



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:28 AM GMT

PDB ID : 3F1F  
Title : Crystal structure of a translation termination complex formed with release factor RF2. This file contains the 50S subunit of one 70S ribosome. The entire crystal structure contains two 70S ribosomes as described in remark 400.  
Authors : Korostelev, A.; Asahara, H.; Lancaster, L.; Laurberg, M.; Hirschi, A.; Noller, H.F.  
Deposited on : 2008-10-27  
Resolution : 3.00 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

---

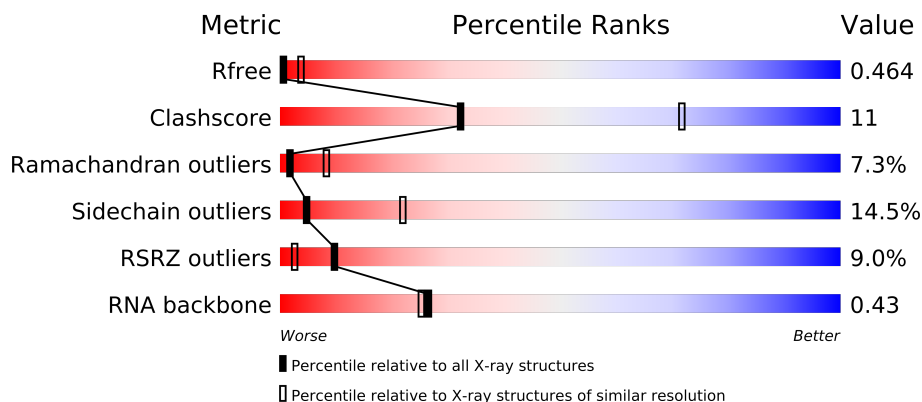
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 Å.

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












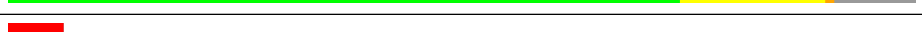




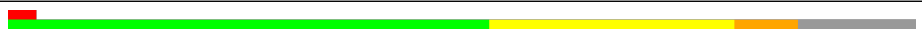
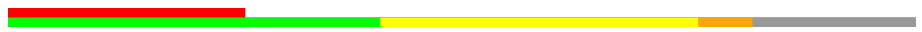



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 1216 (3.00-3.00)                                      |
| Clashscore            | 79885                       | 1594 (3.00-3.00)                                      |
| Ramachandran outliers | 78287                       | 1537 (3.00-3.00)                                      |
| Sidechain outliers    | 78261                       | 1540 (3.00-3.00)                                      |
| RSRZ outliers         | 66119                       | 1217 (3.00-3.00)                                      |
| RNA backbone          | 1838                        | 1070 (3.50-2.50)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 2894   |                  |
| 2   | B     | 124    |                  |
| 3   | D     | 276    |                  |
| 4   | E     | 206    |                  |
| 5   | F     | 210    |                  |
| 6   | G     | 182    |                  |
| 7   | H     | 180    |                  |
| 8   | I     | 148    |                  |
| 9   | K     | 147    |                  |
| 10  | N     | 163    |                  |
| 11  | O     | 122    |                  |
| 12  | P     | 150    |                  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 13  | Q     | 141    |   |
| 14  | R     | 118    |   |
| 15  | S     | 112    |   |
| 16  | T     | 146    |   |
| 17  | U     | 118    |   |
| 18  | V     | 101    |   |
| 19  | W     | 113    |   |
| 20  | X     | 96     |   |
| 21  | Y     | 110    |   |
| 22  | Z     | 206    |   |
| 23  | 0     | 85     |   |
| 24  | 1     | 98     |   |
| 25  | 2     | 72     |   |
| 26  | 3     | 60     |   |
| 27  | 4     | 97     |   |
| 28  | 5     | 60     |   |
| 29  | 6     | 54     |   |
| 30  | 7     | 49     |   |
| 31  | 8     | 65     |  |

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 92692 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1   | A     | 2879     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61997 | 27594 | 11582 | 19943 | 2878 |         |         |       |

- Molecule 2 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2   | B     | 119      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2551  | 1136 | 471 | 826 | 118 |         |         |       |

- Molecule 3 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | D     | 271      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2104  | 1329 | 416 | 356 | 3 |         |         |       |

- Molecule 4 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | E     | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1563  | 988 | 299 | 270 | 6 |         |         |       |

- Molecule 5 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | F     | 202      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1586  | 1011 | 297 | 275 | 3 |         |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| F     | 1       | MET      | -      | INSERTION | UNP Q72I05 |
| F     | 2       | LYS      | -      | INSERTION | UNP Q72I05 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| F     | 3       | GLU      | -      | INSERTION | UNP Q72I05 |
| F     | 4       | VAL      | -      | INSERTION | UNP Q72I05 |
| F     | 5       | ALA      | -      | INSERTION | UNP Q72I05 |

- Molecule 6 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | G     | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1475  | 943 | 268 | 260 | 4 |         |         |       |

- Molecule 7 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | H     | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1222  | 773 | 228 | 220 | 1 |         |         |       |

- Molecule 8 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | I     | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 200 | 207 | 1 |         |         |       |

- Molecule 9 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | K     | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1088  | 692 | 191 | 199 | 6 |         |         |       |

- Molecule 10 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | N     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1096  | 707 | 205 | 181 | 3 |         |         |       |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| N     | 1       | MET      | -      | INSERTION | UNP Q72IN1 |
| N     | 2       | VAL      | -      | INSERTION | UNP Q72IN1 |
| N     | 3       | LYS      | -      | INSERTION | UNP Q72IN1 |
| N     | 4       | SER      | -      | INSERTION | UNP Q72IN1 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| N     | 5       | SER      | -      | INSERTION | UNP Q72IN1 |
| N     | 6       | LEU      | -      | INSERTION | UNP Q72IN1 |
| N     | 7       | ALA      | -      | INSERTION | UNP Q72IN1 |
| N     | 8       | PHE      | -      | INSERTION | UNP Q72IN1 |
| N     | 9       | LEU      | -      | INSERTION | UNP Q72IN1 |
| N     | 10      | ARG      | -      | INSERTION | UNP Q72IN1 |
| N     | 11      | GLY      | -      | INSERTION | UNP Q72IN1 |
| N     | 12      | PRO      | -      | INSERTION | UNP Q72IN1 |
| N     | 13      | PRO      | -      | INSERTION | UNP Q72IN1 |
| N     | 14      | ILE      | -      | INSERTION | UNP Q72IN1 |
| N     | 15      | PRO      | -      | INSERTION | UNP Q72IN1 |
| N     | 16      | ARG      | -      | INSERTION | UNP Q72IN1 |
| N     | 17      | GLN      | -      | INSERTION | UNP Q72IN1 |
| N     | 18      | GLU      | -      | INSERTION | UNP Q72IN1 |
| N     | 19      | GLN      | -      | INSERTION | UNP Q72IN1 |
| N     | 20      | ARG      | -      | INSERTION | UNP Q72IN1 |
| N     | 21      | ARG      | -      | INSERTION | UNP Q72IN1 |
| N     | 22      | ALA      | -      | INSERTION | UNP Q72IN1 |
| N     | 23      | LEU      | -      | INSERTION | UNP Q72IN1 |
| N     | 24      | VAL      | -      | INSERTION | UNP Q72IN1 |

- Molecule 11 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | O     | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 932   | 587 | 171 | 170 | 4 |         |         |       |

- Molecule 12 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | P     | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1114  | 692 | 227 | 193 | 2 |         |         |       |

- Molecule 13 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | Q     | 134      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1064  | 680 | 201 | 178 | 5 |         |         |       |

- Molecule 14 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 14  | R     | 117      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |         |         |       |

- Molecule 15 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 15  | S     | 98       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 770   | 486 | 154 | 130 |         |         |       |

- Molecule 16 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | T     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1143  | 713 | 234 | 195 | 1 |         |         |       |

- Molecule 17 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | U     | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |         |       |

- Molecule 18 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18  | V     | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |

- Molecule 19 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | W     | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 890   | 560 | 175 | 153 | 2 |         |         |       |

- Molecule 20 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 20  | X     | 92       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |         |         |       |

- Molecule 21 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | Y     | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 775   | 500 | 148 | 123 | 4 |         |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | Z     | 187      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1482  | 945 | 264 | 271 | 2 |         |         |       |

- Molecule 23 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23  | 0     | 76       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 605   | 376 | 126 | 102 | 1 |         |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 24  | 1     | 88       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 694   | 435 | 141 | 118 |  |         |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 25  | 2     | 62       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 520   | 325 | 102 | 91 | 2 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26  | 3     | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 467   | 298 | 90 | 78 | 1 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27  | 4     | 30       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 225   | 142 | 36 | 43 | 4 |         |         |       |

There are 27 discrepancies between the modelled and reference sequences:



| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| 4     | 1       | MET      | -      | INSERTION | UNP Q72JR0 |
| 4     | 2       | PRO      | -      | INSERTION | UNP Q72JR0 |
| 4     | 3       | LEU      | -      | INSERTION | UNP Q72JR0 |
| 4     | 4       | GLY      | -      | INSERTION | UNP Q72JR0 |
| 4     | 5       | VAL      | -      | INSERTION | UNP Q72JR0 |
| 4     | 6       | HIS      | -      | INSERTION | UNP Q72JR0 |
| 4     | 7       | PRO      | -      | INSERTION | UNP Q72JR0 |
| 4     | 8       | LEU      | -      | INSERTION | UNP Q72JR0 |
| 4     | 9       | TYR      | -      | INSERTION | UNP Q72JR0 |
| 4     | 10      | THR      | -      | INSERTION | UNP Q72JR0 |
| 4     | 11      | LYS      | -      | INSERTION | UNP Q72JR0 |
| 4     | 12      | ARG      | -      | INSERTION | UNP Q72JR0 |
| 4     | 13      | TRP      | -      | INSERTION | UNP Q72JR0 |
| 4     | 14      | LEU      | -      | INSERTION | UNP Q72JR0 |
| 4     | 15      | ALA      | -      | INSERTION | UNP Q72JR0 |
| 4     | 16      | HIS      | -      | INSERTION | UNP Q72JR0 |
| 4     | 17      | GLY      | -      | INSERTION | UNP Q72JR0 |
| 4     | 18      | GLN      | -      | INSERTION | UNP Q72JR0 |
| 4     | 19      | ASP      | -      | INSERTION | UNP Q72JR0 |
| 4     | 20      | ARG      | -      | INSERTION | UNP Q72JR0 |
| 4     | 21      | ALA      | -      | INSERTION | UNP Q72JR0 |
| 4     | 22      | LYS      | -      | INSERTION | UNP Q72JR0 |
| 4     | 23      | LYS      | -      | INSERTION | UNP Q72JR0 |
| 4     | 24      | GLU      | -      | INSERTION | UNP Q72JR0 |
| 4     | 25      | ALA      | -      | INSERTION | UNP Q72JR0 |
| 4     | 26      | ASN      | -      | INSERTION | UNP Q72JR0 |
| 4     | 27      | VAL      | -      | INSERTION | UNP Q72JR0 |

- Molecule 28 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28  | 5     | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 404   | 255 | 79 | 65 | 5 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29  | 6     | 44       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 380   | 235 | 77 | 64 | 4 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 30  | 7     | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 257 | 104 | 55 | 2 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 31  | 8     | 63       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 507   | 326 | 101 | 78 | 2 |         |         |       |

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 32  | P     | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 32  | K     | 3        | Total | Mg  | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 32  | B     | 35       | Total | Mg  | 0       | 0       |
|     |       |          | 35    | 35  |         |         |
| 32  | 6     | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 32  | W     | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 32  | N     | 4        | Total | Mg  | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 32  | X     | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 32  | 2     | 3        | Total | Mg  | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 32  | S     | 3        | Total | Mg  | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 32  | E     | 6        | Total | Mg  | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 32  | V     | 3        | Total | Mg  | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 32  | A     | 934      | Total | Mg  | 0       | 0       |
|     |       |          | 934   | 934 |         |         |
| 32  | 5     | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 32  | R     | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 32  | 1     | 6        | Total | Mg  | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 32  | D     | 7        | Total | Mg  | 0       | 0       |
|     |       |          | 7     | 7   |         |         |

*Continued on next page...*

*Continued from previous page...*

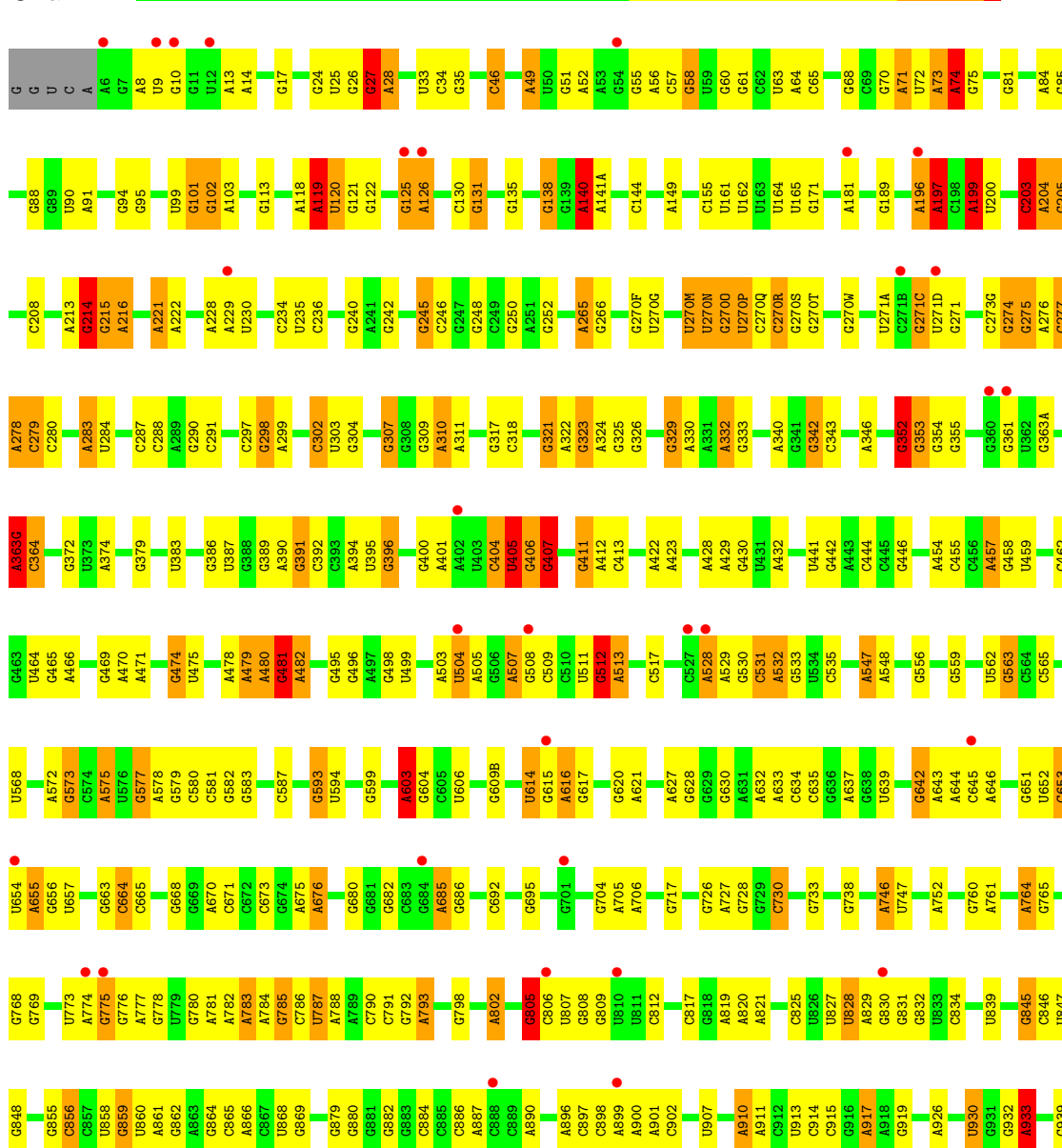
| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 32  | I     | 6        | Total<br>6 | Mg<br>6 | 0       | 0       |
| 32  | Z     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 32  | 4     | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 32  | U     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 32  | 0     | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 32  | G     | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 32  | Q     | 6        | Total<br>6 | Mg<br>6 | 0       | 0       |
| 32  | H     | 4        | Total<br>4 | Mg<br>4 | 0       | 0       |
| 32  | T     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 32  | 8     | 4        | Total<br>4 | Mg<br>4 | 0       | 0       |
| 32  | O     | 6        | Total<br>6 | Mg<br>6 | 0       | 0       |
| 32  | Y     | 3        | Total<br>3 | Mg<br>3 | 0       | 0       |
| 32  | F     | 6        | Total<br>6 | Mg<br>6 | 0       | 0       |

### 3 Residue-property plots

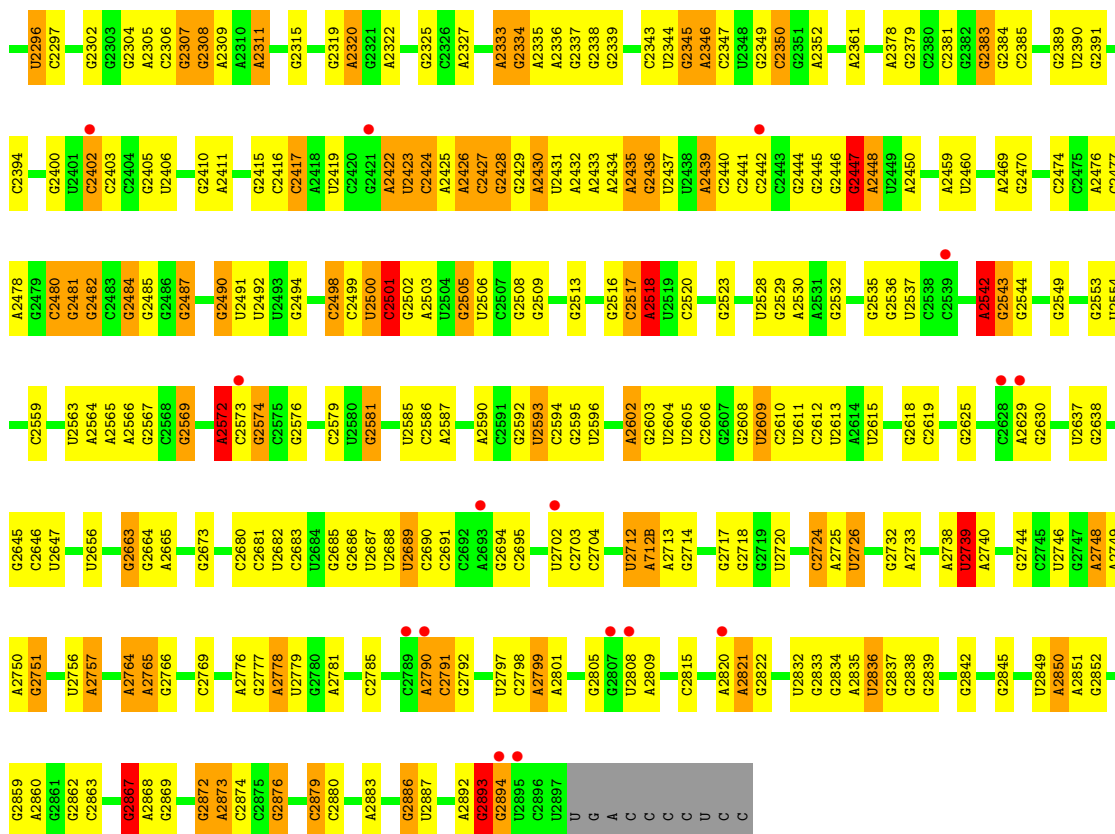
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: 23S rRNA

Chain A:

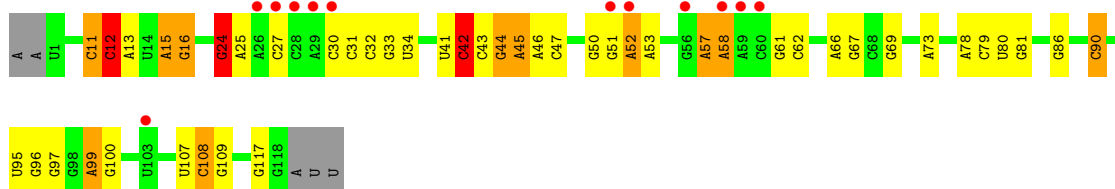


|       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| C2188 | G2110 | A2020 | C1934 | A1700 | C1599 | C1499 | A1395 | G1306 | A1210 | G1110 | U1023 | G940  |
| U2189 | C2111 | C2021 | G1935 | A1701 | C1600 | G1500 | U1396 | G1309 | U1211 | A1111 | G1024 | A941  |
| G2190 | G2112 | U2022 | A1936 | G1705 | G1601 | A1509 | A1397 | G1310 | G1212 | G1112 | U1025 | G942  |
| G2191 | U2113 | G2023 | A1937 | U1706 | U1602 | A1510 | C1399 | G1311 | G1216 | G1117 | U1026 | U943  |
|       | A2114 |       | A1938 | A1729 | C1604 | G1512 | U1405 | U1312 | G1215 | C1116 | A945  | A945  |
| U2197 | G2115 | U2028 | G1939 | U1730 | C1607 | G1513 | U1406 | U1313 | C1217 | A1126 | U1033 | G946  |
| A2198 | G2116 | G2029 | G1828 | A1731 | A1608 | G1519 | C1407 | G1314 | G1218 | A1127 | G1034 |       |
| A2199 | A2117 | A2030 | A1829 | U1732 | A1609 | G1520 | U1408 | A1322 | G1219 | A1128 | U1035 | A953  |
| C2205 | A2119 | C2032 | G1831 | A1733 | A1610 | G1525 | G1414 | U1323 | C1221 | A1129 | G1042 | G954  |
|       | G2120 | A2033 | U1833 | G1734 | G1613 | G1526 | U1415 | G1324 | U1130 | A1130 | C1043 | G956  |
| C2209 | G2121 | U2034 | G1945 | U1735 | A1614 | G1527 | G1416 | G1325 | G1227 | A1131 | A957  | A958  |
| G2210 | U2122 | G2035 | G1948 | C1741 | A1615 | G1528 | U1417 | U1329 | A1241 | U1132 | A1046 | A959  |
| A2212 | G2123 | C2036 | G1949 | G1742 | C1616 | A1528 | G1418 | C1330 | U1242 | U1133 | G1047 | A960  |
|       |       |       | G1950 | G1743 | A1616 | G1529 | G1419 | U1340 | G1244 | A1135 | C1049 | G961  |
| G2215 | A2126 | C2039 | U1951 | G1744 | C1617 | A1530 | U1420 | A1331 | G1245 | G1136 | A1050 |       |
| G2216 | G2127 | G2040 | A1952 | C1843 | A1618 | G1530 | G1421 | G1332 | A1247 | C1140 | G1051 | G964  |
|       | C2128 | C2043 | A1953 | G1750 | G1618 | G1531 | A1439 | C1333 | G1248 | U1141 | G1052 | G965  |
| A2225 | U2129 | C2044 | G1954 | G1754 | G1622 | U1534 | A1437 | G1338 | U1249 | U1142 | G1056 | G966  |
| G2226 | U2130 | U1955 | G1948 | A1847 | G1623 | U1535 | C1428 | U1339 | G1250 | A1143 | G1057 | G967  |
| G2228 | G2132 | G2049 | G1949 | A1848 | A1632 | A1536 | A1448 | G1340 | C1251 | A1144 | G1058 | G972  |
| C2229 | G2133 | U2050 | U1956 | G1761 | A1633 | C1537 | U1447 | U1341 | A1253 | G1144 | G1059 | A973  |
|       | A2134 | A2051 | G1763 | G1764 | G1634 | G1538 | G1449 | A1349 | A1254 | G1151 | U1060 | G974A |
| A2135 | G2135 | G2052 | U1864 | G1774 | G1635 | G1542 | A1498 | C1345 | U1255 | G1154 | U1061 | G974B |
|       | C2136 | G1968 | A1871 | G1775 | C1640 | A1543 | U1448 | G1346 | G1256 | A1155 | U1066 | G975  |
| G2235 | C2139 | A1969 | A1872 | G1776 | A1641 | A1545 | G1447 | G1347 | C1257 | G1160 | G976  | A977  |
| C2236 | G2145 | A1970 | G1878 | G1777 | G1642 | A1546 | G1448 | U1352 | A1262 | G1161 | A1069 | G978  |
| G2237 | C2146 | G1879 | C1877 | A1773 | G1643 | G1551 | A1498 | A1353 | U1263 | G1162 | G1071 | G979  |
| G2238 | G2147 | C1880 | G1774 | G1775 | C1644 | G1552 | A1451 | G1354 | G1264 | G1163 | C1072 | A980  |
| G2239 | G2148 | A1885 | U1775 | G1776 | G1647 | A1553 | C1451 | A1355 | A1265 | A1164 | G981  | A981  |
|       |       | C1886 | G1776 | G1777 | A1648 | G1554 | U1454 | G1356 | G1266 | U1165 | A1073 | G982  |
| U2243 | G2152 | U1889 | U1779 | U1779 | A1654 | G1556 | G1458 | U1357 | U1267 | G1170 | G1074 | A983  |
| U2245 | G2153 | A1889 | A1780 | C1781 | C1657 | C1557 | G1459 | A1358 | C1270 | G1171 | A1077 | G987  |
| G2246 | C2157 | G1839 | A1900 | A1784 | C1658 | A1558 | A1460 | A1360 | A1271 | U1175 | G1078 | A988  |
| G2247 | G2158 | A1901 | A1901 | A1785 | G1661 | G1566 | G1461 | A1365 | A1272 | G1176 | C1079 | A990  |
|       | C2161 | C1902 | G1902 | A1786 | G1662 | C1567 | G1465 | U1372 | U1273 | A1177 | A1085 | A996  |
| G2254 | G2166 | G1903 | G1903 | C1788 | A1668 | C1568 | G1466 | U1373 | A1274 | C1178 | G1087 | G997  |
|       |       | G1906 | G1907 | G1788 | A1669 | A1569 | C1467 | A1374 | A1275 | C1179 | A1088 | G998  |
| G2259 |       | G1907 | G1907 | A1791 | G1674 | A1570 | G1478 | C1375 | U1281 | G1183 | U1089 | U999  |
|       | A2169 | A1913 | A1913 | A1798 | G1678 | A1571 | G1479 | C1375 | U1282 | G1188 | U1090 | A1000 |
| A2273 | A2170 | C1914 | C1914 | U1798 | G1678 | C1574 | G1483 | A1378 | A1286 | U1188 | C1092 | G1003 |
| A2274 | U2172 | G1997 | G1997 | G1799 | G1678 | G1575 | U1483 | A1379 | A1287 | A1189 | U1097 | A1009 |
| G2275 | A2173 | C2085 | C2085 | G1800 | G1682 | U1576 | A1490 | G1380 | U1288 | G1190 | A1098 | A1010 |
| G2276 | C2174 | G2000 | G1920 | A1801 | C1683 | C1577 | G1491 | A1384 | C1289 | G1191 | G1099 | G1011 |
|       | G2175 | U2011 | G1921 | A1802 | U1693 | A1579 | G1492 | A1386 | U1294 | G1195 | C1100 | U1012 |
| A2279 | A2176 | G2012 | U1926 | C1803 | G1694 | C1585 | G1494 | G1386 | U1300 | A1204 | U1101 | C1013 |
| G2280 | C2083 | A2013 | A1927 | A1804 | G1695 | U1585 | A1494 | G1389 | A1301 | U1205 | G1104 | U1019 |
| C2281 | G2182 | A2014 | A1928 | G1811 | G1696 | U1590 | A1495 | G1390 | A1302 | C1208 | U1108 | A1020 |
| G2282 | C2183 | A2015 | G1929 | G1816 | G1697 | U1590 | A1496 | A1393 | G1303 | C1209 | C1109 | G1022 |
| C2283 | G2184 | G2018 | U1931 | U1818 | G1699 | C1598 | C1498 | U1394 |       |       |       |       |
| A2286 |       |       |       |       |       |       |       |       |       |       |       |       |
| A2287 |       |       |       |       |       |       |       |       |       |       |       |       |



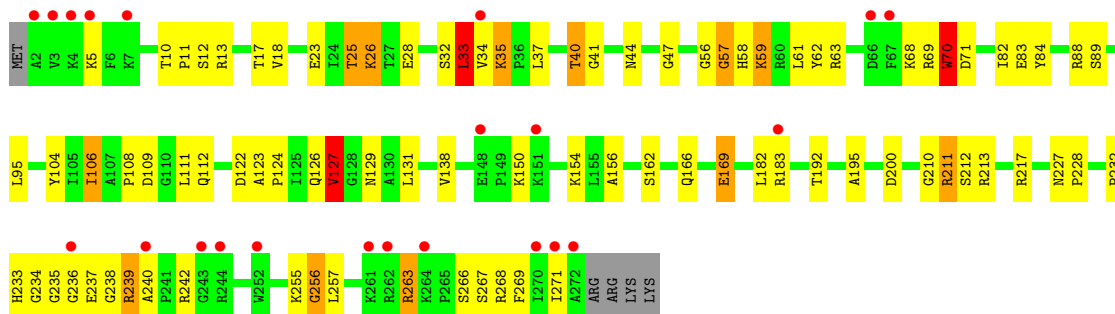
• Molecule 2: 5S rRNA

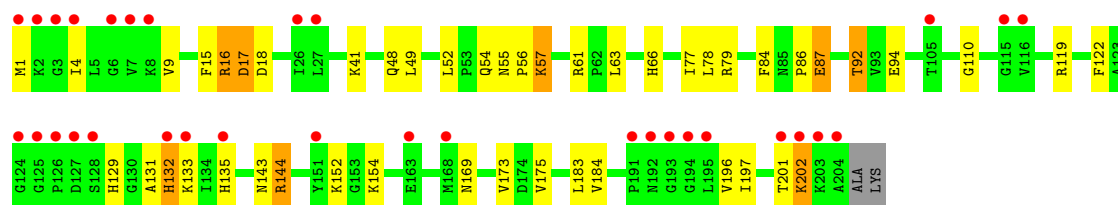
Chain B:



• Molecule 3: 50S ribosomal protein L2

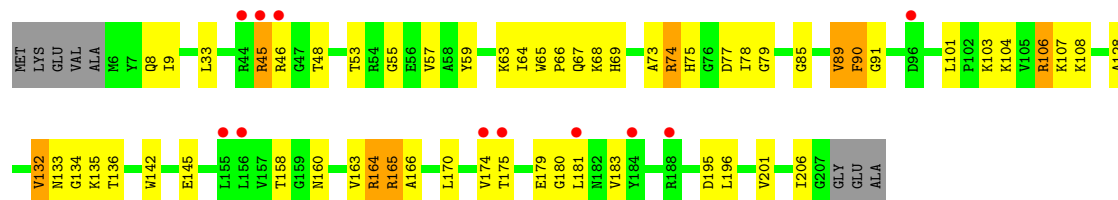
Chain D:





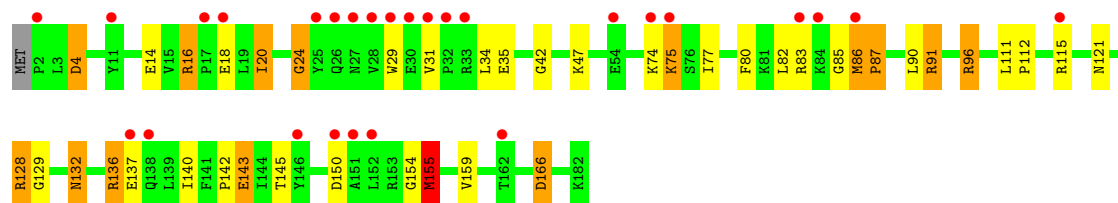
• Molecule 5: 50S ribosomal protein L4

Chain F:



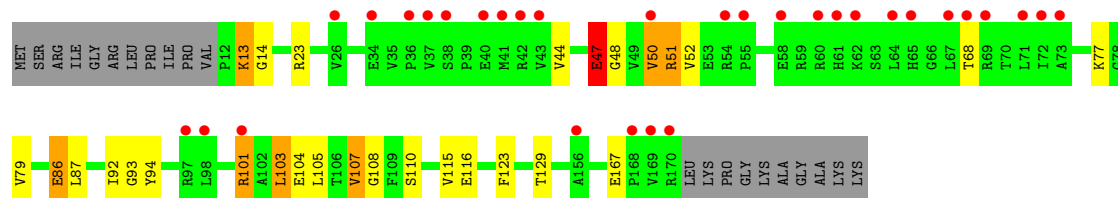
• Molecule 6: 50S ribosomal protein L5

Chain G:



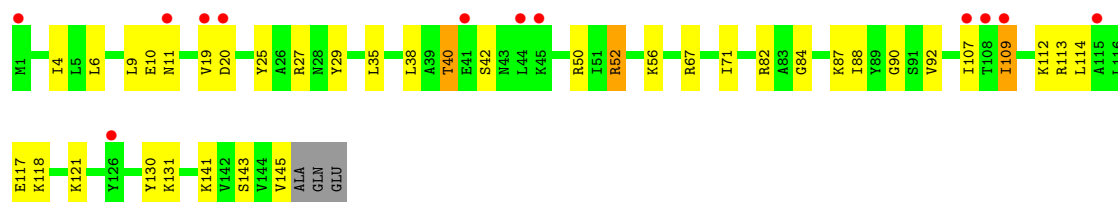
• Molecule 7: 50S ribosomal protein L6

Chain H:



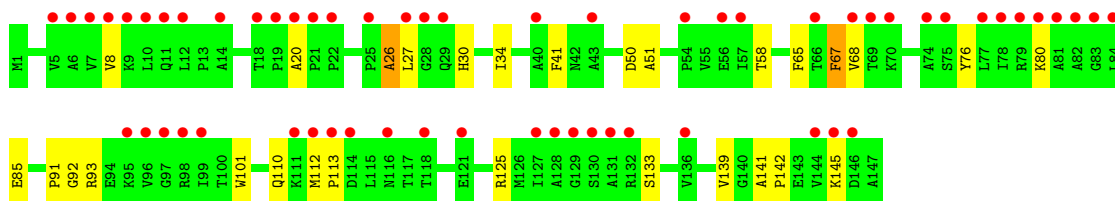
• Molecule 8: 50S ribosomal protein L9

Chain I:



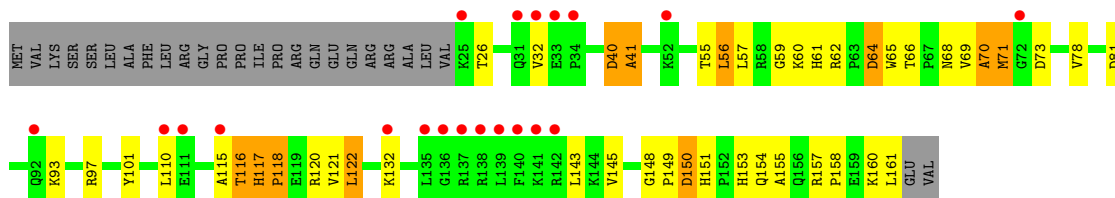
• Molecule 9: 50S ribosomal protein L11

Chain K:



• Molecule 10: 50S ribosomal protein L13

Chain N:



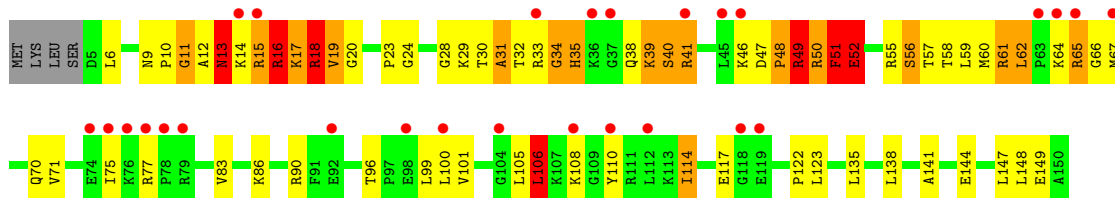
• Molecule 11: 50S ribosomal protein L14

Chain O:



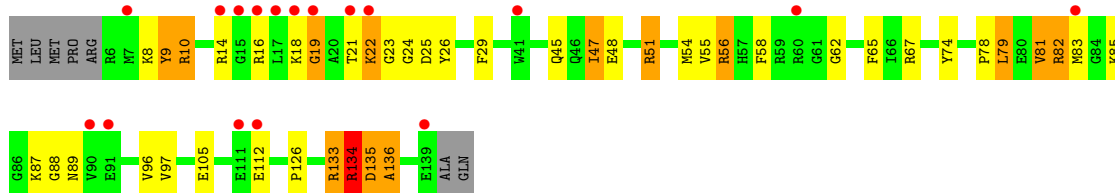
• Molecule 12: 50S ribosomal protein L15

Chain P:



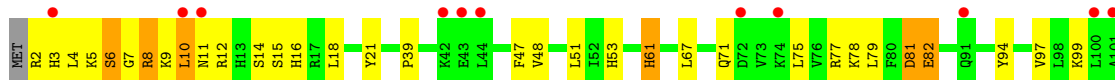
• Molecule 13: 50S ribosomal protein L16

Chain Q:

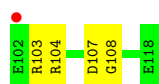


• Molecule 14: 50S ribosomal protein L17

Chain R:

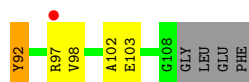
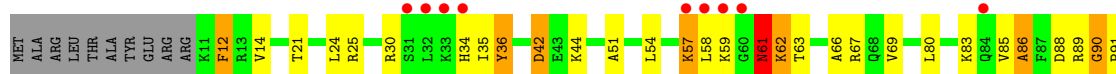






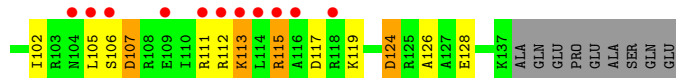
- Molecule 15: 50S ribosomal protein L18

Chain S:



- Molecule 16: 50S ribosomal protein L19

Chain T:



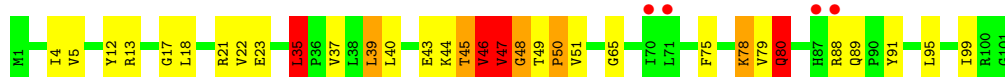
- Molecule 17: 50S ribosomal protein L20

Chain U:



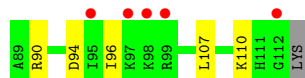
- Molecule 18: 50S ribosomal protein L21

Chain V:



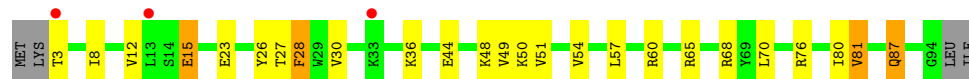
- Molecule 19: 50S ribosomal protein L22

Chain W:



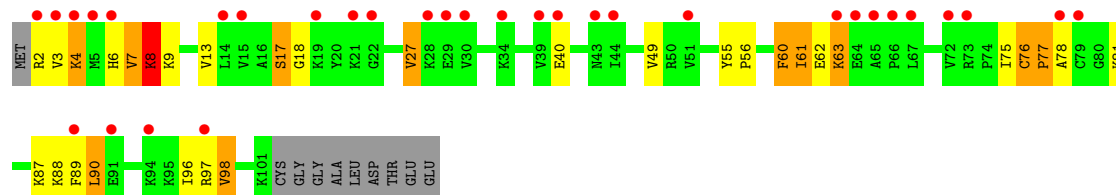
- Molecule 20: 50S ribosomal protein L23

Chain X: 



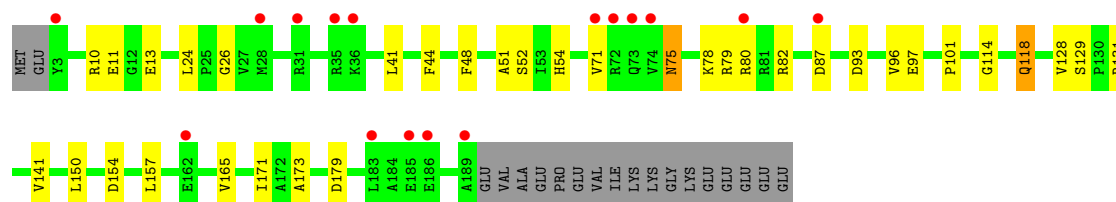
- Molecule 21: 50S ribosomal protein L24

Chain Y: 



- Molecule 22: 50S ribosomal protein L25

Chain Z: 



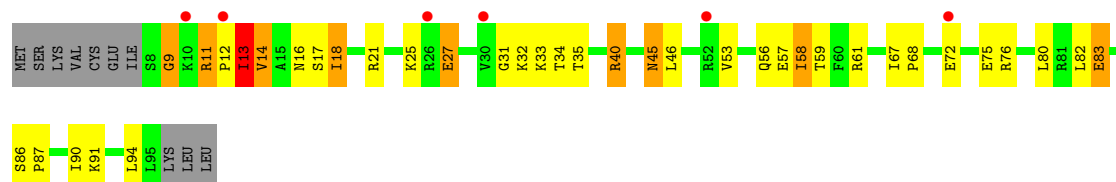
- Molecule 23: 50S ribosomal protein L27

Chain 0: 



- Molecule 24: 50S ribosomal protein L28

Chain 1: 



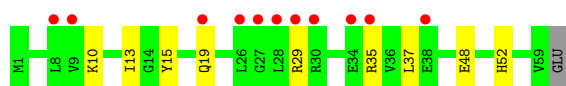
- Molecule 25: 50S ribosomal protein L29

Chain 2: 



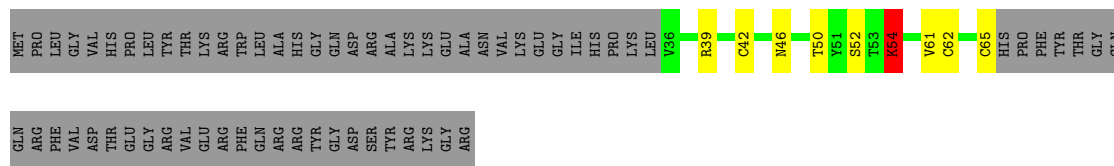
- Molecule 26: 50S ribosomal protein L30

Chain 3: 



- Molecule 27: 50S ribosomal protein L31

Chain 4:



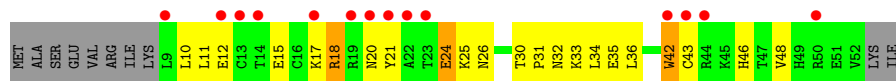
- Molecule 28: 50S ribosomal protein L32

Chain 5:



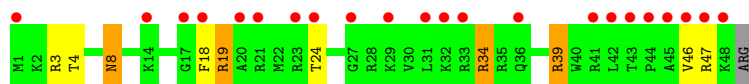
- Molecule 29: 50S ribosomal protein L33

Chain 6:



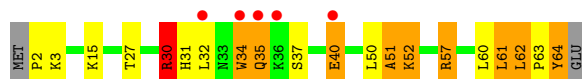
- Molecule 30: 50S ribosomal protein L34

Chain 7:



- Molecule 31: 50S ribosomal protein L35

Chain 8:



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 211.24Å 456.78Å 618.71Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 49.95 – 3.00<br>50.99 – 2.99                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.3 (49.95-3.00)<br>97.2 (50.99-2.99)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.31 (at 3.01Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine)                                      | Depositor        |
| R, $R_{free}$   | 0.280 , 0.316<br>0.462 , 0.464                              | Depositor<br>DCC |
| $R_{free}$ test set   | 10573 reflections (0.92%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 56.2  | Xtriage          |
| Anisotropy  | 0.291   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.09 , -10.0  | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$ | Xtriage          |
| Outliers  | 0 of 1158087 reflections                                    | Xtriage          |
| $F_o, F_c$ correlation  | 0.63  | EDS              |
| Total number of atoms   | 92692   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 82.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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     | 0.65         | 0/69437     | 1.22        | 337/108401 (0.3%) |
| 2   | B     | 0.53         | 0/2853      | 1.12        | 10/4451 (0.2%)    |
| 3   | D     | 0.46         | 0/2154      | 0.67        | 1/2905 (0.0%)     |
| 4   | E     | 0.35         | 0/1596      | 0.58        | 0/2153            |
| 5   | F     | 0.37         | 0/1621      | 0.57        | 0/2194            |
| 6   | G     | 0.28         | 0/1500      | 0.50        | 0/2017            |
| 7   | H     | 0.26         | 0/1245      | 0.48        | 0/1682            |
| 8   | I     | 0.31         | 0/1147      | 0.53        | 0/1552            |
| 9   | K     | 0.24         | 0/1108      | 0.45        | 0/1500            |
| 10  | N     | 0.32         | 0/1123      | 0.55        | 0/1515            |
| 11  | O     | 0.38         | 0/942       | 0.56        | 0/1268            |
| 12  | P     | 0.38         | 0/1131      | 0.71        | 1/1504 (0.1%)     |
| 13  | Q     | 0.38         | 0/1084      | 0.60        | 0/1449            |
| 14  | R     | 0.38         | 0/974       | 0.59        | 0/1302            |
| 15  | S     | 0.28         | 0/778       | 0.50        | 0/1036            |
| 16  | T     | 0.37         | 0/1157      | 0.53        | 0/1544            |
| 17  | U     | 0.37         | 0/982       | 0.53        | 0/1306            |
| 18  | V     | 0.35         | 0/790       | 0.57        | 0/1057            |
| 19  | W     | 0.36         | 0/901       | 0.56        | 0/1209            |
| 20  | X     | 0.40         | 0/739       | 0.55        | 0/993             |
| 21  | Y     | 0.33         | 0/788       | 0.57        | 0/1051            |
| 22  | Z     | 0.28         | 0/1514      | 0.50        | 0/2056            |
| 23  | 0     | 0.34         | 0/613       | 0.54        | 0/816             |
| 24  | 1     | 0.44         | 0/701       | 0.71        | 1/932 (0.1%)      |
| 25  | 2     | 0.37         | 0/522       | 0.62        | 0/690             |
| 26  | 3     | 0.30         | 0/472       | 0.48        | 0/634             |
| 27  | 4     | 0.28         | 0/228       | 0.52        | 0/309             |
| 28  | 5     | 0.32         | 0/418       | 0.55        | 0/567             |
| 29  | 6     | 0.30         | 0/387       | 0.51        | 0/518             |
| 30  | 7     | 0.41         | 0/426       | 0.58        | 0/561             |
| 31  | 8     | 0.46         | 0/515       | 0.66        | 0/679             |
| All | All   | 0.58         | 0/99846     | 1.09        | 350/149851 (0.2%) |

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 |
|-----|-------|---------------------|---------------------|
| 3   | D     | 0                   | 1                   |
| 12  | P     | 0                   | 3                   |
| All | All   | 0                   | 4                   |

There are no bond length outliers.

All (350) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|--------|-------------|----------|
| 1   | A     | 1913   | A    | C1'-O4'-C4' | -12.89 | 99.59       | 109.90   |
| 1   | A     | 1559   | G    | C1'-O4'-C4' | -12.81 | 99.65       | 109.90   |
| 1   | A     | 1379   | A    | C3'-C2'-C1' | -11.68 | 92.16       | 101.50   |
| 1   | A     | 945    | A    | C1'-O4'-C4' | -11.55 | 100.66      | 109.90   |
| 1   | A     | 1559   | G    | O4'-C1'-N9  | 11.02  | 117.02      | 108.20   |
| 1   | A     | 1913   | A    | O4'-C1'-N9  | 11.01  | 117.01      | 108.20   |
| 1   | A     | 1786   | A    | C1'-O4'-C4' | -11.01 | 101.09      | 109.90   |
| 1   | A     | 1698   | A    | C3'-C2'-C1' | -10.42 | 93.16       | 101.50   |
| 1   | A     | 603    | A    | C1'-O4'-C4' | -10.27 | 101.69      | 109.90   |
| 1   | A     | 2609   | U    | C1'-O4'-C4' | -10.13 | 101.80      | 109.90   |
| 1   | A     | 1542   | G    | P-O3'-C3'   | 10.00  | 131.70      | 119.70   |
| 1   | A     | 2447   | G    | P-O3'-C3'   | 9.96   | 131.65      | 119.70   |
| 1   | A     | 1300   | U    | P-O3'-C3'   | 9.93   | 131.62      | 119.70   |
| 1   | A     | 2346   | A    | C3'-C2'-C1' | -9.83  | 93.64       | 101.50   |
| 1   | A     | 802    | A    | O4'-C1'-N9  | -9.46  | 100.63      | 108.20   |
| 1   | A     | 1608   | A    | C1'-O4'-C4' | -9.39  | 102.38      | 109.90   |
| 1   | A     | 74     | A    | P-O3'-C3'   | 9.29   | 130.85      | 119.70   |
| 1   | A     | 2346   | A    | C1'-O4'-C4' | -9.28  | 102.47      | 109.90   |
| 1   | A     | 2275   | C    | P-O3'-C3'   | 9.17   | 130.70      | 119.70   |
| 1   | A     | 676    | A    | C1'-O4'-C4' | -9.11  | 102.61      | 109.90   |
| 1   | A     | 363(G) | A    | P-O3'-C3'   | 9.10   | 130.62      | 119.70   |
| 1   | A     | 933    | A    | O4'-C1'-N9  | 9.04   | 115.44      | 108.20   |
| 1   | A     | 1060   | U    | P-O3'-C3'   | 8.95   | 130.44      | 119.70   |
| 1   | A     | 271(C) | G    | P-O3'-C3'   | 8.84   | 130.31      | 119.70   |
| 1   | A     | 1786   | A    | C3'-C2'-C1' | -8.82  | 94.44       | 101.50   |
| 1   | A     | 945    | A    | O4'-C1'-N9  | 8.73   | 115.19      | 108.20   |
| 1   | A     | 859    | G    | C3'-C2'-C1' | -8.65  | 94.58       | 101.50   |
| 1   | A     | 1204   | A    | C3'-C2'-C1' | -8.61  | 94.61       | 101.50   |
| 1   | A     | 1022   | G    | P-O3'-C3'   | 8.55   | 129.96      | 119.70   |
| 1   | A     | 1698   | A    | O4'-C1'-N9  | 8.55   | 115.04      | 108.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 1   | A     | 2689   | U    | P-O3'-C3'   | 8.54  | 129.95      | 119.70   |
| 1   | A     | 1427   | A    | P-O3'-C3'   | 8.43  | 129.82      | 119.70   |
| 1   | A     | 1460   | A    | C1'-O4'-C4' | -8.36 | 103.21      | 109.90   |
| 1   | A     | 512    | G    | C1'-O4'-C4' | -8.31 | 103.25      | 109.90   |
| 1   | A     | 1379   | A    | C1'-O4'-C4' | -8.27 | 103.29      | 109.90   |
| 1   | A     | 2593   | U    | N3-C4-C5    | -8.22 | 109.67      | 114.60   |
| 1   | A     | 2061   | G    | N9-C1'-C2'  | -8.19 | 102.99      | 112.00   |
| 1   | A     | 265    | A    | C3'-C2'-C1' | -8.19 | 94.95       | 101.50   |
| 1   | A     | 775    | G    | P-O3'-C3'   | 8.14  | 129.47      | 119.70   |
| 1   | A     | 2517   | C    | O4'-C1'-N1  | 8.06  | 114.65      | 108.20   |
| 1   | A     | 1545   | A    | C1'-O4'-C4' | -8.01 | 103.49      | 109.90   |
| 1   | A     | 717    | G    | O4'-C1'-N9  | 7.97  | 114.57      | 108.20   |
| 1   | A     | 974(B) | C    | C3'-C2'-C1' | -7.93 | 95.16       | 101.50   |
| 1   | A     | 481    | G    | P-O3'-C3'   | 7.92  | 129.21      | 119.70   |
| 1   | A     | 214    | G    | C1'-O4'-C4' | -7.92 | 103.57      | 109.90   |
| 1   | A     | 845    | G    | O4'-C1'-N9  | 7.80  | 114.44      | 108.20   |
| 1   | A     | 1913   | A    | C3'-C2'-C1' | -7.73 | 95.31       | 101.50   |
| 1   | A     | 670    | A    | O4'-C1'-N9  | -7.69 | 102.05      | 108.20   |
| 1   | A     | 1698   | A    | C1'-O4'-C4' | -7.68 | 103.76      | 109.90   |
| 1   | A     | 2685   | G    | C5-C6-N1    | -7.67 | 107.67      | 111.50   |
| 1   | A     | 1131   | G    | P-O3'-C3'   | 7.59  | 128.81      | 119.70   |
| 1   | A     | 676    | A    | O4'-C1'-N9  | 7.54  | 114.23      | 108.20   |
| 1   | A     | 199    | A    | C1'-O4'-C4' | -7.49 | 103.91      | 109.90   |
| 1   | A     | 1559   | G    | C3'-C2'-C1' | -7.34 | 95.62       | 101.50   |
| 1   | A     | 1365   | A    | C4'-C3'-C2' | -7.32 | 95.28       | 102.60   |
| 1   | A     | 1913   | A    | O4'-C1'-C2' | -7.29 | 98.51       | 105.80   |
| 1   | A     | 101    | G    | C3'-C2'-C1' | -7.28 | 95.68       | 101.50   |
| 1   | A     | 242    | G    | C3'-C2'-C1' | -7.26 | 95.69       | 101.50   |
| 1   | A     | 1937   | A    | P-O3'-C3'   | 7.25  | 128.40      | 119.70   |
| 1   | A     | 2490   | G    | P-O3'-C3'   | 7.22  | 128.36      | 119.70   |
| 1   | A     | 807    | U    | C4'-C3'-C2' | -7.21 | 95.39       | 102.60   |
| 1   | A     | 1609   | A    | C4'-C3'-C2' | -7.19 | 95.41       | 102.60   |
| 1   | A     | 1385   | G    | P-O3'-C3'   | 7.19  | 128.32      | 119.70   |
| 1   | A     | 1545   | A    | C5'-C4'-O4' | 7.18  | 117.71      | 109.10   |
| 1   | A     | 1332   | G    | N3-C4-N9    | -7.15 | 121.71      | 126.00   |
| 1   | A     | 532    | A    | C1'-O4'-C4' | -7.13 | 104.20      | 109.90   |
| 1   | A     | 1332   | G    | N3-C4-C5    | 7.08  | 132.14      | 128.60   |
| 1   | A     | 1617   | C    | C3'-C2'-C1' | -7.07 | 95.84       | 101.50   |
| 1   | A     | 214    | G    | O4'-C1'-N9  | 7.03  | 113.83      | 108.20   |
| 1   | A     | 2061   | G    | N1-C6-O6    | 7.02  | 124.11      | 119.90   |
| 1   | A     | 1365   | A    | C1'-O4'-C4' | -7.00 | 104.30      | 109.90   |
| 1   | A     | 685    | A    | C1'-O4'-C4' | -6.98 | 104.31      | 109.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 1   | A     | 2790   | A    | C4'-C3'-C2' | -6.97 | 95.63       | 102.60   |
| 1   | A     | 979    | G    | N1-C6-O6    | 6.95  | 124.07      | 119.90   |
| 1   | A     | 1907   | G    | C4'-C3'-C2' | -6.92 | 95.67       | 102.60   |
| 1   | A     | 1962   | C    | N1-C2-O2    | 6.88  | 123.03      | 118.90   |
| 2   | B     | 42     | C    | O4'-C1'-N1  | 6.83  | 113.67      | 108.20   |
| 1   | A     | 2739   | U    | O4'-C1'-N1  | 6.82  | 113.66      | 108.20   |
| 1   | A     | 474    | G    | P-O3'-C3'   | 6.78  | 127.83      | 119.70   |
| 1   | A     | 332    | A    | P-O3'-C3'   | 6.77  | 127.83      | 119.70   |
| 1   | A     | 783    | A    | O4'-C1'-N9  | 6.77  | 113.61      | 108.20   |
| 1   | A     | 1050   | A    | O3'-P-O5'   | -6.76 | 91.15       | 104.00   |
| 1   | A     | 1126   | A    | P-O3'-C3'   | 6.75  | 127.80      | 119.70   |
| 1   | A     | 298    | G    | N1-C6-O6    | 6.74  | 123.94      | 119.90   |
| 1   | A     | 1325   | G    | C1'-O4'-C4' | -6.73 | 104.51      | 109.90   |
| 1   | A     | 196    | A    | C1'-O4'-C4' | -6.72 | 104.52      | 109.90   |
| 1   | A     | 933    | A    | C4'-C3'-C2' | -6.72 | 95.88       | 102.60   |
| 1   | A     | 2311   | A    | C1'-O4'-C4' | -6.68 | 104.55      | 109.90   |
| 1   | A     | 760    | G    | C4'-C3'-C2' | -6.67 | 95.93       | 102.60   |
| 1   | A     | 1614   | A    | O5'-P-OP2   | -6.64 | 99.72       | 105.70   |
| 1   | A     | 1804   | C    | N1-C1'-C2'  | -6.64 | 104.70      | 112.00   |
| 1   | A     | 2346   | A    | O4'-C1'-N9  | 6.63  | 113.51      | 108.20   |
| 1   | A     | 692    | C    | C4'-C3'-C2' | -6.63 | 95.97       | 102.60   |
| 1   | A     | 2593   | U    | O4'-C1'-N1  | 6.58  | 113.47      | 108.20   |
| 3   | D     | 41     | GLY  | N-CA-C      | 6.58  | 129.55      | 113.10   |
| 1   | A     | 1253   | A    | C1'-O4'-C4' | -6.58 | 104.64      | 109.90   |
| 1   | A     | 2724   | C    | O4'-C4'-C3' | -6.55 | 97.45       | 104.00   |
| 1   | A     | 512    | G    | P-O3'-C3'   | 6.54  | 127.54      | 119.70   |
| 1   | A     | 933    | A    | C1'-O4'-C4' | -6.53 | 104.67      | 109.90   |
| 1   | A     | 46     | C    | C4'-C3'-C2' | -6.51 | 96.09       | 102.60   |
| 1   | A     | 783    | A    | C3'-C2'-C1' | -6.50 | 96.30       | 101.50   |
| 1   | A     | 945    | A    | C3'-C2'-C1' | -6.48 | 96.31       | 101.50   |
| 1   | A     | 265    | A    | C1'-O4'-C4' | -6.48 | 104.72      | 109.90   |
| 1   | A     | 1996   | C    | P-O3'-C3'   | 6.45  | 127.44      | 119.70   |
| 1   | A     | 2542   | A    | P-O3'-C3'   | 6.44  | 127.43      | 119.70   |
| 1   | A     | 1899   | G    | C3'-C2'-C1' | 6.44  | 106.65      | 101.50   |
| 1   | A     | 479    | A    | P-O3'-C3'   | 6.42  | 127.40      | 119.70   |
| 1   | A     | 1286   | A    | C1'-O4'-C4' | -6.42 | 104.77      | 109.90   |
| 1   | A     | 2581   | G    | O4'-C1'-N9  | 6.41  | 113.33      | 108.20   |
| 1   | A     | 2445   | G    | C4'-C3'-C2' | -6.38 | 96.22       | 102.60   |
| 1   | A     | 1478   | G    | C4'-C3'-C2' | -6.38 | 96.22       | 102.60   |
| 1   | A     | 1984   | G    | C4'-C3'-C2' | -6.38 | 96.22       | 102.60   |
| 1   | A     | 1902   | C    | O4'-C1'-N1  | -6.37 | 103.11      | 108.20   |
| 1   | A     | 974(B) | C    | C1'-O4'-C4' | -6.35 | 104.82      | 109.90   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1786 | A    | O4'-C1'-C2' | -6.34 | 99.46       | 105.80   |
| 1   | A     | 2494 | G    | C4'-C3'-C2' | -6.31 | 96.29       | 102.60   |
| 1   | A     | 809  | G    | C4'-C3'-C2' | -6.31 | 96.29       | 102.60   |
| 1   | A     | 805  | G    | O4'-C1'-N9  | 6.27  | 113.21      | 108.20   |
| 1   | A     | 1493 | C    | N1-C1'-C2'  | 6.26  | 122.14      | 114.00   |
| 1   | A     | 1543 | A    | C3'-C2'-C1' | -6.26 | 96.49       | 101.50   |
| 1   | A     | 2595 | G    | C4'-C3'-C2' | -6.25 | 96.35       | 102.60   |
| 1   | A     | 2586 | C    | P-O3'-C3'   | -6.25 | 112.20      | 119.70   |
| 1   | A     | 2791 | C    | P-O3'-C3'   | 6.21  | 127.15      | 119.70   |
| 1   | A     | 405  | U    | C3'-C2'-C1' | -6.20 | 96.54       | 101.50   |
| 1   | A     | 1763 | G    | P-O3'-C3'   | 6.20  | 127.14      | 119.70   |
| 1   | A     | 383  | U    | C1'-O4'-C4' | -6.19 | 104.95      | 109.90   |
| 1   | A     | 1570 | A    | O4'-C1'-N9  | -6.19 | 103.25      | 108.20   |
| 1   | A     | 203  | C    | C4'-C3'-C2' | -6.17 | 96.42       | 102.60   |
| 1   | A     | 1954 | G    | O4'-C1'-N9  | -6.17 | 103.26      | 108.20   |
| 1   | A     | 1033 | U    | C1'-O4'-C4' | -6.16 | 104.98      | 109.90   |
| 1   | A     | 1266 | G    | C3'-C2'-C1' | -6.16 | 96.58       | 101.50   |
| 1   | A     | 1975 | G    | C4'-C3'-C2' | -6.14 | 96.45       | 102.60   |
| 2   | B     | 42   | C    | C1'-O4'-C4' | -6.11 | 105.01      | 109.90   |
| 1   | A     | 859  | G    | C4'-C3'-C2' | -6.11 | 96.49       | 102.60   |
| 1   | A     | 1204 | A    | O4'-C1'-N9  | 6.11  | 113.08      | 108.20   |
| 1   | A     | 1603 | A    | P-O3'-C3'   | 6.10  | 127.02      | 119.70   |
| 1   | A     | 1577 | C    | C4'-C3'-C2' | -6.09 | 96.51       | 102.60   |
| 1   | A     | 2593 | U    | N3-C4-O4    | 6.07  | 123.65      | 119.40   |
| 1   | A     | 1962 | C    | P-O3'-C3'   | 6.07  | 126.98      | 119.70   |
| 1   | A     | 1558 | A    | P-O3'-C3'   | 6.06  | 126.97      | 119.70   |
| 1   | A     | 125  | G    | O4'-C1'-N9  | -6.05 | 103.36      | 108.20   |
| 1   | A     | 1108 | U    | P-O3'-C3'   | 6.04  | 126.94      | 119.70   |
| 1   | A     | 1694 | C    | C3'-C2'-C1' | -6.04 | 96.67       | 101.50   |
| 1   | A     | 2447 | G    | N1-C6-O6    | 6.04  | 123.52      | 119.90   |
| 1   | A     | 317  | G    | C4'-C3'-C2' | -6.03 | 96.57       | 102.60   |
| 1   | A     | 1288 | U    | O4'-C1'-N1  | 6.03  | 113.02      | 108.20   |
| 1   | A     | 1936 | A    | C4'-C3'-C2' | -6.01 | 96.59       | 102.60   |
| 1   | A     | 1395 | A    | C1'-O4'-C4' | -6.00 | 105.10      | 109.90   |
| 1   | A     | 404  | C    | C3'-C2'-C1' | -5.99 | 96.71       | 101.50   |
| 1   | A     | 1969 | A    | P-O3'-C3'   | 5.98  | 126.87      | 119.70   |
| 1   | A     | 717  | G    | C4'-C3'-C2' | -5.97 | 96.63       | 102.60   |
| 1   | A     | 989  | G    | O4'-C1'-N9  | 5.95  | 112.96      | 108.20   |
| 1   | A     | 1460 | A    | O4'-C1'-N9  | 5.94  | 112.96      | 108.20   |
| 1   | A     | 310  | A    | C3'-C2'-C1' | 5.94  | 106.25      | 101.50   |
| 1   | A     | 2402 | C    | C1'-O4'-C4' | -5.94 | 105.15      | 109.90   |
| 1   | A     | 1779 | U    | C1'-O4'-C4' | -5.92 | 105.16      | 109.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 1   | A     | 204    | A    | C1'-O4'-C4' | -5.92 | 105.16      | 109.90   |
| 1   | A     | 577    | G    | O4'-C1'-N9  | -5.91 | 103.48      | 108.20   |
| 1   | A     | 1772   | G    | C4'-C3'-C2' | -5.91 | 96.69       | 102.60   |
| 1   | A     | 2500   | U    | C4'-C3'-C2' | -5.90 | 96.70       | 102.60   |
| 1   | A     | 528    | A    | C3'-C2'-C1' | -5.89 | 96.78       | 101.50   |
| 1   | A     | 882    | G    | C3'-C2'-C1' | -5.89 | 96.79       | 101.50   |
| 1   | A     | 2033   | A    | C3'-C2'-C1' | -5.88 | 96.80       | 101.50   |
| 1   | A     | 302    | C    | C1'-O4'-C4' | -5.88 | 105.20      | 109.90   |
| 1   | A     | 2790   | A    | C3'-C2'-C1' | -5.87 | 96.81       | 101.50   |
| 1   | A     | 603    | A    | C3'-C2'-C1' | -5.85 | 96.82       | 101.50   |
| 1   | A     | 2569   | G    | C4'-C3'-C2' | -5.85 | 96.75       | 102.60   |
| 1   | A     | 462    | C    | P-O3'-C3'   | -5.85 | 112.68      | 119.70   |
| 1   | A     | 606    | U    | C4'-C3'-C2' | -5.84 | 96.76       | 102.60   |
| 1   | A     | 974(B) | C    | O4'-C1'-N1  | 5.84  | 112.87      | 108.20   |
| 1   | A     | 746    | A    | O4'-C1'-N9  | 5.83  | 112.87      | 108.20   |
| 1   | A     | 1543   | A    | O4'-C1'-C2' | -5.83 | 99.97       | 105.80   |
| 24  | 1     | 35     | THR  | N-CA-C      | 5.82  | 126.73      | 111.00   |
| 1   | A     | 213    | A    | C4'-C3'-C2' | -5.81 | 96.79       | 102.60   |
| 1   | A     | 2559   | C    | C4'-C3'-C2' | -5.81 | 96.79       | 102.60   |
| 1   | A     | 2333   | A    | P-O3'-C3'   | 5.80  | 126.66      | 119.70   |
| 1   | A     | 651    | G    | C4'-C3'-C2' | -5.80 | 96.80       | 102.60   |
| 1   | A     | 2028   | U    | N3-C4-C5    | -5.79 | 111.12      | 114.60   |
| 1   | A     | 990    | A    | P-O3'-C3'   | 5.79  | 126.65      | 119.70   |
| 1   | A     | 512    | G    | O4'-C1'-N9  | 5.79  | 112.83      | 108.20   |
| 1   | A     | 783    | A    | N1-C6-N6    | 5.78  | 122.07      | 118.60   |
| 1   | A     | 1781   | C    | C1'-O4'-C4' | -5.78 | 105.27      | 109.90   |
| 1   | A     | 49     | A    | C3'-C2'-C1' | -5.76 | 96.89       | 101.50   |
| 1   | A     | 807    | U    | P-O3'-C3'   | 5.75  | 126.60      | 119.70   |
| 1   | A     | 1288   | U    | C1'-O4'-C4' | -5.75 | 105.30      | 109.90   |
| 1   | A     | 2587   | A    | P-O3'-C3'   | 5.75  | 126.59      | 119.70   |
| 1   | A     | 1913   | A    | N9-C1'-C2'  | 5.74  | 121.46      | 114.00   |
| 1   | A     | 933    | A    | O4'-C4'-C3' | -5.72 | 98.28       | 104.00   |
| 1   | A     | 1786   | A    | N1-C6-N6    | 5.72  | 122.03      | 118.60   |
| 1   | A     | 1332   | G    | C2-N3-C4    | -5.71 | 109.04      | 111.90   |
| 1   | A     | 1781   | C    | C3'-C2'-C1' | -5.71 | 96.93       | 101.50   |
| 1   | A     | 2685   | G    | C4'-C3'-C2' | -5.71 | 96.89       | 102.60   |
| 1   | A     | 2523   | G    | C4'-C3'-C2' | -5.71 | 96.89       | 102.60   |
| 1   | A     | 2276   | G    | C4'-C3'-C2' | -5.70 | 96.90       | 102.60   |
| 1   | A     | 559    | G    | P-O3'-C3'   | -5.70 | 112.86      | 119.70   |
| 2   | B     | 42     | C    | C4'-C3'-C2' | -5.70 | 96.90       | 102.60   |
| 1   | A     | 2606   | C    | C3'-C2'-C1' | -5.69 | 96.95       | 101.50   |
| 1   | A     | 203    | C    | C3'-C2'-C1' | -5.69 | 96.95       | 101.50   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1077 | A    | C3'-C2'-C1' | -5.67 | 96.96       | 101.50   |
| 1   | A     | 1204 | A    | C1'-O4'-C4' | -5.66 | 105.37      | 109.90   |
| 1   | A     | 1301 | A    | P-O3'-C3'   | 5.66  | 126.49      | 119.70   |
| 1   | A     | 673  | C    | C4'-C3'-C2' | -5.65 | 96.95       | 102.60   |
| 1   | A     | 2805 | G    | C3'-C2'-C1' | -5.65 | 96.98       | 101.50   |
| 1   | A     | 1493 | C    | C2-N1-C1'   | 5.64  | 125.00      | 118.80   |
| 1   | A     | 352  | G    | P-O3'-C3'   | 5.62  | 126.45      | 119.70   |
| 1   | A     | 240  | G    | O4'-C1'-N9  | -5.62 | 103.70      | 108.20   |
| 1   | A     | 221  | A    | P-O3'-C3'   | 5.62  | 126.44      | 119.70   |
| 1   | A     | 2791 | C    | O4'-C1'-N1  | 5.62  | 112.69      | 108.20   |
| 1   | A     | 197  | A    | P-O3'-C3'   | 5.58  | 126.39      | 119.70   |
| 1   | A     | 1654 | A    | C4'-C3'-C2' | -5.58 | 97.02       | 102.60   |
| 1   | A     | 1899 | G    | C2-N3-C4    | -5.58 | 109.11      | 111.90   |
| 1   | A     | 1800 | C    | C1'-O4'-C4' | -5.58 | 105.44      | 109.90   |
| 1   | A     | 2480 | C    | C1'-O4'-C4' | -5.56 | 105.45      | 109.90   |
| 1   | A     | 2447 | G    | C5-C6-N1    | -5.55 | 108.72      | 111.50   |
| 1   | A     | 825  | C    | C4'-C3'-C2' | -5.55 | 97.05       | 102.60   |
| 1   | A     | 2039 | C    | C4'-C3'-C2' | -5.55 | 97.05       | 102.60   |
| 1   | A     | 2645 | G    | C3'-C2'-C1' | 5.54  | 105.94      | 101.50   |
| 1   | A     | 2032 | G    | C5-N7-C8    | -5.54 | 101.53      | 104.30   |
| 1   | A     | 2391 | G    | C1'-O4'-C4' | -5.54 | 105.47      | 109.90   |
| 1   | A     | 2602 | A    | C1'-O4'-C4' | -5.54 | 105.47      | 109.90   |
| 1   | A     | 2035 | G    | C1'-O4'-C4' | -5.54 | 105.47      | 109.90   |
| 1   | A     | 1378 | A    | P-O3'-C3'   | 5.52  | 126.33      | 119.70   |
| 1   | A     | 2028 | U    | N3-C4-O4    | 5.52  | 123.26      | 119.40   |
| 1   | A     | 1309 | G    | N9-C1'-C2'  | -5.51 | 105.93      | 112.00   |
| 1   | A     | 189  | G    | O4'-C1'-N9  | -5.51 | 103.79      | 108.20   |
| 1   | A     | 2417 | C    | O4'-C4'-C3' | -5.50 | 98.50       | 104.00   |
| 1   | A     | 972  | G    | O4'-C1'-N9  | -5.49 | 103.81      | 108.20   |
| 1   | A     | 1743 | G    | C4'-C3'-C2' | -5.49 | 97.11       | 102.60   |
| 1   | A     | 979  | G    | C6-C5-N7    | -5.49 | 127.11      | 130.40   |
| 1   | A     | 1558 | A    | C1'-O4'-C4' | -5.49 | 105.51      | 109.90   |
| 1   | A     | 1598 | C    | C5'-C4'-C3' | -5.48 | 107.23      | 116.00   |
| 1   | A     | 1930 | G    | C3'-C2'-C1' | -5.48 | 97.12       | 101.50   |
| 1   | A     | 565  | C    | C4'-C3'-C2' | -5.47 | 97.13       | 102.60   |
| 1   | A     | 1578 | U    | C4'-C3'-C2' | -5.47 | 97.13       | 102.60   |
| 1   | A     | 791  | C    | C1'-O4'-C4' | -5.46 | 105.53      | 109.90   |
| 1   | A     | 1349 | A    | O4'-C1'-N9  | 5.45  | 112.56      | 108.20   |
| 1   | A     | 1433 | U    | N1-C1'-C2'  | -5.45 | 106.00      | 112.00   |
| 1   | A     | 820  | A    | C4'-C3'-C2' | -5.45 | 97.15       | 102.60   |
| 1   | A     | 1786 | A    | N9-C1'-C2'  | 5.45  | 121.09      | 114.00   |
| 1   | A     | 1241 | A    | C1'-O4'-C4' | -5.45 | 105.54      | 109.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 717  | G    | C1'-O4'-C4' | -5.44 | 105.55      | 109.90   |
| 1   | A     | 1618 | A    | C4'-C3'-C2' | -5.44 | 97.16       | 102.60   |
| 1   | A     | 1816 | G    | O4'-C1'-N9  | 5.43  | 112.55      | 108.20   |
| 1   | A     | 119  | A    | C1'-O4'-C4' | -5.43 | 105.56      | 109.90   |
| 1   | A     | 2346 | A    | N9-C1'-C2'  | 5.43  | 121.06      | 114.00   |
| 1   | A     | 1379 | A    | O4'-C1'-C2' | -5.42 | 100.38      | 105.80   |
| 1   | A     | 1379 | A    | O4'-C1'-N9  | 5.41  | 112.53      | 108.20   |
| 1   | A     | 298  | G    | C5-C6-O6    | -5.41 | 125.35      | 128.60   |
| 1   | A     | 457  | A    | P-O3'-C3'   | -5.41 | 113.21      | 119.70   |
| 1   | A     | 205  | G    | C3'-C2'-C1' | -5.40 | 97.18       | 101.50   |
| 1   | A     | 1775 | U    | N1-C1'-C2'  | -5.40 | 106.06      | 112.00   |
| 1   | A     | 1264 | G    | P-O3'-C3'   | 5.39  | 126.17      | 119.70   |
| 1   | A     | 834  | C    | C4'-C3'-C2' | -5.38 | 97.22       | 102.60   |
| 1   | A     | 2593 | U    | C6-N1-C2    | -5.38 | 117.77      | 121.00   |
| 1   | A     | 642  | G    | C4'-C3'-C2' | -5.36 | 97.24       | 102.60   |
| 1   | A     | 845  | G    | C1'-O4'-C4' | -5.36 | 105.61      | 109.90   |
| 1   | A     | 1294 | U    | C4'-C3'-C2' | -5.36 | 97.24       | 102.60   |
| 1   | A     | 2673 | G    | C4'-C3'-C2' | -5.36 | 97.24       | 102.60   |
| 1   | A     | 1729 | A    | C1'-O4'-C4' | -5.34 | 105.63      | 109.90   |
| 1   | A     | 2444 | G    | P-O5'-C5'   | -5.34 | 112.35      | 120.90   |
| 1   | A     | 407  | G    | C4'-C3'-C2' | -5.34 | 97.26       | 102.60   |
| 1   | A     | 1258 | C    | O4'-C1'-N1  | -5.34 | 103.93      | 108.20   |
| 2   | B     | 24   | G    | C3'-C2'-C1' | 5.34  | 105.77      | 101.50   |
| 1   | A     | 1613 | G    | C4'-C3'-C2' | -5.32 | 97.28       | 102.60   |
| 1   | A     | 1827 | C    | C4'-C3'-C2' | -5.31 | 97.29       | 102.60   |
| 2   | B     | 11   | C    | C4'-C3'-C2' | -5.31 | 97.29       | 102.60   |
| 12  | P     | 28   | GLY  | N-CA-C      | -5.30 | 99.84       | 113.10   |
| 1   | A     | 102  | G    | C3'-C2'-C1' | 5.30  | 105.74      | 101.50   |
| 1   | A     | 1838 | C    | C1'-O4'-C4' | -5.30 | 105.66      | 109.90   |
| 1   | A     | 1419 | A    | C1'-O4'-C4' | -5.29 | 105.66      | 109.90   |
| 1   | A     | 283  | A    | P-O3'-C3'   | 5.29  | 126.05      | 119.70   |
| 1   | A     | 793  | A    | C4'-C3'-C2' | 5.29  | 107.89      | 102.60   |
| 1   | A     | 323  | G    | P-O3'-C3'   | 5.28  | 126.04      | 119.70   |
| 1   | A     | 783  | A    | N9-C1'-C2'  | -5.28 | 106.19      | 112.00   |
| 1   | A     | 2572 | A    | O4'-C1'-N9  | -5.27 | 103.98      | 108.20   |
| 2   | B     | 117  | G    | C3'-C2'-C1' | -5.27 | 97.29       | 101.50   |
| 1   | A     | 987  | G    | O4'-C1'-N9  | 5.26  | 112.41      | 108.20   |
| 1   | A     | 2428 | G    | P-O3'-C3'   | 5.26  | 126.01      | 119.70   |
| 2   | B     | 12   | C    | C3'-C2'-C1' | 5.25  | 105.70      | 101.50   |
| 1   | A     | 208  | C    | C4'-C3'-C2' | -5.24 | 97.36       | 102.60   |
| 1   | A     | 1069 | A    | C1'-O4'-C4' | -5.23 | 105.71      | 109.90   |
| 1   | A     | 2867 | G    | O4'-C1'-N9  | 5.23  | 112.38      | 108.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1365 | A    | C5'-C4'-O4' | 5.23  | 115.37      | 109.10   |
| 1   | A     | 1151 | G    | C4'-C3'-C2' | -5.22 | 97.38       | 102.60   |
| 1   | A     | 1772 | G    | O4'-C1'-N9  | 5.22  | 112.38      | 108.20   |
| 1   | A     | 1880 | C    | C3'-C2'-C1' | -5.21 | 97.33       | 101.50   |
| 1   | A     | 2613 | U    | C3'-C2'-C1' | -5.21 | 97.33       | 101.50   |
| 1   | A     | 318  | C    | O4'-C1'-N1  | 5.21  | 112.37      | 108.20   |
| 1   | A     | 2184 | G    | C3'-C2'-C1' | -5.21 | 97.33       | 101.50   |
| 1   | A     | 2191 | G    | C3'-C2'-C1' | -5.21 | 97.33       | 101.50   |
| 1   | A     | 2746 | U    | C3'-C2'-C1' | -5.21 | 97.33       | 101.50   |
| 1   | A     | 1962 | C    | C3'-C2'-C1' | 5.21  | 105.66      | 101.50   |
| 1   | A     | 1419 | A    | O4'-C1'-N9  | 5.20  | 112.36      | 108.20   |
| 1   | A     | 71   | A    | O4'-C1'-N9  | -5.20 | 104.04      | 108.20   |
| 1   | A     | 1385 | G    | C1'-O4'-C4' | -5.20 | 105.74      | 109.90   |
| 2   | B     | 58   | A    | C4'-C3'-C2' | -5.19 | 97.41       | 102.60   |
| 1   | A     | 2592 | G    | C4'-C3'-C2' | -5.18 | 97.42       | 102.60   |
| 1   | A     | 979  | G    | C5-C6-O6    | -5.17 | 125.50      | 128.60   |
| 1   | A     | 1571 | A    | C4'-C3'-C2' | -5.17 | 97.43       | 102.60   |
| 1   | A     | 2447 | G    | C3'-C2'-C1' | 5.16  | 105.63      | 101.50   |
| 1   | A     | 379  | G    | C4'-C3'-C2' | -5.16 | 97.44       | 102.60   |
| 1   | A     | 880  | G    | C4'-C3'-C2' | -5.16 | 97.44       | 102.60   |
| 1   | A     | 2751 | G    | C3'-C2'-C1' | -5.16 | 97.38       | 101.50   |
| 1   | A     | 1788 | C    | C4'-C3'-C2' | -5.16 | 97.44       | 102.60   |
| 1   | A     | 1934 | C    | N1-C1'-C2'  | -5.15 | 106.33      | 112.00   |
| 1   | A     | 2390 | U    | P-O3'-C3'   | -5.15 | 113.52      | 119.70   |
| 1   | A     | 1701 | A    | N9-C1'-C2'  | -5.15 | 106.33      | 112.00   |
| 1   | A     | 2592 | G    | O5'-P-OP2   | -5.15 | 101.06      | 105.70   |
| 1   | A     | 1341 | U    | C3'-C2'-C1' | -5.15 | 97.38       | 101.50   |
| 1   | A     | 27   | G    | C5'-C4'-O4' | -5.14 | 102.93      | 109.10   |
| 1   | A     | 2879 | C    | P-O3'-C3'   | 5.14  | 125.87      | 119.70   |
| 1   | A     | 2073 | C    | C4'-C3'-C2' | -5.14 | 97.46       | 102.60   |
| 1   | A     | 2085 | C    | C4'-C3'-C2' | -5.13 | 97.47       | 102.60   |
| 1   | A     | 2501 | C    | C3'-C2'-C1' | 5.13  | 105.60      | 101.50   |
| 1   | A     | 2215 | G    | P-O3'-C3'   | -5.13 | 113.55      | 119.70   |
| 1   | A     | 665  | C    | P-O3'-C3'   | -5.12 | 113.56      | 119.70   |
| 1   | A     | 458  | G    | C3'-C2'-C1' | -5.12 | 97.41       | 101.50   |
| 1   | A     | 1761 | C    | O4'-C1'-N1  | 5.10  | 112.28      | 108.20   |
| 1   | A     | 2487 | G    | C4'-C3'-C2' | -5.10 | 97.50       | 102.60   |
| 1   | A     | 980  | A    | C3'-C2'-C1' | 5.09  | 105.57      | 101.50   |
| 1   | A     | 131  | G    | C4'-C3'-C2' | -5.08 | 97.52       | 102.60   |
| 1   | A     | 614  | U    | C3'-C2'-C1' | 5.07  | 105.56      | 101.50   |
| 1   | A     | 1948 | G    | C4'-C3'-C2' | -5.07 | 97.53       | 102.60   |
| 1   | A     | 307  | G    | C4'-C3'-C2' | -5.07 | 97.53       | 102.60   |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 1   | A     | 1833   | U    | C4'-C3'-C2' | -5.06 | 97.54       | 102.60   |
| 1   | A     | 204    | A    | C3'-C2'-C1' | -5.06 | 97.45       | 101.50   |
| 1   | A     | 1266   | G    | O4'-C1'-N9  | -5.06 | 104.15      | 108.20   |
| 2   | B     | 67     | G    | C4'-C3'-C2' | -5.06 | 97.54       | 102.60   |
| 1   | A     | 695    | G    | N9-C1'-C2'  | -5.05 | 106.44      | 112.00   |
| 1   | A     | 2022   | U    | O4'-C1'-C2' | -5.05 | 100.75      | 105.80   |
| 1   | A     | 131    | G    | O4'-C4'-C3' | -5.05 | 98.95       | 104.00   |
| 1   | A     | 270(M) | U    | C3'-C2'-C1' | 5.05  | 105.54      | 101.50   |
| 1   | A     | 616    | A    | P-O3'-C3'   | 5.05  | 125.75      | 119.70   |
| 1   | A     | 1085   | A    | C3'-C2'-C1' | 5.04  | 105.54      | 101.50   |
| 1   | A     | 140    | A    | C1'-O4'-C4' | -5.04 | 105.87      | 109.90   |
| 1   | A     | 1128   | A    | O4'-C1'-N9  | -5.04 | 104.17      | 108.20   |
| 1   | A     | 2411   | A    | C3'-C2'-C1' | -5.04 | 97.47       | 101.50   |
| 1   | A     | 14     | A    | O4'-C1'-N9  | -5.04 | 104.17      | 108.20   |
| 1   | A     | 1332   | G    | P-O3'-C3'   | -5.03 | 113.66      | 119.70   |
| 1   | A     | 2518   | A    | N1-C6-N6    | 5.03  | 121.62      | 118.60   |
| 1   | A     | 391    | G    | O4'-C1'-N9  | -5.02 | 104.18      | 108.20   |
| 1   | A     | 2893   | G    | C3'-C2'-C1' | 5.02  | 105.51      | 101.50   |
| 1   | A     | 405    | U    | C4'-C3'-C2' | -5.01 | 97.59       | 102.60   |
| 1   | A     | 2011   | U    | P-O3'-C3'   | -5.01 | 113.68      | 119.70   |
| 1   | A     | 1647   | G    | O4'-C1'-N9  | -5.01 | 104.19      | 108.20   |
| 1   | A     | 2197   | U    | C1'-O4'-C4' | -5.01 | 105.89      | 109.90   |
| 1   | A     | 2254   | C    | C4'-C3'-C2' | -5.01 | 97.59       | 102.60   |
| 1   | A     | 1494   | A    | O4'-C1'-N9  | 5.01  | 112.21      | 108.20   |
| 2   | B     | 15     | A    | C1'-O4'-C4' | -5.01 | 105.89      | 109.90   |
| 1   | A     | 302    | C    | O4'-C1'-N1  | 5.00  | 112.20      | 108.20   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 3   | D     | 40  | THR  | Peptide |
| 12  | P     | 51  | PHE  | Peptide |
| 12  | P     | 52  | GLU  | Peptide |
| 12  | P     | 9   | ASN  | Peptide |

## 5.2 Close contacts ⓘ

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

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 61997 | 0        | 0        | 563     | 0            |
| 2   | B     | 2551  | 0        | 0        | 26      | 0            |
| 3   | D     | 2104  | 0        | 0        | 42      | 0            |
| 4   | E     | 1563  | 0        | 0        | 23      | 0            |
| 5   | F     | 1586  | 0        | 0        | 23      | 0            |
| 6   | G     | 1475  | 0        | 0        | 18      | 0            |
| 7   | H     | 1222  | 0        | 0        | 9       | 0            |
| 8   | I     | 1132  | 0        | 0        | 10      | 0            |
| 9   | K     | 1088  | 0        | 0        | 4       | 0            |
| 10  | N     | 1096  | 0        | 0        | 16      | 0            |
| 11  | O     | 932   | 0        | 0        | 8       | 0            |
| 12  | P     | 1114  | 0        | 0        | 50      | 0            |
| 13  | Q     | 1064  | 0        | 0        | 25      | 0            |
| 14  | R     | 960   | 0        | 0        | 17      | 0            |
| 15  | S     | 770   | 0        | 0        | 19      | 0            |
| 16  | T     | 1143  | 0        | 0        | 20      | 0            |
| 17  | U     | 964   | 0        | 0        | 18      | 0            |
| 18  | V     | 779   | 0        | 0        | 16      | 0            |
| 19  | W     | 890   | 0        | 0        | 12      | 0            |
| 20  | X     | 725   | 0        | 0        | 9       | 0            |
| 21  | Y     | 775   | 0        | 0        | 11      | 0            |
| 22  | Z     | 1482  | 0        | 0        | 13      | 0            |
| 23  | 0     | 605   | 0        | 0        | 6       | 0            |
| 24  | 1     | 694   | 0        | 0        | 14      | 0            |
| 25  | 2     | 520   | 0        | 0        | 18      | 0            |
| 26  | 3     | 467   | 0        | 0        | 3       | 0            |
| 27  | 4     | 225   | 0        | 0        | 1       | 0            |
| 28  | 5     | 404   | 0        | 0        | 14      | 0            |
| 29  | 6     | 380   | 0        | 0        | 9       | 0            |
| 30  | 7     | 418   | 0        | 0        | 9       | 0            |
| 31  | 8     | 507   | 0        | 0        | 14      | 0            |
| 32  | 0     | 2     | 0        | 0        | 0       | 0            |
| 32  | 1     | 6     | 0        | 0        | 0       | 0            |
| 32  | 2     | 3     | 0        | 0        | 0       | 0            |
| 32  | 4     | 2     | 0        | 0        | 0       | 0            |
| 32  | 5     | 2     | 0        | 0        | 0       | 0            |
| 32  | 6     | 2     | 0        | 0        | 0       | 0            |
| 32  | 8     | 4     | 0        | 0        | 0       | 0            |
| 32  | A     | 934   | 0        | 0        | 0       | 0            |
| 32  | B     | 35    | 0        | 0        | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 32  | D     | 7     | 0        | 0        | 0       | 0            |
| 32  | E     | 6     | 0        | 0        | 0       | 0            |
| 32  | F     | 6     | 0        | 0        | 0       | 0            |
| 32  | G     | 2     | 0        | 0        | 0       | 0            |
| 32  | H     | 4     | 0        | 0        | 0       | 0            |
| 32  | I     | 6     | 0        | 0        | 0       | 0            |
| 32  | K     | 3     | 0        | 0        | 0       | 0            |
| 32  | N     | 4     | 0        | 0        | 0       | 0            |
| 32  | O     | 6     | 0        | 0        | 0       | 0            |
| 32  | P     | 2     | 0        | 0        | 0       | 0            |
| 32  | Q     | 6     | 0        | 0        | 0       | 0            |
| 32  | R     | 2     | 0        | 0        | 0       | 0            |
| 32  | S     | 3     | 0        | 0        | 0       | 0            |
| 32  | T     | 1     | 0        | 0        | 0       | 0            |
| 32  | U     | 1     | 0        | 0        | 0       | 0            |
| 32  | V     | 3     | 0        | 0        | 0       | 0            |
| 32  | W     | 2     | 0        | 0        | 0       | 0            |
| 32  | X     | 2     | 0        | 0        | 0       | 0            |
| 32  | Y     | 3     | 0        | 0        | 0       | 0            |
| 32  | Z     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 92692 | 0        | 0        | 951     | 0            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (951) close contacts within the same asymmetric unit are listed below.

| Atom-1         | Atom-2          | Distance(Å) | Clash(Å) |
|----------------|-----------------|-------------|----------|
| 1:A:1899:G:N2  | 1:A:1902:C:N4   | 2.20        | 0.90     |
| 1:A:1658:C:OP1 | 4:E:132:HIS:ND1 | 2.07        | 0.87     |
| 3:D:33:LEU:O   | 3:D:35:LYS:N    | 2.17        | 0.77     |
| 12:P:50:ARG:CG | 12:P:51:PHE:N   | 2.50        | 0.75     |
| 1:A:2836:U:C4  | 1:A:2883:A:N6   | 2.54        | 0.74     |
| 1:A:603:A:C2   | 1:A:655:A:C6    | 2.75        | 0.74     |
| 4:E:131:ALA:O  | 4:E:133:LYS:N   | 2.20        | 0.74     |
| 3:D:70:TRP:C   | 3:D:70:TRP:CD1  | 2.60        | 0.74     |
| 25:2:47:ASN:O  | 25:2:49:LYS:N   | 2.22        | 0.72     |
| 1:A:2287:A:N6  | 1:A:2344:U:N3   | 2.39        | 0.71     |
| 25:2:1:MET:SD  | 25:2:1:MET:O    | 2.48        | 0.70     |
| 1:A:27:G:O2'   | 1:A:28:A:C8     | 2.45        | 0.69     |
| 3:D:238:GLY:O  | 3:D:239:ARG:C   | 2.31        | 0.69     |
| 1:A:603:A:N1   | 1:A:655:A:C5    | 2.61        | 0.68     |
| 29:6:30:THR:O  | 29:6:32:ASN:N   | 2.26        | 0.68     |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2          | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 3:D:25:THR:CG2   | 3:D:82:ILE:N    | 2.57        | 0.68     |
| 1:A:2346:A:C2    | 1:A:2383:G:C2   | 2.82        | 0.68     |
| 1:A:2259:G:C2    | 1:A:2282:G:N1   | 2.63        | 0.68     |
| 4:E:132:HIS:CD2  | 4:E:135:HIS:CE1 | 2.82        | 0.67     |
| 1:A:203:C:C6     | 1:A:203:C:C3'   | 2.77        | 0.67     |
| 1:A:1019:U:N3    | 1:A:114(B):A:N6 | 2.42        | 0.67     |
| 15:S:90:GLY:O    | 15:S:92:TYR:N   | 2.27        | 0.67     |
| 12:P:62:LEU:CD1  | 12:P:62:LEU:N   | 2.58        | 0.67     |
| 1:A:2579:C:O2'   | 4:E:131:ALA:CB  | 2.43        | 0.67     |
| 1:A:528:A:C3'    | 1:A:528:A:C8    | 2.75        | 0.66     |
| 4:E:132:HIS:CD2  | 4:E:135:HIS:NE2 | 2.63        | 0.66     |
| 12:P:16:ARG:NE   | 12:P:16:ARG:O   | 2.29        | 0.66     |
| 5:F:67:GLN:O     | 5:F:67:GLN:CG   | 2.44        | 0.66     |
| 6:G:132:ASN:N    | 6:G:132:ASN:ND2 | 2.42        | 0.65     |
| 2:B:80:U:C2      | 2:B:81:G:N2     | 2.64        | 0.65     |
| 1:A:780:G:N2     | 1:A:783:A:N6    | 2.45        | 0.65     |
| 1:A:1678:G:O5'   | 1:A:1678:G:C8   | 2.50        | 0.65     |
| 1:A:276:A:C4     | 1:A:277:C:N4    | 2.65        | 0.65     |
| 12:P:23:PRO:CD   | 12:P:33:ARG:CZ  | 2.76        | 0.64     |
| 1:A:140:A:C8     | 1:A:1408:C:O2'  | 2.50        | 0.64     |
| 12:P:48:PRO:O    | 12:P:49:ARG:C   | 2.36        | 0.64     |
| 1:A:27:G:N2      | 1:A:512:G:O2'   | 2.31        | 0.64     |
| 1:A:643:A:C2     | 1:A:644:A:C4    | 2.86        | 0.64     |
| 20:X:28:PHE:N    | 20:X:28:PHE:CD1 | 2.65        | 0.63     |
| 1:A:1346:G:N2    | 1:A:1600:C:O2   | 2.31        | 0.63     |
| 1:A:1543:A:C8    | 1:A:1543:A:C3'  | 2.81        | 0.63     |
| 24:1:11:ARG:CB   | 24:1:12:PRO:CD  | 2.77        | 0.63     |
| 1:A:1191:G:OP1   | 12:P:35:HIS:CD2 | 2.51        | 0.63     |
| 29:6:15:GLU:OE1  | 29:6:18:ARG:NH1 | 2.32        | 0.63     |
| 12:P:58:THR:O    | 12:P:60:MET:N   | 2.31        | 0.63     |
| 3:D:25:THR:O     | 3:D:26:LYS:C    | 2.37        | 0.63     |
| 12:P:23:PRO:CD   | 12:P:33:ARG:NH2 | 2.62        | 0.63     |
| 1:A:2068:U:N3    | 1:A:2430:A:C2   | 2.67        | 0.62     |
| 8:I:27:ARG:CG    | 8:I:27:ARG:NH1  | 2.61        | 0.62     |
| 1:A:568:U:O4     | 18:V:78:LYS:NZ  | 2.33        | 0.62     |
| 1:A:363(G):A:O2' | 1:A:364:C:OP2   | 2.16        | 0.62     |
| 14:R:11:ASN:OD1  | 14:R:12:ARG:N   | 2.33        | 0.61     |
| 1:A:2439:A:C5'   | 1:A:2439:A:C8   | 2.83        | 0.61     |
| 1:A:1496:A:C8    | 1:A:1577:C:O2'  | 2.54        | 0.61     |
| 31:8:57:ARG:NH1  | 31:8:57:ARG:CB  | 2.64        | 0.61     |
| 31:8:34:TRP:CD1  | 31:8:35:GLN:N   | 2.68        | 0.61     |
| 13:Q:74:TYR:O    | 13:Q:89:ASN:N   | 2.34        | 0.60     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 29:6:15:GLU:OE2 | 29:6:18:ARG:CZ  | 2.48        | 0.60     |
| 13:Q:9:TYR:CD2  | 13:Q:9:TYR:O    | 2.54        | 0.60     |
| 2:B:51:G:N2     | 2:B:52:A:N6     | 2.50        | 0.60     |
| 1:A:848:G:C4    | 1:A:933:A:C8    | 2.89        | 0.60     |
| 1:A:943:U:OP2   | 12:P:38:GLN:CD  | 2.40        | 0.60     |
| 1:A:2798:C:C5   | 1:A:2799:A:C6   | 2.89        | 0.60     |
| 1:A:675:A:C4'   | 5:F:67:GLN:NE2  | 2.65        | 0.59     |
| 25:2:1:MET:SD   | 25:2:1:MET:C    | 2.80        | 0.59     |
| 1:A:2259:G:N2   | 1:A:2282:G:C2   | 2.70        | 0.59     |
| 1:A:1658:C:OP1  | 4:E:132:HIS:O   | 2.20        | 0.59     |
| 3:D:56:GLY:O    | 3:D:57:GLY:O    | 2.19        | 0.59     |
| 3:D:235:GLY:O   | 3:D:237:GLU:N   | 2.35        | 0.59     |
| 13:Q:82:ARG:CG  | 13:Q:82:ARG:NH1 | 2.65        | 0.59     |
| 3:D:17:THR:O    | 3:D:211:ARG:NH2 | 2.36        | 0.59     |
| 1:A:297:C:N4    | 1:A:298:G:C2    | 2.72        | 0.58     |
| 1:A:56:A:C2     | 1:A:57:C:C2     | 2.92        | 0.58     |
| 1:A:2836:U:C5   | 1:A:2883:A:N6   | 2.71        | 0.58     |
| 1:A:2063:C:O2   | 1:A:2450:A:N1   | 2.37        | 0.58     |
| 1:A:2821:A:OP2  | 14:R:5:LYS:NZ   | 2.37        | 0.58     |
| 9:K:67:PHE:N    | 9:K:67:PHE:CD1  | 2.71        | 0.58     |
| 28:5:36:CYS:SG  | 28:5:37:LYS:N   | 2.77        | 0.58     |
| 1:A:1926:U:O2   | 1:A:1928:A:C8   | 2.56        | 0.58     |
| 1:A:1678:G:N2   | 1:A:1989:G:N2   | 2.51        | 0.58     |
| 12:P:65:ARG:NH2 | 31:8:15:LYS:CB  | 2.67        | 0.58     |
| 10:N:59:GLY:O   | 10:N:61:HIS:N   | 2.37        | 0.57     |
| 1:A:1349:A:N6   | 1:A:1598:C:N4   | 2.52        | 0.57     |
| 1:A:2563:U:O2   | 1:A:2565:A:C8   | 2.57        | 0.57     |
| 1:A:1332:G:N2   | 1:A:1609:A:O2'  | 2.38        | 0.57     |
| 31:8:61:LEU:O   | 31:8:63:PRO:CD  | 2.52        | 0.57     |
| 1:A:2720:U:O4   | 1:A:2872:G:C6   | 2.58        | 0.57     |
| 11:O:96:THR:OG1 | 11:O:97:ARG:N   | 2.37        | 0.57     |
| 1:A:2210:G:N2   | 1:A:2211:G:C5'  | 2.67        | 0.57     |
| 5:F:45:ARG:NH1  | 5:F:45:ARG:CG   | 2.66        | 0.57     |
| 6:G:166:ASP:OD1 | 6:G:166:ASP:N   | 2.38        | 0.57     |
| 1:A:996:A:C6    | 1:A:1160:G:N1   | 2.72        | 0.57     |
| 24:1:90:ILE:O   | 24:1:94:LEU:N   | 2.37        | 0.57     |
| 29:6:20:ASN:CG  | 29:6:21:TYR:N   | 2.59        | 0.57     |
| 3:D:71:ASP:N    | 3:D:71:ASP:OD2  | 2.38        | 0.56     |
| 12:P:49:ARG:NH1 | 12:P:49:ARG:CG  | 2.68        | 0.56     |
| 15:S:36:TYR:N   | 15:S:36:TYR:CD1 | 2.73        | 0.56     |
| 1:A:309:G:N3    | 1:A:329:G:O2'   | 2.38        | 0.56     |
| 1:A:1312:U:O2   | 1:A:1603:A:C2   | 2.58        | 0.56     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1252:G:C2    | 1:A:1253:A:C2    | 2.94        | 0.56     |
| 30:7:8:ASN:C     | 30:7:8:ASN:ND2   | 2.59        | 0.56     |
| 1:A:1009:A:C5'   | 1:A:1009:A:C8    | 2.88        | 0.56     |
| 2:B:12:C:O2'     | 23:0:74:ARG:CG   | 2.53        | 0.56     |
| 1:A:2530:A:O2'   | 1:A:2532:G:OP2   | 2.23        | 0.56     |
| 15:S:89:ARG:O    | 15:S:90:GLY:O    | 2.23        | 0.56     |
| 5:F:101:LEU:O    | 5:F:106:ARG:NH1  | 2.39        | 0.56     |
| 1:A:941:A:O2'    | 12:P:35:HIS:CD2  | 2.59        | 0.55     |
| 1:A:1022:G:O2'   | 1:A:1023:U:OP2   | 2.24        | 0.55     |
| 1:A:310:A:O2'    | 1:A:311:A:C2'    | 2.54        | 0.55     |
| 12:P:58:THR:C    | 12:P:60:MET:N    | 2.60        | 0.55     |
| 1:A:1332:G:N2    | 1:A:1610:A:C8    | 2.75        | 0.55     |
| 1:A:1272:A:OP2   | 1:A:1647:G:OP1   | 2.25        | 0.55     |
| 1:A:322:A:C5     | 1:A:340:A:C2     | 2.95        | 0.55     |
| 13:Q:134:ARG:O   | 13:Q:135:ASP:C   | 2.45        | 0.55     |
| 22:Z:52:SER:OG   | 22:Z:54:HIS:CD2  | 2.60        | 0.55     |
| 1:A:2259:G:N2    | 1:A:2282:G:N1    | 2.55        | 0.55     |
| 1:A:1465:G:C2    | 1:A:1466:G:C8    | 2.95        | 0.55     |
| 1:A:2419:U:O4    | 31:8:30:ARG:NH1  | 2.40        | 0.55     |
| 10:N:64:ASP:OD1  | 10:N:64:ASP:N    | 2.39        | 0.55     |
| 17:U:104:GLN:OE1 | 17:U:105:VAL:N   | 2.40        | 0.55     |
| 17:U:75:ASN:N    | 17:U:75:ASN:ND2  | 2.54        | 0.54     |
| 1:A:2821:A:OP2   | 1:A:2822:G:OP2   | 2.25        | 0.54     |
| 1:A:2119:A:C6    | 1:A:2171:A:C2    | 2.95        | 0.54     |
| 1:A:2092:U:C4'   | 1:A:2093:G:O5'   | 2.55        | 0.54     |
| 1:A:441:U:O2     | 5:F:46:ARG:NH2   | 2.41        | 0.54     |
| 1:A:2436:G:C5    | 1:A:2437:U:C5    | 2.95        | 0.54     |
| 1:A:1494:A:O2'   | 1:A:1495:A:C5'   | 2.56        | 0.54     |
| 18:V:49:THR:O    | 18:V:50:PRO:C    | 2.46        | 0.54     |
| 12:P:114:ILE:N   | 12:P:114:ILE:CD1 | 2.69        | 0.54     |
| 1:A:1356:G:C6    | 1:A:1357:U:C4    | 2.95        | 0.54     |
| 1:A:1632:A:C5    | 1:A:1633:G:C6    | 2.96        | 0.54     |
| 1:A:1569:A:C6    | 1:A:1570:A:C6    | 2.95        | 0.54     |
| 5:F:195:ASP:OD1  | 5:F:196:LEU:N    | 2.41        | 0.54     |
| 1:A:81:G:N3      | 21:Y:2:ARG:NH2   | 2.55        | 0.54     |
| 1:A:2518:A:C8    | 1:A:2518:A:C5'   | 2.91        | 0.54     |
| 1:A:1544:C:C6    | 1:A:1544:C:OP1   | 2.61        | 0.54     |
| 19:W:18:ARG:NH1  | 19:W:76:VAL:O    | 2.41        | 0.54     |
| 1:A:2403:C:N3    | 1:A:2415:G:C2    | 2.76        | 0.54     |
| 10:N:116:THR:OG1 | 10:N:117:HIS:N   | 2.41        | 0.54     |
| 30:7:19:ARG:NH1  | 30:7:19:ARG:CG   | 2.70        | 0.54     |
| 6:G:16:ARG:NH1   | 6:G:16:ARG:CG    | 2.71        | 0.54     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:2092:U:C5   | 1:A:2226:C:OP2  | 2.62        | 0.53     |
| 1:A:138:G:N2    | 20:X:44:GLU:OE1 | 2.41        | 0.53     |
| 19:W:25:ARG:NH2 | 19:W:74:ALA:O   | 2.41        | 0.53     |
| 1:A:478:A:C6    | 1:A:480:A:C6    | 2.97        | 0.53     |
| 10:N:157:ARG:N  | 10:N:158:PRO:CD | 2.71        | 0.53     |
| 1:A:562:U:O2    | 1:A:572:A:C4    | 2.62        | 0.53     |
| 1:A:2232:U:OP2  | 24:1:40:ARG:NH2 | 2.41        | 0.53     |
| 12:P:33:ARG:O   | 12:P:34:GLY:O   | 2.27        | 0.53     |
| 12:P:64:LYS:O   | 12:P:66:GLY:N   | 2.41        | 0.53     |
| 11:O:88:ASN:N   | 11:O:92:GLU:O   | 2.41        | 0.53     |
| 1:A:396:G:O4'   | 24:1:18:ILE:CD1 | 2.56        | 0.53     |
| 10:N:40:ASP:CG  | 10:N:41:ALA:N   | 2.60        | 0.53     |
| 1:A:498:G:C2    | 1:A:499:U:C5    | 2.97        | 0.53     |
| 1:A:603:A:C6    | 1:A:655:A:C4    | 2.97        | 0.53     |
| 1:A:2688:U:C5   | 1:A:2720:U:OP2  | 2.62        | 0.53     |
| 5:F:74:ARG:O    | 5:F:75:HIS:CG   | 2.62        | 0.53     |
| 20:X:60:ARG:NH2 | 30:7:47:ARG:NH1 | 2.57        | 0.53     |
| 1:A:2543:G:N2   | 1:A:2765:A:C8   | 2.77        | 0.53     |
| 1:A:1654:A:OP2  | 14:R:3:HIS:CD2  | 2.62        | 0.53     |
| 1:A:864:G:C6    | 1:A:865:C:N4    | 2.77        | 0.53     |
| 1:A:1608:A:O2'  | 1:A:1610:A:OP2  | 2.27        | 0.52     |
| 1:A:2687:U:C4   | 1:A:2688:U:C5   | 2.97        | 0.52     |
| 1:A:2542:A:C8   | 1:A:2544:G:O6   | 2.62        | 0.52     |
| 15:S:12:PHE:N   | 15:S:12:PHE:CD2 | 2.76        | 0.52     |
| 1:A:429:A:C2    | 1:A:430:G:C2    | 2.97        | 0.52     |
| 17:U:57:PHE:O   | 17:U:58:ARG:C   | 2.47        | 0.52     |
| 2:B:66:A:C2     | 2:B:108:C:C2    | 2.98        | 0.52     |
| 28:5:3:LYS:O    | 28:5:4:HIS:C    | 2.48        | 0.52     |
| 7:H:94:TYR:CD1  | 7:H:94:TYR:N    | 2.77        | 0.52     |
| 5:F:89:VAL:O    | 5:F:91:GLY:N    | 2.42        | 0.52     |
| 12:P:58:THR:C   | 12:P:61:ARG:NE  | 2.63        | 0.52     |
| 1:A:2334:G:C2   | 15:S:12:PHE:CE1 | 2.98        | 0.52     |
| 1:A:955:C:OP1   | 13:Q:85:LYS:NZ  | 2.42        | 0.52     |
| 20:X:80:ILE:CG1 | 20:X:80:ILE:O   | 2.57        | 0.52     |
| 13:Q:26:TYR:O   | 13:Q:67:ARG:NH1 | 2.43        | 0.52     |
| 17:U:90:VAL:O   | 17:U:91:ASP:C   | 2.47        | 0.52     |
| 1:A:1110:G:O2'  | 1:A:1111:A:C8   | 2.63        | 0.52     |
| 3:D:242:ARG:CD  | 3:D:242:ARG:N   | 2.72        | 0.52     |
| 1:A:1519:G:C5   | 1:A:1520:U:C5   | 2.98        | 0.52     |
| 1:A:2681:C:C5   | 1:A:2725:A:N6   | 2.78        | 0.52     |
| 1:A:943:U:OP2   | 12:P:38:GLN:OE1 | 2.28        | 0.52     |
| 17:U:90:VAL:CG2 | 17:U:91:ASP:N   | 2.72        | 0.52     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:2484:G:C2    | 1:A:2485:G:C8    | 2.97        | 0.52     |
| 1:A:270(F):G:C6  | 1:A:270(G):U:C4  | 2.98        | 0.52     |
| 6:G:143:GLU:O    | 27:4:54:LYS:NZ   | 2.43        | 0.52     |
| 1:A:1575:C:C2    | 1:A:1576:U:C6    | 2.98        | 0.52     |
| 1:A:2517:C:C6    | 1:A:2542:A:C2    | 2.98        | 0.52     |
| 1:A:464:U:C2     | 1:A:788:A:C6     | 2.98        | 0.52     |
| 1:A:860:U:C5     | 1:A:917:A:N7     | 2.78        | 0.52     |
| 1:A:578:A:O2'    | 1:A:580:C:OP2    | 2.28        | 0.52     |
| 16:T:106:SER:C   | 16:T:107:ASP:OD1 | 2.48        | 0.52     |
| 11:O:105:GLU:OE1 | 11:O:105:GLU:N   | 2.43        | 0.52     |
| 2:B:78:A:C2      | 2:B:99:A:C4      | 2.97        | 0.51     |
| 1:A:1512:G:C5    | 1:A:1513:C:C5    | 2.98        | 0.51     |
| 1:A:2114:A:C5    | 1:A:2115:G:C6    | 2.97        | 0.51     |
| 1:A:2352:A:C2    | 23:0:33:ALA:O    | 2.63        | 0.51     |
| 12:P:40:SER:O    | 12:P:41:ARG:NE   | 2.42        | 0.51     |
| 1:A:866:A:N6     | 1:A:914:C:C4     | 2.78        | 0.51     |
| 2:B:42:C:C4      | 6:G:91:ARG:NH2   | 2.78        | 0.51     |
| 17:U:25:TRP:C    | 17:U:25:TRP:CD1  | 2.82        | 0.51     |
| 1:A:2093:G:C6    | 1:A:2225:A:C8    | 2.98        | 0.51     |
| 1:A:2867:G:OP2   | 16:T:119:LYS:NZ  | 2.43        | 0.51     |
| 1:A:643:A:OP1    | 29:6:42:TRP:NE1  | 2.42        | 0.51     |
| 1:A:2683:C:OP1   | 16:T:53:ARG:NH2  | 2.43        | 0.51     |
| 1:A:2286:A:C8    | 1:A:2287:A:N6    | 2.78        | 0.51     |
| 1:A:1682:G:C6    | 1:A:1683:C:C4    | 2.98        | 0.51     |
| 8:I:87:LYS:CG    | 8:I:88:ILE:N     | 2.73        | 0.51     |
| 1:A:2228:G:OP2   | 3:D:263:ARG:NH1  | 2.44        | 0.51     |
| 5:F:128:ALA:O    | 5:F:142:TRP:NE1  | 2.43        | 0.51     |
| 25:2:17:SER:O    | 25:2:18:PRO:C    | 2.49        | 0.51     |
| 1:A:1301:A:C8    | 1:A:1303:G:C8    | 2.98        | 0.51     |
| 13:Q:55:VAL:CG2  | 13:Q:56:ARG:N    | 2.74        | 0.51     |
| 1:A:1952:A:C5    | 11:O:22:ILE:CD1  | 2.94        | 0.51     |
| 12:P:108:LYS:C   | 12:P:110:TYR:N   | 2.63        | 0.51     |
| 1:A:1126:A:C4'   | 1:A:1127:A:O5'   | 2.59        | 0.51     |
| 18:V:21:ARG:NH2  | 18:V:91:TYR:CZ   | 2.78        | 0.51     |
| 1:A:126:A:C5     | 30:7:18:PHE:CD1  | 2.99        | 0.51     |
| 1:A:70:G:O2'     | 1:A:113:G:O2'    | 2.28        | 0.51     |
| 16:T:3:ARG:O     | 16:T:6:LEU:N     | 2.44        | 0.51     |
| 1:A:459:U:OP2    | 1:A:469:G:N1     | 2.43        | 0.51     |
| 6:G:136:ARG:O    | 6:G:137:GLU:C    | 2.47        | 0.51     |
| 1:A:2536:G:C6    | 1:A:2537:U:C4    | 2.98        | 0.51     |
| 1:A:2572:A:C8    | 4:E:144:ARG:CB   | 2.93        | 0.51     |
| 1:A:1311:G:C2    | 20:X:60:ARG:NH1  | 2.79        | 0.51     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 13:Q:47:ILE:CG2  | 13:Q:48:GLU:N   | 2.74        | 0.51     |
| 1:A:829:A:N7     | 1:A:2247:A:O2'  | 2.43        | 0.51     |
| 1:A:781:A:C2     | 1:A:1776:G:N3   | 2.79        | 0.51     |
| 1:A:2199:A:C8    | 1:A:2205:C:C5   | 3.00        | 0.50     |
| 19:W:84:ARG:O    | 19:W:96:ILE:N   | 2.44        | 0.50     |
| 1:A:768:G:C6     | 1:A:769:G:C5    | 2.99        | 0.50     |
| 12:P:30:THR:CG2  | 12:P:31:ALA:N   | 2.73        | 0.50     |
| 5:F:179:GLU:OE1  | 5:F:179:GLU:N   | 2.44        | 0.50     |
| 3:D:83:GLU:OE1   | 3:D:104:TYR:OH  | 2.30        | 0.50     |
| 30:7:34:ARG:NH1  | 30:7:34:ARG:CG  | 2.73        | 0.50     |
| 3:D:58:HIS:O     | 3:D:59:LYS:C    | 2.48        | 0.50     |
| 1:A:303:U:C2     | 1:A:304:G:C8    | 3.00        | 0.50     |
| 1:A:2851:A:C6    | 1:A:2852:G:C6   | 3.00        | 0.50     |
| 1:A:2029:G:C4    | 1:A:2031:A:OP2  | 2.64        | 0.50     |
| 25:2:48:HIS:O    | 25:2:49:LYS:C   | 2.48        | 0.50     |
| 1:A:1099:G:C6    | 1:A:1100:C:N4   | 2.80        | 0.50     |
| 1:A:2859:G:C6    | 1:A:2860:A:N6   | 2.80        | 0.50     |
| 28:5:40:LYS:NZ   | 28:5:46:CYS:N   | 2.60        | 0.50     |
| 5:F:132:VAL:O    | 5:F:133:ASN:C   | 2.50        | 0.50     |
| 8:I:112:LYS:O    | 8:I:114:LEU:N   | 2.44        | 0.50     |
| 1:A:2018:G:C6    | 1:A:2019:A:C6   | 2.98        | 0.50     |
| 24:1:13:ILE:O    | 24:1:14:VAL:CB  | 2.59        | 0.50     |
| 12:P:51:PHE:O    | 12:P:52:GLU:CB  | 2.59        | 0.50     |
| 1:A:1530:G:N1    | 1:A:1542:G:N2   | 2.60        | 0.50     |
| 1:A:1332:G:C4'   | 1:A:1333:C:OP2  | 2.59        | 0.50     |
| 1:A:864:G:C4     | 1:A:865:C:C5    | 3.00        | 0.50     |
| 22:Z:118:GLN:N   | 22:Z:173:ALA:O  | 2.44        | 0.50     |
| 1:A:2850:A:C8    | 1:A:2869:G:O4'  | 2.64        | 0.50     |
| 1:A:2335:A:C8    | 1:A:2337:G:C5   | 2.99        | 0.50     |
| 1:A:1066:U:O2    | 1:A:1069:A:C8   | 2.65        | 0.50     |
| 1:A:1217:C:C4    | 1:A:1218:C:C5   | 2.99        | 0.50     |
| 1:A:24:G:C6      | 1:A:25:U:C4     | 2.99        | 0.50     |
| 1:A:2845:G:OP1   | 16:T:56:GLY:N   | 2.45        | 0.50     |
| 1:A:214:G:O2'    | 1:A:215:G:O4'   | 2.29        | 0.50     |
| 25:2:3:LEU:O     | 25:2:4:SER:C    | 2.50        | 0.50     |
| 17:U:82:GLY:O    | 17:U:86:ALA:N   | 2.45        | 0.50     |
| 3:D:124:PRO:O    | 3:D:129:ASN:ND2 | 2.45        | 0.50     |
| 1:A:270(Q):C:O2' | 1:A:270(R):C:C6 | 2.65        | 0.50     |
| 16:T:22:PHE:CG   | 16:T:22:PHE:O   | 2.64        | 0.50     |
| 1:A:1176:G:C8    | 1:A:1177:A:C5   | 3.00        | 0.49     |
| 9:K:112:MET:N    | 9:K:113:PRO:CD  | 2.74        | 0.49     |
| 1:A:996:A:N6     | 1:A:1160:G:C6   | 2.79        | 0.49     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 15:S:35:ILE:C   | 15:S:36:TYR:CD1 | 2.85        | 0.49     |
| 21:Y:17:SER:OG  | 21:Y:18:GLY:N   | 2.45        | 0.49     |
| 17:U:92:ARG:O   | 17:U:94:ASN:N   | 2.45        | 0.49     |
| 1:A:390:A:N6    | 12:P:71:VAL:CG2 | 2.75        | 0.49     |
| 1:A:575:A:OP2   | 1:A:2055:C:N4   | 2.45        | 0.49     |
| 25:2:1:MET:SD   | 25:2:5:GLU:OE2  | 2.70        | 0.49     |
| 1:A:1661:G:C6   | 1:A:2000:G:C6   | 2.99        | 0.49     |
| 1:A:663:G:C6    | 1:A:664:C:C4    | 3.00        | 0.49     |
| 1:A:275:G:N2    | 1:A:276:A:C6    | 2.80        | 0.49     |
| 1:A:2446:G:C2   | 1:A:2501:C:C5   | 3.01        | 0.49     |
| 24:1:90:ILE:O   | 24:1:91:LYS:C   | 2.51        | 0.49     |
| 1:A:573:G:N2    | 1:A:2029:G:N2   | 2.61        | 0.49     |
| 13:Q:22:LYS:NZ  | 13:Q:22:LYS:CA  | 2.75        | 0.49     |
| 12:P:55:ARG:CG  | 12:P:56:SER:N   | 2.75        | 0.49     |
| 1:A:2481:G:O2'  | 1:A:2482:G:P    | 2.70        | 0.49     |
| 1:A:2663:G:C6   | 1:A:2664:G:C5   | 3.00        | 0.49     |
| 1:A:996:A:C6    | 1:A:1160:G:C2   | 3.01        | 0.49     |
| 16:T:3:ARG:O    | 16:T:5:ALA:N    | 2.45        | 0.49     |
| 24:1:27:GLU:CB  | 24:1:33:LYS:CG  | 2.90        | 0.49     |
| 2:B:61:G:C6     | 2:B:62:C:C4     | 3.00        | 0.49     |
| 1:A:1658:C:OP1  | 4:E:132:HIS:CE1 | 2.66        | 0.49     |
| 3:D:68:LYS:O    | 3:D:69:ARG:C    | 2.51        | 0.49     |
| 1:A:27:G:O2'    | 1:A:28:A:P      | 2.71        | 0.49     |
| 13:Q:88:GLY:C   | 13:Q:89:ASN:OD1 | 2.50        | 0.49     |
| 1:A:2516:G:C6   | 1:A:2517:C:N4   | 2.80        | 0.49     |
| 1:A:768:G:O2'   | 1:A:1379:A:N6   | 2.46        | 0.49     |
| 1:A:2069:G:C2   | 1:A:2070:G:C8   | 3.01        | 0.49     |
| 1:A:1800:C:OP2  | 3:D:183:ARG:NH2 | 2.46        | 0.49     |
| 1:A:2862:G:C4   | 1:A:2863:C:C5   | 3.01        | 0.49     |
| 4:E:201:THR:CG2 | 4:E:202:LYS:N   | 2.75        | 0.49     |
| 17:U:36:ARG:CG  | 17:U:40:PHE:CE1 | 2.96        | 0.49     |
| 15:S:34:HIS:O   | 15:S:97:ARG:NH2 | 2.46        | 0.48     |
| 1:A:122:G:N2    | 1:A:130:C:C2    | 2.81        | 0.48     |
| 5:F:164:ARG:O   | 5:F:165:ARG:C   | 2.51        | 0.48     |
| 1:A:1525:G:C4   | 1:A:1526:G:C8   | 3.01        | 0.48     |
| 1:A:1615:C:C6   | 1:A:1617:C:C5   | 3.01        | 0.48     |
| 16:T:55:ASN:O   | 16:T:57:PHE:O   | 2.31        | 0.48     |
| 1:A:2134:A:C8   | 1:A:2158:A:C2   | 3.01        | 0.48     |
| 18:V:49:THR:O   | 18:V:51:VAL:N   | 2.45        | 0.48     |
| 1:A:2334:G:C4   | 15:S:12:PHE:CZ  | 3.02        | 0.48     |
| 30:7:18:PHE:CD2 | 30:7:18:PHE:C   | 2.86        | 0.48     |
| 1:A:2176:A:C6   | 1:A:2177:C:N4   | 2.81        | 0.48     |

*Continued on next page...*



*Continued from previous page...*

| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:1607:C:N4   | 1:A:1622:G:OP2  | 2.46        | 0.48     |
| 2:B:16:G:C6     | 2:B:69:G:C2     | 3.01        | 0.48     |
| 1:A:2893:G:C4'  | 1:A:2894:G:C8   | 2.97        | 0.48     |
| 1:A:868:U:C4    | 1:A:869:G:N7    | 2.81        | 0.48     |
| 3:D:25:THR:O    | 3:D:25:THR:CG2  | 2.60        | 0.48     |
| 18:V:79:VAL:O   | 18:V:80:GLN:C   | 2.51        | 0.48     |
| 13:Q:134:ARG:O  | 13:Q:134:ARG:CG | 2.61        | 0.48     |
| 13:Q:22:LYS:O   | 13:Q:24:GLY:N   | 2.46        | 0.48     |
| 1:A:2083:G:C5   | 1:A:2084:C:C4   | 3.02        | 0.48     |
| 1:A:504:U:O2    | 1:A:504:U:O4'   | 2.30        | 0.48     |
| 1:A:2422:A:C4   | 1:A:2424:C:C5   | 3.02        | 0.48     |
| 12:P:50:ARG:O   | 12:P:51:PHE:C   | 2.50        | 0.48     |
| 1:A:603:A:N1    | 1:A:655:A:C4    | 2.82        | 0.48     |
| 2:B:81:G:O6     | 2:B:95:U:O2     | 2.31        | 0.48     |
| 1:A:275:G:O6    | 1:A:363(A):G:C2 | 2.66        | 0.48     |
| 1:A:1022:G:C6   | 1:A:1140:C:C4   | 3.02        | 0.48     |
| 28:5:3:LYS:O    | 28:5:4:HIS:O    | 2.31        | 0.48     |
| 1:A:1359:A:C8   | 1:A:1372:U:O4   | 2.67        | 0.48     |
| 1:A:2212:A:N3   | 1:A:2215:G:N2   | 2.62        | 0.48     |
| 11:O:4:PRO:O    | 11:O:5:GLN:CB   | 2.62        | 0.48     |
| 1:A:783:A:C3'   | 1:A:783:A:C8    | 2.97        | 0.48     |
| 1:A:2280:G:C2   | 1:A:2281:C:C6   | 3.01        | 0.48     |
| 15:S:66:ALA:O   | 15:S:67:ARG:C   | 2.51        | 0.48     |
| 1:A:68:G:N2     | 1:A:74:A:C4     | 2.81        | 0.48     |
| 25:2:13:ALA:O   | 25:2:17:SER:CA  | 2.62        | 0.48     |
| 19:W:45:TYR:OH  | 19:W:49:LYS:NZ  | 2.46        | 0.48     |
| 15:S:102:ALA:O  | 15:S:103:GLU:C  | 2.51        | 0.48     |
| 4:E:48:GLN:NE2  | 4:E:66:HIS:CE1  | 2.82        | 0.48     |
| 7:H:47:GLU:OE1  | 7:H:48:GLY:N    | 2.47        | 0.48     |
| 2:B:43:C:C5     | 2:B:45:A:N6     | 2.82        | 0.48     |
| 10:N:81:ASP:OD1 | 10:N:81:ASP:N   | 2.47        | 0.48     |
| 1:A:1494:A:O2'  | 1:A:1495:A:O5'  | 2.32        | 0.48     |
| 5:F:59:TYR:CE1  | 5:F:85:GLY:O    | 2.67        | 0.48     |
| 1:A:481:G:O2'   | 1:A:482:A:P     | 2.72        | 0.48     |
| 1:A:512:G:O2'   | 1:A:513:A:OP2   | 2.32        | 0.48     |
| 12:P:17:LYS:C   | 12:P:19:VAL:N   | 2.66        | 0.48     |
| 28:5:4:HIS:CB   | 28:5:5:PRO:CD   | 2.91        | 0.48     |
| 1:A:2815:C:O2'  | 28:5:43:HIS:CD2 | 2.66        | 0.48     |
| 1:A:274:G:C2    | 1:A:275:G:N2    | 2.81        | 0.48     |
| 1:A:2018:G:C6   | 1:A:2019:A:C5   | 3.02        | 0.47     |
| 1:A:135:G:N2    | 1:A:144:C:N3    | 2.62        | 0.47     |
| 7:H:101:ARG:N   | 7:H:101:ARG:NE  | 2.62        | 0.47     |

*Continued on next page...*



*Continued from previous page...*

| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:2447:G:C6   | 1:A:2501:C:C2   | 3.02        | 0.47     |
| 1:A:2717:G:C6   | 1:A:2718:G:C5   | 3.02        | 0.47     |
| 1:A:2663:G:C6   | 1:A:2664:G:C4   | 3.02        | 0.47     |
| 12:P:105:LEU:O  | 12:P:106:LEU:CB | 2.62        | 0.47     |
| 1:A:265:A:C6    | 1:A:428:A:C4    | 3.02        | 0.47     |
| 22:Z:150:LEU:O  | 22:Z:171:ILE:N  | 2.47        | 0.47     |
| 1:A:290:G:C5    | 1:A:291:C:C5    | 3.02        | 0.47     |
| 1:A:1843:C:O2'  | 3:D:256:GLY:O   | 2.31        | 0.47     |
| 1:A:2576:G:O2'  | 1:A:2579:C:OP2  | 2.32        | 0.47     |
| 3:D:70:TRP:CD1  | 3:D:71:ASP:N    | 2.82        | 0.47     |
| 1:A:1828:G:OP2  | 3:D:239:ARG:NH1 | 2.47        | 0.47     |
| 1:A:1566:A:OP1  | 3:D:211:ARG:NH1 | 2.47        | 0.47     |
| 9:K:26:ALA:O    | 9:K:30:HIS:ND1  | 2.46        | 0.47     |
| 1:A:1936:A:C3'  | 1:A:1936:A:OP1  | 2.62        | 0.47     |
| 18:V:65:GLY:O   | 18:V:91:TYR:CD2 | 2.67        | 0.47     |
| 31:8:37:SER:OG  | 31:8:40:GLU:N   | 2.47        | 0.47     |
| 1:A:2187:G:C6   | 1:A:2188:C:C4   | 3.02        | 0.47     |
| 1:A:1491:G:C6   | 1:A:1500:G:C2   | 3.02        | 0.47     |
| 1:A:2585:U:C2'  | 1:A:2585:U:O2   | 2.62        | 0.47     |
| 12:P:23:PRO:CB  | 12:P:33:ARG:CG  | 2.92        | 0.47     |
| 1:A:2134:A:C2   | 1:A:2135:A:C8   | 3.03        | 0.47     |
| 1:A:2637:U:C4   | 1:A:2638:G:C6   | 3.02        | 0.47     |
| 1:A:2275:C:C6   | 1:A:2275:C:C5'  | 2.97        | 0.47     |
| 1:A:2228:G:C5   | 1:A:2229:C:C4   | 3.03        | 0.47     |
| 1:A:2245:U:O2   | 1:A:2435:A:C8   | 2.68        | 0.47     |
| 14:R:4:LEU:C    | 14:R:6:SER:N    | 2.67        | 0.47     |
| 1:A:2498:C:OP2  | 1:A:2499:C:OP2  | 2.32        | 0.47     |
| 12:P:16:ARG:NH1 | 12:P:18:ARG:CG  | 2.78        | 0.47     |
| 1:A:2543:G:C2   | 1:A:2765:A:C8   | 3.02        | 0.47     |
| 16:T:58:ASN:ND2 | 16:T:58:ASN:C   | 2.67        | 0.47     |
| 19:W:15:ARG:NH2 | 28:5:20:ARG:NH1 | 2.63        | 0.47     |
| 1:A:2646:C:OP2  | 1:A:2732:G:O2'  | 2.33        | 0.47     |
| 8:I:130:TYR:CD2 | 8:I:131:LYS:N   | 2.83        | 0.47     |
| 2:B:30:C:C5     | 2:B:31:C:C5     | 3.03        | 0.47     |
| 1:A:1142:U:C3'  | 1:A:1142:U:C6   | 2.97        | 0.47     |
| 1:A:2740:A:N6   | 1:A:2764:A:C8   | 2.83        | 0.47     |
| 5:F:107:LYS:O   | 5:F:108:LYS:C   | 2.51        | 0.47     |
| 1:A:2302:G:C6   | 1:A:2315:G:C6   | 3.02        | 0.47     |
| 1:A:1939:U:OP1  | 1:A:2604:U:O2'  | 2.31        | 0.47     |
| 4:E:132:HIS:CG  | 4:E:135:HIS:NE2 | 2.83        | 0.47     |
| 1:A:274:G:C3'   | 1:A:274:G:C8    | 2.98        | 0.47     |
| 30:7:46:VAL:CG1 | 30:7:47:ARG:N   | 2.77        | 0.47     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:1027:A:N6   | 1:A:1126:A:C4    | 2.82        | 0.47     |
| 1:A:1615:C:C5   | 1:A:1617:C:C4    | 3.01        | 0.47     |
| 4:E:152:LYS:O   | 10:N:101:TYR:CD2 | 2.67        | 0.47     |
| 1:A:973:A:OP2   | 18:V:78:LYS:NZ   | 2.47        | 0.47     |
| 8:I:88:ILE:O    | 8:I:121:LYS:NZ   | 2.48        | 0.47     |
| 1:A:2809:A:C2   | 1:A:2892:A:N3    | 2.82        | 0.47     |
| 1:A:1439:A:C2   | 1:A:1553:A:C4    | 3.02        | 0.47     |
| 1:A:8:A:C2      | 1:A:9:U:C2       | 3.03        | 0.47     |
| 1:A:1021:A:C3'  | 1:A:1021:A:C8    | 2.97        | 0.47     |
| 18:V:80:GLN:O   | 18:V:80:GLN:NE2  | 2.48        | 0.47     |
| 22:Z:10:ARG:NH2 | 22:Z:26:GLY:O    | 2.48        | 0.47     |
| 1:A:1264:G:O5'  | 1:A:1264:G:C8    | 2.68        | 0.47     |
| 1:A:1544:C:C3'  | 1:A:1545:A:C5'   | 2.93        | 0.46     |
| 1:A:216:A:C8    | 1:A:432:A:C6     | 3.03        | 0.46     |
| 1:A:274:G:C8    | 1:A:274:G:OP1    | 2.68        | 0.46     |
| 1:A:1519:G:C6   | 1:A:1520:U:C4    | 3.02        | 0.46     |
| 1:A:235:U:C2    | 1:A:236:C:C5     | 3.03        | 0.46     |
| 1:A:422:A:C2    | 1:A:423:A:C4     | 3.03        | 0.46     |
| 8:I:52:ARG:NH1  | 8:I:52:ARG:CG    | 2.77        | 0.46     |
| 1:A:2084:C:C2   | 1:A:2085:C:C5    | 3.04        | 0.46     |
| 24:1:57:GLU:O   | 24:1:58:ILE:CB   | 2.64        | 0.46     |
| 17:U:98:LEU:O   | 17:U:101:ARG:O   | 2.33        | 0.46     |
| 1:A:1731:G:O2'  | 1:A:1732:A:P     | 2.73        | 0.46     |
| 1:A:197:A:C5'   | 1:A:197:A:C8     | 2.98        | 0.46     |
| 1:A:2134:A:C8   | 1:A:2158:A:N1    | 2.83        | 0.46     |
| 1:A:310:A:OP1   | 21:Y:17:SER:O    | 2.32        | 0.46     |
| 2:B:66:A:C6     | 2:B:107:U:C2     | 3.04        | 0.46     |
| 15:S:66:ALA:O   | 15:S:69:VAL:CG1  | 2.64        | 0.46     |
| 1:A:1491:G:N2   | 1:A:1499:C:O2    | 2.48        | 0.46     |
| 24:1:67:ILE:N   | 24:1:68:PRO:CD   | 2.79        | 0.46     |
| 1:A:374:A:C2    | 1:A:401:A:C4     | 3.02        | 0.46     |
| 1:A:2798:C:OP2  | 1:A:2799:A:N7    | 2.49        | 0.46     |
| 1:A:1312:U:C2   | 1:A:1603:A:C2    | 3.04        | 0.46     |
| 1:A:2872:G:C2   | 1:A:2873:A:N6    | 2.84        | 0.46     |
| 13:Q:134:ARG:O  | 13:Q:136:ALA:N   | 2.48        | 0.46     |
| 1:A:1027:A:C6   | 1:A:1126:A:C4    | 3.04        | 0.46     |
| 1:A:1270:C:O2'  | 1:A:1648:C:OP2   | 2.34        | 0.46     |
| 1:A:1322:A:C5   | 1:A:1323:U:C5    | 3.04        | 0.46     |
| 23:O:34:GLY:CA  | 23:O:61:ALA:O    | 2.63        | 0.46     |
| 1:A:2403:C:C4   | 1:A:2415:G:C2    | 3.03        | 0.46     |
| 1:A:1729:A:C5   | 1:A:1731:G:C6    | 3.03        | 0.46     |
| 16:T:124:ASP:O  | 16:T:128:GLU:CB  | 2.64        | 0.46     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:1419:A:C8   | 1:A:1421:G:C6   | 3.04        | 0.46     |
| 1:A:517:C:OP1   | 28:5:16:ARG:NH2 | 2.48        | 0.46     |
| 25:2:50:ILE:CD1 | 25:2:51:ARG:N   | 2.79        | 0.46     |
| 1:A:165:U:C2    | 1:A:171:G:C8    | 3.03        | 0.46     |
| 21:Y:81:LYS:NZ  | 21:Y:98:VAL:CG1 | 2.78        | 0.46     |
| 17:U:92:ARG:O   | 17:U:93:LYS:C   | 2.54        | 0.46     |
| 1:A:512:G:O2'   | 1:A:513:A:P     | 2.74        | 0.46     |
| 1:A:298:G:C8    | 1:A:298:G:O5'   | 2.69        | 0.46     |
| 14:R:8:ARG:NH2  | 14:R:21:TYR:CE1 | 2.84        | 0.46     |
| 3:D:122:ASP:OD2 | 3:D:123:ALA:N   | 2.49        | 0.46     |
| 1:A:953:A:OP2   | 13:Q:16:ARG:NH2 | 2.49        | 0.46     |
| 12:P:33:ARG:C   | 12:P:34:GLY:O   | 2.52        | 0.46     |
| 1:A:2528:U:C6   | 1:A:2530:A:C8   | 3.04        | 0.46     |
| 16:T:57:PHE:CG  | 16:T:58:ASN:N   | 2.83        | 0.46     |
| 19:W:32:ALA:O   | 19:W:33:ARG:C   | 2.55        | 0.46     |
| 1:A:280:C:C2    | 1:A:361:G:C2    | 3.03        | 0.46     |
| 13:Q:18:LYS:O   | 13:Q:19:GLY:O   | 2.34        | 0.46     |
| 1:A:58:G:O2'    | 1:A:73:A:N1     | 2.49        | 0.46     |
| 1:A:582:G:C6    | 1:A:583:G:C6    | 3.04        | 0.46     |
| 1:A:642:G:C3'   | 1:A:642:G:C8    | 2.99        | 0.46     |
| 1:A:1448:G:N2   | 1:A:149(B):A:N6 | 2.64        | 0.45     |
| 1:A:1341:U:OP1  | 1:A:1397:U:N3   | 2.50        | 0.45     |
| 1:A:593:G:C6    | 1:A:594:U:C4    | 3.04        | 0.45     |
| 1:A:1542:G:C8   | 1:A:1543:A:C6   | 3.04        | 0.45     |
| 1:A:832:G:OP1   | 12:P:40:SER:CB  | 2.64        | 0.45     |
| 25:2:17:SER:O   | 25:2:20:GLU:N   | 2.49        | 0.45     |
| 1:A:1775:U:C2'  | 1:A:1776:G:O5'  | 2.65        | 0.45     |
| 2:B:86:G:N2     | 2:B:90:C:C2     | 2.84        | 0.45     |
| 17:U:69:CYS:SG  | 17:U:79:PHE:CB  | 3.05        | 0.45     |
| 5:F:180:GLY:O   | 5:F:181:LEU:C   | 2.54        | 0.45     |
| 1:A:1447:G:N2   | 1:A:1528:A:C2   | 2.84        | 0.45     |
| 1:A:2726:U:O2   | 1:A:2726:U:O4'  | 2.34        | 0.45     |
| 1:A:2798:C:OP2  | 1:A:2799:A:N6   | 2.50        | 0.45     |
| 1:A:2114:A:C3'  | 1:A:2115:G:C8   | 2.99        | 0.45     |
| 5:F:53:THR:C    | 5:F:55:GLY:N    | 2.70        | 0.45     |
| 2:B:57:A:N3     | 6:G:29:TRP:CB   | 2.80        | 0.45     |
| 1:A:2119:A:N1   | 1:A:2171:A:N3   | 2.64        | 0.45     |
| 18:V:47:VAL:O   | 18:V:48:GLY:C   | 2.53        | 0.45     |
| 1:A:1931:U:OP2  | 1:A:1968:G:N1   | 2.49        | 0.45     |
| 24:1:83:GLU:O   | 24:1:86:SER:OG  | 2.34        | 0.45     |
| 16:T:28:VAL:CG2 | 16:T:29:ARG:N   | 2.80        | 0.45     |
| 14:R:81:ASP:N   | 14:R:81:ASP:OD2 | 2.49        | 0.45     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 1:A:1395:A:C6    | 1:A:1398:C:C2   | 3.04        | 0.45     |
| 1:A:855:G:C5     | 1:A:856:C:C5    | 3.04        | 0.45     |
| 1:A:1496:A:C8    | 1:A:1498:C:N3   | 2.84        | 0.45     |
| 31:8:62:LEU:O    | 31:8:63:PRO:C   | 2.52        | 0.45     |
| 18:V:4:ILE:O     | 18:V:39:LEU:N   | 2.50        | 0.45     |
| 1:A:2320:A:C2    | 1:A:2333:A:C8   | 3.04        | 0.45     |
| 20:X:50:LYS:N    | 20:X:87:GLN:NE2 | 2.65        | 0.45     |
| 1:A:64:A:C4      | 1:A:65:C:C6     | 3.05        | 0.45     |
| 1:A:2419:U:O4    | 31:8:30:ARG:CZ  | 2.65        | 0.45     |
| 1:A:1682:G:C5    | 1:A:1683:C:C4   | 3.04        | 0.45     |
| 1:A:1817:G:OP1   | 3:D:88:ARG:NH2  | 2.50        | 0.45     |
| 1:A:8:A:C2       | 1:A:9:U:O2      | 2.69        | 0.45     |
| 14:R:9:LYS:O     | 14:R:10:LEU:CB  | 2.64        | 0.45     |
| 1:A:1831:G:C5    | 1:A:1832:C:C5   | 3.05        | 0.45     |
| 25:2:12:GLU:C    | 25:2:14:ARG:N   | 2.69        | 0.45     |
| 14:R:103:ARG:NH1 | 14:R:108:GLY:O  | 2.50        | 0.45     |
| 1:A:1281:G:C6    | 1:A:1282:U:C4   | 3.04        | 0.45     |
| 1:A:2405:G:OP1   | 12:P:77:ARG:NH2 | 2.50        | 0.45     |
| 1:A:764:A:N3     | 3:D:213:ARG:NH1 | 2.64        | 0.45     |
| 3:D:267:SER:O    | 3:D:269:PHE:N   | 2.50        | 0.45     |
| 12:P:16:ARG:NE   | 12:P:16:ARG:C   | 2.70        | 0.45     |
| 1:A:2862:G:C5    | 1:A:2863:C:C5   | 3.05        | 0.45     |
| 28:5:16:ARG:NH1  | 28:5:17:ASP:OD1 | 2.50        | 0.45     |
| 1:A:900:A:C4     | 1:A:901:A:C8    | 3.04        | 0.45     |
| 1:A:1374:G:C5    | 1:A:1375:C:C5   | 3.04        | 0.45     |
| 1:A:1567:A:C8    | 3:D:84:TYR:CE2  | 3.04        | 0.45     |
| 8:I:109:ILE:CD1  | 8:I:109:ILE:N   | 2.80        | 0.45     |
| 15:S:88:ASP:O    | 15:S:90:GLY:N   | 2.50        | 0.45     |
| 1:A:1056:G:N2    | 1:A:1104:C:N4   | 2.65        | 0.45     |
| 1:A:1374:G:C6    | 1:A:1375:C:C4   | 3.05        | 0.45     |
| 1:A:2074:U:N3    | 1:A:2075:U:C4   | 2.84        | 0.45     |
| 29:6:24:GLU:CD   | 29:6:25:LYS:N   | 2.71        | 0.45     |
| 1:A:2126:A:C2    | 1:A:2173:A:C5   | 3.04        | 0.45     |
| 2:B:46:A:C5      | 2:B:47:C:C4     | 3.04        | 0.45     |
| 4:E:15:PHE:N     | 4:E:15:PHE:CD2  | 2.85        | 0.45     |
| 1:A:1914:C:O4'   | 1:A:1914:C:O2   | 2.35        | 0.45     |
| 1:A:2320:A:C2'   | 1:A:2320:A:N3   | 2.80        | 0.45     |
| 1:A:1567:A:C4    | 3:D:84:TYR:CD2  | 3.04        | 0.45     |
| 1:A:2838:G:C6    | 1:A:2839:G:C5   | 3.05        | 0.45     |
| 15:S:61:ASN:ND2  | 15:S:61:ASN:O   | 2.50        | 0.45     |
| 6:G:74:LYS:O     | 6:G:75:LYS:O    | 2.34        | 0.45     |
| 20:X:15:GLU:N    | 20:X:15:GLU:OE1 | 2.50        | 0.45     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 1:A:325:G:N2     | 1:A:326:G:C4    | 2.85        | 0.45     |
| 3:D:106:ILE:O    | 3:D:108:PRO:CD  | 2.65        | 0.45     |
| 1:A:1816:G:N7    | 3:D:62:TYR:CE1  | 2.86        | 0.45     |
| 4:E:61:ARG:C     | 4:E:63:LEU:N    | 2.70        | 0.45     |
| 31:8:52:LYS:N    | 31:8:52:LYS:CD  | 2.80        | 0.45     |
| 4:E:16:ARG:O     | 4:E:18:ASP:N    | 2.50        | 0.45     |
| 1:A:2119:A:C6    | 1:A:2171:A:N3   | 2.85        | 0.44     |
| 1:A:941:A:O3'    | 12:P:35:HIS:CG  | 2.71        | 0.44     |
| 1:A:1495:A:N3    | 1:A:1496:A:C2   | 2.85        | 0.44     |
| 18:V:47:VAL:O    | 18:V:49:THR:O   | 2.35        | 0.44     |
| 21:Y:7:VAL:CB    | 21:Y:8:LYS:NZ   | 2.80        | 0.44     |
| 14:R:53:HIS:CD2  | 14:R:94:TYR:OH  | 2.70        | 0.44     |
| 1:A:114(B):A:C4  | 1:A:1144:G:N7   | 2.86        | 0.44     |
| 1:A:64:A:C5      | 1:A:65:C:C5     | 3.05        | 0.44     |
| 1:A:2426:A:C3'   | 1:A:2427:C:C5'  | 2.95        | 0.44     |
| 1:A:94:G:C2      | 1:A:95:G:C4     | 3.05        | 0.44     |
| 4:E:55:ASN:O     | 4:E:57:LYS:N    | 2.50        | 0.44     |
| 1:A:352:G:O2'    | 1:A:353:G:O5'   | 2.35        | 0.44     |
| 1:A:910:A:C6     | 1:A:911:A:C6    | 3.06        | 0.44     |
| 1:A:2307:G:C6    | 1:A:2308:G:N1   | 2.86        | 0.44     |
| 1:A:1771:C:O2'   | 1:A:1786:A:C8   | 2.70        | 0.44     |
| 1:A:603:A:C2     | 1:A:655:A:C5    | 3.05        | 0.44     |
| 1:A:1542:G:C5'   | 1:A:1542:G:N3   | 2.81        | 0.44     |
| 1:A:1545:A:C6    | 1:A:1546:A:C2   | 3.04        | 0.44     |
| 1:A:2821:A:C2    | 1:A:2822:G:C4   | 3.05        | 0.44     |
| 16:T:117:ASP:C   | 16:T:119:LYS:N  | 2.70        | 0.44     |
| 8:I:90:GLY:O     | 8:I:121:LYS:NZ  | 2.50        | 0.44     |
| 1:A:270(Q):C:O2' | 1:A:270(R):C:P  | 2.75        | 0.44     |
| 1:A:2070:G:C2    | 1:A:2442:C:C2   | 3.05        | 0.44     |
| 1:A:901:A:C6     | 1:A:902:C:C4    | 3.06        | 0.44     |
| 1:A:1555:G:C6    | 1:A:1556:C:C4   | 3.06        | 0.44     |
| 1:A:56:A:N1      | 1:A:57:C:C2     | 2.86        | 0.44     |
| 1:A:469:G:C6     | 30:7:39:ARG:NH2 | 2.86        | 0.44     |
| 1:A:1338:G:O2'   | 1:A:1393:A:N1   | 2.51        | 0.44     |
| 1:A:1864:U:OP1   | 1:A:2410:G:O2'  | 2.34        | 0.44     |
| 1:A:653:C:C5'    | 1:A:653:C:C6    | 3.01        | 0.44     |
| 1:A:2516:G:C6    | 1:A:2517:C:C4   | 3.06        | 0.44     |
| 2:B:99:A:C6      | 2:B:100:G:C5    | 3.06        | 0.44     |
| 1:A:391:G:C6     | 1:A:411:G:N2    | 2.86        | 0.44     |
| 13:Q:65:PHE:N    | 13:Q:105:GLU:O  | 2.50        | 0.44     |
| 1:A:1088:A:N6    | 9:K:133:SER:CB  | 2.81        | 0.44     |
| 1:A:2593:U:C2    | 1:A:2594:C:C5   | 3.05        | 0.44     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 12:P:12:ALA:O    | 12:P:14:LYS:N   | 2.51        | 0.44     |
| 1:A:2081:C:C5    | 1:A:2237:G:N2   | 2.86        | 0.44     |
| 1:A:1208:C:C4    | 1:A:1209:G:N7   | 2.85        | 0.44     |
| 7:H:103:LEU:O    | 7:H:115:VAL:N   | 2.51        | 0.44     |
| 1:A:278:A:O2'    | 1:A:279:C:OP1   | 2.35        | 0.44     |
| 1:A:587:C:C2'    | 12:P:33:ARG:NH2 | 2.81        | 0.44     |
| 1:A:1346:G:C2    | 1:A:1601:G:C2   | 3.06        | 0.44     |
| 2:B:51:G:N7      | 15:S:62:LYS:NZ  | 2.66        | 0.44     |
| 17:U:39:LEU:O    | 17:U:40:PHE:C   | 2.54        | 0.44     |
| 1:A:2422:A:C6    | 1:A:2424:C:N4   | 2.85        | 0.44     |
| 1:A:1070:A:C2    | 1:A:1097:U:O2'  | 2.70        | 0.44     |
| 1:A:1798:U:C4    | 1:A:1819:A:C2   | 3.06        | 0.44     |
| 2:B:24:G:N3      | 2:B:27:C:N4     | 2.66        | 0.44     |
| 1:A:307:G:O5'    | 1:A:307:G:C8    | 2.71        | 0.44     |
| 1:A:2061:G:C2    | 1:A:2063:C:C4   | 3.06        | 0.44     |
| 1:A:2415:G:C5    | 1:A:2416:C:C4   | 3.05        | 0.44     |
| 1:A:2717:G:C5    | 1:A:2718:G:N7   | 2.85        | 0.44     |
| 2:B:31:C:O2      | 2:B:53:A:N6     | 2.51        | 0.44     |
| 20:X:36:LYS:NZ   | 20:X:54:VAL:O   | 2.51        | 0.44     |
| 1:A:987:G:O2'    | 1:A:1000:A:N3   | 2.50        | 0.44     |
| 1:A:2296:U:O2    | 1:A:2333:A:N3   | 2.50        | 0.44     |
| 1:A:774:A:C2     | 1:A:787:U:O2'   | 2.71        | 0.44     |
| 1:A:1210:A:C4'   | 1:A:1211:U:O5'  | 2.65        | 0.44     |
| 1:A:1210:A:O2'   | 1:A:1211:U:OP2  | 2.35        | 0.44     |
| 14:R:77:ARG:O    | 14:R:78:LYS:C   | 2.57        | 0.44     |
| 18:V:22:VAL:CG1  | 18:V:23:GLU:N   | 2.80        | 0.44     |
| 1:A:2259:G:C2    | 1:A:2282:G:C6   | 3.06        | 0.43     |
| 1:A:2543:G:C6    | 1:A:2544:G:C6   | 3.06        | 0.43     |
| 1:A:1512:G:C6    | 1:A:1513:C:C4   | 3.05        | 0.43     |
| 1:A:406:G:C6     | 1:A:407:G:C5    | 3.05        | 0.43     |
| 1:A:1693:U:O4    | 1:A:1977:A:C5   | 2.71        | 0.43     |
| 3:D:69:ARG:O     | 3:D:70:TRP:CB   | 2.66        | 0.43     |
| 31:8:62:LEU:C    | 31:8:64:TYR:N   | 2.69        | 0.43     |
| 10:N:151:HIS:CE1 | 10:N:157:ARG:NE | 2.86        | 0.43     |
| 3:D:210:GLY:O    | 3:D:213:ARG:N   | 2.51        | 0.43     |
| 20:X:26:TYR:O    | 20:X:81:VAL:N   | 2.50        | 0.43     |
| 21:Y:89:PHE:N    | 21:Y:89:PHE:CD1 | 2.85        | 0.43     |
| 1:A:1695:G:N2    | 1:A:1696:G:C8   | 2.86        | 0.43     |
| 6:G:20:ILE:O     | 6:G:24:GLY:CA   | 2.67        | 0.43     |
| 1:A:199:A:N3     | 1:A:2433:A:C2   | 2.87        | 0.43     |
| 1:A:2432:A:C6    | 1:A:2433:A:C6   | 3.06        | 0.43     |
| 1:A:577:G:C6     | 1:A:578:A:N6    | 2.86        | 0.43     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 3:D:58:HIS:O     | 3:D:59:LYS:O    | 2.36        | 0.43     |
| 5:F:160:ASN:OD1  | 5:F:163:VAL:N   | 2.51        | 0.43     |
| 1:A:245:G:C4     | 1:A:246:C:C5    | 3.06        | 0.43     |
| 10:N:69:VAL:O    | 10:N:70:ALA:CB  | 2.66        | 0.43     |
| 1:A:1267:U:OP2   | 1:A:2012:G:N1   | 2.52        | 0.43     |
| 3:D:232:PRO:O    | 3:D:234:GLY:N   | 2.51        | 0.43     |
| 21:Y:62:GLU:O    | 21:Y:63:LYS:O   | 2.35        | 0.43     |
| 1:A:2111:C:N4    | 1:A:2148:G:N2   | 2.65        | 0.43     |
| 13:Q:10:ARG:NE   | 13:Q:10:ARG:CA  | 2.81        | 0.43     |
| 21:Y:4:LYS:CD    | 21:Y:4:LYS:N    | 2.81        | 0.43     |
| 29:6:15:GLU:OE2  | 29:6:18:ARG:NE  | 2.52        | 0.43     |
| 1:A:1705:G:C6    | 1:A:1706:U:C4   | 3.07        | 0.43     |
| 1:A:234:C:C2     | 1:A:235:U:C5    | 3.06        | 0.43     |
| 1:A:2459:A:C5    | 1:A:2460:U:C5   | 3.07        | 0.43     |
| 1:A:1949:G:C6    | 1:A:1950:G:C6   | 3.07        | 0.43     |
| 1:A:2117:A:O2'   | 1:A:2118:U:C5   | 2.71        | 0.43     |
| 21:Y:76:CYS:SG   | 21:Y:77:PRO:CD  | 3.07        | 0.43     |
| 1:A:1034:G:C6    | 1:A:1035:U:C4   | 3.07        | 0.43     |
| 1:A:277:C:C5     | 1:A:278:A:C8    | 3.06        | 0.43     |
| 12:P:23:PRO:CB   | 12:P:33:ARG:CD  | 2.96        | 0.43     |
| 1:A:321:G:O2'    | 1:A:340:A:O2'   | 2.36        | 0.43     |
| 1:A:1175:U:C2'   | 1:A:1176:G:C5   | 3.02        | 0.43     |
| 1:A:2663:G:C4    | 1:A:2664:G:C8   | 3.06        | 0.43     |
| 1:A:481:G:C4     | 1:A:507:A:C2    | 3.06        | 0.43     |
| 1:A:1731:G:O2'   | 1:A:1732:A:O5'  | 2.36        | 0.43     |
| 1:A:1354:A:C8    | 1:A:1355:G:C8   | 3.06        | 0.43     |
| 1:A:2508:G:C4    | 1:A:2509:G:C8   | 3.07        | 0.43     |
| 1:A:1992:G:C8    | 1:A:1992:G:OP1  | 2.71        | 0.43     |
| 1:A:2777:G:C3'   | 1:A:2777:G:C8   | 3.01        | 0.43     |
| 13:Q:87:LYS:O    | 13:Q:89:ASN:OD1 | 2.36        | 0.43     |
| 1:A:2134:A:N3    | 1:A:2135:A:C8   | 2.87        | 0.43     |
| 1:A:2850:A:C2    | 1:A:2851:A:C4   | 3.07        | 0.43     |
| 1:A:164:U:C2     | 1:A:165:U:C5    | 3.05        | 0.43     |
| 10:N:121:VAL:CG2 | 10:N:122:LEU:N  | 2.82        | 0.43     |
| 1:A:1011:G:OP1   | 17:U:76:TYR:N   | 2.51        | 0.43     |
| 25:2:6:VAL:O     | 25:2:9:GLN:CG   | 2.67        | 0.43     |
| 16:T:111:ARG:O   | 16:T:113:LYS:N  | 2.52        | 0.43     |
| 1:A:2400:G:N2    | 1:A:2417:C:C2   | 2.86        | 0.43     |
| 10:N:118:PRO:C   | 10:N:120:ARG:N  | 2.71        | 0.43     |
| 12:P:58:THR:O    | 12:P:61:ARG:NE  | 2.51        | 0.43     |
| 1:A:1632:A:N7    | 1:A:1633:G:O6   | 2.51        | 0.43     |
| 1:A:2083:G:C6    | 1:A:2084:C:C4   | 3.07        | 0.43     |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2          | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 1:A:1729:A:C2    | 1:A:1731:G:C8   | 3.07        | 0.43     |
| 1:A:1509:A:O3'   | 1:A:1510:A:C8   | 2.71        | 0.43     |
| 4:E:1:MET:O      | 4:E:84:PHE:CG   | 2.71        | 0.43     |
| 1:A:817:C:O2'    | 1:A:839:U:OP1   | 2.37        | 0.43     |
| 13:Q:58:PHE:O    | 13:Q:58:PHE:CD1 | 2.72        | 0.43     |
| 1:A:2131:G:C8    | 1:A:2131:G:OP2  | 2.72        | 0.43     |
| 1:A:663:G:C5     | 1:A:664:C:C5    | 3.07        | 0.43     |
| 1:A:2307:G:C6    | 1:A:2308:G:C6   | 3.06        | 0.43     |
| 1:A:1275:A:C5    | 14:R:16:HIS:ND1 | 2.87        | 0.43     |
| 15:S:85:VAL:O    | 15:S:86:ALA:C   | 2.57        | 0.43     |
| 1:A:270(N):U:O4' | 1:A:270(O):G:C6 | 2.72        | 0.43     |
| 1:A:2574:G:N3    | 4:E:143:ASN:ND2 | 2.67        | 0.43     |
| 7:H:51:ARG:CG    | 7:H:52:VAL:N    | 2.82        | 0.43     |
| 1:A:405:U:C5'    | 1:A:405:U:O2    | 2.67        | 0.43     |
| 16:T:87:ASP:N    | 16:T:87:ASP:OD1 | 2.52        | 0.43     |
| 1:A:884:C:O5'    | 1:A:884:C:C6    | 2.71        | 0.43     |
| 15:S:61:ASN:O    | 15:S:63:THR:N   | 2.52        | 0.43     |
| 1:A:352:G:O2'    | 1:A:353:G:P     | 2.77        | 0.43     |
| 1:A:51:G:O2'     | 1:A:119:A:N1    | 2.52        | 0.43     |
| 1:A:1819:A:O4'   | 1:A:1821:A:C5   | 2.71        | 0.43     |
| 7:H:50:VAL:O     | 7:H:51:ARG:CB   | 2.67        | 0.43     |
| 1:A:2738:A:N1    | 1:A:2739:U:C2   | 2.87        | 0.43     |
| 19:W:88:ARG:NH1  | 19:W:94:ASP:OD1 | 2.51        | 0.43     |
| 1:A:2886:G:C4    | 1:A:2887:U:C5   | 3.07        | 0.43     |
| 4:E:87:GLU:C     | 4:E:87:GLU:CD   | 2.77        | 0.43     |
| 6:G:86:MET:N     | 6:G:87:PRO:CD   | 2.82        | 0.43     |
| 24:1:9:GLY:O     | 24:1:13:ILE:CG2 | 2.67        | 0.42     |
| 24:1:14:VAL:O    | 24:1:14:VAL:CG1 | 2.66        | 0.42     |
| 1:A:2656:U:C5    | 1:A:2664:G:N2   | 2.87        | 0.42     |
| 14:R:7:GLY:O     | 14:R:8:ARG:CB   | 2.66        | 0.42     |
| 1:A:2837:G:C5    | 1:A:2838:G:N7   | 2.87        | 0.42     |
| 15:S:24:LEU:O    | 15:S:86:ALA:CB  | 2.66        | 0.42     |
| 1:A:1427:A:C4'   | 1:A:1428:C:O5'  | 2.67        | 0.42     |
| 1:A:342:G:N3     | 1:A:343:C:C6    | 2.86        | 0.42     |
| 1:A:2832:U:C2    | 1:A:2834:G:C2   | 3.06        | 0.42     |
| 1:A:1306:C:C2    | 1:A:1623:G:C2   | 3.07        | 0.42     |
| 24:1:25:LYS:CB   | 24:1:34:THR:O   | 2.67        | 0.42     |
| 11:O:8:LEU:N     | 11:O:8:LEU:CD2  | 2.82        | 0.42     |
| 1:A:2056:G:C2'   | 1:A:2056:G:N3   | 2.82        | 0.42     |
| 1:A:1952:A:C6    | 11:O:22:ILE:CD1 | 3.02        | 0.42     |
| 1:A:2717:G:C6    | 1:A:2718:G:N7   | 2.87        | 0.42     |
| 17:U:40:PHE:CD2  | 18:V:75:PHE:CD2 | 3.08        | 0.42     |

*Continued on next page...*



*Continued from previous page...*

| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:2212:A:N3   | 1:A:2215:G:C2   | 2.87        | 0.42     |
| 1:A:1729:A:C5   | 1:A:1731:G:C5   | 3.07        | 0.42     |
| 1:A:1981:A:C8   | 1:A:1981:A:C3'  | 3.02        | 0.42     |
| 13:Q:51:ARG:O   | 13:Q:54:MET:N   | 2.52        | 0.42     |
| 1:A:2590:A:C2   | 1:A:2605:U:C2   | 3.07        | 0.42     |
| 2:B:32:C:C4     | 2:B:33:G:N7     | 2.87        | 0.42     |
| 16:T:14:TYR:CD1 | 16:T:14:TYR:N   | 2.87        | 0.42     |
| 1:A:675:A:N6    | 1:A:676:A:N6    | 2.67        | 0.42     |
| 1:A:2119:A:N6   | 1:A:2170:A:C6   | 2.87        | 0.42     |
| 1:A:828:U:C5    | 1:A:829:A:N6    | 2.87        | 0.42     |
| 1:A:1098:A:C8   | 1:A:1099:G:C8   | 3.08        | 0.42     |
| 1:A:2748:A:C6   | 1:A:2749:A:C6   | 3.07        | 0.42     |
| 11:O:64:ARG:NE  | 11:O:101:PRO:O  | 2.51        | 0.42     |
| 1:A:1091:G:C2   | 1:A:1092:C:C2   | 3.08        | 0.42     |
| 18:V:35:LEU:C   | 18:V:37:VAL:N   | 2.70        | 0.42     |
| 1:A:752:A:OP1   | 30:7:3:ARG:NH2  | 2.52        | 0.42     |
| 1:A:680:G:C4    | 1:A:798:G:N2    | 2.88        | 0.42     |
| 23:O:10:THR:OG1 | 23:O:10:THR:O   | 2.37        | 0.42     |
| 1:A:2850:A:C2   | 14:R:61:HIS:CD2 | 3.07        | 0.42     |
| 1:A:2422:A:C4'  | 1:A:2423:U:OP1  | 2.67        | 0.42     |
| 1:A:1314:C:C2   | 1:A:1339:G:N2   | 2.87        | 0.42     |
| 14:R:14:SER:OG  | 14:R:15:SER:N   | 2.51        | 0.42     |
| 1:A:945:A:C4    | 1:A:2448:A:C2   | 3.07        | 0.42     |
| 6:G:31:VAL:O    | 6:G:31:VAL:CG1  | 2.67        | 0.42     |
| 1:A:1990:C:N3   | 1:A:1991:U:C4   | 2.87        | 0.42     |
| 1:A:643:A:N1    | 1:A:644:A:C4    | 2.87        | 0.42     |
| 1:A:973:A:O4'   | 1:A:1188:U:C6   | 2.72        | 0.42     |
| 1:A:2345:G:O2'  | 1:A:2381:C:O2'  | 2.36        | 0.42     |
| 1:A:1842:G:N3   | 1:A:1901:A:C2   | 2.87        | 0.42     |
| 2:B:33:G:C2     | 2:B:50:G:C2     | 3.07        | 0.42     |
| 1:A:635:C:O2'   | 1:A:639:U:OP1   | 2.37        | 0.42     |
| 1:A:120:U:C2    | 1:A:149:A:C6    | 3.07        | 0.42     |
| 1:A:1769:G:C6   | 1:A:1984:G:C6   | 3.08        | 0.42     |
| 21:Y:27:VAL:O   | 21:Y:27:VAL:CG2 | 2.67        | 0.42     |
| 10:N:56:LEU:N   | 10:N:56:LEU:CD1 | 2.82        | 0.42     |
| 1:A:655:A:C8    | 1:A:655:A:C3'   | 3.02        | 0.42     |
| 1:A:2821:A:OP1  | 4:E:110:GLY:N   | 2.53        | 0.42     |
| 1:A:1042:G:C6   | 1:A:1043:C:C4   | 3.08        | 0.42     |
| 1:A:2361:A:OP1  | 31:8:27:THR:OG1 | 2.37        | 0.42     |
| 1:A:2378:A:O2'  | 15:S:21:THR:CG2 | 2.67        | 0.42     |
| 1:A:495:G:O2'   | 19:W:62:HIS:CE1 | 2.73        | 0.42     |
| 13:Q:78:PRO:O   | 13:Q:79:LEU:CB  | 2.67        | 0.42     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 13:Q:112:GLU:OE1 | 13:Q:112:GLU:N  | 2.53        | 0.42     |
| 1:A:2040:C:O2    | 1:A:2040:C:C2'  | 2.66        | 0.42     |
| 25:2:47:ASN:ND2  | 25:2:47:ASN:N   | 2.68        | 0.42     |
| 12:P:16:ARG:O    | 12:P:17:LYS:C   | 2.58        | 0.42     |
| 1:A:1609:A:C6    | 1:A:1616:A:C5   | 3.08        | 0.42     |
| 1:A:33:U:O2'     | 1:A:446:G:N2    | 2.52        | 0.42     |
| 16:T:117:ASP:O   | 16:T:119:LYS:N  | 2.52        | 0.42     |
| 1:A:2892:A:N7    | 1:A:2893:G:C5   | 2.88        | 0.42     |
| 1:A:342:G:C2     | 1:A:343:C:C5    | 3.08        | 0.42     |
| 1:A:1981:A:C5'   | 1:A:1982:C:OP2  | 2.68        | 0.42     |
| 1:A:785:G:C6     | 1:A:786:C:C4    | 3.06        | 0.42     |
| 26:3:19:GLN:NE2  | 26:3:52:HIS:CE1 | 2.88        | 0.42     |
| 28:5:47:PRO:O    | 28:5:48:GLU:CB  | 2.68        | 0.42     |
| 21:Y:60:PHE:O    | 21:Y:61:ILE:C   | 2.58        | 0.42     |
| 1:A:2500:U:C6    | 1:A:2500:U:C3'  | 3.02        | 0.42     |
| 1:A:773:U:C4'    | 3:D:47:GLY:CA   | 2.97        | 0.42     |
| 1:A:531:C:N3     | 1:A:563:G:C8    | 2.88        | 0.42     |
| 1:A:727:A:C6     | 1:A:728:G:C6    | 3.07        | 0.42     |
| 1:A:939:G:C4     | 1:A:940:G:C8    | 3.08        | 0.42     |
| 1:A:1252:G:N3    | 1:A:1253:A:C2   | 2.88        | 0.42     |
| 1:A:391:G:C6     | 1:A:392:C:C4    | 3.08        | 0.42     |
| 19:W:35:ILE:O    | 19:W:36:LEU:C   | 2.58        | 0.42     |
| 1:A:2108:C:O2    | 1:A:2182:G:C2   | 2.72        | 0.42     |
| 31:8:2:PRO:O     | 31:8:3:LYS:CB   | 2.67        | 0.42     |
| 14:R:48:VAL:O    | 14:R:51:LEU:N   | 2.53        | 0.42     |
| 5:F:77:ASP:O     | 5:F:79:GLY:N    | 2.53        | 0.42     |
| 1:A:2842:G:C6    | 1:A:2876:G:C6   | 3.07        | 0.42     |
| 3:D:11:PRO:O     | 3:D:12:SER:C    | 2.59        | 0.42     |
| 12:P:13:ASN:O    | 12:P:13:ASN:ND2 | 2.53        | 0.42     |
| 1:A:2157:G:O2'   | 1:A:2158:A:C8   | 2.73        | 0.42     |
| 1:A:1100:C:C4    | 1:A:1101:U:C5   | 3.08        | 0.42     |
| 1:A:1936:A:N3    | 1:A:1936:A:C5'  | 2.82        | 0.42     |
| 4:E:92:THR:C     | 4:E:94:GLU:N    | 2.72        | 0.42     |
| 2:B:44:G:OP1     | 6:G:96:ARG:NH2  | 2.53        | 0.42     |
| 22:Z:78:LYS:O    | 22:Z:79:ARG:CB  | 2.68        | 0.42     |
| 25:2:2:LYS:O     | 25:2:5:GLU:OE1  | 2.38        | 0.41     |
| 12:P:33:ARG:O    | 12:P:34:GLY:C   | 2.58        | 0.41     |
| 1:A:2171:A:C2    | 1:A:2172:U:N3   | 2.88        | 0.41     |
| 10:N:41:ALA:CB   | 10:N:78:VAL:O   | 2.68        | 0.41     |
| 1:A:2280:G:C5    | 1:A:2281:C:C5   | 3.08        | 0.41     |
| 13:Q:18:LYS:O    | 13:Q:19:GLY:C   | 2.59        | 0.41     |
| 1:A:705:A:C2     | 1:A:706:A:C4    | 3.08        | 0.41     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:1347:G:C5   | 1:A:1348:G:N7   | 2.88        | 0.41     |
| 6:G:150:ASP:OD1 | 6:G:150:ASP:N   | 2.53        | 0.41     |
| 12:P:99:LEU:CD1 | 12:P:99:LEU:N   | 2.83        | 0.41     |
| 8:I:35:LEU:CD2  | 8:I:35:LEU:N    | 2.80        | 0.41     |
| 3:D:32:SER:O    | 3:D:33:LEU:O    | 2.38        | 0.41     |
| 1:A:1099:G:C4   | 1:A:1100:C:C5   | 3.08        | 0.41     |
| 1:A:307:G:C8    | 1:A:307:G:C3'   | 3.03        | 0.41     |
| 19:W:52:GLU:O   | 19:W:54:ALA:N   | 2.53        | 0.41     |
| 1:A:2338:G:C2   | 1:A:2339:G:N7   | 2.88        | 0.41     |
| 1:A:1170:G:C6   | 1:A:1171:G:N7   | 2.89        | 0.41     |
| 1:A:465:G:C6    | 1:A:466:A:N6    | 2.88        | 0.41     |
| 1:A:2703:C:C2   | 1:A:2704:C:C5   | 3.07        | 0.41     |
| 1:A:322:A:C6    | 1:A:340:A:N1    | 2.88        | 0.41     |
| 1:A:51:G:N3     | 1:A:119:A:C2    | 2.88        | 0.41     |
| 6:G:128:ARG:NE  | 6:G:129:GLY:N   | 2.69        | 0.41     |
| 5:F:103:LYS:O   | 5:F:104:LYS:C   | 2.59        | 0.41     |
| 1:A:1733:G:C5   | 1:A:1734:C:C5   | 3.08        | 0.41     |
| 28:5:41:PRO:O   | 28:5:44:THR:OG1 | 2.37        | 0.41     |
| 22:Z:44:PHE:O   | 22:Z:48:PHE:N   | 2.54        | 0.41     |
| 6:G:111:LEU:N   | 6:G:112:PRO:CD  | 2.83        | 0.41     |
| 1:A:276:A:C5    | 1:A:277:C:N4    | 2.88        | 0.41     |
| 1:A:1465:G:N3   | 1:A:1466:G:C8   | 2.88        | 0.41     |
| 1:A:864:G:N2    | 1:A:913:U:C2    | 2.89        | 0.41     |
| 1:A:303:U:O2    | 1:A:304:G:C8    | 2.73        | 0.41     |
| 19:W:14:PRO:O   | 19:W:15:ARG:C   | 2.58        | 0.41     |
| 22:Z:10:ARG:NH2 | 22:Z:26:GLY:N   | 2.68        | 0.41     |
| 24:1:45:ASN:ND2 | 24:1:46:LEU:N   | 2.68        | 0.41     |
| 3:D:109:ASP:N   | 3:D:195:ALA:O   | 2.54        | 0.41     |
| 1:A:354:G:C4    | 1:A:355:G:C8    | 3.08        | 0.41     |
| 1:A:2694:G:C6   | 1:A:2695:C:C4   | 3.08        | 0.41     |
| 6:G:77:ILE:N    | 6:G:82:LEU:O    | 2.54        | 0.41     |
| 1:A:777:A:N3    | 1:A:778:G:C8    | 2.88        | 0.41     |
| 1:A:675:A:OP1   | 5:F:63:LYS:NZ   | 2.54        | 0.41     |
| 12:P:41:ARG:NE  | 12:P:41:ARG:CA  | 2.83        | 0.41     |
| 2:B:57:A:OP2    | 2:B:58:A:OP2    | 2.39        | 0.41     |
| 1:A:1842:G:C2   | 1:A:1901:A:C2   | 3.09        | 0.41     |
| 1:A:1162:G:N3   | 18:V:89:GLN:NE2 | 2.68        | 0.41     |
| 25:2:36:ARG:NH1 | 25:2:36:ARG:CB  | 2.84        | 0.41     |
| 17:U:52:ARG:O   | 17:U:55:ARG:N   | 2.54        | 0.41     |
| 31:8:57:ARG:O   | 31:8:60:LEU:N   | 2.54        | 0.41     |
| 5:F:65:TRP:CH2  | 5:F:75:HIS:CD2  | 3.08        | 0.41     |
| 7:H:93:GLY:O    | 7:H:94:TYR:C    | 2.59        | 0.41     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:580:C:C2     | 1:A:581:C:C5     | 3.08        | 0.41     |
| 1:A:2850:A:N7    | 1:A:2868:A:O2'   | 2.53        | 0.41     |
| 1:A:2338:G:C2    | 1:A:2339:G:C8    | 3.08        | 0.41     |
| 1:A:2044:C:C2    | 1:A:2625:G:C2    | 3.08        | 0.41     |
| 7:H:86:GLU:O     | 7:H:87:LEU:CG    | 2.69        | 0.41     |
| 3:D:126:GLN:O    | 3:D:127:VAL:C    | 2.59        | 0.41     |
| 23:0:60:PHE:CD2  | 23:0:60:PHE:N    | 2.88        | 0.41     |
| 1:A:1154:G:C8    | 1:A:1154:G:O5'   | 2.74        | 0.41     |
| 22:Z:13:GLU:N    | 22:Z:13:GLU:OE1  | 2.54        | 0.41     |
| 22:Z:128:VAL:CG2 | 22:Z:129:SER:N   | 2.83        | 0.41     |
| 1:A:1465:G:C4    | 1:A:1466:G:C8    | 3.08        | 0.41     |
| 1:A:898:C:C2     | 1:A:899:A:C8     | 3.09        | 0.41     |
| 12:P:101:VAL:CA  | 12:P:105:LEU:O   | 2.68        | 0.41     |
| 18:V:45:THR:O    | 18:V:46:VAL:C    | 2.59        | 0.41     |
| 26:3:10:LYS:NZ   | 26:3:15:TYR:OH   | 2.53        | 0.41     |
| 10:N:66:THR:N    | 10:N:71:MET:CE   | 2.84        | 0.41     |
| 1:A:805:G:OP2    | 1:A:806:C:N4     | 2.53        | 0.41     |
| 1:A:60:G:C5      | 1:A:63:U:C5      | 3.08        | 0.41     |
| 1:A:270(P):U:O5' | 1:A:270(P):U:C6  | 2.73        | 0.41     |
| 1:A:1405:U:C2    | 1:A:1406:U:C5    | 3.08        | 0.41     |
| 25:2:2:LYS:O     | 25:2:3:LEU:C     | 2.59        | 0.41     |
| 22:Z:51:ALA:O    | 22:Z:52:SER:OG   | 2.38        | 0.41     |
| 1:A:1374:G:C4    | 1:A:1375:C:C5    | 3.09        | 0.41     |
| 1:A:957:A:N6     | 1:A:2459:A:C8    | 2.89        | 0.41     |
| 1:A:2712:U:O2'   | 1:A:712(B):A:P   | 2.79        | 0.41     |
| 1:A:989:G:N7     | 26:3:13:ILE:CD1  | 2.84        | 0.41     |
| 1:A:2564:A:C2    | 1:A:2647:U:C4'   | 3.04        | 0.41     |
| 3:D:32:SER:C     | 3:D:33:LEU:O     | 2.59        | 0.41     |
| 29:6:32:ASN:N    | 29:6:33:LYS:NZ   | 2.68        | 0.41     |
| 1:A:1989:G:C5    | 1:A:1990:C:C5    | 3.09        | 0.41     |
| 1:A:1543:A:C5    | 1:A:1545:A:O4'   | 2.74        | 0.41     |
| 1:A:1604:C:O2'   | 1:A:1610:A:N1    | 2.54        | 0.41     |
| 1:A:2415:G:C4    | 1:A:2416:C:C5    | 3.09        | 0.41     |
| 1:A:1654:A:N6    | 1:A:2049:G:OP1   | 2.54        | 0.41     |
| 1:A:270(F):G:N1  | 1:A:270(W):G:C6  | 2.89        | 0.41     |
| 1:A:2019:A:N7    | 28:5:9:LYS:NZ    | 2.68        | 0.41     |
| 22:Z:118:GLN:CA  | 22:Z:118:GLN:NE2 | 2.83        | 0.41     |
| 1:A:1871:A:C2'   | 1:A:1872:A:C8    | 3.04        | 0.41     |
| 1:A:404:C:C2     | 1:A:406:G:C5     | 3.09        | 0.41     |
| 1:A:161:U:O2     | 1:A:165:U:O4     | 2.39        | 0.41     |
| 1:A:1551:C:C5    | 1:A:1552:G:N7    | 2.89        | 0.41     |
| 1:A:1116:C:C2    | 1:A:1117:G:C8    | 3.08        | 0.41     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 14:R:47:PHE:O    | 14:R:51:LEU:CD1 | 2.68        | 0.41     |
| 1:A:535:C:O3'    | 17:U:53:ARG:NH1 | 2.54        | 0.41     |
| 1:A:1178:C:C2    | 1:A:1179:C:C5   | 3.09        | 0.41     |
| 1:A:733:G:C8     | 1:A:761:A:N6    | 2.89        | 0.41     |
| 23:O:46:LYS:O    | 23:O:47:PRO:O   | 2.39        | 0.41     |
| 1:A:930:U:O4'    | 1:A:930:U:O2    | 2.36        | 0.41     |
| 1:A:1534:G:C2    | 1:A:1536:A:OP2  | 2.74        | 0.41     |
| 1:A:2283:C:C5    | 1:A:2389:G:C4   | 3.08        | 0.41     |
| 1:A:1389:G:C2    | 1:A:1399:C:O2   | 2.74        | 0.41     |
| 5:F:135:LYS:O    | 5:F:136:THR:C   | 2.59        | 0.41     |
| 22:Z:75:ASN:ND2  | 22:Z:75:ASN:N   | 2.69        | 0.41     |
| 1:A:26:G:C2      | 1:A:27:G:N2     | 2.89        | 0.41     |
| 1:A:780:G:C2     | 1:A:783:A:N6    | 2.88        | 0.41     |
| 13:Q:81:VAL:O    | 13:Q:82:ARG:CZ  | 2.70        | 0.41     |
| 1:A:1603:A:C5    | 1:A:1604:C:C5   | 3.09        | 0.41     |
| 16:T:106:SER:O   | 16:T:107:ASP:CB | 2.69        | 0.41     |
| 1:A:2683:C:P     | 16:T:53:ARG:NH2 | 2.94        | 0.41     |
| 25:2:17:SER:CB   | 25:2:18:PRO:CD  | 2.98        | 0.41     |
| 1:A:2748:A:C4    | 1:A:2757:A:C6   | 3.09        | 0.41     |
| 1:A:280:C:N3     | 1:A:361:G:C2    | 2.89        | 0.41     |
| 14:R:81:ASP:O    | 14:R:82:GLU:CB  | 2.68        | 0.41     |
| 1:A:977:G:O6     | 1:A:987:G:C6    | 2.74        | 0.41     |
| 1:A:270(S):G:OP1 | 8:I:42:SER:OG   | 2.39        | 0.41     |
| 4:E:173:VAL:N    | 4:E:183:LEU:O   | 2.54        | 0.41     |
| 1:A:980:A:C6     | 1:A:981:A:N1    | 2.89        | 0.41     |
| 2:B:96:G:C4      | 2:B:97:G:C8     | 3.08        | 0.41     |
| 1:A:704:G:N2     | 1:A:726:G:C4    | 2.89        | 0.41     |
| 1:A:1900:A:N1    | 1:A:1970:A:C6   | 2.89        | 0.41     |
| 3:D:227:ASN:O    | 3:D:228:PRO:C   | 2.58        | 0.41     |
| 1:A:2776:A:C6    | 1:A:2778:A:C6   | 3.08        | 0.41     |
| 1:A:1385:G:C4    | 1:A:1386:C:C5   | 3.09        | 0.41     |
| 1:A:579:G:C2     | 1:A:1262:A:C4   | 3.09        | 0.41     |
| 1:A:1839:G:C8    | 1:A:1839:G:C5'  | 3.04        | 0.41     |
| 28:5:52:TYR:N    | 28:5:52:TYR:CD1 | 2.89        | 0.41     |
| 19:W:21:VAL:C    | 19:W:23:LEU:N   | 2.75        | 0.41     |
| 10:N:59:GLY:O    | 10:N:62:ARG:N   | 2.54        | 0.40     |
| 1:A:2056:G:N2    | 28:5:4:HIS:O    | 2.54        | 0.40     |
| 1:A:860:U:O2     | 1:A:860:U:O4'   | 2.37        | 0.40     |
| 1:A:901:A:C5     | 1:A:902:C:C4    | 3.09        | 0.40     |
| 1:A:245:G:C5     | 1:A:246:C:C5    | 3.10        | 0.40     |
| 1:A:1265:A:O4'   | 1:A:1267:U:C6   | 2.73        | 0.40     |
| 1:A:728:G:C4     | 1:A:730:C:C5    | 3.09        | 0.40     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 1:A:60:G:N7      | 1:A:63:U:C6     | 2.89        | 0.40     |
| 6:G:154:GLY:O    | 6:G:155:MET:CB  | 2.68        | 0.40     |
| 1:A:2209:C:C2    | 1:A:2216:G:C2   | 3.09        | 0.40     |
| 12:P:29:LYS:N    | 12:P:29:LYS:CD  | 2.84        | 0.40     |
| 3:D:238:GLY:O    | 3:D:240:ALA:N   | 2.54        | 0.40     |
| 12:P:24:GLY:N    | 12:P:33:ARG:NH1 | 2.69        | 0.40     |
| 10:N:61:HIS:CE1  | 10:N:73:ASP:OD2 | 2.74        | 0.40     |
| 1:A:828:U:C3'    | 1:A:828:U:O2    | 2.70        | 0.40     |
| 1:A:2785:C:O2'   | 4:E:66:HIS:CD2  | 2.74        | 0.40     |
| 1:A:977:G:C6     | 1:A:987:G:C6    | 3.09        | 0.40     |
| 1:A:830:G:C4     | 1:A:2448:A:C6   | 3.10        | 0.40     |
| 1:A:2338:G:N3    | 1:A:2339:G:C8   | 2.89        | 0.40     |
| 1:A:733:G:O6     | 1:A:761:A:C8    | 2.74        | 0.40     |
| 1:A:2077:A:C4    | 1:A:2078:C:C5   | 3.10        | 0.40     |
| 1:A:1414:G:C5    | 1:A:1415:U:C5   | 3.10        | 0.40     |
| 1:A:1754:C:OP1   | 16:T:96:ARG:NH1 | 2.54        | 0.40     |
| 31:8:50:LEU:O    | 31:8:51:ALA:CB  | 2.69        | 0.40     |
| 1:A:2014:A:O2'   | 1:A:2015:A:O4'  | 2.38        | 0.40     |
| 12:P:10:PRO:O    | 12:P:11:GLY:C   | 2.59        | 0.40     |
| 1:A:861:A:N3     | 2:B:79:C:O2'    | 2.54        | 0.40     |
| 22:Z:179:ASP:OD2 | 22:Z:179:ASP:C  | 2.59        | 0.40     |
| 1:A:2836:U:C4    | 1:A:2883:A:C6   | 3.10        | 0.40     |
| 1:A:61:G:C5      | 25:2:47:ASN:OD1 | 2.74        | 0.40     |
| 12:P:17:LYS:O    | 12:P:19:VAL:N   | 2.54        | 0.40     |
| 13:Q:88:GLY:O    | 13:Q:89:ASN:CB  | 2.69        | 0.40     |
| 1:A:1416:G:O2'   | 1:A:1417:C:C6   | 2.75        | 0.40     |
| 1:A:389:G:O6     | 12:P:71:VAL:CG2 | 2.69        | 0.40     |
| 1:A:1567:A:O2'   | 3:D:63:ARG:NH2  | 2.54        | 0.40     |
| 6:G:75:LYS:O     | 6:G:83:ARG:O    | 2.39        | 0.40     |
| 1:A:2349:G:C6    | 1:A:2350:C:C5   | 3.09        | 0.40     |
| 15:S:25:ARG:NH2  | 15:S:42:ASP:OD2 | 2.54        | 0.40     |
| 1:A:2505:G:C8    | 1:A:2505:G:C3'  | 3.04        | 0.40     |
| 1:A:273(G):C:C3' | 1:A:274:G:C5'   | 2.99        | 0.40     |
| 29:6:18:ARG:NH1  | 29:6:43:CYS:O   | 2.55        | 0.40     |
| 1:A:996:A:C6     | 1:A:1160:G:C6   | 3.10        | 0.40     |
| 1:A:632:A:N3     | 1:A:2403:C:O2'  | 2.54        | 0.40     |
| 2:B:66:A:N6      | 2:B:107:U:C2    | 2.88        | 0.40     |
| 1:A:1301:A:C4'   | 1:A:1302:A:OP1  | 2.70        | 0.40     |
| 1:A:342:G:C2     | 1:A:343:C:C6    | 3.09        | 0.40     |
| 1:A:2020:A:C5    | 1:A:2022:U:C5   | 3.09        | 0.40     |
| 1:A:287:C:C2     | 1:A:288:C:C5    | 3.09        | 0.40     |
| 1:A:2076:U:C5    | 1:A:2596:U:O2   | 2.75        | 0.40     |

*Continued on next page...*

Continued from previous page...

| Atom-1         | Atom-2        | Distance(Å) | Clash(Å) |
|----------------|---------------|-------------|----------|
| 1:A:394:A:C6   | 1:A:395:U:C4  | 3.09        | 0.40     |
| 1:A:511:U:C5   | 1:A:512:G:C5  | 3.09        | 0.40     |
| 12:P:18:ARG:O  | 12:P:20:GLY:N | 2.53        | 0.40     |
| 1:A:547:A:C2'  | 1:A:548:A:C8  | 3.05        | 0.40     |
| 5:F:89:VAL:CG1 | 5:F:90:PHE:N  | 2.84        | 0.40     |
| 17:U:52:ARG:O  | 17:U:53:ARG:C | 2.58        | 0.40     |
| 1:A:966:G:C6   | 1:A:967:C:N4  | 2.89        | 0.40     |
| 1:A:121:G:N2   | 1:A:131:G:C4  | 2.90        | 0.40     |
| 1:A:1164:G:C6  | 1:A:1165:U:C4 | 3.10        | 0.40     |
| 7:H:13:LYS:CE  | 7:H:14:GLY:N  | 2.84        | 0.40     |
| 1:A:630:G:N2   | 1:A:633:A:OP2 | 2.54        | 0.40     |
| 1:A:2618:G:C6  | 1:A:2619:C:C4 | 3.10        | 0.40     |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 3   | D     | 269/276 (98%) | 208 (77%) | 41 (15%) | 20 (7%)  | 2           | 8  |
| 4   | E     | 202/206 (98%) | 157 (78%) | 37 (18%) | 8 (4%)   | 5           | 25 |
| 5   | F     | 200/210 (95%) | 162 (81%) | 28 (14%) | 10 (5%)  | 3           | 19 |
| 6   | G     | 179/182 (98%) | 128 (72%) | 39 (22%) | 12 (7%)  | 2           | 10 |
| 7   | H     | 157/180 (87%) | 120 (76%) | 30 (19%) | 7 (4%)   | 4           | 22 |
| 8   | I     | 143/148 (97%) | 107 (75%) | 29 (20%) | 7 (5%)   | 3           | 20 |
| 9   | K     | 145/147 (99%) | 101 (70%) | 35 (24%) | 9 (6%)   | 2           | 13 |
| 10  | N     | 135/163 (83%) | 103 (76%) | 17 (13%) | 15 (11%) | 1           | 3  |
| 11  | O     | 120/122 (98%) | 102 (85%) | 14 (12%) | 4 (3%)   | 6           | 32 |
| 12  | P     | 144/150 (96%) | 86 (60%)  | 35 (24%) | 23 (16%) | 0           | 1  |
| 13  | Q     | 132/141 (94%) | 96 (73%)  | 22 (17%) | 14 (11%) | 1           | 3  |
| 14  | R     | 115/118 (98%) | 89 (77%)  | 19 (16%) | 7 (6%)   | 2           | 14 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 15  | S     | 96/112 (86%)    | 56 (58%)   | 29 (30%)  | 11 (12%) | 1           | 3   |
| 16  | T     | 135/146 (92%)   | 91 (67%)   | 30 (22%)  | 14 (10%) | 1           | 4   |
| 17  | U     | 115/118 (98%)   | 92 (80%)   | 19 (16%)  | 4 (4%)   | 6           | 30  |
| 18  | V     | 99/101 (98%)    | 74 (75%)   | 15 (15%)  | 10 (10%) | 1           | 4   |
| 19  | W     | 110/113 (97%)   | 88 (80%)   | 18 (16%)  | 4 (4%)   | 5           | 29  |
| 20  | X     | 90/96 (94%)     | 73 (81%)   | 15 (17%)  | 2 (2%)   | 10          | 45  |
| 21  | Y     | 98/110 (89%)    | 64 (65%)   | 18 (18%)  | 16 (16%) | 0           | 1   |
| 22  | Z     | 185/206 (90%)   | 146 (79%)  | 31 (17%)  | 8 (4%)   | 4           | 23  |
| 23  | 0     | 74/85 (87%)     | 61 (82%)   | 10 (14%)  | 3 (4%)   | 4           | 24  |
| 24  | 1     | 86/98 (88%)     | 59 (69%)   | 16 (19%)  | 11 (13%) | 0           | 2   |
| 25  | 2     | 60/72 (83%)     | 43 (72%)   | 12 (20%)  | 5 (8%)   | 1           | 6   |
| 26  | 3     | 57/60 (95%)     | 50 (88%)   | 5 (9%)    | 2 (4%)   | 6           | 30  |
| 27  | 4     | 28/97 (29%)     | 18 (64%)   | 6 (21%)   | 4 (14%)  | 0           | 1   |
| 28  | 5     | 50/60 (83%)     | 40 (80%)   | 7 (14%)   | 3 (6%)   | 2           | 14  |
| 29  | 6     | 42/54 (78%)     | 27 (64%)   | 10 (24%)  | 5 (12%)  | 1           | 2   |
| 30  | 7     | 46/49 (94%)     | 43 (94%)   | 3 (6%)    | 0        | 100         | 100 |
| 31  | 8     | 61/65 (94%)     | 42 (69%)   | 12 (20%)  | 7 (12%)  | 1           | 3   |
| All | All   | 3373/3685 (92%) | 2526 (75%) | 602 (18%) | 245 (7%) | 2           | 8   |

All (245) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 13  | ARG  |
| 3   | D     | 33  | LEU  |
| 3   | D     | 34  | VAL  |
| 3   | D     | 57  | GLY  |
| 3   | D     | 59  | LYS  |
| 3   | D     | 70  | TRP  |
| 3   | D     | 192 | THR  |
| 3   | D     | 236 | GLY  |
| 4   | E     | 122 | PHE  |
| 4   | E     | 132 | HIS  |
| 5   | F     | 73  | ALA  |
| 5   | F     | 89  | VAL  |
| 6   | G     | 4   | ASP  |
| 6   | G     | 75  | LYS  |

Continued on next page...



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | G     | 87  | PRO  |
| 7   | H     | 47  | GLU  |
| 9   | K     | 20  | ALA  |
| 10  | N     | 40  | ASP  |
| 10  | N     | 149 | PRO  |
| 12  | P     | 46  | LYS  |
| 12  | P     | 47  | ASP  |
| 12  | P     | 49  | ARG  |
| 12  | P     | 52  | GLU  |
| 12  | P     | 59  | LEU  |
| 12  | P     | 141 | ALA  |
| 12  | P     | 149 | GLU  |
| 13  | Q     | 21  | THR  |
| 13  | Q     | 134 | ARG  |
| 13  | Q     | 135 | ASP  |
| 13  | Q     | 136 | ALA  |
| 14  | R     | 6   | SER  |
| 14  | R     | 82  | GLU  |
| 15  | S     | 59  | LYS  |
| 15  | S     | 62  | LYS  |
| 15  | S     | 91  | PRO  |
| 16  | T     | 2   | ASN  |
| 16  | T     | 3   | ARG  |
| 16  | T     | 107 | ASP  |
| 17  | U     | 90  | VAL  |
| 21  | Y     | 8   | LYS  |
| 21  | Y     | 63  | LYS  |
| 21  | Y     | 77  | PRO  |
| 21  | Y     | 78  | ALA  |
| 21  | Y     | 96  | ILE  |
| 22  | Z     | 101 | PRO  |
| 22  | Z     | 141 | VAL  |
| 23  | 0     | 12  | ASN  |
| 23  | 0     | 47  | PRO  |
| 24  | 1     | 11  | ARG  |
| 24  | 1     | 58  | ILE  |
| 24  | 1     | 83  | GLU  |
| 25  | 2     | 44  | LEU  |
| 25  | 2     | 48  | HIS  |
| 26  | 3     | 29  | ARG  |
| 28  | 5     | 4   | HIS  |
| 28  | 5     | 35  | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | 6     | 26  | ASN  |
| 29  | 6     | 31  | PRO  |
| 31  | 8     | 35  | GLN  |
| 31  | 8     | 51  | ALA  |
| 31  | 8     | 62  | LEU  |
| 3   | D     | 26  | LYS  |
| 3   | D     | 169 | GLU  |
| 3   | D     | 256 | GLY  |
| 4   | E     | 17  | ASP  |
| 4   | E     | 86  | PRO  |
| 4   | E     | 129 | HIS  |
| 4   | E     | 144 | ARG  |
| 5   | F     | 66  | PRO  |
| 6   | G     | 24  | GLY  |
| 6   | G     | 142 | PRO  |
| 6   | G     | 155 | MET  |
| 7   | H     | 107 | VAL  |
| 8   | I     | 82  | ARG  |
| 8   | I     | 84  | GLY  |
| 9   | K     | 26  | ALA  |
| 10  | N     | 26  | THR  |
| 10  | N     | 41  | ALA  |
| 10  | N     | 60  | LYS  |
| 10  | N     | 93  | LYS  |
| 10  | N     | 148 | GLY  |
| 10  | N     | 150 | ASP  |
| 11  | O     | 29  | ASN  |
| 11  | O     | 96  | THR  |
| 12  | P     | 11  | GLY  |
| 12  | P     | 15  | ARG  |
| 12  | P     | 16  | ARG  |
| 12  | P     | 17  | LYS  |
| 12  | P     | 18  | ARG  |
| 12  | P     | 19  | VAL  |
| 12  | P     | 34  | GLY  |
| 12  | P     | 39  | LYS  |
| 12  | P     | 56  | SER  |
| 12  | P     | 90  | ARG  |
| 12  | P     | 106 | LEU  |
| 13  | Q     | 10  | ARG  |
| 13  | Q     | 19  | GLY  |
| 13  | Q     | 23  | GLY  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | Q     | 62  | GLY  |
| 13  | Q     | 79  | LEU  |
| 14  | R     | 10  | LEU  |
| 14  | R     | 107 | ASP  |
| 15  | S     | 57  | LYS  |
| 15  | S     | 58  | LEU  |
| 15  | S     | 61  | ASN  |
| 15  | S     | 86  | ALA  |
| 15  | S     | 90  | GLY  |
| 16  | T     | 124 | ASP  |
| 17  | U     | 9   | VAL  |
| 18  | V     | 48  | GLY  |
| 18  | V     | 78  | LYS  |
| 20  | X     | 87  | GLN  |
| 21  | Y     | 3   | VAL  |
| 21  | Y     | 7   | VAL  |
| 21  | Y     | 49  | VAL  |
| 22  | Z     | 80  | ARG  |
| 22  | Z     | 93  | ASP  |
| 24  | 1     | 14  | VAL  |
| 24  | 1     | 16  | ASN  |
| 24  | 1     | 32  | LYS  |
| 27  | 4     | 61  | VAL  |
| 28  | 5     | 51  | TYR  |
| 29  | 6     | 18  | ARG  |
| 29  | 6     | 35  | GLU  |
| 31  | 8     | 30  | ARG  |
| 31  | 8     | 34  | TRP  |
| 3   | D     | 25  | THR  |
| 3   | D     | 35  | LYS  |
| 5   | F     | 48  | THR  |
| 5   | F     | 68  | LYS  |
| 5   | F     | 90  | PHE  |
| 6   | G     | 14  | GLU  |
| 6   | G     | 85  | GLY  |
| 6   | G     | 136 | ARG  |
| 8   | I     | 11  | ASN  |
| 8   | I     | 29  | TYR  |
| 8   | I     | 117 | GLU  |
| 9   | K     | 51  | ALA  |
| 9   | K     | 141 | ALA  |
| 9   | K     | 145 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | N     | 116 | THR  |
| 11  | O     | 26  | LYS  |
| 11  | O     | 94  | ARG  |
| 12  | P     | 13  | ASN  |
| 13  | Q     | 25  | ASP  |
| 13  | Q     | 51  | ARG  |
| 15  | S     | 51  | ALA  |
| 16  | T     | 113 | LYS  |
| 16  | T     | 115 | ARG  |
| 17  | U     | 91  | ASP  |
| 19  | W     | 63  | ASP  |
| 19  | W     | 90  | ARG  |
| 21  | Y     | 17  | SER  |
| 21  | Y     | 40  | GLU  |
| 21  | Y     | 88  | LYS  |
| 24  | 1     | 31  | GLY  |
| 25  | 2     | 3   | LEU  |
| 25  | 2     | 17  | SER  |
| 25  | 2     | 43  | GLN  |
| 27  | 4     | 52  | SER  |
| 31  | 8     | 31  | HIS  |
| 3   | D     | 162 | SER  |
| 3   | D     | 233 | HIS  |
| 4   | E     | 52  | LEU  |
| 5   | F     | 74  | ARG  |
| 5   | F     | 166 | ALA  |
| 7   | H     | 51  | ARG  |
| 7   | H     | 108 | GLY  |
| 8   | I     | 113 | ARG  |
| 10  | N     | 32  | VAL  |
| 12  | P     | 31  | ALA  |
| 13  | Q     | 133 | ARG  |
| 15  | S     | 42  | ASP  |
| 15  | S     | 83  | LYS  |
| 16  | T     | 4   | GLY  |
| 16  | T     | 39  | ARG  |
| 16  | T     | 58  | ASN  |
| 16  | T     | 90  | GLN  |
| 16  | T     | 126 | ALA  |
| 18  | V     | 40  | LEU  |
| 18  | V     | 50  | PRO  |
| 18  | V     | 80  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | W     | 5   | ALA  |
| 20  | X     | 48  | LYS  |
| 21  | Y     | 55  | TYR  |
| 21  | Y     | 90  | LEU  |
| 22  | Z     | 11  | GLU  |
| 23  | 0     | 20  | ARG  |
| 24  | 1     | 13  | ILE  |
| 24  | 1     | 87  | PRO  |
| 26  | 3     | 35  | ARG  |
| 31  | 8     | 40  | GLU  |
| 3   | D     | 44  | ASN  |
| 3   | D     | 239 | ARG  |
| 3   | D     | 268 | ARG  |
| 6   | G     | 96  | ARG  |
| 8   | I     | 40  | THR  |
| 9   | K     | 91  | PRO  |
| 9   | K     | 142 | PRO  |
| 10  | N     | 115 | ALA  |
| 10  | N     | 118 | PRO  |
| 10  | N     | 153 | HIS  |
| 10  | N     | 155 | ALA  |
| 12  | P     | 65  | ARG  |
| 12  | P     | 122 | PRO  |
| 14  | R     | 8   | ARG  |
| 16  | T     | 86  | ILE  |
| 17  | U     | 93  | LYS  |
| 18  | V     | 44  | LYS  |
| 21  | Y     | 98  | VAL  |
| 27  | 4     | 50  | THR  |
| 27  | 4     | 54  | LYS  |
| 29  | 6     | 46  | HIS  |
| 3   | D     | 156 | ALA  |
| 5   | F     | 134 | GLY  |
| 10  | N     | 70  | ALA  |
| 14  | R     | 61  | HIS  |
| 21  | Y     | 56  | PRO  |
| 22  | Z     | 82  | ARG  |
| 22  | Z     | 114 | GLY  |
| 22  | Z     | 165 | VAL  |
| 24  | 1     | 53  | VAL  |
| 6   | G     | 42  | GLY  |
| 7   | H     | 92  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | Q     | 126 | PRO  |
| 16  | T     | 42  | ILE  |
| 18  | V     | 17  | GLY  |
| 18  | V     | 35  | LEU  |
| 21  | Y     | 61  | ILE  |
| 4   | E     | 56  | PRO  |
| 6   | G     | 140 | ILE  |
| 7   | H     | 44  | VAL  |
| 19  | W     | 35  | ILE  |
| 24  | 1     | 9   | GLY  |
| 7   | H     | 50  | VAL  |
| 9   | K     | 34  | ILE  |
| 18  | V     | 46  | VAL  |
| 18  | V     | 47  | VAL  |
| 3   | D     | 127 | VAL  |
| 5   | F     | 132 | VAL  |
| 14  | R     | 39  | PRO  |
| 16  | T     | 37  | GLY  |
| 9   | K     | 92  | GLY  |
| 13  | Q     | 81  | VAL  |
| 12  | P     | 48  | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3   | D     | 213/218 (98%)  | 181 (85%) | 32 (15%) | 4           | 20 |
| 4   | E     | 165/166 (99%)  | 144 (87%) | 21 (13%) | 6           | 27 |
| 5   | F     | 161/166 (97%)  | 142 (88%) | 19 (12%) | 8           | 30 |
| 6   | G     | 155/156 (99%)  | 135 (87%) | 20 (13%) | 6           | 26 |
| 7   | H     | 132/148 (89%)  | 115 (87%) | 17 (13%) | 6           | 26 |
| 8   | I     | 122/124 (98%)  | 101 (83%) | 21 (17%) | 3           | 14 |
| 9   | K     | 111/111 (100%) | 95 (86%)  | 16 (14%) | 5           | 22 |
| 10  | N     | 116/139 (84%)  | 98 (84%)  | 18 (16%) | 4           | 19 |
| 11  | O     | 100/100 (100%) | 86 (86%)  | 14 (14%) | 5           | 23 |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 12  | P     | 112/116 (97%)   | 80 (71%)   | 32 (29%)  | 0           | 3  |
| 13  | Q     | 105/111 (95%)   | 91 (87%)   | 14 (13%)  | 6           | 25 |
| 14  | R     | 100/101 (99%)   | 90 (90%)   | 10 (10%)  | 11          | 39 |
| 15  | S     | 77/88 (88%)     | 66 (86%)   | 11 (14%)  | 5           | 22 |
| 16  | T     | 121/128 (94%)   | 101 (84%)  | 20 (16%)  | 3           | 16 |
| 17  | U     | 93/94 (99%)     | 82 (88%)   | 11 (12%)  | 8           | 30 |
| 18  | V     | 82/82 (100%)    | 68 (83%)   | 14 (17%)  | 3           | 15 |
| 19  | W     | 91/92 (99%)     | 80 (88%)   | 11 (12%)  | 7           | 29 |
| 20  | X     | 74/78 (95%)     | 58 (78%)   | 16 (22%)  | 1           | 8  |
| 21  | Y     | 84/91 (92%)     | 72 (86%)   | 12 (14%)  | 5           | 22 |
| 22  | Z     | 162/179 (90%)   | 151 (93%)  | 11 (7%)   | 22          | 63 |
| 23  | 0     | 61/67 (91%)     | 53 (87%)   | 8 (13%)   | 6           | 25 |
| 24  | 1     | 73/83 (88%)     | 58 (80%)   | 15 (20%)  | 2           | 9  |
| 25  | 2     | 58/67 (87%)     | 45 (78%)   | 13 (22%)  | 1           | 7  |
| 26  | 3     | 51/52 (98%)     | 49 (96%)   | 2 (4%)    | 43          | 85 |
| 27  | 4     | 27/84 (32%)     | 21 (78%)   | 6 (22%)   | 1           | 7  |
| 28  | 5     | 45/52 (86%)     | 41 (91%)   | 4 (9%)    | 14          | 48 |
| 29  | 6     | 43/52 (83%)     | 34 (79%)   | 9 (21%)   | 1           | 8  |
| 30  | 7     | 41/42 (98%)     | 35 (85%)   | 6 (15%)   | 5           | 21 |
| 31  | 8     | 53/55 (96%)     | 47 (89%)   | 6 (11%)   | 9           | 33 |
| All | All   | 2828/3042 (93%) | 2419 (86%) | 409 (14%) | 5           | 22 |

All (409) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 5   | LYS  |
| 3   | D     | 10  | THR  |
| 3   | D     | 18  | VAL  |
| 3   | D     | 23  | GLU  |
| 3   | D     | 28  | GLU  |
| 3   | D     | 33  | LEU  |
| 3   | D     | 37  | LEU  |
| 3   | D     | 40  | THR  |
| 3   | D     | 61  | LEU  |
| 3   | D     | 70  | TRP  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 89  | SER  |
| 3   | D     | 95  | LEU  |
| 3   | D     | 106 | ILE  |
| 3   | D     | 111 | LEU  |
| 3   | D     | 112 | GLN  |
| 3   | D     | 127 | VAL  |
| 3   | D     | 131 | LEU  |
| 3   | D     | 138 | VAL  |
| 3   | D     | 150 | LYS  |
| 3   | D     | 154 | LYS  |
| 3   | D     | 166 | GLN  |
| 3   | D     | 169 | GLU  |
| 3   | D     | 182 | LEU  |
| 3   | D     | 200 | ASP  |
| 3   | D     | 211 | ARG  |
| 3   | D     | 212 | SER  |
| 3   | D     | 217 | ARG  |
| 3   | D     | 255 | LYS  |
| 3   | D     | 257 | LEU  |
| 3   | D     | 263 | ARG  |
| 3   | D     | 266 | SER  |
| 3   | D     | 271 | ILE  |
| 4   | E     | 4   | ILE  |
| 4   | E     | 9   | VAL  |
| 4   | E     | 16  | ARG  |
| 4   | E     | 17  | ASP  |
| 4   | E     | 41  | LYS  |
| 4   | E     | 49  | LEU  |
| 4   | E     | 54  | GLN  |
| 4   | E     | 57  | LYS  |
| 4   | E     | 77  | ILE  |
| 4   | E     | 78  | LEU  |
| 4   | E     | 79  | ARG  |
| 4   | E     | 87  | GLU  |
| 4   | E     | 92  | THR  |
| 4   | E     | 119 | ARG  |
| 4   | E     | 154 | LYS  |
| 4   | E     | 169 | ASN  |
| 4   | E     | 175 | VAL  |
| 4   | E     | 184 | VAL  |
| 4   | E     | 196 | VAL  |
| 4   | E     | 197 | ILE  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | E     | 202 | LYS  |
| 5   | F     | 8   | GLN  |
| 5   | F     | 9   | ILE  |
| 5   | F     | 33  | LEU  |
| 5   | F     | 45  | ARG  |
| 5   | F     | 57  | VAL  |
| 5   | F     | 64  | ILE  |
| 5   | F     | 69  | HIS  |
| 5   | F     | 78  | ILE  |
| 5   | F     | 106 | ARG  |
| 5   | F     | 145 | GLU  |
| 5   | F     | 158 | THR  |
| 5   | F     | 164 | ARG  |
| 5   | F     | 165 | ARG  |
| 5   | F     | 170 | LEU  |
| 5   | F     | 174 | VAL  |
| 5   | F     | 175 | THR  |
| 5   | F     | 183 | VAL  |
| 5   | F     | 201 | VAL  |
| 5   | F     | 206 | ILE  |
| 6   | G     | 4   | ASP  |
| 6   | G     | 16  | ARG  |
| 6   | G     | 18  | GLU  |
| 6   | G     | 20  | ILE  |
| 6   | G     | 34  | LEU  |
| 6   | G     | 35  | GLU  |
| 6   | G     | 47  | LYS  |
| 6   | G     | 80  | PHE  |
| 6   | G     | 86  | MET  |
| 6   | G     | 90  | LEU  |
| 6   | G     | 91  | ARG  |
| 6   | G     | 115 | ARG  |
| 6   | G     | 121 | ASN  |
| 6   | G     | 128 | ARG  |
| 6   | G     | 132 | ASN  |
| 6   | G     | 143 | GLU  |
| 6   | G     | 145 | THR  |
| 6   | G     | 155 | MET  |
| 6   | G     | 159 | VAL  |
| 6   | G     | 166 | ASP  |
| 7   | H     | 13  | LYS  |
| 7   | H     | 23  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | H     | 47  | GLU  |
| 7   | H     | 68  | THR  |
| 7   | H     | 77  | LYS  |
| 7   | H     | 79  | VAL  |
| 7   | H     | 86  | GLU  |
| 7   | H     | 101 | ARG  |
| 7   | H     | 103 | LEU  |
| 7   | H     | 104 | GLU  |
| 7   | H     | 105 | LEU  |
| 7   | H     | 107 | VAL  |
| 7   | H     | 110 | SER  |
| 7   | H     | 116 | GLU  |
| 7   | H     | 123 | PHE  |
| 7   | H     | 129 | THR  |
| 7   | H     | 167 | GLU  |
| 8   | I     | 4   | ILE  |
| 8   | I     | 6   | LEU  |
| 8   | I     | 9   | LEU  |
| 8   | I     | 10  | GLU  |
| 8   | I     | 19  | VAL  |
| 8   | I     | 20  | ASP  |
| 8   | I     | 25  | TYR  |
| 8   | I     | 38  | LEU  |
| 8   | I     | 40  | THR  |
| 8   | I     | 50  | ARG  |
| 8   | I     | 52  | ARG  |
| 8   | I     | 56  | LYS  |
| 8   | I     | 67  | ARG  |
| 8   | I     | 71  | ILE  |
| 8   | I     | 92  | VAL  |
| 8   | I     | 107 | ILE  |
| 8   | I     | 109 | ILE  |
| 8   | I     | 118 | LYS  |
| 8   | I     | 141 | LYS  |
| 8   | I     | 143 | SER  |
| 8   | I     | 145 | VAL  |
| 9   | K     | 8   | VAL  |
| 9   | K     | 27  | LEU  |
| 9   | K     | 41  | PHE  |
| 9   | K     | 50  | ASP  |
| 9   | K     | 58  | THR  |
| 9   | K     | 65  | PHE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | K     | 67  | PHE  |
| 9   | K     | 68  | VAL  |
| 9   | K     | 76  | TYR  |
| 9   | K     | 80  | LYS  |
| 9   | K     | 85  | GLU  |
| 9   | K     | 93  | ARG  |
| 9   | K     | 101 | TRP  |
| 9   | K     | 110 | GLN  |
| 9   | K     | 125 | ARG  |
| 9   | K     | 139 | VAL  |
| 10  | N     | 55  | THR  |
| 10  | N     | 56  | LEU  |
| 10  | N     | 57  | LEU  |
| 10  | N     | 64  | ASP  |
| 10  | N     | 65  | TRP  |
| 10  | N     | 68  | ASN  |
| 10  | N     | 71  | MET  |
| 10  | N     | 97  | ARG  |
| 10  | N     | 110 | LEU  |
| 10  | N     | 117 | HIS  |
| 10  | N     | 122 | LEU  |
| 10  | N     | 132 | LYS  |
| 10  | N     | 143 | LEU  |
| 10  | N     | 145 | VAL  |
| 10  | N     | 150 | ASP  |
| 10  | N     | 154 | GLN  |
| 10  | N     | 160 | LYS  |
| 10  | N     | 161 | LEU  |
| 11  | O     | 8   | LEU  |
| 11  | O     | 9   | GLU  |
| 11  | O     | 19  | ILE  |
| 11  | O     | 24  | VAL  |
| 11  | O     | 32  | TYR  |
| 11  | O     | 45  | GLU  |
| 11  | O     | 47  | ILE  |
| 11  | O     | 53  | LYS  |
| 11  | O     | 65  | THR  |
| 11  | O     | 73  | ASP  |
| 11  | O     | 75  | SER  |
| 11  | O     | 77  | ILE  |
| 11  | O     | 104 | ARG  |
| 11  | O     | 114 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | P     | 6   | LEU  |
| 12  | P     | 13  | ASN  |
| 12  | P     | 15  | ARG  |
| 12  | P     | 16  | ARG  |
| 12  | P     | 18  | ARG  |
| 12  | P     | 32  | THR  |
| 12  | P     | 35  | HIS  |
| 12  | P     | 39  | LYS  |
| 12  | P     | 40  | SER  |
| 12  | P     | 41  | ARG  |
| 12  | P     | 49  | ARG  |
| 12  | P     | 50  | ARG  |
| 12  | P     | 51  | PHE  |
| 12  | P     | 57  | THR  |
| 12  | P     | 61  | ARG  |
| 12  | P     | 62  | LEU  |
| 12  | P     | 67  | MET  |
| 12  | P     | 70  | GLN  |
| 12  | P     | 75  | ILE  |
| 12  | P     | 83  | VAL  |
| 12  | P     | 86  | LYS  |
| 12  | P     | 96  | THR  |
| 12  | P     | 100 | LEU  |
| 12  | P     | 106 | LEU  |
| 12  | P     | 114 | ILE  |
| 12  | P     | 117 | GLU  |
| 12  | P     | 123 | LEU  |
| 12  | P     | 135 | LEU  |
| 12  | P     | 138 | LEU  |
| 12  | P     | 144 | GLU  |
| 12  | P     | 147 | LEU  |
| 12  | P     | 148 | LEU  |
| 13  | Q     | 8   | LYS  |
| 13  | Q     | 9   | TYR  |
| 13  | Q     | 14  | ARG  |
| 13  | Q     | 22  | LYS  |
| 13  | Q     | 29  | PHE  |
| 13  | Q     | 45  | GLN  |
| 13  | Q     | 47  | ILE  |
| 13  | Q     | 56  | ARG  |
| 13  | Q     | 82  | ARG  |
| 13  | Q     | 83  | MET  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | Q     | 96  | VAL  |
| 13  | Q     | 97  | VAL  |
| 13  | Q     | 133 | ARG  |
| 13  | Q     | 134 | ARG  |
| 14  | R     | 2   | ARG  |
| 14  | R     | 18  | LEU  |
| 14  | R     | 67  | LEU  |
| 14  | R     | 71  | GLN  |
| 14  | R     | 75  | LEU  |
| 14  | R     | 79  | LEU  |
| 14  | R     | 81  | ASP  |
| 14  | R     | 97  | VAL  |
| 14  | R     | 99  | LYS  |
| 14  | R     | 104 | ARG  |
| 15  | S     | 12  | PHE  |
| 15  | S     | 14  | VAL  |
| 15  | S     | 30  | ARG  |
| 15  | S     | 36  | TYR  |
| 15  | S     | 44  | LYS  |
| 15  | S     | 54  | LEU  |
| 15  | S     | 57  | LYS  |
| 15  | S     | 61  | ASN  |
| 15  | S     | 80  | LEU  |
| 15  | S     | 92  | TYR  |
| 15  | S     | 98  | VAL  |
| 16  | T     | 15  | VAL  |
| 16  | T     | 17  | THR  |
| 16  | T     | 19  | LEU  |
| 16  | T     | 27  | THR  |
| 16  | T     | 28  | VAL  |
| 16  | T     | 30  | VAL  |
| 16  | T     | 31  | SER  |
| 16  | T     | 50  | ILE  |
| 16  | T     | 51  | ARG  |
| 16  | T     | 58  | ASN  |
| 16  | T     | 62  | THR  |
| 16  | T     | 85  | LYS  |
| 16  | T     | 86  | ILE  |
| 16  | T     | 87  | ASP  |
| 16  | T     | 88  | ILE  |
| 16  | T     | 98  | LYS  |
| 16  | T     | 102 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | T     | 105 | LEU  |
| 16  | T     | 112 | ARG  |
| 16  | T     | 115 | ARG  |
| 17  | U     | 27  | LEU  |
| 17  | U     | 31  | SER  |
| 17  | U     | 60  | LEU  |
| 17  | U     | 75  | ASN  |
| 17  | U     | 80  | ILE  |
| 17  | U     | 83  | LEU  |
| 17  | U     | 88  | ILE  |
| 17  | U     | 92  | ARG  |
| 17  | U     | 97  | ASP  |
| 17  | U     | 104 | GLN  |
| 17  | U     | 112 | ARG  |
| 18  | V     | 5   | VAL  |
| 18  | V     | 12  | TYR  |
| 18  | V     | 13  | ARG  |
| 18  | V     | 18  | LEU  |
| 18  | V     | 35  | LEU  |
| 18  | V     | 39  | LEU  |
| 18  | V     | 43  | GLU  |
| 18  | V     | 45  | THR  |
| 18  | V     | 46  | VAL  |
| 18  | V     | 47  | VAL  |
| 18  | V     | 80  | GLN  |
| 18  | V     | 88  | ARG  |
| 18  | V     | 95  | LEU  |
| 18  | V     | 99  | ILE  |
| 19  | W     | 1   | MET  |
| 19  | W     | 11  | ARG  |
| 19  | W     | 19  | LEU  |
| 19  | W     | 27  | LYS  |
| 19  | W     | 39  | THR  |
| 19  | W     | 61  | ASN  |
| 19  | W     | 64  | MET  |
| 19  | W     | 69  | LEU  |
| 19  | W     | 88  | ARG  |
| 19  | W     | 107 | LEU  |
| 19  | W     | 110 | LYS  |
| 20  | X     | 3   | THR  |
| 20  | X     | 8   | ILE  |
| 20  | X     | 12  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | X     | 15  | GLU  |
| 20  | X     | 23  | GLU  |
| 20  | X     | 27  | THR  |
| 20  | X     | 28  | PHE  |
| 20  | X     | 30  | VAL  |
| 20  | X     | 49  | VAL  |
| 20  | X     | 51  | VAL  |
| 20  | X     | 57  | LEU  |
| 20  | X     | 65  | ARG  |
| 20  | X     | 68  | ARG  |
| 20  | X     | 70  | LEU  |
| 20  | X     | 76  | ARG  |
| 20  | X     | 81  | VAL  |
| 21  | Y     | 4   | LYS  |
| 21  | Y     | 6   | HIS  |
| 21  | Y     | 8   | LYS  |
| 21  | Y     | 9   | LYS  |
| 21  | Y     | 13  | VAL  |
| 21  | Y     | 27  | VAL  |
| 21  | Y     | 60  | PHE  |
| 21  | Y     | 75  | ILE  |
| 21  | Y     | 76  | CYS  |
| 21  | Y     | 87  | LYS  |
| 21  | Y     | 90  | LEU  |
| 21  | Y     | 97  | ARG  |
| 22  | Z     | 24  | LEU  |
| 22  | Z     | 41  | LEU  |
| 22  | Z     | 71  | VAL  |
| 22  | Z     | 75  | ASN  |
| 22  | Z     | 87  | ASP  |
| 22  | Z     | 96  | VAL  |
| 22  | Z     | 97  | GLU  |
| 22  | Z     | 118 | GLN  |
| 22  | Z     | 131 | ARG  |
| 22  | Z     | 154 | ASP  |
| 22  | Z     | 157 | LEU  |
| 23  | 0     | 11  | LYS  |
| 23  | 0     | 17  | GLN  |
| 23  | 0     | 21  | LEU  |
| 23  | 0     | 25  | ARG  |
| 23  | 0     | 32  | ARG  |
| 23  | 0     | 64  | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | 0     | 80  | HIS  |
| 23  | 0     | 84  | LEU  |
| 24  | 1     | 13  | ILE  |
| 24  | 1     | 17  | SER  |
| 24  | 1     | 18  | ILE  |
| 24  | 1     | 21  | ARG  |
| 24  | 1     | 27  | GLU  |
| 24  | 1     | 40  | ARG  |
| 24  | 1     | 45  | ASN  |
| 24  | 1     | 56  | GLN  |
| 24  | 1     | 59  | THR  |
| 24  | 1     | 61  | ARG  |
| 24  | 1     | 72  | GLU  |
| 24  | 1     | 75  | GLU  |
| 24  | 1     | 76  | ARG  |
| 24  | 1     | 80  | LEU  |
| 24  | 1     | 82  | LEU  |
| 25  | 2     | 1   | MET  |
| 25  | 2     | 2   | LYS  |
| 25  | 2     | 5   | GLU  |
| 25  | 2     | 9   | GLN  |
| 25  | 2     | 16  | LEU  |
| 25  | 2     | 17  | SER  |
| 25  | 2     | 24  | LEU  |
| 25  | 2     | 36  | ARG  |
| 25  | 2     | 49  | LYS  |
| 25  | 2     | 50  | ILE  |
| 25  | 2     | 53  | LEU  |
| 25  | 2     | 59  | ARG  |
| 25  | 2     | 61  | LEU  |
| 26  | 3     | 37  | LEU  |
| 26  | 3     | 48  | GLU  |
| 27  | 4     | 39  | ARG  |
| 27  | 4     | 42  | CYS  |
| 27  | 4     | 46  | ASN  |
| 27  | 4     | 54  | LYS  |
| 27  | 4     | 62  | CYS  |
| 27  | 4     | 65  | CYS  |
| 28  | 5     | 3   | LYS  |
| 28  | 5     | 33  | CYS  |
| 28  | 5     | 51  | TYR  |
| 28  | 5     | 52  | TYR  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | 6     | 10  | LEU  |
| 29  | 6     | 11  | LEU  |
| 29  | 6     | 12  | GLU  |
| 29  | 6     | 17  | LYS  |
| 29  | 6     | 24  | GLU  |
| 29  | 6     | 34  | LEU  |
| 29  | 6     | 36  | LEU  |
| 29  | 6     | 42  | TRP  |
| 29  | 6     | 48  | VAL  |
| 30  | 7     | 4   | THR  |
| 30  | 7     | 8   | ASN  |
| 30  | 7     | 19  | ARG  |
| 30  | 7     | 24  | THR  |
| 30  | 7     | 34  | ARG  |
| 30  | 7     | 39  | ARG  |
| 31  | 8     | 30  | ARG  |
| 31  | 8     | 32  | LEU  |
| 31  | 8     | 52  | LYS  |
| 31  | 8     | 57  | ARG  |
| 31  | 8     | 61  | LEU  |
| 31  | 8     | 64  | TYR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 2878/2894 (99%) | 589 (20%)         | 178 (6%)        |
| 2   | B     | 118/124 (95%)   | 17 (14%)          | 6 (5%)          |
| All | All   | 2996/3018 (99%) | 606 (20%)         | 184 (6%)        |

All (606) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | G    |
| 1   | A     | 13  | A    |
| 1   | A     | 17  | G    |
| 1   | A     | 27  | G    |
| 1   | A     | 28  | A    |
| 1   | A     | 34  | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 35     | G    |
| 1   | A     | 46     | C    |
| 1   | A     | 49     | A    |
| 1   | A     | 52     | A    |
| 1   | A     | 55     | G    |
| 1   | A     | 58     | G    |
| 1   | A     | 71     | A    |
| 1   | A     | 72     | U    |
| 1   | A     | 73     | A    |
| 1   | A     | 74     | A    |
| 1   | A     | 75     | G    |
| 1   | A     | 84     | A    |
| 1   | A     | 85     | G    |
| 1   | A     | 88     | G    |
| 1   | A     | 91     | A    |
| 1   | A     | 99     | U    |
| 1   | A     | 101    | G    |
| 1   | A     | 102    | G    |
| 1   | A     | 103    | A    |
| 1   | A     | 118    | A    |
| 1   | A     | 119    | A    |
| 1   | A     | 120    | U    |
| 1   | A     | 126    | A    |
| 1   | A     | 138    | G    |
| 1   | A     | 140    | A    |
| 1   | A     | 141(A) | A    |
| 1   | A     | 155    | C    |
| 1   | A     | 162    | U    |
| 1   | A     | 181    | A    |
| 1   | A     | 196    | A    |
| 1   | A     | 197    | A    |
| 1   | A     | 199    | A    |
| 1   | A     | 200    | U    |
| 1   | A     | 204    | A    |
| 1   | A     | 205    | G    |
| 1   | A     | 214    | G    |
| 1   | A     | 215    | G    |
| 1   | A     | 216    | A    |
| 1   | A     | 221    | A    |
| 1   | A     | 222    | A    |
| 1   | A     | 228    | A    |
| 1   | A     | 229    | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 230    | U    |
| 1   | A     | 245    | G    |
| 1   | A     | 248    | G    |
| 1   | A     | 250    | G    |
| 1   | A     | 252    | G    |
| 1   | A     | 266    | G    |
| 1   | A     | 270(M) | U    |
| 1   | A     | 270(N) | U    |
| 1   | A     | 270(O) | G    |
| 1   | A     | 270(P) | U    |
| 1   | A     | 270(R) | C    |
| 1   | A     | 270(T) | G    |
| 1   | A     | 271(D) | U    |
| 1   | A     | 271    | G    |
| 1   | A     | 274    | G    |
| 1   | A     | 275    | G    |
| 1   | A     | 277    | C    |
| 1   | A     | 278    | A    |
| 1   | A     | 279    | C    |
| 1   | A     | 284    | U    |
| 1   | A     | 299    | A    |
| 1   | A     | 302    | C    |
| 1   | A     | 323    | G    |
| 1   | A     | 324    | A    |
| 1   | A     | 329    | G    |
| 1   | A     | 330    | A    |
| 1   | A     | 333    | G    |
| 1   | A     | 342    | G    |
| 1   | A     | 346    | A    |
| 1   | A     | 352    | G    |
| 1   | A     | 353    | G    |
| 1   | A     | 364    | C    |
| 1   | A     | 372    | G    |
| 1   | A     | 386    | G    |
| 1   | A     | 387    | U    |
| 1   | A     | 396    | G    |
| 1   | A     | 400    | G    |
| 1   | A     | 405    | U    |
| 1   | A     | 406    | G    |
| 1   | A     | 407    | G    |
| 1   | A     | 411    | G    |
| 1   | A     | 412    | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 413    | C    |
| 1   | A     | 442    | G    |
| 1   | A     | 444    | C    |
| 1   | A     | 454    | A    |
| 1   | A     | 455    | C    |
| 1   | A     | 457    | A    |
| 1   | A     | 470    | A    |
| 1   | A     | 471    | A    |
| 1   | A     | 474    | G    |
| 1   | A     | 475    | U    |
| 1   | A     | 479    | A    |
| 1   | A     | 480    | A    |
| 1   | A     | 481    | G    |
| 1   | A     | 482    | A    |
| 1   | A     | 496    | G    |
| 1   | A     | 504    | U    |
| 1   | A     | 505    | A    |
| 1   | A     | 507    | A    |
| 1   | A     | 508    | G    |
| 1   | A     | 509    | C    |
| 1   | A     | 512    | G    |
| 1   | A     | 513    | A    |
| 1   | A     | 530    | G    |
| 1   | A     | 531    | C    |
| 1   | A     | 532    | A    |
| 1   | A     | 533    | G    |
| 1   | A     | 547    | A    |
| 1   | A     | 556    | G    |
| 1   | A     | 563    | G    |
| 1   | A     | 573    | G    |
| 1   | A     | 575    | A    |
| 1   | A     | 593    | G    |
| 1   | A     | 599    | G    |
| 1   | A     | 603    | A    |
| 1   | A     | 604    | G    |
| 1   | A     | 609(B) | G    |
| 1   | A     | 615    | G    |
| 1   | A     | 617    | G    |
| 1   | A     | 620    | G    |
| 1   | A     | 621    | A    |
| 1   | A     | 627    | A    |
| 1   | A     | 628    | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 634 | C    |
| 1   | A     | 637 | A    |
| 1   | A     | 645 | C    |
| 1   | A     | 646 | A    |
| 1   | A     | 652 | U    |
| 1   | A     | 653 | C    |
| 1   | A     | 654 | U    |
| 1   | A     | 655 | A    |
| 1   | A     | 656 | G    |
| 1   | A     | 657 | U    |
| 1   | A     | 664 | C    |
| 1   | A     | 668 | G    |
| 1   | A     | 671 | C    |
| 1   | A     | 682 | G    |
| 1   | A     | 685 | A    |
| 1   | A     | 686 | G    |
| 1   | A     | 730 | C    |
| 1   | A     | 738 | G    |
| 1   | A     | 746 | A    |
| 1   | A     | 747 | U    |
| 1   | A     | 764 | A    |
| 1   | A     | 765 | G    |
| 1   | A     | 776 | G    |
| 1   | A     | 782 | A    |
| 1   | A     | 784 | A    |
| 1   | A     | 785 | G    |
| 1   | A     | 787 | U    |
| 1   | A     | 792 | G    |
| 1   | A     | 793 | A    |
| 1   | A     | 802 | A    |
| 1   | A     | 805 | G    |
| 1   | A     | 808 | G    |
| 1   | A     | 812 | C    |
| 1   | A     | 819 | A    |
| 1   | A     | 821 | A    |
| 1   | A     | 827 | U    |
| 1   | A     | 828 | U    |
| 1   | A     | 831 | G    |
| 1   | A     | 845 | G    |
| 1   | A     | 846 | C    |
| 1   | A     | 847 | U    |
| 1   | A     | 856 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 859    | G    |
| 1   | A     | 862    | G    |
| 1   | A     | 879    | G    |
| 1   | A     | 886    | C    |
| 1   | A     | 887    | A    |
| 1   | A     | 890    | A    |
| 1   | A     | 896    | A    |
| 1   | A     | 897    | C    |
| 1   | A     | 907    | U    |
| 1   | A     | 910    | A    |
| 1   | A     | 915    | C    |
| 1   | A     | 917    | A    |
| 1   | A     | 919    | G    |
| 1   | A     | 926    | A    |
| 1   | A     | 932    | G    |
| 1   | A     | 933    | A    |
| 1   | A     | 941    | A    |
| 1   | A     | 942    | G    |
| 1   | A     | 945    | A    |
| 1   | A     | 946    | G    |
| 1   | A     | 956    | G    |
| 1   | A     | 959    | A    |
| 1   | A     | 961    | C    |
| 1   | A     | 972    | G    |
| 1   | A     | 974(A) | G    |
| 1   | A     | 974(B) | C    |
| 1   | A     | 975    | G    |
| 1   | A     | 983    | A    |
| 1   | A     | 990    | A    |
| 1   | A     | 996    | A    |
| 1   | A     | 997    | G    |
| 1   | A     | 999    | U    |
| 1   | A     | 1003   | G    |
| 1   | A     | 1009   | A    |
| 1   | A     | 1010   | A    |
| 1   | A     | 1011   | G    |
| 1   | A     | 1012   | U    |
| 1   | A     | 1013   | C    |
| 1   | A     | 1022   | G    |
| 1   | A     | 1023   | U    |
| 1   | A     | 1025   | G    |
| 1   | A     | 1026   | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 1046   | A    |
| 1   | A     | 1047   | G    |
| 1   | A     | 1048   | A    |
| 1   | A     | 1049   | C    |
| 1   | A     | 1060   | U    |
| 1   | A     | 1061   | U    |
| 1   | A     | 1069   | A    |
| 1   | A     | 1070   | A    |
| 1   | A     | 1071   | G    |
| 1   | A     | 1072   | C    |
| 1   | A     | 1074   | G    |
| 1   | A     | 1078   | U    |
| 1   | A     | 1079   | C    |
| 1   | A     | 1088   | A    |
| 1   | A     | 1090   | U    |
| 1   | A     | 1100   | C    |
| 1   | A     | 1110   | G    |
| 1   | A     | 1112   | G    |
| 1   | A     | 1127   | A    |
| 1   | A     | 1129   | A    |
| 1   | A     | 1130   | U    |
| 1   | A     | 1131   | G    |
| 1   | A     | 1132   | A    |
| 1   | A     | 1135   | C    |
| 1   | A     | 1136   | G    |
| 1   | A     | 114(B) | A    |
| 1   | A     | 1144   | G    |
| 1   | A     | 1155   | A    |
| 1   | A     | 1175   | U    |
| 1   | A     | 1176   | G    |
| 1   | A     | 1190   | G    |
| 1   | A     | 1195   | G    |
| 1   | A     | 1204   | A    |
| 1   | A     | 1205   | U    |
| 1   | A     | 1210   | A    |
| 1   | A     | 1211   | U    |
| 1   | A     | 1212   | G    |
| 1   | A     | 1221   | C    |
| 1   | A     | 1227   | G    |
| 1   | A     | 1244   | G    |
| 1   | A     | 1248   | G    |
| 1   | A     | 1250   | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 1253   | A    |
| 1   | A     | 1254   | A    |
| 1   | A     | 1256   | G    |
| 1   | A     | 1265   | A    |
| 1   | A     | 1271   | G    |
| 1   | A     | 1272   | A    |
| 1   | A     | 1273   | U    |
| 1   | A     | 1274   | A    |
| 1   | A     | 1286   | A    |
| 1   | A     | 1287   | A    |
| 1   | A     | 1288   | U    |
| 1   | A     | 1289   | C    |
| 1   | A     | 1300   | U    |
| 1   | A     | 1301   | A    |
| 1   | A     | 1302   | A    |
| 1   | A     | 1306   | C    |
| 1   | A     | 1311   | G    |
| 1   | A     | 1313   | U    |
| 1   | A     | 1314   | C    |
| 1   | A     | 1329   | U    |
| 1   | A     | 1330   | C    |
| 1   | A     | 1332   | G    |
| 1   | A     | 1345   | C    |
| 1   | A     | 1349   | A    |
| 1   | A     | 1352   | U    |
| 1   | A     | 1359   | A    |
| 1   | A     | 1360   | A    |
| 1   | A     | 1378   | A    |
| 1   | A     | 1379   | A    |
| 1   | A     | 1380   | G    |
| 1   | A     | 1384   | A    |
| 1   | A     | 1385   | G    |
| 1   | A     | 1386   | C    |
| 1   | A     | 1394   | U    |
| 1   | A     | 1396   | U    |
| 1   | A     | 1397   | U    |
| 1   | A     | 1416   | G    |
| 1   | A     | 1420   | U    |
| 1   | A     | 1421   | G    |
| 1   | A     | 1427   | A    |
| 1   | A     | 1428   | C    |
| 1   | A     | 144(B) | A    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1451 | C    |
| 1   | A     | 1453 | A    |
| 1   | A     | 1454 | U    |
| 1   | A     | 1458 | C    |
| 1   | A     | 1460 | A    |
| 1   | A     | 1461 | G    |
| 1   | A     | 1467 | C    |
| 1   | A     | 1479 | G    |
| 1   | A     | 1483 | G    |
| 1   | A     | 1490 | A    |
| 1   | A     | 1493 | C    |
| 1   | A     | 1494 | A    |
| 1   | A     | 1495 | A    |
| 1   | A     | 1496 | A    |
| 1   | A     | 1497 | U    |
| 1   | A     | 1498 | C    |
| 1   | A     | 1509 | A    |
| 1   | A     | 1510 | A    |
| 1   | A     | 1535 | U    |
| 1   | A     | 1538 | G    |
| 1   | A     | 1542 | G    |
| 1   | A     | 1543 | A    |
| 1   | A     | 1544 | C    |
| 1   | A     | 1545 | A    |
| 1   | A     | 1554 | A    |
| 1   | A     | 1558 | A    |
| 1   | A     | 1559 | G    |
| 1   | A     | 1566 | A    |
| 1   | A     | 1569 | A    |
| 1   | A     | 1579 | A    |
| 1   | A     | 1585 | C    |
| 1   | A     | 1603 | A    |
| 1   | A     | 1609 | A    |
| 1   | A     | 1610 | A    |
| 1   | A     | 1617 | C    |
| 1   | A     | 1618 | A    |
| 1   | A     | 1633 | G    |
| 1   | A     | 1640 | C    |
| 1   | A     | 1648 | C    |
| 1   | A     | 1668 | A    |
| 1   | A     | 1669 | A    |
| 1   | A     | 1674 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1678 | G    |
| 1   | A     | 1696 | G    |
| 1   | A     | 1698 | A    |
| 1   | A     | 1699 | G    |
| 1   | A     | 1729 | A    |
| 1   | A     | 1730 | U    |
| 1   | A     | 1731 | G    |
| 1   | A     | 1732 | A    |
| 1   | A     | 1750 | G    |
| 1   | A     | 1762 | A    |
| 1   | A     | 1763 | G    |
| 1   | A     | 1764 | G    |
| 1   | A     | 1773 | A    |
| 1   | A     | 1776 | G    |
| 1   | A     | 1784 | A    |
| 1   | A     | 1791 | A    |
| 1   | A     | 1800 | C    |
| 1   | A     | 1801 | G    |
| 1   | A     | 1802 | A    |
| 1   | A     | 1811 | G    |
| 1   | A     | 1816 | G    |
| 1   | A     | 1829 | A    |
| 1   | A     | 1833 | U    |
| 1   | A     | 1839 | G    |
| 1   | A     | 1840 | G    |
| 1   | A     | 1847 | A    |
| 1   | A     | 1848 | A    |
| 1   | A     | 1878 | G    |
| 1   | A     | 1889 | A    |
| 1   | A     | 1900 | A    |
| 1   | A     | 1902 | C    |
| 1   | A     | 1903 | G    |
| 1   | A     | 1906 | G    |
| 1   | A     | 1913 | A    |
| 1   | A     | 1914 | C    |
| 1   | A     | 1919 | A    |
| 1   | A     | 1929 | G    |
| 1   | A     | 1930 | G    |
| 1   | A     | 1936 | A    |
| 1   | A     | 1937 | A    |
| 1   | A     | 1938 | A    |
| 1   | A     | 1939 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1940 | U    |
| 1   | A     | 1941 | C    |
| 1   | A     | 1942 | C    |
| 1   | A     | 1945 | G    |
| 1   | A     | 1955 | U    |
| 1   | A     | 1963 | U    |
| 1   | A     | 1967 | C    |
| 1   | A     | 1970 | A    |
| 1   | A     | 1971 | A    |
| 1   | A     | 1972 | A    |
| 1   | A     | 1980 | G    |
| 1   | A     | 1982 | C    |
| 1   | A     | 1991 | U    |
| 1   | A     | 1992 | G    |
| 1   | A     | 1993 | U    |
| 1   | A     | 1997 | G    |
| 1   | A     | 2020 | A    |
| 1   | A     | 2023 | G    |
| 1   | A     | 2031 | A    |
| 1   | A     | 2033 | A    |
| 1   | A     | 2036 | C    |
| 1   | A     | 2043 | C    |
| 1   | A     | 2051 | A    |
| 1   | A     | 2052 | G    |
| 1   | A     | 2055 | C    |
| 1   | A     | 2056 | G    |
| 1   | A     | 2060 | A    |
| 1   | A     | 2061 | G    |
| 1   | A     | 2062 | A    |
| 1   | A     | 2063 | C    |
| 1   | A     | 2069 | G    |
| 1   | A     | 2078 | C    |
| 1   | A     | 2083 | G    |
| 1   | A     | 2093 | G    |
| 1   | A     | 2108 | C    |
| 1   | A     | 2118 | U    |
| 1   | A     | 2119 | A    |
| 1   | A     | 2120 | G    |
| 1   | A     | 2126 | A    |
| 1   | A     | 2127 | G    |
| 1   | A     | 2131 | G    |
| 1   | A     | 2133 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2145 | C    |
| 1   | A     | 2146 | C    |
| 1   | A     | 2147 | G    |
| 1   | A     | 2158 | A    |
| 1   | A     | 2159 | G    |
| 1   | A     | 2166 | G    |
| 1   | A     | 2171 | A    |
| 1   | A     | 2173 | A    |
| 1   | A     | 2198 | A    |
| 1   | A     | 2199 | A    |
| 1   | A     | 2210 | G    |
| 1   | A     | 2211 | G    |
| 1   | A     | 2212 | A    |
| 1   | A     | 2213 | U    |
| 1   | A     | 2215 | G    |
| 1   | A     | 2225 | A    |
| 1   | A     | 2226 | C    |
| 1   | A     | 2235 | G    |
| 1   | A     | 2238 | G    |
| 1   | A     | 2239 | G    |
| 1   | A     | 2243 | U    |
| 1   | A     | 2273 | A    |
| 1   | A     | 2275 | C    |
| 1   | A     | 2276 | G    |
| 1   | A     | 2279 | G    |
| 1   | A     | 2283 | C    |
| 1   | A     | 2287 | A    |
| 1   | A     | 2297 | C    |
| 1   | A     | 2304 | G    |
| 1   | A     | 2305 | A    |
| 1   | A     | 2306 | C    |
| 1   | A     | 2307 | G    |
| 1   | A     | 2308 | G    |
| 1   | A     | 2309 | A    |
| 1   | A     | 2311 | A    |
| 1   | A     | 2319 | G    |
| 1   | A     | 2320 | A    |
| 1   | A     | 2322 | A    |
| 1   | A     | 2325 | G    |
| 1   | A     | 2327 | A    |
| 1   | A     | 2334 | G    |
| 1   | A     | 2336 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2343 | C    |
| 1   | A     | 2345 | G    |
| 1   | A     | 2347 | C    |
| 1   | A     | 2350 | C    |
| 1   | A     | 2379 | G    |
| 1   | A     | 2383 | G    |
| 1   | A     | 2384 | G    |
| 1   | A     | 2385 | C    |
| 1   | A     | 2394 | C    |
| 1   | A     | 2402 | C    |
| 1   | A     | 2406 | U    |
| 1   | A     | 2423 | U    |
| 1   | A     | 2424 | C    |
| 1   | A     | 2425 | A    |
| 1   | A     | 2427 | C    |
| 1   | A     | 2428 | G    |
| 1   | A     | 2429 | G    |
| 1   | A     | 2430 | A    |
| 1   | A     | 2431 | U    |
| 1   | A     | 2434 | A    |
| 1   | A     | 2435 | A    |
| 1   | A     | 2436 | G    |
| 1   | A     | 2439 | A    |
| 1   | A     | 2440 | C    |
| 1   | A     | 2441 | C    |
| 1   | A     | 2447 | G    |
| 1   | A     | 2448 | A    |
| 1   | A     | 2469 | A    |
| 1   | A     | 2470 | G    |
| 1   | A     | 2474 | C    |
| 1   | A     | 2476 | A    |
| 1   | A     | 2477 | C    |
| 1   | A     | 2478 | A    |
| 1   | A     | 2480 | C    |
| 1   | A     | 2482 | G    |
| 1   | A     | 2484 | G    |
| 1   | A     | 2487 | G    |
| 1   | A     | 2491 | U    |
| 1   | A     | 2492 | U    |
| 1   | A     | 2498 | C    |
| 1   | A     | 2501 | C    |
| 1   | A     | 2502 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 2503   | A    |
| 1   | A     | 2505   | G    |
| 1   | A     | 2506   | U    |
| 1   | A     | 2513   | G    |
| 1   | A     | 2518   | A    |
| 1   | A     | 2520   | C    |
| 1   | A     | 2529   | G    |
| 1   | A     | 2535   | G    |
| 1   | A     | 2542   | A    |
| 1   | A     | 2543   | G    |
| 1   | A     | 2549   | G    |
| 1   | A     | 2553   | G    |
| 1   | A     | 2554   | U    |
| 1   | A     | 2566   | A    |
| 1   | A     | 2567   | G    |
| 1   | A     | 2569   | G    |
| 1   | A     | 2572   | A    |
| 1   | A     | 2573   | C    |
| 1   | A     | 2574   | G    |
| 1   | A     | 2602   | A    |
| 1   | A     | 2603   | G    |
| 1   | A     | 2608   | G    |
| 1   | A     | 2609   | U    |
| 1   | A     | 2610   | C    |
| 1   | A     | 2611   | U    |
| 1   | A     | 2612   | C    |
| 1   | A     | 2615   | U    |
| 1   | A     | 2629   | A    |
| 1   | A     | 2630   | G    |
| 1   | A     | 2663   | G    |
| 1   | A     | 2665   | A    |
| 1   | A     | 2680   | C    |
| 1   | A     | 2682   | U    |
| 1   | A     | 2686   | G    |
| 1   | A     | 2690   | C    |
| 1   | A     | 2691   | C    |
| 1   | A     | 2702   | U    |
| 1   | A     | 2712   | U    |
| 1   | A     | 712(B) | A    |
| 1   | A     | 2713   | A    |
| 1   | A     | 2714   | G    |
| 1   | A     | 2724   | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2726 | U    |
| 1   | A     | 2733 | A    |
| 1   | A     | 2739 | U    |
| 1   | A     | 2744 | G    |
| 1   | A     | 2748 | A    |
| 1   | A     | 2751 | G    |
| 1   | A     | 2757 | A    |
| 1   | A     | 2764 | A    |
| 1   | A     | 2765 | A    |
| 1   | A     | 2766 | G    |
| 1   | A     | 2769 | C    |
| 1   | A     | 2778 | A    |
| 1   | A     | 2779 | U    |
| 1   | A     | 2781 | A    |
| 1   | A     | 2790 | A    |
| 1   | A     | 2791 | C    |
| 1   | A     | 2792 | G    |
| 1   | A     | 2797 | U    |
| 1   | A     | 2799 | A    |
| 1   | A     | 2801 | A    |
| 1   | A     | 2808 | U    |
| 1   | A     | 2820 | A    |
| 1   | A     | 2821 | A    |
| 1   | A     | 2833 | G    |
| 1   | A     | 2835 | A    |
| 1   | A     | 2836 | U    |
| 1   | A     | 2849 | U    |
| 1   | A     | 2850 | A    |
| 1   | A     | 2867 | G    |
| 1   | A     | 2872 | G    |
| 1   | A     | 2873 | A    |
| 1   | A     | 2874 | C    |
| 1   | A     | 2876 | G    |
| 1   | A     | 2880 | C    |
| 1   | A     | 2886 | G    |
| 1   | A     | 2893 | G    |
| 1   | A     | 2894 | G    |
| 2   | B     | 12   | C    |
| 2   | B     | 13   | A    |
| 2   | B     | 15   | A    |
| 2   | B     | 16   | G    |
| 2   | B     | 24   | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 25  | A    |
| 2   | B     | 41  | U    |
| 2   | B     | 42  | C    |
| 2   | B     | 44  | G    |
| 2   | B     | 45  | A    |
| 2   | B     | 52  | A    |
| 2   | B     | 57  | A    |
| 2   | B     | 73  | A    |
| 2   | B     | 90  | C    |
| 2   | B     | 99  | A    |
| 2   | B     | 108 | C    |
| 2   | B     | 109 | G    |

All (184) RNA pucker outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 27     | G    |
| 1   | A     | 52     | A    |
| 1   | A     | 74     | A    |
| 1   | A     | 84     | A    |
| 1   | A     | 90     | U    |
| 1   | A     | 99     | U    |
| 1   | A     | 101    | G    |
| 1   | A     | 102    | G    |
| 1   | A     | 119    | A    |
| 1   | A     | 120    | U    |
| 1   | A     | 125    | G    |
| 1   | A     | 126    | A    |
| 1   | A     | 196    | A    |
| 1   | A     | 199    | A    |
| 1   | A     | 203    | C    |
| 1   | A     | 221    | A    |
| 1   | A     | 270(N) | U    |
| 1   | A     | 270(O) | G    |
| 1   | A     | 271(A) | U    |
| 1   | A     | 271(C) | G    |
| 1   | A     | 278    | A    |
| 1   | A     | 283    | A    |
| 1   | A     | 321    | G    |
| 1   | A     | 323    | G    |
| 1   | A     | 332    | A    |
| 1   | A     | 333    | G    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 352    | G    |
| 1   | A     | 363(G) | A    |
| 1   | A     | 405    | U    |
| 1   | A     | 457    | A    |
| 1   | A     | 470    | A    |
| 1   | A     | 474    | G    |
| 1   | A     | 479    | A    |
| 1   | A     | 481    | G    |
| 1   | A     | 503    | A    |
| 1   | A     | 504    | U    |
| 1   | A     | 512    | G    |
| 1   | A     | 529    | A    |
| 1   | A     | 532    | A    |
| 1   | A     | 547    | A    |
| 1   | A     | 603    | A    |
| 1   | A     | 614    | U    |
| 1   | A     | 616    | A    |
| 1   | A     | 620    | G    |
| 1   | A     | 627    | A    |
| 1   | A     | 652    | U    |
| 1   | A     | 653    | C    |
| 1   | A     | 685    | A    |
| 1   | A     | 746    | A    |
| 1   | A     | 764    | A    |
| 1   | A     | 775    | G    |
| 1   | A     | 776    | G    |
| 1   | A     | 790    | C    |
| 1   | A     | 827    | U    |
| 1   | A     | 846    | C    |
| 1   | A     | 858    | U    |
| 1   | A     | 859    | G    |
| 1   | A     | 930    | U    |
| 1   | A     | 932    | G    |
| 1   | A     | 933    | A    |
| 1   | A     | 945    | A    |
| 1   | A     | 974(A) | G    |
| 1   | A     | 989    | G    |
| 1   | A     | 1009   | A    |
| 1   | A     | 1022   | G    |
| 1   | A     | 1025   | G    |
| 1   | A     | 1026   | U    |
| 1   | A     | 1033   | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1047 | G    |
| 1   | A     | 1048 | A    |
| 1   | A     | 1060 | U    |
| 1   | A     | 1069 | A    |
| 1   | A     | 1070 | A    |
| 1   | A     | 1071 | G    |
| 1   | A     | 1087 | G    |
| 1   | A     | 1126 | A    |
| 1   | A     | 1131 | G    |
| 1   | A     | 1176 | G    |
| 1   | A     | 1210 | A    |
| 1   | A     | 1220 | A    |
| 1   | A     | 1247 | A    |
| 1   | A     | 1252 | G    |
| 1   | A     | 1253 | A    |
| 1   | A     | 1266 | G    |
| 1   | A     | 1273 | U    |
| 1   | A     | 1286 | A    |
| 1   | A     | 1288 | U    |
| 1   | A     | 1300 | U    |
| 1   | A     | 1301 | A    |
| 1   | A     | 1365 | A    |
| 1   | A     | 1378 | A    |
| 1   | A     | 1384 | A    |
| 1   | A     | 1385 | G    |
| 1   | A     | 1396 | U    |
| 1   | A     | 1427 | A    |
| 1   | A     | 1451 | C    |
| 1   | A     | 1458 | C    |
| 1   | A     | 1459 | G    |
| 1   | A     | 1460 | A    |
| 1   | A     | 1493 | C    |
| 1   | A     | 1494 | A    |
| 1   | A     | 1542 | G    |
| 1   | A     | 1544 | C    |
| 1   | A     | 1545 | A    |
| 1   | A     | 1558 | A    |
| 1   | A     | 1559 | G    |
| 1   | A     | 1579 | A    |
| 1   | A     | 1602 | U    |
| 1   | A     | 1607 | C    |
| 1   | A     | 1608 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1609 | A    |
| 1   | A     | 1617 | C    |
| 1   | A     | 1635 | G    |
| 1   | A     | 1729 | A    |
| 1   | A     | 1784 | A    |
| 1   | A     | 1786 | A    |
| 1   | A     | 1800 | C    |
| 1   | A     | 1816 | G    |
| 1   | A     | 1839 | G    |
| 1   | A     | 1899 | G    |
| 1   | A     | 1913 | A    |
| 1   | A     | 1929 | G    |
| 1   | A     | 1936 | A    |
| 1   | A     | 1937 | A    |
| 1   | A     | 1939 | U    |
| 1   | A     | 1941 | C    |
| 1   | A     | 1962 | C    |
| 1   | A     | 1996 | C    |
| 1   | A     | 2014 | A    |
| 1   | A     | 2031 | A    |
| 1   | A     | 2036 | C    |
| 1   | A     | 2062 | A    |
| 1   | A     | 2092 | U    |
| 1   | A     | 2111 | C    |
| 1   | A     | 2126 | A    |
| 1   | A     | 2145 | C    |
| 1   | A     | 2158 | A    |
| 1   | A     | 2172 | U    |
| 1   | A     | 2197 | U    |
| 1   | A     | 2211 | G    |
| 1   | A     | 2225 | A    |
| 1   | A     | 2249 | U    |
| 1   | A     | 2266 | A    |
| 1   | A     | 2275 | C    |
| 1   | A     | 2282 | G    |
| 1   | A     | 2296 | U    |
| 1   | A     | 2311 | A    |
| 1   | A     | 2384 | G    |
| 1   | A     | 2394 | C    |
| 1   | A     | 2422 | A    |
| 1   | A     | 2423 | U    |
| 1   | A     | 2426 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2427 | C    |
| 1   | A     | 2439 | A    |
| 1   | A     | 2447 | G    |
| 1   | A     | 2481 | G    |
| 1   | A     | 2490 | G    |
| 1   | A     | 2491 | U    |
| 1   | A     | 2502 | G    |
| 1   | A     | 2518 | A    |
| 1   | A     | 2573 | C    |
| 1   | A     | 2581 | G    |
| 1   | A     | 2602 | A    |
| 1   | A     | 2609 | U    |
| 1   | A     | 2611 | U    |
| 1   | A     | 2629 | A    |
| 1   | A     | 2689 | U    |
| 1   | A     | 2690 | C    |
| 1   | A     | 2750 | A    |
| 1   | A     | 2756 | U    |
| 1   | A     | 2781 | A    |
| 1   | A     | 2791 | C    |
| 1   | A     | 2835 | A    |
| 1   | A     | 2849 | U    |
| 1   | A     | 2867 | G    |
| 1   | A     | 2873 | A    |
| 1   | A     | 2879 | C    |
| 1   | A     | 2893 | G    |
| 2   | B     | 11   | C    |
| 2   | B     | 12   | C    |
| 2   | B     | 15   | A    |
| 2   | B     | 24   | G    |
| 2   | B     | 34   | U    |
| 2   | B     | 44   | G    |

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 1060 ligands modelled in this entry, 1060 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 2879/2894 (99%) | 0.13   | 122 (4%) 35 7 | 14, 64, 186, 278      | 0     |
| 2   | B     | 119/124 (95%)   | 0.36   | 12 (10%) 7 2  | 69, 100, 144, 222     | 0     |
| 3   | D     | 271/276 (98%)   | 0.50   | 22 (8%) 12 3  | 27, 51, 99, 162       | 0     |
| 4   | E     | 204/206 (99%)   | 0.65   | 32 (15%) 3 1  | 36, 69, 126, 159      | 0     |
| 5   | F     | 202/210 (96%)   | 0.21   | 11 (5%) 25 5  | 38, 71, 131, 153      | 0     |
| 6   | G     | 181/182 (99%)   | 0.62   | 27 (14%) 3 1  | 88, 121, 164, 179     | 0     |
| 7   | H     | 159/180 (88%)   | 0.88   | 31 (19%) 2 1  | 97, 139, 185, 202     | 0     |
| 8   | I     | 145/148 (97%)   | 0.42   | 12 (8%) 11 3  | 54, 106, 147, 198     | 0     |
| 9   | K     | 147/147 (100%)  | 1.86   | 59 (40%) 1 0  | 177, 205, 225, 240    | 0     |
| 10  | N     | 137/163 (84%)   | 0.71   | 20 (14%) 3 1  | 55, 87, 131, 153      | 0     |
| 11  | O     | 122/122 (100%)  | 0.09   | 1 (0%) 83 26  | 32, 61, 101, 118      | 0     |
| 12  | P     | 146/150 (97%)   | 0.84   | 27 (18%) 2 1  | 35, 89, 148, 203      | 0     |
| 13  | Q     | 134/141 (95%)   | 0.64   | 17 (12%) 4 1  | 44, 79, 136, 188      | 0     |
| 14  | R     | 117/118 (99%)   | 0.60   | 12 (10%) 7 2  | 31, 63, 114, 165      | 0     |
| 15  | S     | 98/112 (87%)    | 0.65   | 10 (10%) 7 2  | 66, 105, 140, 169     | 0     |
| 16  | T     | 137/146 (93%)   | 0.67   | 21 (15%) 3 1  | 41, 76, 136, 156      | 0     |
| 17  | U     | 117/118 (99%)   | 0.49   | 10 (8%) 11 3  | 45, 78, 124, 159      | 0     |
| 18  | V     | 101/101 (100%)  | 0.21   | 4 (3%) 36 7   | 63, 99, 144, 220      | 0     |
| 19  | W     | 112/113 (99%)   | 0.50   | 14 (12%) 5 1  | 39, 64, 111, 163      | 0     |
| 20  | X     | 92/96 (95%)     | 0.26   | 3 (3%) 44 8   | 50, 79, 122, 149      | 0     |
| 21  | Y     | 100/110 (90%)   | 1.66   | 32 (32%) 1 0  | 75, 112, 179, 200     | 0     |
| 22  | Z     | 187/206 (90%)   | 0.43   | 16 (8%) 11 3  | 83, 119, 156, 196     | 0     |
| 23  | 0     | 76/85 (89%)     | 0.38   | 5 (6%) 18 4   | 56, 78, 115, 150      | 0     |
| 24  | 1     | 88/98 (89%)     | 0.46   | 6 (6%) 17 4   | 31, 66, 119, 177      | 0     |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 25  | 2     | 62/72 (86%)     | 0.46   | 4 (6%) 18 4   | 55, 90, 131, 165      | 0     |
| 26  | 3     | 59/60 (98%)     | 0.81   | 11 (18%) 2 1  | 65, 85, 145, 166      | 0     |
| 27  | 4     | 30/97 (30%)     | -0.26  | 0 100 100     | 101, 135, 178, 183    | 0     |
| 28  | 5     | 52/60 (86%)     | 0.32   | 2 (3%) 38 7   | 49, 79, 147, 166      | 0     |
| 29  | 6     | 44/54 (81%)     | 1.75   | 14 (31%) 1 0  | 106, 136, 175, 224    | 0     |
| 30  | 7     | 48/49 (97%)     | 2.07   | 22 (45%) 1 0  | 38, 57, 119, 143      | 0     |
| 31  | 8     | 63/65 (96%)     | 0.59   | 5 (7%) 13 3   | 42, 59, 117, 156      | 0     |
| All | All   | 6429/6703 (95%) | 0.41   | 584 (9%) 10 2 | 14, 76, 182, 278      | 0     |

All (584) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 9   | K     | 83   | GLY  | 11.1 |
| 28  | 5     | 53   | ALA  | 10.4 |
| 1   | A     | 2132 | U    | 10.2 |
| 1   | A     | 2175 | C    | 9.3  |
| 7   | H     | 170  | ARG  | 9.2  |
| 9   | K     | 56   | GLU  | 9.0  |
| 21  | Y     | 91   | GLU  | 8.8  |
| 19  | W     | 1    | MET  | 8.7  |
| 21  | Y     | 79   | CYS  | 8.6  |
| 1   | A     | 2129 | C    | 8.6  |
| 13  | Q     | 91   | GLU  | 8.5  |
| 9   | K     | 97   | GLY  | 8.3  |
| 9   | K     | 84   | LEU  | 7.9  |
| 29  | 6     | 21   | TYR  | 7.8  |
| 22  | Z     | 72   | ARG  | 7.6  |
| 9   | K     | 82   | ALA  | 7.5  |
| 4   | E     | 204  | ALA  | 7.5  |
| 9   | K     | 78   | ILE  | 7.1  |
| 29  | 6     | 12   | GLU  | 7.1  |
| 30  | 7     | 47   | ARG  | 6.8  |
| 1   | A     | 615  | G    | 6.8  |
| 9   | K     | 9    | LYS  | 6.8  |
| 13  | Q     | 60   | ARG  | 6.7  |
| 15  | S     | 32   | LEU  | 6.5  |
| 6   | G     | 83   | ARG  | 6.5  |
| 21  | Y     | 4    | LYS  | 6.4  |
| 9   | K     | 8    | VAL  | 6.4  |
| 1   | A     | 10   | G    | 6.3  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 29  | 6     | 13     | CYS  | 6.3  |
| 1   | A     | 504    | U    | 6.3  |
| 1   | A     | 2122   | U    | 6.1  |
| 16  | T     | 112    | ARG  | 6.0  |
| 16  | T     | 115    | ARG  | 6.0  |
| 4   | E     | 203    | LYS  | 6.0  |
| 9   | K     | 128    | ALA  | 5.9  |
| 7   | H     | 64     | LEU  | 5.8  |
| 1   | A     | 1590   | U    | 5.8  |
| 7   | H     | 41     | MET  | 5.8  |
| 16  | T     | 113    | LYS  | 5.8  |
| 21  | Y     | 78     | ALA  | 5.8  |
| 15  | S     | 33     | LYS  | 5.7  |
| 7   | H     | 73     | ALA  | 5.7  |
| 1   | A     | 2152   | G    | 5.7  |
| 1   | A     | 1535   | U    | 5.6  |
| 29  | 6     | 20     | ASN  | 5.5  |
| 9   | K     | 12     | LEU  | 5.5  |
| 6   | G     | 84     | LYS  | 5.5  |
| 9   | K     | 7      | VAL  | 5.4  |
| 7   | H     | 169    | VAL  | 5.4  |
| 1   | A     | 2161   | C    | 5.4  |
| 21  | Y     | 28     | LYS  | 5.4  |
| 21  | Y     | 2      | ARG  | 5.4  |
| 10  | N     | 138    | ARG  | 5.4  |
| 3   | D     | 262    | ARG  | 5.3  |
| 7   | H     | 61     | HIS  | 5.3  |
| 13  | Q     | 19     | GLY  | 5.3  |
| 30  | 7     | 48     | LYS  | 5.2  |
| 21  | Y     | 5      | MET  | 5.2  |
| 1   | A     | 1536   | A    | 5.1  |
| 9   | K     | 6      | ALA  | 5.1  |
| 1   | A     | 2808   | U    | 5.1  |
| 2   | B     | 59     | A    | 5.0  |
| 1   | A     | 2128   | C    | 5.0  |
| 30  | 7     | 43     | THR  | 4.9  |
| 6   | G     | 26     | GLN  | 4.9  |
| 6   | G     | 28     | VAL  | 4.9  |
| 1   | A     | 271(D) | U    | 4.9  |
| 7   | H     | 60     | ARG  | 4.9  |
| 1   | A     | 2629   | A    | 4.9  |
| 21  | Y     | 66     | PRO  | 4.8  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 9   | K     | 80   | LYS  | 4.8  |
| 1   | A     | 1963 | U    | 4.8  |
| 29  | 6     | 22   | ALA  | 4.7  |
| 30  | 7     | 46   | VAL  | 4.7  |
| 16  | T     | 93   | ARG  | 4.7  |
| 22  | Z     | 73   | GLN  | 4.7  |
| 29  | 6     | 42   | TRP  | 4.7  |
| 14  | R     | 101  | ALA  | 4.7  |
| 1   | A     | 2112 | G    | 4.7  |
| 13  | Q     | 16   | ARG  | 4.7  |
| 30  | 7     | 42   | LEU  | 4.7  |
| 4   | E     | 133  | LYS  | 4.6  |
| 9   | K     | 19   | PRO  | 4.5  |
| 1   | A     | 1217 | C    | 4.5  |
| 19  | W     | 112  | GLY  | 4.5  |
| 15  | S     | 59   | LYS  | 4.5  |
| 21  | Y     | 64   | GLU  | 4.5  |
| 8   | I     | 109  | ILE  | 4.4  |
| 17  | U     | 89   | GLU  | 4.4  |
| 1   | A     | 2123 | G    | 4.4  |
| 3   | D     | 271  | ILE  | 4.3  |
| 14  | R     | 102  | GLU  | 4.3  |
| 17  | U     | 12   | ARG  | 4.3  |
| 1   | A     | 830  | G    | 4.3  |
| 19  | W     | 84   | ARG  | 4.3  |
| 3   | D     | 261  | LYS  | 4.3  |
| 9   | K     | 98   | ARG  | 4.3  |
| 6   | G     | 137  | GLU  | 4.3  |
| 14  | R     | 74   | LYS  | 4.3  |
| 21  | Y     | 97   | ARG  | 4.3  |
| 15  | S     | 31   | SER  | 4.3  |
| 9   | K     | 146  | ASP  | 4.3  |
| 10  | N     | 141  | LYS  | 4.2  |
| 9   | K     | 144  | VAL  | 4.2  |
| 7   | H     | 72   | ILE  | 4.2  |
| 1   | A     | 2153 | G    | 4.2  |
| 1   | A     | 806  | C    | 4.2  |
| 6   | G     | 74   | LYS  | 4.2  |
| 9   | K     | 75   | SER  | 4.2  |
| 12  | P     | 92   | GLU  | 4.2  |
| 1   | A     | 229  | A    | 4.2  |
| 6   | G     | 138  | GLN  | 4.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 16  | T     | 111  | ARG  | 4.1  |
| 9   | K     | 79   | ARG  | 4.1  |
| 4   | E     | 163  | GLU  | 4.1  |
| 30  | 7     | 29   | LYS  | 4.1  |
| 6   | G     | 32   | PRO  | 4.1  |
| 2   | B     | 29   | A    | 4.1  |
| 4   | E     | 132  | HIS  | 4.1  |
| 1   | A     | 2127 | G    | 4.1  |
| 6   | G     | 86   | MET  | 4.1  |
| 7   | H     | 65   | HIS  | 4.1  |
| 12  | P     | 76   | LYS  | 4.0  |
| 21  | Y     | 22   | GLY  | 4.0  |
| 1   | A     | 645  | C    | 4.0  |
| 2   | B     | 30   | C    | 4.0  |
| 1   | A     | 1657 | C    | 4.0  |
| 6   | G     | 30   | GLU  | 4.0  |
| 21  | Y     | 73   | ARG  | 4.0  |
| 7   | H     | 34   | GLU  | 4.0  |
| 31  | 8     | 35   | GLN  | 4.0  |
| 3   | D     | 272  | ALA  | 4.0  |
| 30  | 7     | 45   | ALA  | 4.0  |
| 11  | O     | 90   | GLN  | 3.9  |
| 6   | G     | 75   | LYS  | 3.9  |
| 10  | N     | 92   | GLN  | 3.9  |
| 9   | K     | 131  | ALA  | 3.9  |
| 8   | I     | 41   | GLU  | 3.9  |
| 22  | Z     | 74   | VAL  | 3.9  |
| 9   | K     | 145  | LYS  | 3.9  |
| 25  | 2     | 56   | GLN  | 3.9  |
| 26  | 3     | 35   | ARG  | 3.9  |
| 7   | H     | 68   | THR  | 3.9  |
| 17  | U     | 16   | LYS  | 3.9  |
| 29  | 6     | 14   | THR  | 3.8  |
| 29  | 6     | 9    | LEU  | 3.8  |
| 7   | H     | 43   | VAL  | 3.8  |
| 15  | S     | 60   | GLY  | 3.8  |
| 15  | S     | 34   | HIS  | 3.8  |
| 1   | A     | 9    | U    | 3.8  |
| 3   | D     | 270  | ILE  | 3.8  |
| 6   | G     | 146  | TYR  | 3.8  |
| 12  | P     | 110  | TYR  | 3.8  |
| 9   | K     | 25   | PRO  | 3.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 9   | K     | 118  | THR  | 3.8  |
| 1   | A     | 964  | C    | 3.8  |
| 16  | T     | 78   | LEU  | 3.8  |
| 13  | Q     | 112  | GLU  | 3.8  |
| 21  | Y     | 6    | HIS  | 3.8  |
| 8   | I     | 45   | LYS  | 3.7  |
| 30  | 7     | 32   | LYS  | 3.7  |
| 6   | G     | 33   | ARG  | 3.7  |
| 9   | K     | 96   | VAL  | 3.7  |
| 13  | Q     | 17   | LEU  | 3.7  |
| 9   | K     | 130  | SER  | 3.7  |
| 9   | K     | 10   | LEU  | 3.7  |
| 3   | D     | 5    | LYS  | 3.7  |
| 6   | G     | 2    | PRO  | 3.7  |
| 1   | A     | 1553 | A    | 3.7  |
| 12  | P     | 118  | GLY  | 3.7  |
| 22  | Z     | 186  | GLU  | 3.7  |
| 9   | K     | 18   | THR  | 3.7  |
| 30  | 7     | 33   | ARG  | 3.6  |
| 1   | A     | 1058 | G    | 3.6  |
| 1   | A     | 1033 | U    | 3.6  |
| 1   | A     | 2068 | U    | 3.6  |
| 1   | A     | 2249 | U    | 3.6  |
| 9   | K     | 27   | LEU  | 3.6  |
| 30  | 7     | 23   | ARG  | 3.6  |
| 6   | G     | 150  | ASP  | 3.6  |
| 10  | N     | 33   | GLU  | 3.6  |
| 1   | A     | 1052 | C    | 3.6  |
| 1   | A     | 1642 | G    | 3.6  |
| 1   | A     | 2190 | G    | 3.6  |
| 6   | G     | 29   | TRP  | 3.6  |
| 1   | A     | 2189 | U    | 3.6  |
| 16  | T     | 114  | LEU  | 3.5  |
| 1   | A     | 2121 | G    | 3.5  |
| 21  | Y     | 43   | ASN  | 3.5  |
| 1   | A     | 1741 | C    | 3.5  |
| 8   | I     | 108  | THR  | 3.5  |
| 1   | A     | 1078 | U    | 3.5  |
| 10  | N     | 142  | ARG  | 3.5  |
| 9   | K     | 99   | ILE  | 3.5  |
| 7   | H     | 38   | SER  | 3.5  |
| 26  | 3     | 19   | GLN  | 3.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 508  | G    | 3.5  |
| 7   | H     | 101  | ARG  | 3.5  |
| 24  | 1     | 52   | ARG  | 3.5  |
| 29  | 6     | 23   | THR  | 3.5  |
| 7   | H     | 97   | ARG  | 3.5  |
| 1   | A     | 1420 | U    | 3.5  |
| 15  | S     | 58   | LEU  | 3.5  |
| 2   | B     | 51   | G    | 3.4  |
| 9   | K     | 127  | ILE  | 3.4  |
| 14  | R     | 100  | LEU  | 3.4  |
| 21  | Y     | 3    | VAL  | 3.4  |
| 1   | A     | 2273 | A    | 3.4  |
| 2   | B     | 52   | A    | 3.4  |
| 9   | K     | 21   | PRO  | 3.4  |
| 13  | Q     | 14   | ARG  | 3.4  |
| 15  | S     | 57   | LYS  | 3.4  |
| 4   | E     | 126  | PRO  | 3.4  |
| 22  | Z     | 189  | ALA  | 3.4  |
| 9   | K     | 77   | LEU  | 3.4  |
| 12  | P     | 79   | ARG  | 3.4  |
| 10  | N     | 139  | LEU  | 3.4  |
| 12  | P     | 46   | LYS  | 3.4  |
| 6   | G     | 25   | TYR  | 3.3  |
| 1   | A     | 2250 | G    | 3.3  |
| 9   | K     | 81   | ALA  | 3.3  |
| 4   | E     | 3    | GLY  | 3.3  |
| 4   | E     | 7    | VAL  | 3.3  |
| 13  | Q     | 18   | LYS  | 3.3  |
| 4   | E     | 135  | HIS  | 3.3  |
| 8   | I     | 20   | ASP  | 3.3  |
| 31  | 8     | 40   | GLU  | 3.3  |
| 6   | G     | 17   | PRO  | 3.3  |
| 25  | 2     | 3    | LEU  | 3.3  |
| 1   | A     | 1116 | C    | 3.3  |
| 1   | A     | 6    | A    | 3.3  |
| 22  | Z     | 87   | ASP  | 3.3  |
| 9   | K     | 69   | THR  | 3.3  |
| 1   | A     | 1643 | G    | 3.3  |
| 7   | H     | 62   | LYS  | 3.3  |
| 9   | K     | 113  | PRO  | 3.3  |
| 6   | G     | 152  | LEU  | 3.3  |
| 21  | Y     | 63   | LYS  | 3.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | E     | 191  | PRO  | 3.2  |
| 8   | I     | 115  | ALA  | 3.2  |
| 16  | T     | 79   | HIS  | 3.2  |
| 1   | A     | 1641 | A    | 3.2  |
| 9   | K     | 95   | LYS  | 3.2  |
| 31  | 8     | 36   | LYS  | 3.2  |
| 9   | K     | 66   | THR  | 3.2  |
| 1   | A     | 1886 | C    | 3.2  |
| 1   | A     | 1059 | G    | 3.2  |
| 12  | P     | 75   | ILE  | 3.2  |
| 10  | N     | 136  | GLY  | 3.2  |
| 22  | Z     | 185  | GLU  | 3.2  |
| 26  | 3     | 26   | LEU  | 3.2  |
| 30  | 7     | 21   | ARG  | 3.2  |
| 26  | 3     | 27   | GLY  | 3.2  |
| 1   | A     | 1026 | U    | 3.2  |
| 1   | A     | 2895 | U    | 3.2  |
| 9   | K     | 132  | ARG  | 3.2  |
| 1   | A     | 2402 | C    | 3.2  |
| 19  | W     | 9    | TYR  | 3.1  |
| 1   | A     | 2573 | C    | 3.1  |
| 1   | A     | 2790 | A    | 3.1  |
| 26  | 3     | 30   | ARG  | 3.1  |
| 13  | Q     | 15   | GLY  | 3.1  |
| 30  | 7     | 14   | LYS  | 3.1  |
| 4   | E     | 1    | MET  | 3.1  |
| 22  | Z     | 28   | MET  | 3.1  |
| 1   | A     | 1574 | C    | 3.1  |
| 21  | Y     | 14   | LEU  | 3.1  |
| 12  | P     | 64   | LYS  | 3.1  |
| 31  | 8     | 34   | TRP  | 3.1  |
| 1   | A     | 1906 | G    | 3.1  |
| 3   | D     | 183  | ARG  | 3.1  |
| 19  | W     | 85   | VAL  | 3.1  |
| 1   | A     | 2136 | C    | 3.1  |
| 1   | A     | 125  | G    | 3.1  |
| 7   | H     | 55   | PRO  | 3.1  |
| 26  | 3     | 34   | GLU  | 3.1  |
| 1   | A     | 1077 | A    | 3.1  |
| 1   | A     | 2274 | A    | 3.1  |
| 1   | A     | 2191 | G    | 3.1  |
| 29  | 6     | 44   | ARG  | 3.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 2   | B     | 58     | A    | 3.0  |
| 12  | P     | 15     | ARG  | 3.0  |
| 17  | U     | 58     | ARG  | 3.0  |
| 7   | H     | 69     | ARG  | 3.0  |
| 22  | Z     | 3      | TYR  | 3.0  |
| 6   | G     | 115    | ARG  | 3.0  |
| 15  | S     | 97     | ARG  | 3.0  |
| 1   | A     | 888    | C    | 3.0  |
| 6   | G     | 54     | GLU  | 3.0  |
| 24  | 1     | 72     | GLU  | 3.0  |
| 4   | E     | 168    | MET  | 3.0  |
| 4   | E     | 193    | GLY  | 3.0  |
| 21  | Y     | 65     | ALA  | 3.0  |
| 9   | K     | 11     | GLN  | 2.9  |
| 23  | 0     | 18     | ALA  | 2.9  |
| 9   | K     | 57     | ILE  | 2.9  |
| 15  | S     | 84     | GLN  | 2.9  |
| 22  | Z     | 31     | ARG  | 2.9  |
| 21  | Y     | 29     | GLU  | 2.9  |
| 26  | 3     | 28     | LEU  | 2.9  |
| 1   | A     | 271(B) | C    | 2.9  |
| 24  | 1     | 10     | LYS  | 2.9  |
| 9   | K     | 68     | VAL  | 2.9  |
| 21  | Y     | 94     | LYS  | 2.9  |
| 1   | A     | 1060   | U    | 2.9  |
| 7   | H     | 54     | ARG  | 2.8  |
| 12  | P     | 14     | LYS  | 2.9  |
| 12  | P     | 63     | PRO  | 2.8  |
| 30  | 7     | 24     | THR  | 2.8  |
| 9   | K     | 136    | VAL  | 2.8  |
| 13  | Q     | 21     | THR  | 2.8  |
| 1   | A     | 2101   | G    | 2.8  |
| 1   | A     | 2807   | G    | 2.8  |
| 10  | N     | 31     | GLN  | 2.8  |
| 10  | N     | 137    | ARG  | 2.8  |
| 7   | H     | 37     | VAL  | 2.8  |
| 9   | K     | 28     | GLY  | 2.8  |
| 22  | Z     | 80     | ARG  | 2.8  |
| 30  | 7     | 18     | PHE  | 2.8  |
| 3   | D     | 4      | LYS  | 2.8  |
| 30  | 7     | 41     | ARG  | 2.8  |
| 21  | Y     | 40     | GLU  | 2.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 9   | K     | 74   | ALA  | 2.8  |
| 1   | A     | 1205 | U    | 2.8  |
| 7   | H     | 42   | ARG  | 2.8  |
| 19  | W     | 82   | LEU  | 2.8  |
| 7   | H     | 50   | VAL  | 2.8  |
| 3   | D     | 66   | ASP  | 2.7  |
| 4   | E     | 125  | GLY  | 2.7  |
| 16  | T     | 109  | GLU  | 2.7  |
| 17  | U     | 11   | ARG  | 2.7  |
| 10  | N     | 115  | ALA  | 2.7  |
| 19  | W     | 78   | GLU  | 2.7  |
| 1   | A     | 527  | C    | 2.7  |
| 3   | D     | 264  | LYS  | 2.7  |
| 16  | T     | 37   | GLY  | 2.7  |
| 12  | P     | 33   | ARG  | 2.7  |
| 12  | P     | 77   | ARG  | 2.7  |
| 30  | 7     | 31   | LEU  | 2.7  |
| 19  | W     | 98   | LYS  | 2.7  |
| 6   | G     | 162  | THR  | 2.7  |
| 12  | P     | 100  | LEU  | 2.7  |
| 30  | 7     | 44   | PRO  | 2.7  |
| 1   | A     | 684  | G    | 2.7  |
| 29  | 6     | 43   | CYS  | 2.7  |
| 3   | D     | 148  | GLU  | 2.7  |
| 1   | A     | 196  | A    | 2.7  |
| 14  | R     | 72   | ASP  | 2.7  |
| 1   | A     | 1921 | G    | 2.7  |
| 21  | Y     | 34   | LYS  | 2.7  |
| 1   | A     | 1218 | C    | 2.7  |
| 1   | A     | 126  | A    | 2.7  |
| 4   | E     | 192  | ASN  | 2.7  |
| 6   | G     | 18   | GLU  | 2.7  |
| 14  | R     | 42   | LYS  | 2.6  |
| 13  | Q     | 90   | VAL  | 2.6  |
| 9   | K     | 54   | PRO  | 2.6  |
| 9   | K     | 111  | LYS  | 2.6  |
| 19  | W     | 97   | LYS  | 2.6  |
| 20  | X     | 33   | LYS  | 2.6  |
| 1   | A     | 1885 | A    | 2.6  |
| 10  | N     | 132  | LYS  | 2.6  |
| 1   | A     | 1658 | C    | 2.6  |
| 26  | 3     | 8    | LEU  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 2160 | G    | 2.6  |
| 1   | A     | 1439 | A    | 2.6  |
| 7   | H     | 168  | PRO  | 2.6  |
| 14  | R     | 44   | LEU  | 2.6  |
| 5   | F     | 184  | TYR  | 2.6  |
| 7   | H     | 36   | PRO  | 2.6  |
| 26  | 3     | 9    | VAL  | 2.6  |
| 4   | E     | 27   | LEU  | 2.6  |
| 6   | G     | 27   | ASN  | 2.6  |
| 17  | U     | 9    | VAL  | 2.6  |
| 5   | F     | 44   | ARG  | 2.6  |
| 9   | K     | 116  | ASN  | 2.6  |
| 17  | U     | 17   | ILE  | 2.6  |
| 18  | V     | 70   | ILE  | 2.6  |
| 13  | Q     | 139  | GLU  | 2.6  |
| 5   | F     | 155  | LEU  | 2.6  |
| 9   | K     | 29   | GLN  | 2.6  |
| 13  | Q     | 22   | LYS  | 2.5  |
| 4   | E     | 105  | THR  | 2.5  |
| 21  | Y     | 89   | PHE  | 2.5  |
| 1   | A     | 2169 | A    | 2.5  |
| 6   | G     | 151  | ALA  | 2.5  |
| 21  | Y     | 21   | LYS  | 2.5  |
| 23  | 0     | 17   | GLN  | 2.5  |
| 29  | 6     | 19   | ARG  | 2.5  |
| 1   | A     | 12   | U    | 2.5  |
| 5   | F     | 156  | LEU  | 2.5  |
| 23  | 0     | 41   | ARG  | 2.5  |
| 2   | B     | 60   | C    | 2.5  |
| 8   | I     | 107  | ILE  | 2.5  |
| 3   | D     | 243  | GLY  | 2.5  |
| 5   | F     | 188  | ARG  | 2.5  |
| 16  | T     | 35   | LYS  | 2.5  |
| 19  | W     | 8    | ARG  | 2.5  |
| 18  | V     | 87   | HIS  | 2.5  |
| 1   | A     | 810  | U    | 2.5  |
| 3   | D     | 151  | LYS  | 2.5  |
| 4   | E     | 2    | LYS  | 2.5  |
| 9   | K     | 20   | ALA  | 2.5  |
| 29  | 6     | 50   | ARG  | 2.5  |
| 10  | N     | 110  | LEU  | 2.5  |
| 10  | N     | 25   | LYS  | 2.5  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 21  | Y     | 19   | LYS  | 2.5  |
| 1   | A     | 181  | A    | 2.5  |
| 4   | E     | 26   | ILE  | 2.5  |
| 10  | N     | 111  | GLU  | 2.5  |
| 1   | A     | 1962 | C    | 2.5  |
| 1   | A     | 2102 | U    | 2.5  |
| 3   | D     | 3    | VAL  | 2.5  |
| 7   | H     | 71   | LEU  | 2.4  |
| 12  | P     | 74   | GLU  | 2.4  |
| 9   | K     | 14   | ALA  | 2.4  |
| 16  | T     | 118  | ARG  | 2.4  |
| 9   | K     | 121  | GLU  | 2.4  |
| 20  | X     | 13   | LEU  | 2.4  |
| 16  | T     | 94   | ALA  | 2.4  |
| 12  | P     | 112  | LEU  | 2.4  |
| 1   | A     | 1554 | A    | 2.4  |
| 1   | A     | 2820 | A    | 2.4  |
| 1   | A     | 2110 | G    | 2.4  |
| 12  | P     | 65   | ARG  | 2.4  |
| 21  | Y     | 15   | VAL  | 2.4  |
| 21  | Y     | 67   | LEU  | 2.4  |
| 1   | A     | 1415 | U    | 2.4  |
| 21  | Y     | 72   | VAL  | 2.4  |
| 29  | 6     | 17   | LYS  | 2.4  |
| 1   | A     | 775  | G    | 2.4  |
| 1   | A     | 1754 | C    | 2.4  |
| 1   | A     | 2442 | C    | 2.4  |
| 2   | B     | 27   | C    | 2.4  |
| 9   | K     | 112  | MET  | 2.4  |
| 16  | T     | 116  | ALA  | 2.4  |
| 23  | 0     | 40   | GLN  | 2.4  |
| 1   | A     | 1183 | G    | 2.4  |
| 1   | A     | 1215 | G    | 2.4  |
| 3   | D     | 34   | VAL  | 2.4  |
| 3   | D     | 240  | ALA  | 2.4  |
| 22  | Z     | 162  | GLU  | 2.4  |
| 31  | 8     | 32   | LEU  | 2.4  |
| 10  | N     | 140  | PHE  | 2.4  |
| 16  | T     | 104  | ASN  | 2.4  |
| 25  | 2     | 9    | GLN  | 2.4  |
| 4   | E     | 8    | LYS  | 2.4  |
| 14  | R     | 3    | HIS  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | 7     | 17   | GLY  | 2.4  |
| 9   | K     | 5    | VAL  | 2.3  |
| 10  | N     | 34   | PRO  | 2.3  |
| 16  | T     | 21   | GLU  | 2.3  |
| 4   | E     | 128  | SER  | 2.3  |
| 8   | I     | 126  | TYR  | 2.3  |
| 10  | N     | 32   | VAL  | 2.3  |
| 12  | P     | 36   | LYS  | 2.3  |
| 13  | Q     | 41   | TRP  | 2.3  |
| 1   | A     | 1555 | G    | 2.3  |
| 5   | F     | 175  | THR  | 2.3  |
| 12  | P     | 45   | LEU  | 2.3  |
| 12  | P     | 78   | PRO  | 2.3  |
| 24  | 1     | 26   | ARG  | 2.3  |
| 1   | A     | 2275 | C    | 2.3  |
| 21  | Y     | 39   | VAL  | 2.3  |
| 13  | Q     | 7    | MET  | 2.3  |
| 7   | H     | 40   | GLU  | 2.3  |
| 26  | 3     | 29   | ARG  | 2.3  |
| 4   | E     | 115  | GLY  | 2.3  |
| 4   | E     | 127  | ASP  | 2.3  |
| 6   | G     | 31   | VAL  | 2.3  |
| 4   | E     | 124  | GLY  | 2.3  |
| 7   | H     | 58   | GLU  | 2.3  |
| 1   | A     | 2148 | G    | 2.3  |
| 25  | 2     | 8    | LYS  | 2.3  |
| 12  | P     | 98   | GLU  | 2.3  |
| 4   | E     | 202  | LYS  | 2.3  |
| 22  | Z     | 183  | LEU  | 2.3  |
| 9   | K     | 129  | GLY  | 2.3  |
| 5   | F     | 174  | VAL  | 2.3  |
| 21  | Y     | 30   | VAL  | 2.3  |
| 19  | W     | 83   | LYS  | 2.3  |
| 1   | A     | 774  | A    | 2.3  |
| 5   | F     | 96   | ASP  | 2.3  |
| 1   | A     | 2139 | C    | 2.3  |
| 2   | B     | 28   | C    | 2.3  |
| 12  | P     | 108  | LYS  | 2.3  |
| 18  | V     | 88   | ARG  | 2.3  |
| 30  | 7     | 27   | GLY  | 2.3  |
| 17  | U     | 5    | LYS  | 2.2  |
| 19  | W     | 41   | LYS  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | Q     | 111  | GLU  | 2.2  |
| 1   | A     | 1644 | C    | 2.2  |
| 1   | A     | 2628 | C    | 2.2  |
| 1   | A     | 2702 | U    | 2.2  |
| 7   | H     | 156  | ALA  | 2.2  |
| 23  | O     | 16   | SER  | 2.2  |
| 4   | E     | 116  | VAL  | 2.2  |
| 1   | A     | 402  | A    | 2.2  |
| 1   | A     | 2789 | C    | 2.2  |
| 4   | E     | 6    | GLY  | 2.2  |
| 1   | A     | 360  | G    | 2.2  |
| 4   | E     | 195  | LEU  | 2.2  |
| 18  | V     | 71   | LEU  | 2.2  |
| 4   | E     | 4    | ILE  | 2.2  |
| 12  | P     | 37   | GLY  | 2.2  |
| 10  | N     | 72   | GLY  | 2.2  |
| 14  | R     | 91   | GLN  | 2.2  |
| 1   | A     | 361  | G    | 2.2  |
| 5   | F     | 45   | ARG  | 2.2  |
| 19  | W     | 95   | ILE  | 2.2  |
| 20  | X     | 3    | THR  | 2.2  |
| 12  | P     | 41   | ARG  | 2.2  |
| 19  | W     | 99   | ARG  | 2.2  |
| 22  | Z     | 35   | ARG  | 2.2  |
| 22  | Z     | 36   | LYS  | 2.2  |
| 2   | B     | 26   | A    | 2.2  |
| 24  | 1     | 12   | PRO  | 2.2  |
| 1   | A     | 958  | U    | 2.2  |
| 8   | I     | 44   | LEU  | 2.2  |
| 24  | 1     | 30   | VAL  | 2.2  |
| 1   | A     | 899  | A    | 2.2  |
| 1   | A     | 2894 | G    | 2.2  |
| 3   | D     | 67   | PHE  | 2.2  |
| 1   | A     | 2211 | G    | 2.2  |
| 8   | I     | 19   | VAL  | 2.2  |
| 1   | A     | 54   | G    | 2.2  |
| 2   | B     | 56   | G    | 2.2  |
| 30  | 7     | 20   | ALA  | 2.2  |
| 30  | 7     | 36   | GLN  | 2.1  |
| 1   | A     | 701  | G    | 2.1  |
| 1   | A     | 1857 | G    | 2.1  |
| 1   | A     | 2170 | A    | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 14  | R     | 43   | GLU  | 2.1  |
| 13  | Q     | 83   | MET  | 2.1  |
| 16  | T     | 77   | PRO  | 2.1  |
| 3   | D     | 244  | ARG  | 2.1  |
| 6   | G     | 11   | TYR  | 2.1  |
| 12  | P     | 67   | MET  | 2.1  |
| 21  | Y     | 51   | VAL  | 2.1  |
| 3   | D     | 2    | ALA  | 2.1  |
| 14  | R     | 11   | ASN  | 2.1  |
| 3   | D     | 236  | GLY  | 2.1  |
| 8   | I     | 1    | MET  | 2.1  |
| 28  | 5     | 48   | GLU  | 2.1  |
| 8   | I     | 11   | ASN  | 2.1  |
| 7   | H     | 98   | LEU  | 2.1  |
| 1   | A     | 1534 | G    | 2.1  |
| 16  | T     | 106  | SER  | 2.1  |
| 5   | F     | 181  | LEU  | 2.1  |
| 3   | D     | 7    | LYS  | 2.1  |
| 9   | K     | 40   | ALA  | 2.1  |
| 17  | U     | 70   | ARG  | 2.1  |
| 26  | 3     | 38   | GLU  | 2.1  |
| 30  | 7     | 1    | MET  | 2.1  |
| 22  | Z     | 71   | VAL  | 2.1  |
| 12  | P     | 119  | GLU  | 2.1  |
| 1   | A     | 2421 | G    | 2.1  |
| 4   | E     | 194  | GLY  | 2.1  |
| 16  | T     | 96   | ARG  | 2.1  |
| 9   | K     | 22   | PRO  | 2.0  |
| 2   | B     | 103  | U    | 2.0  |
| 7   | H     | 26   | VAL  | 2.0  |
| 16  | T     | 95   | ARG  | 2.0  |
| 16  | T     | 105  | LEU  | 2.0  |
| 9   | K     | 70   | LYS  | 2.0  |
| 12  | P     | 104  | GLY  | 2.0  |
| 9   | K     | 114  | ASP  | 2.0  |
| 1   | A     | 1938 | A    | 2.0  |
| 4   | E     | 201  | THR  | 2.0  |
| 5   | F     | 46   | ARG  | 2.0  |
| 1   | A     | 2100 | G    | 2.0  |
| 1   | A     | 2539 | C    | 2.0  |
| 3   | D     | 252  | TRP  | 2.0  |
| 4   | E     | 151  | TYR  | 2.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 2693 | A    | 2.0  |
| 21  | Y     | 44   | ILE  | 2.0  |
| 1   | A     | 654  | U    | 2.0  |
| 9   | K     | 43   | ALA  | 2.0  |
| 17  | U     | 19   | LYS  | 2.0  |
| 7   | H     | 67   | LEU  | 2.0  |
| 10  | N     | 52   | LYS  | 2.0  |
| 1   | A     | 528  | A    | 2.0  |
| 10  | N     | 135  | LEU  | 2.0  |
| 14  | R     | 10   | LEU  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 32  | MG   | D     | 5005 | 1/1   | 0.55 | -    | 10,10,10,10                | 0     |
| 32  | MG   | H     | 5026 | 1/1   | 0.21 | -    | 54,54,54,54                | 0     |
| 32  | MG   | P     | 5050 | 1/1   | 0.46 | -    | 68,68,68,68                | 0     |
| 32  | MG   | A     | 5362 | 1/1   | 1.22 | -    | 74,74,74,74                | 0     |
| 32  | MG   | A     | 5527 | 1/1   | 0.30 | -    | 32,32,32,32                | 0     |
| 32  | MG   | A     | 6022 | 1/1   | 0.11 | -    | 53,53,53,53                | 0     |
| 32  | MG   | A     | 5530 | 1/1   | 0.38 | -    | 67,67,67,67                | 0     |
| 32  | MG   | D     | 5008 | 1/1   | 2.57 | -    | 55,55,55,55                | 0     |
| 32  | MG   | A     | 5382 | 1/1   | 0.18 | -    | 7,7,7,7                    | 0     |
| 32  | MG   | A     | 5297 | 1/1   | 0.10 | -    | 54,54,54,54                | 0     |
| 32  | MG   | A     | 5667 | 1/1   | 1.16 | -    | 74,74,74,74                | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5686 | 1/1   | 0.62 | -    | 64,64,64,64                 | 0     |
| 32  | MG   | A     | 5743 | 1/1   | 0.10 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | A     | 5399 | 1/1   | 0.70 | -    | 73,73,73,73                 | 0     |
| 32  | MG   | I     | 6059 | 1/1   | 0.12 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5998 | 1/1   | 0.54 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | A     | 5778 | 1/1   | 1.41 | -    | 59,59,59,59                 | 0     |
| 32  | MG   | A     | 5199 | 1/1   | 0.19 | -    | 35,35,35,35                 | 0     |
| 32  | MG   | A     | 5816 | 1/1   | 0.19 | -    | 37,37,37,37                 | 0     |
| 32  | MG   | A     | 5938 | 1/1   | 0.33 | -    | 29,29,29,29                 | 0     |
| 32  | MG   | A     | 5620 | 1/1   | 1.51 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5100 | 1/1   | 0.84 | -    | 103,103,103,103             | 0     |
| 32  | MG   | A     | 5262 | 1/1   | 0.46 | -    | 83,83,83,83                 | 0     |
| 32  | MG   | A     | 5794 | 1/1   | 0.25 | -    | 72,72,72,72                 | 0     |
| 32  | MG   | A     | 5349 | 1/1   | 0.57 | -    | 75,75,75,75                 | 0     |
| 32  | MG   | 1     | 5084 | 1/1   | 0.21 | -    | 87,87,87,87                 | 0     |
| 32  | MG   | A     | 5265 | 1/1   | 0.31 | -    | 40,40,40,40                 | 0     |
| 32  | MG   | A     | 5312 | 1/1   | 0.15 | -    | 32,32,32,32                 | 0     |
| 32  | MG   | A     | 6008 | 1/1   | 0.26 | -    | 27,27,27,27                 | 0     |
| 32  | MG   | A     | 5730 | 1/1   | 0.36 | -    | 33,33,33,33                 | 0     |
| 32  | MG   | B     | 6029 | 1/1   | 0.18 | -    | 84,84,84,84                 | 0     |
| 32  | MG   | A     | 5706 | 1/1   | 1.13 | -    | 32,32,32,32                 | 0     |
| 32  | MG   | A     | 5483 | 1/1   | 0.39 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5390 | 1/1   | 0.16 | -    | 31,31,31,31                 | 0     |
| 32  | MG   | B     | 6056 | 1/1   | 0.14 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | A     | 5506 | 1/1   | 0.20 | -    | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 5259 | 1/1   | 0.24 | -    | 77,77,77,77                 | 0     |
| 32  | MG   | Q     | 5053 | 1/1   | 0.53 | -    | 46,46,46,46                 | 0     |
| 32  | MG   | A     | 5048 | 1/1   | 0.27 | -    | 11,11,11,11                 | 0     |
| 32  | MG   | A     | 5878 | 1/1   | 0.43 | -    | 32,32,32,32                 | 0     |
| 32  | MG   | A     | 5895 | 1/1   | 0.34 | -    | 84,84,84,84                 | 0     |
| 32  | MG   | A     | 5332 | 1/1   | 0.27 | -    | 26,26,26,26                 | 0     |
| 32  | MG   | A     | 5443 | 1/1   | 0.18 | -    | 17,17,17,17                 | 0     |
| 32  | MG   | A     | 5479 | 1/1   | 0.32 | -    | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 5640 | 1/1   | 0.24 | -    | 36,36,36,36                 | 0     |
| 32  | MG   | A     | 5465 | 1/1   | 0.50 | -    | 85,85,85,85                 | 0     |
| 32  | MG   | A     | 6017 | 1/1   | 1.97 | -    | 59,59,59,59                 | 0     |
| 32  | MG   | A     | 5932 | 1/1   | 0.20 | -    | 28,28,28,28                 | 0     |
| 32  | MG   | A     | 6001 | 1/1   | 0.33 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | A     | 5200 | 1/1   | 0.48 | -    | 40,40,40,40                 | 0     |
| 32  | MG   | A     | 5277 | 1/1   | 0.24 | -    | 96,96,96,96                 | 0     |
| 32  | MG   | A     | 5852 | 1/1   | 0.44 | -    | 58,58,58,58                 | 0     |
| 32  | MG   | 4     | 5098 | 1/1   | 0.10 | -    | 31,31,31,31                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5839 | 1/1   | 0.20 | -    | 70,70,70,70                 | 0     |
| 32  | MG   | A     | 5751 | 1/1   | 0.20 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | A     | 5887 | 1/1   | 1.04 | -    | 97,97,97,97                 | 0     |
| 32  | MG   | F     | 5021 | 1/1   | 0.29 | -    | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 5285 | 1/1   | 0.17 | -    | 85,85,85,85                 | 0     |
| 32  | MG   | A     | 5148 | 1/1   | 0.16 | -    | 83,83,83,83                 | 0     |
| 32  | MG   | B     | 6044 | 1/1   | 0.25 | -    | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 5708 | 1/1   | 0.23 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 5850 | 1/1   | 0.76 | -    | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 5755 | 1/1   | 0.46 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 5423 | 1/1   | 0.09 | -    | 77,77,77,77                 | 0     |
| 32  | MG   | A     | 5930 | 1/1   | 0.12 | -    | 12,12,12,12                 | 0     |
| 32  | MG   | A     | 5670 | 1/1   | 0.15 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5948 | 1/1   | 0.55 | -    | 62,62,62,62                 | 0     |
| 32  | MG   | D     | 5004 | 1/1   | 0.43 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 5508 | 1/1   | 0.09 | -    | 8,8,8,8                     | 0     |
| 32  | MG   | A     | 5641 | 1/1   | 0.27 | -    | 27,27,27,27                 | 0     |
| 32  | MG   | A     | 5459 | 1/1   | 0.22 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5369 | 1/1   | 0.26 | -    | 29,29,29,29                 | 0     |
| 32  | MG   | A     | 5639 | 1/1   | 0.11 | -    | 16,16,16,16                 | 0     |
| 32  | MG   | A     | 5138 | 1/1   | 0.28 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5381 | 1/1   | 1.16 | -    | 36,36,36,36                 | 0     |
| 32  | MG   | A     | 5109 | 1/1   | 0.20 | -    | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 5830 | 1/1   | 0.48 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | A     | 5375 | 1/1   | 0.27 | -    | 17,17,17,17                 | 0     |
| 32  | MG   | A     | 5781 | 1/1   | 0.25 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 5692 | 1/1   | 0.52 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 5718 | 1/1   | 0.29 | -    | 103,103,103,103             | 0     |
| 32  | MG   | A     | 5741 | 1/1   | 0.14 | -    | 30,30,30,30                 | 0     |
| 32  | MG   | A     | 6012 | 1/1   | 0.11 | -    | 22,22,22,22                 | 0     |
| 32  | MG   | A     | 5810 | 1/1   | 0.10 | -    | 33,33,33,33                 | 0     |
| 32  | MG   | A     | 5589 | 1/1   | 0.29 | -    | 68,68,68,68                 | 0     |
| 32  | MG   | A     | 5979 | 1/1   | 0.29 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5942 | 1/1   | 0.25 | -    | 31,31,31,31                 | 0     |
| 32  | MG   | A     | 5131 | 1/1   | 1.43 | -    | 49,49,49,49                 | 0     |
| 32  | MG   | A     | 5974 | 1/1   | 0.17 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5485 | 1/1   | 0.37 | -    | 41,41,41,41                 | 0     |
| 32  | MG   | A     | 5378 | 1/1   | 1.02 | -    | 31,31,31,31                 | 0     |
| 32  | MG   | A     | 5319 | 1/1   | 0.18 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5298 | 1/1   | 0.33 | -    | 69,69,69,69                 | 0     |
| 32  | MG   | A     | 5572 | 1/1   | 1.05 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 5828 | 1/1   | 0.80 | -    | 53,53,53,53                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5689 | 1/1   | 0.16 | -    | 13,13,13,13                 | 0     |
| 32  | MG   | A     | 5359 | 1/1   | 0.65 | -    | 64,64,64,64                 | 0     |
| 32  | MG   | A     | 5550 | 1/1   | 0.25 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 5740 | 1/1   | 0.21 | -    | 26,26,26,26                 | 0     |
| 32  | MG   | A     | 5566 | 1/1   | 0.42 | -    | 73,73,73,73                 | 0     |
| 32  | MG   | A     | 5515 | 1/1   | 2.02 | -    | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 5993 | 1/1   | 0.32 | -    | 46,46,46,46                 | 0     |
| 32  | MG   | A     | 5286 | 1/1   | 0.46 | -    | 76,76,76,76                 | 0     |
| 32  | MG   | A     | 5926 | 1/1   | 0.27 | -    | 28,28,28,28                 | 0     |
| 32  | MG   | 1     | 5082 | 1/1   | 0.58 | -    | 37,37,37,37                 | 0     |
| 32  | MG   | A     | 5981 | 1/1   | 0.43 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5824 | 1/1   | 0.76 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5414 | 1/1   | 0.26 | -    | 66,66,66,66                 | 0     |
| 32  | MG   | A     | 5552 | 1/1   | 0.70 | -    | 75,75,75,75                 | 0     |
| 32  | MG   | A     | 5698 | 1/1   | 0.70 | -    | 12,12,12,12                 | 0     |
| 32  | MG   | A     | 5154 | 1/1   | 0.19 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5717 | 1/1   | 0.15 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5171 | 1/1   | 0.41 | -    | 71,71,71,71                 | 0     |
| 32  | MG   | A     | 5940 | 1/1   | 0.47 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5221 | 1/1   | 0.29 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | N     | 5040 | 1/1   | 0.40 | -    | 72,72,72,72                 | 0     |
| 32  | MG   | A     | 5422 | 1/1   | 0.34 | -    | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 5595 | 1/1   | 0.10 | -    | 41,41,41,41                 | 0     |
| 32  | MG   | A     | 5145 | 1/1   | 0.27 | -    | 80,80,80,80                 | 0     |
| 32  | MG   | A     | 5517 | 1/1   | 0.07 | -    | 20,20,20,20                 | 0     |
| 32  | MG   | A     | 5695 | 1/1   | 0.73 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 5504 | 1/1   | 0.34 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 6007 | 1/1   | 0.42 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5978 | 1/1   | 0.45 | -    | 76,76,76,76                 | 0     |
| 32  | MG   | A     | 5279 | 1/1   | 0.43 | -    | 26,26,26,26                 | 0     |
| 32  | MG   | A     | 5862 | 1/1   | 0.34 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5548 | 1/1   | 0.17 | -    | 24,24,24,24                 | 0     |
| 32  | MG   | A     | 5301 | 1/1   | 0.45 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 5933 | 1/1   | 0.13 | -    | 9,9,9,9                     | 0     |
| 32  | MG   | A     | 5642 | 1/1   | 1.58 | -    | 42,42,42,42                 | 0     |
| 32  | MG   | A     | 5409 | 1/1   | 0.37 | -    | 84,84,84,84                 | 0     |
| 32  | MG   | A     | 5995 | 1/1   | 0.41 | -    | 70,70,70,70                 | 0     |
| 32  | MG   | A     | 5368 | 1/1   | 0.22 | -    | 39,39,39,39                 | 0     |
| 32  | MG   | A     | 5873 | 1/1   | 0.54 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 5885 | 1/1   | 0.15 | -    | 18,18,18,18                 | 0     |
| 32  | MG   | B     | 5434 | 1/1   | 0.48 | -    | 59,59,59,59                 | 0     |
| 32  | MG   | A     | 5487 | 1/1   | 0.20 | -    | 42,42,42,42                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 32  | MG   | A     | 6010 | 1/1   | 0.34 | -    | 39,39,39,39                | 0     |
| 32  | MG   | A     | 5220 | 1/1   | 0.19 | -    | 40,40,40,40                | 0     |
| 32  | MG   | A     | 5913 | 1/1   | 0.22 | -    | 15,15,15,15                | 0     |
| 32  | MG   | A     | 5341 | 1/1   | 0.16 | -    | 80,80,80,80                | 0     |
| 32  | MG   | A     | 5407 | 1/1   | 0.23 | -    | 25,25,25,25                | 0     |
| 32  | MG   | A     | 5602 | 1/1   | 0.45 | -    | 61,61,61,61                | 0     |
| 32  | MG   | A     | 5288 | 1/1   | 0.59 | -    | 76,76,76,76                | 0     |
| 32  | MG   | A     | 5325 | 1/1   | 0.29 | -    | 28,28,28,28                | 0     |
| 32  | MG   | A     | 5195 | 1/1   | 0.18 | -    | 49,49,49,49                | 0     |
| 32  | MG   | A     | 5968 | 1/1   | 0.35 | -    | 50,50,50,50                | 0     |
| 32  | MG   | A     | 5472 | 1/1   | 0.12 | -    | 48,48,48,48                | 0     |
| 32  | MG   | A     | 6023 | 1/1   | 0.22 | -    | 56,56,56,56                | 0     |
| 32  | MG   | A     | 5842 | 1/1   | 0.62 | -    | 70,70,70,70                | 0     |
| 32  | MG   | A     | 5733 | 1/1   | 0.78 | -    | 61,61,61,61                | 0     |
| 32  | MG   | A     | 5217 | 1/1   | 1.31 | -    | 48,48,48,48                | 0     |
| 32  | MG   | A     | 5769 | 1/1   | 0.20 | -    | 19,19,19,19                | 0     |
| 32  | MG   | A     | 5973 | 1/1   | 0.59 | -    | 54,54,54,54                | 0     |
| 32  | MG   | A     | 5281 | 1/1   | 0.37 | -    | 83,83,83,83                | 0     |
| 32  | MG   | A     | 5554 | 1/1   | 0.21 | -    | 35,35,35,35                | 0     |
| 32  | MG   | A     | 5256 | 1/1   | 0.41 | -    | 52,52,52,52                | 0     |
| 32  | MG   | A     | 5159 | 1/1   | 0.30 | -    | 35,35,35,35                | 0     |
| 32  | MG   | A     | 5457 | 1/1   | 0.17 | -    | 24,24,24,24                | 0     |
| 32  | MG   | B     | 6053 | 1/1   | 0.62 | -    | 50,50,50,50                | 0     |
| 32  | MG   | A     | 5618 | 1/1   | 0.17 | -    | 49,49,49,49                | 0     |
| 32  | MG   | D     | 5003 | 1/1   | 0.41 | -    | 57,57,57,57                | 0     |
| 32  | MG   | A     | 5308 | 1/1   | 0.21 | -    | 13,13,13,13                | 0     |
| 32  | MG   | A     | 5723 | 1/1   | 2.23 | -    | 71,71,71,71                | 0     |
| 32  | MG   | A     | 5127 | 1/1   | 0.25 | -    | 97,97,97,97                | 0     |
| 32  | MG   | A     | 5236 | 1/1   | 0.21 | -    | 35,35,35,35                | 0     |
| 32  | MG   | A     | 5649 | 1/1   | 0.19 | -    | 29,29,29,29                | 0     |
| 32  | MG   | A     | 5394 | 1/1   | 0.09 | -    | 18,18,18,18                | 0     |
| 32  | MG   | A     | 5739 | 1/1   | 0.23 | -    | 68,68,68,68                | 0     |
| 32  | MG   | A     | 5207 | 1/1   | 0.50 | -    | 54,54,54,54                | 0     |
| 32  | MG   | A     | 5786 | 1/1   | 0.34 | -    | 80,80,80,80                | 0     |
| 32  | MG   | I     | 5032 | 1/1   | 2.74 | -    | 53,53,53,53                | 0     |
| 32  | MG   | A     | 5453 | 1/1   | 0.44 | -    | 68,68,68,68                | 0     |
| 32  | MG   | A     | 5683 | 1/1   | 0.28 | -    | 32,32,32,32                | 0     |
| 32  | MG   | A     | 5821 | 1/1   | 1.20 | -    | 29,29,29,29                | 0     |
| 32  | MG   | A     | 5546 | 1/1   | 0.39 | -    | 63,63,63,63                | 0     |
| 32  | MG   | A     | 5079 | 1/1   | 0.18 | -    | 30,30,30,30                | 0     |
| 32  | MG   | E     | 5012 | 1/1   | 0.13 | -    | 53,53,53,53                | 0     |
| 32  | MG   | A     | 5130 | 1/1   | 0.12 | -    | 58,58,58,58                | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5117 | 1/1   | 0.56 | -    | 36,36,36,36                 | 0     |
| 32  | MG   | A     | 5280 | 1/1   | 0.48 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 5299 | 1/1   | 0.42 | -    | 80,80,80,80                 | 0     |
| 32  | MG   | A     | 5989 | 1/1   | 0.47 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 6015 | 1/1   | 0.50 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5327 | 1/1   | 0.34 | -    | 69,69,69,69                 | 0     |
| 32  | MG   | O     | 5042 | 1/1   | 0.24 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 5242 | 1/1   | 0.10 | -    | 41,41,41,41                 | 0     |
| 32  | MG   | A     | 5108 | 1/1   | 0.32 | -    | 37,37,37,37                 | 0     |
| 32  | MG   | A     | 5638 | 1/1   | 0.30 | -    | 40,40,40,40                 | 0     |
| 32  | MG   | A     | 5282 | 1/1   | 0.10 | -    | 36,36,36,36                 | 0     |
| 32  | MG   | I     | 5033 | 1/1   | 0.54 | -    | 32,32,32,32                 | 0     |
| 32  | MG   | A     | 5737 | 1/1   | 0.30 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5643 | 1/1   | 0.78 | -    | 19,19,19,19                 | 0     |
| 32  | MG   | A     | 5356 | 1/1   | 0.12 | -    | 21,21,21,21                 | 0     |
| 32  | MG   | A     | 5190 | 1/1   | 0.74 | -    | 89,89,89,89                 | 0     |
| 32  | MG   | A     | 5615 | 1/1   | 0.23 | -    | 62,62,62,62                 | 0     |
| 32  | MG   | A     | 5668 | 1/1   | 0.24 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 5334 | 1/1   | 0.55 | -    | 39,39,39,39                 | 0     |
| 32  | MG   | 2     | 5087 | 1/1   | 0.48 | -    | 62,62,62,62                 | 0     |
| 32  | MG   | A     | 5337 | 1/1   | 0.48 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 5469 | 1/1   | 0.16 | -    | 32,32,32,32                 | 0     |
| 32  | MG   | W     | 5068 | 1/1   | 0.24 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | A     | 5402 | 1/1   | 0.36 | -    | 33,33,33,33                 | 0     |
| 32  | MG   | A     | 5267 | 1/1   | 0.40 | -    | 32,32,32,32                 | 0     |
| 32  | MG   | V     | 5066 | 1/1   | 0.20 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5996 | 1/1   | 1.40 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | A     | 5579 | 1/1   | 0.13 | -    | 26,26,26,26                 | 0     |
| 32  | MG   | A     | 5818 | 1/1   | 0.23 | -    | 34,34,34,34                 | 0     |
| 32  | MG   | A     | 6011 | 1/1   | 0.93 | -    | 40,40,40,40                 | 0     |
| 32  | MG   | A     | 5524 | 1/1   | 0.52 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5866 | 1/1   | 0.08 | -    | 28,28,28,28                 | 0     |
| 32  | MG   | A     | 5907 | 1/1   | 0.20 | -    | 37,37,37,37                 | 0     |
| 32  | MG   | A     | 5797 | 1/1   | 0.16 | -    | 72,72,72,72                 | 0     |
| 32  | MG   | A     | 5788 | 1/1   | 1.68 | -    | 73,73,73,73                 | 0     |
| 32  | MG   | A     | 5310 | 1/1   | 0.54 | -    | 39,39,39,39                 | 0     |
| 32  | MG   | A     | 5915 | 1/1   | 0.29 | -    | 28,28,28,28                 | 0     |
| 32  | MG   | A     | 5703 | 1/1   | 0.17 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | A     | 5522 | 1/1   | 0.20 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 5582 | 1/1   | 0.20 | -    | 75,75,75,75                 | 0     |
| 32  | MG   | A     | 5619 | 1/1   | 0.26 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | A     | 5861 | 1/1   | 0.26 | -    | 45,45,45,45                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5569 | 1/1   | 0.17 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 5934 | 1/1   | 0.37 | -    | 12,12,12,12                 | 0     |
| 32  | MG   | A     | 5395 | 1/1   | 0.34 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5181 | 1/1   | 0.68 | -    | 80,80,80,80                 | 0     |
| 32  | MG   | A     | 5146 | 1/1   | 0.35 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5405 | 1/1   | 0.25 | -    | 35,35,35,35                 | 0     |
| 32  | MG   | A     | 5543 | 1/1   | 0.10 | -    | 13,13,13,13                 | 0     |
| 32  | MG   | A     | 5732 | 1/1   | 0.48 | -    | 31,31,31,31                 | 0     |
| 32  | MG   | A     | 5452 | 1/1   | 0.26 | -    | 16,16,16,16                 | 0     |
| 32  | MG   | A     | 5482 | 1/1   | 0.29 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | A     | 5971 | 1/1   | 0.40 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5553 | 1/1   | 0.25 | -    | 69,69,69,69                 | 0     |
| 32  | MG   | A     | 5811 | 1/1   | 0.83 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5243 | 1/1   | 0.53 | -    | 46,46,46,46                 | 0     |
| 32  | MG   | A     | 5943 | 1/1   | 0.24 | -    | 16,16,16,16                 | 0     |
| 32  | MG   | A     | 5466 | 1/1   | 0.95 | -    | 76,76,76,76                 | 0     |
| 32  | MG   | A     | 5392 | 1/1   | 0.15 | -    | 12,12,12,12                 | 0     |
| 32  | MG   | A     | 5560 | 1/1   | 0.15 | -    | 22,22,22,22                 | 0     |
| 32  | MG   | A     | 5523 | 1/1   | 0.25 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5827 | 1/1   | 0.56 | -    | 86,86,86,86                 | 0     |
| 32  | MG   | 6     | 5092 | 1/1   | 0.21 | -    | 57,57,57,57                 | 0     |
| 32  | MG   | 1     | 5080 | 1/1   | 0.19 | -    | 31,31,31,31                 | 0     |
| 32  | MG   | A     | 5140 | 1/1   | 0.75 | -    | 78,78,78,78                 | 0     |
| 32  | MG   | A     | 6018 | 1/1   | 1.84 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | A     | 5379 | 1/1   | 0.38 | -    | 15,15,15,15                 | 0     |
| 32  | MG   | A     | 5518 | 1/1   | 0.24 | -    | 34,34,34,34                 | 0     |
| 32  | MG   | E     | 5017 | 1/1   | 0.15 | -    | 71,71,71,71                 | 0     |
| 32  | MG   | A     | 5946 | 1/1   | 0.91 | -    | 68,68,68,68                 | 0     |
| 32  | MG   | A     | 5338 | 1/1   | 0.65 | -    | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 5669 | 1/1   | 0.72 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 5701 | 1/1   | 0.25 | -    | 40,40,40,40                 | 0     |
| 32  | MG   | A     | 5584 | 1/1   | 0.18 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | A     | 5424 | 1/1   | 0.53 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5765 | 1/1   | 0.15 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5838 | 1/1   | 0.22 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5905 | 1/1   | 0.33 | -    | 40,40,40,40                 | 0     |
| 32  | MG   | A     | 5149 | 1/1   | 0.15 | -    | 76,76,76,76                 | 0     |
| 32  | MG   | A     | 5936 | 1/1   | 0.21 | -    | 20,20,20,20                 | 0     |
| 32  | MG   | A     | 5959 | 1/1   | 0.15 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5590 | 1/1   | 0.48 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 5684 | 1/1   | 0.46 | -    | 29,29,29,29                 | 0     |
| 32  | MG   | A     | 5611 | 1/1   | 0.33 | -    | 82,82,82,82                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 6014 | 1/1   | 0.15 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 5884 | 1/1   | 0.38 | -    | 32,32,32,32                 | 0     |
| 32  | MG   | A     | 5241 | 1/1   | 0.18 | -    | 41,41,41,41                 | 0     |
| 32  | MG   | K     | 5037 | 1/1   | 0.34 | -    | 72,72,72,72                 | 0     |
| 32  | MG   | A     | 5597 | 1/1   | 0.30 | -    | 92,92,92,92                 | 0     |
| 32  | MG   | A     | 5564 | 1/1   | 0.17 | -    | 10,10,10,10                 | 0     |
| 32  | MG   | A     | 5963 | 1/1   | 0.28 | -    | 85,85,85,85                 | 0     |
| 32  | MG   | A     | 5826 | 1/1   | 0.18 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | A     | 5872 | 1/1   | 0.21 | -    | 36,36,36,36                 | 0     |
| 32  | MG   | A     | 5831 | 1/1   | 0.43 | -    | 59,59,59,59                 | 0     |
| 32  | MG   | A     | 5446 | 1/1   | 0.20 | -    | 33,33,33,33                 | 0     |
| 32  | MG   | A     | 5404 | 1/1   | 0.06 | -    | 28,28,28,28                 | 0     |
| 32  | MG   | Z     | 5076 | 1/1   | 0.17 | -    | 81,81,81,81                 | 0     |
| 32  | MG   | A     | 5661 | 1/1   | 0.37 | -    | 40,40,40,40                 | 0     |
| 32  | MG   | T     | 5061 | 1/1   | 1.12 | -    | 81,81,81,81                 | 0     |
| 32  | MG   | A     | 5353 | 1/1   | 1.09 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5218 | 1/1   | 0.32 | -    | 32,32,32,32                 | 0     |
| 32  | MG   | A     | 5015 | 1/1   | 0.61 | -    | 27,27,27,27                 | 0     |
| 32  | MG   | A     | 5115 | 1/1   | 0.22 | -    | 39,39,39,39                 | 0     |
| 32  | MG   | A     | 5266 | 1/1   | 0.18 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | B     | 6054 | 1/1   | 1.30 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5585 | 1/1   | 0.17 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 6013 | 1/1   | 0.14 | -    | 26,26,26,26                 | 0     |
| 32  | MG   | A     | 5588 | 1/1   | 0.74 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5204 | 1/1   | 0.27 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | R     | 5057 | 1/1   | 0.42 | -    | 34,34,34,34                 | 0     |
| 32  | MG   | A     | 5766 | 1/1   | 0.35 | -    | 37,37,37,37                 | 0     |
| 32  | MG   | A     | 5232 | 1/1   | 0.26 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 5903 | 1/1   | 0.76 | -    | 32,32,32,32                 | 0     |
| 32  | MG   | A     | 5320 | 1/1   | 0.21 | -    | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 5748 | 1/1   | 0.75 | -    | 28,28,28,28                 | 0     |
| 32  | MG   | A     | 5805 | 1/1   | 0.30 | -    | 28,28,28,28                 | 0     |
| 32  | MG   | E     | 5011 | 1/1   | 0.14 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | Y     | 5072 | 1/1   | 0.69 | -    | 68,68,68,68                 | 0     |
| 32  | MG   | A     | 5206 | 1/1   | 0.21 | -    | 23,23,23,23                 | 0     |
| 32  | MG   | A     | 5756 | 1/1   | 0.38 | -    | 12,12,12,12                 | 0     |
| 32  | MG   | A     | 5623 | 1/1   | 0.13 | -    | 12,12,12,12                 | 0     |
| 32  | MG   | A     | 5501 | 1/1   | 1.11 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5287 | 1/1   | 0.67 | -    | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 5784 | 1/1   | 0.60 | -    | 59,59,59,59                 | 0     |
| 32  | MG   | A     | 5581 | 1/1   | 0.23 | -    | 32,32,32,32                 | 0     |
| 32  | MG   | A     | 5009 | 1/1   | 0.27 | -    | 36,36,36,36                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5955 | 1/1   | 0.35 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5644 | 1/1   | 0.28 | -    | 15,15,15,15                 | 0     |
| 32  | MG   | A     | 5444 | 1/1   | 0.49 | -    | 37,37,37,37                 | 0     |
| 32  | MG   | A     | 5997 | 1/1   | 0.16 | -    | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 5495 | 1/1   | 0.11 | -    | 11,11,11,11                 | 0     |
| 32  | MG   | W     | 5067 | 1/1   | 1.83 | -    | 80,80,80,80                 | 0     |
| 32  | MG   | A     | 5777 | 1/1   | 2.80 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5652 | 1/1   | 0.44 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5764 | 1/1   | 0.16 | -    | 33,33,33,33                 | 0     |
| 32  | MG   | A     | 5099 | 1/1   | 0.42 | -    | 75,75,75,75                 | 0     |
| 32  | MG   | A     | 5844 | 1/1   | 0.98 | -    | 64,64,64,64                 | 0     |
| 32  | MG   | A     | 5386 | 1/1   | 0.24 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 5316 | 1/1   | 0.16 | -    | 31,31,31,31                 | 0     |
| 32  | MG   | A     | 5804 | 1/1   | 0.18 | -    | 77,77,77,77                 | 0     |
| 32  | MG   | A     | 5728 | 1/1   | 0.31 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | Q     | 5055 | 1/1   | 0.25 | -    | 57,57,57,57                 | 0     |
| 32  | MG   | A     | 5984 | 1/1   | 0.23 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5658 | 1/1   | 0.73 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | V     | 5064 | 1/1   | 0.15 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 5745 | 1/1   | 0.19 | -    | 30,30,30,30                 | 0     |
| 32  | MG   | A     | 5910 | 1/1   | 0.11 | -    | 12,12,12,12                 | 0     |
| 32  | MG   | A     | 5167 | 1/1   | 0.16 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | 8     | 5093 | 1/1   | 0.17 | -    | 30,30,30,30                 | 0     |
| 32  | MG   | A     | 5796 | 1/1   | 0.45 | -    | 79,79,79,79                 | 0     |
| 32  | MG   | 5     | 5090 | 1/1   | 0.27 | -    | 49,49,49,49                 | 0     |
| 32  | MG   | A     | 5746 | 1/1   | 0.12 | -    | 5,5,5,5                     | 0     |
| 32  | MG   | A     | 5690 | 1/1   | 0.33 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | A     | 5833 | 1/1   | 0.21 | -    | 26,26,26,26                 | 0     |
| 32  | MG   | A     | 5336 | 1/1   | 0.33 | -    | 42,42,42,42                 | 0     |
| 32  | MG   | A     | 5304 | 1/1   | 0.39 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5364 | 1/1   | 0.26 | -    | 46,46,46,46                 | 0     |
| 32  | MG   | A     | 5937 | 1/1   | 0.42 | -    | 71,71,71,71                 | 0     |
| 32  | MG   | B     | 6030 | 1/1   | 0.67 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5498 | 1/1   | 0.26 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 5854 | 1/1   | 0.94 | -    | 76,76,76,76                 | 0     |
| 32  | MG   | A     | 5185 | 1/1   | 0.21 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5179 | 1/1   | 0.15 | -    | 37,37,37,37                 | 0     |
| 32  | MG   | A     | 5592 | 1/1   | 0.11 | -    | 21,21,21,21                 | 0     |
| 32  | MG   | A     | 5541 | 1/1   | 1.02 | -    | 73,73,73,73                 | 0     |
| 32  | MG   | A     | 5985 | 1/1   | 0.21 | -    | 80,80,80,80                 | 0     |
| 32  | MG   | A     | 5436 | 1/1   | 0.22 | -    | 42,42,42,42                 | 0     |
| 32  | MG   | A     | 5178 | 1/1   | 0.14 | -    | 43,43,43,43                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5813 | 1/1   | 0.23 | -    | 24,24,24,24                 | 0     |
| 32  | MG   | A     | 5374 | 1/1   | 0.59 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | A     | 5843 | 1/1   | 0.36 | -    | 71,71,71,71                 | 0     |
| 32  | MG   | A     | 5782 | 1/1   | 0.43 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5754 | 1/1   | 0.57 | -    | 36,36,36,36                 | 0     |
| 32  | MG   | A     | 5919 | 1/1   | 0.52 | -    | 34,34,34,34                 | 0     |
| 32  | MG   | B     | 6043 | 1/1   | 0.50 | -    | 84,84,84,84                 | 0     |
| 32  | MG   | A     | 5467 | 1/1   | 0.26 | -    | 39,39,39,39                 | 0     |
| 32  | MG   | A     | 5815 | 1/1   | 0.19 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | A     | 5819 | 1/1   | 0.52 | -    | 66,66,66,66                 | 0     |
| 32  | MG   | A     | 5376 | 1/1   | 0.71 | -    | 27,27,27,27                 | 0     |
| 32  | MG   | A     | 5863 | 1/1   | 0.74 | -    | 31,31,31,31                 | 0     |
| 32  | MG   | A     | 5271 | 1/1   | 0.27 | -    | 57,57,57,57                 | 0     |
| 32  | MG   | A     | 5897 | 1/1   | 0.13 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5917 | 1/1   | 0.25 | -    | 30,30,30,30                 | 0     |
| 32  | MG   | A     | 5726 | 1/1   | 0.19 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5606 | 1/1   | 0.14 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 5223 | 1/1   | 0.13 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 5219 | 1/1   | 0.21 | -    | 72,72,72,72                 | 0     |
| 32  | MG   | A     | 5537 | 1/1   | 1.38 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | B     | 6025 | 1/1   | 0.24 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | B     | 6039 | 1/1   | 0.13 | -    | 46,46,46,46                 | 0     |
| 32  | MG   | A     | 5847 | 1/1   | 0.67 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 5350 | 1/1   | 0.13 | -    | 14,14,14,14                 | 0     |
| 32  | MG   | A     | 5118 | 1/1   | 0.44 | -    | 74,74,74,74                 | 0     |
| 32  | MG   | A     | 5858 | 1/1   | 0.29 | -    | 29,29,29,29                 | 0     |
| 32  | MG   | A     | 5132 | 1/1   | 0.23 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | V     | 5065 | 1/1   | 0.61 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | A     | 5531 | 1/1   | 0.14 | -    | 18,18,18,18                 | 0     |
| 32  | MG   | A     | 5853 | 1/1   | 0.28 | -    | 49,49,49,49                 | 0     |
| 32  | MG   | A     | 5587 | 1/1   | 0.31 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | A     | 5429 | 1/1   | 0.27 | -    | 66,66,66,66                 | 0     |
| 32  | MG   | O     | 5043 | 1/1   | 2.03 | -    | 62,62,62,62                 | 0     |
| 32  | MG   | D     | 5007 | 1/1   | 0.41 | -    | 11,11,11,11                 | 0     |
| 32  | MG   | A     | 5888 | 1/1   | 0.82 | -    | 69,69,69,69                 | 0     |
| 32  | MG   | A     | 5571 | 1/1   | 0.63 | -    | 30,30,30,30                 | 0     |
| 32  | MG   | A     | 5525 | 1/1   | 0.37 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5461 | 1/1   | 0.18 | -    | 46,46,46,46                 | 0     |
| 32  | MG   | A     | 5645 | 1/1   | 0.09 | -    | 12,12,12,12                 | 0     |
| 32  | MG   | A     | 5210 | 1/1   | 0.20 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 6021 | 1/1   | 0.22 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5426 | 1/1   | 0.22 | -    | 47,47,47,47                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | 1     | 5085 | 1/1   | 0.09 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 5687 | 1/1   | 0.23 | -    | 12,12,12,12                 | 0     |
| 32  | MG   | A     | 5918 | 1/1   | 0.73 | -    | 71,71,71,71                 | 0     |
| 32  | MG   | A     | 5447 | 1/1   | 2.02 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5719 | 1/1   | 0.26 | -    | 89,89,89,89                 | 0     |
| 32  | MG   | A     | 5691 | 1/1   | 0.35 | -    | 73,73,73,73                 | 0     |
| 32  | MG   | A     | 5450 | 1/1   | 0.77 | -    | 70,70,70,70                 | 0     |
| 32  | MG   | A     | 5776 | 1/1   | 0.15 | -    | 5,5,5,5                     | 0     |
| 32  | MG   | A     | 5150 | 1/1   | 0.10 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | B     | 6058 | 1/1   | 0.20 | -    | 59,59,59,59                 | 0     |
| 32  | MG   | A     | 5290 | 1/1   | 0.92 | -    | 57,57,57,57                 | 0     |
| 32  | MG   | A     | 5648 | 1/1   | 1.39 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 5294 | 1/1   | 0.31 | -    | 35,35,35,35                 | 0     |
| 32  | MG   | A     | 5617 | 1/1   | 0.22 | -    | 77,77,77,77                 | 0     |
| 32  | MG   | A     | 5928 | 1/1   | 0.64 | -    | 46,46,46,46                 | 0     |
| 32  | MG   | A     | 5835 | 1/1   | 0.59 | -    | 57,57,57,57                 | 0     |
| 32  | MG   | A     | 5440 | 1/1   | 0.11 | -    | 46,46,46,46                 | 0     |
| 32  | MG   | A     | 5725 | 1/1   | 0.15 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5742 | 1/1   | 0.17 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5657 | 1/1   | 0.25 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 5410 | 1/1   | 0.51 | -    | 40,40,40,40                 | 0     |
| 32  | MG   | A     | 5492 | 1/1   | 0.11 | -    | 86,86,86,86                 | 0     |
| 32  | MG   | A     | 5110 | 1/1   | 0.46 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5393 | 1/1   | 0.16 | -    | 25,25,25,25                 | 0     |
| 32  | MG   | A     | 5180 | 1/1   | 0.83 | -    | 73,73,73,73                 | 0     |
| 32  | MG   | 8     | 5094 | 1/1   | 1.28 | -    | 57,57,57,57                 | 0     |
| 32  | MG   | 2     | 5088 | 1/1   | 0.12 | -    | 36,36,36,36                 | 0     |
| 32  | MG   | A     | 5951 | 1/1   | 0.47 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5229 | 1/1   | 0.56 | -    | 68,68,68,68                 | 0     |
| 32  | MG   | A     | 5194 | 1/1   | 0.28 | -    | 68,68,68,68                 | 0     |
| 32  | MG   | A     | 5906 | 1/1   | 0.17 | -    | 29,29,29,29                 | 0     |
| 32  | MG   | A     | 5484 | 1/1   | 0.84 | -    | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 5675 | 1/1   | 0.10 | -    | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 5883 | 1/1   | 0.45 | -    | 25,25,25,25                 | 0     |
| 32  | MG   | A     | 5625 | 1/1   | 0.12 | -    | 2,2,2,2                     | 0     |
| 32  | MG   | A     | 5947 | 1/1   | 0.30 | -    | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 5137 | 1/1   | 0.22 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5849 | 1/1   | 0.35 | -    | 71,71,71,71                 | 0     |
| 32  | MG   | A     | 5198 | 1/1   | 0.47 | -    | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 5274 | 1/1   | 0.38 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5677 | 1/1   | 0.84 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5700 | 1/1   | 0.29 | -    | 40,40,40,40                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5254 | 1/1   | 0.37 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5893 | 1/1   | 0.52 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | Q     | 5054 | 1/1   | 0.50 | -    | 80,80,80,80                 | 0     |
| 32  | MG   | A     | 5551 | 1/1   | 0.24 | -    | 18,18,18,18                 | 0     |
| 32  | MG   | F     | 5023 | 1/1   | 0.39 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | O     | 5046 | 1/1   | 0.23 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 5945 | 1/1   | 0.21 | -    | 36,36,36,36                 | 0     |
| 32  | MG   | A     | 5608 | 1/1   | 0.23 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 5408 | 1/1   | 0.20 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5832 | 1/1   | 0.15 | -    | 29,29,29,29                 | 0     |
| 32  | MG   | B     | 6035 | 1/1   | 0.32 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 5889 | 1/1   | 0.19 | -    | 36,36,36,36                 | 0     |
| 32  | MG   | A     | 5455 | 1/1   | 0.33 | -    | 40,40,40,40                 | 0     |
| 32  | MG   | A     | 5817 | 1/1   | 0.36 | -    | 28,28,28,28                 | 0     |
| 32  | MG   | A     | 5442 | 1/1   | 0.26 | -    | 22,22,22,22                 | 0     |
| 32  | MG   | A     | 5793 | 1/1   | 0.21 | -    | 69,69,69,69                 | 0     |
| 32  | MG   | A     | 5134 | 1/1   | 0.21 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5306 | 1/1   | 0.22 | -    | 25,25,25,25                 | 0     |
| 32  | MG   | A     | 5533 | 1/1   | 1.31 | -    | 70,70,70,70                 | 0     |
| 32  | MG   | I     | 5031 | 1/1   | 0.34 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 5715 | 1/1   | 0.92 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 5976 | 1/1   | 0.18 | -    | 27,27,27,27                 | 0     |
| 32  | MG   | A     | 5163 | 1/1   | 0.20 | -    | 29,29,29,29                 | 0     |
| 32  | MG   | A     | 5511 | 1/1   | 0.24 | -    | 19,19,19,19                 | 0     |
| 32  | MG   | A     | 5291 | 1/1   | 0.21 | -    | 39,39,39,39                 | 0     |
| 32  | MG   | A     | 5795 | 1/1   | 0.50 | -    | 94,94,94,94                 | 0     |
| 32  | MG   | Y     | 5073 | 1/1   | 0.27 | -    | 42,42,42,42                 | 0     |
| 32  | MG   | A     | 5246 | 1/1   | 0.21 | -    | 42,42,42,42                 | 0     |
| 32  | MG   | N     | 5039 | 1/1   | 0.39 | -    | 46,46,46,46                 | 0     |
| 32  | MG   | A     | 5471 | 1/1   | 0.18 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 5868 | 1/1   | 0.95 | -    | 72,72,72,72                 | 0     |
| 32  | MG   | A     | 5713 | 1/1   | 0.10 | -    | 39,39,39,39                 | 0     |
| 32  | MG   | A     | 5462 | 1/1   | 0.12 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 5143 | 1/1   | 0.26 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 5542 | 1/1   | 0.14 | -    | 24,24,24,24                 | 0     |
| 32  | MG   | I     | 5034 | 1/1   | 0.11 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 5058 | 1/1   | 0.65 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | A     | 5260 | 1/1   | 0.38 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5330 | 1/1   | 0.32 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | 1     | 5083 | 1/1   | 0.75 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | A     | 5237 | 1/1   | 0.32 | -    | 29,29,29,29                 | 0     |
| 32  | MG   | A     | 5612 | 1/1   | 0.54 | -    | 61,61,61,61                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5679 | 1/1   | 0.26 | -    | 18,18,18,18                 | 0     |
| 32  | MG   | A     | 5825 | 1/1   | 0.25 | -    | 34,34,34,34                 | 0     |
| 32  | MG   | A     | 5966 | 1/1   | 0.28 | -    | 37,37,37,37                 | 0     |
| 32  | MG   | A     | 5478 | 1/1   | 0.34 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 5406 | 1/1   | 0.17 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | B     | 6033 | 1/1   | 1.33 | -    | 81,81,81,81                 | 0     |
| 32  | MG   | A     | 5388 | 1/1   | 0.48 | -    | 9,9,9,9                     | 0     |
| 32  | MG   | A     | 5705 | 1/1   | 0.27 | -    | 9,9,9,9                     | 0     |
| 32  | MG   | A     | 5920 | 1/1   | 0.36 | -    | 59,59,59,59                 | 0     |
| 32  | MG   | A     | 5512 | 1/1   | 0.42 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 5562 | 1/1   | 0.56 | -    | 77,77,77,77                 | 0     |
| 32  | MG   | A     | 5488 | 1/1   | 0.24 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5663 | 1/1   | 0.11 | -    | 39,39,39,39                 | 0     |
| 32  | MG   | A     | 5174 | 1/1   | 0.50 | -    | 23,23,23,23                 | 0     |
| 32  | MG   | A     | 5969 | 1/1   | 0.18 | -    | 11,11,11,11                 | 0     |
| 32  | MG   | A     | 5846 | 1/1   | 0.27 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 5961 | 1/1   | 0.12 | -    | 62,62,62,62                 | 0     |
| 32  | MG   | A     | 5896 | 1/1   | 0.13 | -    | 30,30,30,30                 | 0     |
| 32  | MG   | A     | 5859 | 1/1   | 0.29 | -    | 28,28,28,28                 | 0     |
| 32  | MG   | A     | 5245 | 1/1   | 0.60 | -    | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 5845 | 1/1   | 0.56 | -    | 35,35,35,35                 | 0     |
| 32  | MG   | A     | 5384 | 1/1   | 0.18 | -    | 22,22,22,22                 | 0     |
| 32  | MG   | A     | 5707 | 1/1   | 0.18 | -    | 26,26,26,26                 | 0     |
| 32  | MG   | A     | 5437 | 1/1   | 1.01 | -    | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 5357 | 1/1   | 0.25 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | B     | 6045 | 1/1   | 0.28 | -    | 39,39,39,39                 | 0     |
| 32  | MG   | A     | 5880 | 1/1   | 0.73 | -    | 21,21,21,21                 | 0     |
| 32  | MG   | A     | 5272 | 1/1   | 0.25 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 5300 | 1/1   | 0.20 | -    | 29,29,29,29                 | 0     |
| 32  | MG   | A     | 5761 | 1/1   | 0.27 | -    | 24,24,24,24                 | 0     |
| 32  | MG   | A     | 5674 | 1/1   | 0.32 | -    | 69,69,69,69                 | 0     |
| 32  | MG   | G     | 5024 | 1/1   | 0.96 | -    | 64,64,64,64                 | 0     |
| 32  | MG   | A     | 5062 | 1/1   | 0.34 | -    | 59,59,59,59                 | 0     |
| 32  | MG   | A     | 5952 | 1/1   | 0.14 | -    | 17,17,17,17                 | 0     |
| 32  | MG   | E     | 5013 | 1/1   | 0.37 | -    | 79,79,79,79                 | 0     |
| 32  | MG   | A     | 5752 | 1/1   | 1.52 | -    | 16,16,16,16                 | 0     |
| 32  | MG   | A     | 5875 | 1/1   | 0.66 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5251 | 1/1   | 0.52 | -    | 91,91,91,91                 | 0     |
| 32  | MG   | A     | 5503 | 1/1   | 0.20 | -    | 64,64,64,64                 | 0     |
| 32  | MG   | A     | 5803 | 1/1   | 0.15 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 5268 | 1/1   | 0.32 | -    | 36,36,36,36                 | 0     |
| 32  | MG   | A     | 5324 | 1/1   | 0.48 | -    | 35,35,35,35                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5186 | 1/1   | 0.14 | -    | 27,27,27,27                 | 0     |
| 32  | MG   | A     | 5613 | 1/1   | 0.39 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 5135 | 1/1   | 0.32 | -    | 58,58,58,58                 | 0     |
| 32  | MG   | 2     | 5086 | 1/1   | 0.86 | -    | 76,76,76,76                 | 0     |
| 32  | MG   | A     | 5235 | 1/1   | 1.55 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5823 | 1/1   | 0.08 | -    | 25,25,25,25                 | 0     |
| 32  | MG   | A     | 5445 | 1/1   | 0.41 | -    | 59,59,59,59                 | 0     |
| 32  | MG   | A     | 5499 | 1/1   | 0.40 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 5387 | 1/1   | 0.11 | -    | 30,30,30,30                 | 0     |
| 32  | MG   | A     | 5575 | 1/1   | 0.69 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5490 | 1/1   | 0.08 | -    | 73,73,73,73                 | 0     |
| 32  | MG   | A     | 5603 | 1/1   | 0.21 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 5806 | 1/1   | 0.15 | -    | 70,70,70,70                 | 0     |
| 32  | MG   | A     | 5209 | 1/1   | 0.16 | -    | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 5870 | 1/1   | 0.28 | -    | 25,25,25,25                 | 0     |
| 32  | MG   | N     | 5041 | 1/1   | 0.24 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 5799 | 1/1   | 1.05 | -    | 83,83,83,83                 | 0     |
| 32  | MG   | A     | 5594 | 1/1   | 0.07 | -    | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 5211 | 1/1   | 0.56 | -    | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 5801 | 1/1   | 0.18 | -    | 88,88,88,88                 | 0     |
| 32  | MG   | A     | 5877 | 1/1   | 0.26 | -    | 36,36,36,36                 | 0     |
| 32  | MG   | A     | 5202 | 1/1   | 0.23 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5284 | 1/1   | 0.69 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | B     | 6041 | 1/1   | 0.41 | -    | 78,78,78,78                 | 0     |
| 32  | MG   | A     | 5335 | 1/1   | 0.77 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5113 | 1/1   | 0.39 | -    | 33,33,33,33                 | 0     |
| 32  | MG   | A     | 5365 | 1/1   | 0.19 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | Q     | 5051 | 1/1   | 0.28 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 5681 | 1/1   | 0.29 | -    | 24,24,24,24                 | 0     |
| 32  | MG   | A     | 5904 | 1/1   | 0.89 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5514 | 1/1   | 0.19 | -    | 21,21,21,21                 | 0     |
| 32  | MG   | B     | 6046 | 1/1   | 0.12 | -    | 27,27,27,27                 | 0     |
| 32  | MG   | A     | 5468 | 1/1   | 0.14 | -    | 73,73,73,73                 | 0     |
| 32  | MG   | A     | 5152 | 1/1   | 0.22 | -    | 57,57,57,57                 | 0     |
| 32  | MG   | A     | 5396 | 1/1   | 0.21 | -    | 34,34,34,34                 | 0     |
| 32  | MG   | N     | 5038 | 1/1   | 0.49 | -    | 70,70,70,70                 | 0     |
| 32  | MG   | A     | 5155 | 1/1   | 0.48 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | A     | 5449 | 1/1   | 0.14 | -    | 17,17,17,17                 | 0     |
| 32  | MG   | A     | 5712 | 1/1   | 0.17 | -    | 19,19,19,19                 | 0     |
| 32  | MG   | A     | 5168 | 1/1   | 0.13 | -    | 29,29,29,29                 | 0     |
| 32  | MG   | A     | 5593 | 1/1   | 0.55 | -    | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 5565 | 1/1   | 0.19 | -    | 31,31,31,31                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | B     | 6034 | 1/1   | 0.17 | -    | 82,82,82,82                 | 0     |
| 32  | MG   | A     | 5970 | 1/1   | 0.26 | -    | 7,7,7,7                     | 0     |
| 32  | MG   | A     | 5112 | 1/1   | 0.16 | -    | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 5438 | 1/1   | 0.35 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 5763 | 1/1   | 0.32 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | A     | 5775 | 1/1   | 0.49 | -    | 37,37,37,37                 | 0     |
| 32  | MG   | A     | 5164 | 1/1   | 0.28 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | A     | 5456 | 1/1   | 0.20 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 5721 | 1/1   | 0.21 | -    | 62,62,62,62                 | 0     |
| 32  | MG   | A     | 5257 | 1/1   | 0.51 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5432 | 1/1   | 0.17 | -    | 20,20,20,20                 | 0     |
| 32  | MG   | A     | 5172 | 1/1   | 0.58 | -    | 62,62,62,62                 | 0     |
| 32  | MG   | A     | 5986 | 1/1   | 0.16 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5660 | 1/1   | 0.63 | -    | 33,33,33,33                 | 0     |
| 32  | MG   | A     | 5351 | 1/1   | 0.13 | -    | 7,7,7,7                     | 0     |
| 32  | MG   | A     | 5736 | 1/1   | 0.69 | -    | 24,24,24,24                 | 0     |
| 32  | MG   | A     | 5634 | 1/1   | 0.34 | -    | 27,27,27,27                 | 0     |
| 32  | MG   | A     | 5075 | 1/1   | 0.23 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5757 | 1/1   | 0.89 | -    | 71,71,71,71                 | 0     |
| 32  | MG   | A     | 5779 | 1/1   | 0.22 | -    | 20,20,20,20                 | 0     |
| 32  | MG   | A     | 5532 | 1/1   | 0.67 | -    | 73,73,73,73                 | 0     |
| 32  | MG   | A     | 5977 | 1/1   | 0.56 | -    | 88,88,88,88                 | 0     |
| 32  | MG   | A     | 5258 | 1/1   | 0.36 | -    | 80,80,80,80                 | 0     |
| 32  | MG   | A     | 5463 | 1/1   | 0.28 | -    | 37,37,37,37                 | 0     |
| 32  | MG   | A     | 5249 | 1/1   | 0.43 | -    | 103,103,103,103             | 0     |
| 32  | MG   | A     | 5122 | 1/1   | 0.23 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | A     | 5165 | 1/1   | 0.21 | -    | 59,59,59,59                 | 0     |
| 32  | MG   | A     | 5253 | 1/1   | 0.24 | -    | 21,21,21,21                 | 0     |
| 32  | MG   | A     | 5419 | 1/1   | 0.22 | -    | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 5505 | 1/1   | 0.19 | -    | 23,23,23,23                 | 0     |
| 32  | MG   | A     | 5711 | 1/1   | 1.18 | -    | 66,66,66,66                 | 0     |
| 32  | MG   | A     | 5326 | 1/1   | 0.17 | -    | 20,20,20,20                 | 0     |
| 32  | MG   | A     | 5502 | 1/1   | 0.18 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | A     | 5656 | 1/1   | 0.25 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5856 | 1/1   | 0.57 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | O     | 5077 | 1/1   | 0.77 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5637 | 1/1   | 0.29 | -    | 23,23,23,23                 | 0     |
| 32  | MG   | A     | 5367 | 1/1   | 0.69 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5182 | 1/1   | 0.08 | -    | 76,76,76,76                 | 0     |
| 32  | MG   | S     | 5059 | 1/1   | 0.61 | -    | 46,46,46,46                 | 0     |
| 32  | MG   | A     | 5867 | 1/1   | 0.09 | -    | 30,30,30,30                 | 0     |
| 32  | MG   | A     | 5921 | 1/1   | 0.24 | -    | 22,22,22,22                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | D     | 5002 | 1/1   | 0.46 | -    | 82,82,82,82                 | 0     |
| 32  | MG   | A     | 5627 | 1/1   | 0.22 | -    | 62,62,62,62                 | 0     |
| 32  | MG   | A     | 5651 | 1/1   | 0.12 | -    | 31,31,31,31                 | 0     |
| 32  | MG   | A     | 5881 | 1/1   | 0.62 | -    | 27,27,27,27                 | 0     |
| 32  | MG   | A     | 5343 | 1/1   | 0.41 | -    | 79,79,79,79                 | 0     |
| 32  | MG   | A     | 5477 | 1/1   | 0.26 | -    | 79,79,79,79                 | 0     |
| 32  | MG   | B     | 6028 | 1/1   | 0.31 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | A     | 5372 | 1/1   | 0.43 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5604 | 1/1   | 0.21 | -    | 62,62,62,62                 | 0     |
| 32  | MG   | A     | 5967 | 1/1   | 0.41 | -    | 25,25,25,25                 | 0     |
| 32  | MG   | F     | 5018 | 1/1   | 0.22 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5773 | 1/1   | 0.99 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5837 | 1/1   | 0.16 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 5871 | 1/1   | 0.17 | -    | 42,42,42,42                 | 0     |
| 32  | MG   | A     | 5240 | 1/1   | 0.42 | -    | 49,49,49,49                 | 0     |
| 32  | MG   | B     | 6049 | 1/1   | 0.70 | -    | 72,72,72,72                 | 0     |
| 32  | MG   | A     | 5360 | 1/1   | 0.18 | -    | 57,57,57,57                 | 0     |
| 32  | MG   | A     | 5655 | 1/1   | 0.13 | -    | 57,57,57,57                 | 0     |
| 32  | MG   | A     | 5724 | 1/1   | 0.66 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 5659 | 1/1   | 0.58 | -    | 23,23,23,23                 | 0     |
| 32  | MG   | A     | 5476 | 1/1   | 0.13 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5311 | 1/1   | 0.26 | -    | 36,36,36,36                 | 0     |
| 32  | MG   | A     | 5925 | 1/1   | 0.17 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 5999 | 1/1   | 0.35 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | A     | 5567 | 1/1   | 0.09 | -    | 22,22,22,22                 | 0     |
| 32  | MG   | A     | 5269 | 1/1   | 0.13 | -    | 23,23,23,23                 | 0     |
| 32  | MG   | A     | 5563 | 1/1   | 0.28 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | E     | 5014 | 1/1   | 0.48 | -    | 22,22,22,22                 | 0     |
| 32  | MG   | 1     | 5081 | 1/1   | 0.09 | -    | 9,9,9,9                     | 0     |
| 32  | MG   | A     | 5114 | 1/1   | 0.66 | -    | 86,86,86,86                 | 0     |
| 32  | MG   | A     | 5191 | 1/1   | 0.54 | -    | 78,78,78,78                 | 0     |
| 32  | MG   | O     | 5047 | 1/1   | 0.18 | -    | 86,86,86,86                 | 0     |
| 32  | MG   | A     | 5425 | 1/1   | 0.38 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 5147 | 1/1   | 0.09 | -    | 74,74,74,74                 | 0     |
| 32  | MG   | A     | 5731 | 1/1   | 0.17 | -    | 37,37,37,37                 | 0     |
| 32  | MG   | P     | 5329 | 1/1   | 0.26 | -    | 24,24,24,24                 | 0     |
| 32  | MG   | A     | 5709 | 1/1   | 0.21 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 5792 | 1/1   | 0.33 | -    | 70,70,70,70                 | 0     |
| 32  | MG   | A     | 6005 | 1/1   | 0.27 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 5441 | 1/1   | 0.41 | -    | 31,31,31,31                 | 0     |
| 32  | MG   | A     | 5144 | 1/1   | 0.28 | -    | 66,66,66,66                 | 0     |
| 32  | MG   | A     | 5891 | 1/1   | 0.22 | -    | 63,63,63,63                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5354 | 1/1   | 0.34 | -    | 42,42,42,42                 | 0     |
| 32  | MG   | A     | 5931 | 1/1   | 0.41 | -    | 34,34,34,34                 | 0     |
| 32  | MG   | B     | 6037 | 1/1   | 0.17 | -    | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 5710 | 1/1   | 0.15 | -    | 12,12,12,12                 | 0     |
| 32  | MG   | U     | 5063 | 1/1   | 1.22 | -    | 83,83,83,83                 | 0     |
| 32  | MG   | A     | 5507 | 1/1   | 0.16 | -    | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 5263 | 1/1   | 0.34 | -    | 69,69,69,69                 | 0     |
| 32  | MG   | A     | 5820 | 1/1   | 0.29 | -    | 7,7,7,7                     | 0     |
| 32  | MG   | A     | 5166 | 1/1   | 0.61 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | A     | 5622 | 1/1   | 0.84 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5296 | 1/1   | 0.26 | -    | 86,86,86,86                 | 0     |
| 32  | MG   | A     | 5944 | 1/1   | 1.69 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5598 | 1/1   | 0.64 | -    | 59,59,59,59                 | 0     |
| 32  | MG   | A     | 5886 | 1/1   | 0.59 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5519 | 1/1   | 0.47 | -    | 86,86,86,86                 | 0     |
| 32  | MG   | A     | 5636 | 1/1   | 0.61 | -    | 72,72,72,72                 | 0     |
| 32  | MG   | A     | 5678 | 1/1   | 0.22 | -    | 35,35,35,35                 | 0     |
| 32  | MG   | A     | 5935 | 1/1   | 0.23 | -    | 8,8,8,8                     | 0     |
| 32  | MG   | A     | 5309 | 1/1   | 0.38 | -    | 33,33,33,33                 | 0     |
| 32  | MG   | A     | 5318 | 1/1   | 0.69 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5673 | 1/1   | 0.26 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5184 | 1/1   | 0.37 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5954 | 1/1   | 0.19 | -    | 25,25,25,25                 | 0     |
| 32  | MG   | A     | 5123 | 1/1   | 2.03 | -    | 88,88,88,88                 | 0     |
| 32  | MG   | A     | 5744 | 1/1   | 1.29 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | X     | 5070 | 1/1   | 0.21 | -    | 25,25,25,25                 | 0     |
| 32  | MG   | A     | 5400 | 1/1   | 0.50 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5521 | 1/1   | 0.18 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | A     | 5361 | 1/1   | 0.76 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5558 | 1/1   | 0.44 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5192 | 1/1   | 0.14 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5103 | 1/1   | 1.48 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 5568 | 1/1   | 0.26 | -    | 18,18,18,18                 | 0     |
| 32  | MG   | A     | 5295 | 1/1   | 0.20 | -    | 73,73,73,73                 | 0     |
| 32  | MG   | A     | 5734 | 1/1   | 0.93 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | A     | 5912 | 1/1   | 0.74 | -    | 40,40,40,40                 | 0     |
| 32  | MG   | A     | 5840 | 1/1   | 0.17 | -    | 64,64,64,64                 | 0     |
| 32  | MG   | A     | 5513 | 1/1   | 0.55 | -    | 59,59,59,59                 | 0     |
| 32  | MG   | A     | 5183 | 1/1   | 0.17 | -    | 40,40,40,40                 | 0     |
| 32  | MG   | A     | 5292 | 1/1   | 0.35 | -    | 34,34,34,34                 | 0     |
| 32  | MG   | A     | 5857 | 1/1   | 0.32 | -    | 49,49,49,49                 | 0     |
| 32  | MG   | A     | 5729 | 1/1   | 1.05 | -    | 36,36,36,36                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | H     | 5027 | 1/1   | 0.36 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 5346 | 1/1   | 0.15 | -    | 28,28,28,28                 | 0     |
| 32  | MG   | A     | 5451 | 1/1   | 0.31 | -    | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 5544 | 1/1   | 0.32 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5129 | 1/1   | 0.35 | -    | 74,74,74,74                 | 0     |
| 32  | MG   | A     | 5216 | 1/1   | 1.05 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5869 | 1/1   | 0.20 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | A     | 5980 | 1/1   | 0.30 | -    | 46,46,46,46                 | 0     |
| 32  | MG   | A     | 5785 | 1/1   | 0.13 | -    | 74,74,74,74                 | 0     |
| 32  | MG   | A     | 5535 | 1/1   | 0.30 | -    | 71,71,71,71                 | 0     |
| 32  | MG   | A     | 5339 | 1/1   | 0.47 | -    | 81,81,81,81                 | 0     |
| 32  | MG   | A     | 5960 | 1/1   | 0.43 | -    | 80,80,80,80                 | 0     |
| 32  | MG   | A     | 5621 | 1/1   | 0.30 | -    | 64,64,64,64                 | 0     |
| 32  | MG   | A     | 5352 | 1/1   | 1.08 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 6006 | 1/1   | 0.18 | -    | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 5420 | 1/1   | 0.11 | -    | 74,74,74,74                 | 0     |
| 32  | MG   | A     | 5234 | 1/1   | 0.16 | -    | 33,33,33,33                 | 0     |
| 32  | MG   | K     | 5036 | 1/1   | 0.27 | -    | 83,83,83,83                 | 0     |
| 32  | MG   | A     | 5412 | 1/1   | 0.32 | -    | 57,57,57,57                 | 0     |
| 32  | MG   | A     | 5894 | 1/1   | 0.22 | -    | 65,65,65,65                 | 0     |
| 32  | MG   | B     | 6050 | 1/1   | 0.16 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | B     | 6052 | 1/1   | 0.18 | -    | 33,33,33,33                 | 0     |
| 32  | MG   | A     | 5941 | 1/1   | 1.15 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 5899 | 1/1   | 0.16 | -    | 29,29,29,29                 | 0     |
| 32  | MG   | A     | 5671 | 1/1   | 0.23 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | A     | 5953 | 1/1   | 0.17 | -    | 35,35,35,35                 | 0     |
| 32  | MG   | A     | 5431 | 1/1   | 0.39 | -    | 70,70,70,70                 | 0     |
| 32  | MG   | A     | 5570 | 1/1   | 1.20 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5529 | 1/1   | 0.74 | -    | 117,117,117,117             | 0     |
| 32  | MG   | A     | 5366 | 1/1   | 0.41 | -    | 57,57,57,57                 | 0     |
| 32  | MG   | A     | 5808 | 1/1   | 0.34 | -    | 70,70,70,70                 | 0     |
| 32  | MG   | B     | 6038 | 1/1   | 0.16 | -    | 103,103,103,103             | 0     |
| 32  | MG   | A     | 5682 | 1/1   | 0.38 | -    | 29,29,29,29                 | 0     |
| 32  | MG   | A     | 5250 | 1/1   | 1.89 | -    | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 5489 | 1/1   | 0.17 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 5666 | 1/1   | 0.52 | -    | 62,62,62,62                 | 0     |
| 32  | MG   | A     | 5735 | 1/1   | 1.56 | -    | 42,42,42,42                 | 0     |
| 32  | MG   | S     | 5060 | 1/1   | 0.15 | -    | 42,42,42,42                 | 0     |
| 32  | MG   | A     | 5188 | 1/1   | 0.88 | -    | 57,57,57,57                 | 0     |
| 32  | MG   | A     | 5693 | 1/1   | 0.43 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5665 | 1/1   | 0.14 | -    | 34,34,34,34                 | 0     |
| 32  | MG   | A     | 5983 | 1/1   | 0.70 | -    | 42,42,42,42                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5591 | 1/1   | 0.18 | -    | 57,57,57,57                 | 0     |
| 32  | MG   | A     | 5509 | 1/1   | 0.18 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5908 | 1/1   | 0.22 | -    | 18,18,18,18                 | 0     |
| 32  | MG   | A     | 5227 | 1/1   | 0.35 | -    | 59,59,59,59                 | 0     |
| 32  | MG   | A     | 5892 | 1/1   | 0.97 | -    | 85,85,85,85                 | 0     |
| 32  | MG   | 6     | 5091 | 1/1   | 0.31 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5704 | 1/1   | 0.27 | -    | 8,8,8,8                     | 0     |
| 32  | MG   | A     | 5972 | 1/1   | 0.86 | -    | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 5212 | 1/1   | 1.64 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | B     | 6026 | 1/1   | 0.17 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | B     | 6024 | 1/1   | 0.23 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | H     | 5028 | 1/1   | 0.15 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 6016 | 1/1   | 0.61 | -    | 41,41,41,41                 | 0     |
| 32  | MG   | A     | 5370 | 1/1   | 0.22 | -    | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 5228 | 1/1   | 0.26 | -    | 33,33,33,33                 | 0     |
| 32  | MG   | A     | 5841 | 1/1   | 0.14 | -    | 72,72,72,72                 | 0     |
| 32  | MG   | A     | 5774 | 1/1   | 0.70 | -    | 30,30,30,30                 | 0     |
| 32  | MG   | A     | 5214 | 1/1   | 0.17 | -    | 46,46,46,46                 | 0     |
| 32  | MG   | A     | 5125 | 1/1   | 0.13 | -    | 41,41,41,41                 | 0     |
| 32  | MG   | A     | 5270 | 1/1   | 0.25 | -    | 20,20,20,20                 | 0     |
| 32  | MG   | A     | 5500 | 1/1   | 0.12 | -    | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 5631 | 1/1   | 0.12 | -    | 12,12,12,12                 | 0     |
| 32  | MG   | A     | 5238 | 1/1   | 0.48 | -    | 41,41,41,41                 | 0     |
| 32  | MG   | A     | 5231 | 1/1   | 0.52 | -    | 64,64,64,64                 | 0     |
| 32  | MG   | A     | 5758 | 1/1   | 0.21 | -    | 35,35,35,35                 | 0     |
| 32  | MG   | B     | 6047 | 1/1   | 0.34 | -    | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 5464 | 1/1   | 0.32 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 5720 | 1/1   | 0.25 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 5559 | 1/1   | 0.23 | -    | 21,21,21,21                 | 0     |
| 32  | MG   | A     | 5958 | 1/1   | 0.09 | -    | 71,71,71,71                 | 0     |
| 32  | MG   | A     | 5233 | 1/1   | 0.22 | -    | 22,22,22,22                 | 0     |
| 32  | MG   | A     | 5949 | 1/1   | 0.65 | -    | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 5371 | 1/1   | 0.36 | -    | 34,34,34,34                 | 0     |
| 32  | MG   | A     | 5812 | 1/1   | 0.30 | -    | 28,28,28,28                 | 0     |
| 32  | MG   | A     | 5317 | 1/1   | 0.90 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5215 | 1/1   | 0.16 | -    | 22,22,22,22                 | 0     |
| 32  | MG   | A     | 6000 | 1/1   | 0.60 | -    | 73,73,73,73                 | 0     |
| 32  | MG   | A     | 5293 | 1/1   | 0.67 | -    | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 6019 | 1/1   | 0.37 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5770 | 1/1   | 0.30 | -    | 12,12,12,12                 | 0     |
| 32  | MG   | A     | 5128 | 1/1   | 0.24 | -    | 98,98,98,98                 | 0     |
| 32  | MG   | A     | 5699 | 1/1   | 1.66 | -    | 52,52,52,52                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5851 | 1/1   | 0.44 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5255 | 1/1   | 0.22 | -    | 22,22,22,22                 | 0     |
| 32  | MG   | A     | 5994 | 1/1   | 0.85 | -    | 62,62,62,62                 | 0     |
| 32  | MG   | A     | 5814 | 1/1   | 1.56 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5417 | 1/1   | 0.09 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | D     | 5001 | 1/1   | 0.66 | -    | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 5616 | 1/1   | 0.14 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5340 | 1/1   | 0.21 | -    | 41,41,41,41                 | 0     |
| 32  | MG   | A     | 5650 | 1/1   | 0.20 | -    | 10,10,10,10                 | 0     |
| 32  | MG   | A     | 5385 | 1/1   | 0.70 | -    | 68,68,68,68                 | 0     |
| 32  | MG   | A     | 5380 | 1/1   | 0.33 | -    | 9,9,9,9                     | 0     |
| 32  | MG   | A     | 5790 | 1/1   | 1.48 | -    | 62,62,62,62                 | 0     |
| 32  | MG   | A     | 5239 | 1/1   | 0.18 | -    | 31,31,31,31                 | 0     |
| 32  | MG   | A     | 5142 | 1/1   | 0.97 | -    | 73,73,73,73                 | 0     |
| 32  | MG   | A     | 5787 | 1/1   | 0.07 | -    | 80,80,80,80                 | 0     |
| 32  | MG   | I     | 5030 | 1/1   | 1.19 | -    | 78,78,78,78                 | 0     |
| 32  | MG   | A     | 5276 | 1/1   | 0.19 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 5716 | 1/1   | 0.92 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 5497 | 1/1   | 0.15 | -    | 23,23,23,23                 | 0     |
| 32  | MG   | A     | 5555 | 1/1   | 0.27 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | A     | 5965 | 1/1   | 0.34 | -    | 78,78,78,78                 | 0     |
| 32  | MG   | A     | 5539 | 1/1   | 0.16 | -    | 31,31,31,31                 | 0     |
| 32  | MG   | A     | 5929 | 1/1   | 0.27 | -    | 40,40,40,40                 | 0     |
| 32  | MG   | A     | 5771 | 1/1   | 0.40 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | B     | 6057 | 1/1   | 0.12 | -    | 23,23,23,23                 | 0     |
| 32  | MG   | A     | 5111 | 1/1   | 0.76 | -    | 87,87,87,87                 | 0     |
| 32  | MG   | A     | 5303 | 1/1   | 0.24 | -    | 27,27,27,27                 | 0     |
| 32  | MG   | A     | 5836 | 1/1   | 0.15 | -    | 23,23,23,23                 | 0     |
| 32  | MG   | A     | 5573 | 1/1   | 0.45 | -    | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 5261 | 1/1   | 0.41 | -    | 80,80,80,80                 | 0     |
| 32  | MG   | A     | 5313 | 1/1   | 1.49 | -    | 27,27,27,27                 | 0     |
| 32  | MG   | A     | 5157 | 1/1   | 0.30 | -    | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 5628 | 1/1   | 0.31 | -    | 70,70,70,70                 | 0     |
| 32  | MG   | A     | 5153 | 1/1   | 0.62 | -    | 78,78,78,78                 | 0     |
| 32  | MG   | B     | 6055 | 1/1   | 0.22 | -    | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 5964 | 1/1   | 0.24 | -    | 62,62,62,62                 | 0     |
| 32  | MG   | A     | 5189 | 1/1   | 0.33 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5314 | 1/1   | 0.84 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 5333 | 1/1   | 0.42 | -    | 31,31,31,31                 | 0     |
| 32  | MG   | A     | 5510 | 1/1   | 0.42 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 5398 | 1/1   | 0.17 | -    | 17,17,17,17                 | 0     |
| 32  | MG   | A     | 5647 | 1/1   | 0.12 | -    | 7,7,7,7                     | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5923 | 1/1   | 0.22 | -    | 14,14,14,14                 | 0     |
| 32  | MG   | A     | 5654 | 1/1   | 0.18 | -    | 28,28,28,28                 | 0     |
| 32  | MG   | A     | 5428 | 1/1   | 0.23 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 5175 | 1/1   | 0.35 | -    | 24,24,24,24                 | 0     |
| 32  | MG   | A     | 5226 | 1/1   | 0.24 | -    | 27,27,27,27                 | 0     |
| 32  | MG   | A     | 5911 | 1/1   | 0.36 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | B     | 6040 | 1/1   | 0.44 | -    | 74,74,74,74                 | 0     |
| 32  | MG   | A     | 5780 | 1/1   | 0.42 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5538 | 1/1   | 1.67 | -    | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 5373 | 1/1   | 0.18 | -    | 15,15,15,15                 | 0     |
| 32  | MG   | A     | 5536 | 1/1   | 0.82 | -    | 42,42,42,42                 | 0     |
| 32  | MG   | A     | 5605 | 1/1   | 0.12 | -    | 28,28,28,28                 | 0     |
| 32  | MG   | A     | 5783 | 1/1   | 0.35 | -    | 49,49,49,49                 | 0     |
| 32  | MG   | A     | 5540 | 1/1   | 0.14 | -    | 21,21,21,21                 | 0     |
| 32  | MG   | A     | 5120 | 1/1   | 0.97 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | A     | 5962 | 1/1   | 0.49 | -    | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 5676 | 1/1   | 0.20 | -    | 71,71,71,71                 | 0     |
| 32  | MG   | A     | 5141 | 1/1   | 0.20 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5900 | 1/1   | 0.24 | -    | 74,74,74,74                 | 0     |
| 32  | MG   | A     | 5161 | 1/1   | 0.41 | -    | 57,57,57,57                 | 0     |
| 32  | MG   | B     | 6042 | 1/1   | 0.13 | -    | 41,41,41,41                 | 0     |
| 32  | MG   | A     | 5411 | 1/1   | 0.30 | -    | 40,40,40,40                 | 0     |
| 32  | MG   | A     | 5534 | 1/1   | 0.31 | -    | 46,46,46,46                 | 0     |
| 32  | MG   | A     | 5990 | 1/1   | 0.37 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5278 | 1/1   | 1.32 | -    | 77,77,77,77                 | 0     |
| 32  | MG   | A     | 5391 | 1/1   | 0.39 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5991 | 1/1   | 0.26 | -    | 25,25,25,25                 | 0     |
| 32  | MG   | A     | 5957 | 1/1   | 0.09 | -    | 36,36,36,36                 | 0     |
| 32  | MG   | A     | 5273 | 1/1   | 0.40 | -    | 8,8,8,8                     | 0     |
| 32  | MG   | K     | 5035 | 1/1   | 0.18 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5822 | 1/1   | 0.24 | -    | 23,23,23,23                 | 0     |
| 32  | MG   | A     | 5694 | 1/1   | 0.18 | -    | 30,30,30,30                 | 0     |
| 32  | MG   | A     | 5865 | 1/1   | 0.32 | -    | 31,31,31,31                 | 0     |
| 32  | MG   | A     | 5633 | 1/1   | 0.16 | -    | 30,30,30,30                 | 0     |
| 32  | MG   | A     | 5767 | 1/1   | 1.78 | -    | 57,57,57,57                 | 0     |
| 32  | MG   | A     | 5403 | 1/1   | 0.53 | -    | 22,22,22,22                 | 0     |
| 32  | MG   | A     | 5481 | 1/1   | 0.38 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5328 | 1/1   | 0.21 | -    | 40,40,40,40                 | 0     |
| 32  | MG   | A     | 5160 | 1/1   | 0.56 | -    | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 5496 | 1/1   | 0.98 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5415 | 1/1   | 0.14 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 5561 | 1/1   | 0.37 | -    | 46,46,46,46                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5289 | 1/1   | 0.29 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5355 | 1/1   | 0.17 | -    | 24,24,24,24                 | 0     |
| 32  | MG   | A     | 5576 | 1/1   | 0.37 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5696 | 1/1   | 1.18 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5071 | 1/1   | 1.97 | -    | 72,72,72,72                 | 0     |
| 32  | MG   | A     | 5225 | 1/1   | 0.26 | -    | 19,19,19,19                 | 0     |
| 32  | MG   | A     | 5473 | 1/1   | 0.15 | -    | 75,75,75,75                 | 0     |
| 32  | MG   | A     | 5302 | 1/1   | 0.31 | -    | 19,19,19,19                 | 0     |
| 32  | MG   | H     | 5029 | 1/1   | 0.59 | -    | 77,77,77,77                 | 0     |
| 32  | MG   | A     | 5470 | 1/1   | 1.19 | -    | 115,115,115,115             | 0     |
| 32  | MG   | A     | 5789 | 1/1   | 2.05 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5102 | 1/1   | 0.31 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5156 | 1/1   | 0.22 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | B     | 6048 | 1/1   | 0.50 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | A     | 5975 | 1/1   | 0.42 | -    | 103,103,103,103             | 0     |
| 32  | MG   | A     | 5344 | 1/1   | 0.14 | -    | 72,72,72,72                 | 0     |
| 32  | MG   | A     | 5664 | 1/1   | 0.16 | -    | 58,58,58,58                 | 0     |
| 32  | MG   | 8     | 5095 | 1/1   | 0.65 | -    | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 5556 | 1/1   | 0.26 | -    | 75,75,75,75                 | 0     |
| 32  | MG   | A     | 5829 | 1/1   | 0.26 | -    | 68,68,68,68                 | 0     |
| 32  | MG   | A     | 5105 | 1/1   | 0.17 | -    | 40,40,40,40                 | 0     |
| 32  | MG   | A     | 5162 | 1/1   | 0.18 | -    | 26,26,26,26                 | 0     |
| 32  | MG   | A     | 5601 | 1/1   | 0.12 | -    | 34,34,34,34                 | 0     |
| 32  | MG   | A     | 5909 | 1/1   | 0.23 | -    | 13,13,13,13                 | 0     |
| 32  | MG   | B     | 6051 | 1/1   | 0.52 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5264 | 1/1   | 0.48 | -    | 66,66,66,66                 | 0     |
| 32  | MG   | A     | 5922 | 1/1   | 0.16 | -    | 34,34,34,34                 | 0     |
| 32  | MG   | A     | 6009 | 1/1   | 0.18 | -    | 26,26,26,26                 | 0     |
| 32  | MG   | A     | 5607 | 1/1   | 0.13 | -    | 68,68,68,68                 | 0     |
| 32  | MG   | A     | 5208 | 1/1   | 0.31 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | O     | 5045 | 1/1   | 3.12 | -    | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 5176 | 1/1   | 0.79 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5807 | 1/1   | 0.17 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5126 | 1/1   | 0.20 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5363 | 1/1   | 0.18 | -    | 21,21,21,21                 | 0     |
| 32  | MG   | A     | 5448 | 1/1   | 0.24 | -    | 31,31,31,31                 | 0     |
| 32  | MG   | A     | 5458 | 1/1   | 0.46 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 5244 | 1/1   | 0.92 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 6060 | 1/1   | 0.43 | -    | 57,57,57,57                 | 0     |
| 32  | MG   | A     | 5101 | 1/1   | 0.31 | -    | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 5193 | 1/1   | 0.72 | -    | 30,30,30,30                 | 0     |
| 32  | MG   | A     | 5834 | 1/1   | 0.64 | -    | 50,50,50,50                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5653 | 1/1   | 0.38 | -    | 75,75,75,75                 | 0     |
| 32  | MG   | A     | 5170 | 1/1   | 0.21 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | 5     | 5089 | 1/1   | 0.30 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5528 | 1/1   | 0.35 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5809 | 1/1   | 0.34 | -    | 77,77,77,77                 | 0     |
| 32  | MG   | A     | 5914 | 1/1   | 2.29 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5624 | 1/1   | 0.26 | -    | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 5583 | 1/1   | 0.14 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | A     | 5252 | 1/1   | 0.52 | -    | 35,35,35,35                 | 0     |
| 32  | MG   | G     | 5025 | 1/1   | 1.03 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5454 | 1/1   | 1.27 | -    | 42,42,42,42                 | 0     |
| 32  | MG   | Y     | 5074 | 1/1   | 2.26 | -    | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 5646 | 1/1   | 0.17 | -    | 7,7,7,7                     | 0     |
| 32  | MG   | A     | 5389 | 1/1   | 1.09 | -    | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 5205 | 1/1   | 0.32 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5629 | 1/1   | 0.14 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | A     | 5610 | 1/1   | 0.17 | -    | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 5685 | 1/1   | 0.88 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5224 | 1/1   | 0.53 | -    | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 5203 | 1/1   | 0.29 | -    | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 5749 | 1/1   | 1.92 | -    | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 5800 | 1/1   | 0.23 | -    | 68,68,68,68                 | 0     |
| 32  | MG   | A     | 5275 | 1/1   | 0.10 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5901 | 1/1   | 1.00 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | A     | 5987 | 1/1   | 0.13 | -    | 69,69,69,69                 | 0     |
| 32  | MG   | B     | 6031 | 1/1   | 0.23 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5430 | 1/1   | 0.62 | -    | 73,73,73,73                 | 0     |
| 32  | MG   | A     | 5626 | 1/1   | 0.38 | -    | 61,61,61,61                 | 0     |
| 32  | MG   | Q     | 5052 | 1/1   | 0.72 | -    | 18,18,18,18                 | 0     |
| 32  | MG   | A     | 5213 | 1/1   | 0.29 | -    | 26,26,26,26                 | 0     |
| 32  | MG   | A     | 5753 | 1/1   | 0.29 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 5860 | 1/1   | 0.88 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5383 | 1/1   | 0.19 | -    | 4,4,4,4                     | 0     |
| 32  | MG   | A     | 5526 | 1/1   | 0.47 | -    | 68,68,68,68                 | 0     |
| 32  | MG   | A     | 5680 | 1/1   | 0.24 | -    | 40,40,40,40                 | 0     |
| 32  | MG   | A     | 5124 | 1/1   | 2.57 | -    | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 5898 | 1/1   | 0.21 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5802 | 1/1   | 0.15 | -    | 42,42,42,42                 | 0     |
| 32  | MG   | A     | 5397 | 1/1   | 0.19 | -    | 8,8,8,8                     | 0     |
| 32  | MG   | A     | 5714 | 1/1   | 0.60 | -    | 42,42,42,42                 | 0     |
| 32  | MG   | A     | 5187 | 1/1   | 0.17 | -    | 29,29,29,29                 | 0     |
| 32  | MG   | A     | 5119 | 1/1   | 0.22 | -    | 30,30,30,30                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5697 | 1/1   | 1.58 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 5630 | 1/1   | 0.58 | -    | 30,30,30,30                 | 0     |
| 32  | MG   | A     | 5342 | 1/1   | 0.25 | -    | 71,71,71,71                 | 0     |
| 32  | MG   | A     | 5722 | 1/1   | 0.09 | -    | 22,22,22,22                 | 0     |
| 32  | MG   | A     | 5480 | 1/1   | 1.56 | -    | 75,75,75,75                 | 0     |
| 32  | MG   | A     | 5688 | 1/1   | 0.17 | -    | 62,62,62,62                 | 0     |
| 32  | MG   | A     | 5578 | 1/1   | 0.17 | -    | 36,36,36,36                 | 0     |
| 32  | MG   | A     | 5882 | 1/1   | 0.41 | -    | 33,33,33,33                 | 0     |
| 32  | MG   | F     | 5019 | 1/1   | 0.60 | -    | 59,59,59,59                 | 0     |
| 32  | MG   | A     | 5107 | 1/1   | 0.55 | -    | 73,73,73,73                 | 0     |
| 32  | MG   | A     | 5358 | 1/1   | 0.39 | -    | 31,31,31,31                 | 0     |
| 32  | MG   | A     | 5474 | 1/1   | 0.26 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | E     | 5010 | 1/1   | 0.14 | -    | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 5760 | 1/1   | 0.22 | -    | 23,23,23,23                 | 0     |
| 32  | MG   | A     | 5798 | 1/1   | 0.15 | -    | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 5759 | 1/1   | 0.31 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 5345 | 1/1   | 0.22 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5305 | 1/1   | 0.25 | -    | 12,12,12,12                 | 0     |
| 32  | MG   | A     | 5772 | 1/1   | 0.41 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | A     | 5702 | 1/1   | 0.43 | -    | 39,39,39,39                 | 0     |
| 32  | MG   | A     | 5323 | 1/1   | 0.17 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5377 | 1/1   | 1.20 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | S     | 6036 | 1/1   | 0.23 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5116 | 1/1   | 0.29 | -    | 59,59,59,59                 | 0     |
| 32  | MG   | A     | 5049 | 1/1   | 0.63 | -    | 20,20,20,20                 | 0     |
| 32  | MG   | A     | 5196 | 1/1   | 0.27 | -    | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 5307 | 1/1   | 0.20 | -    | 17,17,17,17                 | 0     |
| 32  | MG   | A     | 5586 | 1/1   | 0.17 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5321 | 1/1   | 0.34 | -    | 70,70,70,70                 | 0     |
| 32  | MG   | A     | 5577 | 1/1   | 0.26 | -    | 71,71,71,71                 | 0     |
| 32  | MG   | A     | 6003 | 1/1   | 0.86 | -    | 66,66,66,66                 | 0     |
| 32  | MG   | A     | 5879 | 1/1   | 0.73 | -    | 85,85,85,85                 | 0     |
| 32  | MG   | A     | 5902 | 1/1   | 0.47 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5435 | 1/1   | 0.63 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5283 | 1/1   | 0.27 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5549 | 1/1   | 0.23 | -    | 11,11,11,11                 | 0     |
| 32  | MG   | A     | 5791 | 1/1   | 0.22 | -    | 77,77,77,77                 | 0     |
| 32  | MG   | A     | 5491 | 1/1   | 0.12 | -    | 101,101,101,101             | 0     |
| 32  | MG   | A     | 5982 | 1/1   | 0.49 | -    | 68,68,68,68                 | 0     |
| 32  | MG   | A     | 5557 | 1/1   | 0.71 | -    | 59,59,59,59                 | 0     |
| 32  | MG   | A     | 5006 | 1/1   | 0.47 | -    | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 5874 | 1/1   | 0.20 | -    | 32,32,32,32                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5927 | 1/1   | 0.36 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | A     | 5727 | 1/1   | 0.35 | -    | 27,27,27,27                 | 0     |
| 32  | MG   | B     | 6032 | 1/1   | 0.22 | -    | 72,72,72,72                 | 0     |
| 32  | MG   | A     | 5848 | 1/1   | 0.21 | -    | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 5416 | 1/1   | 0.17 | -    | 64,64,64,64                 | 0     |
| 32  | MG   | A     | 5635 | 1/1   | 0.21 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | A     | 5614 | 1/1   | 0.13 | -    | 36,36,36,36                 | 0     |
| 32  | MG   | A     | 5201 | 1/1   | 0.30 | -    | 85,85,85,85                 | 0     |
| 32  | MG   | A     | 5427 | 1/1   | 0.56 | -    | 69,69,69,69                 | 0     |
| 32  | MG   | A     | 5855 | 1/1   | 1.14 | -    | 94,94,94,94                 | 0     |
| 32  | MG   | A     | 5133 | 1/1   | 0.55 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | A     | 5139 | 1/1   | 0.15 | -    | 71,71,71,71                 | 0     |
| 32  | MG   | A     | 5864 | 1/1   | 0.24 | -    | 31,31,31,31                 | 0     |
| 32  | MG   | A     | 5177 | 1/1   | 0.25 | -    | 69,69,69,69                 | 0     |
| 32  | MG   | A     | 5574 | 1/1   | 0.32 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 5939 | 1/1   | 0.32 | -    | 68,68,68,68                 | 0     |
| 32  | MG   | A     | 5248 | 1/1   | 0.24 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5747 | 1/1   | 0.15 | -    | 37,37,37,37                 | 0     |
| 32  | MG   | A     | 5348 | 1/1   | 0.32 | -    | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 5750 | 1/1   | 0.14 | -    | 12,12,12,12                 | 0     |
| 32  | MG   | A     | 5401 | 1/1   | 0.32 | -    | 36,36,36,36                 | 0     |
| 32  | MG   | A     | 5230 | 1/1   | 0.23 | -    | 24,24,24,24                 | 0     |
| 32  | MG   | A     | 5516 | 1/1   | 0.55 | -    | 48,48,48,48                 | 0     |
| 32  | MG   | A     | 5956 | 1/1   | 0.14 | -    | 49,49,49,49                 | 0     |
| 32  | MG   | A     | 5768 | 1/1   | 0.06 | -    | 18,18,18,18                 | 0     |
| 32  | MG   | A     | 5596 | 1/1   | 0.38 | -    | 34,34,34,34                 | 0     |
| 32  | MG   | B     | 6027 | 1/1   | 0.45 | -    | 100,100,100,100             | 0     |
| 32  | MG   | A     | 5662 | 1/1   | 0.13 | -    | 62,62,62,62                 | 0     |
| 32  | MG   | A     | 5347 | 1/1   | 0.12 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 5121 | 1/1   | 0.82 | -    | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 5545 | 1/1   | 0.80 | -    | 57,57,57,57                 | 0     |
| 32  | MG   | 4     | 5097 | 1/1   | 0.08 | -    | 29,29,29,29                 | 0     |
| 32  | MG   | A     | 5486 | 1/1   | 0.16 | -    | 22,22,22,22                 | 0     |
| 32  | MG   | A     | 6002 | 1/1   | 0.46 | -    | 62,62,62,62                 | 0     |
| 32  | MG   | 0     | 5078 | 1/1   | 0.32 | -    | 37,37,37,37                 | 0     |
| 32  | MG   | A     | 5173 | 1/1   | 0.15 | -    | 29,29,29,29                 | 0     |
| 32  | MG   | A     | 5421 | 1/1   | 0.69 | -    | 90,90,90,90                 | 0     |
| 32  | MG   | A     | 5988 | 1/1   | 0.14 | -    | 66,66,66,66                 | 0     |
| 32  | MG   | A     | 5016 | 1/1   | 0.26 | -    | 51,51,51,51                 | 0     |
| 32  | MG   | X     | 5069 | 1/1   | 3.51 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5222 | 1/1   | 0.13 | -    | 23,23,23,23                 | 0     |
| 32  | MG   | A     | 5315 | 1/1   | 0.65 | -    | 46,46,46,46                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 5331 | 1/1   | 0.12 | -    | 23,23,23,23                 | 0     |
| 32  | MG   | A     | 5876 | 1/1   | 0.29 | -    | 22,22,22,22                 | 0     |
| 32  | MG   | A     | 5197 | 1/1   | 0.16 | -    | 70,70,70,70                 | 0     |
| 32  | MG   | A     | 5738 | 1/1   | 0.26 | -    | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 5106 | 1/1   | 0.14 | -    | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 5494 | 1/1   | 0.14 | -    | 98,98,98,98                 | 0     |
| 32  | MG   | A     | 5439 | 1/1   | 0.44 | -    | 37,37,37,37                 | 0     |
| 32  | MG   | O     | 5044 | 1/1   | 0.09 | -    | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 5992 | 1/1   | 0.26 | -    | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 5158 | 1/1   | 0.15 | -    | 37,37,37,37                 | 0     |
| 32  | MG   | A     | 5418 | 1/1   | 0.14 | -    | 79,79,79,79                 | 0     |
| 32  | MG   | A     | 5580 | 1/1   | 0.47 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5475 | 1/1   | 0.54 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 5599 | 1/1   | 0.26 | -    | 82,82,82,82                 | 0     |
| 32  | MG   | A     | 5493 | 1/1   | 0.15 | -    | 49,49,49,49                 | 0     |
| 32  | MG   | A     | 5322 | 1/1   | 0.18 | -    | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 5916 | 1/1   | 0.11 | -    | 38,38,38,38                 | 0     |
| 32  | MG   | A     | 5924 | 1/1   | 0.24 | -    | 17,17,17,17                 | 0     |
| 32  | MG   | A     | 5413 | 1/1   | 0.23 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 5460 | 1/1   | 0.20 | -    | 60,60,60,60                 | 0     |
| 32  | MG   | Q     | 5056 | 1/1   | 0.26 | -    | 13,13,13,13                 | 0     |
| 32  | MG   | F     | 5020 | 1/1   | 1.20 | -    | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 6020 | 1/1   | 0.47 | -    | 49,49,49,49                 | 0     |
| 32  | MG   | 8     | 5096 | 1/1   | 0.16 | -    | 49,49,49,49                 | 0     |
| 32  | MG   | A     | 5672 | 1/1   | 0.09 | -    | 69,69,69,69                 | 0     |
| 32  | MG   | A     | 5136 | 1/1   | 0.21 | -    | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 5104 | 1/1   | 0.26 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5762 | 1/1   | 0.21 | -    | 46,46,46,46                 | 0     |
| 32  | MG   | A     | 5433 | 1/1   | 0.51 | -    | 70,70,70,70                 | 0     |
| 32  | MG   | A     | 5547 | 1/1   | 0.14 | -    | 26,26,26,26                 | 0     |
| 32  | MG   | A     | 5151 | 1/1   | 0.09 | -    | 86,86,86,86                 | 0     |
| 32  | MG   | A     | 6004 | 1/1   | 2.16 | -    | 71,71,71,71                 | 0     |
| 32  | MG   | A     | 5169 | 1/1   | 0.56 | -    | 31,31,31,31                 | 0     |
| 32  | MG   | F     | 5022 | 1/1   | 0.35 | -    | 63,63,63,63                 | 0     |
| 32  | MG   | R     | 5520 | 1/1   | 0.24 | -    | 89,89,89,89                 | 0     |
| 32  | MG   | A     | 5632 | 1/1   | 0.67 | -    | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 5600 | 1/1   | 0.18 | -    | 33,33,33,33                 | 0     |
| 32  | MG   | A     | 5890 | 1/1   | 0.57 | -    | 86,86,86,86                 | 0     |
| 32  | MG   | A     | 5950 | 1/1   | 1.06 | -    | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 5247 | 1/1   | 0.55 | -    | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 5609 | 1/1   | 0.47 | -    | 46,46,46,46                 | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.