     |
| 51  | 9     | 1383 | A2M  | O4'-C1' | 8.97  | 1.62        | 1.42     |
| 48  | 5     | 1534 | A2M  | C2'-C1' | -8.94 | 1.31        | 1.53     |
| 48  | 5     | 3724 | A2M  | O4'-C1' | 8.94  | 1.62        | 1.42     |
| 51  | 9     | 166  | A2M  | C2'-C1' | -8.93 | 1.31        | 1.53     |
| 51  | 9     | 99   | A2M  | O4'-C1' | 8.92  | 1.62        | 1.42     |
| 48  | 5     | 398  | A2M  | O4'-C1' | 8.92  | 1.62        | 1.42     |
| 48  | 5     | 3825 | A2M  | C2'-C1' | -8.90 | 1.31        | 1.53     |
| 48  | 5     | 4523 | A2M  | C2'-C1' | -8.88 | 1.31        | 1.53     |
| 51  | 9     | 159  | A2M  | O4'-C1' | 8.88  | 1.62        | 1.42     |
| 48  | 5     | 3718 | A2M  | O4'-C1' | 8.88  | 1.62        | 1.42     |
| 51  | 9     | 484  | A2M  | O4'-C1' | 8.87  | 1.62        | 1.42     |
| 48  | 5     | 3760 | A2M  | C2'-C1' | -8.85 | 1.31        | 1.53     |
| 48  | 5     | 3867 | A2M  | C2'-C1' | -8.84 | 1.31        | 1.53     |
| 48  | 5     | 3760 | A2M  | O4'-C1' | 8.83  | 1.62        | 1.42     |
| 48  | 5     | 2815 | A2M  | C2'-C1' | -8.76 | 1.31        | 1.53     |
| 51  | 9     | 484  | A2M  | C2'-C1' | -8.76 | 1.31        | 1.53     |
| 51  | 9     | 1383 | A2M  | C2'-C1' | -8.75 | 1.31        | 1.53     |
| 48  | 5     | 4571 | A2M  | O4'-C1' | 8.74  | 1.62        | 1.42     |
| 51  | 9     | 468  | A2M  | O4'-C1' | 8.73  | 1.62        | 1.42     |
| 48  | 5     | 4447 | 5MC  | C6-C5   | 8.73  | 1.48        | 1.34     |
| 51  | 9     | 27   | A2M  | C2'-C1' | -8.72 | 1.31        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 51  | 9     | 1031 | A2M  | O4'-C1' | 8.72  | 1.62        | 1.42     |
| 51  | 9     | 512  | A2M  | O4'-C1' | 8.71  | 1.62        | 1.42     |
| 48  | 5     | 1534 | A2M  | O4'-C1' | 8.70  | 1.62        | 1.42     |
| 48  | 5     | 3785 | A2M  | C2'-C1' | -8.69 | 1.31        | 1.53     |
| 48  | 5     | 3825 | A2M  | O4'-C1' | 8.69  | 1.62        | 1.42     |
| 48  | 5     | 3830 | A2M  | C2'-C1' | -8.67 | 1.31        | 1.53     |
| 48  | 5     | 2363 | A2M  | O4'-C1' | 8.66  | 1.62        | 1.42     |
| 48  | 5     | 1871 | A2M  | C2'-C1' | -8.65 | 1.31        | 1.53     |
| 51  | 9     | 1678 | A2M  | O4'-C1' | 8.62  | 1.61        | 1.42     |
| 48  | 5     | 1524 | A2M  | C2'-C1' | -8.58 | 1.32        | 1.53     |
| 51  | 9     | 1678 | A2M  | C2'-C1' | -8.58 | 1.32        | 1.53     |
| 48  | 5     | 2787 | A2M  | C2'-C1' | -8.56 | 1.32        | 1.53     |
| 48  | 5     | 400  | A2M  | C2'-C1' | -8.50 | 1.32        | 1.53     |
| 51  | 9     | 27   | A2M  | O4'-C1' | 8.48  | 1.61        | 1.42     |
| 51  | 9     | 166  | A2M  | O4'-C1' | 8.48  | 1.61        | 1.42     |
| 48  | 5     | 400  | A2M  | O4'-C1' | 8.47  | 1.61        | 1.42     |
| 48  | 5     | 2815 | A2M  | O4'-C1' | 8.43  | 1.61        | 1.42     |
| 48  | 5     | 1326 | A2M  | O4'-C1' | 8.43  | 1.61        | 1.42     |
| 48  | 5     | 2787 | A2M  | O4'-C1' | 8.41  | 1.61        | 1.42     |
| 48  | 5     | 4523 | A2M  | O4'-C1' | 8.40  | 1.61        | 1.42     |
| 51  | 9     | 668  | A2M  | O4'-C1' | 8.40  | 1.61        | 1.42     |
| 48  | 5     | 3830 | A2M  | O4'-C1' | 8.39  | 1.61        | 1.42     |
| 48  | 5     | 3867 | A2M  | O4'-C1' | 8.34  | 1.61        | 1.42     |
| 48  | 5     | 1871 | A2M  | O4'-C1' | 8.33  | 1.61        | 1.42     |
| 51  | 9     | 668  | A2M  | C2'-C1' | -8.27 | 1.32        | 1.53     |
| 48  | 5     | 1524 | A2M  | O4'-C1' | 8.18  | 1.60        | 1.42     |
| 48  | 5     | 3785 | A2M  | O4'-C1' | 8.09  | 1.60        | 1.42     |
| 51  | 9     | 1248 | B8N  | C4-C5   | 8.03  | 1.65        | 1.47     |
| 48  | 5     | 1322 | 1MA  | C2-N3   | 7.54  | 1.44        | 1.30     |
| 51  | 9     | 1248 | B8N  | C6-N1   | 7.54  | 1.54        | 1.36     |
| 51  | 9     | 1248 | B8N  | C4-N3   | -7.46 | 1.27        | 1.40     |
| 51  | 9     | 1442 | OMU  | C2-N1   | 7.14  | 1.49        | 1.38     |
| 51  | 9     | 668  | A2M  | O4'-C4' | -7.11 | 1.29        | 1.45     |
| 48  | 5     | 2837 | OMU  | C2-N1   | 7.10  | 1.49        | 1.38     |
| 48  | 5     | 4530 | UR3  | C2-N1   | 7.04  | 1.48        | 1.38     |
| 48  | 5     | 3818 | UY1  | C2-N3   | 7.00  | 1.49        | 1.37     |
| 48  | 5     | 1524 | A2M  | O4'-C4' | -6.87 | 1.29        | 1.45     |
| 48  | 5     | 4620 | OMU  | C2-N1   | 6.84  | 1.49        | 1.38     |
| 48  | 5     | 4571 | A2M  | O4'-C4' | -6.83 | 1.29        | 1.45     |
| 48  | 5     | 1534 | A2M  | O4'-C4' | -6.78 | 1.29        | 1.45     |
| 51  | 9     | 428  | OMU  | C2-N1   | 6.74  | 1.49        | 1.38     |
| 48  | 5     | 4499 | OMG  | C4-N3   | 6.71  | 1.49        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 51  | 9     | 509  | OMG  | C4-N3   | 6.66  | 1.49        | 1.34     |
| 51  | 9     | 683  | OMG  | C4-N3   | 6.66  | 1.49        | 1.34     |
| 51  | 9     | 428  | OMU  | C2-N3   | 6.66  | 1.49        | 1.38     |
| 48  | 5     | 3867 | A2M  | O4'-C4' | -6.65 | 1.30        | 1.45     |
| 51  | 9     | 436  | OMG  | C4-N3   | 6.64  | 1.49        | 1.34     |
| 51  | 9     | 116  | OMU  | C2-N1   | 6.64  | 1.48        | 1.38     |
| 48  | 5     | 3925 | OMU  | C2-N1   | 6.63  | 1.48        | 1.38     |
| 51  | 9     | 1391 | OMC  | C2-N3   | 6.60  | 1.49        | 1.36     |
| 48  | 5     | 4306 | OMU  | C2-N1   | 6.60  | 1.48        | 1.38     |
| 48  | 5     | 2876 | OMG  | C4-N3   | 6.59  | 1.49        | 1.34     |
| 48  | 5     | 1517 | 2MG  | C2-N3   | 6.59  | 1.44        | 1.32     |
| 48  | 5     | 4227 | OMU  | C2-N1   | 6.58  | 1.48        | 1.38     |
| 51  | 9     | 1248 | B8N  | C2-N1   | 6.57  | 1.58        | 1.39     |
| 48  | 5     | 4623 | OMG  | C4-N3   | 6.56  | 1.49        | 1.34     |
| 48  | 5     | 4637 | OMG  | C4-N3   | 6.55  | 1.49        | 1.34     |
| 48  | 5     | 400  | A2M  | O4'-C4' | -6.52 | 1.30        | 1.45     |
| 48  | 5     | 2815 | A2M  | O4'-C4' | -6.52 | 1.30        | 1.45     |
| 51  | 9     | 172  | OMU  | C2-N3   | 6.51  | 1.49        | 1.38     |
| 51  | 9     | 1639 | G7M  | C2-N2   | 6.50  | 1.49        | 1.34     |
| 48  | 5     | 1625 | OMG  | C4-N3   | 6.50  | 1.49        | 1.34     |
| 48  | 5     | 4196 | OMG  | C4-N3   | 6.50  | 1.49        | 1.34     |
| 48  | 5     | 2363 | A2M  | O4'-C4' | -6.49 | 1.30        | 1.45     |
| 48  | 5     | 1340 | OMC  | C2-N3   | 6.45  | 1.49        | 1.36     |
| 48  | 5     | 1326 | A2M  | O4'-C4' | -6.44 | 1.30        | 1.45     |
| 48  | 5     | 1871 | A2M  | O4'-C4' | -6.44 | 1.30        | 1.45     |
| 48  | 5     | 3760 | A2M  | O4'-C4' | -6.44 | 1.30        | 1.45     |
| 51  | 9     | 159  | A2M  | O4'-C4' | -6.43 | 1.30        | 1.45     |
| 48  | 5     | 3899 | OMG  | C4-N3   | 6.43  | 1.49        | 1.34     |
| 51  | 9     | 517  | OMC  | C2-N3   | 6.43  | 1.49        | 1.36     |
| 51  | 9     | 1031 | A2M  | O4'-C4' | -6.43 | 1.30        | 1.45     |
| 48  | 5     | 373  | OMG  | C4-N3   | 6.43  | 1.49        | 1.34     |
| 51  | 9     | 27   | A2M  | O4'-C4' | -6.40 | 1.30        | 1.45     |
| 48  | 5     | 3782 | 5MC  | C5-C4   | 6.40  | 1.49        | 1.44     |
| 51  | 9     | 484  | A2M  | O4'-C4' | -6.39 | 1.30        | 1.45     |
| 51  | 9     | 172  | OMU  | C2-N1   | 6.38  | 1.48        | 1.38     |
| 48  | 5     | 3718 | A2M  | O4'-C4' | -6.38 | 1.30        | 1.45     |
| 51  | 9     | 644  | OMG  | C4-N3   | 6.37  | 1.48        | 1.34     |
| 48  | 5     | 2422 | OMC  | C2-N3   | 6.35  | 1.49        | 1.36     |
| 48  | 5     | 3887 | OMC  | C2-N3   | 6.35  | 1.48        | 1.36     |
| 51  | 9     | 468  | A2M  | O4'-C4' | -6.34 | 1.30        | 1.45     |
| 48  | 5     | 4498 | OMU  | C2-N1   | 6.34  | 1.48        | 1.38     |
| 51  | 9     | 1639 | G7M  | C4-N3   | 6.34  | 1.48        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 48  | 5     | 4370 | OMG  | C4-N3   | 6.34  | 1.48        | 1.34     |
| 51  | 9     | 1326 | OMU  | C2-N1   | 6.33  | 1.48        | 1.38     |
| 48  | 5     | 398  | A2M  | O4'-C4' | -6.33 | 1.30        | 1.45     |
| 48  | 5     | 2787 | A2M  | O4'-C4' | -6.32 | 1.30        | 1.45     |
| 51  | 9     | 1337 | 4AC  | C6-C5   | 6.31  | 1.49        | 1.35     |
| 48  | 5     | 1522 | OMG  | C4-N3   | 6.31  | 1.48        | 1.34     |
| 51  | 9     | 1703 | OMC  | C2-N3   | 6.31  | 1.48        | 1.36     |
| 48  | 5     | 4523 | A2M  | O4'-C4' | -6.31 | 1.31        | 1.45     |
| 51  | 9     | 121  | OMU  | C2-N1   | 6.29  | 1.48        | 1.38     |
| 48  | 5     | 3627 | OMG  | C4-N3   | 6.28  | 1.48        | 1.34     |
| 51  | 9     | 517  | OMC  | C6-C5   | 6.27  | 1.49        | 1.35     |
| 48  | 5     | 4228 | OMG  | C4-N3   | 6.27  | 1.48        | 1.34     |
| 48  | 5     | 2861 | OMC  | C2-N3   | 6.24  | 1.48        | 1.36     |
| 48  | 5     | 3830 | A2M  | O4'-C4' | -6.23 | 1.31        | 1.45     |
| 51  | 9     | 1328 | OMG  | C4-N3   | 6.23  | 1.48        | 1.34     |
| 51  | 9     | 1442 | OMU  | C2-N3   | 6.23  | 1.48        | 1.38     |
| 51  | 9     | 99   | A2M  | O4'-C4' | -6.20 | 1.31        | 1.45     |
| 48  | 5     | 2364 | OMG  | C4-N3   | 6.19  | 1.48        | 1.34     |
| 48  | 5     | 3792 | OMG  | C4-N3   | 6.19  | 1.48        | 1.34     |
| 51  | 9     | 512  | A2M  | O4'-C4' | -6.18 | 1.31        | 1.45     |
| 48  | 5     | 3825 | A2M  | O4'-C4' | -6.16 | 1.31        | 1.45     |
| 51  | 9     | 116  | OMU  | C2-N3   | 6.16  | 1.48        | 1.38     |
| 51  | 9     | 1678 | A2M  | O4'-C4' | -6.15 | 1.31        | 1.45     |
| 48  | 5     | 1316 | OMG  | C4-N3   | 6.15  | 1.48        | 1.34     |
| 48  | 5     | 4447 | 5MC  | C4-N3   | 6.15  | 1.44        | 1.34     |
| 51  | 9     | 166  | A2M  | O4'-C4' | -6.14 | 1.31        | 1.45     |
| 51  | 9     | 1326 | OMU  | C2-N3   | 6.14  | 1.48        | 1.38     |
| 48  | 5     | 1340 | OMC  | C6-C5   | 6.14  | 1.49        | 1.35     |
| 51  | 9     | 121  | OMU  | C2-N3   | 6.14  | 1.48        | 1.38     |
| 48  | 5     | 2837 | OMU  | C2-N3   | 6.13  | 1.48        | 1.38     |
| 48  | 5     | 1322 | 1MA  | C4-N3   | 6.13  | 1.48        | 1.35     |
| 48  | 5     | 3724 | A2M  | O4'-C4' | -6.11 | 1.31        | 1.45     |
| 48  | 5     | 2424 | OMG  | C4-N3   | 6.11  | 1.48        | 1.34     |
| 48  | 5     | 4498 | OMU  | C2-N3   | 6.10  | 1.48        | 1.38     |
| 48  | 5     | 4620 | OMU  | C2-N3   | 6.10  | 1.48        | 1.38     |
| 48  | 5     | 3785 | A2M  | O4'-C4' | -6.08 | 1.31        | 1.45     |
| 51  | 9     | 1490 | OMG  | C4-N3   | 6.07  | 1.48        | 1.34     |
| 51  | 9     | 174  | OMC  | C2-N3   | 6.06  | 1.48        | 1.36     |
| 48  | 5     | 4618 | OMG  | C4-N3   | 6.05  | 1.48        | 1.34     |
| 51  | 9     | 1383 | A2M  | O4'-C4' | -6.05 | 1.31        | 1.45     |
| 48  | 5     | 4392 | OMG  | C4-N3   | 6.04  | 1.48        | 1.34     |
| 50  | 8     | 75   | OMG  | C4-N3   | 6.04  | 1.48        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 51  | 9     | 174  | OMC  | C6-C5 | 6.04 | 1.49        | 1.35     |
| 48  | 5     | 2804 | OMC  | C2-N3 | 6.04 | 1.48        | 1.36     |
| 51  | 9     | 1391 | OMC  | C6-C5 | 6.03 | 1.49        | 1.35     |
| 48  | 5     | 4227 | OMU  | C2-N3 | 6.03 | 1.48        | 1.38     |
| 48  | 5     | 4536 | OMC  | C6-C5 | 6.01 | 1.49        | 1.35     |
| 48  | 5     | 2365 | OMC  | C2-N3 | 6.01 | 1.48        | 1.36     |
| 48  | 5     | 3925 | OMU  | C2-N3 | 6.01 | 1.48        | 1.38     |
| 48  | 5     | 3841 | OMC  | C2-N3 | 6.00 | 1.48        | 1.36     |
| 51  | 9     | 1337 | 4AC  | C4-N3 | 5.97 | 1.42        | 1.32     |
| 51  | 9     | 1842 | 4AC  | C4-N3 | 5.95 | 1.42        | 1.32     |
| 48  | 5     | 3869 | OMC  | C6-C5 | 5.94 | 1.48        | 1.35     |
| 48  | 5     | 4494 | OMG  | C4-N3 | 5.93 | 1.47        | 1.34     |
| 48  | 5     | 3841 | OMC  | C6-C5 | 5.92 | 1.48        | 1.35     |
| 48  | 5     | 4306 | OMU  | C6-C5 | 5.91 | 1.48        | 1.35     |
| 51  | 9     | 1703 | OMC  | C6-C5 | 5.90 | 1.48        | 1.35     |
| 48  | 5     | 2365 | OMC  | C6-C5 | 5.88 | 1.48        | 1.35     |
| 48  | 5     | 2861 | OMC  | C6-C5 | 5.88 | 1.48        | 1.35     |
| 48  | 5     | 4306 | OMU  | C2-N3 | 5.88 | 1.48        | 1.38     |
| 51  | 9     | 172  | OMU  | C6-C5 | 5.87 | 1.48        | 1.35     |
| 48  | 5     | 4456 | OMC  | C2-N3 | 5.87 | 1.48        | 1.36     |
| 48  | 5     | 2824 | OMC  | C2-N3 | 5.85 | 1.48        | 1.36     |
| 51  | 9     | 1842 | 4AC  | C6-C5 | 5.84 | 1.48        | 1.35     |
| 48  | 5     | 2422 | OMC  | C6-C5 | 5.84 | 1.48        | 1.35     |
| 48  | 5     | 2351 | OMC  | C6-C5 | 5.80 | 1.48        | 1.35     |
| 48  | 5     | 3701 | OMC  | C6-C5 | 5.79 | 1.48        | 1.35     |
| 51  | 9     | 116  | OMU  | C6-C5 | 5.78 | 1.48        | 1.35     |
| 48  | 5     | 2824 | OMC  | C6-C5 | 5.77 | 1.48        | 1.35     |
| 48  | 5     | 4447 | 5MC  | C2-N3 | 5.75 | 1.47        | 1.36     |
| 51  | 9     | 1326 | OMU  | C6-C5 | 5.74 | 1.48        | 1.35     |
| 48  | 5     | 3869 | OMC  | C2-N3 | 5.73 | 1.47        | 1.36     |
| 51  | 9     | 1248 | B8N  | C6-C5 | 5.70 | 1.43        | 1.35     |
| 48  | 5     | 3808 | OMC  | C2-N3 | 5.69 | 1.47        | 1.36     |
| 51  | 9     | 436  | OMG  | C2-N3 | 5.67 | 1.46        | 1.33     |
| 48  | 5     | 2804 | OMC  | C6-C5 | 5.66 | 1.48        | 1.35     |
| 48  | 5     | 4536 | OMC  | C2-N3 | 5.66 | 1.47        | 1.36     |
| 48  | 5     | 4456 | OMC  | C6-C5 | 5.65 | 1.48        | 1.35     |
| 48  | 5     | 4498 | OMU  | C6-C5 | 5.64 | 1.48        | 1.35     |
| 48  | 5     | 4227 | OMU  | C6-C5 | 5.64 | 1.48        | 1.35     |
| 48  | 5     | 3925 | OMU  | C6-C5 | 5.64 | 1.48        | 1.35     |
| 48  | 5     | 4620 | OMU  | C6-C5 | 5.62 | 1.48        | 1.35     |
| 48  | 5     | 3808 | OMC  | C6-C5 | 5.57 | 1.48        | 1.35     |
| 51  | 9     | 683  | OMG  | C2-N3 | 5.55 | 1.46        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 48  | 5     | 3701 | OMC  | C2-N3  | 5.54  | 1.47        | 1.36     |
| 48  | 5     | 4530 | UR3  | C6-C5  | 5.52  | 1.47        | 1.35     |
| 51  | 9     | 428  | OMU  | C6-C5  | 5.52  | 1.47        | 1.35     |
| 48  | 5     | 2351 | OMC  | C2-N3  | 5.51  | 1.47        | 1.36     |
| 48  | 5     | 4196 | OMG  | C2-N3  | 5.49  | 1.46        | 1.33     |
| 51  | 9     | 1442 | OMU  | C6-C5  | 5.48  | 1.47        | 1.35     |
| 48  | 5     | 1625 | OMG  | C2-N3  | 5.44  | 1.46        | 1.33     |
| 48  | 5     | 237  | B9B  | C2-N2  | 5.40  | 1.44        | 1.33     |
| 48  | 5     | 4499 | OMG  | C2-N3  | 5.39  | 1.46        | 1.33     |
| 48  | 5     | 4447 | 5MC  | C5-C4  | 5.38  | 1.48        | 1.44     |
| 48  | 5     | 3782 | 5MC  | C4-N3  | 5.36  | 1.42        | 1.34     |
| 48  | 5     | 3887 | OMC  | C6-C5  | 5.35  | 1.47        | 1.35     |
| 48  | 5     | 3818 | UY1  | C1'-C5 | -5.35 | 1.38        | 1.50     |
| 51  | 9     | 509  | OMG  | C2-N3  | 5.34  | 1.46        | 1.33     |
| 48  | 5     | 4623 | OMG  | C2-N3  | 5.31  | 1.46        | 1.33     |
| 48  | 5     | 2837 | OMU  | C6-C5  | 5.31  | 1.47        | 1.35     |
| 51  | 9     | 1337 | 4AC  | C2-N3  | 5.29  | 1.46        | 1.36     |
| 51  | 9     | 1328 | OMG  | C2-N3  | 5.27  | 1.46        | 1.33     |
| 51  | 9     | 121  | OMU  | C6-C5  | 5.25  | 1.47        | 1.35     |
| 51  | 9     | 1639 | G7M  | C2-N3  | 5.20  | 1.45        | 1.33     |
| 48  | 5     | 3782 | 5MC  | C2-N3  | 5.18  | 1.46        | 1.36     |
| 48  | 5     | 373  | OMG  | C2-N3  | 5.18  | 1.45        | 1.33     |
| 48  | 5     | 4637 | OMG  | C2-N3  | 5.15  | 1.45        | 1.33     |
| 48  | 5     | 2876 | OMG  | C2-N3  | 5.15  | 1.45        | 1.33     |
| 48  | 5     | 3627 | OMG  | C2-N3  | 5.10  | 1.45        | 1.33     |
| 48  | 5     | 4370 | OMG  | C2-N3  | 5.09  | 1.45        | 1.33     |
| 48  | 5     | 2364 | OMG  | C2-N3  | 5.08  | 1.45        | 1.33     |
| 51  | 9     | 644  | OMG  | C2-N3  | 5.08  | 1.45        | 1.33     |
| 51  | 9     | 1842 | 4AC  | C2-N3  | 5.07  | 1.46        | 1.36     |
| 48  | 5     | 1517 | 2MG  | C2-N2  | 5.07  | 1.44        | 1.33     |
| 48  | 5     | 2424 | OMG  | C2-N3  | 5.06  | 1.45        | 1.33     |
| 48  | 5     | 3899 | OMG  | C2-N3  | 5.05  | 1.45        | 1.33     |
| 48  | 5     | 1316 | OMG  | C2-N3  | 5.03  | 1.45        | 1.33     |
| 48  | 5     | 4392 | OMG  | C2-N3  | 5.02  | 1.45        | 1.33     |
| 50  | 8     | 75   | OMG  | C2-N3  | 5.01  | 1.45        | 1.33     |
| 48  | 5     | 3792 | OMG  | C2-N3  | 4.99  | 1.45        | 1.33     |
| 48  | 5     | 1340 | OMC  | C4-N4  | 4.97  | 1.45        | 1.33     |
| 51  | 9     | 1391 | OMC  | C4-N4  | 4.89  | 1.45        | 1.33     |
| 48  | 5     | 4618 | OMG  | C2-N3  | 4.89  | 1.45        | 1.33     |
| 48  | 5     | 1522 | OMG  | C2-N3  | 4.89  | 1.45        | 1.33     |
| 48  | 5     | 4494 | OMG  | C2-N3  | 4.88  | 1.45        | 1.33     |
| 48  | 5     | 1517 | 2MG  | C4-N3  | 4.88  | 1.45        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 51  | 9     | 1703 | OMC  | C2-N1 | 4.87  | 1.50        | 1.40     |
| 51  | 9     | 1337 | 4AC  | C4-N4 | 4.84  | 1.47        | 1.39     |
| 51  | 9     | 1703 | OMC  | C4-N3 | 4.81  | 1.44        | 1.34     |
| 51  | 9     | 517  | OMC  | C4-N3 | 4.76  | 1.44        | 1.34     |
| 48  | 5     | 3887 | OMC  | C4-N3 | 4.73  | 1.43        | 1.34     |
| 51  | 9     | 174  | OMC  | C4-N3 | 4.71  | 1.43        | 1.34     |
| 48  | 5     | 4228 | OMG  | C2-N3 | 4.69  | 1.44        | 1.33     |
| 48  | 5     | 3818 | UY1  | C6-N1 | 4.67  | 1.44        | 1.36     |
| 48  | 5     | 2422 | OMC  | C4-N3 | 4.67  | 1.43        | 1.34     |
| 48  | 5     | 1625 | OMG  | C2-N2 | 4.64  | 1.45        | 1.34     |
| 51  | 9     | 1490 | OMG  | C2-N3 | 4.63  | 1.44        | 1.33     |
| 48  | 5     | 2861 | OMC  | C4-N3 | 4.62  | 1.43        | 1.34     |
| 51  | 9     | 166  | A2M  | C6-N6 | 4.61  | 1.46        | 1.34     |
| 51  | 9     | 1703 | OMC  | C4-N4 | 4.55  | 1.44        | 1.33     |
| 48  | 5     | 3869 | OMC  | C4-N4 | 4.53  | 1.44        | 1.33     |
| 48  | 5     | 2365 | OMC  | C4-N3 | 4.52  | 1.43        | 1.34     |
| 51  | 9     | 644  | OMG  | C2-N2 | 4.51  | 1.44        | 1.34     |
| 48  | 5     | 4196 | OMG  | C2-N2 | 4.50  | 1.44        | 1.34     |
| 48  | 5     | 3869 | OMC  | C4-N3 | 4.50  | 1.43        | 1.34     |
| 51  | 9     | 1639 | G7M  | C5-N7 | -4.49 | 1.34        | 1.39     |
| 51  | 9     | 517  | OMC  | C4-N4 | 4.49  | 1.44        | 1.33     |
| 48  | 5     | 4456 | OMC  | C4-N3 | 4.48  | 1.43        | 1.34     |
| 48  | 5     | 2861 | OMC  | C2-N1 | 4.46  | 1.49        | 1.40     |
| 48  | 5     | 4456 | OMC  | C4-N4 | 4.46  | 1.44        | 1.33     |
| 48  | 5     | 2824 | OMC  | C4-N4 | 4.45  | 1.44        | 1.33     |
| 51  | 9     | 174  | OMC  | C4-N4 | 4.45  | 1.44        | 1.33     |
| 48  | 5     | 2422 | OMC  | C2-N1 | 4.44  | 1.49        | 1.40     |
| 48  | 5     | 4499 | OMG  | C2-N2 | 4.44  | 1.44        | 1.34     |
| 51  | 9     | 683  | OMG  | C2-N2 | 4.44  | 1.44        | 1.34     |
| 48  | 5     | 2861 | OMC  | C4-N4 | 4.44  | 1.44        | 1.33     |
| 51  | 9     | 1391 | OMC  | C4-N3 | 4.43  | 1.43        | 1.34     |
| 51  | 9     | 436  | OMG  | C2-N2 | 4.43  | 1.44        | 1.34     |
| 48  | 5     | 2365 | OMC  | C4-N4 | 4.42  | 1.44        | 1.33     |
| 48  | 5     | 4571 | A2M  | C6-N6 | 4.42  | 1.45        | 1.34     |
| 48  | 5     | 4623 | OMG  | C2-N2 | 4.42  | 1.44        | 1.34     |
| 51  | 9     | 517  | OMC  | C2-N1 | 4.41  | 1.49        | 1.40     |
| 48  | 5     | 4530 | UR3  | C2-N3 | 4.41  | 1.47        | 1.39     |
| 51  | 9     | 1678 | A2M  | C6-N6 | 4.40  | 1.45        | 1.34     |
| 48  | 5     | 2422 | OMC  | C4-N4 | 4.38  | 1.44        | 1.33     |
| 48  | 5     | 3825 | A2M  | C6-N6 | 4.38  | 1.45        | 1.34     |
| 48  | 5     | 2424 | OMG  | C2-N2 | 4.38  | 1.44        | 1.34     |
| 51  | 9     | 1842 | 4AC  | C7-N4 | 4.37  | 1.46        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 51  | 9     | 1490 | OMG  | C2-N2 | 4.37 | 1.44        | 1.34     |
| 48  | 5     | 3887 | OMC  | C4-N4 | 4.37 | 1.44        | 1.33     |
| 48  | 5     | 3701 | OMC  | C4-N3 | 4.36 | 1.43        | 1.34     |
| 48  | 5     | 3841 | OMC  | C4-N4 | 4.34 | 1.44        | 1.33     |
| 48  | 5     | 1340 | OMC  | C4-N3 | 4.34 | 1.43        | 1.34     |
| 50  | 8     | 75   | OMG  | C2-N2 | 4.34 | 1.44        | 1.34     |
| 48  | 5     | 2364 | OMG  | C2-N2 | 4.34 | 1.44        | 1.34     |
| 48  | 5     | 4447 | 5MC  | C6-N1 | 4.34 | 1.45        | 1.38     |
| 48  | 5     | 373  | OMG  | C2-N2 | 4.32 | 1.44        | 1.34     |
| 51  | 9     | 509  | OMG  | C2-N2 | 4.32 | 1.44        | 1.34     |
| 51  | 9     | 1328 | OMG  | C2-N2 | 4.30 | 1.44        | 1.34     |
| 51  | 9     | 174  | OMC  | C2-N1 | 4.29 | 1.49        | 1.40     |
| 48  | 5     | 4370 | OMG  | C2-N2 | 4.29 | 1.44        | 1.34     |
| 48  | 5     | 2824 | OMC  | C2-N1 | 4.28 | 1.49        | 1.40     |
| 48  | 5     | 2804 | OMC  | C4-N4 | 4.28 | 1.44        | 1.33     |
| 48  | 5     | 398  | A2M  | C6-N6 | 4.27 | 1.45        | 1.34     |
| 48  | 5     | 3899 | OMG  | C2-N2 | 4.27 | 1.44        | 1.34     |
| 51  | 9     | 1391 | OMC  | C2-N1 | 4.27 | 1.49        | 1.40     |
| 48  | 5     | 3808 | OMC  | C2-N1 | 4.27 | 1.49        | 1.40     |
| 51  | 9     | 468  | A2M  | C6-N6 | 4.27 | 1.45        | 1.34     |
| 48  | 5     | 4536 | OMC  | C4-N4 | 4.26 | 1.44        | 1.33     |
| 48  | 5     | 2351 | OMC  | C4-N3 | 4.25 | 1.43        | 1.34     |
| 48  | 5     | 3841 | OMC  | C4-N3 | 4.24 | 1.42        | 1.34     |
| 48  | 5     | 4228 | OMG  | C2-N2 | 4.23 | 1.44        | 1.34     |
| 48  | 5     | 3701 | OMC  | C2-N1 | 4.23 | 1.48        | 1.40     |
| 48  | 5     | 3627 | OMG  | C2-N2 | 4.21 | 1.44        | 1.34     |
| 48  | 5     | 4618 | OMG  | C2-N2 | 4.20 | 1.44        | 1.34     |
| 48  | 5     | 2804 | OMC  | C4-N3 | 4.20 | 1.42        | 1.34     |
| 48  | 5     | 3724 | A2M  | C6-N6 | 4.20 | 1.44        | 1.34     |
| 48  | 5     | 2824 | OMC  | C4-N3 | 4.19 | 1.42        | 1.34     |
| 51  | 9     | 512  | A2M  | C6-N6 | 4.19 | 1.44        | 1.34     |
| 48  | 5     | 3808 | OMC  | C4-N3 | 4.18 | 1.42        | 1.34     |
| 48  | 5     | 3792 | OMG  | C2-N2 | 4.18 | 1.44        | 1.34     |
| 48  | 5     | 3782 | 5MC  | C6-N1 | 4.17 | 1.45        | 1.38     |
| 48  | 5     | 4494 | OMG  | C2-N2 | 4.17 | 1.43        | 1.34     |
| 51  | 9     | 484  | A2M  | C6-N6 | 4.17 | 1.44        | 1.34     |
| 51  | 9     | 668  | A2M  | C6-N6 | 4.16 | 1.44        | 1.34     |
| 51  | 9     | 159  | A2M  | C6-N6 | 4.16 | 1.44        | 1.34     |
| 48  | 5     | 3760 | A2M  | C6-N6 | 4.16 | 1.44        | 1.34     |
| 48  | 5     | 3808 | OMC  | C4-N4 | 4.15 | 1.44        | 1.33     |
| 51  | 9     | 27   | A2M  | C6-N6 | 4.14 | 1.44        | 1.34     |
| 51  | 9     | 1842 | 4AC  | C4-N4 | 4.11 | 1.46        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 48  | 5     | 1524 | A2M  | C6-N6 | 4.10  | 1.44        | 1.34     |
| 51  | 9     | 1337 | 4AC  | C7-N4 | 4.08  | 1.45        | 1.37     |
| 48  | 5     | 1522 | OMG  | C2-N2 | 4.08  | 1.43        | 1.34     |
| 48  | 5     | 2876 | OMG  | C2-N2 | 4.08  | 1.43        | 1.34     |
| 48  | 5     | 2351 | OMC  | C2-N1 | 4.07  | 1.48        | 1.40     |
| 48  | 5     | 3867 | A2M  | C6-N6 | 4.05  | 1.44        | 1.34     |
| 48  | 5     | 2351 | OMC  | C4-N4 | 4.05  | 1.43        | 1.33     |
| 48  | 5     | 3701 | OMC  | C4-N4 | 4.05  | 1.43        | 1.33     |
| 51  | 9     | 1383 | A2M  | C6-N6 | 4.04  | 1.44        | 1.34     |
| 48  | 5     | 4536 | OMC  | C2-N1 | 4.03  | 1.48        | 1.40     |
| 48  | 5     | 2787 | A2M  | C6-N6 | 4.02  | 1.44        | 1.34     |
| 48  | 5     | 4536 | OMC  | C4-N3 | 4.01  | 1.42        | 1.34     |
| 48  | 5     | 2804 | OMC  | C2-N1 | 4.01  | 1.48        | 1.40     |
| 48  | 5     | 1871 | A2M  | C6-N6 | 4.01  | 1.44        | 1.34     |
| 48  | 5     | 1316 | OMG  | C2-N2 | 4.01  | 1.43        | 1.34     |
| 48  | 5     | 1534 | A2M  | C6-N6 | 4.00  | 1.44        | 1.34     |
| 48  | 5     | 4447 | 5MC  | C4-N4 | 3.99  | 1.44        | 1.34     |
| 48  | 5     | 3782 | 5MC  | C4-N4 | 3.98  | 1.44        | 1.34     |
| 51  | 9     | 1031 | A2M  | C6-N6 | 3.98  | 1.44        | 1.34     |
| 48  | 5     | 4523 | A2M  | C6-N6 | 3.98  | 1.44        | 1.34     |
| 48  | 5     | 1340 | OMC  | C2-N1 | 3.97  | 1.48        | 1.40     |
| 48  | 5     | 400  | A2M  | C6-N6 | 3.97  | 1.44        | 1.34     |
| 48  | 5     | 4637 | OMG  | C2-N2 | 3.96  | 1.43        | 1.34     |
| 48  | 5     | 2363 | A2M  | C6-N6 | 3.94  | 1.44        | 1.34     |
| 48  | 5     | 3841 | OMC  | C2-N1 | 3.94  | 1.48        | 1.40     |
| 51  | 9     | 99   | A2M  | C6-N6 | 3.93  | 1.44        | 1.34     |
| 48  | 5     | 1326 | A2M  | C6-N6 | 3.93  | 1.44        | 1.34     |
| 48  | 5     | 2815 | A2M  | C6-N6 | 3.92  | 1.44        | 1.34     |
| 51  | 9     | 1842 | 4AC  | C2-N1 | 3.92  | 1.48        | 1.40     |
| 48  | 5     | 3718 | A2M  | C6-N6 | 3.90  | 1.44        | 1.34     |
| 48  | 5     | 3785 | A2M  | C6-N6 | 3.88  | 1.44        | 1.34     |
| 51  | 9     | 1639 | G7M  | C5-C6 | 3.86  | 1.54        | 1.43     |
| 48  | 5     | 1322 | 1MA  | C5-C6 | 3.85  | 1.54        | 1.43     |
| 48  | 5     | 4293 | PSU  | C6-C5 | 3.85  | 1.39        | 1.35     |
| 48  | 5     | 3734 | PSU  | C6-C5 | 3.85  | 1.39        | 1.35     |
| 48  | 5     | 2365 | OMC  | C2-N1 | 3.82  | 1.48        | 1.40     |
| 48  | 5     | 1517 | 2MG  | C2-N1 | 3.82  | 1.42        | 1.36     |
| 48  | 5     | 3869 | OMC  | C2-N1 | 3.80  | 1.48        | 1.40     |
| 48  | 5     | 4392 | OMG  | C5-N7 | -3.80 | 1.31        | 1.39     |
| 48  | 5     | 3887 | OMC  | C2-N1 | 3.80  | 1.48        | 1.40     |
| 48  | 5     | 4456 | OMC  | C2-N1 | 3.79  | 1.48        | 1.40     |
| 48  | 5     | 2876 | OMG  | C5-N7 | -3.79 | 1.31        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 51  | 9     | 1248 | B8N  | O4-C4 | -3.76 | 1.15        | 1.23     |
| 48  | 5     | 4392 | OMG  | C2-N2 | 3.76  | 1.43        | 1.34     |
| 48  | 5     | 4306 | OMU  | O2-C2 | -3.76 | 1.16        | 1.23     |
| 48  | 5     | 3830 | A2M  | C6-N6 | 3.75  | 1.43        | 1.34     |
| 48  | 5     | 373  | OMG  | C5-N7 | -3.75 | 1.31        | 1.39     |
| 48  | 5     | 4637 | OMG  | C5-N7 | -3.74 | 1.31        | 1.39     |
| 51  | 9     | 801  | PSU  | C6-C5 | 3.73  | 1.39        | 1.35     |
| 48  | 5     | 4447 | 5MC  | C2-N1 | 3.72  | 1.47        | 1.40     |
| 48  | 5     | 1683 | PSU  | C6-C5 | 3.71  | 1.39        | 1.35     |
| 48  | 5     | 3782 | 5MC  | C2-N1 | 3.70  | 1.47        | 1.40     |
| 51  | 9     | 484  | A2M  | C5-C4 | -3.69 | 1.32        | 1.39     |
| 48  | 5     | 3899 | OMG  | C5-N7 | -3.68 | 1.31        | 1.39     |
| 48  | 5     | 237  | B9B  | O6-C6 | 3.66  | 1.40        | 1.34     |
| 51  | 9     | 436  | OMG  | C5-N7 | -3.66 | 1.31        | 1.39     |
| 51  | 9     | 99   | A2M  | C5-C4 | -3.65 | 1.32        | 1.39     |
| 51  | 9     | 1337 | 4AC  | C5-C4 | 3.65  | 1.49        | 1.41     |
| 51  | 9     | 1842 | 4AC  | C5-C4 | 3.64  | 1.49        | 1.41     |
| 48  | 5     | 4456 | OMC  | O2-C2 | -3.64 | 1.16        | 1.23     |
| 48  | 5     | 2824 | OMC  | O2-C2 | -3.64 | 1.16        | 1.23     |
| 48  | 5     | 4420 | PSU  | C6-C5 | 3.63  | 1.39        | 1.35     |
| 51  | 9     | 644  | OMG  | C5-N7 | -3.63 | 1.31        | 1.39     |
| 48  | 5     | 3853 | PSU  | C6-C5 | 3.62  | 1.39        | 1.35     |
| 48  | 5     | 2787 | A2M  | C5-C4 | -3.62 | 1.32        | 1.39     |
| 48  | 5     | 3718 | A2M  | C5-C4 | -3.61 | 1.32        | 1.39     |
| 48  | 5     | 4296 | PSU  | C6-C5 | 3.60  | 1.39        | 1.35     |
| 48  | 5     | 4196 | OMG  | C5-N7 | -3.60 | 1.31        | 1.39     |
| 48  | 5     | 1862 | PSU  | C6-C5 | 3.58  | 1.39        | 1.35     |
| 48  | 5     | 4457 | PSU  | C6-C5 | 3.58  | 1.39        | 1.35     |
| 48  | 5     | 2861 | OMC  | O2-C2 | -3.58 | 1.17        | 1.23     |
| 51  | 9     | 1238 | PSU  | C6-C5 | 3.57  | 1.39        | 1.35     |
| 48  | 5     | 400  | A2M  | C5-N7 | -3.57 | 1.32        | 1.39     |
| 48  | 5     | 4306 | OMU  | O4-C4 | -3.56 | 1.17        | 1.24     |
| 48  | 5     | 3792 | OMG  | C5-N7 | -3.56 | 1.31        | 1.39     |
| 48  | 5     | 4628 | PSU  | C6-C5 | 3.56  | 1.39        | 1.35     |
| 48  | 5     | 1871 | A2M  | C5-C4 | -3.56 | 1.32        | 1.39     |
| 48  | 5     | 1625 | OMG  | C5-N7 | -3.55 | 1.32        | 1.39     |
| 51  | 9     | 1850 | MA6  | C5-C4 | -3.55 | 1.32        | 1.39     |
| 51  | 9     | 109  | PSU  | C6-C5 | 3.55  | 1.39        | 1.35     |
| 51  | 9     | 822  | PSU  | C6-C5 | 3.54  | 1.39        | 1.35     |
| 51  | 9     | 34   | PSU  | C6-C5 | 3.54  | 1.39        | 1.35     |
| 48  | 5     | 3869 | OMC  | O2-C2 | -3.53 | 1.17        | 1.23     |
| 48  | 5     | 1326 | A2M  | C5-N7 | -3.53 | 1.32        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 48  | 5     | 4536 | OMC  | O2-C2 | -3.52 | 1.17        | 1.23     |
| 48  | 5     | 2632 | PSU  | C6-C5 | 3.52  | 1.39        | 1.35     |
| 51  | 9     | 1692 | PSU  | C6-C5 | 3.52  | 1.39        | 1.35     |
| 48  | 5     | 1534 | A2M  | C5-C4 | -3.52 | 1.32        | 1.39     |
| 51  | 9     | 1244 | PSU  | C6-C5 | 3.51  | 1.39        | 1.35     |
| 48  | 5     | 1322 | 1MA  | C2-N1 | 3.51  | 1.43        | 1.35     |
| 48  | 5     | 4571 | A2M  | C5-C4 | -3.51 | 1.32        | 1.39     |
| 51  | 9     | 1367 | PSU  | C6-C5 | 3.51  | 1.39        | 1.35     |
| 48  | 5     | 4523 | A2M  | C5-N7 | -3.50 | 1.32        | 1.39     |
| 48  | 5     | 4620 | OMU  | O2-C2 | -3.47 | 1.16        | 1.23     |
| 48  | 5     | 4494 | OMG  | C5-N7 | -3.47 | 1.32        | 1.39     |
| 48  | 5     | 1316 | OMG  | C5-N7 | -3.46 | 1.32        | 1.39     |
| 48  | 5     | 3925 | OMU  | O4-C4 | -3.46 | 1.17        | 1.24     |
| 48  | 5     | 4521 | PSU  | C6-C5 | 3.46  | 1.39        | 1.35     |
| 48  | 5     | 3701 | OMC  | O2-C2 | -3.46 | 1.17        | 1.23     |
| 51  | 9     | 105  | PSU  | C6-C5 | 3.45  | 1.39        | 1.35     |
| 51  | 9     | 1232 | PSU  | C6-C5 | 3.45  | 1.39        | 1.35     |
| 48  | 5     | 2804 | OMC  | O2-C2 | -3.45 | 1.17        | 1.23     |
| 51  | 9     | 1031 | A2M  | C5-C4 | -3.44 | 1.32        | 1.39     |
| 51  | 9     | 1442 | OMU  | C4-N3 | 3.44  | 1.44        | 1.38     |
| 50  | 8     | 75   | OMG  | C5-N7 | -3.43 | 1.32        | 1.39     |
| 48  | 5     | 3764 | PSU  | C6-C5 | 3.43  | 1.39        | 1.35     |
| 51  | 9     | 1851 | MA6  | C5-C4 | -3.43 | 1.33        | 1.39     |
| 51  | 9     | 428  | OMU  | C4-N3 | 3.43  | 1.44        | 1.38     |
| 51  | 9     | 509  | OMG  | C5-N7 | -3.42 | 1.32        | 1.39     |
| 48  | 5     | 373  | OMG  | O6-C6 | -3.42 | 1.17        | 1.23     |
| 48  | 5     | 3925 | OMU  | O2-C2 | -3.42 | 1.17        | 1.23     |
| 48  | 5     | 1782 | PSU  | C6-C5 | 3.41  | 1.39        | 1.35     |
| 48  | 5     | 2424 | OMG  | C5-N7 | -3.40 | 1.32        | 1.39     |
| 48  | 5     | 2787 | A2M  | C5-N7 | -3.40 | 1.32        | 1.39     |
| 51  | 9     | 1004 | PSU  | C6-C5 | 3.40  | 1.39        | 1.35     |
| 51  | 9     | 609  | PSU  | C6-C5 | 3.39  | 1.39        | 1.35     |
| 51  | 9     | 1326 | OMU  | C4-N3 | 3.39  | 1.44        | 1.38     |
| 48  | 5     | 4227 | OMU  | O2-C2 | -3.39 | 1.17        | 1.23     |
| 48  | 5     | 1522 | OMG  | O6-C6 | -3.38 | 1.17        | 1.23     |
| 51  | 9     | 683  | OMG  | C5-N7 | -3.38 | 1.32        | 1.39     |
| 48  | 5     | 2837 | OMU  | O2-C2 | -3.38 | 1.17        | 1.23     |
| 51  | 9     | 1174 | PSU  | C6-C5 | 3.38  | 1.39        | 1.35     |
| 51  | 9     | 1045 | PSU  | C6-C5 | 3.38  | 1.39        | 1.35     |
| 48  | 5     | 1340 | OMC  | O2-C2 | -3.38 | 1.17        | 1.23     |
| 48  | 5     | 3627 | OMG  | C5-N7 | -3.38 | 1.32        | 1.39     |
| 48  | 5     | 3841 | OMC  | O2-C2 | -3.37 | 1.17        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 51  | 9     | 1046 | PSU  | C6-C5   | 3.37  | 1.39        | 1.35     |
| 48  | 5     | 2365 | OMC  | O2-C2   | -3.37 | 1.17        | 1.23     |
| 51  | 9     | 468  | A2M  | O3'-C3' | -3.37 | 1.34        | 1.43     |
| 51  | 9     | 1842 | 4AC  | O2-C2   | -3.37 | 1.17        | 1.23     |
| 51  | 9     | 218  | PSU  | C6-C5   | 3.37  | 1.39        | 1.35     |
| 51  | 9     | 1177 | PSU  | C6-C5   | 3.37  | 1.39        | 1.35     |
| 51  | 9     | 572  | PSU  | C6-C5   | 3.36  | 1.39        | 1.35     |
| 51  | 9     | 121  | OMU  | O4-C4   | -3.36 | 1.18        | 1.24     |
| 48  | 5     | 3808 | OMC  | O2-C2   | -3.35 | 1.17        | 1.23     |
| 48  | 5     | 4532 | PSU  | C6-C5   | 3.35  | 1.39        | 1.35     |
| 48  | 5     | 1524 | A2M  | C5-C4   | -3.35 | 1.33        | 1.39     |
| 48  | 5     | 2815 | A2M  | C5-C4   | -3.35 | 1.33        | 1.39     |
| 48  | 5     | 4618 | OMG  | C5-N7   | -3.35 | 1.32        | 1.39     |
| 48  | 5     | 3782 | 5MC  | O2-C2   | -3.35 | 1.17        | 1.23     |
| 48  | 5     | 1522 | OMG  | C5-N7   | -3.34 | 1.32        | 1.39     |
| 48  | 5     | 4499 | OMG  | C5-N7   | -3.34 | 1.32        | 1.39     |
| 48  | 5     | 3830 | A2M  | C5-N7   | -3.33 | 1.33        | 1.39     |
| 51  | 9     | 1337 | 4AC  | O2-C2   | -3.33 | 1.17        | 1.23     |
| 51  | 9     | 172  | OMU  | C4-N3   | 3.32  | 1.44        | 1.38     |
| 48  | 5     | 4618 | OMG  | O6-C6   | -3.32 | 1.17        | 1.23     |
| 48  | 5     | 2363 | A2M  | C5-N7   | -3.32 | 1.33        | 1.39     |
| 48  | 5     | 237  | B9B  | C5-C4   | -3.32 | 1.33        | 1.39     |
| 48  | 5     | 2351 | OMC  | O2-C2   | -3.32 | 1.17        | 1.23     |
| 51  | 9     | 1850 | MA6  | C5-N7   | -3.32 | 1.33        | 1.39     |
| 48  | 5     | 4552 | PSU  | C6-C5   | 3.32  | 1.39        | 1.35     |
| 51  | 9     | 174  | OMC  | O2-C2   | -3.32 | 1.17        | 1.23     |
| 48  | 5     | 3830 | A2M  | C5-C4   | -3.31 | 1.33        | 1.39     |
| 48  | 5     | 3867 | A2M  | C5-C4   | -3.31 | 1.33        | 1.39     |
| 48  | 5     | 1316 | OMG  | O6-C6   | -3.31 | 1.17        | 1.23     |
| 51  | 9     | 1081 | PSU  | C6-C5   | 3.30  | 1.38        | 1.35     |
| 48  | 5     | 3825 | A2M  | C5-N7   | -3.30 | 1.33        | 1.39     |
| 48  | 5     | 1871 | A2M  | C5-N7   | -3.30 | 1.33        | 1.39     |
| 51  | 9     | 1326 | OMU  | O2-C2   | -3.29 | 1.17        | 1.23     |
| 51  | 9     | 27   | A2M  | C5-N7   | -3.29 | 1.33        | 1.39     |
| 48  | 5     | 4498 | OMU  | O4-C4   | -3.29 | 1.18        | 1.24     |
| 48  | 5     | 3785 | A2M  | C5-C4   | -3.29 | 1.33        | 1.39     |
| 48  | 5     | 3867 | A2M  | C5-N7   | -3.29 | 1.33        | 1.39     |
| 51  | 9     | 1490 | OMG  | C5-N7   | -3.28 | 1.32        | 1.39     |
| 51  | 9     | 1337 | 4AC  | C6-N1   | 3.28  | 1.45        | 1.38     |
| 48  | 5     | 4623 | OMG  | C5-N7   | -3.27 | 1.32        | 1.39     |
| 48  | 5     | 1534 | A2M  | C5-N7   | -3.27 | 1.33        | 1.39     |
| 48  | 5     | 1677 | PSU  | C6-C5   | 3.27  | 1.38        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 48  | 5     | 4370 | OMG  | C5-N7   | -3.27 | 1.32        | 1.39     |
| 48  | 5     | 2363 | A2M  | C5-C4   | -3.26 | 1.33        | 1.39     |
| 48  | 5     | 2422 | OMC  | O2-C2   | -3.26 | 1.17        | 1.23     |
| 48  | 5     | 4498 | OMU  | C4-N3   | 3.26  | 1.44        | 1.38     |
| 51  | 9     | 1337 | 4AC  | C2-N1   | 3.26  | 1.46        | 1.40     |
| 48  | 5     | 1322 | 1MA  | C4-N9   | -3.26 | 1.29        | 1.38     |
| 48  | 5     | 4498 | OMU  | O2-C2   | -3.25 | 1.17        | 1.23     |
| 48  | 5     | 3718 | A2M  | C5-N7   | -3.25 | 1.33        | 1.39     |
| 48  | 5     | 4196 | OMG  | O6-C6   | -3.24 | 1.17        | 1.23     |
| 48  | 5     | 4392 | OMG  | O6-C6   | -3.24 | 1.17        | 1.23     |
| 48  | 5     | 4620 | OMU  | O4-C4   | -3.24 | 1.18        | 1.24     |
| 48  | 5     | 3762 | PSU  | C6-C5   | 3.24  | 1.38        | 1.35     |
| 51  | 9     | 1678 | A2M  | C5-C4   | -3.23 | 1.33        | 1.39     |
| 51  | 9     | 668  | A2M  | C5-C4   | -3.23 | 1.33        | 1.39     |
| 51  | 9     | 509  | OMG  | O6-C6   | -3.23 | 1.17        | 1.23     |
| 51  | 9     | 649  | PSU  | C6-C5   | 3.23  | 1.38        | 1.35     |
| 51  | 9     | 512  | A2M  | O2'-C2' | 3.22  | 1.50        | 1.42     |
| 48  | 5     | 1625 | OMG  | O6-C6   | -3.22 | 1.17        | 1.23     |
| 48  | 5     | 3785 | A2M  | C5-N7   | -3.22 | 1.33        | 1.39     |
| 48  | 5     | 3639 | PSU  | C6-C5   | 3.22  | 1.38        | 1.35     |
| 48  | 5     | 3869 | OMC  | C6-N1   | 3.21  | 1.45        | 1.38     |
| 51  | 9     | 1328 | OMG  | C5-N7   | -3.21 | 1.32        | 1.39     |
| 48  | 5     | 4442 | PSU  | C6-C5   | 3.21  | 1.38        | 1.35     |
| 48  | 5     | 4494 | OMG  | O6-C6   | -3.21 | 1.17        | 1.23     |
| 51  | 9     | 1678 | A2M  | O2'-C2' | 3.21  | 1.50        | 1.42     |
| 48  | 5     | 1860 | PSU  | C6-C5   | 3.20  | 1.38        | 1.35     |
| 48  | 5     | 400  | A2M  | C5-C4   | -3.20 | 1.33        | 1.39     |
| 48  | 5     | 398  | A2M  | C5-C4   | -3.20 | 1.33        | 1.39     |
| 48  | 5     | 4228 | OMG  | C5-N7   | -3.19 | 1.32        | 1.39     |
| 48  | 5     | 4361 | PSU  | C6-C5   | 3.19  | 1.38        | 1.35     |
| 51  | 9     | 815  | PSU  | C6-C5   | 3.18  | 1.38        | 1.35     |
| 48  | 5     | 2861 | OMC  | C6-N1   | 3.18  | 1.45        | 1.38     |
| 48  | 5     | 4447 | 5MC  | O2-C2   | -3.17 | 1.17        | 1.23     |
| 48  | 5     | 4623 | OMG  | O6-C6   | -3.17 | 1.17        | 1.23     |
| 48  | 5     | 2422 | OMC  | C6-N1   | 3.17  | 1.45        | 1.38     |
| 48  | 5     | 1326 | A2M  | O2'-C2' | 3.17  | 1.50        | 1.42     |
| 51  | 9     | 1391 | OMC  | C6-N1   | 3.17  | 1.45        | 1.38     |
| 48  | 5     | 1781 | PSU  | C6-C5   | 3.17  | 1.38        | 1.35     |
| 48  | 5     | 3724 | A2M  | C5-C4   | -3.17 | 1.33        | 1.39     |
| 51  | 9     | 668  | A2M  | C5-N7   | -3.16 | 1.33        | 1.39     |
| 48  | 5     | 2508 | PSU  | C6-C5   | 3.15  | 1.38        | 1.35     |
| 51  | 9     | 119  | PSU  | C6-C5   | 3.15  | 1.38        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 48  | 5     | 4370 | OMG  | O6-C6   | -3.13 | 1.17        | 1.23     |
| 48  | 5     | 1326 | A2M  | C5-C4   | -3.13 | 1.33        | 1.39     |
| 48  | 5     | 2364 | OMG  | C5-N7   | -3.13 | 1.32        | 1.39     |
| 48  | 5     | 2824 | OMC  | C6-N1   | 3.13  | 1.45        | 1.38     |
| 48  | 5     | 1517 | 2MG  | C4-N9   | -3.13 | 1.30        | 1.38     |
| 51  | 9     | 1643 | PSU  | C6-C5   | 3.12  | 1.38        | 1.35     |
| 51  | 9     | 517  | OMC  | C6-N1   | 3.12  | 1.45        | 1.38     |
| 48  | 5     | 3841 | OMC  | C6-N1   | 3.12  | 1.45        | 1.38     |
| 51  | 9     | 1850 | MA6  | C6-N6   | 3.12  | 1.45        | 1.36     |
| 48  | 5     | 4227 | OMU  | C4-N3   | 3.11  | 1.43        | 1.38     |
| 51  | 9     | 1445 | PSU  | C6-C5   | 3.11  | 1.38        | 1.35     |
| 48  | 5     | 4571 | A2M  | C5-N7   | -3.11 | 1.33        | 1.39     |
| 48  | 5     | 4227 | OMU  | O4-C4   | -3.11 | 1.18        | 1.24     |
| 51  | 9     | 1383 | A2M  | C5-C4   | -3.11 | 1.33        | 1.39     |
| 48  | 5     | 1340 | OMC  | C6-N1   | 3.11  | 1.45        | 1.38     |
| 48  | 5     | 3760 | A2M  | C5-C4   | -3.10 | 1.33        | 1.39     |
| 51  | 9     | 1347 | PSU  | C6-C5   | 3.10  | 1.38        | 1.35     |
| 48  | 5     | 2364 | OMG  | O6-C6   | -3.10 | 1.17        | 1.23     |
| 48  | 5     | 2837 | OMU  | O4-C4   | -3.10 | 1.18        | 1.24     |
| 48  | 5     | 1524 | A2M  | C5-N7   | -3.09 | 1.33        | 1.39     |
| 48  | 5     | 4353 | PSU  | C6-C5   | 3.09  | 1.38        | 1.35     |
| 51  | 9     | 512  | A2M  | C5-N7   | -3.09 | 1.33        | 1.39     |
| 51  | 9     | 116  | OMU  | C4-N3   | 3.09  | 1.43        | 1.38     |
| 48  | 5     | 3724 | A2M  | C5-N7   | -3.09 | 1.33        | 1.39     |
| 48  | 5     | 2365 | OMC  | C6-N1   | 3.08  | 1.45        | 1.38     |
| 48  | 5     | 2351 | OMC  | C6-N1   | 3.08  | 1.45        | 1.38     |
| 48  | 5     | 4571 | A2M  | O3'-C3' | -3.07 | 1.35        | 1.43     |
| 48  | 5     | 4523 | A2M  | O3'-C3' | -3.07 | 1.35        | 1.43     |
| 48  | 5     | 4228 | OMG  | O6-C6   | -3.07 | 1.17        | 1.23     |
| 51  | 9     | 159  | A2M  | C5-C4   | -3.06 | 1.33        | 1.39     |
| 48  | 5     | 1677 | PSU  | O4'-C1' | -3.06 | 1.39        | 1.43     |
| 51  | 9     | 1678 | A2M  | C5-N7   | -3.06 | 1.33        | 1.39     |
| 48  | 5     | 398  | A2M  | C5-N7   | -3.05 | 1.33        | 1.39     |
| 51  | 9     | 468  | A2M  | C5-C4   | -3.05 | 1.33        | 1.39     |
| 48  | 5     | 4637 | OMG  | O6-C6   | -3.05 | 1.17        | 1.23     |
| 48  | 5     | 3718 | A2M  | O2'-C2' | 3.04  | 1.50        | 1.42     |
| 51  | 9     | 1391 | OMC  | O2-C2   | -3.04 | 1.18        | 1.23     |
| 51  | 9     | 1851 | MA6  | C6-N6   | 3.04  | 1.45        | 1.36     |
| 48  | 5     | 3887 | OMC  | O2-C2   | -3.04 | 1.18        | 1.23     |
| 51  | 9     | 814  | PSU  | C6-C5   | 3.03  | 1.38        | 1.35     |
| 51  | 9     | 121  | OMU  | O2-C2   | -3.03 | 1.17        | 1.23     |
| 51  | 9     | 1703 | OMC  | C6-N1   | 3.03  | 1.45        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 48  | 5     | 4571 | A2M  | O2'-C2' | 3.03  | 1.50        | 1.42     |
| 51  | 9     | 99   | A2M  | C5-N7   | -3.03 | 1.33        | 1.39     |
| 48  | 5     | 4523 | A2M  | C5-C4   | -3.02 | 1.33        | 1.39     |
| 48  | 5     | 3627 | OMG  | O6-C6   | -3.02 | 1.17        | 1.23     |
| 48  | 5     | 4403 | PSU  | C6-C5   | 3.02  | 1.38        | 1.35     |
| 48  | 5     | 2424 | OMG  | O6-C6   | -3.02 | 1.17        | 1.23     |
| 51  | 9     | 436  | OMG  | O6-C6   | -3.01 | 1.17        | 1.23     |
| 48  | 5     | 3701 | OMC  | C6-N1   | 3.01  | 1.45        | 1.38     |
| 51  | 9     | 159  | A2M  | O3'-C3' | -3.01 | 1.35        | 1.43     |
| 48  | 5     | 3792 | OMG  | O6-C6   | -3.01 | 1.17        | 1.23     |
| 51  | 9     | 174  | OMC  | C6-N1   | 3.00  | 1.45        | 1.38     |
| 51  | 9     | 166  | A2M  | C5-C4   | -3.00 | 1.33        | 1.39     |
| 48  | 5     | 3818 | UY1  | C4-N3   | 3.00  | 1.44        | 1.38     |
| 51  | 9     | 166  | A2M  | O3'-C3' | -3.00 | 1.35        | 1.43     |
| 51  | 9     | 512  | A2M  | C5-C4   | -2.99 | 1.33        | 1.39     |
| 51  | 9     | 1383 | A2M  | O2'-C2' | 2.99  | 1.50        | 1.42     |
| 51  | 9     | 517  | OMC  | O2-C2   | -2.98 | 1.18        | 1.23     |
| 51  | 9     | 1383 | A2M  | C5-N7   | -2.98 | 1.33        | 1.39     |
| 48  | 5     | 4500 | PSU  | C6-C5   | 2.97  | 1.38        | 1.35     |
| 48  | 5     | 2876 | OMG  | O6-C6   | -2.97 | 1.17        | 1.23     |
| 48  | 5     | 2363 | A2M  | O2'-C2' | 2.96  | 1.49        | 1.42     |
| 51  | 9     | 172  | OMU  | O2-C2   | -2.96 | 1.17        | 1.23     |
| 51  | 9     | 1490 | OMG  | C4-N9   | -2.95 | 1.30        | 1.38     |
| 48  | 5     | 2804 | OMC  | C6-N1   | 2.95  | 1.45        | 1.38     |
| 51  | 9     | 484  | A2M  | O2'-C2' | 2.94  | 1.49        | 1.42     |
| 48  | 5     | 3808 | OMC  | C6-N1   | 2.93  | 1.45        | 1.38     |
| 48  | 5     | 3760 | A2M  | C5-N7   | -2.93 | 1.33        | 1.39     |
| 48  | 5     | 1534 | A2M  | O2'-C2' | 2.93  | 1.49        | 1.42     |
| 51  | 9     | 172  | OMU  | O4-C4   | -2.93 | 1.18        | 1.24     |
| 51  | 9     | 428  | OMU  | O4-C4   | -2.93 | 1.18        | 1.24     |
| 48  | 5     | 2815 | A2M  | C5-N7   | -2.93 | 1.33        | 1.39     |
| 48  | 5     | 1326 | A2M  | O3'-C3' | -2.93 | 1.35        | 1.43     |
| 48  | 5     | 3825 | A2M  | C5-C4   | -2.93 | 1.33        | 1.39     |
| 48  | 5     | 4523 | A2M  | C8-N9   | -2.92 | 1.32        | 1.37     |
| 48  | 5     | 3760 | A2M  | O2'-C2' | 2.92  | 1.49        | 1.42     |
| 48  | 5     | 2837 | OMU  | C4-N3   | 2.92  | 1.43        | 1.38     |
| 51  | 9     | 159  | A2M  | O2'-C2' | 2.92  | 1.49        | 1.42     |
| 48  | 5     | 4536 | OMC  | C6-N1   | 2.92  | 1.45        | 1.38     |
| 48  | 5     | 4579 | PSU  | C6-C5   | 2.91  | 1.38        | 1.35     |
| 48  | 5     | 4499 | OMG  | O6-C6   | -2.91 | 1.18        | 1.23     |
| 48  | 5     | 398  | A2M  | O3'-C3' | -2.91 | 1.35        | 1.43     |
| 51  | 9     | 116  | OMU  | O2-C2   | -2.91 | 1.17        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 48  | 5     | 3899 | OMG  | O6-C6   | -2.91 | 1.18        | 1.23     |
| 48  | 5     | 1524 | A2M  | O2'-C2' | 2.90  | 1.49        | 1.42     |
| 48  | 5     | 1517 | 2MG  | O6-C6   | -2.90 | 1.18        | 1.23     |
| 51  | 9     | 512  | A2M  | O3'-C3' | -2.90 | 1.35        | 1.43     |
| 51  | 9     | 863  | PSU  | C6-C5   | 2.90  | 1.38        | 1.35     |
| 51  | 9     | 166  | A2M  | C5-N7   | -2.89 | 1.33        | 1.39     |
| 51  | 9     | 1442 | OMU  | O4-C4   | -2.89 | 1.18        | 1.24     |
| 48  | 5     | 1792 | PSU  | C6-C5   | 2.89  | 1.38        | 1.35     |
| 48  | 5     | 3760 | A2M  | O3'-C3' | -2.89 | 1.35        | 1.43     |
| 48  | 5     | 3851 | PSU  | C6-C5   | 2.88  | 1.38        | 1.35     |
| 48  | 5     | 3887 | OMC  | C6-N1   | 2.88  | 1.44        | 1.38     |
| 48  | 5     | 3830 | A2M  | O3'-C3' | -2.87 | 1.35        | 1.43     |
| 51  | 9     | 686  | PSU  | C6-C5   | 2.87  | 1.38        | 1.35     |
| 51  | 9     | 668  | A2M  | O3'-C3' | -2.87 | 1.35        | 1.43     |
| 48  | 5     | 1517 | 2MG  | C5-N7   | -2.86 | 1.33        | 1.39     |
| 51  | 9     | 1832 | 6MZ  | C5-C4   | -2.86 | 1.34        | 1.39     |
| 48  | 5     | 3724 | A2M  | O3'-C3' | -2.86 | 1.35        | 1.43     |
| 51  | 9     | 166  | A2M  | O2'-C2' | 2.85  | 1.49        | 1.42     |
| 48  | 5     | 2363 | A2M  | O3'-C3' | -2.85 | 1.35        | 1.43     |
| 51  | 9     | 668  | A2M  | O2'-C2' | 2.85  | 1.49        | 1.42     |
| 51  | 9     | 1490 | OMG  | O6-C6   | -2.85 | 1.18        | 1.23     |
| 51  | 9     | 1031 | A2M  | C5-N7   | -2.85 | 1.33        | 1.39     |
| 48  | 5     | 2815 | A2M  | O2'-C2' | 2.85  | 1.49        | 1.42     |
| 48  | 5     | 3867 | A2M  | O3'-C3' | -2.85 | 1.35        | 1.43     |
| 48  | 5     | 1534 | A2M  | O3'-C3' | -2.84 | 1.35        | 1.43     |
| 50  | 8     | 75   | OMG  | O6-C6   | -2.84 | 1.18        | 1.23     |
| 51  | 9     | 1328 | OMG  | O6-C6   | -2.84 | 1.18        | 1.23     |
| 48  | 5     | 3818 | UY1  | O2-C2   | -2.84 | 1.17        | 1.23     |
| 48  | 5     | 3825 | A2M  | O2'-C2' | 2.84  | 1.49        | 1.42     |
| 51  | 9     | 1842 | 4AC  | C6-N1   | 2.84  | 1.44        | 1.38     |
| 48  | 5     | 1322 | 1MA  | C5-N7   | -2.84 | 1.33        | 1.39     |
| 51  | 9     | 468  | A2M  | C5-N7   | -2.83 | 1.33        | 1.39     |
| 51  | 9     | 1851 | MA6  | C5-N7   | -2.82 | 1.33        | 1.39     |
| 48  | 5     | 3920 | PSU  | C6-C5   | 2.82  | 1.38        | 1.35     |
| 51  | 9     | 1703 | OMC  | O2-C2   | -2.82 | 1.18        | 1.23     |
| 48  | 5     | 4220 | 6MZ  | C5-N7   | -2.82 | 1.33        | 1.39     |
| 51  | 9     | 121  | OMU  | C4-N3   | 2.82  | 1.43        | 1.38     |
| 48  | 5     | 2787 | A2M  | O2'-C2' | 2.82  | 1.49        | 1.42     |
| 48  | 5     | 398  | A2M  | O2'-C2' | 2.81  | 1.49        | 1.42     |
| 48  | 5     | 237  | B9B  | C5-N7   | -2.81 | 1.34        | 1.39     |
| 48  | 5     | 4423 | PSU  | C6-C5   | 2.80  | 1.38        | 1.35     |
| 48  | 5     | 3830 | A2M  | O2'-C2' | 2.80  | 1.49        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 51  | 9     | 1326 | OMU  | O4-C4   | -2.79 | 1.19        | 1.24     |
| 51  | 9     | 1383 | A2M  | O3'-C3' | -2.79 | 1.36        | 1.43     |
| 51  | 9     | 159  | A2M  | C5-N7   | -2.79 | 1.34        | 1.39     |
| 51  | 9     | 1850 | MA6  | C8-N9   | -2.79 | 1.32        | 1.37     |
| 51  | 9     | 683  | OMG  | O6-C6   | -2.79 | 1.18        | 1.23     |
| 48  | 5     | 4523 | A2M  | O2'-C2' | 2.78  | 1.49        | 1.42     |
| 51  | 9     | 116  | OMU  | O4-C4   | -2.78 | 1.19        | 1.24     |
| 48  | 5     | 4220 | 6MZ  | C5-C4   | -2.78 | 1.34        | 1.39     |
| 48  | 5     | 2787 | A2M  | O3'-C3' | -2.77 | 1.36        | 1.43     |
| 48  | 5     | 4530 | UR3  | C6-N1   | 2.77  | 1.44        | 1.38     |
| 48  | 5     | 1744 | PSU  | C6-C5   | 2.76  | 1.38        | 1.35     |
| 48  | 5     | 3715 | PSU  | C6-C5   | 2.76  | 1.38        | 1.35     |
| 51  | 9     | 27   | A2M  | O2'-C2' | 2.76  | 1.49        | 1.42     |
| 51  | 9     | 99   | A2M  | O2'-C2' | 2.76  | 1.49        | 1.42     |
| 51  | 9     | 468  | A2M  | O2'-C2' | 2.75  | 1.49        | 1.42     |
| 48  | 5     | 4456 | OMC  | C6-N1   | 2.75  | 1.44        | 1.38     |
| 51  | 9     | 1678 | A2M  | C8-N9   | -2.74 | 1.32        | 1.37     |
| 48  | 5     | 3818 | UY1  | O4-C4   | -2.74 | 1.18        | 1.23     |
| 51  | 9     | 1639 | G7M  | C2-N1   | 2.74  | 1.44        | 1.37     |
| 48  | 5     | 3695 | PSU  | C6-C5   | 2.73  | 1.38        | 1.35     |
| 51  | 9     | 484  | A2M  | C5-N7   | -2.73 | 1.34        | 1.39     |
| 48  | 5     | 4299 | PSU  | C6-C5   | 2.73  | 1.38        | 1.35     |
| 48  | 5     | 1871 | A2M  | O2'-C2' | 2.73  | 1.49        | 1.42     |
| 51  | 9     | 428  | OMU  | O2-C2   | -2.72 | 1.18        | 1.23     |
| 48  | 5     | 400  | A2M  | O3'-C3' | -2.72 | 1.36        | 1.43     |
| 51  | 9     | 1639 | G7M  | C6-N1   | 2.71  | 1.43        | 1.38     |
| 48  | 5     | 3724 | A2M  | O2'-C2' | 2.70  | 1.49        | 1.42     |
| 48  | 5     | 2815 | A2M  | O3'-C3' | -2.69 | 1.36        | 1.43     |
| 51  | 9     | 99   | A2M  | O3'-C3' | -2.69 | 1.36        | 1.43     |
| 48  | 5     | 3825 | A2M  | O3'-C3' | -2.69 | 1.36        | 1.43     |
| 48  | 5     | 4530 | UR3  | O2-C2   | -2.69 | 1.17        | 1.22     |
| 48  | 5     | 4220 | 6MZ  | C8-N9   | -2.68 | 1.33        | 1.37     |
| 51  | 9     | 99   | A2M  | C8-N9   | -2.68 | 1.33        | 1.37     |
| 48  | 5     | 400  | A2M  | O2'-C2' | 2.68  | 1.49        | 1.42     |
| 48  | 5     | 3867 | A2M  | O2'-C2' | 2.67  | 1.49        | 1.42     |
| 48  | 5     | 1871 | A2M  | O3'-C3' | -2.67 | 1.36        | 1.43     |
| 51  | 9     | 27   | A2M  | C5-C4   | -2.67 | 1.34        | 1.39     |
| 51  | 9     | 1031 | A2M  | O3'-C3' | -2.66 | 1.36        | 1.43     |
| 48  | 5     | 1524 | A2M  | O3'-C3' | -2.66 | 1.36        | 1.43     |
| 48  | 5     | 3718 | A2M  | O3'-C3' | -2.65 | 1.36        | 1.43     |
| 51  | 9     | 27   | A2M  | O3'-C3' | -2.65 | 1.36        | 1.43     |
| 48  | 5     | 3724 | A2M  | C8-N9   | -2.64 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 51  | 9     | 1639 | G7M  | O6-C6   | -2.64 | 1.18        | 1.23     |
| 48  | 5     | 3760 | A2M  | C8-N9   | -2.64 | 1.33        | 1.37     |
| 51  | 9     | 1442 | OMU  | O2-C2   | -2.62 | 1.18        | 1.23     |
| 51  | 9     | 644  | OMG  | C2-N1   | 2.62  | 1.44        | 1.37     |
| 48  | 5     | 1326 | A2M  | C8-N9   | -2.62 | 1.33        | 1.37     |
| 51  | 9     | 1031 | A2M  | O2'-C2' | 2.61  | 1.49        | 1.42     |
| 51  | 9     | 484  | A2M  | O3'-C3' | -2.61 | 1.36        | 1.43     |
| 51  | 9     | 468  | A2M  | C8-N9   | -2.60 | 1.33        | 1.37     |
| 48  | 5     | 3785 | A2M  | O2'-C2' | 2.60  | 1.49        | 1.42     |
| 48  | 5     | 237  | B9B  | C8-N9   | -2.60 | 1.33        | 1.37     |
| 48  | 5     | 4499 | OMG  | C2-N1   | 2.60  | 1.43        | 1.37     |
| 51  | 9     | 1842 | 4AC  | O7-C7   | -2.59 | 1.17        | 1.23     |
| 48  | 5     | 4530 | UR3  | O4-C4   | -2.58 | 1.18        | 1.23     |
| 48  | 5     | 3818 | UY1  | O4'-C1' | -2.57 | 1.40        | 1.43     |
| 48  | 5     | 1534 | A2M  | C8-N9   | -2.57 | 1.33        | 1.37     |
| 48  | 5     | 2364 | OMG  | C5-C6   | 2.57  | 1.54        | 1.44     |
| 48  | 5     | 398  | A2M  | C8-N9   | -2.56 | 1.33        | 1.37     |
| 48  | 5     | 1517 | 2MG  | C6-N1   | 2.55  | 1.43        | 1.38     |
| 48  | 5     | 2363 | A2M  | C8-N9   | -2.54 | 1.33        | 1.37     |
| 51  | 9     | 1248 | B8N  | C32-C33 | 2.52  | 1.58        | 1.53     |
| 48  | 5     | 3825 | A2M  | C8-N9   | -2.51 | 1.33        | 1.37     |
| 51  | 9     | 644  | OMG  | O6-C6   | -2.50 | 1.18        | 1.23     |
| 48  | 5     | 3627 | OMG  | C5-C6   | 2.50  | 1.53        | 1.44     |
| 48  | 5     | 2815 | A2M  | C8-N9   | -2.50 | 1.33        | 1.37     |
| 51  | 9     | 1703 | OMC  | C5-C4   | 2.50  | 1.48        | 1.42     |
| 51  | 9     | 1678 | A2M  | O3'-C3' | -2.49 | 1.36        | 1.43     |
| 48  | 5     | 1316 | OMG  | C4-N9   | -2.48 | 1.31        | 1.38     |
| 51  | 9     | 484  | A2M  | C8-N9   | -2.48 | 1.33        | 1.37     |
| 51  | 9     | 668  | A2M  | C8-N9   | -2.47 | 1.33        | 1.37     |
| 48  | 5     | 1316 | OMG  | C5-C6   | 2.47  | 1.53        | 1.44     |
| 48  | 5     | 1871 | A2M  | C8-N9   | -2.46 | 1.33        | 1.37     |
| 51  | 9     | 1851 | MA6  | C8-N9   | -2.45 | 1.33        | 1.37     |
| 48  | 5     | 4306 | OMU  | C4-N3   | 2.45  | 1.42        | 1.38     |
| 50  | 8     | 75   | OMG  | C4-N9   | -2.45 | 1.31        | 1.38     |
| 50  | 8     | 75   | OMG  | C2-N1   | 2.45  | 1.43        | 1.37     |
| 48  | 5     | 4228 | OMG  | C5-C6   | 2.45  | 1.53        | 1.44     |
| 51  | 9     | 159  | A2M  | C8-N9   | -2.44 | 1.33        | 1.37     |
| 51  | 9     | 517  | OMC  | C5-C4   | 2.44  | 1.48        | 1.42     |
| 48  | 5     | 1524 | A2M  | C8-N9   | -2.44 | 1.33        | 1.37     |
| 51  | 9     | 1832 | 6MZ  | C5-N7   | -2.43 | 1.34        | 1.39     |
| 48  | 5     | 2365 | OMC  | C5-C4   | 2.43  | 1.48        | 1.42     |
| 51  | 9     | 1337 | 4AC  | O7-C7   | -2.43 | 1.17        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 51  | 9     | 27   | A2M  | C8-N9   | -2.42 | 1.33        | 1.37     |
| 48  | 5     | 1522 | OMG  | C5-C6   | 2.42  | 1.53        | 1.44     |
| 48  | 5     | 4392 | OMG  | C5-C6   | 2.42  | 1.53        | 1.44     |
| 48  | 5     | 3925 | OMU  | C4-N3   | 2.41  | 1.42        | 1.38     |
| 48  | 5     | 4620 | OMU  | C4-N3   | 2.41  | 1.42        | 1.38     |
| 48  | 5     | 2364 | OMG  | C2-N1   | 2.41  | 1.43        | 1.37     |
| 48  | 5     | 2876 | OMG  | C2-N1   | 2.40  | 1.43        | 1.37     |
| 48  | 5     | 1871 | A2M  | C4-N9   | -2.40 | 1.32        | 1.37     |
| 48  | 5     | 1522 | OMG  | C2-N1   | 2.40  | 1.43        | 1.37     |
| 48  | 5     | 4571 | A2M  | C8-N9   | -2.39 | 1.33        | 1.37     |
| 48  | 5     | 1625 | OMG  | C6-N1   | 2.39  | 1.43        | 1.38     |
| 51  | 9     | 1031 | A2M  | C8-N9   | -2.38 | 1.33        | 1.37     |
| 48  | 5     | 2787 | A2M  | C8-N9   | -2.37 | 1.33        | 1.37     |
| 48  | 5     | 4392 | OMG  | C4-N9   | -2.36 | 1.32        | 1.38     |
| 48  | 5     | 4623 | OMG  | C4-N9   | -2.36 | 1.32        | 1.38     |
| 48  | 5     | 3792 | OMG  | C4-N9   | -2.36 | 1.32        | 1.38     |
| 48  | 5     | 2876 | OMG  | C5-C6   | 2.36  | 1.53        | 1.44     |
| 51  | 9     | 644  | OMG  | C5-C6   | 2.36  | 1.53        | 1.44     |
| 48  | 5     | 400  | A2M  | C8-N9   | -2.36 | 1.33        | 1.37     |
| 51  | 9     | 683  | OMG  | C5-C6   | 2.36  | 1.53        | 1.44     |
| 48  | 5     | 3830 | A2M  | C8-N9   | -2.36 | 1.33        | 1.37     |
| 48  | 5     | 3718 | A2M  | C4-N9   | -2.36 | 1.32        | 1.37     |
| 48  | 5     | 4494 | OMG  | C4-N9   | -2.35 | 1.32        | 1.38     |
| 51  | 9     | 1328 | OMG  | C2-N1   | 2.34  | 1.43        | 1.37     |
| 51  | 9     | 683  | OMG  | C2-N1   | 2.33  | 1.43        | 1.37     |
| 48  | 5     | 4228 | OMG  | C2-N1   | 2.33  | 1.43        | 1.37     |
| 48  | 5     | 4456 | OMC  | C5-C4   | 2.33  | 1.48        | 1.42     |
| 51  | 9     | 436  | OMG  | C2-N1   | 2.32  | 1.43        | 1.37     |
| 48  | 5     | 4618 | OMG  | C5-C6   | 2.32  | 1.53        | 1.44     |
| 48  | 5     | 3715 | PSU  | C4-C5   | -2.32 | 1.37        | 1.44     |
| 51  | 9     | 174  | OMC  | C5-C4   | 2.32  | 1.48        | 1.42     |
| 48  | 5     | 2824 | OMC  | C5-C4   | 2.31  | 1.48        | 1.42     |
| 50  | 8     | 75   | OMG  | C5-C6   | 2.30  | 1.53        | 1.44     |
| 48  | 5     | 1625 | OMG  | C2-N1   | 2.30  | 1.43        | 1.37     |
| 48  | 5     | 4637 | OMG  | C5-C6   | 2.29  | 1.53        | 1.44     |
| 51  | 9     | 801  | PSU  | O4'-C1' | -2.29 | 1.40        | 1.43     |
| 51  | 9     | 512  | A2M  | C8-N9   | -2.29 | 1.33        | 1.37     |
| 48  | 5     | 1340 | OMC  | C5-C4   | 2.28  | 1.48        | 1.42     |
| 48  | 5     | 3627 | OMG  | C4-N9   | -2.27 | 1.32        | 1.38     |
| 48  | 5     | 3899 | OMG  | C5-C6   | 2.27  | 1.52        | 1.44     |
| 48  | 5     | 4370 | OMG  | C5-C6   | 2.27  | 1.52        | 1.44     |
| 48  | 5     | 4618 | OMG  | C2-N1   | 2.27  | 1.43        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 51  | 9     | 1490 | OMG  | C5-C6   | 2.26  | 1.52        | 1.44     |
| 48  | 5     | 1522 | OMG  | C4-N9   | -2.26 | 1.32        | 1.38     |
| 48  | 5     | 4370 | OMG  | C2-N1   | 2.26  | 1.43        | 1.37     |
| 48  | 5     | 1316 | OMG  | C2-N1   | 2.25  | 1.43        | 1.37     |
| 51  | 9     | 1639 | G7M  | C8-N7   | 2.25  | 1.36        | 1.33     |
| 48  | 5     | 2424 | OMG  | C4-N9   | -2.25 | 1.32        | 1.38     |
| 48  | 5     | 3627 | OMG  | C2-N1   | 2.25  | 1.43        | 1.37     |
| 48  | 5     | 4499 | OMG  | C4-N9   | -2.24 | 1.32        | 1.38     |
| 48  | 5     | 2422 | OMC  | C5-C4   | 2.24  | 1.48        | 1.42     |
| 48  | 5     | 4370 | OMG  | C4-N9   | -2.23 | 1.32        | 1.38     |
| 48  | 5     | 4494 | OMG  | C2-N1   | 2.23  | 1.43        | 1.37     |
| 48  | 5     | 2861 | OMC  | C5-C4   | 2.22  | 1.48        | 1.42     |
| 48  | 5     | 4500 | PSU  | O4'-C1' | -2.21 | 1.40        | 1.43     |
| 48  | 5     | 2424 | OMG  | C5-C6   | 2.21  | 1.52        | 1.44     |
| 48  | 5     | 373  | OMG  | C2-N1   | 2.21  | 1.43        | 1.37     |
| 48  | 5     | 3715 | PSU  | O4'-C1' | -2.21 | 1.40        | 1.43     |
| 48  | 5     | 3867 | A2M  | C8-N9   | -2.20 | 1.33        | 1.37     |
| 48  | 5     | 4623 | OMG  | C5-C6   | 2.19  | 1.52        | 1.44     |
| 48  | 5     | 2804 | OMC  | C5-C4   | 2.19  | 1.48        | 1.42     |
| 51  | 9     | 1328 | OMG  | C4-N9   | -2.19 | 1.32        | 1.38     |
| 48  | 5     | 4618 | OMG  | C4-N9   | -2.19 | 1.32        | 1.38     |
| 48  | 5     | 4637 | OMG  | C4-N9   | -2.18 | 1.32        | 1.38     |
| 48  | 5     | 1517 | 2MG  | CM2-N2  | 2.18  | 1.49        | 1.45     |
| 48  | 5     | 4494 | OMG  | C5-C6   | 2.18  | 1.52        | 1.44     |
| 48  | 5     | 3841 | OMC  | C5-C4   | 2.18  | 1.48        | 1.42     |
| 48  | 5     | 373  | OMG  | C5-C6   | 2.18  | 1.52        | 1.44     |
| 48  | 5     | 4637 | OMG  | C2-N1   | 2.18  | 1.42        | 1.37     |
| 51  | 9     | 1238 | PSU  | C4-C5   | -2.18 | 1.38        | 1.44     |
| 48  | 5     | 2351 | OMC  | C5-C4   | 2.17  | 1.48        | 1.42     |
| 51  | 9     | 1832 | 6MZ  | C8-N9   | -2.16 | 1.33        | 1.37     |
| 48  | 5     | 3701 | OMC  | C5-C4   | 2.15  | 1.47        | 1.42     |
| 48  | 5     | 4196 | OMG  | C5-C6   | 2.14  | 1.52        | 1.44     |
| 51  | 9     | 428  | OMU  | C6-N1   | 2.14  | 1.43        | 1.38     |
| 51  | 9     | 822  | PSU  | O4'-C1' | -2.14 | 1.40        | 1.43     |
| 48  | 5     | 2424 | OMG  | C2-N1   | 2.13  | 1.42        | 1.37     |
| 51  | 9     | 822  | PSU  | C4-C5   | -2.13 | 1.38        | 1.44     |
| 48  | 5     | 3925 | OMU  | C5-C4   | 2.12  | 1.48        | 1.43     |
| 48  | 5     | 3785 | A2M  | O3'-C3' | -2.12 | 1.37        | 1.43     |
| 48  | 5     | 2364 | OMG  | C4-N9   | -2.12 | 1.32        | 1.38     |
| 51  | 9     | 509  | OMG  | C2-N1   | 2.12  | 1.42        | 1.37     |
| 48  | 5     | 3851 | PSU  | O4'-C1' | -2.11 | 1.40        | 1.43     |
| 51  | 9     | 1031 | A2M  | C4-N9   | -2.11 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 51  | 9     | 1326 | OMU  | C5-C4   | 2.10  | 1.48        | 1.43     |
| 48  | 5     | 3808 | OMC  | C5-C4   | 2.10  | 1.47        | 1.42     |
| 51  | 9     | 172  | OMU  | C5-C4   | 2.10  | 1.48        | 1.43     |
| 48  | 5     | 3734 | PSU  | C4-C5   | -2.09 | 1.38        | 1.44     |
| 48  | 5     | 4392 | OMG  | C2-N1   | 2.09  | 1.42        | 1.37     |
| 51  | 9     | 166  | A2M  | C8-N9   | -2.09 | 1.34        | 1.37     |
| 51  | 9     | 1383 | A2M  | C8-N9   | -2.09 | 1.34        | 1.37     |
| 48  | 5     | 237  | B9B  | C4-N9   | -2.09 | 1.33        | 1.37     |
| 48  | 5     | 4499 | OMG  | C5-C6   | 2.09  | 1.52        | 1.44     |
| 51  | 9     | 1490 | OMG  | C6-N1   | 2.09  | 1.42        | 1.38     |
| 51  | 9     | 1328 | OMG  | C5-C6   | 2.08  | 1.52        | 1.44     |
| 48  | 5     | 2363 | A2M  | C4-N9   | -2.08 | 1.33        | 1.37     |
| 51  | 9     | 1850 | MA6  | C5-C6   | -2.08 | 1.36        | 1.41     |
| 51  | 9     | 509  | OMG  | C4-N9   | -2.08 | 1.32        | 1.38     |
| 48  | 5     | 4530 | UR3  | C5-C4   | 2.08  | 1.49        | 1.43     |
| 48  | 5     | 3785 | A2M  | C4-N9   | -2.07 | 1.33        | 1.37     |
| 48  | 5     | 4536 | OMC  | C5-C4   | 2.07  | 1.47        | 1.42     |
| 48  | 5     | 3899 | OMG  | C2-N1   | 2.07  | 1.42        | 1.37     |
| 48  | 5     | 4623 | OMG  | C2-N1   | 2.07  | 1.42        | 1.37     |
| 48  | 5     | 4530 | UR3  | C4-N3   | 2.06  | 1.44        | 1.40     |
| 48  | 5     | 4227 | OMU  | C5-C4   | 2.06  | 1.48        | 1.43     |
| 48  | 5     | 4306 | OMU  | C6-N1   | 2.05  | 1.43        | 1.38     |
| 51  | 9     | 1248 | B8N  | O35-C34 | 2.04  | 1.28        | 1.22     |
| 51  | 9     | 1391 | OMC  | C5-C4   | 2.04  | 1.47        | 1.42     |
| 48  | 5     | 4293 | PSU  | C4-C5   | -2.04 | 1.38        | 1.44     |
| 48  | 5     | 1781 | PSU  | C4-C5   | -2.04 | 1.38        | 1.44     |
| 48  | 5     | 4571 | A2M  | C4-N9   | -2.04 | 1.33        | 1.37     |
| 48  | 5     | 4628 | PSU  | C4-C5   | -2.04 | 1.38        | 1.44     |
| 48  | 5     | 1522 | OMG  | C6-N1   | 2.03  | 1.42        | 1.38     |
| 48  | 5     | 4353 | PSU  | C4-C5   | -2.03 | 1.38        | 1.44     |
| 48  | 5     | 4521 | PSU  | O4'-C1' | -2.02 | 1.41        | 1.43     |
| 48  | 5     | 3718 | A2M  | C8-N9   | -2.02 | 1.34        | 1.37     |
| 48  | 5     | 3785 | A2M  | C8-N9   | -2.02 | 1.34        | 1.37     |
| 51  | 9     | 1328 | OMG  | C6-N1   | 2.02  | 1.42        | 1.38     |
| 48  | 5     | 4498 | OMU  | C5-C4   | 2.02  | 1.48        | 1.43     |
| 48  | 5     | 4620 | OMU  | C6-N1   | 2.02  | 1.42        | 1.38     |
| 48  | 5     | 4296 | PSU  | C4-C5   | -2.02 | 1.38        | 1.44     |
| 48  | 5     | 4196 | OMG  | C2-N1   | 2.02  | 1.42        | 1.37     |
| 48  | 5     | 4499 | OMG  | C6-N1   | 2.02  | 1.42        | 1.38     |
| 51  | 9     | 686  | PSU  | C4-C5   | -2.01 | 1.38        | 1.44     |
| 48  | 5     | 4500 | PSU  | C4-C5   | -2.01 | 1.38        | 1.44     |
| 48  | 5     | 3899 | OMG  | C4-N9   | -2.00 | 1.33        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 51  | 9     | 683  | OMG  | C6-N1 | 2.00  | 1.42        | 1.38     |
| 48  | 5     | 4498 | OMU  | C6-N1 | 2.00  | 1.42        | 1.38     |
| 51  | 9     | 1045 | PSU  | C4-C5 | -2.00 | 1.38        | 1.44     |
| 51  | 9     | 1383 | A2M  | C4-N9 | -2.00 | 1.33        | 1.37     |

All (1007) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 51  | 9     | 1851 | MA6  | N1-C6-N6  | -15.95 | 97.42       | 116.86   |
| 51  | 9     | 1850 | MA6  | N1-C6-N6  | -13.25 | 100.72      | 116.86   |
| 51  | 9     | 1851 | MA6  | C5-C6-N6  | 10.76  | 142.36      | 125.33   |
| 51  | 9     | 1850 | MA6  | C5-C6-N6  | 9.04   | 139.64      | 125.33   |
| 51  | 9     | 1851 | MA6  | C4-N9-C1' | -7.48  | 109.14      | 126.63   |
| 51  | 9     | 512  | A2M  | N6-C6-N1  | -7.37  | 101.95      | 118.38   |
| 51  | 9     | 484  | A2M  | N6-C6-N1  | -7.33  | 102.06      | 118.38   |
| 51  | 9     | 1678 | A2M  | N6-C6-N1  | -7.25  | 102.23      | 118.38   |
| 48  | 5     | 1517 | 2MG  | N1-C2-N2  | 7.24   | 123.96      | 116.56   |
| 48  | 5     | 3760 | A2M  | N6-C6-N1  | -7.09  | 102.59      | 118.38   |
| 48  | 5     | 4571 | A2M  | N6-C6-N1  | -7.09  | 102.59      | 118.38   |
| 48  | 5     | 2363 | A2M  | N6-C6-N1  | -7.06  | 102.65      | 118.38   |
| 51  | 9     | 1383 | A2M  | N6-C6-N1  | -7.02  | 102.74      | 118.38   |
| 48  | 5     | 4523 | A2M  | N6-C6-N1  | -6.96  | 102.89      | 118.38   |
| 51  | 9     | 99   | A2M  | N6-C6-N1  | -6.95  | 102.89      | 118.38   |
| 51  | 9     | 668  | A2M  | N6-C6-N1  | -6.94  | 102.93      | 118.38   |
| 48  | 5     | 398  | A2M  | N6-C6-N1  | -6.91  | 102.98      | 118.38   |
| 51  | 9     | 159  | A2M  | N6-C6-N1  | -6.90  | 103.00      | 118.38   |
| 48  | 5     | 3718 | A2M  | N6-C6-N1  | -6.79  | 103.26      | 118.38   |
| 51  | 9     | 1850 | MA6  | C4-N9-C1' | -6.76  | 110.83      | 126.63   |
| 48  | 5     | 2815 | A2M  | N6-C6-N1  | -6.74  | 103.36      | 118.38   |
| 51  | 9     | 468  | A2M  | N6-C6-N1  | -6.72  | 103.41      | 118.38   |
| 51  | 9     | 1851 | MA6  | C1'-N9-C8 | 6.71   | 141.99      | 127.09   |
| 51  | 9     | 27   | A2M  | N6-C6-N1  | -6.70  | 103.44      | 118.38   |
| 48  | 5     | 3785 | A2M  | N6-C6-N1  | -6.70  | 103.45      | 118.38   |
| 48  | 5     | 3867 | A2M  | N6-C6-N1  | -6.66  | 103.54      | 118.38   |
| 48  | 5     | 3830 | A2M  | N6-C6-N1  | -6.63  | 103.61      | 118.38   |
| 48  | 5     | 1524 | A2M  | N6-C6-N1  | -6.57  | 103.74      | 118.38   |
| 48  | 5     | 1534 | A2M  | N6-C6-N1  | -6.57  | 103.75      | 118.38   |
| 48  | 5     | 3724 | A2M  | N6-C6-N1  | -6.51  | 103.88      | 118.38   |
| 48  | 5     | 1322 | 1MA  | C1'-N9-C8 | -6.50  | 108.26      | 126.73   |
| 51  | 9     | 1031 | A2M  | N6-C6-N1  | -6.44  | 104.04      | 118.38   |
| 48  | 5     | 2787 | A2M  | N6-C6-N1  | -6.43  | 104.06      | 118.38   |
| 48  | 5     | 1326 | A2M  | N6-C6-N1  | -6.42  | 104.08      | 118.38   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 51  | 9     | 166  | A2M  | N6-C6-N1  | -6.38 | 104.16      | 118.38   |
| 48  | 5     | 1517 | 2MG  | C2-N3-C4  | 6.34  | 119.94      | 112.00   |
| 48  | 5     | 2876 | OMG  | C5-C4-N3  | -6.31 | 118.35      | 128.39   |
| 51  | 9     | 166  | A2M  | N3-C2-N1  | -6.26 | 119.11      | 128.58   |
| 48  | 5     | 237  | B9B  | C5-C4-N3  | -6.18 | 120.67      | 127.18   |
| 51  | 9     | 512  | A2M  | C5-C6-N6  | 6.16  | 138.54      | 123.29   |
| 51  | 9     | 484  | A2M  | N3-C2-N1  | -6.16 | 119.26      | 128.58   |
| 48  | 5     | 1871 | A2M  | N6-C6-N1  | -6.13 | 104.72      | 118.38   |
| 48  | 5     | 4498 | OMU  | C4-N3-C2  | -6.11 | 119.03      | 126.61   |
| 51  | 9     | 512  | A2M  | N3-C2-N1  | -6.08 | 119.38      | 128.58   |
| 48  | 5     | 373  | OMG  | C5-C4-N3  | -6.08 | 118.72      | 128.39   |
| 48  | 5     | 3830 | A2M  | N3-C2-N1  | -6.06 | 119.41      | 128.58   |
| 48  | 5     | 1625 | OMG  | C5-C4-N3  | -6.04 | 118.77      | 128.39   |
| 51  | 9     | 1326 | OMU  | C4-N3-C2  | -6.04 | 119.11      | 126.61   |
| 51  | 9     | 1832 | 6MZ  | N1-C2-N3  | -6.02 | 119.46      | 128.58   |
| 48  | 5     | 3825 | A2M  | N6-C6-N1  | -6.02 | 104.97      | 118.38   |
| 48  | 5     | 1871 | A2M  | N3-C2-N1  | -6.01 | 119.48      | 128.58   |
| 51  | 9     | 484  | A2M  | C5-C6-N6  | 5.99  | 138.13      | 123.29   |
| 51  | 9     | 1248 | B8N  | C1'-C5-C4 | 5.99  | 126.70      | 117.61   |
| 48  | 5     | 2837 | OMU  | C4-N3-C2  | -5.99 | 119.18      | 126.61   |
| 51  | 9     | 1490 | OMG  | C1'-N9-C4 | -5.97 | 108.86      | 126.49   |
| 51  | 9     | 1031 | A2M  | N3-C2-N1  | -5.95 | 119.58      | 128.58   |
| 48  | 5     | 4196 | OMG  | C5-C4-N3  | -5.94 | 118.94      | 128.39   |
| 48  | 5     | 3867 | A2M  | N3-C2-N1  | -5.89 | 119.67      | 128.58   |
| 51  | 9     | 1851 | MA6  | C5-C4-N3  | -5.85 | 118.66      | 126.72   |
| 51  | 9     | 1851 | MA6  | N1-C2-N3  | -5.85 | 119.73      | 128.58   |
| 51  | 9     | 1678 | A2M  | C5-C6-N6  | 5.84  | 137.75      | 123.29   |
| 48  | 5     | 1326 | A2M  | N3-C2-N1  | -5.83 | 119.75      | 128.58   |
| 51  | 9     | 1383 | A2M  | N3-C2-N1  | -5.83 | 119.76      | 128.58   |
| 48  | 5     | 4521 | PSU  | N1-C2-N3  | 5.82  | 121.31      | 115.17   |
| 48  | 5     | 3925 | OMU  | C4-N3-C2  | -5.82 | 119.39      | 126.61   |
| 48  | 5     | 4571 | A2M  | N3-C2-N1  | -5.81 | 119.78      | 128.58   |
| 48  | 5     | 2364 | OMG  | C5-C4-N3  | -5.81 | 119.14      | 128.39   |
| 51  | 9     | 218  | PSU  | N1-C2-N3  | 5.80  | 121.29      | 115.17   |
| 48  | 5     | 2815 | A2M  | N3-C2-N1  | -5.80 | 119.80      | 128.58   |
| 48  | 5     | 4392 | OMG  | C5-C4-N3  | -5.80 | 119.16      | 128.39   |
| 48  | 5     | 4227 | OMU  | C4-N3-C2  | -5.79 | 119.43      | 126.61   |
| 51  | 9     | 686  | PSU  | C4-N3-C2  | -5.78 | 118.40      | 126.37   |
| 48  | 5     | 2787 | A2M  | C5-C4-N3  | -5.77 | 118.78      | 126.72   |
| 51  | 9     | 468  | A2M  | N3-C2-N1  | -5.77 | 119.85      | 128.58   |
| 48  | 5     | 4523 | A2M  | N3-C2-N1  | -5.75 | 119.87      | 128.58   |
| 51  | 9     | 668  | A2M  | N3-C2-N1  | -5.75 | 119.88      | 128.58   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 51  | 9     | 683  | OMG  | C5-C4-N3  | -5.75 | 119.24      | 128.39   |
| 48  | 5     | 4523 | A2M  | C5-C6-N6  | 5.73  | 137.47      | 123.29   |
| 51  | 9     | 1490 | OMG  | C1'-N9-C8 | 5.72  | 142.98      | 126.73   |
| 48  | 5     | 4637 | OMG  | C5-C4-N3  | -5.72 | 119.29      | 128.39   |
| 51  | 9     | 1850 | MA6  | C1'-N9-C8 | 5.71  | 139.77      | 127.09   |
| 48  | 5     | 1524 | A2M  | N3-C2-N1  | -5.71 | 119.94      | 128.58   |
| 48  | 5     | 3718 | A2M  | N3-C2-N1  | -5.68 | 119.99      | 128.58   |
| 48  | 5     | 3899 | OMG  | C5-C4-N3  | -5.67 | 119.36      | 128.39   |
| 51  | 9     | 1383 | A2M  | C5-C6-N6  | 5.66  | 137.29      | 123.29   |
| 48  | 5     | 2363 | A2M  | C5-C6-N6  | 5.65  | 137.28      | 123.29   |
| 48  | 5     | 1534 | A2M  | N3-C2-N1  | -5.65 | 120.03      | 128.58   |
| 48  | 5     | 400  | A2M  | N6-C6-N1  | -5.65 | 105.79      | 118.38   |
| 48  | 5     | 4620 | OMU  | C4-N3-C2  | -5.63 | 119.62      | 126.61   |
| 48  | 5     | 3760 | A2M  | C5-C6-N6  | 5.63  | 137.22      | 123.29   |
| 48  | 5     | 4571 | A2M  | C5-C6-N6  | 5.62  | 137.20      | 123.29   |
| 48  | 5     | 4306 | OMU  | C4-N3-C2  | -5.62 | 119.64      | 126.61   |
| 48  | 5     | 4220 | 6MZ  | N1-C2-N3  | -5.61 | 120.09      | 128.58   |
| 51  | 9     | 27   | A2M  | N3-C2-N1  | -5.60 | 120.10      | 128.58   |
| 51  | 9     | 27   | A2M  | C5-C6-N6  | 5.60  | 137.16      | 123.29   |
| 51  | 9     | 436  | OMG  | C5-C4-N3  | -5.59 | 119.49      | 128.39   |
| 48  | 5     | 3762 | PSU  | C4-N3-C2  | -5.59 | 118.67      | 126.37   |
| 48  | 5     | 3853 | PSU  | N1-C2-N3  | 5.58  | 121.05      | 115.17   |
| 51  | 9     | 218  | PSU  | C4-N3-C2  | -5.58 | 118.69      | 126.37   |
| 48  | 5     | 4628 | PSU  | N1-C2-N3  | 5.56  | 121.03      | 115.17   |
| 51  | 9     | 172  | OMU  | C4-N3-C2  | -5.56 | 119.71      | 126.61   |
| 51  | 9     | 159  | A2M  | C5-C6-N6  | 5.56  | 137.04      | 123.29   |
| 51  | 9     | 1678 | A2M  | N3-C2-N1  | -5.55 | 120.17      | 128.58   |
| 51  | 9     | 668  | A2M  | C5-C6-N6  | 5.55  | 137.04      | 123.29   |
| 48  | 5     | 2787 | A2M  | N3-C2-N1  | -5.54 | 120.19      | 128.58   |
| 51  | 9     | 1442 | OMU  | C4-N3-C2  | -5.54 | 119.73      | 126.61   |
| 51  | 9     | 121  | OMU  | C4-N3-C2  | -5.54 | 119.73      | 126.61   |
| 48  | 5     | 398  | A2M  | C5-C4-N3  | -5.53 | 119.10      | 126.72   |
| 51  | 9     | 99   | A2M  | C5-C6-N6  | 5.51  | 136.92      | 123.29   |
| 48  | 5     | 3718 | A2M  | C5-C6-N6  | 5.50  | 136.90      | 123.29   |
| 48  | 5     | 3760 | A2M  | N3-C2-N1  | -5.49 | 120.26      | 128.58   |
| 48  | 5     | 1677 | PSU  | N1-C2-N3  | 5.49  | 120.96      | 115.17   |
| 48  | 5     | 398  | A2M  | N3-C2-N1  | -5.48 | 120.28      | 128.58   |
| 48  | 5     | 1524 | A2M  | C5-C6-N6  | 5.48  | 136.85      | 123.29   |
| 48  | 5     | 1677 | PSU  | C4-N3-C2  | -5.46 | 118.85      | 126.37   |
| 48  | 5     | 1683 | PSU  | N1-C2-N3  | 5.46  | 120.92      | 115.17   |
| 51  | 9     | 1174 | PSU  | N1-C2-N3  | 5.46  | 120.92      | 115.17   |
| 48  | 5     | 1322 | 1MA  | C1'-N9-C4 | 5.46  | 142.60      | 126.49   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 48  | 5     | 2363 | A2M  | N3-C2-N1 | -5.46 | 120.32      | 128.58   |
| 48  | 5     | 400  | A2M  | C5-C4-N3 | -5.45 | 119.21      | 126.72   |
| 51  | 9     | 509  | OMG  | C5-C4-N3 | -5.45 | 119.71      | 128.39   |
| 48  | 5     | 3785 | A2M  | N3-C2-N1 | -5.45 | 120.33      | 128.58   |
| 51  | 9     | 822  | PSU  | N1-C2-N3 | 5.45  | 120.91      | 115.17   |
| 48  | 5     | 1534 | A2M  | C5-C6-N6 | 5.44  | 136.76      | 123.29   |
| 48  | 5     | 4442 | PSU  | N1-C2-N3 | 5.44  | 120.91      | 115.17   |
| 48  | 5     | 3724 | A2M  | N3-C2-N1 | -5.44 | 120.35      | 128.58   |
| 51  | 9     | 1045 | PSU  | N1-C2-N3 | 5.44  | 120.90      | 115.17   |
| 48  | 5     | 3825 | A2M  | C5-C4-N3 | -5.44 | 119.23      | 126.72   |
| 48  | 5     | 4353 | PSU  | N1-C2-N3 | 5.43  | 120.90      | 115.17   |
| 51  | 9     | 1643 | PSU  | C4-N3-C2 | -5.43 | 118.89      | 126.37   |
| 48  | 5     | 4628 | PSU  | C4-N3-C2 | -5.43 | 118.89      | 126.37   |
| 51  | 9     | 1248 | B8N  | C5-C4-N3 | 5.43  | 126.00      | 116.15   |
| 51  | 9     | 99   | A2M  | N3-C2-N1 | -5.42 | 120.37      | 128.58   |
| 51  | 9     | 428  | OMU  | C4-N3-C2 | -5.42 | 119.88      | 126.61   |
| 51  | 9     | 686  | PSU  | N1-C2-N3 | 5.41  | 120.87      | 115.17   |
| 51  | 9     | 166  | A2M  | C5-C6-N6 | 5.41  | 136.67      | 123.29   |
| 48  | 5     | 3851 | PSU  | N1-C2-N3 | 5.40  | 120.86      | 115.17   |
| 48  | 5     | 3830 | A2M  | C5-C6-N6 | 5.39  | 136.63      | 123.29   |
| 51  | 9     | 468  | A2M  | C5-C6-N6 | 5.38  | 136.62      | 123.29   |
| 48  | 5     | 2815 | A2M  | C5-C6-N6 | 5.38  | 136.61      | 123.29   |
| 48  | 5     | 3920 | PSU  | C4-N3-C2 | -5.38 | 118.97      | 126.37   |
| 48  | 5     | 4370 | OMG  | C5-C4-N3 | -5.37 | 119.84      | 128.39   |
| 48  | 5     | 1326 | A2M  | C5-C6-N6 | 5.37  | 136.58      | 123.29   |
| 48  | 5     | 3920 | PSU  | N1-C2-N3 | 5.36  | 120.83      | 115.17   |
| 51  | 9     | 109  | PSU  | N1-C2-N3 | 5.36  | 120.82      | 115.17   |
| 51  | 9     | 159  | A2M  | N3-C2-N1 | -5.36 | 120.47      | 128.58   |
| 51  | 9     | 1850 | MA6  | N1-C2-N3 | -5.35 | 120.48      | 128.58   |
| 48  | 5     | 398  | A2M  | C5-C6-N6 | 5.33  | 136.50      | 123.29   |
| 48  | 5     | 3760 | A2M  | C5-C4-N3 | -5.33 | 119.37      | 126.72   |
| 51  | 9     | 1850 | MA6  | C5-C4-N3 | -5.33 | 119.37      | 126.72   |
| 48  | 5     | 3867 | A2M  | C5-C6-N6 | 5.32  | 136.46      | 123.29   |
| 48  | 5     | 3762 | PSU  | N1-C2-N3 | 5.32  | 120.78      | 115.17   |
| 51  | 9     | 644  | OMG  | C5-C4-N3 | -5.32 | 119.93      | 128.39   |
| 51  | 9     | 105  | PSU  | N1-C2-N3 | 5.32  | 120.78      | 115.17   |
| 51  | 9     | 1045 | PSU  | C4-N3-C2 | -5.31 | 119.06      | 126.37   |
| 51  | 9     | 1643 | PSU  | N1-C2-N3 | 5.30  | 120.76      | 115.17   |
| 48  | 5     | 3724 | A2M  | C5-C4-N3 | -5.30 | 119.42      | 126.72   |
| 48  | 5     | 4361 | PSU  | N1-C2-N3 | 5.29  | 120.75      | 115.17   |
| 51  | 9     | 116  | OMU  | C4-N3-C2 | -5.29 | 120.04      | 126.61   |
| 51  | 9     | 1248 | B8N  | C4-N3-C2 | -5.28 | 119.12      | 125.62   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 51  | 9     | 815  | PSU  | N1-C2-N3 | 5.27  | 120.73      | 115.17   |
| 48  | 5     | 4623 | OMG  | C5-C4-N3 | -5.27 | 120.00      | 128.39   |
| 48  | 5     | 3764 | PSU  | N1-C2-N3 | 5.27  | 120.72      | 115.17   |
| 51  | 9     | 1244 | PSU  | C4-N3-C2 | -5.27 | 119.12      | 126.37   |
| 48  | 5     | 4228 | OMG  | C5-C4-N3 | -5.26 | 120.02      | 128.39   |
| 48  | 5     | 4494 | OMG  | C5-C4-N3 | -5.26 | 120.02      | 128.39   |
| 51  | 9     | 1081 | PSU  | N1-C2-N3 | 5.26  | 120.71      | 115.17   |
| 48  | 5     | 3853 | PSU  | C4-N3-C2 | -5.24 | 119.15      | 126.37   |
| 48  | 5     | 1871 | A2M  | C5-C6-N6 | 5.24  | 136.26      | 123.29   |
| 48  | 5     | 3785 | A2M  | C5-C6-N6 | 5.24  | 136.26      | 123.29   |
| 48  | 5     | 400  | A2M  | N3-C2-N1 | -5.24 | 120.66      | 128.58   |
| 48  | 5     | 3792 | OMG  | C5-C4-N3 | -5.23 | 120.07      | 128.39   |
| 48  | 5     | 3764 | PSU  | C4-N3-C2 | -5.22 | 119.17      | 126.37   |
| 51  | 9     | 814  | PSU  | C4-N3-C2 | -5.22 | 119.19      | 126.37   |
| 48  | 5     | 4423 | PSU  | C4-N3-C2 | -5.20 | 119.20      | 126.37   |
| 51  | 9     | 34   | PSU  | N1-C2-N3 | 5.20  | 120.65      | 115.17   |
| 48  | 5     | 4361 | PSU  | C4-N3-C2 | -5.19 | 119.23      | 126.37   |
| 51  | 9     | 822  | PSU  | C4-N3-C2 | -5.19 | 119.23      | 126.37   |
| 51  | 9     | 109  | PSU  | C4-N3-C2 | -5.18 | 119.23      | 126.37   |
| 51  | 9     | 815  | PSU  | C4-N3-C2 | -5.18 | 119.23      | 126.37   |
| 48  | 5     | 4299 | PSU  | C4-N3-C2 | -5.17 | 119.25      | 126.37   |
| 51  | 9     | 1031 | A2M  | C5-C6-N6 | 5.17  | 136.09      | 123.29   |
| 51  | 9     | 1850 | MA6  | C4-C5-C6 | 5.17  | 121.26      | 115.91   |
| 48  | 5     | 2424 | OMG  | C5-C4-N3 | -5.17 | 120.16      | 128.39   |
| 51  | 9     | 1347 | PSU  | C4-N3-C2 | -5.17 | 119.25      | 126.37   |
| 50  | 8     | 75   | OMG  | C5-C4-N3 | -5.16 | 120.17      | 128.39   |
| 48  | 5     | 4296 | PSU  | N1-C2-N3 | 5.16  | 120.61      | 115.17   |
| 51  | 9     | 1004 | PSU  | N1-C2-N3 | 5.15  | 120.60      | 115.17   |
| 48  | 5     | 4552 | PSU  | C4-N3-C2 | -5.15 | 119.28      | 126.37   |
| 51  | 9     | 1174 | PSU  | C4-N3-C2 | -5.15 | 119.28      | 126.37   |
| 48  | 5     | 1683 | PSU  | C4-N3-C2 | -5.15 | 119.28      | 126.37   |
| 51  | 9     | 814  | PSU  | N1-C2-N3 | 5.14  | 120.59      | 115.17   |
| 48  | 5     | 4420 | PSU  | N1-C2-N3 | 5.13  | 120.58      | 115.17   |
| 48  | 5     | 4499 | OMG  | C5-C4-N3 | -5.12 | 120.23      | 128.39   |
| 48  | 5     | 2363 | A2M  | C5-C4-N3 | -5.12 | 119.67      | 126.72   |
| 51  | 9     | 668  | A2M  | C5-C4-N3 | -5.12 | 119.67      | 126.72   |
| 48  | 5     | 2632 | PSU  | N1-C2-N3 | 5.12  | 120.56      | 115.17   |
| 51  | 9     | 1244 | PSU  | N1-C2-N3 | 5.12  | 120.56      | 115.17   |
| 48  | 5     | 1782 | PSU  | N1-C2-N3 | 5.11  | 120.56      | 115.17   |
| 48  | 5     | 1522 | OMG  | C5-C4-N3 | -5.11 | 120.25      | 128.39   |
| 48  | 5     | 3695 | PSU  | N1-C2-N3 | 5.11  | 120.56      | 115.17   |
| 48  | 5     | 4618 | OMG  | C5-C4-N3 | -5.11 | 120.27      | 128.39   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 51  | 9     | 609  | PSU  | N1-C2-N3 | 5.10  | 120.55      | 115.17   |
| 48  | 5     | 3825 | A2M  | N3-C2-N1 | -5.10 | 120.86      | 128.58   |
| 48  | 5     | 3785 | A2M  | C5-C4-N3 | -5.09 | 119.70      | 126.72   |
| 48  | 5     | 3695 | PSU  | C4-N3-C2 | -5.08 | 119.38      | 126.37   |
| 48  | 5     | 3851 | PSU  | C4-N3-C2 | -5.08 | 119.38      | 126.37   |
| 48  | 5     | 3724 | A2M  | C5-C6-N6 | 5.06  | 135.82      | 123.29   |
| 48  | 5     | 1860 | PSU  | N1-C2-N3 | 5.06  | 120.51      | 115.17   |
| 51  | 9     | 119  | PSU  | C4-N3-C2 | -5.06 | 119.41      | 126.37   |
| 51  | 9     | 1232 | PSU  | N1-C2-N3 | 5.05  | 120.50      | 115.17   |
| 51  | 9     | 99   | A2M  | C5-C4-N3 | -5.05 | 119.76      | 126.72   |
| 48  | 5     | 3867 | A2M  | C5-C4-N3 | -5.05 | 119.76      | 126.72   |
| 48  | 5     | 1322 | 1MA  | N1-C2-N3 | -5.04 | 120.00      | 126.00   |
| 48  | 5     | 1744 | PSU  | C4-N3-C2 | -5.04 | 119.43      | 126.37   |
| 48  | 5     | 4423 | PSU  | N1-C2-N3 | 5.03  | 120.47      | 115.17   |
| 48  | 5     | 4442 | PSU  | C4-N3-C2 | -5.03 | 119.44      | 126.37   |
| 48  | 5     | 1781 | PSU  | C4-N3-C2 | -5.02 | 119.45      | 126.37   |
| 48  | 5     | 4521 | PSU  | C4-N3-C2 | -5.02 | 119.45      | 126.37   |
| 48  | 5     | 4500 | PSU  | N1-C2-N3 | 5.02  | 120.46      | 115.17   |
| 51  | 9     | 119  | PSU  | N1-C2-N3 | 5.02  | 120.46      | 115.17   |
| 48  | 5     | 4353 | PSU  | C4-N3-C2 | -5.02 | 119.46      | 126.37   |
| 48  | 5     | 4579 | PSU  | C4-N3-C2 | -5.02 | 119.46      | 126.37   |
| 48  | 5     | 4523 | A2M  | C5-C4-N3 | -5.01 | 119.81      | 126.72   |
| 51  | 9     | 649  | PSU  | C4-N3-C2 | -5.01 | 119.47      | 126.37   |
| 48  | 5     | 4420 | PSU  | C4-N3-C2 | -5.00 | 119.48      | 126.37   |
| 48  | 5     | 3825 | A2M  | C5-C6-N6 | 5.00  | 135.68      | 123.29   |
| 48  | 5     | 1862 | PSU  | N1-C2-N3 | 5.00  | 120.44      | 115.17   |
| 51  | 9     | 1238 | PSU  | C4-N3-C2 | -5.00 | 119.49      | 126.37   |
| 51  | 9     | 27   | A2M  | C5-C4-N3 | -4.99 | 119.84      | 126.72   |
| 48  | 5     | 1744 | PSU  | N1-C2-N3 | 4.99  | 120.44      | 115.17   |
| 51  | 9     | 1328 | OMG  | C5-C4-N3 | -4.99 | 120.45      | 128.39   |
| 48  | 5     | 1625 | OMG  | C2-N3-C4 | 4.99  | 120.89      | 112.30   |
| 48  | 5     | 2787 | A2M  | C5-C6-N6 | 4.98  | 135.63      | 123.29   |
| 48  | 5     | 4293 | PSU  | C4-N3-C2 | -4.98 | 119.52      | 126.37   |
| 48  | 5     | 1792 | PSU  | C4-N3-C2 | -4.97 | 119.52      | 126.37   |
| 51  | 9     | 105  | PSU  | C4-N3-C2 | -4.97 | 119.52      | 126.37   |
| 48  | 5     | 1782 | PSU  | C4-N3-C2 | -4.97 | 119.52      | 126.37   |
| 51  | 9     | 1081 | PSU  | C4-N3-C2 | -4.97 | 119.52      | 126.37   |
| 51  | 9     | 484  | A2M  | C5-C4-N3 | -4.97 | 119.87      | 126.72   |
| 48  | 5     | 2632 | PSU  | C4-N3-C2 | -4.96 | 119.53      | 126.37   |
| 51  | 9     | 1046 | PSU  | N1-C2-N3 | 4.96  | 120.40      | 115.17   |
| 48  | 5     | 1316 | OMG  | C5-C4-N3 | -4.96 | 120.49      | 128.39   |
| 48  | 5     | 4403 | PSU  | C4-N3-C2 | -4.96 | 119.54      | 126.37   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 51  | 9     | 609  | PSU  | C4-N3-C2 | -4.96 | 119.55      | 126.37   |
| 51  | 9     | 1004 | PSU  | C4-N3-C2 | -4.95 | 119.55      | 126.37   |
| 48  | 5     | 4457 | PSU  | C4-N3-C2 | -4.94 | 119.56      | 126.37   |
| 51  | 9     | 863  | PSU  | C4-N3-C2 | -4.94 | 119.57      | 126.37   |
| 48  | 5     | 3639 | PSU  | N1-C2-N3 | 4.92  | 120.36      | 115.17   |
| 48  | 5     | 4296 | PSU  | C4-N3-C2 | -4.92 | 119.60      | 126.37   |
| 48  | 5     | 3734 | PSU  | N1-C2-N3 | 4.92  | 120.35      | 115.17   |
| 48  | 5     | 1862 | PSU  | C4-N3-C2 | -4.91 | 119.61      | 126.37   |
| 48  | 5     | 4403 | PSU  | N1-C2-N3 | 4.90  | 120.34      | 115.17   |
| 51  | 9     | 572  | PSU  | N1-C2-N3 | 4.90  | 120.34      | 115.17   |
| 51  | 9     | 1238 | PSU  | N1-C2-N3 | 4.90  | 120.34      | 115.17   |
| 51  | 9     | 1347 | PSU  | N1-C2-N3 | 4.90  | 120.34      | 115.17   |
| 51  | 9     | 1678 | A2M  | C5-C4-N3 | -4.89 | 119.98      | 126.72   |
| 48  | 5     | 4552 | PSU  | N1-C2-N3 | 4.89  | 120.33      | 115.17   |
| 48  | 5     | 2508 | PSU  | C4-N3-C2 | -4.89 | 119.63      | 126.37   |
| 48  | 5     | 4500 | PSU  | C4-N3-C2 | -4.88 | 119.64      | 126.37   |
| 48  | 5     | 3639 | PSU  | C4-N3-C2 | -4.88 | 119.65      | 126.37   |
| 48  | 5     | 4220 | 6MZ  | C5-C4-N3 | -4.87 | 120.01      | 126.72   |
| 48  | 5     | 2508 | PSU  | N1-C2-N3 | 4.87  | 120.30      | 115.17   |
| 51  | 9     | 1232 | PSU  | C4-N3-C2 | -4.86 | 119.68      | 126.37   |
| 48  | 5     | 4532 | PSU  | C4-N3-C2 | -4.85 | 119.69      | 126.37   |
| 51  | 9     | 1367 | PSU  | C4-N3-C2 | -4.84 | 119.70      | 126.37   |
| 48  | 5     | 2364 | OMG  | C2-N3-C4 | 4.83  | 120.62      | 112.30   |
| 51  | 9     | 512  | A2M  | C5-C4-N3 | -4.83 | 120.06      | 126.72   |
| 48  | 5     | 1534 | A2M  | C5-C4-N3 | -4.83 | 120.07      | 126.72   |
| 48  | 5     | 2815 | A2M  | C5-C4-N3 | -4.82 | 120.09      | 126.72   |
| 48  | 5     | 4299 | PSU  | N1-C2-N3 | 4.80  | 120.23      | 115.17   |
| 48  | 5     | 3818 | UY1  | N1-C2-N3 | 4.80  | 120.23      | 115.17   |
| 48  | 5     | 3830 | A2M  | C5-C4-N3 | -4.80 | 120.11      | 126.72   |
| 48  | 5     | 4530 | UR3  | C4-N3-C2 | -4.80 | 120.72      | 124.58   |
| 48  | 5     | 1316 | OMG  | C2-N3-C4 | 4.80  | 120.56      | 112.30   |
| 48  | 5     | 1781 | PSU  | N1-C2-N3 | 4.79  | 120.22      | 115.17   |
| 51  | 9     | 649  | PSU  | N1-C2-N3 | 4.78  | 120.21      | 115.17   |
| 51  | 9     | 1367 | PSU  | N1-C2-N3 | 4.78  | 120.21      | 115.17   |
| 48  | 5     | 1524 | A2M  | C5-C4-N3 | -4.77 | 120.15      | 126.72   |
| 51  | 9     | 468  | A2M  | C5-C4-N3 | -4.77 | 120.15      | 126.72   |
| 51  | 9     | 1832 | 6MZ  | C5-C4-N3 | -4.76 | 120.16      | 126.72   |
| 48  | 5     | 4579 | PSU  | N1-C2-N3 | 4.76  | 120.19      | 115.17   |
| 48  | 5     | 4196 | OMG  | C2-N3-C4 | 4.76  | 120.49      | 112.30   |
| 48  | 5     | 1860 | PSU  | C4-N3-C2 | -4.75 | 119.83      | 126.37   |
| 48  | 5     | 1792 | PSU  | N1-C2-N3 | 4.74  | 120.17      | 115.17   |
| 51  | 9     | 1692 | PSU  | C4-N3-C2 | -4.74 | 119.84      | 126.37   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 48  | 5     | 4293 | PSU  | N1-C2-N3  | 4.74  | 120.17      | 115.17   |
| 48  | 5     | 3734 | PSU  | C4-N3-C2  | -4.73 | 119.85      | 126.37   |
| 48  | 5     | 3818 | UY1  | C4-N3-C2  | -4.73 | 119.86      | 126.37   |
| 48  | 5     | 4571 | A2M  | C5-C4-N3  | -4.73 | 120.20      | 126.72   |
| 51  | 9     | 572  | PSU  | C4-N3-C2  | -4.73 | 119.86      | 126.37   |
| 51  | 9     | 1046 | PSU  | C4-N3-C2  | -4.72 | 119.87      | 126.37   |
| 48  | 5     | 1522 | OMG  | C2-N3-C4  | 4.71  | 120.42      | 112.30   |
| 48  | 5     | 3627 | OMG  | C5-C4-N3  | -4.71 | 120.89      | 128.39   |
| 48  | 5     | 3899 | OMG  | C2-N3-C4  | 4.71  | 120.41      | 112.30   |
| 48  | 5     | 4392 | OMG  | C2-N3-C4  | 4.70  | 120.39      | 112.30   |
| 48  | 5     | 373  | OMG  | C2-N3-C4  | 4.69  | 120.38      | 112.30   |
| 48  | 5     | 1326 | A2M  | C5-C4-N3  | -4.68 | 120.27      | 126.72   |
| 51  | 9     | 159  | A2M  | C5-C4-N3  | -4.68 | 120.27      | 126.72   |
| 48  | 5     | 3715 | PSU  | N1-C2-N3  | 4.67  | 120.09      | 115.17   |
| 51  | 9     | 1851 | MA6  | C4-C5-C6  | 4.67  | 120.74      | 115.91   |
| 51  | 9     | 1851 | MA6  | N9-C8-N7  | -4.66 | 107.33      | 113.94   |
| 51  | 9     | 1177 | PSU  | N1-C2-N3  | 4.65  | 120.07      | 115.17   |
| 51  | 9     | 34   | PSU  | C4-N3-C2  | -4.64 | 119.98      | 126.37   |
| 48  | 5     | 4618 | OMG  | C2-N3-C4  | 4.64  | 120.29      | 112.30   |
| 51  | 9     | 1639 | G7M  | C2-N3-C4  | 4.61  | 120.24      | 112.30   |
| 48  | 5     | 400  | A2M  | C5-C6-N6  | 4.61  | 134.70      | 123.29   |
| 51  | 9     | 1445 | PSU  | N1-C2-N3  | 4.61  | 120.03      | 115.17   |
| 48  | 5     | 3718 | A2M  | C5-C4-N3  | -4.61 | 120.38      | 126.72   |
| 51  | 9     | 863  | PSU  | N1-C2-N3  | 4.60  | 120.02      | 115.17   |
| 51  | 9     | 166  | A2M  | C5-C4-N3  | -4.59 | 120.40      | 126.72   |
| 51  | 9     | 683  | OMG  | C2-N3-C4  | 4.59  | 120.20      | 112.30   |
| 50  | 8     | 75   | OMG  | C2-N3-C4  | 4.57  | 120.17      | 112.30   |
| 51  | 9     | 1177 | PSU  | C4-N3-C2  | -4.57 | 120.08      | 126.37   |
| 51  | 9     | 1850 | MA6  | N9-C8-N7  | -4.57 | 107.46      | 113.94   |
| 48  | 5     | 4228 | OMG  | C2-N3-C4  | 4.56  | 120.16      | 112.30   |
| 48  | 5     | 4623 | OMG  | C2-N3-C4  | 4.56  | 120.16      | 112.30   |
| 51  | 9     | 1692 | PSU  | N1-C2-N3  | 4.55  | 119.97      | 115.17   |
| 51  | 9     | 1850 | MA6  | N3-C4-N9  | 4.53  | 134.88      | 127.17   |
| 48  | 5     | 1625 | OMG  | N9-C4-N3  | 4.53  | 135.01      | 125.95   |
| 48  | 5     | 3715 | PSU  | C4-N3-C2  | -4.50 | 120.17      | 126.37   |
| 48  | 5     | 4306 | OMU  | N3-C2-N1  | 4.50  | 120.75      | 114.89   |
| 48  | 5     | 4370 | OMG  | C2-N3-C4  | 4.49  | 120.04      | 112.30   |
| 51  | 9     | 1328 | OMG  | C1'-N9-C4 | -4.48 | 113.26      | 126.49   |
| 51  | 9     | 1832 | 6MZ  | N9-C8-N7  | -4.46 | 107.60      | 113.94   |
| 48  | 5     | 3792 | OMG  | C2-N3-C4  | 4.46  | 119.98      | 112.30   |
| 48  | 5     | 4637 | OMG  | C2-N3-C4  | 4.46  | 119.97      | 112.30   |
| 48  | 5     | 3627 | OMG  | C1'-N9-C4 | -4.45 | 113.33      | 126.49   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 51  | 9     | 1383 | A2M  | C5-C4-N3  | -4.43 | 120.61      | 126.72   |
| 51  | 9     | 1445 | PSU  | C4-N3-C2  | -4.43 | 120.27      | 126.37   |
| 48  | 5     | 237  | B9B  | O6-C6-C5  | 4.40  | 122.55      | 116.73   |
| 48  | 5     | 1524 | A2M  | N9-C8-N7  | -4.39 | 107.71      | 113.94   |
| 48  | 5     | 4494 | OMG  | C2-N3-C4  | 4.38  | 119.85      | 112.30   |
| 48  | 5     | 4571 | A2M  | N9-C8-N7  | -4.37 | 107.74      | 113.94   |
| 48  | 5     | 2876 | OMG  | N9-C4-N3  | 4.35  | 134.66      | 125.95   |
| 51  | 9     | 1031 | A2M  | C5-C4-N3  | -4.34 | 120.74      | 126.72   |
| 51  | 9     | 1326 | OMU  | N3-C2-N1  | 4.34  | 120.54      | 114.89   |
| 48  | 5     | 4532 | PSU  | N1-C2-N3  | 4.33  | 119.74      | 115.17   |
| 48  | 5     | 4623 | OMG  | C1'-N9-C4 | -4.30 | 113.78      | 126.49   |
| 48  | 5     | 2876 | OMG  | C2-N3-C4  | 4.30  | 119.70      | 112.30   |
| 51  | 9     | 801  | PSU  | N1-C2-N3  | 4.29  | 119.70      | 115.17   |
| 48  | 5     | 2424 | OMG  | C2-N3-C4  | 4.29  | 119.69      | 112.30   |
| 48  | 5     | 4457 | PSU  | N1-C2-N3  | 4.29  | 119.69      | 115.17   |
| 48  | 5     | 4420 | PSU  | O2-C2-N1  | -4.25 | 118.40      | 122.79   |
| 51  | 9     | 1851 | MA6  | N3-C4-N9  | 4.24  | 134.37      | 127.17   |
| 51  | 9     | 815  | PSU  | O2-C2-N1  | -4.23 | 118.43      | 122.79   |
| 48  | 5     | 4499 | OMG  | C2-N3-C4  | 4.23  | 119.58      | 112.30   |
| 51  | 9     | 1678 | A2M  | N9-C8-N7  | -4.22 | 107.94      | 113.94   |
| 51  | 9     | 801  | PSU  | C4-N3-C2  | -4.21 | 120.57      | 126.37   |
| 48  | 5     | 3925 | OMU  | C5-C4-N3  | 4.20  | 120.68      | 114.80   |
| 48  | 5     | 237  | B9B  | N9-C8-N7  | -4.19 | 108.00      | 113.94   |
| 51  | 9     | 1328 | OMG  | C1'-N9-C8 | 4.18  | 138.61      | 126.73   |
| 51  | 9     | 1328 | OMG  | C2-N3-C4  | 4.18  | 119.50      | 112.30   |
| 48  | 5     | 1534 | A2M  | N9-C8-N7  | -4.17 | 108.02      | 113.94   |
| 48  | 5     | 3627 | OMG  | C2-N3-C4  | 4.17  | 119.48      | 112.30   |
| 48  | 5     | 4498 | OMU  | C5-C4-N3  | 4.17  | 120.64      | 114.80   |
| 51  | 9     | 644  | OMG  | C2-N3-C4  | 4.16  | 119.47      | 112.30   |
| 48  | 5     | 2787 | A2M  | N9-C8-N7  | -4.15 | 108.05      | 113.94   |
| 51  | 9     | 1490 | OMG  | C5-C4-N3  | -4.14 | 121.80      | 128.39   |
| 51  | 9     | 863  | PSU  | O2-C2-N1  | -4.14 | 118.52      | 122.79   |
| 48  | 5     | 1517 | 2MG  | C2-N1-C6  | -4.14 | 119.55      | 124.55   |
| 51  | 9     | 116  | OMU  | N3-C2-N1  | 4.13  | 120.27      | 114.89   |
| 51  | 9     | 1490 | OMG  | C2-N3-C4  | 4.11  | 119.38      | 112.30   |
| 48  | 5     | 1316 | OMG  | C1'-N9-C4 | -4.10 | 114.38      | 126.49   |
| 48  | 5     | 237  | B9B  | C4-C5-C6  | 4.10  | 119.24      | 115.22   |
| 48  | 5     | 1871 | A2M  | C5-C4-N3  | -4.09 | 121.08      | 126.72   |
| 51  | 9     | 436  | OMG  | C2-N3-C4  | 4.09  | 119.35      | 112.30   |
| 51  | 9     | 436  | OMG  | N9-C4-N3  | 4.09  | 134.13      | 125.95   |
| 48  | 5     | 3853 | PSU  | O2-C2-N1  | -4.08 | 118.58      | 122.79   |
| 48  | 5     | 4620 | OMU  | C5-C4-N3  | 4.08  | 120.51      | 114.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 50  | 8     | 75   | OMG  | C1'-N9-C4  | -4.07 | 114.47      | 126.49   |
| 48  | 5     | 4220 | 6MZ  | N9-C8-N7   | -4.05 | 108.20      | 113.94   |
| 48  | 5     | 4227 | OMU  | C5-C4-N3   | 4.04  | 120.46      | 114.80   |
| 48  | 5     | 3627 | OMG  | C1'-N9-C8  | 4.04  | 138.20      | 126.73   |
| 48  | 5     | 3718 | A2M  | N9-C8-N7   | -4.03 | 108.22      | 113.94   |
| 48  | 5     | 3715 | PSU  | O2-C2-N1   | -4.03 | 118.64      | 122.79   |
| 48  | 5     | 1522 | OMG  | C1'-N9-C4  | -4.02 | 114.62      | 126.49   |
| 48  | 5     | 3818 | UY1  | C6-C5-C4   | 4.01  | 120.88      | 118.17   |
| 48  | 5     | 4370 | OMG  | C1'-N9-C4  | -4.01 | 114.65      | 126.49   |
| 48  | 5     | 4228 | OMG  | C1'-N9-C4  | -4.01 | 114.65      | 126.49   |
| 48  | 5     | 3867 | A2M  | N9-C8-N7   | -4.00 | 108.26      | 113.94   |
| 51  | 9     | 686  | PSU  | O2-C2-N1   | -4.00 | 118.66      | 122.79   |
| 51  | 9     | 1442 | OMU  | N3-C2-N1   | 4.00  | 120.09      | 114.89   |
| 48  | 5     | 400  | A2M  | N3-C4-N9   | 3.98  | 133.94      | 127.17   |
| 48  | 5     | 4623 | OMG  | C1'-N9-C8  | 3.98  | 138.05      | 126.73   |
| 48  | 5     | 1871 | A2M  | N9-C8-N7   | -3.98 | 108.29      | 113.94   |
| 48  | 5     | 3760 | A2M  | N9-C8-N7   | -3.97 | 108.30      | 113.94   |
| 48  | 5     | 1517 | 2MG  | C5-C4-N3   | -3.96 | 122.09      | 128.39   |
| 51  | 9     | 512  | A2M  | N9-C8-N7   | -3.96 | 108.32      | 113.94   |
| 48  | 5     | 4498 | OMU  | N3-C2-N1   | 3.95  | 120.04      | 114.89   |
| 48  | 5     | 2815 | A2M  | N9-C8-N7   | -3.95 | 108.33      | 113.94   |
| 51  | 9     | 509  | OMG  | C2-N3-C4   | 3.95  | 119.11      | 112.30   |
| 48  | 5     | 398  | A2M  | N9-C8-N7   | -3.94 | 108.35      | 113.94   |
| 48  | 5     | 3785 | A2M  | O4'-C1'-N9 | 3.94  | 115.65      | 108.09   |
| 51  | 9     | 1248 | B8N  | N3-C2-N1   | 3.93  | 121.52      | 116.72   |
| 51  | 9     | 428  | OMU  | C5-C4-N3   | 3.93  | 120.30      | 114.80   |
| 48  | 5     | 2837 | OMU  | C5-C4-N3   | 3.92  | 120.30      | 114.80   |
| 48  | 5     | 4523 | A2M  | N9-C8-N7   | -3.92 | 108.37      | 113.94   |
| 51  | 9     | 1031 | A2M  | N9-C8-N7   | -3.91 | 108.39      | 113.94   |
| 48  | 5     | 3899 | OMG  | C1'-N9-C4  | -3.91 | 114.94      | 126.49   |
| 51  | 9     | 572  | PSU  | O2-C2-N1   | -3.90 | 118.76      | 122.79   |
| 48  | 5     | 2424 | OMG  | C1'-N9-C4  | -3.90 | 114.98      | 126.49   |
| 48  | 5     | 2837 | OMU  | N3-C2-N1   | 3.89  | 119.95      | 114.89   |
| 51  | 9     | 99   | A2M  | N9-C8-N7   | -3.89 | 108.42      | 113.94   |
| 48  | 5     | 3830 | A2M  | N9-C8-N7   | -3.89 | 108.42      | 113.94   |
| 51  | 9     | 683  | OMG  | N9-C4-N3   | 3.89  | 133.73      | 125.95   |
| 51  | 9     | 668  | A2M  | N9-C8-N7   | -3.87 | 108.45      | 113.94   |
| 48  | 5     | 4637 | OMG  | N9-C4-N3   | 3.87  | 133.69      | 125.95   |
| 51  | 9     | 121  | OMU  | C5-C4-N3   | 3.86  | 120.21      | 114.80   |
| 48  | 5     | 373  | OMG  | N9-C4-N3   | 3.86  | 133.67      | 125.95   |
| 50  | 8     | 75   | OMG  | C1'-N9-C8  | 3.86  | 137.69      | 126.73   |
| 51  | 9     | 1639 | G7M  | C5-C4-N3   | -3.85 | 120.86      | 128.15   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 51  | 9     | 1643 | PSU  | O2-C2-N1  | -3.85 | 118.82      | 122.79   |
| 48  | 5     | 237  | B9B  | N3-C2-N1  | -3.85 | 119.59      | 125.48   |
| 48  | 5     | 2787 | A2M  | N3-C4-N9  | 3.84  | 133.70      | 127.17   |
| 48  | 5     | 4499 | OMG  | N9-C4-N3  | 3.83  | 133.61      | 125.95   |
| 48  | 5     | 4620 | OMU  | N3-C2-N1  | 3.82  | 119.87      | 114.89   |
| 51  | 9     | 468  | A2M  | N9-C8-N7  | -3.81 | 108.53      | 113.94   |
| 51  | 9     | 166  | A2M  | N9-C8-N7  | -3.81 | 108.53      | 113.94   |
| 48  | 5     | 3925 | OMU  | N3-C2-N1  | 3.81  | 119.85      | 114.89   |
| 51  | 9     | 1851 | MA6  | C2-N3-C4  | 3.80  | 121.12      | 111.83   |
| 51  | 9     | 509  | OMG  | N9-C4-N3  | 3.80  | 133.55      | 125.95   |
| 48  | 5     | 4227 | OMU  | N3-C2-N1  | 3.80  | 119.84      | 114.89   |
| 48  | 5     | 4392 | OMG  | C1'-N9-C4 | -3.79 | 115.28      | 126.49   |
| 51  | 9     | 1383 | A2M  | N9-C8-N7  | -3.78 | 108.57      | 113.94   |
| 48  | 5     | 4306 | OMU  | C5-C4-N3  | 3.77  | 120.07      | 114.80   |
| 51  | 9     | 1639 | G7M  | C5-C6-N1  | 3.76  | 119.62      | 111.84   |
| 48  | 5     | 1517 | 2MG  | N9-C8-N7  | -3.76 | 106.43      | 113.40   |
| 48  | 5     | 4220 | 6MZ  | C4-C5-C6  | 3.74  | 119.89      | 116.78   |
| 51  | 9     | 609  | PSU  | O2-C2-N1  | -3.74 | 118.93      | 122.79   |
| 48  | 5     | 4500 | PSU  | O2-C2-N1  | -3.74 | 118.94      | 122.79   |
| 48  | 5     | 4228 | OMG  | C1'-N9-C8 | 3.74  | 137.34      | 126.73   |
| 51  | 9     | 159  | A2M  | N9-C8-N7  | -3.73 | 108.65      | 113.94   |
| 48  | 5     | 1522 | OMG  | C1'-N9-C8 | 3.73  | 137.32      | 126.73   |
| 48  | 5     | 4392 | OMG  | C1'-N9-C8 | 3.72  | 137.29      | 126.73   |
| 51  | 9     | 172  | OMU  | C5-C4-N3  | 3.71  | 120.00      | 114.80   |
| 48  | 5     | 237  | B9B  | C2-N1-C6  | 3.71  | 121.12      | 115.96   |
| 48  | 5     | 1326 | A2M  | N9-C8-N7  | -3.70 | 108.68      | 113.94   |
| 48  | 5     | 4196 | OMG  | N9-C4-N3  | 3.70  | 133.35      | 125.95   |
| 48  | 5     | 3715 | PSU  | C6-C5-C4  | 3.70  | 120.67      | 118.17   |
| 48  | 5     | 1316 | OMG  | C1'-N9-C8 | 3.69  | 137.20      | 126.73   |
| 48  | 5     | 2424 | OMG  | C1'-N9-C8 | 3.69  | 137.20      | 126.73   |
| 48  | 5     | 237  | B9B  | N2-C2-N3  | 3.69  | 122.75      | 117.22   |
| 48  | 5     | 3785 | A2M  | N9-C8-N7  | -3.68 | 108.71      | 113.94   |
| 51  | 9     | 172  | OMU  | N3-C2-N1  | 3.68  | 119.68      | 114.89   |
| 48  | 5     | 4618 | OMG  | C1'-N9-C4 | -3.67 | 115.64      | 126.49   |
| 48  | 5     | 2363 | A2M  | N9-C8-N7  | -3.67 | 108.73      | 113.94   |
| 51  | 9     | 1326 | OMU  | C5-C4-N3  | 3.64  | 119.90      | 114.80   |
| 48  | 5     | 3899 | OMG  | C1'-N9-C8 | 3.63  | 137.04      | 126.73   |
| 51  | 9     | 1832 | 6MZ  | C2-N3-C4  | 3.62  | 120.68      | 111.83   |
| 48  | 5     | 4521 | PSU  | C6-C5-C4  | 3.62  | 120.61      | 118.17   |
| 48  | 5     | 4499 | OMG  | C1'-N9-C4 | -3.61 | 115.83      | 126.49   |
| 48  | 5     | 2787 | A2M  | C2-N3-C4  | 3.61  | 120.64      | 111.83   |
| 48  | 5     | 4637 | OMG  | C1'-N9-C4 | -3.60 | 115.84      | 126.49   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 48  | 5     | 4494 | OMG  | C1'-N9-C4  | -3.60 | 115.85      | 126.49   |
| 51  | 9     | 484  | A2M  | C2-N3-C4   | 3.58  | 120.59      | 111.83   |
| 48  | 5     | 3825 | A2M  | N3-C4-N9   | 3.56  | 133.22      | 127.17   |
| 51  | 9     | 512  | A2M  | C2-N3-C4   | 3.56  | 120.52      | 111.83   |
| 51  | 9     | 668  | A2M  | C2-N3-C4   | 3.54  | 120.47      | 111.83   |
| 48  | 5     | 3792 | OMG  | C1'-N9-C4  | -3.54 | 116.04      | 126.49   |
| 48  | 5     | 3782 | 5MC  | C5-C6-N1   | -3.53 | 119.47      | 123.31   |
| 48  | 5     | 4530 | UR3  | C5-C4-N3   | 3.53  | 119.69      | 115.04   |
| 48  | 5     | 1862 | PSU  | O2-C2-N1   | -3.53 | 119.14      | 122.79   |
| 48  | 5     | 4628 | PSU  | O2-C2-N1   | -3.53 | 119.15      | 122.79   |
| 48  | 5     | 3825 | A2M  | N9-C8-N7   | -3.52 | 108.94      | 113.94   |
| 51  | 9     | 121  | OMU  | N3-C2-N1   | 3.52  | 119.48      | 114.89   |
| 48  | 5     | 3724 | A2M  | N3-C4-N9   | 3.51  | 133.15      | 127.17   |
| 51  | 9     | 428  | OMU  | O4-C4-C5   | -3.51 | 119.11      | 125.16   |
| 48  | 5     | 3867 | A2M  | C2-N3-C4   | 3.51  | 120.40      | 111.83   |
| 48  | 5     | 2364 | OMG  | N9-C4-N3   | 3.51  | 132.96      | 125.95   |
| 48  | 5     | 400  | A2M  | N9-C8-N7   | -3.50 | 108.97      | 113.94   |
| 51  | 9     | 509  | OMG  | C1'-N9-C4  | -3.50 | 116.14      | 126.49   |
| 48  | 5     | 398  | A2M  | C2-N3-C4   | 3.50  | 120.38      | 111.83   |
| 48  | 5     | 3818 | UY1  | C6-N1-C2   | -3.50 | 119.44      | 122.69   |
| 51  | 9     | 436  | OMG  | C1'-N9-C4  | -3.49 | 116.17      | 126.49   |
| 48  | 5     | 4623 | OMG  | C2-N1-C6   | -3.48 | 118.79      | 125.11   |
| 51  | 9     | 484  | A2M  | N9-C8-N7   | -3.47 | 109.01      | 113.94   |
| 48  | 5     | 3899 | OMG  | N9-C4-N3   | 3.47  | 132.90      | 125.95   |
| 51  | 9     | 1850 | MA6  | C4-N9-C8   | 3.47  | 109.38      | 105.74   |
| 48  | 5     | 2815 | A2M  | C2-N3-C4   | 3.47  | 120.30      | 111.83   |
| 51  | 9     | 218  | PSU  | C6-C5-C4   | 3.46  | 120.51      | 118.17   |
| 48  | 5     | 4392 | OMG  | C2-N1-C6   | -3.46 | 118.83      | 125.11   |
| 48  | 5     | 4370 | OMG  | C1'-N9-C8  | 3.46  | 136.57      | 126.73   |
| 48  | 5     | 4571 | A2M  | C2-N3-C4   | 3.46  | 120.27      | 111.83   |
| 48  | 5     | 3830 | A2M  | C2'-C1'-N9 | -3.45 | 108.07      | 113.75   |
| 48  | 5     | 3792 | OMG  | N9-C4-N3   | 3.45  | 132.86      | 125.95   |
| 48  | 5     | 1677 | PSU  | O2-C2-N1   | -3.45 | 119.23      | 122.79   |
| 48  | 5     | 1625 | OMG  | C2-N1-C6   | -3.45 | 118.85      | 125.11   |
| 48  | 5     | 2364 | OMG  | C1'-N9-C4  | -3.45 | 116.30      | 126.49   |
| 48  | 5     | 4447 | 5MC  | C5-C6-N1   | -3.45 | 119.57      | 123.31   |
| 48  | 5     | 1625 | OMG  | O6-C6-C5   | -3.44 | 117.45      | 126.53   |
| 48  | 5     | 373  | OMG  | C1'-N9-C4  | -3.44 | 116.32      | 126.49   |
| 51  | 9     | 644  | OMG  | C1'-N9-C4  | -3.44 | 116.33      | 126.49   |
| 48  | 5     | 4494 | OMG  | C1'-N9-C8  | 3.44  | 136.49      | 126.73   |
| 51  | 9     | 116  | OMU  | C5-C4-N3   | 3.43  | 119.61      | 114.80   |
| 48  | 5     | 3762 | PSU  | O2-C2-N1   | -3.42 | 119.26      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 48  | 5     | 398  | A2M  | N3-C4-N9   | 3.42  | 132.99      | 127.17   |
| 48  | 5     | 3724 | A2M  | N9-C8-N7   | -3.42 | 109.09      | 113.94   |
| 48  | 5     | 1322 | 1MA  | N9-C8-N7   | -3.42 | 107.06      | 113.40   |
| 51  | 9     | 822  | PSU  | C6-C5-C4   | 3.42  | 120.48      | 118.17   |
| 48  | 5     | 3785 | A2M  | C2-N3-C4   | 3.41  | 120.17      | 111.83   |
| 48  | 5     | 3920 | PSU  | O2-C2-N1   | -3.41 | 119.27      | 122.79   |
| 48  | 5     | 4523 | A2M  | N3-C4-N9   | 3.41  | 132.97      | 127.17   |
| 48  | 5     | 4521 | PSU  | O2-C2-N1   | -3.41 | 119.27      | 122.79   |
| 51  | 9     | 1678 | A2M  | C2-N3-C4   | 3.40  | 120.14      | 111.83   |
| 51  | 9     | 1174 | PSU  | O2-C2-N1   | -3.38 | 119.30      | 122.79   |
| 48  | 5     | 3760 | A2M  | C2-N3-C4   | 3.38  | 120.09      | 111.83   |
| 51  | 9     | 166  | A2M  | C2-N3-C4   | 3.38  | 120.09      | 111.83   |
| 48  | 5     | 2424 | OMG  | C2-N1-C6   | -3.37 | 118.99      | 125.11   |
| 48  | 5     | 4392 | OMG  | N9-C4-N3   | 3.37  | 132.70      | 125.95   |
| 51  | 9     | 644  | OMG  | C1'-N9-C8  | 3.37  | 136.29      | 126.73   |
| 48  | 5     | 2876 | OMG  | C2-N1-C6   | -3.36 | 119.01      | 125.11   |
| 51  | 9     | 99   | A2M  | C2-N3-C4   | 3.36  | 120.03      | 111.83   |
| 48  | 5     | 3724 | A2M  | C2-N3-C4   | 3.35  | 120.02      | 111.83   |
| 48  | 5     | 2363 | A2M  | C2-N3-C4   | 3.35  | 120.01      | 111.83   |
| 51  | 9     | 683  | OMG  | C2-N1-C6   | -3.34 | 119.06      | 125.11   |
| 48  | 5     | 1517 | 2MG  | N2-C2-N3   | -3.33 | 116.26      | 120.51   |
| 48  | 5     | 3830 | A2M  | N3-C4-N9   | 3.33  | 132.82      | 127.17   |
| 51  | 9     | 1639 | G7M  | O6-C6-C5   | -3.32 | 120.59      | 128.01   |
| 48  | 5     | 2364 | OMG  | C2-N1-C6   | -3.32 | 119.08      | 125.11   |
| 51  | 9     | 468  | A2M  | C2-N3-C4   | 3.32  | 119.95      | 111.83   |
| 48  | 5     | 4370 | OMG  | N9-C8-N7   | -3.32 | 107.24      | 113.40   |
| 48  | 5     | 1322 | 1MA  | C2-N3-C4   | 3.32  | 119.03      | 112.53   |
| 51  | 9     | 436  | OMG  | C2-N1-C6   | -3.31 | 119.11      | 125.11   |
| 48  | 5     | 3718 | A2M  | C2'-C1'-N9 | -3.31 | 108.31      | 113.75   |
| 48  | 5     | 1524 | A2M  | C2-N3-C4   | 3.31  | 119.91      | 111.83   |
| 51  | 9     | 683  | OMG  | C1'-N9-C4  | -3.30 | 116.74      | 126.49   |
| 48  | 5     | 4370 | OMG  | N9-C4-N3   | 3.30  | 132.55      | 125.95   |
| 48  | 5     | 3830 | A2M  | C2-N3-C4   | 3.29  | 119.88      | 111.83   |
| 48  | 5     | 4220 | 6MZ  | C2-N3-C4   | 3.29  | 119.86      | 111.83   |
| 51  | 9     | 509  | OMG  | C1'-N9-C8  | 3.28  | 136.05      | 126.73   |
| 48  | 5     | 1744 | PSU  | O2-C2-N1   | -3.28 | 119.41      | 122.79   |
| 48  | 5     | 4523 | A2M  | C2-N3-C4   | 3.27  | 119.81      | 111.83   |
| 48  | 5     | 4618 | OMG  | C1'-N9-C8  | 3.26  | 136.00      | 126.73   |
| 48  | 5     | 1534 | A2M  | C2-N3-C4   | 3.26  | 119.79      | 111.83   |
| 51  | 9     | 822  | PSU  | O2-C2-N1   | -3.25 | 119.43      | 122.79   |
| 48  | 5     | 1782 | PSU  | O2-C2-N1   | -3.25 | 119.43      | 122.79   |
| 51  | 9     | 1442 | OMU  | C5-C4-N3   | 3.25  | 119.35      | 114.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | 5     | 1326 | A2M  | C2-N3-C4    | 3.25  | 119.76      | 111.83   |
| 48  | 5     | 1792 | PSU  | O2-C2-N1    | -3.24 | 119.45      | 122.79   |
| 51  | 9     | 1851 | MA6  | C5-N7-C8    | 3.24  | 108.54      | 103.45   |
| 51  | 9     | 119  | PSU  | O2-C2-N1    | -3.24 | 119.45      | 122.79   |
| 48  | 5     | 3825 | A2M  | C2-N3-C4    | 3.24  | 119.74      | 111.83   |
| 48  | 5     | 2787 | A2M  | C5-N7-C8    | 3.24  | 108.54      | 103.45   |
| 48  | 5     | 4499 | OMG  | C2-N1-C6    | -3.24 | 119.24      | 125.11   |
| 51  | 9     | 1850 | MA6  | C2-N1-C6    | 3.23  | 119.71      | 111.83   |
| 48  | 5     | 3627 | OMG  | N9-C8-N7    | -3.23 | 107.42      | 113.40   |
| 48  | 5     | 4353 | PSU  | C6-C5-C4    | 3.22  | 120.34      | 118.17   |
| 50  | 8     | 75   | OMG  | C2-N1-C6    | -3.21 | 119.28      | 125.11   |
| 48  | 5     | 3867 | A2M  | N3-C4-N9    | 3.21  | 132.62      | 127.17   |
| 51  | 9     | 1442 | OMU  | O4-C4-C5    | -3.21 | 119.63      | 125.16   |
| 51  | 9     | 34   | PSU  | C6-N1-C2    | -3.21 | 119.72      | 122.69   |
| 51  | 9     | 1031 | A2M  | C2-N3-C4    | 3.20  | 119.66      | 111.83   |
| 51  | 9     | 428  | OMU  | N3-C2-N1    | 3.20  | 119.06      | 114.89   |
| 48  | 5     | 4618 | OMG  | C2-N1-C6    | -3.19 | 119.32      | 125.11   |
| 48  | 5     | 237  | B9B  | C5-C6-N1    | -3.19 | 119.22      | 123.49   |
| 48  | 5     | 4637 | OMG  | N9-C8-N7    | -3.19 | 107.48      | 113.40   |
| 51  | 9     | 1832 | 6MZ  | C5-N7-C8    | 3.19  | 108.46      | 103.45   |
| 51  | 9     | 683  | OMG  | CM2-O2'-C2' | 3.18  | 122.65      | 114.47   |
| 48  | 5     | 4623 | OMG  | N9-C4-N3    | 3.18  | 132.32      | 125.95   |
| 51  | 9     | 1383 | A2M  | C2-N3-C4    | 3.18  | 119.61      | 111.83   |
| 48  | 5     | 2363 | A2M  | N3-C4-N9    | 3.18  | 132.58      | 127.17   |
| 48  | 5     | 4637 | OMG  | C2-N1-C6    | -3.18 | 119.35      | 125.11   |
| 51  | 9     | 27   | A2M  | C2-N3-C4    | 3.17  | 119.57      | 111.83   |
| 51  | 9     | 468  | A2M  | N3-C4-N9    | 3.17  | 132.55      | 127.17   |
| 51  | 9     | 1490 | OMG  | N9-C8-N7    | -3.16 | 107.53      | 113.40   |
| 48  | 5     | 3760 | A2M  | N3-C4-N9    | 3.16  | 132.54      | 127.17   |
| 51  | 9     | 1851 | MA6  | C2-N1-C6    | 3.16  | 119.55      | 111.83   |
| 48  | 5     | 4370 | OMG  | C2-N1-C6    | -3.16 | 119.38      | 125.11   |
| 51  | 9     | 1850 | MA6  | C2-N3-C4    | 3.16  | 119.55      | 111.83   |
| 48  | 5     | 3792 | OMG  | C1'-N9-C8   | 3.15  | 135.69      | 126.73   |
| 48  | 5     | 4423 | PSU  | O2-C2-N1    | -3.15 | 119.54      | 122.79   |
| 48  | 5     | 3718 | A2M  | C2-N3-C4    | 3.14  | 119.49      | 111.83   |
| 51  | 9     | 1678 | A2M  | C5-N7-C8    | 3.13  | 108.37      | 103.45   |
| 48  | 5     | 4623 | OMG  | C5-C6-N1    | 3.13  | 121.22      | 113.25   |
| 48  | 5     | 4228 | OMG  | N9-C4-N3    | 3.13  | 132.21      | 125.95   |
| 48  | 5     | 1524 | A2M  | C5-N7-C8    | 3.12  | 108.36      | 103.45   |
| 51  | 9     | 159  | A2M  | C2-N3-C4    | 3.12  | 119.44      | 111.83   |
| 48  | 5     | 3760 | A2M  | C5-N7-C8    | 3.12  | 108.35      | 103.45   |
| 48  | 5     | 4618 | OMG  | N9-C8-N7    | -3.12 | 107.62      | 113.40   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 48  | 5     | 4637 | OMG  | C1'-N9-C8 | 3.12  | 135.58      | 126.73   |
| 48  | 5     | 237  | B9B  | N3-C4-N9  | 3.11  | 130.94      | 126.99   |
| 51  | 9     | 27   | A2M  | N9-C8-N7  | -3.11 | 109.52      | 113.94   |
| 48  | 5     | 400  | A2M  | C6-C5-C4  | 3.11  | 121.43      | 117.18   |
| 48  | 5     | 2364 | OMG  | N9-C8-N7  | -3.11 | 107.63      | 113.40   |
| 48  | 5     | 4196 | OMG  | C2-N1-C6  | -3.11 | 119.47      | 125.11   |
| 48  | 5     | 373  | OMG  | C2-N1-C6  | -3.11 | 119.47      | 125.11   |
| 48  | 5     | 373  | OMG  | C1'-N9-C8 | 3.10  | 135.53      | 126.73   |
| 51  | 9     | 644  | OMG  | N9-C4-N3  | 3.09  | 132.14      | 125.95   |
| 51  | 9     | 683  | OMG  | N9-C8-N7  | -3.09 | 107.67      | 113.40   |
| 51  | 9     | 27   | A2M  | N3-C4-N9  | 3.09  | 132.42      | 127.17   |
| 48  | 5     | 1524 | A2M  | N3-C4-N9  | 3.09  | 132.42      | 127.17   |
| 48  | 5     | 1326 | A2M  | N3-C4-N9  | 3.09  | 132.41      | 127.17   |
| 48  | 5     | 400  | A2M  | C2-N3-C4  | 3.08  | 119.36      | 111.83   |
| 51  | 9     | 512  | A2M  | C5-N7-C8  | 3.08  | 108.29      | 103.45   |
| 51  | 9     | 1328 | OMG  | C2-N1-C6  | -3.08 | 119.53      | 125.11   |
| 48  | 5     | 1316 | OMG  | N9-C8-N7  | -3.07 | 107.71      | 113.40   |
| 51  | 9     | 509  | OMG  | C2-N1-C6  | -3.06 | 119.55      | 125.11   |
| 51  | 9     | 686  | PSU  | C6-C5-C4  | 3.06  | 120.24      | 118.17   |
| 48  | 5     | 4494 | OMG  | N9-C4-N3  | 3.05  | 132.06      | 125.95   |
| 48  | 5     | 1522 | OMG  | C2-N1-C6  | -3.05 | 119.58      | 125.11   |
| 48  | 5     | 4442 | PSU  | O2-C2-N1  | -3.05 | 119.65      | 122.79   |
| 48  | 5     | 373  | OMG  | N9-C8-N7  | -3.04 | 107.77      | 113.40   |
| 48  | 5     | 2364 | OMG  | C1'-N9-C8 | 3.03  | 135.35      | 126.73   |
| 48  | 5     | 3851 | PSU  | O2-C2-N1  | -3.03 | 119.66      | 122.79   |
| 48  | 5     | 4618 | OMG  | N9-C4-N3  | 3.03  | 132.00      | 125.95   |
| 48  | 5     | 4494 | OMG  | C2-N1-C6  | -3.02 | 119.63      | 125.11   |
| 51  | 9     | 218  | PSU  | O2-C2-N1  | -3.02 | 119.67      | 122.79   |
| 48  | 5     | 3785 | A2M  | N3-C4-N9  | 3.02  | 132.30      | 127.17   |
| 48  | 5     | 1534 | A2M  | C5-N7-C8  | 3.01  | 108.19      | 103.45   |
| 48  | 5     | 4500 | PSU  | C6-C5-C4  | 3.01  | 120.21      | 118.17   |
| 51  | 9     | 1328 | OMG  | N9-C4-N3  | 3.00  | 131.96      | 125.95   |
| 48  | 5     | 1871 | A2M  | C2-N3-C4  | 3.00  | 119.17      | 111.83   |
| 48  | 5     | 4499 | OMG  | O6-C6-C5  | -3.00 | 118.61      | 126.53   |
| 48  | 5     | 3899 | OMG  | N9-C8-N7  | -3.00 | 107.84      | 113.40   |
| 48  | 5     | 4499 | OMG  | N9-C8-N7  | -2.99 | 107.85      | 113.40   |
| 48  | 5     | 1625 | OMG  | C1'-N9-C4 | -2.99 | 117.66      | 126.49   |
| 48  | 5     | 1625 | OMG  | N9-C8-N7  | -2.98 | 107.88      | 113.40   |
| 48  | 5     | 1316 | OMG  | C2-N1-C6  | -2.97 | 119.72      | 125.11   |
| 48  | 5     | 4220 | 6MZ  | C5-N7-C8  | 2.97  | 108.12      | 103.45   |
| 48  | 5     | 3851 | PSU  | C6-N1-C2  | -2.97 | 119.93      | 122.69   |
| 51  | 9     | 1248 | B8N  | O4-C4-N3  | -2.96 | 115.18      | 119.99   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 51  | 9     | 644  | OMG  | C2-N1-C6   | -2.96 | 119.75      | 125.11   |
| 51  | 9     | 1326 | OMU  | O2-C2-N1   | -2.96 | 118.95      | 122.80   |
| 51  | 9     | 1445 | PSU  | C6-N1-C2   | -2.95 | 119.95      | 122.69   |
| 51  | 9     | 668  | A2M  | C5-N7-C8   | 2.95  | 108.09      | 103.45   |
| 51  | 9     | 436  | OMG  | C1'-N9-C8  | 2.95  | 135.11      | 126.73   |
| 51  | 9     | 1851 | MA6  | C4-N9-C8   | 2.95  | 108.83      | 105.74   |
| 48  | 5     | 237  | B9B  | C5-N7-C8   | 2.95  | 108.08      | 103.45   |
| 48  | 5     | 4499 | OMG  | C1'-N9-C8  | 2.95  | 135.10      | 126.73   |
| 48  | 5     | 3920 | PSU  | C6-C5-C4   | 2.94  | 120.16      | 118.17   |
| 48  | 5     | 4228 | OMG  | N9-C8-N7   | -2.94 | 107.95      | 113.40   |
| 48  | 5     | 3627 | OMG  | C2-N1-C6   | -2.94 | 119.78      | 125.11   |
| 48  | 5     | 1860 | PSU  | O2-C2-N1   | -2.93 | 119.77      | 122.79   |
| 51  | 9     | 668  | A2M  | O4'-C1'-N9 | -2.92 | 102.47      | 108.09   |
| 51  | 9     | 436  | OMG  | O6-C6-C5   | -2.92 | 118.82      | 126.53   |
| 48  | 5     | 2837 | OMU  | O2-C2-N1   | -2.92 | 118.99      | 122.80   |
| 48  | 5     | 2424 | OMG  | N9-C4-N3   | 2.92  | 131.79      | 125.95   |
| 48  | 5     | 4523 | A2M  | C5-N7-C8   | 2.92  | 108.04      | 103.45   |
| 51  | 9     | 1850 | MA6  | C5-N7-C8   | 2.92  | 108.04      | 103.45   |
| 51  | 9     | 814  | PSU  | O2-C2-N1   | -2.92 | 119.78      | 122.79   |
| 48  | 5     | 4196 | OMG  | C1'-N9-C4  | -2.91 | 117.89      | 126.49   |
| 51  | 9     | 99   | A2M  | N3-C4-N9   | 2.90  | 132.10      | 127.17   |
| 48  | 5     | 4498 | OMU  | O4-C4-C5   | -2.90 | 120.16      | 125.16   |
| 48  | 5     | 4196 | OMG  | C1'-N9-C8  | 2.90  | 134.97      | 126.73   |
| 51  | 9     | 1328 | OMG  | N9-C8-N7   | -2.90 | 108.03      | 113.40   |
| 51  | 9     | 1045 | PSU  | O2-C2-N1   | -2.90 | 119.80      | 122.79   |
| 48  | 5     | 1316 | OMG  | N9-C4-N3   | 2.89  | 131.73      | 125.95   |
| 48  | 5     | 398  | A2M  | C5-N7-C8   | 2.88  | 107.98      | 103.45   |
| 51  | 9     | 116  | OMU  | O2-C2-N1   | -2.88 | 119.05      | 122.80   |
| 48  | 5     | 1625 | OMG  | C5-C6-N1   | 2.88  | 120.57      | 113.25   |
| 51  | 9     | 436  | OMG  | N9-C8-N7   | -2.87 | 108.07      | 113.40   |
| 48  | 5     | 4571 | A2M  | C5-N7-C8   | 2.87  | 107.96      | 103.45   |
| 48  | 5     | 4623 | OMG  | N9-C8-N7   | -2.87 | 108.08      | 113.40   |
| 51  | 9     | 1238 | PSU  | C6-C5-C4   | 2.87  | 120.11      | 118.17   |
| 48  | 5     | 1522 | OMG  | N9-C8-N7   | -2.86 | 108.09      | 113.40   |
| 48  | 5     | 1522 | OMG  | N9-C4-N3   | 2.86  | 131.67      | 125.95   |
| 48  | 5     | 4499 | OMG  | C5-C6-N1   | 2.86  | 120.52      | 113.25   |
| 51  | 9     | 512  | A2M  | C4-C5-N7   | -2.86 | 107.32      | 110.58   |
| 48  | 5     | 2815 | A2M  | C5-N7-C8   | 2.85  | 107.94      | 103.45   |
| 51  | 9     | 105  | PSU  | C6-N1-C2   | -2.85 | 120.05      | 122.69   |
| 48  | 5     | 3792 | OMG  | O6-C6-C5   | -2.85 | 119.01      | 126.53   |
| 48  | 5     | 2424 | OMG  | N9-C8-N7   | -2.85 | 108.12      | 113.40   |
| 51  | 9     | 668  | A2M  | N3-C4-N9   | 2.85  | 132.01      | 127.17   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 51  | 9     | 512  | A2M  | C5-C4-N9   | 2.84  | 108.91      | 105.81   |
| 48  | 5     | 4637 | OMG  | O6-C6-C5   | -2.84 | 119.03      | 126.53   |
| 48  | 5     | 1326 | A2M  | C5-N7-C8   | 2.84  | 107.91      | 103.45   |
| 48  | 5     | 2815 | A2M  | N3-C4-N9   | 2.84  | 131.99      | 127.17   |
| 51  | 9     | 1842 | 4AC  | O2-C2-N3   | -2.83 | 117.86      | 122.33   |
| 51  | 9     | 1004 | PSU  | O2-C2-N1   | -2.83 | 119.87      | 122.79   |
| 48  | 5     | 3825 | A2M  | C6-C5-C4   | 2.83  | 121.04      | 117.18   |
| 48  | 5     | 4228 | OMG  | C2-N1-C6   | -2.82 | 119.99      | 125.11   |
| 50  | 8     | 75   | OMG  | N9-C4-N3   | 2.82  | 131.59      | 125.95   |
| 48  | 5     | 1534 | A2M  | N3-C4-N9   | 2.82  | 131.96      | 127.17   |
| 51  | 9     | 1244 | PSU  | O2-C2-N1   | -2.81 | 119.89      | 122.79   |
| 48  | 5     | 4498 | OMU  | O2-C2-N1   | -2.81 | 119.14      | 122.80   |
| 51  | 9     | 436  | OMG  | C5-C6-N1   | 2.81  | 120.41      | 113.25   |
| 51  | 9     | 683  | OMG  | C1'-N9-C8  | 2.81  | 134.71      | 126.73   |
| 51  | 9     | 1639 | G7M  | C2-N1-C6   | -2.80 | 120.03      | 125.11   |
| 51  | 9     | 1045 | PSU  | C6-C5-C4   | 2.80  | 120.06      | 118.17   |
| 50  | 8     | 75   | OMG  | N9-C8-N7   | -2.80 | 108.21      | 113.40   |
| 51  | 9     | 1678 | A2M  | N3-C4-N9   | 2.80  | 131.93      | 127.17   |
| 48  | 5     | 4196 | OMG  | C5-C6-N1   | 2.80  | 120.37      | 113.25   |
| 51  | 9     | 683  | OMG  | C5-C6-N1   | 2.79  | 120.36      | 113.25   |
| 48  | 5     | 1316 | OMG  | C5-C6-N1   | 2.79  | 120.36      | 113.25   |
| 48  | 5     | 2837 | OMU  | C2'-C1'-N1 | -2.79 | 108.94      | 114.24   |
| 48  | 5     | 4579 | PSU  | O2-C2-N1   | -2.79 | 119.91      | 122.79   |
| 48  | 5     | 4623 | OMG  | O6-C6-C5   | -2.79 | 119.17      | 126.53   |
| 48  | 5     | 2424 | OMG  | O6-C6-C5   | -2.79 | 119.17      | 126.53   |
| 51  | 9     | 649  | PSU  | O2-C2-N1   | -2.79 | 119.91      | 122.79   |
| 48  | 5     | 3853 | PSU  | C6-N1-C2   | -2.78 | 120.11      | 122.69   |
| 51  | 9     | 822  | PSU  | C6-N1-C2   | -2.78 | 120.11      | 122.69   |
| 51  | 9     | 1326 | OMU  | O4-C4-C5   | -2.78 | 120.37      | 125.16   |
| 51  | 9     | 121  | OMU  | O4-C4-C5   | -2.77 | 120.39      | 125.16   |
| 48  | 5     | 4392 | OMG  | C5-C6-N1   | 2.76  | 120.29      | 113.25   |
| 51  | 9     | 815  | PSU  | C6-N1-C2   | -2.76 | 120.13      | 122.69   |
| 48  | 5     | 2837 | OMU  | O4-C4-C5   | -2.76 | 120.40      | 125.16   |
| 48  | 5     | 3639 | PSU  | O2-C2-N1   | -2.76 | 119.95      | 122.79   |
| 48  | 5     | 1683 | PSU  | C6-N1-C2   | -2.75 | 120.14      | 122.69   |
| 51  | 9     | 509  | OMG  | C5-C6-N1   | 2.74  | 120.22      | 113.25   |
| 51  | 9     | 34   | PSU  | O2-C2-N1   | -2.73 | 119.97      | 122.79   |
| 48  | 5     | 4370 | OMG  | C5-C6-N1   | 2.72  | 120.19      | 113.25   |
| 48  | 5     | 4353 | PSU  | C6-N1-C2   | -2.72 | 120.17      | 122.69   |
| 48  | 5     | 1683 | PSU  | O2-C2-N1   | -2.72 | 119.98      | 122.79   |
| 51  | 9     | 1832 | 6MZ  | N3-C4-N9   | 2.71  | 131.78      | 127.17   |
| 48  | 5     | 3792 | OMG  | N9-C8-N7   | -2.71 | 108.38      | 113.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | 5     | 4220 | 6MZ  | C4-C5-N7    | -2.70 | 107.49      | 110.58   |
| 48  | 5     | 3718 | A2M  | N3-C4-N9    | 2.70  | 131.76      | 127.17   |
| 48  | 5     | 3899 | OMG  | C2-N1-C6    | -2.70 | 120.22      | 125.11   |
| 48  | 5     | 4618 | OMG  | C5-C6-N1    | 2.70  | 120.11      | 113.25   |
| 50  | 8     | 75   | OMG  | C5-C6-N1    | 2.69  | 120.11      | 113.25   |
| 51  | 9     | 509  | OMG  | O6-C6-C5    | -2.68 | 119.45      | 126.53   |
| 51  | 9     | 1232 | PSU  | C6-N1-C2    | -2.68 | 120.20      | 122.69   |
| 51  | 9     | 166  | A2M  | C5-N7-C8    | 2.68  | 107.66      | 103.45   |
| 48  | 5     | 3830 | A2M  | C5-N7-C8    | 2.68  | 107.66      | 103.45   |
| 48  | 5     | 1522 | OMG  | C5-C6-N1    | 2.68  | 120.07      | 113.25   |
| 48  | 5     | 1781 | PSU  | O2-C2-N1    | -2.68 | 120.03      | 122.79   |
| 48  | 5     | 2632 | PSU  | C6-N1-C2    | -2.68 | 120.21      | 122.69   |
| 48  | 5     | 3825 | A2M  | C5-N7-C8    | 2.67  | 107.65      | 103.45   |
| 48  | 5     | 2632 | PSU  | O2-C2-N1    | -2.67 | 120.03      | 122.79   |
| 51  | 9     | 1046 | PSU  | O2-C2-N1    | -2.67 | 120.04      | 122.79   |
| 48  | 5     | 1517 | 2MG  | C5-C6-N1    | 2.67  | 120.04      | 113.25   |
| 48  | 5     | 2424 | OMG  | C5-C6-N1    | 2.66  | 120.03      | 113.25   |
| 48  | 5     | 3785 | A2M  | C5-N7-C8    | 2.66  | 107.63      | 103.45   |
| 51  | 9     | 1832 | 6MZ  | C4-C5-C6    | 2.66  | 118.99      | 116.78   |
| 48  | 5     | 4637 | OMG  | C5-C6-N1    | 2.66  | 120.02      | 113.25   |
| 51  | 9     | 109  | PSU  | C6-N1-C2    | -2.66 | 120.22      | 122.69   |
| 51  | 9     | 1244 | PSU  | C6-C5-C4    | 2.65  | 119.97      | 118.17   |
| 48  | 5     | 3867 | A2M  | C5-N7-C8    | 2.65  | 107.62      | 103.45   |
| 48  | 5     | 4392 | OMG  | N9-C8-N7    | -2.65 | 108.49      | 113.40   |
| 51  | 9     | 1174 | PSU  | C6-N1-C2    | -2.65 | 120.23      | 122.69   |
| 51  | 9     | 1328 | OMG  | O6-C6-C5    | -2.65 | 119.55      | 126.53   |
| 48  | 5     | 4521 | PSU  | C6-N1-C2    | -2.64 | 120.24      | 122.69   |
| 48  | 5     | 4628 | PSU  | C6-C5-C4    | 2.64  | 119.96      | 118.17   |
| 48  | 5     | 4494 | OMG  | N9-C8-N7    | -2.64 | 108.50      | 113.40   |
| 48  | 5     | 1517 | 2MG  | O6-C6-C5    | -2.64 | 119.55      | 126.53   |
| 48  | 5     | 373  | OMG  | C5-C6-N1    | 2.64  | 119.98      | 113.25   |
| 48  | 5     | 237  | B9B  | C4-C5-N7    | -2.64 | 107.56      | 110.58   |
| 48  | 5     | 1871 | A2M  | C2'-C1'-N9  | -2.64 | 109.41      | 113.75   |
| 51  | 9     | 121  | OMU  | CM2-O2'-C2' | 2.64  | 121.24      | 114.47   |
| 48  | 5     | 2787 | A2M  | C6-C5-C4    | 2.64  | 120.78      | 117.18   |
| 48  | 5     | 2364 | OMG  | C5-C6-N1    | 2.63  | 119.96      | 113.25   |
| 48  | 5     | 4442 | PSU  | C6-C5-C4    | 2.63  | 119.95      | 118.17   |
| 48  | 5     | 3792 | OMG  | C2-N1-C6    | -2.63 | 120.35      | 125.11   |
| 48  | 5     | 1322 | 1MA  | C5-C4-N3    | -2.62 | 123.41      | 127.27   |
| 48  | 5     | 4220 | 6MZ  | N3-C4-N9    | 2.62  | 131.63      | 127.17   |
| 51  | 9     | 484  | A2M  | N3-C4-N9    | 2.62  | 131.62      | 127.17   |
| 48  | 5     | 2363 | A2M  | C5-N7-C8    | 2.61  | 107.56      | 103.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 51  | 9     | 468  | A2M  | C5-N7-C8    | 2.61  | 107.55      | 103.45   |
| 51  | 9     | 1490 | OMG  | O6-C6-C5    | -2.61 | 119.65      | 126.53   |
| 48  | 5     | 3627 | OMG  | C5-C6-N1    | 2.60  | 119.88      | 113.25   |
| 48  | 5     | 3764 | PSU  | O2-C2-N1    | -2.60 | 120.11      | 122.79   |
| 51  | 9     | 1328 | OMG  | C5-C6-N1    | 2.60  | 119.87      | 113.25   |
| 48  | 5     | 1524 | A2M  | C4'-O4'-C1' | -2.60 | 103.72      | 109.47   |
| 48  | 5     | 3760 | A2M  | C4-C5-N7    | -2.60 | 107.61      | 110.58   |
| 48  | 5     | 3925 | OMU  | O4-C4-C5    | -2.59 | 120.70      | 125.16   |
| 51  | 9     | 1678 | A2M  | C4-C5-N7    | -2.59 | 107.63      | 110.58   |
| 51  | 9     | 1046 | PSU  | C6-N1-C2    | -2.59 | 120.29      | 122.69   |
| 51  | 9     | 159  | A2M  | N3-C4-N9    | 2.58  | 131.56      | 127.17   |
| 48  | 5     | 1860 | PSU  | C6-N1-C2    | -2.58 | 120.30      | 122.69   |
| 48  | 5     | 4571 | A2M  | N3-C4-N9    | 2.58  | 131.55      | 127.17   |
| 48  | 5     | 4530 | UR3  | C6-N1-C2    | -2.58 | 119.69      | 121.80   |
| 51  | 9     | 1639 | G7M  | N9-C4-N3    | 2.57  | 131.10      | 125.95   |
| 48  | 5     | 1871 | A2M  | N3-C4-N9    | 2.56  | 131.53      | 127.17   |
| 51  | 9     | 1383 | A2M  | C5-N7-C8    | 2.56  | 107.48      | 103.45   |
| 51  | 9     | 1639 | G7M  | CN7-N7-C5   | 2.56  | 129.99      | 126.80   |
| 48  | 5     | 3695 | PSU  | C6-N1-C2    | -2.56 | 120.31      | 122.69   |
| 48  | 5     | 1517 | 2MG  | C8-N7-C5    | 2.56  | 108.81      | 104.26   |
| 48  | 5     | 1782 | PSU  | C6-C5-C4    | 2.56  | 119.90      | 118.17   |
| 48  | 5     | 4361 | PSU  | O2-C2-N1    | -2.55 | 120.15      | 122.79   |
| 51  | 9     | 99   | A2M  | C5-N7-C8    | 2.55  | 107.46      | 103.45   |
| 51  | 9     | 1850 | MA6  | C6-C5-N7    | -2.55 | 129.37      | 133.43   |
| 51  | 9     | 1832 | 6MZ  | C4-C5-N7    | -2.55 | 107.67      | 110.58   |
| 51  | 9     | 1031 | A2M  | N3-C4-N9    | 2.55  | 131.50      | 127.17   |
| 51  | 9     | 644  | OMG  | N9-C8-N7    | -2.55 | 108.68      | 113.40   |
| 51  | 9     | 484  | A2M  | C5-N7-C8    | 2.54  | 107.45      | 103.45   |
| 48  | 5     | 4442 | PSU  | C6-N1-C2    | -2.54 | 120.33      | 122.69   |
| 51  | 9     | 572  | PSU  | C6-N1-C2    | -2.54 | 120.33      | 122.69   |
| 48  | 5     | 4392 | OMG  | O6-C6-C5    | -2.54 | 119.84      | 126.53   |
| 48  | 5     | 4620 | OMU  | O4-C4-C5    | -2.53 | 120.79      | 125.16   |
| 48  | 5     | 4618 | OMG  | O6-C6-C5    | -2.53 | 119.85      | 126.53   |
| 48  | 5     | 2876 | OMG  | N9-C8-N7    | -2.53 | 108.71      | 113.40   |
| 51  | 9     | 1347 | PSU  | O2-C2-N1    | -2.52 | 120.19      | 122.79   |
| 48  | 5     | 3627 | OMG  | N9-C4-N3    | 2.52  | 131.00      | 125.95   |
| 51  | 9     | 159  | A2M  | C5-N7-C8    | 2.52  | 107.41      | 103.45   |
| 48  | 5     | 4500 | PSU  | C6-N1-C2    | -2.52 | 120.36      | 122.69   |
| 48  | 5     | 4299 | PSU  | O2-C2-N1    | -2.52 | 120.19      | 122.79   |
| 48  | 5     | 1625 | OMG  | C1'-N9-C8   | 2.52  | 133.88      | 126.73   |
| 51  | 9     | 1367 | PSU  | C6-N1-C2    | -2.51 | 120.36      | 122.69   |
| 48  | 5     | 4227 | OMU  | O4-C4-C5    | -2.51 | 120.84      | 125.16   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 51  | 9     | 172  | OMU  | O4-C4-C5    | -2.51 | 120.84      | 125.16   |
| 51  | 9     | 428  | OMU  | O2-C2-N1    | -2.50 | 119.54      | 122.80   |
| 51  | 9     | 815  | PSU  | C6-C5-C4    | 2.50  | 119.86      | 118.17   |
| 48  | 5     | 1871 | A2M  | C5-N7-C8    | 2.50  | 107.37      | 103.45   |
| 48  | 5     | 1524 | A2M  | C4-N9-C8    | 2.49  | 108.35      | 105.74   |
| 48  | 5     | 2364 | OMG  | C8-N7-C5    | 2.49  | 108.69      | 104.26   |
| 51  | 9     | 801  | PSU  | C6-N1-C2    | -2.49 | 120.38      | 122.69   |
| 48  | 5     | 1522 | OMG  | C2'-C1'-N9  | -2.49 | 109.52      | 114.24   |
| 48  | 5     | 4494 | OMG  | C5-C6-N1    | 2.49  | 119.58      | 113.25   |
| 48  | 5     | 237  | B9B  | C2-N3-C4    | 2.48  | 120.16      | 113.51   |
| 51  | 9     | 1445 | PSU  | O2-C2-N1    | -2.48 | 120.23      | 122.79   |
| 51  | 9     | 172  | OMU  | O2-C2-N1    | -2.48 | 119.57      | 122.80   |
| 48  | 5     | 2824 | OMC  | O2-C2-N3    | -2.48 | 118.42      | 122.33   |
| 51  | 9     | 1177 | PSU  | C6-N1-C2    | -2.48 | 120.39      | 122.69   |
| 48  | 5     | 373  | OMG  | C8-N7-C5    | 2.48  | 108.67      | 104.26   |
| 51  | 9     | 468  | A2M  | C5'-C4'-C3' | -2.47 | 106.31      | 115.21   |
| 48  | 5     | 4370 | OMG  | C8-N7-C5    | 2.47  | 108.66      | 104.26   |
| 48  | 5     | 4353 | PSU  | O2-C2-N1    | -2.47 | 120.24      | 122.79   |
| 51  | 9     | 484  | A2M  | C5-C4-N9    | 2.47  | 108.50      | 105.81   |
| 51  | 9     | 1692 | PSU  | O2-C2-N1    | -2.46 | 120.25      | 122.79   |
| 51  | 9     | 116  | OMU  | O4-C4-C5    | -2.46 | 120.92      | 125.16   |
| 48  | 5     | 4552 | PSU  | O2-C2-N1    | -2.46 | 120.25      | 122.79   |
| 48  | 5     | 4196 | OMG  | N9-C8-N7    | -2.46 | 108.84      | 113.40   |
| 48  | 5     | 4227 | OMU  | O2-C2-N1    | -2.46 | 119.60      | 122.80   |
| 48  | 5     | 400  | A2M  | C5-N7-C8    | 2.46  | 107.31      | 103.45   |
| 48  | 5     | 3899 | OMG  | C5-C6-N1    | 2.46  | 119.51      | 113.25   |
| 48  | 5     | 3792 | OMG  | C5-C6-N1    | 2.45  | 119.50      | 113.25   |
| 51  | 9     | 668  | A2M  | C4-C5-N7    | -2.45 | 107.78      | 110.58   |
| 51  | 9     | 801  | PSU  | O2-C2-N1    | -2.45 | 120.26      | 122.79   |
| 51  | 9     | 1248 | B8N  | C31-N3-C4   | 2.45  | 120.64      | 117.18   |
| 51  | 9     | 683  | OMG  | C8-N7-C5    | 2.45  | 108.62      | 104.26   |
| 48  | 5     | 4228 | OMG  | C5-C6-N1    | 2.44  | 119.46      | 113.25   |
| 48  | 5     | 4447 | 5MC  | CM5-C5-C6   | -2.44 | 119.55      | 122.85   |
| 51  | 9     | 166  | A2M  | N3-C4-N9    | 2.44  | 131.31      | 127.17   |
| 48  | 5     | 3715 | PSU  | C6-N1-C2    | -2.43 | 120.43      | 122.69   |
| 48  | 5     | 3627 | OMG  | C8-N7-C5    | 2.43  | 108.58      | 104.26   |
| 48  | 5     | 4420 | PSU  | C6-N1-C2    | -2.42 | 120.44      | 122.69   |
| 51  | 9     | 1081 | PSU  | C6-C5-C4    | 2.42  | 119.81      | 118.17   |
| 48  | 5     | 3899 | OMG  | C8-N7-C5    | 2.42  | 108.57      | 104.26   |
| 51  | 9     | 1383 | A2M  | N3-C4-N9    | 2.42  | 131.28      | 127.17   |
| 50  | 8     | 75   | OMG  | O6-C6-C5    | -2.41 | 120.16      | 126.53   |
| 48  | 5     | 3718 | A2M  | C5-N7-C8    | 2.41  | 107.24      | 103.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | 5     | 1517 | 2MG  | C4-C5-N7    | -2.41 | 106.85      | 110.67   |
| 51  | 9     | 609  | PSU  | C6-N1-C2    | -2.41 | 120.46      | 122.69   |
| 51  | 9     | 1004 | PSU  | C6-N1-C2    | -2.40 | 120.46      | 122.69   |
| 48  | 5     | 4296 | PSU  | C6-N1-C2    | -2.40 | 120.47      | 122.69   |
| 51  | 9     | 644  | OMG  | C5-C6-N1    | 2.39  | 119.34      | 113.25   |
| 48  | 5     | 3734 | PSU  | C6-C5-C4    | 2.39  | 119.78      | 118.17   |
| 48  | 5     | 4196 | OMG  | O6-C6-C5    | -2.38 | 120.24      | 126.53   |
| 51  | 9     | 119  | PSU  | C6-N1-C2    | -2.38 | 120.49      | 122.69   |
| 51  | 9     | 1367 | PSU  | O2-C2-N1    | -2.37 | 120.34      | 122.79   |
| 48  | 5     | 4637 | OMG  | C8-N7-C5    | 2.37  | 108.48      | 104.26   |
| 51  | 9     | 1045 | PSU  | C6-N1-C2    | -2.37 | 120.49      | 122.69   |
| 48  | 5     | 237  | B9B  | C5-C4-N9    | 2.36  | 108.38      | 105.81   |
| 48  | 5     | 4494 | OMG  | O6-C6-C5    | -2.36 | 120.31      | 126.53   |
| 48  | 5     | 4293 | PSU  | C6-N1-C2    | -2.36 | 120.50      | 122.69   |
| 51  | 9     | 1031 | A2M  | C5-N7-C8    | 2.35  | 107.15      | 103.45   |
| 51  | 9     | 1832 | 6MZ  | C4-N9-C8    | 2.35  | 108.20      | 105.74   |
| 48  | 5     | 3764 | PSU  | C6-N1-C2    | -2.35 | 120.52      | 122.69   |
| 51  | 9     | 1347 | PSU  | C6-N1-C2    | -2.35 | 120.52      | 122.69   |
| 48  | 5     | 1316 | OMG  | C8-N7-C5    | 2.34  | 108.43      | 104.26   |
| 48  | 5     | 4220 | 6MZ  | C5-C4-N9    | 2.34  | 108.36      | 105.81   |
| 48  | 5     | 4457 | PSU  | O2-C2-N1    | -2.34 | 120.38      | 122.79   |
| 48  | 5     | 1517 | 2MG  | C6-C5-N7    | 2.34  | 134.54      | 130.29   |
| 48  | 5     | 3734 | PSU  | C6-N1-C2    | -2.33 | 120.53      | 122.69   |
| 48  | 5     | 1340 | OMC  | C5-C4-N3    | -2.33 | 117.39      | 121.32   |
| 48  | 5     | 2876 | OMG  | C5-C6-N1    | 2.33  | 119.19      | 113.25   |
| 48  | 5     | 3760 | A2M  | C6-C5-C4    | 2.33  | 120.36      | 117.18   |
| 48  | 5     | 1781 | PSU  | C6-C5-C4    | 2.32  | 119.74      | 118.17   |
| 48  | 5     | 398  | A2M  | C6-C5-C4    | 2.32  | 120.35      | 117.18   |
| 51  | 9     | 822  | PSU  | O4'-C1'-C2' | 2.32  | 108.36      | 105.15   |
| 48  | 5     | 4618 | OMG  | C8-N7-C5    | 2.32  | 108.39      | 104.26   |
| 48  | 5     | 1517 | 2MG  | N1-C2-N3    | -2.32 | 119.78      | 123.68   |
| 48  | 5     | 3695 | PSU  | O2-C2-N1    | -2.31 | 120.40      | 122.79   |
| 51  | 9     | 509  | OMG  | N9-C8-N7    | -2.31 | 109.12      | 113.40   |
| 48  | 5     | 4370 | OMG  | O6-C6-C5    | -2.31 | 120.44      | 126.53   |
| 51  | 9     | 668  | A2M  | C5-C4-N9    | 2.31  | 108.32      | 105.81   |
| 51  | 9     | 814  | PSU  | C6-N1-C2    | -2.31 | 120.55      | 122.69   |
| 48  | 5     | 3724 | A2M  | C6-C5-C4    | 2.30  | 120.32      | 117.18   |
| 48  | 5     | 1534 | A2M  | C6-C5-C4    | 2.30  | 120.32      | 117.18   |
| 48  | 5     | 3899 | OMG  | O6-C6-C5    | -2.30 | 120.46      | 126.53   |
| 48  | 5     | 3718 | A2M  | O4'-C1'-N9  | 2.30  | 112.50      | 108.09   |
| 48  | 5     | 3762 | PSU  | C6-N1-C2    | -2.30 | 120.56      | 122.69   |
| 51  | 9     | 1490 | OMG  | C2-N1-C6    | -2.30 | 120.95      | 125.11   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | 5     | 3724 | A2M  | C5-N7-C8    | 2.29  | 107.05      | 103.45   |
| 48  | 5     | 3701 | OMC  | O2-C2-N3    | -2.29 | 118.72      | 122.33   |
| 51  | 9     | 468  | A2M  | C4-N9-C8    | 2.29  | 108.14      | 105.74   |
| 48  | 5     | 3734 | PSU  | O2-C2-N1    | -2.29 | 120.43      | 122.79   |
| 51  | 9     | 27   | A2M  | C5-N7-C8    | 2.28  | 107.04      | 103.45   |
| 51  | 9     | 683  | OMG  | O6-C6-C5    | -2.28 | 120.51      | 126.53   |
| 48  | 5     | 1522 | OMG  | O6-C6-C5    | -2.28 | 120.52      | 126.53   |
| 48  | 5     | 2364 | OMG  | O6-C6-C5    | -2.28 | 120.52      | 126.53   |
| 48  | 5     | 373  | OMG  | O6-C6-C5    | -2.28 | 120.52      | 126.53   |
| 48  | 5     | 2876 | OMG  | C8-N7-C5    | 2.27  | 108.31      | 104.26   |
| 51  | 9     | 1081 | PSU  | O4'-C1'-C2' | 2.27  | 108.29      | 105.15   |
| 48  | 5     | 1871 | A2M  | C4-N9-C8    | 2.27  | 108.12      | 105.74   |
| 51  | 9     | 512  | A2M  | N3-C4-N9    | 2.27  | 131.03      | 127.17   |
| 51  | 9     | 166  | A2M  | C5-C4-N9    | 2.27  | 108.28      | 105.81   |
| 48  | 5     | 4228 | OMG  | O6-C6-C5    | -2.26 | 120.56      | 126.53   |
| 51  | 9     | 1081 | PSU  | O2-C2-N1    | -2.26 | 120.45      | 122.79   |
| 51  | 9     | 1177 | PSU  | O2-C2-N1    | -2.26 | 120.46      | 122.79   |
| 48  | 5     | 2508 | PSU  | O2-C2-N1    | -2.26 | 120.46      | 122.79   |
| 48  | 5     | 1862 | PSU  | C6-C5-C4    | 2.26  | 119.70      | 118.17   |
| 51  | 9     | 1383 | A2M  | C2'-C3'-C4' | -2.26 | 97.14       | 101.99   |
| 51  | 9     | 814  | PSU  | C6-C5-C4    | 2.25  | 119.69      | 118.17   |
| 48  | 5     | 3715 | PSU  | O4'-C1'-C2' | 2.25  | 108.26      | 105.15   |
| 51  | 9     | 1383 | A2M  | C2'-C1'-N9  | -2.25 | 110.06      | 113.75   |
| 51  | 9     | 1081 | PSU  | C6-N1-C2    | -2.24 | 120.61      | 122.69   |
| 48  | 5     | 4523 | A2M  | C4-N9-C8    | 2.24  | 108.09      | 105.74   |
| 51  | 9     | 218  | PSU  | C5-C6-N1    | -2.24 | 119.03      | 122.14   |
| 51  | 9     | 218  | PSU  | C6-N1-C2    | -2.24 | 120.61      | 122.69   |
| 51  | 9     | 1490 | OMG  | C5-C6-N1    | 2.24  | 118.95      | 113.25   |
| 48  | 5     | 4571 | A2M  | C5-C4-N9    | 2.24  | 108.25      | 105.81   |
| 48  | 5     | 1534 | A2M  | C4-C5-N7    | -2.23 | 108.03      | 110.58   |
| 48  | 5     | 1517 | 2MG  | C1'-N9-C8   | -2.22 | 120.41      | 126.73   |
| 48  | 5     | 3627 | OMG  | O6-C6-C5    | -2.22 | 120.67      | 126.53   |
| 48  | 5     | 2508 | PSU  | C6-N1-C2    | -2.22 | 120.63      | 122.69   |
| 51  | 9     | 27   | A2M  | C6-C5-C4    | 2.22  | 120.21      | 117.18   |
| 48  | 5     | 4618 | OMG  | N2-C2-N1    | 2.21  | 121.44      | 116.76   |
| 48  | 5     | 2815 | A2M  | C4-C5-N7    | -2.21 | 108.06      | 110.58   |
| 51  | 9     | 1238 | PSU  | C5-C6-N1    | -2.20 | 119.09      | 122.14   |
| 48  | 5     | 2876 | OMG  | O6-C6-C5    | -2.20 | 120.73      | 126.53   |
| 48  | 5     | 3818 | UY1  | O4'-C1'-C2' | 2.20  | 108.41      | 104.56   |
| 48  | 5     | 4571 | A2M  | C4-C5-N7    | -2.19 | 108.07      | 110.58   |
| 48  | 5     | 1534 | A2M  | C2'-C1'-N9  | 2.19  | 117.36      | 113.75   |
| 51  | 9     | 484  | A2M  | C4-C5-N7    | -2.19 | 108.08      | 110.58   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | 5     | 4628 | PSU  | C6-N1-C2    | -2.19 | 120.66      | 122.69   |
| 51  | 9     | 1639 | G7M  | N2-C2-N1    | 2.19  | 121.38      | 116.76   |
| 48  | 5     | 4228 | OMG  | C8-N7-C5    | 2.18  | 108.15      | 104.26   |
| 51  | 9     | 99   | A2M  | C6-C5-C4    | 2.18  | 120.16      | 117.18   |
| 48  | 5     | 2876 | OMG  | C6-C5-C4    | 2.18  | 122.11      | 118.83   |
| 48  | 5     | 398  | A2M  | C4-C5-N7    | -2.18 | 108.09      | 110.58   |
| 51  | 9     | 119  | PSU  | C6-C5-C4    | 2.18  | 119.64      | 118.17   |
| 51  | 9     | 1248 | B8N  | O4-C4-C5    | -2.18 | 118.81      | 122.58   |
| 48  | 5     | 3639 | PSU  | C6-N1-C2    | -2.18 | 120.67      | 122.69   |
| 51  | 9     | 649  | PSU  | C6-N1-C2    | -2.18 | 120.67      | 122.69   |
| 48  | 5     | 3920 | PSU  | C6-N1-C2    | -2.18 | 120.67      | 122.69   |
| 48  | 5     | 4306 | OMU  | O2-C2-N1    | -2.18 | 119.96      | 122.80   |
| 51  | 9     | 668  | A2M  | C2'-C1'-N9  | 2.17  | 117.33      | 113.75   |
| 48  | 5     | 4494 | OMG  | N2-C2-N1    | 2.17  | 121.35      | 116.76   |
| 51  | 9     | 159  | A2M  | C5-C4-N9    | 2.16  | 108.17      | 105.81   |
| 48  | 5     | 3782 | 5MC  | CM5-C5-C6   | -2.16 | 119.92      | 122.85   |
| 51  | 9     | 1031 | A2M  | C4-N9-C8    | 2.16  | 108.01      | 105.74   |
| 51  | 9     | 109  | PSU  | O2-C2-N1    | -2.16 | 120.56      | 122.79   |
| 50  | 8     | 75   | OMG  | C8-N7-C5    | 2.16  | 108.11      | 104.26   |
| 48  | 5     | 1316 | OMG  | O6-C6-C5    | -2.16 | 120.83      | 126.53   |
| 51  | 9     | 1244 | PSU  | C6-N1-C2    | -2.16 | 120.69      | 122.69   |
| 51  | 9     | 159  | A2M  | C4-C5-N7    | -2.15 | 108.12      | 110.58   |
| 48  | 5     | 237  | B9B  | C61-O6-C6   | 2.15  | 121.41      | 117.66   |
| 48  | 5     | 4579 | PSU  | C6-N1-C2    | -2.15 | 120.69      | 122.69   |
| 48  | 5     | 1522 | OMG  | C8-N7-C5    | 2.15  | 108.09      | 104.26   |
| 48  | 5     | 3825 | A2M  | C2'-C1'-N9  | -2.15 | 110.21      | 113.75   |
| 48  | 5     | 1524 | A2M  | C6-C5-C4    | 2.15  | 120.11      | 117.18   |
| 51  | 9     | 1643 | PSU  | C6-N1-C2    | -2.14 | 120.70      | 122.69   |
| 48  | 5     | 1524 | A2M  | C4-C5-N7    | -2.14 | 108.13      | 110.58   |
| 48  | 5     | 1744 | PSU  | C6-N1-C2    | -2.14 | 120.71      | 122.69   |
| 48  | 5     | 1782 | PSU  | C6-N1-C2    | -2.13 | 120.71      | 122.69   |
| 51  | 9     | 166  | A2M  | C4-C5-N7    | -2.13 | 108.15      | 110.58   |
| 48  | 5     | 4571 | A2M  | C4-N9-C8    | 2.13  | 107.97      | 105.74   |
| 48  | 5     | 237  | B9B  | C4-N9-C8    | 2.13  | 107.97      | 105.74   |
| 51  | 9     | 99   | A2M  | C5-C4-N9    | 2.13  | 108.13      | 105.81   |
| 48  | 5     | 4552 | PSU  | C6-N1-C2    | -2.13 | 120.72      | 122.69   |
| 48  | 5     | 1625 | OMG  | C8-N7-C5    | 2.13  | 108.05      | 104.26   |
| 51  | 9     | 668  | A2M  | C3'-C2'-C1' | 2.13  | 106.88      | 102.81   |
| 48  | 5     | 398  | A2M  | C2'-C1'-N9  | -2.12 | 110.26      | 113.75   |
| 48  | 5     | 373  | OMG  | C2'-C1'-N9  | -2.12 | 110.22      | 114.24   |
| 50  | 8     | 75   | OMG  | N2-C2-N1    | 2.12  | 121.23      | 116.76   |
| 51  | 9     | 1678 | A2M  | C4-N9-C8    | 2.11  | 107.95      | 105.74   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | 5     | 2861 | OMC  | O2-C2-N3    | -2.11 | 119.01      | 122.33   |
| 48  | 5     | 4423 | PSU  | C6-N1-C2    | -2.10 | 120.74      | 122.69   |
| 51  | 9     | 1383 | A2M  | C5-C4-N9    | 2.10  | 108.10      | 105.81   |
| 51  | 9     | 1391 | OMC  | O2-C2-N3    | -2.10 | 119.02      | 122.33   |
| 48  | 5     | 1677 | PSU  | C6-C5-C4    | 2.10  | 119.59      | 118.17   |
| 48  | 5     | 1522 | OMG  | N2-C2-N1    | 2.10  | 121.19      | 116.76   |
| 51  | 9     | 1678 | A2M  | C5-C4-N9    | 2.10  | 108.10      | 105.81   |
| 51  | 9     | 1347 | PSU  | O4-C4-C5    | -2.10 | 118.80      | 124.01   |
| 48  | 5     | 4361 | PSU  | C6-N1-C2    | -2.09 | 120.75      | 122.69   |
| 51  | 9     | 1046 | PSU  | O4'-C1'-C2' | 2.09  | 108.05      | 105.15   |
| 48  | 5     | 3760 | A2M  | C5-C4-N9    | 2.08  | 108.08      | 105.81   |
| 51  | 9     | 105  | PSU  | O2-C2-N1    | -2.08 | 120.64      | 122.79   |
| 48  | 5     | 4530 | UR3  | C1'-N1-C2   | 2.08  | 120.44      | 117.04   |
| 48  | 5     | 4403 | PSU  | C6-N1-C2    | -2.07 | 120.77      | 122.69   |
| 51  | 9     | 121  | OMU  | C1'-N1-C2   | 2.07  | 121.32      | 117.59   |
| 48  | 5     | 4403 | PSU  | O4'-C1'-C2' | 2.07  | 108.02      | 105.15   |
| 51  | 9     | 1832 | 6MZ  | C5-C4-N9    | 2.07  | 108.06      | 105.81   |
| 48  | 5     | 4293 | PSU  | O4-C4-C5    | -2.07 | 118.87      | 124.01   |
| 48  | 5     | 4521 | PSU  | C5-C6-N1    | -2.06 | 119.28      | 122.14   |
| 48  | 5     | 4521 | PSU  | O4'-C1'-C2' | 2.06  | 108.01      | 105.15   |
| 48  | 5     | 4628 | PSU  | O4'-C1'-C2' | 2.06  | 108.00      | 105.15   |
| 51  | 9     | 1337 | 4AC  | C5-C4-N4    | 2.06  | 126.41      | 122.94   |
| 51  | 9     | 644  | OMG  | C8-N7-C5    | 2.06  | 107.92      | 104.26   |
| 48  | 5     | 3830 | A2M  | C4-N9-C8    | 2.06  | 107.90      | 105.74   |
| 48  | 5     | 4196 | OMG  | C8-N7-C5    | 2.05  | 107.92      | 104.26   |
| 51  | 9     | 1639 | G7M  | N9-C8-N7    | -2.05 | 107.50      | 112.48   |
| 48  | 5     | 3887 | OMC  | C2'-C1'-N1  | -2.05 | 110.34      | 114.24   |
| 51  | 9     | 686  | PSU  | O4-C4-C5    | -2.05 | 118.91      | 124.01   |
| 48  | 5     | 1862 | PSU  | C6-N1-C2    | -2.05 | 120.79      | 122.69   |
| 48  | 5     | 4523 | A2M  | C6-C5-C4    | 2.05  | 119.98      | 117.18   |
| 48  | 5     | 2787 | A2M  | C4-C5-N7    | -2.04 | 108.25      | 110.58   |
| 48  | 5     | 2363 | A2M  | C6-C5-C4    | 2.04  | 119.96      | 117.18   |
| 48  | 5     | 4532 | PSU  | O2-C2-N1    | -2.04 | 120.69      | 122.79   |
| 48  | 5     | 1340 | OMC  | C6-C5-C4    | 2.04  | 120.87      | 117.53   |
| 51  | 9     | 1842 | 4AC  | C6-C5-C4    | 2.04  | 119.45      | 117.00   |
| 48  | 5     | 3762 | PSU  | C6-C5-C4    | 2.03  | 119.54      | 118.17   |
| 48  | 5     | 4361 | PSU  | C6-C5-C4    | 2.03  | 119.54      | 118.17   |
| 48  | 5     | 3718 | A2M  | C6-C5-C4    | 2.03  | 119.95      | 117.18   |
| 48  | 5     | 1781 | PSU  | C6-N1-C2    | -2.03 | 120.81      | 122.69   |
| 48  | 5     | 3853 | PSU  | O4'-C1'-C2' | 2.02  | 107.95      | 105.15   |
| 48  | 5     | 3627 | OMG  | C4-C5-N7    | -2.02 | 107.47      | 110.67   |
| 48  | 5     | 4370 | OMG  | N2-C2-N1    | 2.02  | 121.02      | 116.76   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | 5     | 4523 | A2M  | C4-C5-N7    | -2.02 | 108.28      | 110.58   |
| 51  | 9     | 686  | PSU  | C6-N1-C2    | -2.02 | 120.82      | 122.69   |
| 51  | 9     | 218  | PSU  | O4'-C1'-C2' | 2.01  | 107.94      | 105.15   |
| 48  | 5     | 3830 | A2M  | C6-C5-C4    | 2.01  | 119.92      | 117.18   |
| 48  | 5     | 3764 | PSU  | C6-C5-C4    | 2.01  | 119.53      | 118.17   |
| 48  | 5     | 4620 | OMU  | O2-C2-N1    | -2.00 | 120.19      | 122.80   |
| 48  | 5     | 3785 | A2M  | C5-C4-N9    | 2.00  | 107.99      | 105.81   |

There are no chirality outliers.

All (103) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 48  | 5     | 237  | B9B  | C5-C6-O6-C61    |
| 48  | 5     | 237  | B9B  | N1-C6-O6-C61    |
| 48  | 5     | 1781 | PSU  | C3'-C4'-C5'-O5' |
| 48  | 5     | 2424 | OMG  | O4'-C4'-C5'-O5' |
| 48  | 5     | 2424 | OMG  | C1'-C2'-O2'-CM2 |
| 48  | 5     | 3701 | OMC  | C2'-C1'-N1-C2   |
| 48  | 5     | 3701 | OMC  | C2'-C1'-N1-C6   |
| 48  | 5     | 4228 | OMG  | C3'-C2'-O2'-CM2 |
| 48  | 5     | 4500 | PSU  | O4'-C4'-C5'-O5' |
| 51  | 9     | 34   | PSU  | O4'-C4'-C5'-O5' |
| 51  | 9     | 121  | OMU  | C1'-C2'-O2'-CM2 |
| 51  | 9     | 166  | A2M  | C3'-C4'-C5'-O5' |
| 51  | 9     | 683  | OMG  | C1'-C2'-O2'-CM2 |
| 51  | 9     | 1248 | B8N  | C31-C32-C33-N34 |
| 51  | 9     | 1328 | OMG  | C1'-C2'-O2'-CM2 |
| 51  | 9     | 1851 | MA6  | O4'-C4'-C5'-O5' |
| 48  | 5     | 2364 | OMG  | O4'-C4'-C5'-O5' |
| 48  | 5     | 4500 | PSU  | C3'-C4'-C5'-O5' |
| 51  | 9     | 99   | A2M  | O4'-C4'-C5'-O5' |
| 51  | 9     | 166  | A2M  | O4'-C4'-C5'-O5' |
| 51  | 9     | 801  | PSU  | C3'-C4'-C5'-O5' |
| 51  | 9     | 822  | PSU  | C3'-C4'-C5'-O5' |
| 48  | 5     | 1781 | PSU  | O4'-C4'-C5'-O5' |
| 48  | 5     | 2424 | OMG  | C3'-C4'-C5'-O5' |
| 48  | 5     | 2815 | A2M  | O4'-C4'-C5'-O5' |
| 48  | 5     | 3760 | A2M  | C3'-C4'-C5'-O5' |
| 51  | 9     | 34   | PSU  | C3'-C4'-C5'-O5' |
| 51  | 9     | 822  | PSU  | O4'-C4'-C5'-O5' |
| 51  | 9     | 1045 | PSU  | C3'-C4'-C5'-O5' |
| 51  | 9     | 1442 | OMU  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 51  | 9     | 1639 | G7M  | O4'-C4'-C5'-O5' |
| 51  | 9     | 1639 | G7M  | C3'-C4'-C5'-O5' |
| 51  | 9     | 1703 | OMC  | O4'-C4'-C5'-O5' |
| 48  | 5     | 3818 | UY1  | O4'-C4'-C5'-O5' |
| 51  | 9     | 668  | A2M  | O4'-C4'-C5'-O5' |
| 51  | 9     | 668  | A2M  | C3'-C4'-C5'-O5' |
| 51  | 9     | 1045 | PSU  | O4'-C4'-C5'-O5' |
| 51  | 9     | 1851 | MA6  | C3'-C4'-C5'-O5' |
| 48  | 5     | 3760 | A2M  | O4'-C4'-C5'-O5' |
| 48  | 5     | 3785 | A2M  | O4'-C4'-C5'-O5' |
| 48  | 5     | 3785 | A2M  | C3'-C4'-C5'-O5' |
| 48  | 5     | 3818 | UY1  | C3'-C4'-C5'-O5' |
| 51  | 9     | 99   | A2M  | C3'-C4'-C5'-O5' |
| 51  | 9     | 172  | OMU  | O4'-C4'-C5'-O5' |
| 51  | 9     | 801  | PSU  | O4'-C4'-C5'-O5' |
| 48  | 5     | 4447 | 5MC  | C2'-C1'-N1-C6   |
| 51  | 9     | 428  | OMU  | C2'-C1'-N1-C6   |
| 48  | 5     | 2364 | OMG  | C3'-C4'-C5'-O5' |
| 51  | 9     | 172  | OMU  | C3'-C4'-C5'-O5' |
| 51  | 9     | 1442 | OMU  | C3'-C4'-C5'-O5' |
| 51  | 9     | 1490 | OMG  | O4'-C4'-C5'-O5' |
| 48  | 5     | 2787 | A2M  | C2'-C1'-N9-C4   |
| 48  | 5     | 2787 | A2M  | C2'-C1'-N9-C8   |
| 48  | 5     | 3818 | UY1  | C4'-C5'-O5'-P   |
| 48  | 5     | 1625 | OMG  | C3'-C2'-O2'-CM2 |
| 48  | 5     | 2815 | A2M  | C3'-C4'-C5'-O5' |
| 51  | 9     | 512  | A2M  | O4'-C4'-C5'-O5' |
| 51  | 9     | 1248 | B8N  | C32-C33-C34-O35 |
| 48  | 5     | 1534 | A2M  | C4'-C5'-O5'-P   |
| 51  | 9     | 668  | A2M  | C2'-C1'-N9-C8   |
| 51  | 9     | 1832 | 6MZ  | N1-C6-N6-C9     |
| 48  | 5     | 4447 | 5MC  | O4'-C1'-N1-C6   |
| 48  | 5     | 3792 | OMG  | C3'-C4'-C5'-O5' |
| 51  | 9     | 683  | OMG  | C3'-C4'-C5'-O5' |
| 51  | 9     | 1248 | B8N  | N3-C31-C32-C33  |
| 51  | 9     | 1832 | 6MZ  | C5-C6-N6-C9     |
| 51  | 9     | 1248 | B8N  | C32-C33-C34-O36 |
| 51  | 9     | 428  | OMU  | O4'-C1'-N1-C6   |
| 51  | 9     | 1490 | OMG  | C4'-C5'-O5'-P   |
| 48  | 5     | 4447 | 5MC  | O4'-C1'-N1-C2   |
| 48  | 5     | 4447 | 5MC  | C2'-C1'-N1-C2   |
| 48  | 5     | 1524 | A2M  | C3'-C2'-O2'-CM' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 51  | 9     | 1031 | A2M  | C3'-C2'-O2'-CM' |
| 48  | 5     | 1326 | A2M  | C4'-C5'-O5'-P   |
| 51  | 9     | 34   | PSU  | O4'-C1'-C5-C4   |
| 51  | 9     | 1445 | PSU  | O4'-C1'-C5-C4   |
| 51  | 9     | 468  | A2M  | C3'-C4'-C5'-O5' |
| 48  | 5     | 3701 | OMC  | O4'-C1'-N1-C6   |
| 48  | 5     | 3792 | OMG  | O4'-C4'-C5'-O5' |
| 51  | 9     | 644  | OMG  | C4'-C5'-O5'-P   |
| 48  | 5     | 3851 | PSU  | C3'-C4'-C5'-O5' |
| 48  | 5     | 4499 | OMG  | C3'-C2'-O2'-CM2 |
| 48  | 5     | 1322 | 1MA  | C2'-C1'-N9-C4   |
| 51  | 9     | 1851 | MA6  | C4'-C5'-O5'-P   |
| 51  | 9     | 428  | OMU  | C2'-C1'-N1-C2   |
| 48  | 5     | 3701 | OMC  | O4'-C1'-N1-C2   |
| 48  | 5     | 2364 | OMG  | C1'-C2'-O2'-CM2 |
| 48  | 5     | 2837 | OMU  | C3'-C4'-C5'-O5' |
| 51  | 9     | 863  | PSU  | C3'-C4'-C5'-O5' |
| 51  | 9     | 1703 | OMC  | C3'-C4'-C5'-O5' |
| 51  | 9     | 34   | PSU  | O4'-C1'-C5-C6   |
| 51  | 9     | 428  | OMU  | O4'-C1'-N1-C2   |
| 48  | 5     | 2787 | A2M  | O4'-C1'-N9-C8   |
| 48  | 5     | 3867 | A2M  | C3'-C4'-C5'-O5' |
| 48  | 5     | 1322 | 1MA  | C2'-C1'-N9-C8   |
| 48  | 5     | 3760 | A2M  | C3'-C2'-O2'-CM' |
| 48  | 5     | 4494 | OMG  | C3'-C2'-O2'-CM2 |
| 48  | 5     | 1534 | A2M  | O4'-C4'-C5'-O5' |
| 51  | 9     | 683  | OMG  | O4'-C4'-C5'-O5' |
| 51  | 9     | 863  | PSU  | O4'-C4'-C5'-O5' |
| 48  | 5     | 3785 | A2M  | C2'-C1'-N9-C8   |
| 48  | 5     | 373  | OMG  | C4'-C5'-O5'-P   |
| 48  | 5     | 2351 | OMC  | C2'-C1'-N1-C2   |

There are no ring outliers.

55 monomers are involved in 79 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 48  | 5     | 4196 | OMG  | 1       | 0            |
| 51  | 9     | 172  | OMU  | 2       | 0            |
| 48  | 5     | 1871 | A2M  | 1       | 0            |
| 51  | 9     | 484  | A2M  | 1       | 0            |
| 48  | 5     | 4420 | PSU  | 1       | 0            |
| 51  | 9     | 1442 | OMU  | 3       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 51  | 9     | 1850 | MA6  | 1       | 0            |
| 51  | 9     | 1367 | PSU  | 1       | 0            |
| 51  | 9     | 1391 | OMC  | 1       | 0            |
| 48  | 5     | 3701 | OMC  | 1       | 0            |
| 48  | 5     | 4447 | 5MC  | 1       | 0            |
| 48  | 5     | 3867 | A2M  | 2       | 0            |
| 51  | 9     | 1337 | 4AC  | 1       | 0            |
| 48  | 5     | 373  | OMG  | 1       | 0            |
| 48  | 5     | 4456 | OMC  | 1       | 0            |
| 51  | 9     | 1692 | PSU  | 2       | 0            |
| 51  | 9     | 166  | A2M  | 1       | 0            |
| 48  | 5     | 3818 | UY1  | 2       | 0            |
| 48  | 5     | 4370 | OMG  | 1       | 0            |
| 48  | 5     | 2424 | OMG  | 1       | 0            |
| 51  | 9     | 109  | PSU  | 2       | 0            |
| 51  | 9     | 1347 | PSU  | 1       | 0            |
| 51  | 9     | 686  | PSU  | 1       | 0            |
| 48  | 5     | 3899 | OMG  | 1       | 0            |
| 48  | 5     | 2351 | OMC  | 2       | 0            |
| 51  | 9     | 1328 | OMG  | 1       | 0            |
| 51  | 9     | 1842 | 4AC  | 2       | 0            |
| 51  | 9     | 159  | A2M  | 1       | 0            |
| 51  | 9     | 1639 | G7M  | 1       | 0            |
| 50  | 8     | 75   | OMG  | 2       | 0            |
| 51  | 9     | 1703 | OMC  | 1       | 0            |
| 51  | 9     | 863  | PSU  | 3       | 0            |
| 51  | 9     | 1232 | PSU  | 2       | 0            |
| 48  | 5     | 1340 | OMC  | 1       | 0            |
| 48  | 5     | 1316 | OMG  | 1       | 0            |
| 48  | 5     | 3808 | OMC  | 2       | 0            |
| 51  | 9     | 27   | A2M  | 1       | 0            |
| 51  | 9     | 218  | PSU  | 3       | 0            |
| 51  | 9     | 174  | OMC  | 1       | 0            |
| 51  | 9     | 1445 | PSU  | 2       | 0            |
| 51  | 9     | 116  | OMU  | 2       | 0            |
| 48  | 5     | 3792 | OMG  | 2       | 0            |
| 48  | 5     | 3718 | A2M  | 1       | 0            |
| 51  | 9     | 121  | OMU  | 1       | 0            |
| 51  | 9     | 1490 | OMG  | 2       | 0            |
| 48  | 5     | 1322 | 1MA  | 1       | 0            |
| 48  | 5     | 2364 | OMG  | 2       | 0            |
| 51  | 9     | 1244 | PSU  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 48  | 5     | 400  | A2M  | 2       | 0            |
| 51  | 9     | 105  | PSU  | 2       | 0            |
| 51  | 9     | 1326 | OMU  | 1       | 0            |
| 48  | 5     | 4637 | OMG  | 1       | 0            |
| 51  | 9     | 801  | PSU  | 1       | 0            |
| 48  | 5     | 2876 | OMG  | 1       | 0            |
| 51  | 9     | 34   | PSU  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 323 ligands modelled in this entry, 320 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 91  | SF4  | jj    | 601 | 87   | 0,12,12      | -    | -           | -           |      |             |
| 91  | SF4  | jj    | 602 | 87   | 0,12,12      | -    | -           | -           |      |             |
| 90  | ZVM  | ii    | 501 | 88   | 30,31,31     | 4.96 | 21 (70%)    | 32,46,46    | 3.11 | 7 (21%)     |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 91  | SF4  | jj    | 601 | 87   | -       | -         | 0/6/5/5 |
| 91  | SF4  | jj    | 602 | 87   | -       | -         | 0/6/5/5 |
| 90  | ZVM  | ii    | 501 | 88   | 2/2/8/8 | 0/4/50/50 | 0/3/5/5 |

All (21) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 90  | ii    | 501 | ZVM  | O01-C01 | 12.83 | 1.39        | 1.22     |
| 90  | ii    | 501 | ZVM  | O02-C15 | 9.69  | 1.39        | 1.22     |
| 90  | ii    | 501 | ZVM  | C13-C14 | 8.13  | 1.52        | 1.38     |
| 90  | ii    | 501 | ZVM  | C10-C09 | 7.54  | 1.53        | 1.39     |
| 90  | ii    | 501 | ZVM  | C03-N01 | 7.44  | 1.38        | 1.27     |
| 90  | ii    | 501 | ZVM  | C12-C11 | 6.49  | 1.52        | 1.38     |
| 90  | ii    | 501 | ZVM  | C04-N02 | -5.99 | 1.42        | 1.47     |
| 90  | ii    | 501 | ZVM  | C03-N03 | 5.42  | 1.47        | 1.37     |
| 90  | ii    | 501 | ZVM  | C05-C04 | 5.30  | 1.59        | 1.54     |
| 90  | ii    | 501 | ZVM  | C02-C03 | -4.97 | 1.40        | 1.52     |
| 90  | ii    | 501 | ZVM  | C08-C05 | -4.27 | 1.45        | 1.54     |
| 90  | ii    | 501 | ZVM  | C17-N03 | 4.25  | 1.49        | 1.40     |
| 90  | ii    | 501 | ZVM  | C11-C10 | -4.19 | 1.31        | 1.38     |
| 90  | ii    | 501 | ZVM  | C14-C09 | -4.16 | 1.31        | 1.39     |
| 90  | ii    | 501 | ZVM  | C21-C22 | -4.06 | 1.33        | 1.39     |
| 90  | ii    | 501 | ZVM  | C06-C05 | -3.93 | 1.45        | 1.54     |
| 90  | ii    | 501 | ZVM  | C12-C13 | -2.98 | 1.31        | 1.38     |
| 90  | ii    | 501 | ZVM  | C15-N02 | 2.98  | 1.40        | 1.36     |
| 90  | ii    | 501 | ZVM  | C02-C01 | -2.56 | 1.46        | 1.51     |
| 90  | ii    | 501 | ZVM  | C07-C06 | 2.18  | 1.65        | 1.53     |
| 90  | ii    | 501 | ZVM  | C07-C08 | 2.12  | 1.65        | 1.53     |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 90  | ii    | 501 | ZVM  | C05-C04-N01 | 11.95 | 121.33      | 109.91   |
| 90  | ii    | 501 | ZVM  | O01-C01-C02 | -9.29 | 118.89      | 126.79   |
| 90  | ii    | 501 | ZVM  | C05-C04-N02 | 4.49  | 119.42      | 111.94   |
| 90  | ii    | 501 | ZVM  | N02-C04-N01 | 4.29  | 119.25      | 113.37   |
| 90  | ii    | 501 | ZVM  | C21-C22-C17 | 2.77  | 121.99      | 118.81   |
| 90  | ii    | 501 | ZVM  | C22-C01-C02 | 2.70  | 120.36      | 116.72   |
| 90  | ii    | 501 | ZVM  | C02-C15-N02 | 2.48  | 119.16      | 116.89   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 90  | ii    | 501 | ZVM  | C04  |
| 90  | ii    | 501 | ZVM  | C02  |

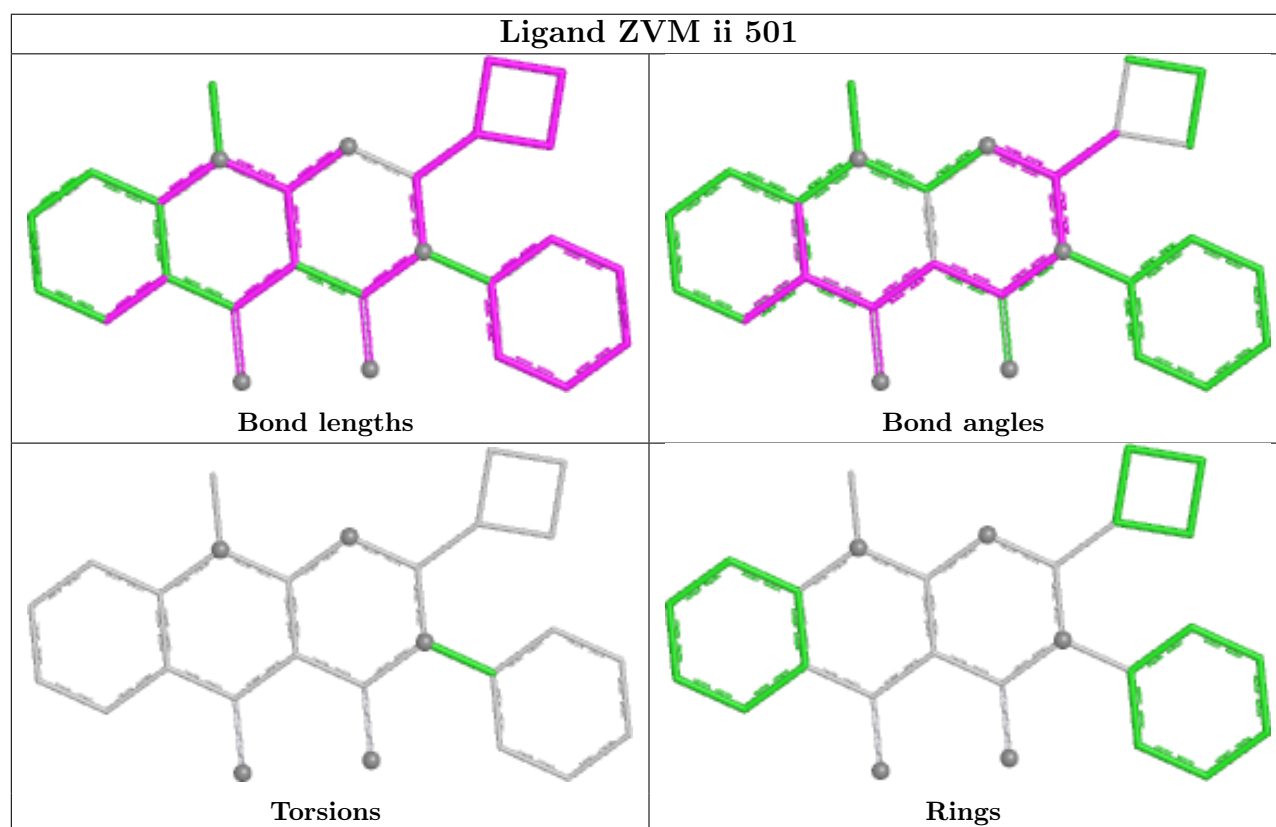
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 91  | jj    | 601 | SF4  | 4       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 48  | 5     | 23               |
| 51  | 9     | 3                |
| 47  | 3     | 2                |
| 46  | 2     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | 5     | 2113:G    | O3'    | 2258:C    | P      | 41.98        |
| 1     | 5     | 1219:G    | O3'    | 1233:G    | P      | 19.96        |
| 1     | 5     | 1406(C):G | O3'    | 1411:C    | P      | 16.99        |
| 1     | 5     | 1696:C    | O3'    | 1720:C    | P      | 16.41        |
| 1     | 5     | 990:C     | O3'    | 1064:G    | P      | 15.53        |
| 1     | 5     | 523:C     | O3'    | 638:G     | P      | 15.09        |
| 1     | 5     | 4138:C    | O3'    | 4146:G    | P      | 15.05        |
| 1     | 5     | 1364:U    | O3'    | 1368:A    | P      | 14.32        |
| 1     | 5     | 4777:C    | O3'    | 4859:C    | P      | 14.25        |
| 1     | 5     | 4101:C    | O3'    | 4107:G    | P      | 13.97        |
| 1     | 5     | 5022:U    | O3'    | 5028:G    | P      | 13.74        |
| 1     | 5     | 182:G     | O3'    | 189:G     | P      | 13.69        |
| 1     | 5     | 760:G     | O3'    | 904:C     | P      | 13.62        |
| 1     | 5     | 2901:G    | O3'    | 3597:G    | P      | 12.67        |
| 1     | 5     | 3948:C    | O3'    | 4065:G    | P      | 12.45        |
| 1     | 9     | 890:U     | O3'    | 894:G     | P      | 12.31        |
| 1     | 5     | 1180:C    | O3'    | 1183:C    | P      | 9.35         |
| 1     | 5     | 4729:A    | O3'    | 4735:G    | P      | 8.97         |
| 1     | 5     | 1980:U    | O3'    | 1981:G    | P      | 7.17         |
| 1     | 5     | 1981:G    | O3'    | 1982:G    | P      | 6.96         |
| 1     | 5     | 512:U     | O3'    | 515:C     | P      | 6.64         |
| 1     | 5     | 4740:G    | O3'    | 4743:G    | P      | 6.62         |
| 1     | 5     | 500:G     | O3'    | 504:G     | P      | 6.28         |
| 1     | 3     | 19:G      | O3'    | 20:U      | P      | 5.95         |
| 1     | 3     | 16:C      | O3'    | 18:U      | P      | 5.54         |
| 1     | 2     | 16:C      | O3'    | 18:G      | P      | 5.42         |
| 1     | 5     | 1100:U    | O3'    | 1168:G    | P      | 4.14         |
| 1     | 9     | 873:G     | O3'    | 874:G     | P      | 3.50         |
| 1     | 9     | 900:C     | O3'    | 901:G     | P      | 3.23         |

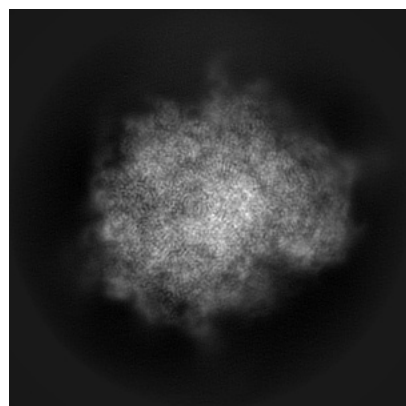
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40344. These allow visual inspection of the internal detail of the map and identification of artifacts.

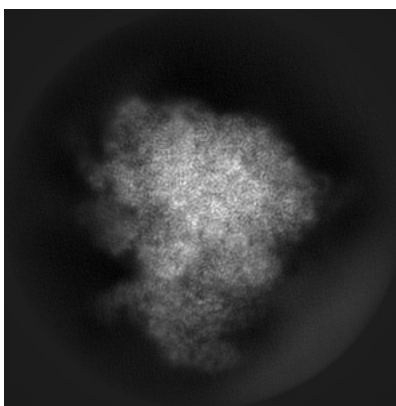
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

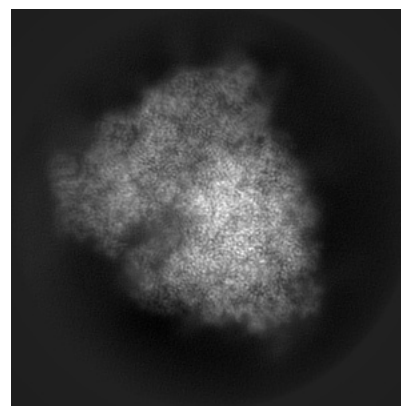
#### 6.1.1 Primary map



X

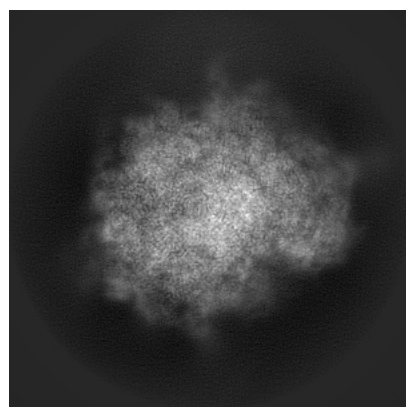


Y

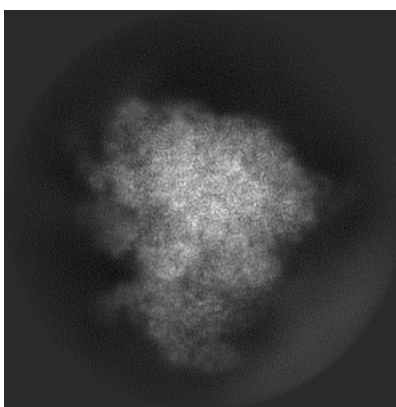


Z

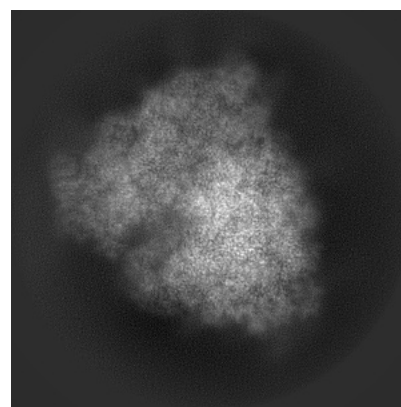
#### 6.1.2 Raw map



X



Y

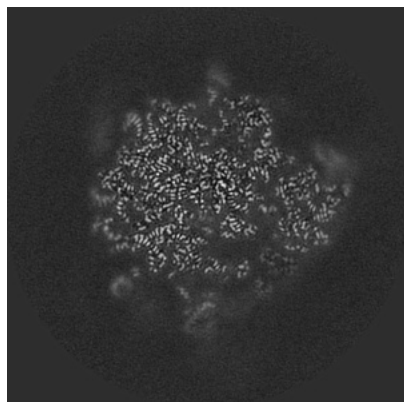


Z

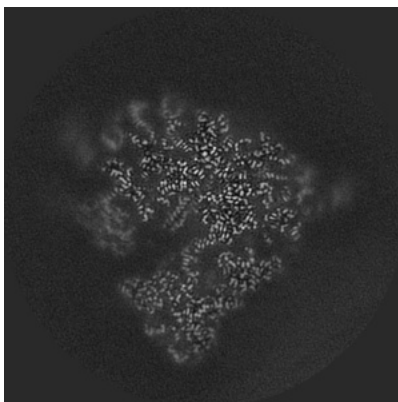
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

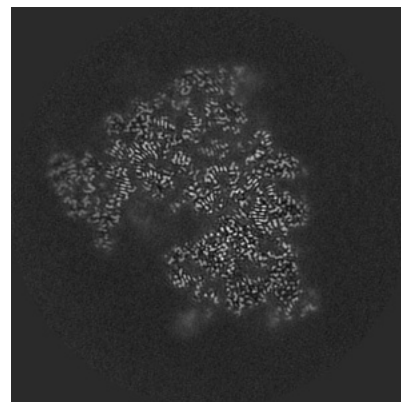
### 6.2.1 Primary map



X Index: 240

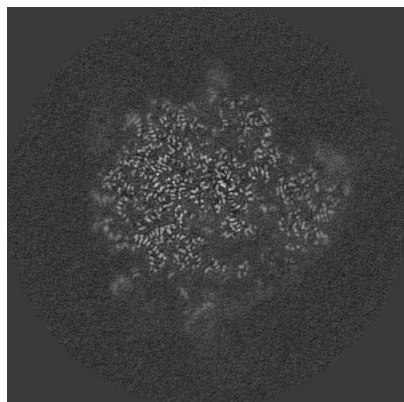


Y Index: 240

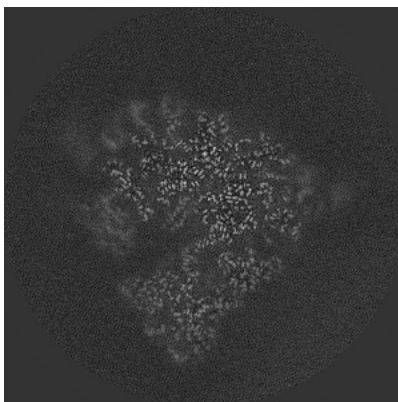


Z Index: 240

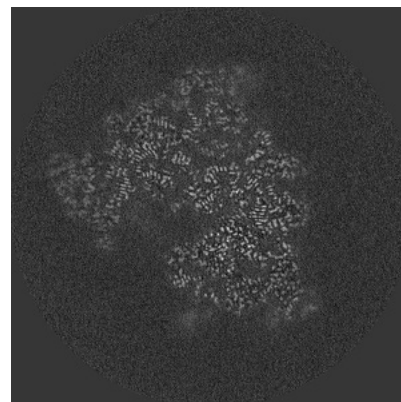
### 6.2.2 Raw map



X Index: 240



Y Index: 240

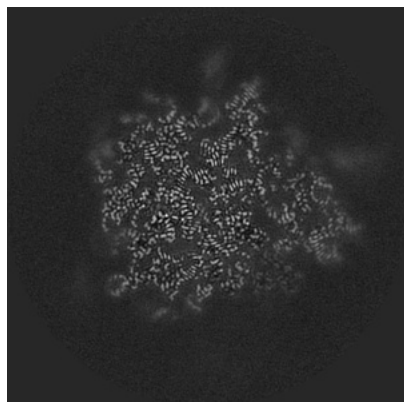


Z Index: 240

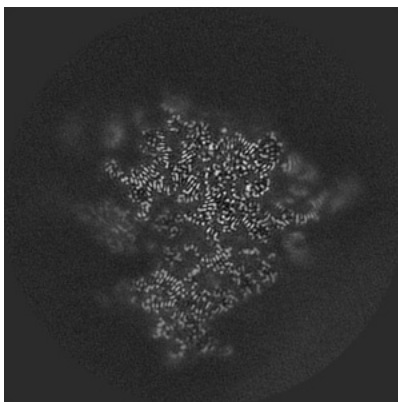
The images above show central slices of the map in three orthogonal directions.

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

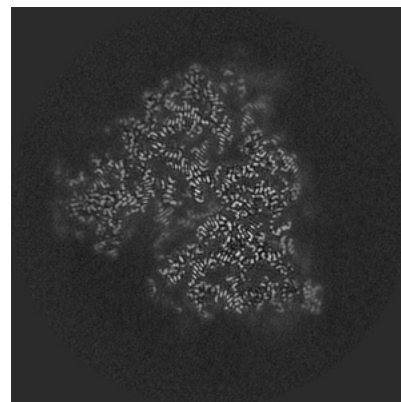
### 6.3.1 Primary map



X Index: 261

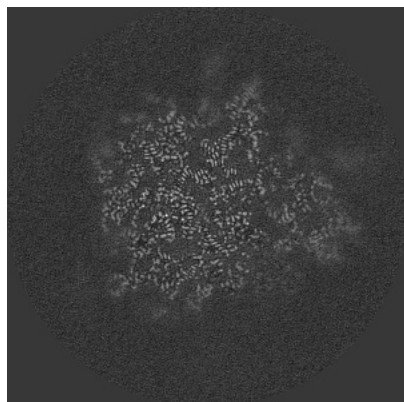


Y Index: 250

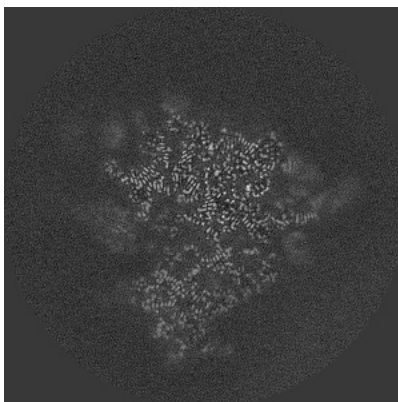


Z Index: 227

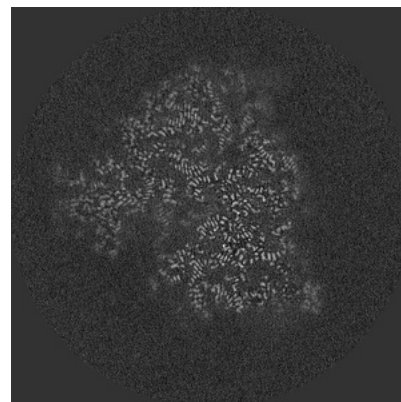
### 6.3.2 Raw map



X Index: 261



Y Index: 250

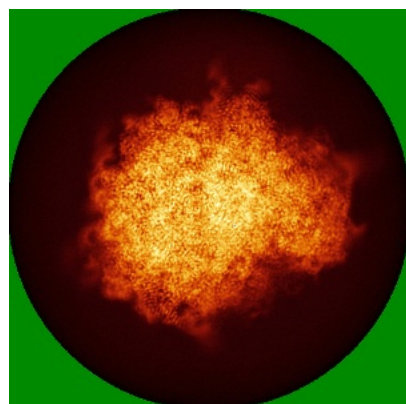


Z Index: 228

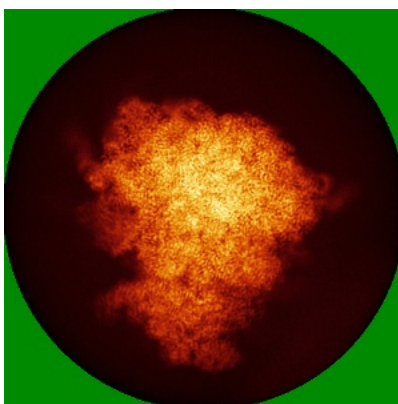
The images above show the largest variance slices of the map in three orthogonal directions.

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

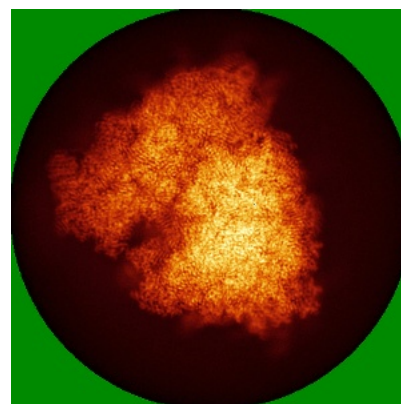
### 6.4.1 Primary map



X

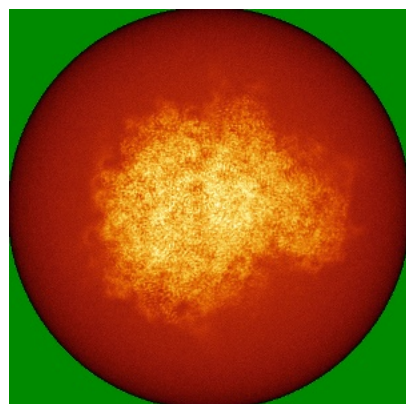


Y

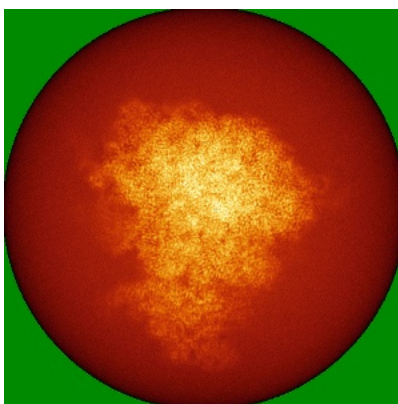


Z

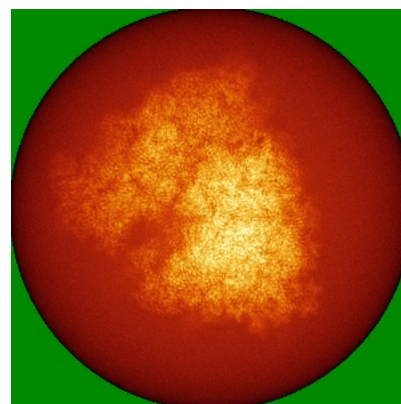
### 6.4.2 Raw map



X



Y

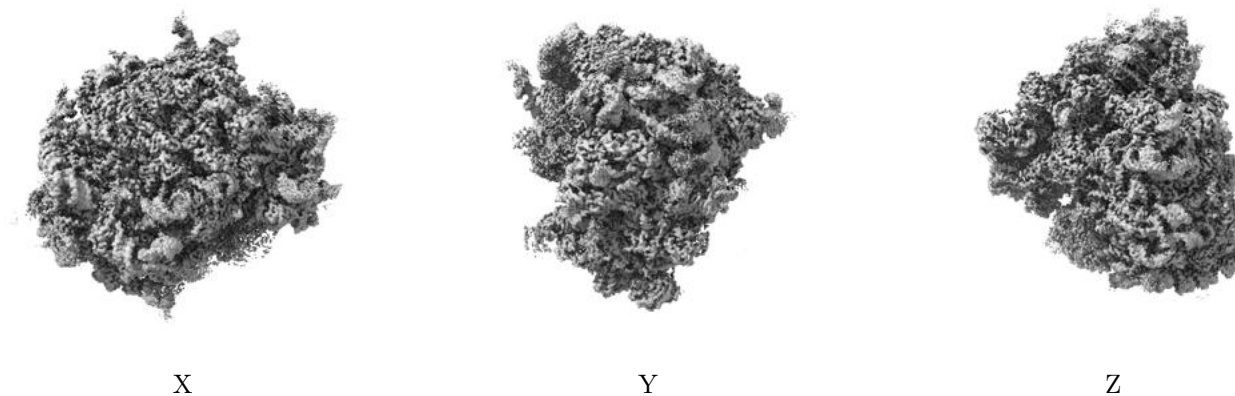


Z

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.

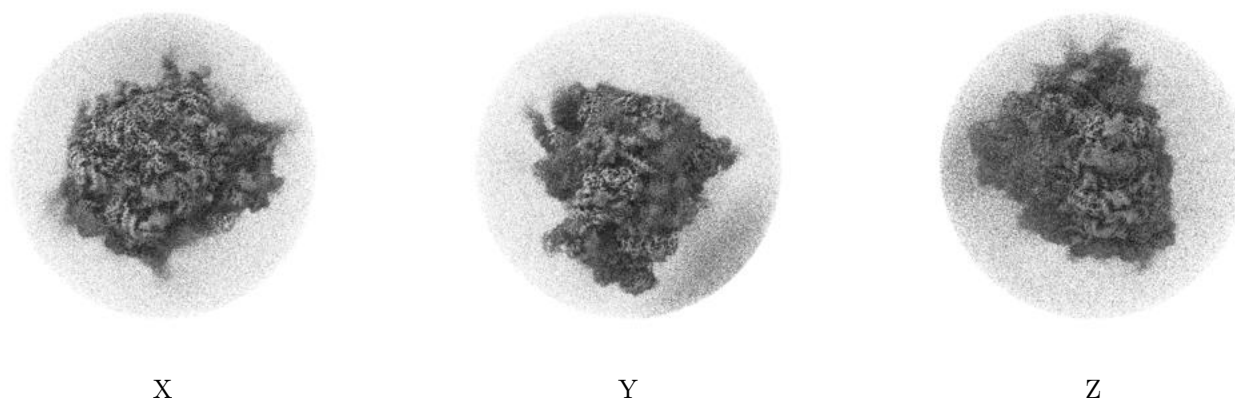
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

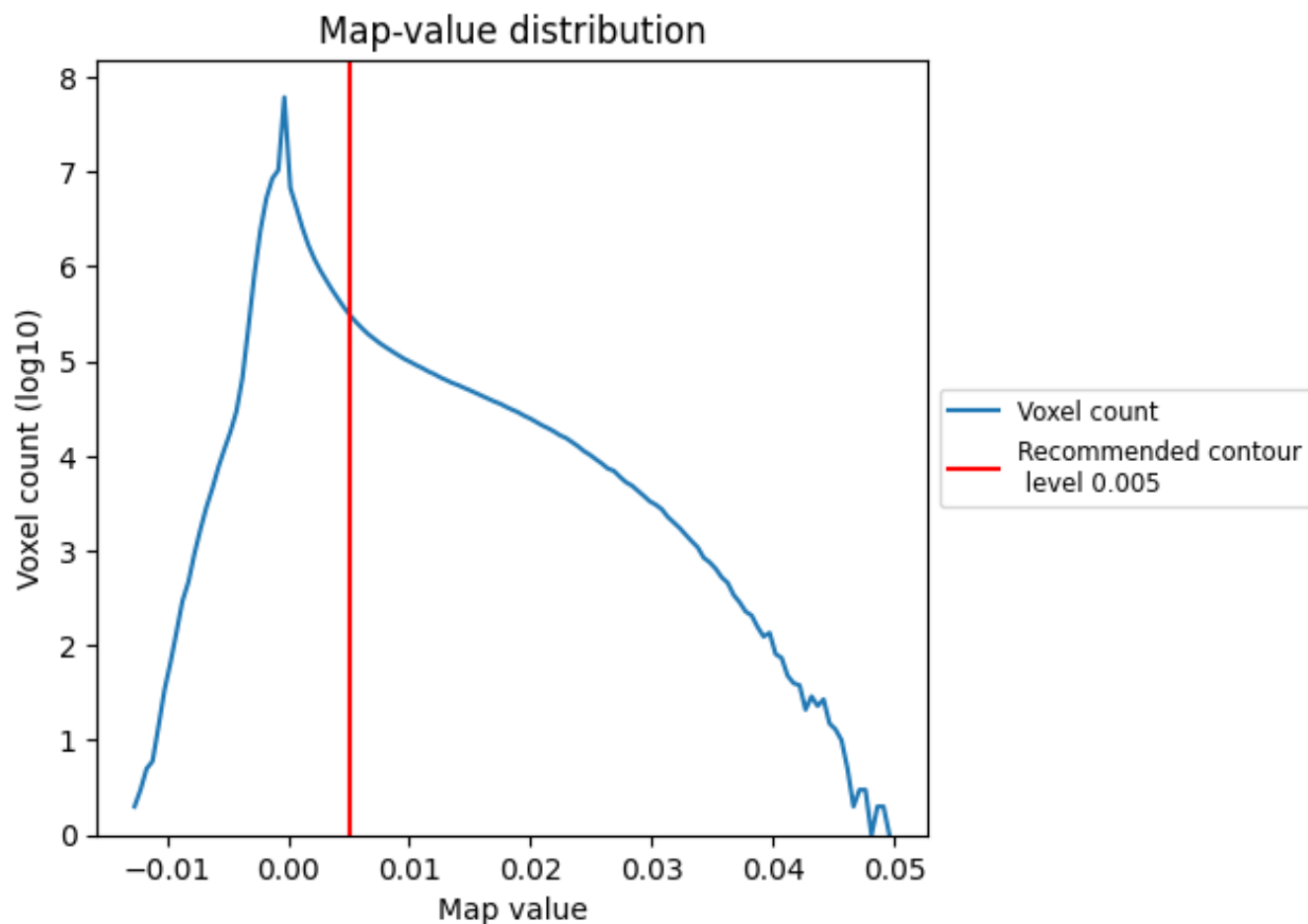
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

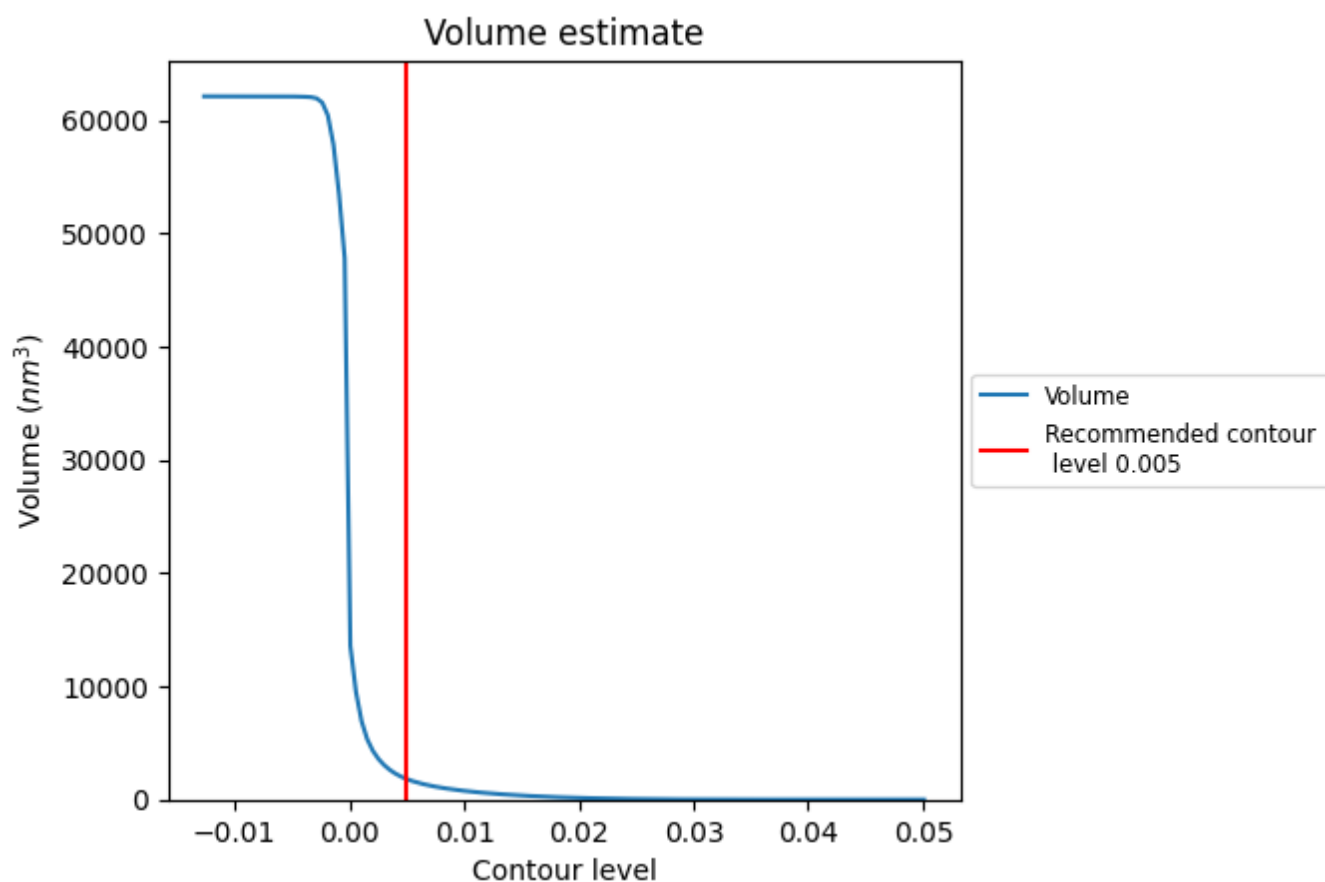
This section contains the results of statistical analysis of the map.

### 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.

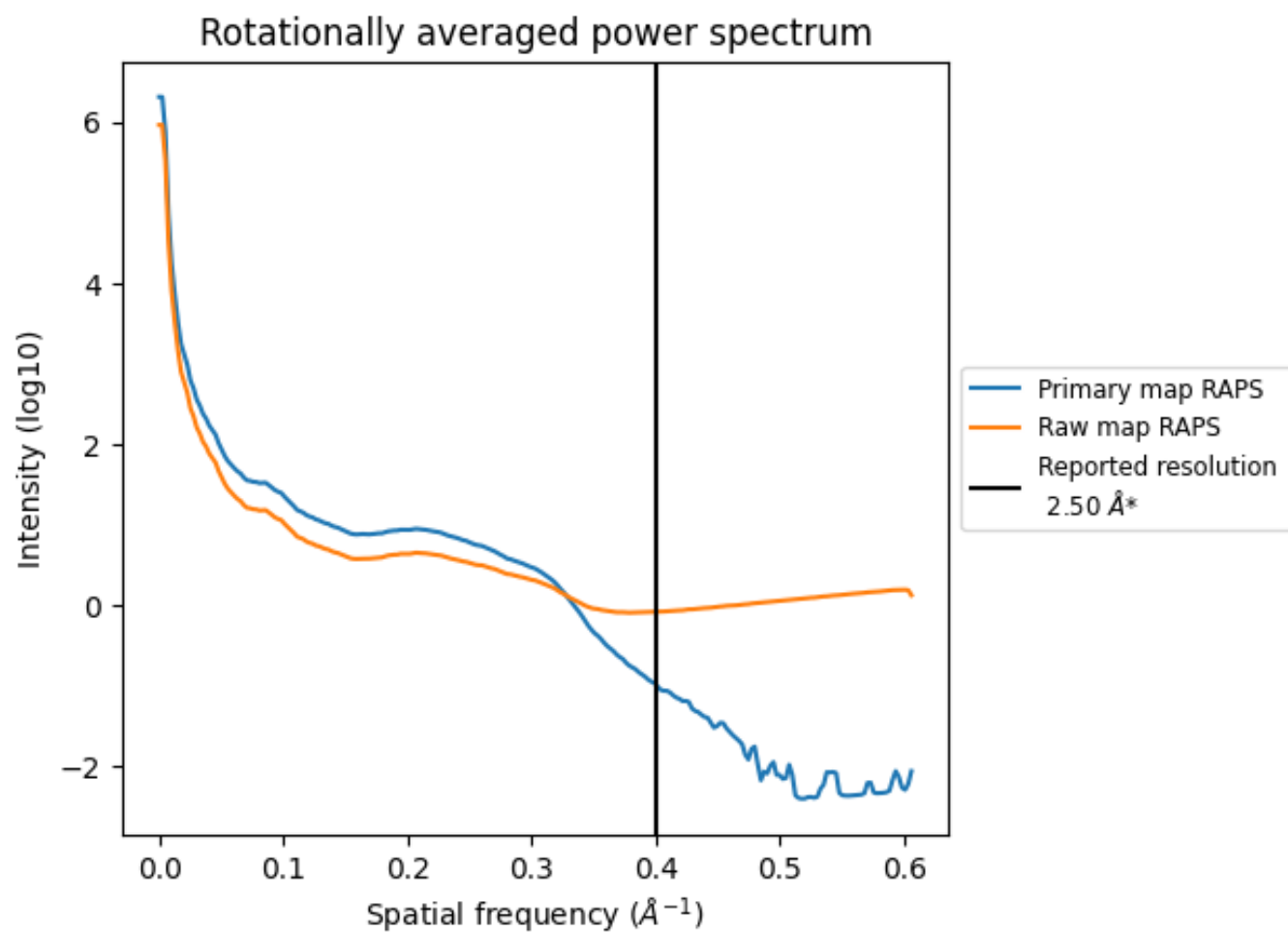
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1812 nm<sup>3</sup>; this corresponds to an approximate mass of 1637 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 ⓘ

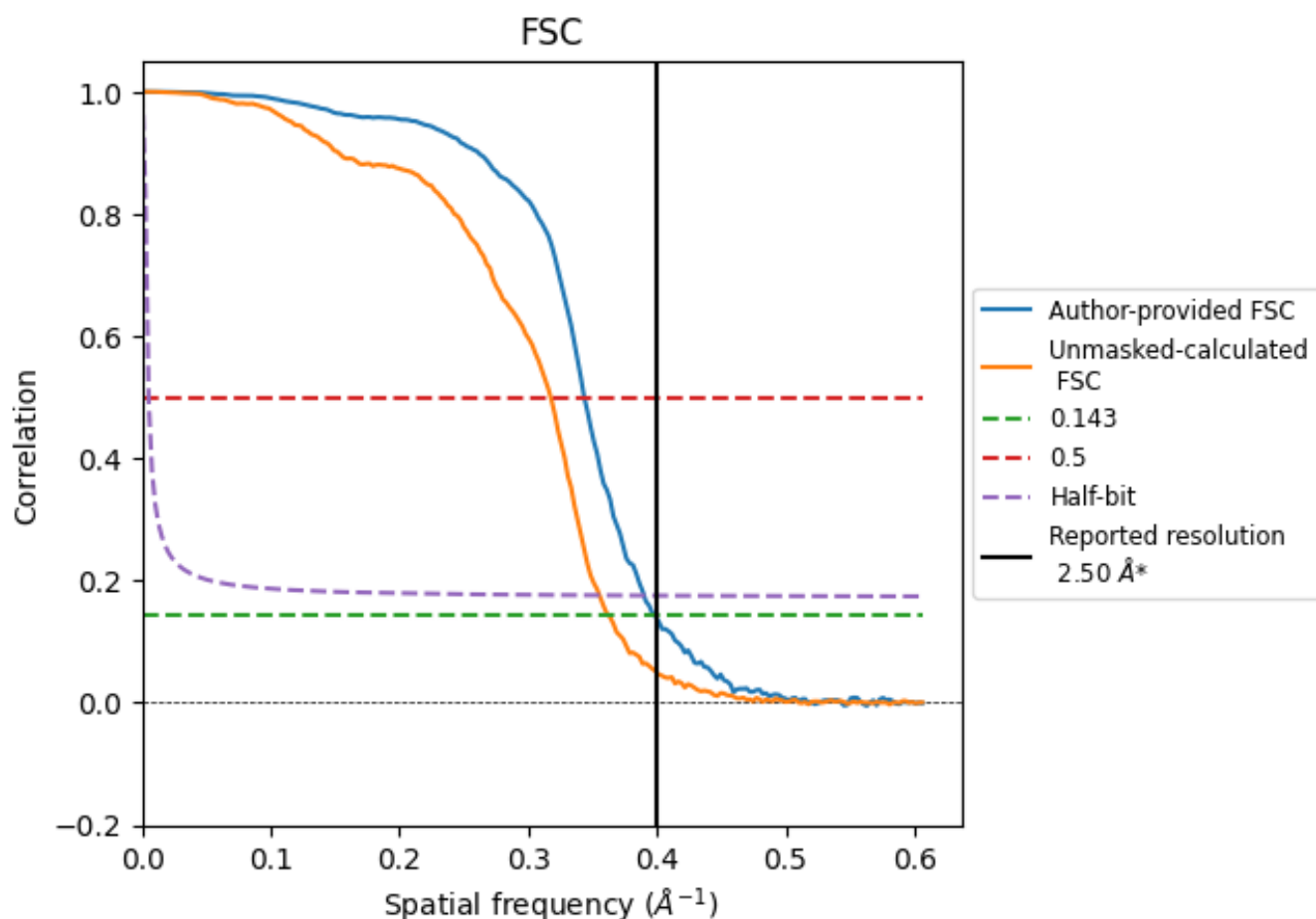


\*Reported resolution corresponds to spatial frequency of 0.400 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.400 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

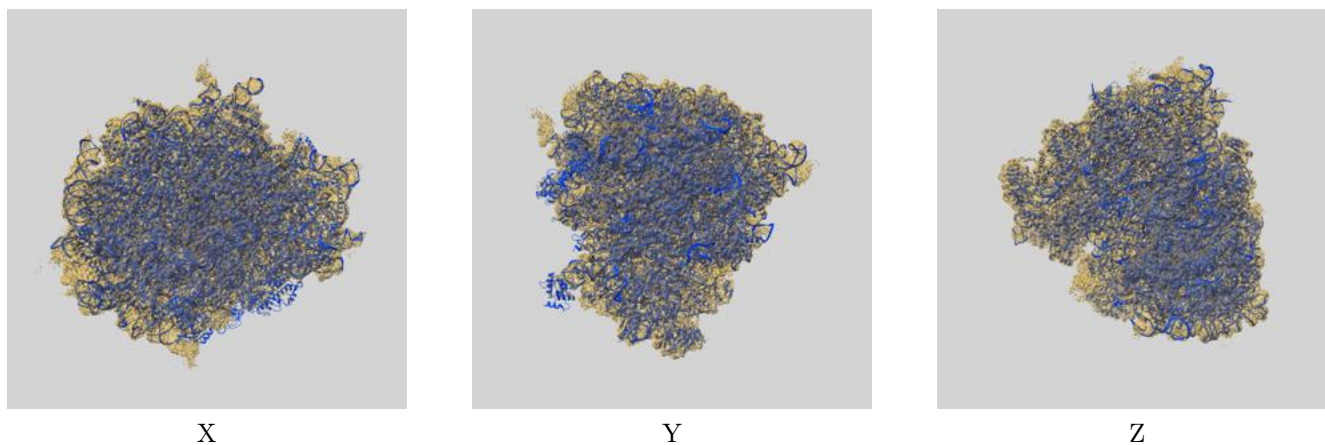
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.50                               | -    | -        |
| Author-provided FSC curve | 2.51                               | 2.91 | 2.56     |
| Unmasked-calculated*      | 2.76                               | 3.15 | 2.81     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.76 differs from the reported value 2.5 by more than 10 %

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

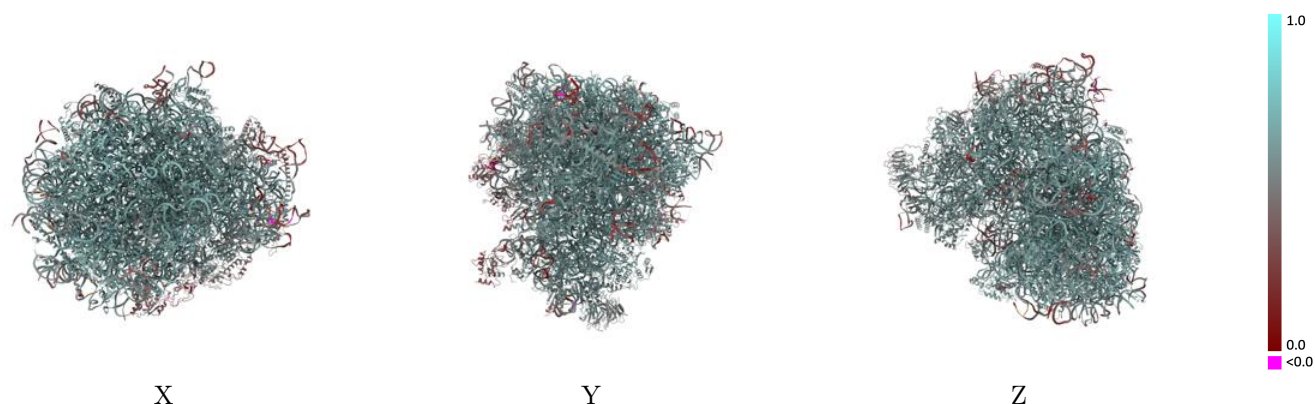
This section contains information regarding the fit between EMDB map EMD-40344 and PDB model 8SCB. Per-residue inclusion information can be found in section [3](#) on page [27](#).

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



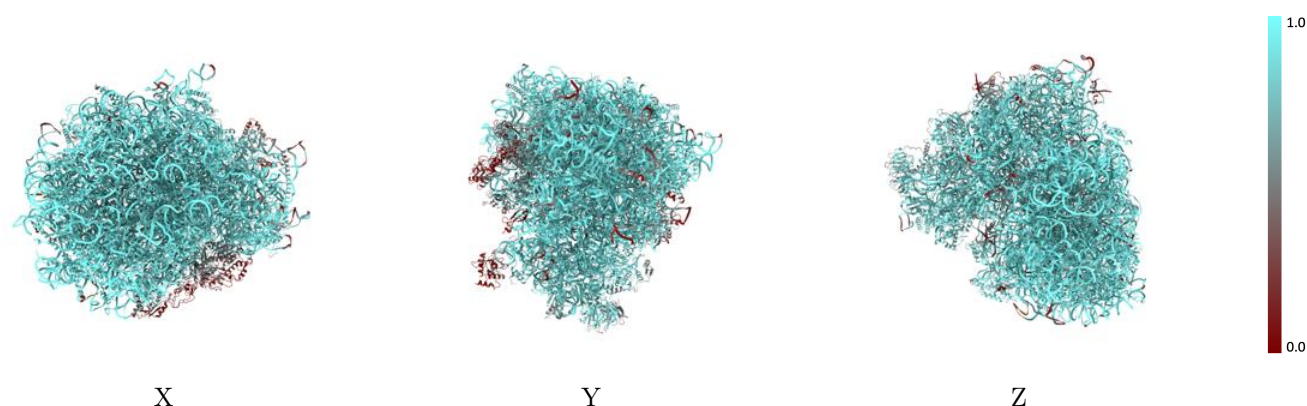
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



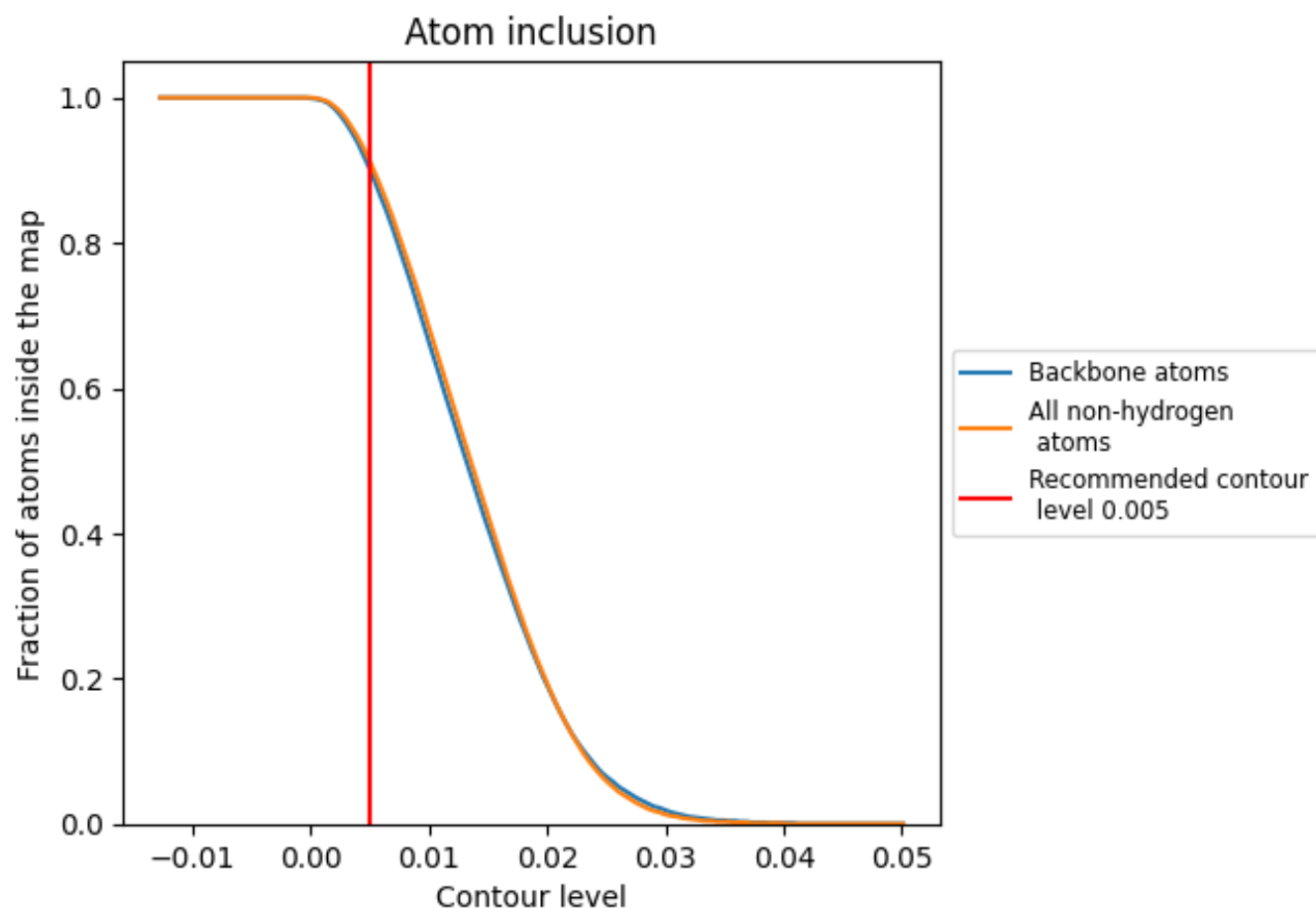
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.005) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9140   |  0.5890   |
| 1     |  0.9590   |  0.6230   |
| 2     |  0.9490   |  0.5410   |
| 3     |  0.5710   |  0.3940   |
| 5     |  0.9750   |  0.6070   |
| 7     |  0.9950   |  0.6350   |
| 8     |  0.9630   |  0.6010   |
| 9     |  0.9380   |  0.5680   |
| A     |  0.9860   |  0.6570   |
| AA    |  0.8810   |  0.5860   |
| B     |  0.9700   |  0.6410   |
| BB    |  0.9000   |  0.5920   |
| C     |  0.9670   |  0.6410   |
| CC    |  0.9270   |  0.6040   |
| D     |  0.9380  |  0.6090  |
| DD    |  0.8180 |  0.5420 |
| E     |  0.9520 |  0.6100 |
| EE    |  0.9280 |  0.5870 |
| F     |  0.9690 |  0.6450 |
| FF    |  0.9060 |  0.5780 |
| G     |  0.9140 |  0.5970 |
| GG    |  0.7990 |  0.5030 |
| H     |  0.9330 |  0.6160 |
| HH    |  0.5830 |  0.4750 |
| I     |  0.9590 |  0.6300 |
| II    |  0.8730 |  0.5680 |
| J     |  0.9180 |  0.5910 |
| JJ    |  0.9020 |  0.5760 |
| KK    |  0.8390 |  0.5400 |
| L     |  0.9210 |  0.6130 |
| LL    |  0.9440 |  0.6250 |
| M     |  0.9470 |  0.6130 |
| MM    |  0.1120 |  0.3190 |
| N     |  0.9900 |  0.6560 |
| NN    |  0.9280 |  0.6010 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| O     |  0.9690   |  0.6370   |
| OO    |  0.9570   |  0.6170   |
| P     |  0.9640   |  0.6460   |
| PP    |  0.8780   |  0.5590   |
| Q     |  0.9730   |  0.6490   |
| QQ    |  0.9080   |  0.5780   |
| R     |  0.9000   |  0.6030   |
| RR    |  0.7450   |  0.5440   |
| S     |  0.9760   |  0.6450   |
| SS    |  0.8830   |  0.5660   |
| T     |  0.9440   |  0.6210   |
| TT    |  0.9120   |  0.5790   |
| U     |  0.8820   |  0.5490   |
| UU    |  0.7490   |  0.5170   |
| V     |  0.9730   |  0.6440   |
| VV    |  0.8760   |  0.5780   |
| W     |  0.9490   |  0.6300   |
| WW    |  0.9550  |  0.6150  |
| X     |  0.9530 |  0.6240 |
| XX    |  0.9590 |  0.6230 |
| Y     |  0.9390 |  0.6220 |
| YY    |  0.8960 |  0.5620 |
| Z     |  0.9460 |  0.6140 |
| ZZ    |  0.8430 |  0.5540 |
| a     |  0.9660 |  0.6480 |
| aa    |  0.9420 |  0.6160 |
| b     |  0.8450 |  0.5830 |
| bb    |  0.8470 |  0.5730 |
| c     |  0.9440 |  0.6220 |
| cc    |  0.8400 |  0.5680 |
| d     |  0.9650 |  0.6330 |
| dd    |  0.9490 |  0.5990 |
| e     |  0.9830 |  0.6530 |
| ee    |  0.9060 |  0.5680 |
| f     |  0.9790 |  0.6560 |
| ff    |  0.2530 |  0.3490 |
| g     |  0.9350 |  0.6170 |
| gg    |  0.7550 |  0.5030 |
| h     |  0.9380 |  0.6160 |
| hh    |  0.9920 |  0.6100 |
| i     |  0.9210 |  0.6070 |
| ii    |  0.7390 |  0.5290 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| j     |  0.9940 |  0.6520 |
| jj    |  0.4420 |  0.5120 |
| k     |  0.8460 |  0.5750 |
| l     |  0.9860 |  0.6370 |
| m     |  0.9490 |  0.6270 |
| n     |  0.9750 |  0.6320 |
| o     |  0.9610 |  0.6380 |
| p     |  0.9580 |  0.6370 |
| r     |  0.9660 |  0.6340 |
| s     |  0.1770 |  0.2900 |
| t     |  0.4670 |  0.3450 |