



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:01 PM EDT

PDB ID : 4JI3 / pdb\_00004ji3  
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*  
Authors : Demirci, H.; Wang, L.; Murphy, F.V.; Murphy, E.L.; Carr, J.; Blanchard, S.;  
Jogl, G.; Dahlberg, A.E.; Gregory, S.T.  
Deposited on : 2013-03-05  
Resolution : 3.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

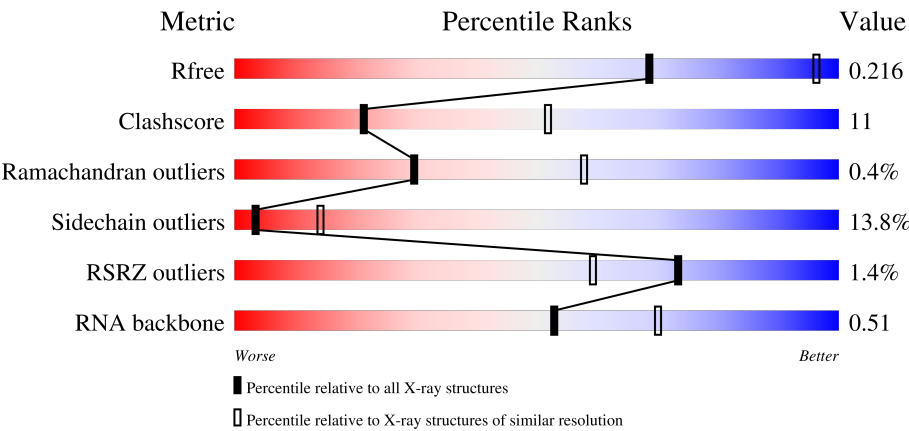
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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.



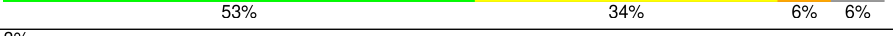
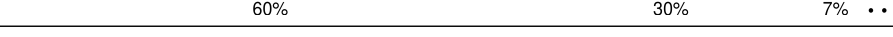
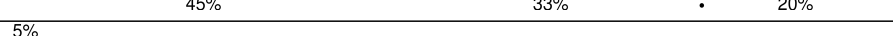
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 1099 (3.40-3.32)                                      |
| Clashscore            | 190562                      | 1116 (3.40-3.32)                                      |
| Ramachandran outliers | 187476                      | 1101 (3.40-3.32)                                      |
| Sidechain outliers    | 187428                      | 1101 (3.40-3.32)                                      |
| RSRZ outliers         | 180081                      | 1099 (3.40-3.32)                                      |
| RNA backbone          | 3983                        | 1110 (3.72-3.00)                                      |

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

| Mol | Chain | Length | Quality of chain                             |
|-----|-------|--------|----------------------------------------------|
| 1   | A     | 1522   | <div><div>55%35%10%</div><div></div></div>   |
| 2   | B     | 256    | <div><div>52%31%8%9%</div><div></div></div>  |
| 3   | C     | 239    | <div><div>44%36%6%14%</div><div></div></div> |
| 4   | D     | 209    | <div><div>66%28%6%</div><div>4%</div></div>  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 5   | E     | 162    |    |
| 6   | F     | 101    |    |
| 7   | G     | 156    |    |
| 8   | H     | 138    |    |
| 9   | I     | 128    |    |
| 10  | J     | 105    |    |
| 11  | K     | 129    |    |
| 12  | L     | 135    |    |
| 13  | M     | 126    |    |
| 14  | N     | 61     |    |
| 15  | O     | 89     |    |
| 16  | P     | 88     |   |
| 17  | Q     | 105    |  |
| 18  | R     | 88     |  |
| 19  | S     | 93     |  |
| 20  | T     | 106    |  |
| 21  | U     | 27     |  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 23  | MG   | A     | 1683 | -         | -        | -       | X                |
| 23  | MG   | A     | 1771 | -         | -        | -       | X                |
| 23  | MG   | A     | 1800 | -         | -        | -       | X                |
| 23  | MG   | A     | 1801 | -         | -        | -       | X                |
| 23  | MG   | A     | 1805 | -         | -        | -       | X                |
| 23  | MG   | A     | 1823 | -         | -        | -       | X                |
| 23  | MG   | A     | 1829 | -         | -        | -       | X                |

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52101 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | A     | 1511     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32487 | 14468 | 6008 | 10500 | 1511 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference   |
|-------|---------|----------|--------|----------|-------------|
| A     | 1534    | C        | A      | conflict | GB M26923.1 |
| A     | 1535    | A        | C      | conflict | GB M26923.1 |

- Molecule 2 is a protein called RIBOSOMAL PROTEIN S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1900  | 1213 | 341 | 341 | 5 |         |         |       |

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | C     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1016 | 314 | 281 | 1 |         |         |       |

- Molecule 4 is a protein called RIBOSOMAL PROTEIN S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | D     | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |

- Molecule 5 is a protein called RIBOSOMAL PROTEIN S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | E     | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 724 | 217 | 201 | 4 |         |         |       |

- Molecule 6 is a protein called RIBOSOMAL PROTEIN S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |

- Molecule 7 is a protein called RIBOSOMAL PROTEIN S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | G     | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |

- Molecule 8 is a protein called RIBOSOMAL PROTEIN S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |

- Molecule 9 is a protein called RIBOSOMAL PROTEIN S9.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 9   | I     | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1010  | 639 | 197 | 174 |         |         |       |

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | J     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 792   | 498 | 156 | 137 | 1 |         |         |       |

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | K     | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 864   | 537 | 164 | 160 | 3 |         |         |       |

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | L     | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 977   | 617 | 196 | 163 | 1 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| L     | 94      | TRP      | PRO    | conflict | UNP F6DEQ7 |

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | M     | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 937   | 579 | 193 | 163 | 2 |         |         |       |

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S14.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14  | N     | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |

- Molecule 15 is a protein called RIBOSOMAL PROTEIN S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | O     | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 729   | 457 | 146 | 124 | 2 |         |         |       |

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | P     | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 700   | 443 | 139 | 117 | 1 |         |         |       |

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | Q     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 823   | 528 | 151 | 142 | 2 |         |         |       |

- Molecule 18 is a protein called RIBOSOMAL PROTEIN S18.

| Mol | Chain | Residues | Atoms |     |     |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|--|---------|---------|-------|
| 18  | R     | 70       | Total | C   | N   | O  |  | 0       | 0       | 0     |
|     |       |          | 574   | 367 | 112 | 95 |  |         |         |       |

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | S     | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 647   | 414 | 119 | 112 | 2 |         |         |       |

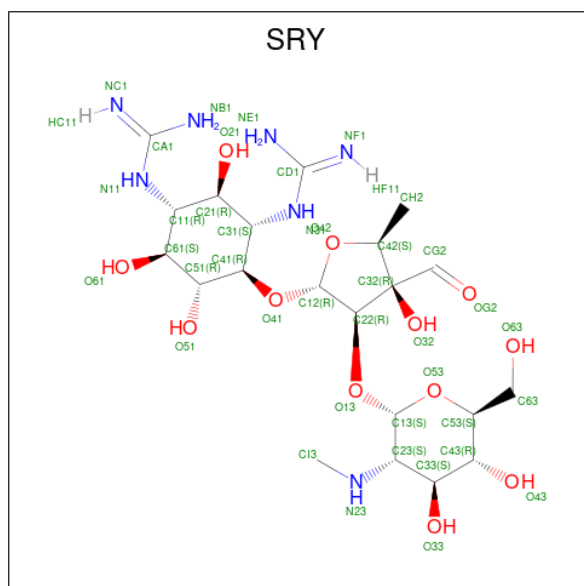
- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | T     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |

- Molecule 21 is a protein called RIBOSOMAL PROTEIN THX.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21  | U     | 24       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 208   | 128 | 50 | 30 |         |         |       |

- Molecule 22 is STREPTOMYCIN (CCD ID: SRY) (formula:  $C_{21}H_{39}N_7O_{12}$ ).



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 22  | A     | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 40    | 21 | 7 | 12 |         |         |

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 23  | A     | 231      | Total | Mg  | 0       | 0       |
|     |       |          | 231   | 231 |         |         |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 23  | B     | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 23  | C     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 23  | D     | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 23  | E     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 23  | F     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 23  | H     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 23  | K     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 23  | L     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 23  | N     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 23  | P     | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 23  | Q     | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 24  | D     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 24  | N     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

- Molecule 25 is water.

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 25  | A     | 223      | Total<br>223 | O<br>223 | 0       | 0       |
| 25  | D     | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 25  | E     | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 25  | L     | 1        | Total<br>1   | O<br>1   | 0       | 0       |

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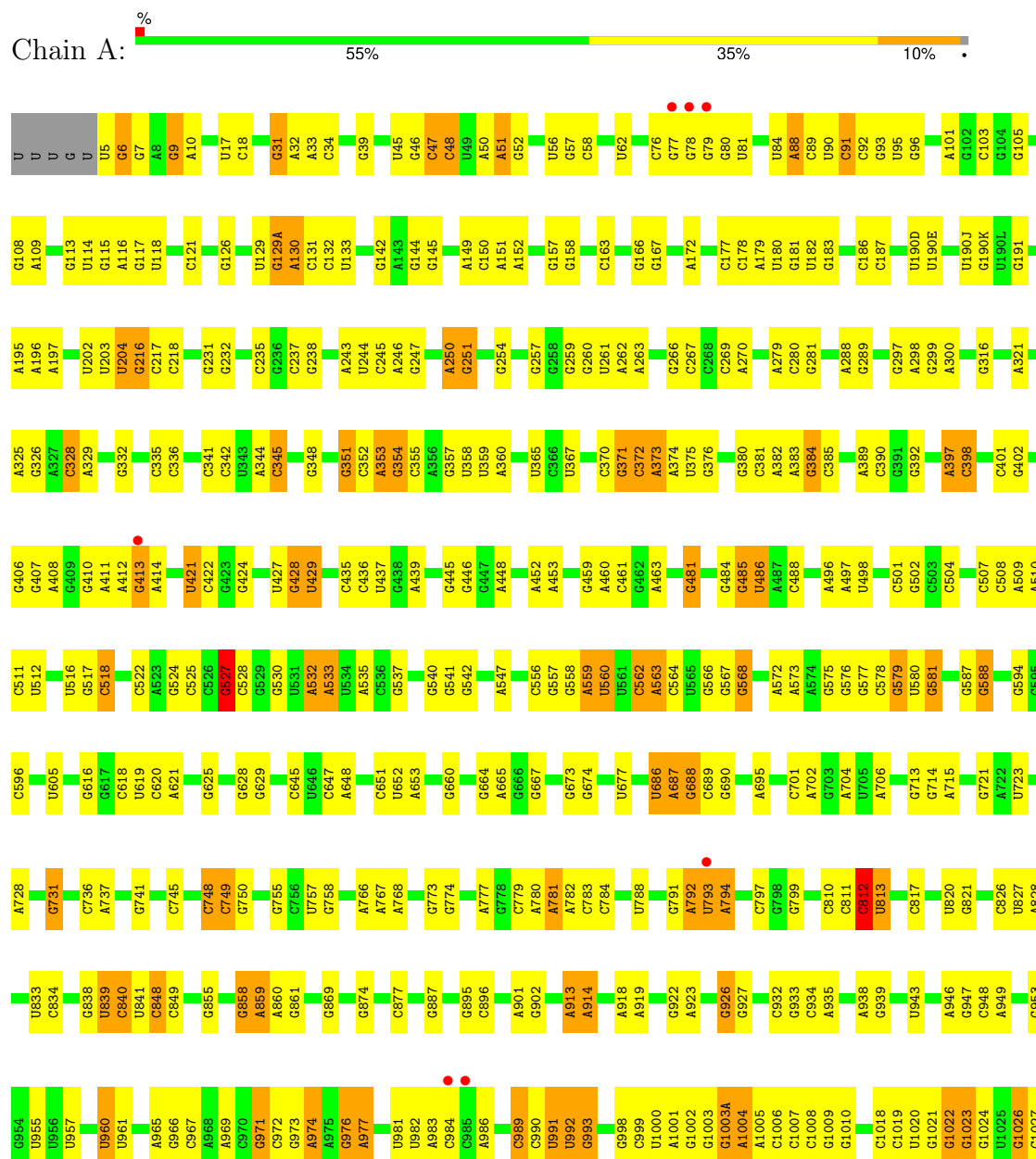
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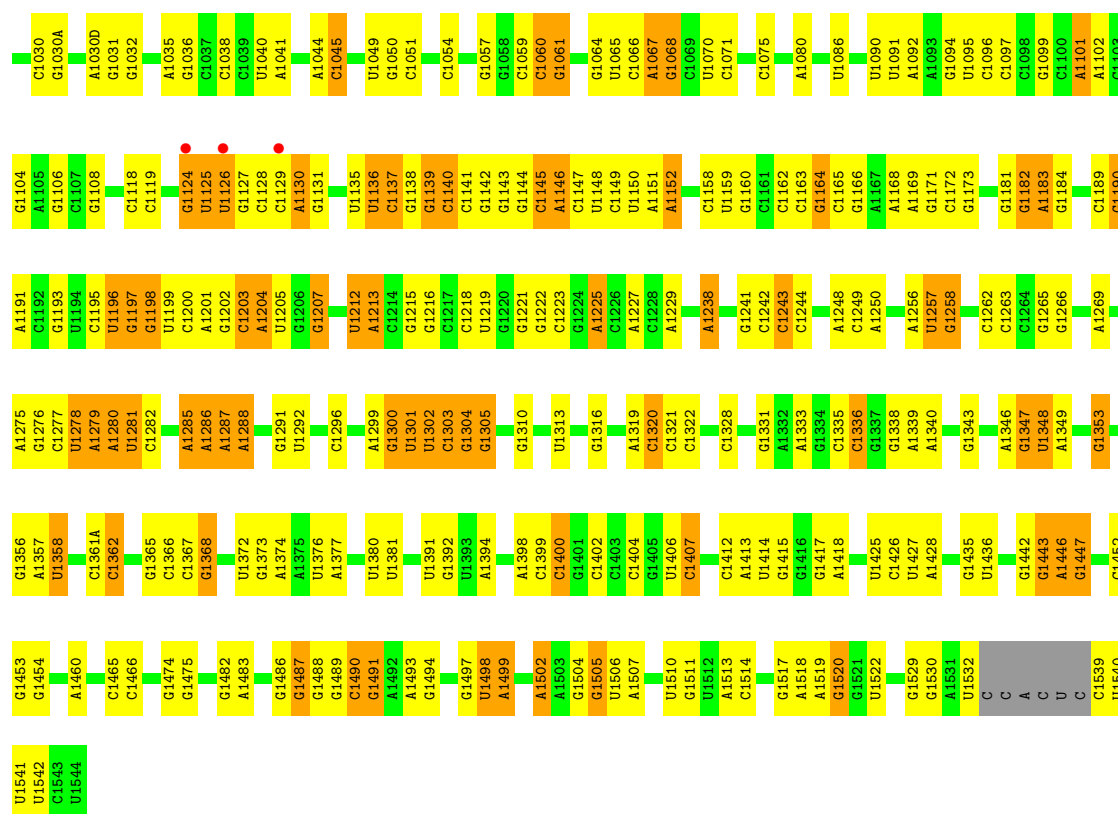
| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 25  | N     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 25  | Q     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 25  | T     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 25  | U     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

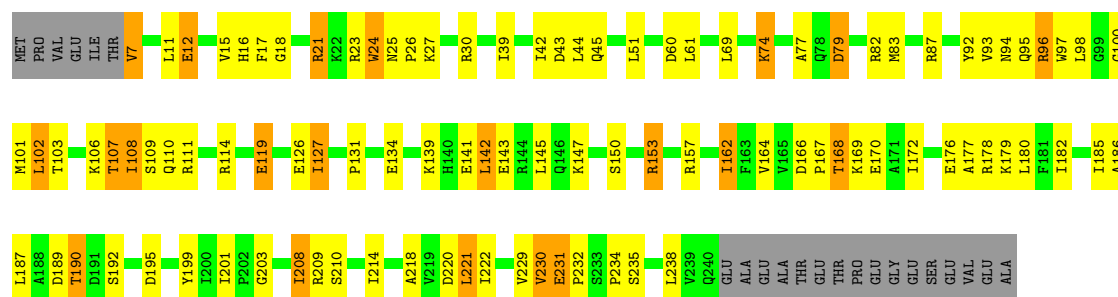
#### • Molecule 1: 16S rRNA





### • Molecule 2: RIBOSOMAL PROTEIN S2

Chain B: 52% 31% 8% 9%



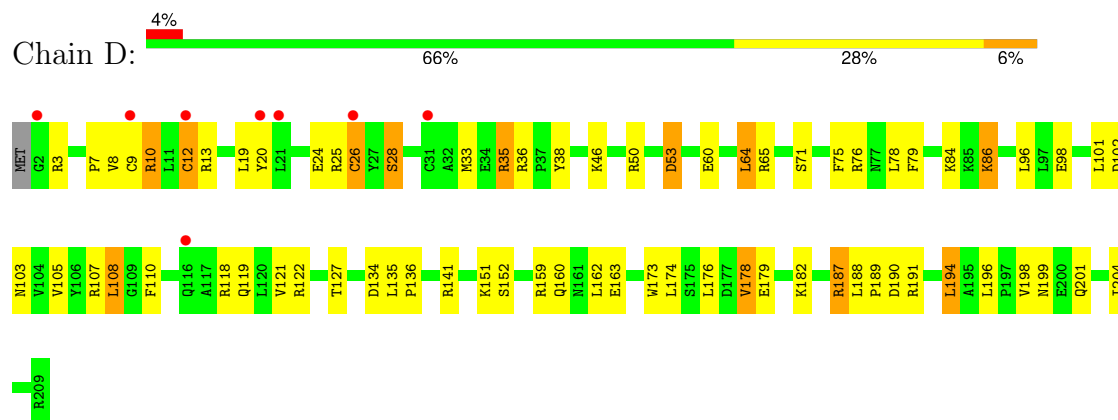
### • Molecule 3: RIBOSOMAL PROTEIN S3

Chain C: 44% 36% 6% 14%

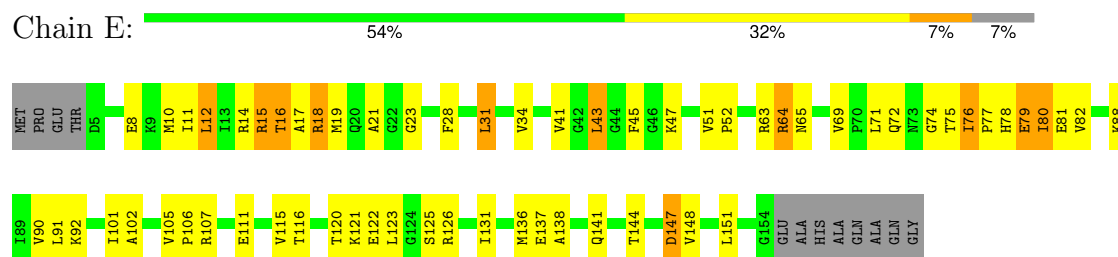


VAL  
ARG  
VAL  
LYS  
LYS  
GLU  
GLU

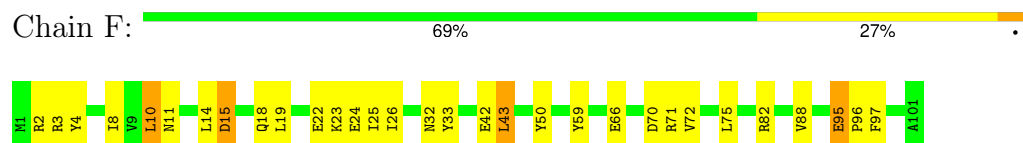
• Molecule 4: RIBOSOMAL PROTEIN S4



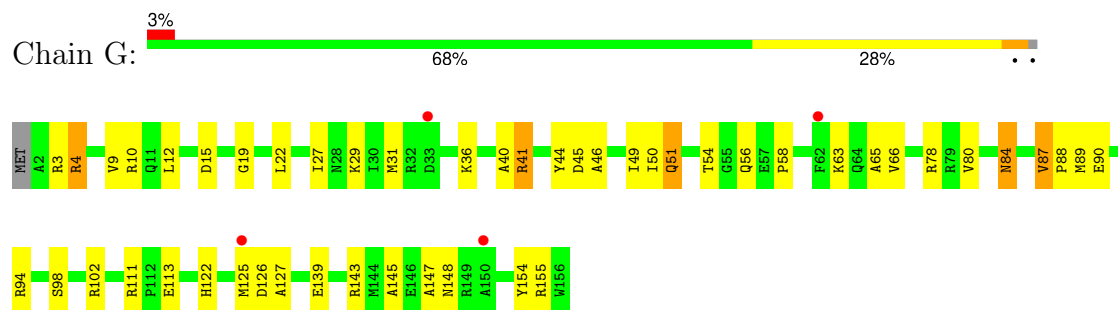
• Molecule 5: RIBOSOMAL PROTEIN S5



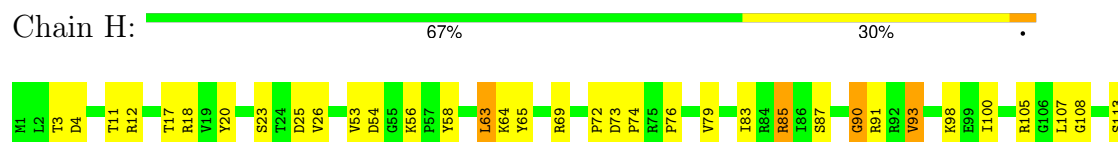
• Molecule 6: RIBOSOMAL PROTEIN S6



• Molecule 7: RIBOSOMAL PROTEIN S7

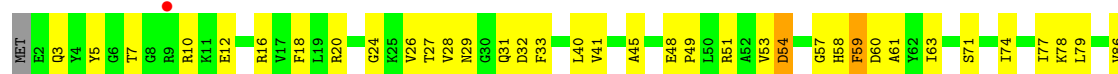


• Molecule 8: RIBOSOMAL PROTEIN S8





• Molecule 9: RIBOSOMAL PROTEIN S9



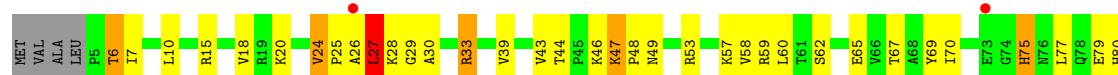
• Molecule 10: RIBOSOMAL PROTEIN S10



• Molecule 11: RIBOSOMAL PROTEIN S11

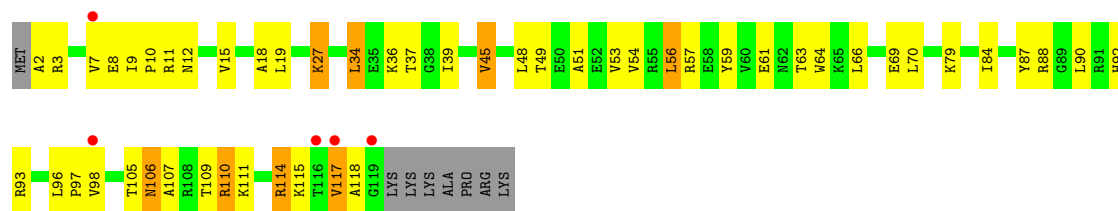


• Molecule 12: RIBOSOMAL PROTEIN S12

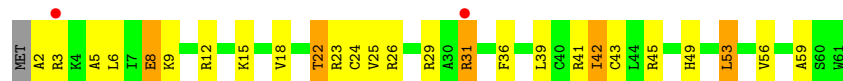


• Molecule 13: RIBOSOMAL PROTEIN S13





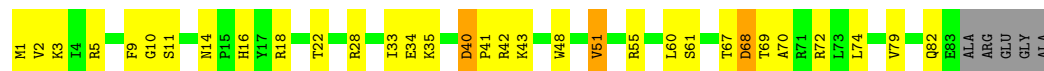
• Molecule 14: RIBOSOMAL PROTEIN S14



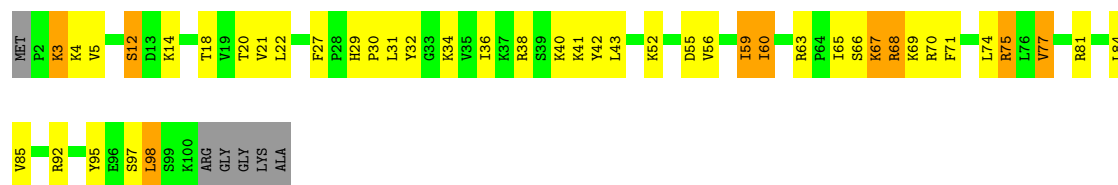
• Molecule 15: RIBOSOMAL PROTEIN S15



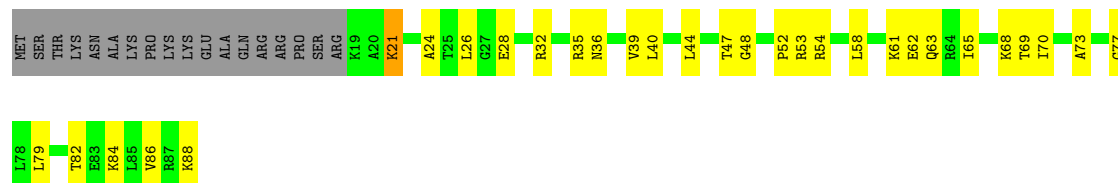
• Molecule 16: RIBOSOMAL PROTEIN S16



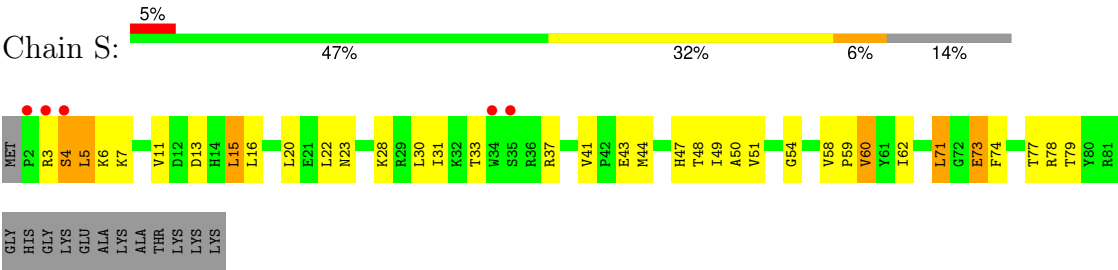
• Molecule 17: RIBOSOMAL PROTEIN S17



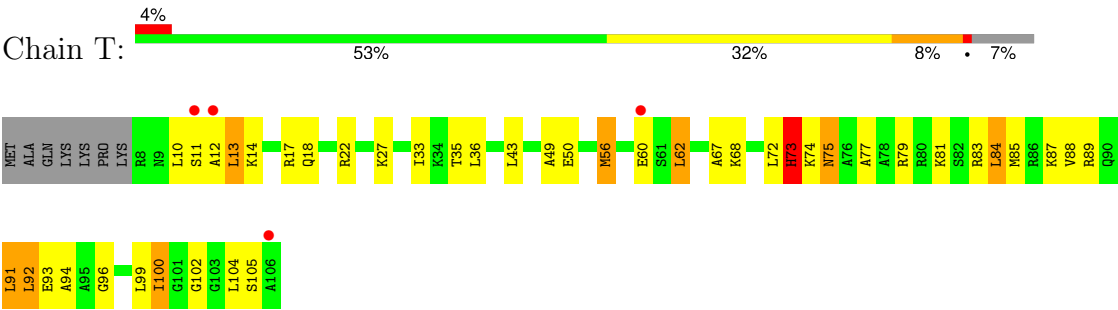
• Molecule 18: RIBOSOMAL PROTEIN S18



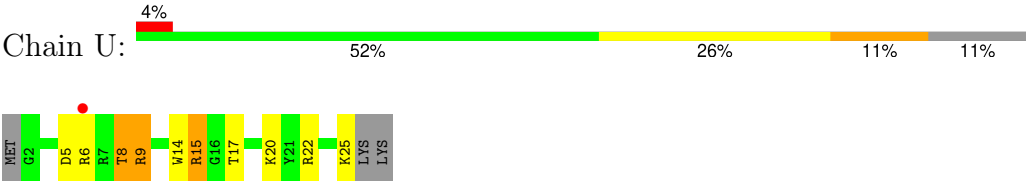
• Molecule 19: RIBOSOMAL PROTEIN S19



• Molecule 20: RIBOSOMAL PROTEIN S20



• Molecule 21: RIBOSOMAL PROTEIN THX



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 41 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 402.98Å 402.98Å 173.12Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 34.00 – 3.35<br>34.00 – 3.35                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 87.8 (34.00-3.35)<br>87.7 (34.00-3.35)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.07                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.12 (at 3.32Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX dev_1119                                             | Depositor        |
| R, $R_{free}$                                                           | 0.168 , 0.215<br>0.169 , 0.216                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 8999 reflections (4.43%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 116.5                                                       | Xtriage          |
| Anisotropy                                                              | 0.285                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 104.0                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 52101                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 144.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M2G, UR3, 5MC, 2MG, 4OC, ZN, PSU, SRY, 7MG, MA6, 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     | 0.27         | 0/36018     | 0.47        | 1/56209 (0.0%)  |
| 2   | B     | 0.48         | 0/1935      | 0.93        | 4/2609 (0.2%)   |
| 3   | C     | 0.43         | 0/1636      | 0.87        | 3/2205 (0.1%)   |
| 4   | D     | 0.48         | 0/1733      | 0.98        | 6/2318 (0.3%)   |
| 5   | E     | 0.67         | 0/1162      | 1.06        | 4/1564 (0.3%)   |
| 6   | F     | 0.39         | 0/856       | 0.86        | 2/1154 (0.2%)   |
| 7   | G     | 0.40         | 0/1276      | 0.90        | 4/1709 (0.2%)   |
| 8   | H     | 0.61         | 0/1136      | 1.04        | 4/1527 (0.3%)   |
| 9   | I     | 0.45         | 0/1029      | 0.90        | 2/1379 (0.1%)   |
| 10  | J     | 0.39         | 0/805       | 0.96        | 2/1082 (0.2%)   |
| 11  | K     | 0.49         | 0/879       | 1.05        | 7/1187 (0.6%)   |
| 12  | L     | 0.55         | 0/994       | 1.12        | 10/1331 (0.8%)  |
| 13  | M     | 0.45         | 0/947       | 0.91        | 0/1270          |
| 14  | N     | 0.43         | 0/501       | 0.98        | 3/664 (0.5%)    |
| 15  | O     | 0.50         | 0/740       | 0.83        | 0/987           |
| 16  | P     | 0.54         | 0/716       | 0.96        | 3/963 (0.3%)    |
| 17  | Q     | 0.56         | 0/836       | 1.02        | 4/1117 (0.4%)   |
| 18  | R     | 0.44         | 0/579       | 0.91        | 0/768           |
| 19  | S     | 0.37         | 0/661       | 0.99        | 5/890 (0.6%)    |
| 20  | T     | 0.54         | 0/765       | 1.01        | 5/1007 (0.5%)   |
| 21  | U     | 0.36         | 0/212       | 0.72        | 0/277           |
| All | All   | 0.36         | 0/55416     | 0.66        | 69/82217 (0.1%) |

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   | C     | 0                   | 1                   |
| 8   | H     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 12  | L     | 0                   | 1                   |
| 20  | T     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

There are no bond length outliers.

All (69) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 12  | L     | 26  | ALA  | N-CA-C  | -10.20 | 98.58       | 111.02   |
| 4   | D     | 26  | CYS  | N-CA-C  | -9.43  | 101.77      | 113.18   |
| 12  | L     | 24  | VAL  | CA-C-N  | -8.11  | 110.96      | 121.91   |
| 12  | L     | 24  | VAL  | C-N-CA  | -8.11  | 110.96      | 121.91   |
| 8   | H     | 100 | ILE  | CA-C-N  | 7.50   | 127.26      | 119.76   |
| 8   | H     | 100 | ILE  | C-N-CA  | 7.50   | 127.26      | 119.76   |
| 11  | K     | 114 | VAL  | CA-C-N  | -7.24  | 113.03      | 120.85   |
| 11  | K     | 114 | VAL  | C-N-CA  | -7.24  | 113.03      | 120.85   |
| 10  | J     | 55  | LYS  | N-CA-C  | 7.04   | 118.42      | 108.00   |
| 9   | I     | 54  | ASP  | N-CA-C  | 7.03   | 119.13      | 110.91   |
| 11  | K     | 49  | GLY  | N-CA-C  | 7.02   | 122.61      | 113.27   |
| 19  | S     | 6   | LYS  | N-CA-C  | 6.82   | 118.10      | 108.00   |
| 16  | P     | 40  | ASP  | CA-C-N  | 6.81   | 126.77      | 119.28   |
| 16  | P     | 40  | ASP  | C-N-CA  | 6.81   | 126.77      | 119.28   |
| 4   | D     | 12  | CYS  | N-CA-C  | -6.80  | 102.94      | 111.11   |
| 20  | T     | 94  | ALA  | N-CA-C  | -6.79  | 96.05       | 107.80   |
| 8   | H     | 73  | ASP  | CA-C-N  | 6.75   | 126.89      | 119.87   |
| 8   | H     | 73  | ASP  | C-N-CA  | 6.75   | 126.89      | 119.87   |
| 7   | G     | 111 | ARG  | CA-C-N  | 6.75   | 126.37      | 119.56   |
| 7   | G     | 111 | ARG  | C-N-CA  | 6.75   | 126.37      | 119.56   |
| 9   | I     | 57  | GLY  | N-CA-C  | -6.74  | 105.59      | 115.63   |
| 14  | N     | 31  | ARG  | N-CA-C  | 6.67   | 119.16      | 111.02   |
| 12  | L     | 119 | LYS  | N-CA-C  | -6.66  | 100.43      | 110.28   |
| 11  | K     | 120 | ARG  | CA-C-N  | 6.59   | 126.55      | 120.03   |
| 11  | K     | 120 | ARG  | C-N-CA  | 6.59   | 126.55      | 120.03   |
| 14  | N     | 12  | ARG  | CB-CA-C | -6.54  | 109.05      | 116.63   |
| 2   | B     | 12  | GLU  | N-CA-C  | 6.44   | 124.52      | 110.80   |
| 3   | C     | 167 | TRP  | N-CA-C  | 6.38   | 115.83      | 108.49   |
| 19  | S     | 6   | LYS  | CB-CA-C | -6.34  | 107.46      | 116.34   |
| 12  | L     | 30  | ALA  | CA-C-N  | 6.33   | 125.75      | 118.85   |
| 12  | L     | 30  | ALA  | C-N-CA  | 6.33   | 125.75      | 118.85   |
| 12  | L     | 27  | LEU  | CB-CA-C | -6.12  | 107.78      | 116.34   |
| 11  | K     | 80  | VAL  | N-CA-C  | 6.09   | 117.06      | 108.17   |
| 17  | Q     | 12  | SER  | N-CA-C  | 6.07   | 118.33      | 108.26   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | L     | 105 | TYR  | CB-CA-C     | -5.98 | 109.69      | 116.63   |
| 5   | E     | 23  | GLY  | N-CA-C      | 5.94  | 119.42      | 110.75   |
| 4   | D     | 28  | SER  | CA-C-N      | -5.93 | 115.66      | 121.65   |
| 4   | D     | 28  | SER  | C-N-CA      | -5.93 | 115.66      | 121.65   |
| 16  | P     | 51  | VAL  | N-CA-C      | 5.91  | 121.64      | 109.34   |
| 19  | S     | 4   | SER  | N-CA-C      | 5.86  | 118.44      | 108.02   |
| 19  | S     | 30  | LEU  | CB-CA-C     | -5.81 | 108.88      | 115.79   |
| 20  | T     | 73  | HIS  | CB-CA-C     | -5.75 | 108.95      | 115.79   |
| 14  | N     | 22  | THR  | N-CA-C      | 5.68  | 117.14      | 111.07   |
| 17  | Q     | 67  | LYS  | N-CA-C      | -5.64 | 102.05      | 110.23   |
| 5   | E     | 64  | ARG  | N-CA-C      | -5.50 | 102.35      | 110.48   |
| 19  | S     | 73  | GLU  | N-CA-C      | -5.43 | 106.16      | 112.89   |
| 11  | K     | 91  | ARG  | N-CA-C      | -5.41 | 105.28      | 111.07   |
| 4   | D     | 33  | MET  | N-CA-C      | -5.37 | 105.59      | 111.82   |
| 2   | B     | 230 | VAL  | N-CA-C      | 5.36  | 116.33      | 109.30   |
| 5   | E     | 15  | ARG  | N-CA-C      | 5.31  | 119.92      | 113.38   |
| 17  | Q     | 98  | LEU  | N-CA-C      | 5.31  | 118.77      | 111.54   |
| 4   | D     | 196 | LEU  | N-CA-C      | 5.30  | 116.08      | 109.57   |
| 5   | E     | 17  | ALA  | N-CA-C      | 5.27  | 117.67      | 110.55   |
| 6   | F     | 11  | ASN  | CA-C-N      | 5.26  | 124.93      | 119.56   |
| 6   | F     | 11  | ASN  | C-N-CA      | 5.26  | 124.93      | 119.56   |
| 17  | Q     | 14  | LYS  | N-CA-C      | 5.21  | 119.27      | 113.01   |
| 20  | T     | 75  | ASN  | N-CA-C      | -5.20 | 106.61      | 113.17   |
| 10  | J     | 62  | HIS  | N-CA-C      | 5.17  | 117.88      | 109.24   |
| 20  | T     | 92  | LEU  | CA-C-N      | -5.16 | 115.14      | 122.77   |
| 20  | T     | 92  | LEU  | C-N-CA      | -5.16 | 115.14      | 122.77   |
| 1   | A     | 812 | C    | C4'-C3'-O3' | 5.15  | 117.13      | 109.40   |
| 2   | B     | 172 | ILE  | CB-CA-C     | -5.14 | 105.20      | 112.14   |
| 12  | L     | 115 | LYS  | CA-C-N      | -5.13 | 115.72      | 122.85   |
| 12  | L     | 115 | LYS  | C-N-CA      | -5.13 | 115.72      | 122.85   |
| 2   | B     | 23  | ARG  | N-CA-C      | -5.09 | 99.95       | 110.80   |
| 7   | G     | 87  | VAL  | CA-C-N      | 5.04  | 124.94      | 119.85   |
| 7   | G     | 87  | VAL  | C-N-CA      | 5.04  | 124.94      | 119.85   |
| 3   | C     | 194 | GLY  | N-CA-C      | 5.03  | 117.38      | 110.58   |
| 3   | C     | 155 | GLY  | N-CA-C      | 5.02  | 120.78      | 112.66   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 3   | C     | 166 | GLU  | Peptide |
| 8   | H     | 90  | GLY  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 12  | L     | 27  | LEU  | Peptide |
| 20  | T     | 93  | GLU  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 32487 | 0        | 16421    | 446     | 0            |
| 2   | B     | 1900  | 0        | 1951     | 60      | 0            |
| 3   | C     | 1612  | 0        | 1677     | 67      | 0            |
| 4   | D     | 1703  | 0        | 1763     | 48      | 0            |
| 5   | E     | 1146  | 0        | 1207     | 38      | 0            |
| 6   | F     | 843   | 0        | 857      | 14      | 0            |
| 7   | G     | 1257  | 0        | 1296     | 33      | 0            |
| 8   | H     | 1116  | 0        | 1177     | 25      | 0            |
| 9   | I     | 1010  | 0        | 1037     | 29      | 0            |
| 10  | J     | 792   | 0        | 835      | 41      | 0            |
| 11  | K     | 864   | 0        | 881      | 25      | 0            |
| 12  | L     | 977   | 0        | 1060     | 38      | 0            |
| 13  | M     | 937   | 0        | 995      | 29      | 0            |
| 14  | N     | 492   | 0        | 529      | 16      | 0            |
| 15  | O     | 729   | 0        | 768      | 21      | 0            |
| 16  | P     | 700   | 0        | 720      | 20      | 0            |
| 17  | Q     | 823   | 0        | 891      | 36      | 0            |
| 18  | R     | 574   | 0        | 644      | 18      | 0            |
| 19  | S     | 647   | 0        | 673      | 22      | 0            |
| 20  | T     | 763   | 0        | 861      | 34      | 0            |
| 21  | U     | 208   | 0        | 221      | 7       | 0            |
| 22  | A     | 40    | 0        | 37       | 4       | 0            |
| 23  | A     | 231   | 0        | 0        | 0       | 0            |
| 23  | B     | 2     | 0        | 0        | 0       | 0            |
| 23  | C     | 1     | 0        | 0        | 0       | 0            |
| 23  | D     | 2     | 0        | 0        | 0       | 0            |
| 23  | E     | 1     | 0        | 0        | 0       | 0            |
| 23  | F     | 1     | 0        | 0        | 0       | 0            |
| 23  | H     | 1     | 0        | 0        | 0       | 0            |
| 23  | K     | 1     | 0        | 0        | 0       | 0            |
| 23  | L     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 23  | N     | 1     | 0        | 0        | 0       | 0            |
| 23  | P     | 2     | 0        | 0        | 0       | 0            |
| 23  | Q     | 2     | 0        | 0        | 0       | 0            |
| 24  | D     | 1     | 0        | 0        | 0       | 0            |
| 24  | N     | 1     | 0        | 0        | 0       | 0            |
| 25  | A     | 223   | 0        | 0        | 3       | 0            |
| 25  | D     | 1     | 0        | 0        | 0       | 0            |
| 25  | E     | 4     | 0        | 0        | 0       | 0            |
| 25  | L     | 1     | 0        | 0        | 0       | 0            |
| 25  | N     | 1     | 0        | 0        | 0       | 0            |
| 25  | Q     | 1     | 0        | 0        | 0       | 0            |
| 25  | T     | 1     | 0        | 0        | 0       | 0            |
| 25  | U     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 52101 | 0        | 36501    | 944     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (944) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1443:G:H5''  | 1:A:1446:A:H5'    | 1.43                     | 0.99              |
| 1:A:279:A:OP2    | 17:Q:95:TYR:OH    | 1.88                     | 0.89              |
| 17:Q:29:HIS:HD2  | 17:Q:32:TYR:H     | 1.11                     | 0.89              |
| 1:A:411:A:H62    | 1:A:413:G:H21     | 1.23                     | 0.87              |
| 1:A:298:A:N6     | 25:A:2054:HOH:O   | 2.06                     | 0.85              |
| 3:C:180:ALA:HB3  | 3:C:203:PHE:HE1   | 1.42                     | 0.84              |
| 1:A:235:C:N4     | 25:A:1986:HOH:O   | 2.14                     | 0.81              |
| 1:A:130:A:OP2    | 1:A:190(E):U:O2'  | 2.00                     | 0.80              |
| 1:A:542:G:OP1    | 4:D:10:ARG:NH2    | 2.14                     | 0.79              |
| 1:A:1057:G:H5''  | 3:C:154:SER:HB2   | 1.65                     | 0.79              |
| 1:A:527:7MG:OP2  | 22:A:1601:SRY:O32 | 1.99                     | 0.79              |
| 1:A:664:G:H22    | 1:A:741:G:H1      | 1.30                     | 0.79              |
| 15:O:39:LEU:HD12 | 15:O:56:LEU:HB2   | 1.63                     | 0.77              |
| 20:T:56:MET:HE2  | 20:T:85:MET:HA    | 1.66                     | 0.77              |
| 4:D:3:ARG:HH21   | 4:D:118:ARG:HH12  | 1.31                     | 0.76              |
| 17:Q:66:SER:O    | 17:Q:70:ARG:NH1   | 2.19                     | 0.76              |
| 1:A:1491:G:H5'   | 12:L:94:TRP:HZ2   | 1.51                     | 0.75              |
| 1:A:412:A:O2'    | 4:D:35:ARG:NH2    | 2.19                     | 0.75              |
| 17:Q:29:HIS:CD2  | 17:Q:32:TYR:H     | 1.99                     | 0.74              |
| 20:T:56:MET:HE1  | 20:T:104:LEU:HD21 | 1.70                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1412:C:H2'   | 1:A:1413:A:C8    | 2.23                     | 0.73              |
| 1:A:1266:G:N2    | 1:A:1269:A:OP2   | 2.22                     | 0.73              |
| 1:A:427:U:OP2    | 4:D:36:ARG:NH2   | 2.22                     | 0.73              |
| 8:H:83:ILE:HG13  | 8:H:137:VAL:HG22 | 1.70                     | 0.73              |
| 1:A:1158:C:N3    | 1:A:1181:G:N2    | 2.37                     | 0.72              |
| 12:L:24:VAL:HG13 | 12:L:98:TYR:HE2  | 1.55                     | 0.72              |
| 1:A:677:U:H3     | 1:A:713:G:H22    | 1.37                     | 0.71              |
| 1:A:838:G:H1     | 1:A:848:C:H42    | 1.36                     | 0.71              |
| 1:A:1195:C:H3'   | 1:A:1196:U:H5''  | 1.72                     | 0.71              |
| 1:A:92:C:H2'     | 1:A:93:G:H8      | 1.56                     | 0.70              |
| 5:E:78:HIS:HD2   | 8:H:107:LEU:HD12 | 1.54                     | 0.70              |
| 1:A:1373:G:H5''  | 7:G:36:LYS:HE2   | 1.73                     | 0.70              |
| 1:A:1222:G:OP2   | 1:A:1322:C:N4    | 2.22                     | 0.70              |
| 1:A:1200:C:O2    | 1:A:1205:U:N3    | 2.18                     | 0.70              |
| 1:A:560:U:H5'    | 1:A:566:G:N2     | 2.06                     | 0.70              |
| 3:C:43:LEU:HD22  | 3:C:47:LEU:HD22  | 1.74                     | 0.70              |
| 1:A:1328:C:OP1   | 21:U:20:LYS:NZ   | 2.23                     | 0.69              |
| 10:J:8:LEU:HB3   | 10:J:96:ILE:HG23 | 1.72                     | 0.69              |
| 3:C:125:GLU:HG3  | 3:C:189:ALA:HB1  | 1.75                     | 0.69              |
| 3:C:180:ALA:HB3  | 3:C:203:PHE:CE1  | 2.27                     | 0.69              |
| 1:A:537:G:OP1    | 12:L:113:ARG:NH2 | 2.25                     | 0.69              |
| 5:E:12:LEU:HD13  | 5:E:31:LEU:HB2   | 1.75                     | 0.69              |
| 1:A:1414:U:H2'   | 1:A:1415:G:H8    | 1.58                     | 0.68              |
| 4:D:107:ARG:HH21 | 4:D:194:LEU:HD12 | 1.58                     | 0.68              |
| 7:G:51:GLN:HG2   | 7:G:58:PRO:HD3   | 1.74                     | 0.68              |
| 1:A:972:C:H4'    | 10:J:57:LYS:HG2  | 1.75                     | 0.68              |
| 1:A:976:G:OP2    | 1:A:1358:U:O2'   | 2.07                     | 0.68              |
| 11:K:57:THR:HG23 | 11:K:60:ALA:H    | 1.58                     | 0.68              |
| 20:T:49:ALA:HB3  | 20:T:99:LEU:HD23 | 1.75                     | 0.68              |
| 1:A:1442:G:N7    | 1:A:1446:A:N6    | 2.42                     | 0.68              |
| 1:A:517:G:N1     | 1:A:533:A:OP2    | 2.19                     | 0.68              |
| 1:A:859:A:OP2    | 1:A:869:G:N1     | 2.23                     | 0.68              |
| 7:G:15:ASP:OD2   | 7:G:44:TYR:OH    | 2.12                     | 0.68              |
| 4:D:13:ARG:NH1   | 4:D:38:TYR:O     | 2.27                     | 0.68              |
| 1:A:1391:U:H2'   | 1:A:1392:G:C8    | 2.30                     | 0.67              |
| 1:A:1035:A:H2'   | 1:A:1036:G:H8    | 1.60                     | 0.67              |
| 2:B:114:ARG:NH1  | 2:B:141:GLU:OE1  | 2.27                     | 0.67              |
| 12:L:28:LYS:HD2  | 12:L:33:ARG:HH12 | 1.59                     | 0.67              |
| 1:A:991:U:O4     | 1:A:1212:U:O2'   | 2.12                     | 0.67              |
| 1:A:113:G:H1'    | 1:A:354:G:H5'    | 1.76                     | 0.67              |
| 8:H:119:LEU:HD11 | 8:H:127:LEU:HD12 | 1.76                     | 0.67              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1417:G:O2'   | 1:A:1483:A:N6     | 2.28                     | 0.67              |
| 16:P:18:ARG:HD3  | 16:P:35:LYS:HD2   | 1.75                     | 0.66              |
| 16:P:67:THR:HG22 | 16:P:69:THR:H     | 1.59                     | 0.66              |
| 2:B:15:VAL:HG13  | 2:B:209:ARG:HG2   | 1.77                     | 0.66              |
| 10:J:48:THR:HA   | 10:J:62:HIS:HB3   | 1.77                     | 0.66              |
| 1:A:427:U:OP1    | 4:D:13:ARG:NH2    | 2.28                     | 0.66              |
| 11:K:90:GLY:HA2  | 11:K:93:GLN:HB2   | 1.76                     | 0.66              |
| 13:M:11:ARG:HA   | 13:M:45:VAL:HG11  | 1.78                     | 0.66              |
| 1:A:1412:C:H2'   | 1:A:1413:A:H8     | 1.59                     | 0.66              |
| 1:A:1356:G:H2'   | 1:A:1357:A:C8     | 2.31                     | 0.66              |
| 5:E:80:ILE:HD13  | 5:E:138:ALA:HB1   | 1.78                     | 0.66              |
| 11:K:110:ASP:HB2 | 18:R:88:LYS:HG2   | 1.76                     | 0.66              |
| 3:C:157:ILE:HD13 | 3:C:164:ARG:HB2   | 1.78                     | 0.65              |
| 3:C:134:ILE:HD11 | 3:C:153:VAL:HB    | 1.78                     | 0.65              |
| 6:F:10:LEU:HD12  | 6:F:59:TYR:HB3    | 1.78                     | 0.65              |
| 1:A:250:A:H4'    | 1:A:251:G:O5'     | 1.96                     | 0.64              |
| 3:C:26:LYS:HZ2   | 10:J:45:ARG:HD2   | 1.61                     | 0.64              |
| 1:A:579:G:H5'    | 1:A:728:A:H1'     | 1.77                     | 0.64              |
| 15:O:70:LEU:HD13 | 15:O:78:TYR:HA    | 1.79                     | 0.64              |
| 1:A:144:G:H1     | 1:A:178:C:H42     | 1.45                     | 0.64              |
| 1:A:1135:U:H4'   | 1:A:1136:U:H5     | 1.61                     | 0.64              |
| 12:L:25:PRO:HB3  | 12:L:27:LEU:HD22  | 1.79                     | 0.64              |
| 2:B:101:MET:HA   | 2:B:108:ILE:HD12  | 1.79                     | 0.64              |
| 1:A:1316:G:H4'   | 14:N:18:VAL:HG11  | 1.79                     | 0.64              |
| 5:E:81:GLU:HG2   | 5:E:90:VAL:HG22   | 1.80                     | 0.64              |
| 12:L:28:LYS:HE3  | 12:L:62:SER:HA    | 1.79                     | 0.64              |
| 1:A:993:G:O6     | 1:A:1045:C:N4     | 2.31                     | 0.64              |
| 1:A:1510:U:H2'   | 1:A:1511:G:C8     | 2.33                     | 0.64              |
| 18:R:48:GLY:HA3  | 18:R:82:THR:HA    | 1.80                     | 0.64              |
| 1:A:1399:C:H4'   | 1:A:1400:5MC:H5'' | 1.80                     | 0.63              |
| 3:C:20:SER:OG    | 3:C:36:ASP:OD1    | 2.15                     | 0.63              |
| 1:A:259:G:OP2    | 20:T:83:ARG:NH1   | 2.31                     | 0.63              |
| 5:E:8:GLU:HB3    | 5:E:34:VAL:HG22   | 1.81                     | 0.63              |
| 13:M:96:LEU:O    | 13:M:110:ARG:NH1  | 2.31                     | 0.63              |
| 20:T:67:ALA:HA   | 20:T:73:HIS:H     | 1.62                     | 0.63              |
| 1:A:1291:G:OP1   | 7:G:41:ARG:NH2    | 2.32                     | 0.63              |
| 3:C:88:ARG:HG3   | 3:C:100:ALA:HA    | 1.81                     | 0.63              |
| 1:A:17:U:H2'     | 1:A:18:C:C6       | 2.34                     | 0.63              |
| 1:A:1305:G:N2    | 1:A:1331:G:H1'    | 2.14                     | 0.63              |
| 9:I:54:ASP:O     | 9:I:58:HIS:ND1    | 2.32                     | 0.62              |
| 1:A:421:U:O2     | 3:C:126:ARG:NH1   | 2.31                     | 0.62              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:372:C:H4'     | 1:A:373:A:O5'    | 1.99                     | 0.62              |
| 1:A:1189:C:H5''   | 3:C:5:ILE:HG12   | 1.80                     | 0.62              |
| 10:J:61:GLU:OE1   | 14:N:45:ARG:NH1  | 2.32                     | 0.62              |
| 13:M:10:PRO:HB2   | 13:M:18:ALA:HB1  | 1.81                     | 0.62              |
| 3:C:188:LEU:HD21  | 3:C:195:VAL:HG23 | 1.82                     | 0.62              |
| 11:K:27:ASN:OD1   | 11:K:28:THR:N    | 2.32                     | 0.62              |
| 19:S:50:ALA:HA    | 19:S:59:PRO:HA   | 1.82                     | 0.62              |
| 2:B:16:HIS:ND1    | 2:B:17:PHE:O     | 2.26                     | 0.62              |
| 2:B:79:ASP:HB2    | 2:B:238:LEU:HD13 | 1.80                     | 0.62              |
| 2:B:21:ARG:HA     | 2:B:39:ILE:HA    | 1.82                     | 0.62              |
| 5:E:147:ASP:N     | 5:E:147:ASP:OD1  | 2.32                     | 0.61              |
| 13:M:15:VAL:HG21  | 13:M:48:LEU:HD21 | 1.82                     | 0.61              |
| 1:A:1149:C:O2'    | 1:A:1280:A:N1    | 2.27                     | 0.61              |
| 3:C:121:ALA:HA    | 3:C:124:ILE:HD12 | 1.82                     | 0.61              |
| 1:A:1238:A:H5'    | 1:A:1336:C:H41   | 1.64                     | 0.61              |
| 1:A:1435:G:H2'    | 1:A:1436:U:C6    | 2.35                     | 0.61              |
| 1:A:56:U:H2'      | 1:A:57:G:C8      | 2.36                     | 0.61              |
| 1:A:90:U:H2'      | 1:A:91:C:C6      | 2.36                     | 0.61              |
| 13:M:117:VAL:HG12 | 13:M:118:ALA:H   | 1.66                     | 0.61              |
| 1:A:103:C:OP1     | 20:T:17:ARG:NH1  | 2.34                     | 0.60              |
| 1:A:524:G:H2'     | 1:A:525:C:C6     | 2.35                     | 0.60              |
| 1:A:76:C:H2'      | 1:A:77:G:C8      | 2.36                     | 0.60              |
| 3:C:34:LEU:HD22   | 3:C:38:ARG:HE    | 1.65                     | 0.60              |
| 1:A:1035:A:H2'    | 1:A:1036:G:C8    | 2.36                     | 0.60              |
| 1:A:1491:G:H5'    | 12:L:94:TRP:CZ2  | 2.35                     | 0.60              |
| 1:A:527:7MG:O2'   | 1:A:535:A:N1     | 2.32                     | 0.60              |
| 1:A:1407:5MC:HN41 | 1:A:1494:G:H1    | 1.49                     | 0.60              |
| 1:A:748:C:H4'     | 1:A:749:C:O5'    | 2.01                     | 0.60              |
| 4:D:64:LEU:HG     | 4:D:198:VAL:HG11 | 1.83                     | 0.60              |
| 1:A:76:C:H2'      | 1:A:77:G:H8      | 1.66                     | 0.60              |
| 1:A:80:G:H1       | 1:A:89:C:H42     | 1.48                     | 0.60              |
| 1:A:1229:A:OP2    | 13:M:114:ARG:NH1 | 2.34                     | 0.60              |
| 1:A:411:A:N6      | 1:A:413:G:H21    | 1.96                     | 0.60              |
| 1:A:1502:A:H2     | 1:A:1505:G:H1    | 1.50                     | 0.60              |
| 22:A:1601:SRV:H61 | 12:L:47:LYS:HD2  | 1.82                     | 0.60              |
| 5:E:43:LEU:HD22   | 5:E:136:MET:HG3  | 1.84                     | 0.60              |
| 1:A:686:U:HO2'    | 1:A:687:A:H8     | 1.49                     | 0.60              |
| 1:A:1442:G:N2     | 1:A:1447:G:N7    | 2.50                     | 0.60              |
| 12:L:113:ARG:NH1  | 12:L:116:SER:H   | 2.00                     | 0.59              |
| 1:A:736:C:H2'     | 1:A:737:A:C8     | 2.37                     | 0.59              |
| 7:G:84:ASN:OD1    | 7:G:84:ASN:N     | 2.36                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:O:32:LEU:HD12 | 15:O:63:ARG:HB2   | 1.85                     | 0.59              |
| 20:T:89:ARG:HG3  | 20:T:104:LEU:HD13 | 1.84                     | 0.59              |
| 3:C:46:GLU:O     | 3:C:83:ARG:NH2    | 2.34                     | 0.59              |
| 12:L:89:ARG:HG2  | 12:L:97:ARG:HA    | 1.84                     | 0.59              |
| 17:Q:5:VAL:HG22  | 17:Q:60:ILE:HG13  | 1.84                     | 0.59              |
| 1:A:1425:U:H3    | 1:A:1475:G:H1     | 1.49                     | 0.59              |
| 1:A:84:U:H2'     | 1:A:88:A:O4'      | 2.02                     | 0.59              |
| 1:A:1145:C:O2'   | 1:A:1146:A:O5'    | 2.20                     | 0.59              |
| 1:A:558:G:OP2    | 1:A:559:A:O2'     | 2.14                     | 0.59              |
| 1:A:673:G:H2'    | 1:A:674:G:C8      | 2.37                     | 0.59              |
| 1:A:957:U:H4'    | 19:S:79:THR:HB    | 1.85                     | 0.59              |
| 3:C:155:GLY:HA3  | 3:C:163:ALA:HB1   | 1.84                     | 0.59              |
| 20:T:33:ILE:HD13 | 20:T:62:LEU:HB3   | 1.85                     | 0.59              |
| 1:A:1241:G:H2'   | 1:A:1242:C:C6     | 2.37                     | 0.59              |
| 6:F:15:ASP:OD2   | 6:F:18:GLN:NE2    | 2.36                     | 0.59              |
| 17:Q:43:LEU:HD12 | 17:Q:68:ARG:HB3   | 1.83                     | 0.59              |
| 1:A:512:U:OP1    | 4:D:46:LYS:NZ     | 2.36                     | 0.59              |
| 1:A:1068:G:H8    | 1:A:1068:G:OP2    | 1.85                     | 0.58              |
| 7:G:27:ILE:HD12  | 7:G:40:ALA:HA     | 1.84                     | 0.58              |
| 8:H:64:LYS:HG2   | 8:H:79:VAL:HG21   | 1.85                     | 0.58              |
| 15:O:3:ILE:HD13  | 15:O:34:LEU:HD13  | 1.85                     | 0.58              |
| 1:A:191:G:O2'    | 20:T:102:GLY:O    | 2.17                     | 0.58              |
| 1:A:955:U:H1'    | 1:A:1227:A:N6     | 2.18                     | 0.58              |
| 1:A:1064:G:H1'   | 1:A:1190:G:H21    | 1.67                     | 0.58              |
| 1:A:1303:C:H2'   | 1:A:1304:G:H5'    | 1.86                     | 0.58              |
| 1:A:1221:G:O3'   | 19:S:77:THR:HG21  | 2.03                     | 0.58              |
| 9:I:63:ILE:HG21  | 9:I:77:ILE:HG12   | 1.85                     | 0.58              |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:H     | 1.68                     | 0.58              |
| 2:B:17:PHE:HD1   | 2:B:18:GLY:H      | 1.51                     | 0.58              |
| 5:E:101:ILE:O    | 5:E:120:THR:HB    | 2.03                     | 0.58              |
| 11:K:13:GLN:HA   | 11:K:76:GLY:HA3   | 1.84                     | 0.58              |
| 1:A:522:C:OP2    | 12:L:69:TYR:OH    | 2.20                     | 0.58              |
| 1:A:1060:C:OP1   | 14:N:45:ARG:NH2   | 2.36                     | 0.58              |
| 10:J:50:ILE:HB   | 14:N:41:ARG:HH21  | 1.69                     | 0.58              |
| 10:J:53:PRO:HB3  | 14:N:42:ILE:HD12  | 1.85                     | 0.58              |
| 1:A:373:A:H1'    | 1:A:481:G:H1'     | 1.86                     | 0.57              |
| 7:G:22:LEU:HD21  | 7:G:66:VAL:HG11   | 1.85                     | 0.57              |
| 1:A:1196:U:OP1   | 1:A:1197:G:H5'    | 2.04                     | 0.57              |
| 10:J:84:GLN:HG3  | 10:J:85:LEU:HD22  | 1.85                     | 0.57              |
| 13:M:34:LEU:HD12 | 13:M:39:ILE:HB    | 1.87                     | 0.57              |
| 1:A:562:C:H1'    | 12:L:15:ARG:HG3   | 1.87                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1366:C:H2'   | 1:A:1367:C:C6     | 2.39                     | 0.57              |
| 10:J:54:PHE:O    | 10:J:55:LYS:HG3   | 2.04                     | 0.57              |
| 12:L:70:ILE:HG12 | 12:L:100:ILE:HD12 | 1.86                     | 0.57              |
| 1:A:407:G:O4'    | 4:D:119:GLN:NE2   | 2.38                     | 0.57              |
| 1:A:989:C:H42    | 1:A:1216:G:H1     | 1.52                     | 0.57              |
| 19:S:11:VAL:HG21 | 19:S:41:VAL:HG13  | 1.85                     | 0.57              |
| 1:A:261:U:OP2    | 20:T:79:ARG:NH2   | 2.38                     | 0.57              |
| 3:C:26:LYS:NZ    | 10:J:45:ARG:HD2   | 2.20                     | 0.57              |
| 8:H:17:THR:OG1   | 8:H:18:ARG:NH1    | 2.38                     | 0.57              |
| 1:A:1021:G:N2    | 1:A:1022:G:O2'    | 2.38                     | 0.57              |
| 1:A:95:U:H2'     | 1:A:96:G:C8       | 2.40                     | 0.57              |
| 1:A:578:C:O2'    | 1:A:728:A:N3      | 2.34                     | 0.56              |
| 1:A:1338:G:H2'   | 1:A:1339:A:C8     | 2.40                     | 0.56              |
| 4:D:3:ARG:HH11   | 4:D:71:SER:H      | 1.51                     | 0.56              |
| 4:D:102:ASP:OD1  | 4:D:103:ASN:N     | 2.38                     | 0.56              |
| 13:M:107:ALA:HB3 | 13:M:111:LYS:HE3  | 1.87                     | 0.56              |
| 2:B:18:GLY:HA2   | 2:B:42:ILE:HG13   | 1.87                     | 0.56              |
| 3:C:19:GLU:OE1   | 3:C:54:ARG:NE     | 2.37                     | 0.56              |
| 1:A:926:G:N2     | 1:A:1542:U:OP1    | 2.38                     | 0.56              |
| 1:A:1006:C:N4    | 1:A:1023:G:O6     | 2.38                     | 0.56              |
| 1:A:1343:G:H4'   | 9:I:122:ALA:HB3   | 1.88                     | 0.56              |
| 1:A:1368:G:H5''  | 9:I:112:LYS:HB3   | 1.87                     | 0.56              |
| 11:K:12:ARG:HB3  | 11:K:14:VAL:HG22  | 1.87                     | 0.56              |
| 1:A:793:U:H3'    | 1:A:794:A:H5''    | 1.87                     | 0.56              |
| 1:A:1086:U:H3    | 1:A:1099:G:H22    | 1.52                     | 0.56              |
| 20:T:67:ALA:HB2  | 20:T:77:ALA:HB2   | 1.86                     | 0.56              |
| 2:B:231:GLU:HG3  | 2:B:232:PRO:HD2   | 1.86                     | 0.56              |
| 9:I:95:LYS:HE3   | 9:I:98:PRO:HG2    | 1.88                     | 0.56              |
| 1:A:1040:U:H2'   | 1:A:1041:A:H8     | 1.71                     | 0.56              |
| 3:C:156:ARG:H    | 3:C:163:ALA:HA    | 1.70                     | 0.56              |
| 19:S:22:LEU:HD21 | 19:S:28:LYS:H     | 1.71                     | 0.56              |
| 1:A:1372:U:H2'   | 1:A:1373:G:O4'    | 2.06                     | 0.56              |
| 2:B:69:LEU:HD21  | 2:B:93:VAL:HG23   | 1.88                     | 0.56              |
| 2:B:139:LYS:NZ   | 2:B:143:GLU:OE2   | 2.37                     | 0.56              |
| 15:O:4:THR:OG1   | 15:O:7:GLU:OE2    | 2.22                     | 0.56              |
| 20:T:60:GLU:HG3  | 20:T:81:LYS:HD2   | 1.88                     | 0.56              |
| 1:A:1493:A:HO2'  | 1:A:1494:G:H8     | 1.54                     | 0.55              |
| 17:Q:12:SER:HB3  | 17:Q:20:THR:HB    | 1.89                     | 0.55              |
| 2:B:24:TRP:CZ3   | 2:B:26:PRO:HA     | 2.40                     | 0.55              |
| 10:J:32:ALA:O    | 10:J:34:VAL:HG23  | 2.07                     | 0.55              |
| 1:A:279:A:H5'    | 1:A:279:A:H8      | 1.71                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1090:U:H2'  | 1:A:1091:U:H6    | 1.72                     | 0.55              |
| 3:C:20:SER:HB2  | 3:C:40:ARG:HH12  | 1.71                     | 0.55              |
| 3:C:24:ALA:HB2  | 3:C:32:LEU:HD12  | 1.88                     | 0.55              |
| 4:D:53:ASP:OD1  | 4:D:53:ASP:N     | 2.33                     | 0.55              |
| 1:A:7:G:H5'     | 1:A:298:A:O4'    | 2.06                     | 0.55              |
| 1:A:257:G:H1    | 1:A:269:C:H42    | 1.55                     | 0.55              |
| 1:A:1020:U:H2'  | 1:A:1021:G:H8    | 1.70                     | 0.55              |
| 9:I:71:SER:HA   | 9:I:74:ILE:HD12  | 1.89                     | 0.55              |
| 1:A:1392:G:H21  | 1:A:1502:A:H8    | 1.54                     | 0.55              |
| 15:O:56:LEU:HA  | 15:O:59:MET:HE2  | 1.89                     | 0.55              |
| 1:A:1104:G:O5'  | 2:B:111:ARG:HD2  | 2.07                     | 0.55              |
| 1:A:1143:G:H2'  | 1:A:1144:G:C8    | 2.42                     | 0.55              |
| 1:A:1148:U:H2'  | 1:A:1149:C:O4'   | 2.07                     | 0.55              |
| 10:J:6:ILE:HB   | 10:J:72:VAL:HB   | 1.87                     | 0.55              |
| 1:A:118:U:H3'   | 1:A:288:A:H61    | 1.71                     | 0.55              |
| 1:A:990:C:H42   | 1:A:1215:G:H1    | 1.55                     | 0.55              |
| 1:A:1313:U:O4   | 19:S:4:SER:OG    | 2.19                     | 0.55              |
| 5:E:144:THR:O   | 5:E:148:VAL:HG23 | 2.07                     | 0.55              |
| 16:P:68:ASP:OD1 | 16:P:68:ASP:N    | 2.37                     | 0.55              |
| 1:A:1163:C:H2'  | 1:A:1164:G:C8    | 2.42                     | 0.54              |
| 1:A:279:A:H5''  | 1:A:281:G:O4'    | 2.06                     | 0.54              |
| 10:J:57:LYS:O   | 10:J:60:ARG:NH1  | 2.41                     | 0.54              |
| 1:A:381:C:H2'   | 1:A:382:A:O4'    | 2.06                     | 0.54              |
| 1:A:410:G:OP2   | 4:D:25:ARG:NE    | 2.29                     | 0.54              |
| 7:G:45:ASP:O    | 7:G:49:ILE:HG12  | 2.07                     | 0.54              |
| 3:C:20:SER:HB2  | 3:C:40:ARG:HH22  | 1.71                     | 0.54              |
| 3:C:39:ILE:HD12 | 3:C:57:ILE:HD13  | 1.90                     | 0.54              |
| 1:A:518:C:H2'   | 1:A:530:G:C8     | 2.43                     | 0.54              |
| 7:G:9:VAL:HG13  | 7:G:94:ARG:HH21  | 1.73                     | 0.54              |
| 1:A:1368:G:OP2  | 9:I:112:LYS:HD3  | 2.07                     | 0.54              |
| 5:E:11:ILE:HD13 | 5:E:105:VAL:HG13 | 1.89                     | 0.54              |
| 1:A:9:G:OP2     | 5:E:121:LYS:NZ   | 2.23                     | 0.54              |
| 2:B:87:ARG:HD3  | 2:B:234:PRO:HD2  | 1.90                     | 0.54              |
| 4:D:65:ARG:HG3  | 4:D:75:PHE:CD1   | 2.43                     | 0.54              |
| 3:C:167:TRP:HE3 | 3:C:168:ALA:N    | 2.06                     | 0.54              |
| 1:A:974:A:OP2   | 14:N:29:ARG:NH2  | 2.41                     | 0.53              |
| 1:A:108:G:H5'   | 1:A:109:A:H5''   | 1.89                     | 0.53              |
| 1:A:736:C:H2'   | 1:A:737:A:H8     | 1.74                     | 0.53              |
| 3:C:34:LEU:HD13 | 3:C:38:ARG:HH21  | 1.73                     | 0.53              |
| 1:A:1010:G:H1   | 1:A:1019:C:H42   | 1.56                     | 0.53              |
| 1:A:1225:A:H4'  | 19:S:78:ARG:HD3  | 1.89                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:121:ALA:HB1  | 3:C:189:ALA:HB2  | 1.89                     | 0.53              |
| 13:M:88:ARG:HD3  | 19:S:3:ARG:HH21  | 1.73                     | 0.53              |
| 1:A:689:C:H2'    | 1:A:690:G:O4'    | 2.09                     | 0.53              |
| 1:A:714:G:H2'    | 1:A:715:A:C8     | 2.42                     | 0.53              |
| 1:A:955:U:H1'    | 1:A:1227:A:H61   | 1.74                     | 0.53              |
| 1:A:1223:C:OP2   | 19:S:78:ARG:NH2  | 2.42                     | 0.53              |
| 1:A:974:A:OP1    | 1:A:974:A:H8     | 1.91                     | 0.53              |
| 5:E:74:GLY:HA3   | 5:E:116:THR:HG22 | 1.90                     | 0.53              |
| 12:L:97:ARG:HB2  | 12:L:98:TYR:CE1  | 2.43                     | 0.53              |
| 2:B:168:THR:HG23 | 2:B:192:SER:HA   | 1.90                     | 0.53              |
| 1:A:179:A:H2'    | 1:A:180:U:C6     | 2.43                     | 0.53              |
| 1:A:1303:C:C2'   | 1:A:1304:G:H5'   | 2.39                     | 0.53              |
| 1:A:1367:C:H5'   | 10:J:60:ARG:HE   | 1.74                     | 0.53              |
| 16:P:14:ASN:HA   | 16:P:42:ARG:NH1  | 2.24                     | 0.53              |
| 1:A:235:C:H5'    | 17:Q:70:ARG:HG3  | 1.91                     | 0.53              |
| 1:A:1147:C:O2    | 9:I:16:ARG:NH1   | 2.42                     | 0.53              |
| 1:A:237:C:OP2    | 17:Q:40:LYS:NZ   | 2.42                     | 0.53              |
| 1:A:359:U:H2'    | 1:A:360:A:C8     | 2.44                     | 0.53              |
| 1:A:1256:A:H5'   | 1:A:1258:G:H1'   | 1.91                     | 0.53              |
| 1:A:1296:C:H4'   | 1:A:1302:U:C5    | 2.43                     | 0.53              |
| 3:C:167:TRP:HE3  | 3:C:168:ALA:H    | 1.56                     | 0.53              |
| 6:F:33:TYR:HA    | 6:F:71:ARG:NH2   | 2.24                     | 0.52              |
| 1:A:1427:U:H2'   | 1:A:1428:A:C8    | 2.44                     | 0.52              |
| 3:C:150:LYS:HG3  | 3:C:169:ALA:HB2  | 1.91                     | 0.52              |
| 1:A:407:G:H2'    | 1:A:408:A:C8     | 2.45                     | 0.52              |
| 1:A:1101:A:H4'   | 1:A:1102:A:O5'   | 2.10                     | 0.52              |
| 1:A:1300:G:O2'   | 1:A:1301:U:O5'   | 2.27                     | 0.52              |
| 12:L:60:LEU:HD11 | 12:L:85:ILE:HD12 | 1.91                     | 0.52              |
| 16:P:10:GLY:HA3  | 16:P:14:ASN:O    | 2.10                     | 0.52              |
| 17:Q:21:VAL:HG21 | 17:Q:59:ILE:HD11 | 1.90                     | 0.52              |
| 3:C:77:ILE:HD11  | 3:C:103:VAL:HG21 | 1.91                     | 0.52              |
| 5:E:122:GLU:O    | 5:E:126:ARG:NH1  | 2.42                     | 0.52              |
| 12:L:6:THR:O     | 12:L:10:LEU:HD12 | 2.09                     | 0.52              |
| 10:J:8:LEU:HG    | 10:J:70:ARG:HB2  | 1.91                     | 0.52              |
| 13:M:39:ILE:HD12 | 13:M:56:LEU:HG   | 1.91                     | 0.52              |
| 1:A:1061:G:H1    | 1:A:1195:C:H42   | 1.57                     | 0.52              |
| 1:A:1243:C:H2'   | 1:A:1244:C:C6    | 2.45                     | 0.52              |
| 6:F:43:LEU:HD21  | 18:R:35:ARG:HH12 | 1.74                     | 0.52              |
| 8:H:87:SER:HB2   | 8:H:93:VAL:H     | 1.75                     | 0.52              |
| 1:A:56:U:H2'     | 1:A:57:G:H8      | 1.74                     | 0.52              |
| 1:A:1435:G:H2'   | 1:A:1436:U:H6    | 1.74                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1198:G:H2'   | 1:A:1199:U:C6     | 2.44                     | 0.51              |
| 10:J:77:PRO:HB2  | 10:J:82:ILE:HD11  | 1.91                     | 0.51              |
| 1:A:401:C:H2'    | 1:A:402:G:H8      | 1.75                     | 0.51              |
| 18:R:39:VAL:HG13 | 18:R:40:LEU:HD23  | 1.92                     | 0.51              |
| 21:U:17:THR:O    | 21:U:22:ARG:NH1   | 2.43                     | 0.51              |
| 1:A:580:U:H2'    | 1:A:581:G:O4'     | 2.10                     | 0.51              |
| 1:A:1007:C:O2    | 1:A:1023:G:N1     | 2.44                     | 0.51              |
| 1:A:1499:A:H1'   | 1:A:1520:G:H5'    | 1.92                     | 0.51              |
| 11:K:19:ALA:HB2  | 11:K:80:VAL:HG21  | 1.91                     | 0.51              |
| 19:S:49:ILE:HG21 | 19:S:71:LEU:HD11  | 1.92                     | 0.51              |
| 1:A:316:G:OP2    | 1:A:351:G:O2'     | 2.29                     | 0.51              |
| 1:A:1275:A:H2'   | 1:A:1276:G:O4'    | 2.10                     | 0.51              |
| 13:M:37:THR:HG21 | 13:M:56:LEU:HA    | 1.91                     | 0.51              |
| 16:P:70:ALA:O    | 16:P:74:LEU:HG    | 2.10                     | 0.51              |
| 10:J:51:ARG:CZ   | 10:J:61:GLU:HB2   | 2.41                     | 0.51              |
| 12:L:24:VAL:HG13 | 12:L:98:TYR:CE2   | 2.41                     | 0.51              |
| 18:R:88:LYS:OXT  | 18:R:88:LYS:NZ    | 2.31                     | 0.51              |
| 20:T:50:GLU:HA   | 20:T:100:ILE:HB   | 1.92                     | 0.51              |
| 6:F:18:GLN:O     | 6:F:22:GLU:HG2    | 2.10                     | 0.51              |
| 9:I:112:LYS:HE3  | 9:I:117:HIS:O     | 2.11                     | 0.51              |
| 1:A:947:G:H2'    | 1:A:948:C:O4'     | 2.11                     | 0.51              |
| 1:A:126:G:OP1    | 1:A:605:U:O2'     | 2.28                     | 0.51              |
| 1:A:1030(A):G:N2 | 1:A:1030(D):A:OP2 | 2.44                     | 0.51              |
| 1:A:1221:G:OP2   | 19:S:37:ARG:NH2   | 2.43                     | 0.51              |
| 1:A:972:C:OP1    | 10:J:57:LYS:NZ    | 2.26                     | 0.51              |
| 1:A:1130:A:O2'   | 9:I:3:GLN:NE2     | 2.44                     | 0.51              |
| 11:K:84:VAL:HG21 | 11:K:95:ILE:HD11  | 1.93                     | 0.51              |
| 4:D:3:ARG:NH1    | 4:D:71:SER:H      | 2.09                     | 0.50              |
| 1:A:216:G:H2'    | 1:A:217:C:C6      | 2.46                     | 0.50              |
| 1:A:397:A:H5'    | 1:A:398:C:OP1     | 2.11                     | 0.50              |
| 1:A:413:G:O6     | 4:D:36:ARG:HD3    | 2.11                     | 0.50              |
| 1:A:1080:A:O3'   | 5:E:16:THR:OG1    | 2.29                     | 0.50              |
| 1:A:1136:U:H5''  | 1:A:1137:C:OP2    | 2.11                     | 0.50              |
| 12:L:85:ILE:HG23 | 12:L:98:TYR:HB3   | 1.92                     | 0.50              |
| 19:S:23:ASN:OD1  | 19:S:47:HIS:NE2   | 2.21                     | 0.50              |
| 1:A:177:C:H2'    | 1:A:178:C:H6      | 1.75                     | 0.50              |
| 1:A:355:C:H5'    | 1:A:389:A:OP2     | 2.12                     | 0.50              |
| 1:A:540:G:H2'    | 1:A:541:G:O4'     | 2.11                     | 0.50              |
| 1:A:706:A:O4'    | 11:K:29:ILE:HD11  | 2.11                     | 0.50              |
| 1:A:335:C:H2'    | 1:A:336:C:C6      | 2.46                     | 0.50              |
| 1:A:918:A:H2'    | 1:A:919:A:C8      | 2.46                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1414:U:H2'   | 1:A:1415:G:C8    | 2.43                     | 0.50              |
| 4:D:36:ARG:HA    | 4:D:38:TYR:CE2   | 2.45                     | 0.50              |
| 1:A:532:A:N6     | 3:C:158:GLY:O    | 2.43                     | 0.50              |
| 18:R:73:ALA:HB3  | 18:R:79:LEU:HD12 | 1.93                     | 0.50              |
| 1:A:382:A:H2'    | 1:A:383:A:C8     | 2.47                     | 0.50              |
| 1:A:1460:A:OP2   | 20:T:27:LYS:NZ   | 2.44                     | 0.50              |
| 2:B:92:TYR:CD1   | 2:B:94:ASN:HB2   | 2.47                     | 0.50              |
| 1:A:1145:C:HO2'  | 1:A:1146:A:P     | 2.34                     | 0.50              |
| 1:A:1285:A:H4'   | 1:A:1286:A:O5'   | 2.10                     | 0.50              |
| 2:B:7:VAL:HG11   | 2:B:221:LEU:HD23 | 1.93                     | 0.50              |
| 19:S:15:LEU:HD23 | 19:S:33:THR:HG21 | 1.94                     | 0.50              |
| 1:A:452:A:H2'    | 1:A:453:A:C8     | 2.46                     | 0.50              |
| 1:A:686:U:O2'    | 1:A:687:A:H8     | 1.94                     | 0.50              |
| 1:A:992:U:H4'    | 1:A:993:G:O5'    | 2.10                     | 0.50              |
| 1:A:1124:G:H3'   | 1:A:1145:C:H5    | 1.76                     | 0.50              |
| 1:A:1427:U:H2'   | 1:A:1428:A:H8    | 1.76                     | 0.50              |
| 13:M:3:ARG:HH21  | 13:M:7:VAL:HG12  | 1.77                     | 0.50              |
| 1:A:1067:A:N1    | 1:A:1108:G:O2'   | 2.43                     | 0.49              |
| 1:A:1488:G:H2'   | 1:A:1489:G:C8    | 2.47                     | 0.49              |
| 9:I:32:ASP:OD1   | 9:I:33:PHE:N     | 2.45                     | 0.49              |
| 1:A:413:G:H2'    | 1:A:428:G:N2     | 2.27                     | 0.49              |
| 1:A:1152:A:H5''  | 10:J:13:HIS:ND1  | 2.26                     | 0.49              |
| 1:A:1172:C:H2'   | 1:A:1173:G:C8    | 2.47                     | 0.49              |
| 3:C:54:ARG:HD3   | 3:C:56:ASP:OD2   | 2.12                     | 0.49              |
| 20:T:50:GLU:HB2  | 20:T:99:LEU:HD11 | 1.95                     | 0.49              |
| 1:A:279:A:C6     | 17:Q:98:LEU:HD13 | 2.48                     | 0.49              |
| 1:A:401:C:H2'    | 1:A:402:G:C8     | 2.47                     | 0.49              |
| 1:A:501:C:H2'    | 1:A:502:G:C8     | 2.47                     | 0.49              |
| 3:C:55:VAL:HG22  | 3:C:68:VAL:HG23  | 1.94                     | 0.49              |
| 3:C:150:LYS:HA   | 3:C:169:ALA:HA   | 1.94                     | 0.49              |
| 15:O:45:VAL:HG12 | 15:O:46:HIS:H    | 1.76                     | 0.49              |
| 1:A:943:U:H1'    | 9:I:124:GLN:HE22 | 1.77                     | 0.49              |
| 1:A:1425:U:H2'   | 1:A:1426:C:C6    | 2.48                     | 0.49              |
| 1:A:1490:C:H5'   | 1:A:1491:G:OP2   | 2.12                     | 0.49              |
| 4:D:20:TYR:HD2   | 4:D:26:CYS:HB3   | 1.77                     | 0.49              |
| 7:G:139:GLU:O    | 7:G:143:ARG:HB2  | 2.12                     | 0.49              |
| 1:A:620:C:N1     | 4:D:135:LEU:HD13 | 2.28                     | 0.49              |
| 1:A:750:G:H1'    | 15:O:23:GLY:H    | 1.77                     | 0.49              |
| 1:A:1021:G:C2    | 1:A:1022:G:H1'   | 2.48                     | 0.49              |
| 10:J:50:ILE:HG12 | 10:J:60:ARG:HH11 | 1.77                     | 0.49              |
| 17:Q:67:LYS:HA   | 17:Q:70:ARG:HH12 | 1.76                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:833:U:H2'    | 1:A:834:C:C6     | 2.47                     | 0.49              |
| 1:A:839:U:H5'    | 1:A:840:C:H5     | 1.78                     | 0.49              |
| 11:K:92:GLU:HB3  | 11:K:96:ARG:NH2  | 2.28                     | 0.49              |
| 21:U:14:TRP:CE3  | 21:U:15:ARG:HG2  | 2.48                     | 0.49              |
| 1:A:1262:C:H2'   | 1:A:1263:C:C6    | 2.48                     | 0.49              |
| 4:D:9:CYS:O      | 4:D:12:CYS:HB2   | 2.12                     | 0.49              |
| 12:L:27:LEU:C    | 12:L:29:GLY:N    | 2.67                     | 0.49              |
| 17:Q:74:LEU:HG   | 17:Q:75:ARG:HG2  | 1.94                     | 0.49              |
| 1:A:452:A:O2'    | 1:A:453:A:O4'    | 2.20                     | 0.49              |
| 1:A:1426:C:H42   | 1:A:1474:G:H1    | 1.60                     | 0.49              |
| 3:C:150:LYS:HB3  | 3:C:201:TYR:HB2  | 1.95                     | 0.49              |
| 3:C:186:PHE:HD1  | 3:C:199:LYS:HG2  | 1.77                     | 0.49              |
| 15:O:54:ARG:HD3  | 15:O:58:MET:HE2  | 1.95                     | 0.49              |
| 1:A:1125:U:OP2   | 1:A:1145:C:N4    | 2.45                     | 0.49              |
| 1:A:57:G:H2'     | 1:A:58:C:C6      | 2.48                     | 0.49              |
| 1:A:151:A:H2'    | 1:A:152:A:O4'    | 2.13                     | 0.49              |
| 1:A:1203:C:O2'   | 1:A:1204:A:OP1   | 2.31                     | 0.49              |
| 1:A:269:C:H2'    | 1:A:270:A:C8     | 2.47                     | 0.48              |
| 1:A:558:G:H3'    | 1:A:559:A:H3'    | 1.95                     | 0.48              |
| 1:A:1218:C:H2'   | 1:A:1219:U:C6    | 2.48                     | 0.48              |
| 3:C:186:PHE:CD1  | 3:C:199:LYS:HG2  | 2.48                     | 0.48              |
| 14:N:8:GLU:OE2   | 14:N:9:LYS:N     | 2.45                     | 0.48              |
| 1:A:459:G:H1'    | 1:A:463:A:H61    | 1.77                     | 0.48              |
| 11:K:54:ARG:NH1  | 11:K:54:ARG:HB3  | 2.28                     | 0.48              |
| 12:L:39:VAL:H    | 12:L:57:LYS:HB2  | 1.78                     | 0.48              |
| 17:Q:29:HIS:CG   | 17:Q:30:PRO:HD2  | 2.48                     | 0.48              |
| 1:A:1139:G:O2'   | 1:A:1140:C:O5'   | 2.29                     | 0.48              |
| 2:B:16:HIS:HB3   | 2:B:210:SER:HB2  | 1.94                     | 0.48              |
| 1:A:157:G:H2'    | 1:A:158:G:H8     | 1.78                     | 0.48              |
| 1:A:1347:G:O2'   | 1:A:1348:U:P     | 2.71                     | 0.48              |
| 2:B:189:ASP:OD1  | 2:B:189:ASP:N    | 2.46                     | 0.48              |
| 11:K:33:THR:HA   | 11:K:39:PRO:HA   | 1.96                     | 0.48              |
| 19:S:13:ASP:HA   | 19:S:16:LEU:HB3  | 1.95                     | 0.48              |
| 1:A:410:G:H2'    | 1:A:429:U:C5     | 2.48                     | 0.48              |
| 1:A:1248:A:H2'   | 1:A:1249:C:C6    | 2.48                     | 0.48              |
| 1:A:1488:G:H2'   | 1:A:1489:G:H8    | 1.79                     | 0.48              |
| 5:E:69:VAL:HG12  | 5:E:71:LEU:HG    | 1.96                     | 0.48              |
| 7:G:122:HIS:O    | 7:G:126:ASP:HB2  | 2.14                     | 0.48              |
| 12:L:33:ARG:HG2  | 12:L:60:LEU:HD12 | 1.94                     | 0.48              |
| 12:L:75:HIS:CD2  | 12:L:77:LEU:HB2  | 2.49                     | 0.48              |
| 4:D:187:ARG:HH22 | 4:D:188:LEU:HD12 | 1.79                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1376:U:OP1    | 7:G:98:SER:OG    | 2.25                     | 0.48              |
| 1:A:103:C:O2'     | 1:A:172:A:N1     | 2.45                     | 0.48              |
| 1:A:243:A:C2      | 1:A:246:A:C8     | 3.01                     | 0.48              |
| 1:A:254:G:OP1     | 17:Q:67:LYS:O    | 2.31                     | 0.48              |
| 1:A:781:A:O2'     | 1:A:1522:U:O2    | 2.30                     | 0.48              |
| 1:A:923:A:OP1     | 5:E:21:ALA:HB2   | 2.14                     | 0.48              |
| 6:F:23:LYS:NZ     | 6:F:42:GLU:OE2   | 2.44                     | 0.48              |
| 17:Q:29:HIS:HD2   | 17:Q:32:TYR:N    | 1.93                     | 0.48              |
| 1:A:149:A:H2'     | 1:A:150:C:H6     | 1.78                     | 0.48              |
| 1:A:1279:A:H2     | 10:J:43:ARG:HH12 | 1.60                     | 0.48              |
| 1:A:1418:A:N6     | 1:A:1482:G:O2'   | 2.46                     | 0.48              |
| 5:E:51:VAL:HB     | 5:E:52:PRO:HD3   | 1.96                     | 0.48              |
| 1:A:297:G:N2      | 1:A:300:A:OP2    | 2.43                     | 0.48              |
| 1:A:376:G:H5''    | 16:P:5:ARG:HB2   | 1.96                     | 0.48              |
| 1:A:625:G:H4'     | 16:P:16:HIS:CD2  | 2.48                     | 0.48              |
| 9:I:45:ALA:O      | 9:I:78:LYS:HE2   | 2.14                     | 0.48              |
| 10:J:54:PHE:C     | 10:J:55:LYS:HG3  | 2.38                     | 0.48              |
| 1:A:647:C:H2'     | 1:A:648:A:H8     | 1.78                     | 0.47              |
| 1:A:1018:C:H2'    | 1:A:1019:C:O4'   | 2.14                     | 0.47              |
| 1:A:1300:G:O2'    | 1:A:1301:U:P     | 2.72                     | 0.47              |
| 2:B:98:LEU:HB2    | 2:B:101:MET:HG3  | 1.95                     | 0.47              |
| 6:F:50:TYR:CE1    | 18:R:77:GLY:HA2  | 2.48                     | 0.47              |
| 9:I:24:GLY:HA2    | 9:I:59:PHE:O     | 2.14                     | 0.47              |
| 1:A:31:G:N2       | 1:A:48:C:OP1     | 2.36                     | 0.47              |
| 1:A:95:U:H2'      | 1:A:96:G:H8      | 1.79                     | 0.47              |
| 1:A:279:A:H5'     | 1:A:279:A:C8     | 2.49                     | 0.47              |
| 1:A:374:A:C6      | 1:A:375:U:C4     | 3.02                     | 0.47              |
| 1:A:983:A:O5'     | 14:N:3:ARG:NH2   | 2.48                     | 0.47              |
| 3:C:148:GLY:HA3   | 3:C:172:ARG:O    | 2.15                     | 0.47              |
| 1:A:279:A:OP1     | 1:A:280:C:O2'    | 2.29                     | 0.47              |
| 1:A:1090:U:H2'    | 1:A:1091:U:C6    | 2.48                     | 0.47              |
| 2:B:162:ILE:HG23  | 2:B:164:VAL:HG23 | 1.94                     | 0.47              |
| 8:H:4:ASP:CG      | 8:H:85:ARG:HH11  | 2.22                     | 0.47              |
| 12:L:25:PRO:HA    | 12:L:27:LEU:HB2  | 1.96                     | 0.47              |
| 13:M:2:ALA:O      | 13:M:10:PRO:HD2  | 2.15                     | 0.47              |
| 1:A:731:G:H5'     | 1:A:766:A:H4'    | 1.96                     | 0.47              |
| 1:A:953:G:H5'     | 1:A:965:A:H61    | 1.78                     | 0.47              |
| 12:L:113:ARG:HH11 | 12:L:116:SER:H   | 1.62                     | 0.47              |
| 1:A:132:C:H2'     | 1:A:133:U:H6     | 1.79                     | 0.47              |
| 1:A:1026:G:H5'    | 1:A:1027:C:OP2   | 2.14                     | 0.47              |
| 1:A:1513:A:H2'    | 1:A:1514:C:C6    | 2.49                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:36:ARG:HD2   | 4:D:38:TYR:OH    | 2.15                     | 0.47              |
| 1:A:244:U:H4'    | 1:A:245:C:H5''   | 1.97                     | 0.47              |
| 4:D:79:PHE:HE1   | 4:D:204:ILE:HD13 | 1.78                     | 0.47              |
| 9:I:118:LYS:O    | 9:I:120:ARG:N    | 2.40                     | 0.47              |
| 10:J:6:ILE:HD13  | 10:J:72:VAL:HB   | 1.96                     | 0.47              |
| 19:S:51:VAL:HG21 | 19:S:71:LEU:HD22 | 1.96                     | 0.47              |
| 21:U:6:ARG:HB2   | 21:U:15:ARG:NH2  | 2.30                     | 0.47              |
| 1:A:177:C:H2'    | 1:A:178:C:C6     | 2.50                     | 0.47              |
| 1:A:371:G:O2'    | 1:A:372:C:H5'    | 2.15                     | 0.47              |
| 7:G:15:ASP:HB3   | 7:G:19:GLY:H     | 1.80                     | 0.47              |
| 18:R:53:ARG:HD3  | 18:R:63:GLN:HB2  | 1.96                     | 0.47              |
| 1:A:1002:G:H2'   | 1:A:1003:G:C8    | 2.49                     | 0.47              |
| 1:A:1338:G:C6    | 1:A:1339:A:C6    | 3.03                     | 0.47              |
| 2:B:79:ASP:OD2   | 2:B:79:ASP:N     | 2.48                     | 0.47              |
| 7:G:65:ALA:HB1   | 7:G:127:ALA:HB3  | 1.96                     | 0.47              |
| 1:A:157:G:H2'    | 1:A:158:G:C8     | 2.50                     | 0.47              |
| 1:A:299:G:H2'    | 1:A:300:A:C8     | 2.50                     | 0.47              |
| 3:C:30:ARG:HB3   | 14:N:36:PHE:O    | 2.15                     | 0.47              |
| 16:P:43:LYS:HG2  | 16:P:48:TRP:CD2  | 2.50                     | 0.47              |
| 1:A:190(J):U:H2' | 1:A:190(K):G:C8  | 2.49                     | 0.46              |
| 1:A:960:U:H1'    | 1:A:1223:C:H5'   | 1.96                     | 0.46              |
| 1:A:972:C:P      | 10:J:57:LYS:HD3  | 2.55                     | 0.46              |
| 1:A:1031:G:H2'   | 1:A:1032:G:C8    | 2.50                     | 0.46              |
| 1:A:1278:U:H5'   | 1:A:1279:A:O4'   | 2.15                     | 0.46              |
| 2:B:25:ASN:O     | 2:B:26:PRO:C     | 2.58                     | 0.46              |
| 6:F:25:ILE:HG21  | 6:F:82:ARG:HD2   | 1.96                     | 0.46              |
| 11:K:18:ARG:HB3  | 11:K:20:TYR:CE1  | 2.50                     | 0.46              |
| 12:L:25:PRO:C    | 12:L:27:LEU:HB2  | 2.39                     | 0.46              |
| 16:P:74:LEU:O    | 16:P:79:VAL:HG23 | 2.14                     | 0.46              |
| 21:U:9:ARG:HD2   | 21:U:22:ARG:HD2  | 1.96                     | 0.46              |
| 1:A:92:C:H2'     | 1:A:93:G:C8      | 2.45                     | 0.46              |
| 1:A:556:C:H2'    | 1:A:557:G:O4'    | 2.15                     | 0.46              |
| 3:C:180:ALA:HB2  | 3:C:206:GLU:O    | 2.15                     | 0.46              |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:N    | 2.29                     | 0.46              |
| 17:Q:59:ILE:HG23 | 17:Q:71:PHE:CD1  | 2.50                     | 0.46              |
| 1:A:384:G:H2'    | 1:A:385:C:C6     | 2.50                     | 0.46              |
| 1:A:628:G:H2'    | 1:A:629:G:O4'    | 2.16                     | 0.46              |
| 1:A:1486:G:H2'   | 1:A:1487:G:O4'   | 2.14                     | 0.46              |
| 3:C:123:GLN:HG3  | 3:C:128:PHE:HD1  | 1.81                     | 0.46              |
| 16:P:43:LYS:HG2  | 16:P:48:TRP:CG   | 2.51                     | 0.46              |
| 19:S:60:VAL:HG11 | 19:S:74:PHE:HB3  | 1.98                     | 0.46              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:A:1150:U:O4      | 1:A:1151:A:N6    | 2.48                     | 0.46              |
| 1:A:1320:C:H1'     | 19:S:73:GLU:HG2  | 1.97                     | 0.46              |
| 5:E:102:ALA:HB1    | 5:E:106:PRO:HG2  | 1.98                     | 0.46              |
| 8:H:17:THR:HG22    | 8:H:63:LEU:HG    | 1.97                     | 0.46              |
| 11:K:54:ARG:H      | 11:K:54:ARG:HG2  | 1.31                     | 0.46              |
| 12:L:28:LYS:HD2    | 12:L:33:ARG:NH1  | 2.29                     | 0.46              |
| 1:A:992:U:H3       | 1:A:1044:A:H62   | 1.63                     | 0.46              |
| 1:A:1051:C:H42     | 1:A:1207:2MG:HN1 | 1.62                     | 0.46              |
| 22:A:1601:SRY:HH21 | 12:L:48:PRO:HG3  | 1.98                     | 0.46              |
| 3:C:88:ARG:HE      | 3:C:101:LEU:H    | 1.63                     | 0.46              |
| 10:J:49:VAL:HG13   | 14:N:41:ARG:HB2  | 1.97                     | 0.46              |
| 17:Q:81:ARG:HB3    | 17:Q:84:LEU:HD12 | 1.98                     | 0.46              |
| 1:A:237:C:H2'      | 1:A:238:G:C8     | 2.50                     | 0.46              |
| 4:D:86:LYS:H       | 4:D:86:LYS:HD2   | 1.79                     | 0.46              |
| 7:G:29:LYS:HD2     | 7:G:29:LYS:HA    | 1.68                     | 0.46              |
| 10:J:51:ARG:NE     | 10:J:61:GLU:HB2  | 2.31                     | 0.46              |
| 11:K:18:ARG:HD3    | 11:K:35:PRO:HA   | 1.98                     | 0.46              |
| 16:P:34:GLU:OE1    | 16:P:55:ARG:NH1  | 2.40                     | 0.46              |
| 1:A:269:C:H2'      | 1:A:270:A:H8     | 1.80                     | 0.46              |
| 1:A:688:G:O2'      | 1:A:704:A:N1     | 2.45                     | 0.46              |
| 2:B:24:TRP:HB2     | 2:B:190:THR:HG22 | 1.97                     | 0.46              |
| 2:B:95:GLN:HG3     | 2:B:147:LYS:O    | 2.15                     | 0.46              |
| 9:I:5:TYR:HE1      | 9:I:7:THR:HG1    | 1.62                     | 0.46              |
| 11:K:34:ASP:HB2    | 11:K:35:PRO:HD2  | 1.98                     | 0.46              |
| 1:A:933:G:OP2      | 7:G:3:ARG:HB3    | 2.16                     | 0.46              |
| 1:A:946:A:O2'      | 1:A:1333:A:N3    | 2.46                     | 0.46              |
| 1:A:1141:C:H2'     | 1:A:1142:G:C8    | 2.51                     | 0.46              |
| 1:A:1392:G:N2      | 1:A:1502:A:H8    | 2.12                     | 0.46              |
| 2:B:82:ARG:HG3     | 2:B:92:TYR:CZ    | 2.51                     | 0.46              |
| 3:C:119:ARG:HE     | 3:C:140:ARG:NH2  | 2.14                     | 0.46              |
| 15:O:39:LEU:CD1    | 15:O:56:LEU:HB2  | 2.40                     | 0.46              |
| 1:A:452:A:O2'      | 16:P:72:ARG:HD2  | 2.16                     | 0.46              |
| 1:A:1376:U:H2'     | 1:A:1377:A:C8    | 2.51                     | 0.46              |
| 2:B:98:LEU:HD12    | 2:B:101:MET:HE3  | 1.98                     | 0.46              |
| 6:F:97:PHE:HB2     | 18:R:32:ARG:NH1  | 2.31                     | 0.46              |
| 20:T:10:LEU:O      | 20:T:13:LEU:HD22 | 2.16                     | 0.46              |
| 20:T:87:LYS:O      | 20:T:91:LEU:HB2  | 2.16                     | 0.46              |
| 1:A:79:G:H2'       | 1:A:80:G:C8      | 2.51                     | 0.46              |
| 1:A:791:G:N2       | 1:A:792:A:H62    | 2.13                     | 0.46              |
| 1:A:939:G:H5''     | 7:G:102:ARG:HH12 | 1.81                     | 0.46              |
| 2:B:119:GLU:OE1    | 2:B:153:ARG:NH2  | 2.48                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:218:ALA:O    | 2:B:222:ILE:HG13 | 2.16                     | 0.46              |
| 7:G:9:VAL:HG12   | 7:G:10:ARG:O     | 2.16                     | 0.46              |
| 11:K:23:ALA:O    | 11:K:86:GLY:HA3  | 2.16                     | 0.46              |
| 12:L:24:VAL:HG12 | 12:L:24:VAL:O    | 2.16                     | 0.46              |
| 13:M:92:HIS:CE1  | 13:M:98:VAL:HG21 | 2.50                     | 0.46              |
| 17:Q:97:SER:O    | 17:Q:98:LEU:HD12 | 2.15                     | 0.46              |
| 18:R:58:LEU:HD13 | 18:R:62:GLU:HB3  | 1.98                     | 0.46              |
| 1:A:812:C:H4'    | 1:A:813:U:O5'    | 2.16                     | 0.45              |
| 1:A:939:G:H5''   | 7:G:102:ARG:NH1  | 2.31                     | 0.45              |
| 1:A:1031:G:H2'   | 1:A:1032:G:H8    | 1.80                     | 0.45              |
| 1:A:977:A:O2'    | 1:A:981:U:N3     | 2.40                     | 0.45              |
| 6:F:8:ILE:HD13   | 6:F:88:VAL:HG22  | 1.98                     | 0.45              |
| 2:B:178:ARG:HH21 | 8:H:74:PRO:HB3   | 1.81                     | 0.45              |
| 5:E:107:ARG:O    | 5:E:111:GLU:HB2  | 2.17                     | 0.45              |
| 9:I:95:LYS:HE3   | 9:I:95:LYS:HA    | 1.97                     | 0.45              |
| 10:J:49:VAL:HG12 | 10:J:50:ILE:O    | 2.17                     | 0.45              |
| 14:N:5:ALA:O     | 14:N:8:GLU:HB3   | 2.16                     | 0.45              |
| 14:N:29:ARG:HH12 | 14:N:41:ARG:HH11 | 1.65                     | 0.45              |
| 15:O:45:VAL:HB   | 15:O:46:HIS:ND1  | 2.31                     | 0.45              |
| 1:A:594:G:H1     | 1:A:645:C:H42    | 1.65                     | 0.45              |
| 1:A:667:G:H4'    | 15:O:51:HIS:CE1  | 2.51                     | 0.45              |
| 2:B:189:ASP:HB3  | 2:B:203:GLY:O    | 2.16                     | 0.45              |
| 4:D:190:ASP:O    | 4:D:194:LEU:HD22 | 2.17                     | 0.45              |
| 12:L:59:ARG:HD3  | 12:L:65:GLU:HG3  | 1.99                     | 0.45              |
| 15:O:26:GLU:HG3  | 15:O:81:LEU:HG   | 1.97                     | 0.45              |
| 17:Q:95:TYR:HA   | 17:Q:98:LEU:HD11 | 1.99                     | 0.45              |
| 20:T:92:LEU:O    | 20:T:96:GLY:HA2  | 2.17                     | 0.45              |
| 1:A:660:G:H1     | 1:A:745:C:H42    | 1.65                     | 0.45              |
| 2:B:167:PRO:HG3  | 2:B:186:ALA:HB1  | 1.98                     | 0.45              |
| 10:J:25:GLU:HA   | 10:J:28:ARG:HG3  | 1.98                     | 0.45              |
| 20:T:67:ALA:O    | 20:T:73:HIS:ND1  | 2.49                     | 0.45              |
| 1:A:328:C:H2'    | 1:A:328:C:O2     | 2.17                     | 0.45              |
| 1:A:357:G:C2     | 1:A:358:U:C5     | 3.04                     | 0.45              |
| 1:A:382:A:H2'    | 1:A:383:A:H8     | 1.82                     | 0.45              |
| 1:A:522:C:H41    | 12:L:53:ARG:HH22 | 1.64                     | 0.45              |
| 1:A:1040:U:H2'   | 1:A:1041:A:C8    | 2.50                     | 0.45              |
| 3:C:67:THR:HA    | 3:C:102:ASN:HB2  | 1.99                     | 0.45              |
| 9:I:28:VAL:N     | 9:I:31:GLN:O     | 2.49                     | 0.45              |
| 17:Q:29:HIS:CD2  | 17:Q:31:LEU:H    | 2.33                     | 0.45              |
| 1:A:435:C:H2'    | 1:A:436:C:C6     | 2.52                     | 0.45              |
| 1:A:587:G:O2'    | 1:A:588:G:OP2    | 2.30                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:101:LEU:O    | 4:D:105:VAL:HG23 | 2.16                     | 0.45              |
| 10:J:40:LEU:HD23 | 10:J:41:PRO:HD2  | 1.98                     | 0.45              |
| 11:K:57:THR:CG2  | 11:K:60:ALA:H    | 2.29                     | 0.45              |
| 12:L:25:PRO:CA   | 12:L:27:LEU:HB2  | 2.47                     | 0.45              |
| 21:U:5:ASP:HB3   | 21:U:8:THR:OG1   | 2.16                     | 0.45              |
| 1:A:446:G:H1     | 1:A:488:C:H42    | 1.64                     | 0.45              |
| 1:A:913:A:H1'    | 1:A:914:A:OP2    | 2.16                     | 0.45              |
| 1:A:1096:C:H2'   | 1:A:1097:C:H6    | 1.81                     | 0.45              |
| 1:A:1193:G:OP1   | 3:C:167:TRP:NE1  | 2.45                     | 0.45              |
| 3:C:112:SER:O    | 3:C:116:VAL:HG23 | 2.16                     | 0.45              |
| 9:I:93:ARG:HB3   | 9:I:93:ARG:NH1   | 2.31                     | 0.45              |
| 2:B:51:LEU:HG    | 2:B:201:ILE:HG23 | 1.99                     | 0.45              |
| 2:B:180:LEU:HA   | 2:B:180:LEU:HD23 | 1.74                     | 0.45              |
| 3:C:77:ILE:HA    | 3:C:84:ILE:HB    | 1.99                     | 0.45              |
| 3:C:188:LEU:HD23 | 3:C:196:LEU:O    | 2.17                     | 0.45              |
| 4:D:60:GLU:OE2   | 4:D:199:ASN:N    | 2.31                     | 0.45              |
| 5:E:28:PHE:CD2   | 5:E:51:VAL:HG22  | 2.52                     | 0.45              |
| 13:M:57:ARG:O    | 13:M:61:GLU:HB2  | 2.16                     | 0.45              |
| 1:A:838:G:H1     | 1:A:848:C:N4     | 2.09                     | 0.45              |
| 1:A:1502:A:H2    | 1:A:1505:G:N1    | 2.12                     | 0.45              |
| 3:C:11:ARG:NH1   | 3:C:177:THR:O    | 2.50                     | 0.45              |
| 4:D:173:TRP:CD2  | 4:D:189:PRO:HB3  | 2.52                     | 0.45              |
| 5:E:90:VAL:O     | 5:E:91:LEU:HD23  | 2.17                     | 0.45              |
| 1:A:31:G:H2'     | 1:A:48:C:N4      | 2.32                     | 0.44              |
| 1:A:390:C:O3'    | 16:P:28:ARG:NH2  | 2.50                     | 0.44              |
| 1:A:788:U:O2'    | 1:A:1539:C:O2    | 2.34                     | 0.44              |
| 1:A:1426:C:H2'   | 1:A:1427:U:C6    | 2.53                     | 0.44              |
| 2:B:43:ASP:OD2   | 2:B:45:GLN:HG2   | 2.17                     | 0.44              |
| 2:B:107:THR:O    | 2:B:110:GLN:HB2  | 2.16                     | 0.44              |
| 3:C:14:ILE:HG22  | 3:C:15:THR:HG23  | 2.00                     | 0.44              |
| 4:D:178:VAL:HG23 | 4:D:179:GLU:OE2  | 2.17                     | 0.44              |
| 13:M:63:THR:HG23 | 13:M:64:TRP:CD2  | 2.53                     | 0.44              |
| 15:O:6:GLU:OE2   | 15:O:6:GLU:N     | 2.26                     | 0.44              |
| 1:A:410:G:H2'    | 1:A:429:U:C4     | 2.52                     | 0.44              |
| 1:A:858:G:O6     | 1:A:869:G:C8     | 2.71                     | 0.44              |
| 1:A:1059:C:OP2   | 3:C:199:LYS:NZ   | 2.46                     | 0.44              |
| 1:A:89:C:H2'     | 1:A:90:U:O4'     | 2.17                     | 0.44              |
| 1:A:1124:G:H5'   | 10:J:35:SER:O    | 2.18                     | 0.44              |
| 4:D:7:PRO:HG2    | 4:D:10:ARG:HD2   | 1.99                     | 0.44              |
| 4:D:187:ARG:NH2  | 4:D:188:LEU:HD12 | 2.31                     | 0.44              |
| 5:E:88:LYS:HB3   | 5:E:123:LEU:HB2  | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 18:R:61:LYS:O    | 18:R:65:ILE:HG13 | 2.17                     | 0.44              |
| 1:A:973:G:H3'    | 1:A:974:A:H5''   | 1.99                     | 0.44              |
| 1:A:1190:G:OP1   | 3:C:4:LYS:HA     | 2.16                     | 0.44              |
| 3:C:134:ILE:O    | 3:C:138:VAL:HG23 | 2.18                     | 0.44              |
| 8:H:12:ARG:NH1   | 8:H:25:ASP:O     | 2.50                     | 0.44              |
| 8:H:113:SER:HB2  | 8:H:134:ILE:HD11 | 1.98                     | 0.44              |
| 12:L:77:LEU:HD21 | 12:L:107:ALA:HB2 | 1.98                     | 0.44              |
| 1:A:1165:C:H2'   | 1:A:1166:G:C8    | 2.51                     | 0.44              |
| 1:A:1181:G:O2'   | 1:A:1182:G:H5'   | 2.17                     | 0.44              |
| 4:D:84:LYS:HD3   | 4:D:84:LYS:HA    | 1.67                     | 0.44              |
| 14:N:26:ARG:HB3  | 14:N:43:CYS:SG   | 2.57                     | 0.44              |
| 16:P:9:PHE:CE1   | 16:P:18:ARG:HD2  | 2.53                     | 0.44              |
| 17:Q:75:ARG:HH22 | 17:Q:77:VAL:HG13 | 1.81                     | 0.44              |
| 1:A:579:G:H2'    | 1:A:580:U:H6     | 1.83                     | 0.44              |
| 1:A:1304:G:C6    | 1:A:1305:G:N1    | 2.85                     | 0.44              |
| 1:A:1286:A:H5'   | 21:U:25:LYS:NZ   | 2.33                     | 0.44              |
| 3:C:6:HIS:CD2    | 3:C:8:ILE:HB     | 2.52                     | 0.44              |
| 3:C:25:GLY:O     | 3:C:29:TYR:HB2   | 2.18                     | 0.44              |
| 3:C:83:ARG:HA    | 3:C:86:VAL:HB    | 1.99                     | 0.44              |
| 1:A:33:A:H2'     | 1:A:34:C:C6      | 2.53                     | 0.44              |
| 1:A:579:G:H2'    | 1:A:580:U:C6     | 2.52                     | 0.44              |
| 1:A:820:U:H4'    | 1:A:821:G:OP2    | 2.17                     | 0.44              |
| 1:A:1049:U:C5    | 14:N:2:ALA:HA    | 2.53                     | 0.44              |
| 1:A:1075:C:H5'   | 2:B:103:THR:HG21 | 2.00                     | 0.44              |
| 8:H:120:THR:H    | 8:H:123:GLU:HB2  | 1.83                     | 0.44              |
| 9:I:89:ASN:HB3   | 9:I:92:TYR:CE1   | 2.52                     | 0.44              |
| 13:M:2:ALA:N     | 13:M:9:ILE:HG23  | 2.32                     | 0.44              |
| 20:T:13:LEU:HD23 | 20:T:14:LYS:N    | 2.32                     | 0.44              |
| 20:T:56:MET:HG3  | 20:T:88:VAL:HG21 | 1.99                     | 0.44              |
| 20:T:89:ARG:NH2  | 20:T:105:SER:O   | 2.46                     | 0.44              |
| 1:A:1339:A:H2'   | 1:A:1340:A:O4'   | 2.18                     | 0.44              |
| 4:D:24:GLU:HG2   | 4:D:25:ARG:N     | 2.32                     | 0.44              |
| 4:D:135:LEU:HA   | 4:D:136:PRO:HD3  | 1.89                     | 0.44              |
| 7:G:50:ILE:O     | 7:G:54:THR:OG1   | 2.26                     | 0.44              |
| 12:L:46:LYS:N    | 12:L:92:ASP:O    | 2.50                     | 0.44              |
| 18:R:36:ASN:O    | 18:R:40:LEU:HG   | 2.16                     | 0.44              |
| 1:A:114:U:H1'    | 1:A:353:A:H1'    | 2.00                     | 0.43              |
| 1:A:695:A:H61    | 1:A:797:C:H1'    | 1.83                     | 0.43              |
| 1:A:1213:A:N1    | 1:A:1215:G:H1'   | 2.33                     | 0.43              |
| 2:B:119:GLU:HA   | 2:B:142:LEU:HD11 | 1.99                     | 0.43              |
| 10:J:19:SER:OG   | 10:J:91:PRO:HG3  | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:40:LEU:HD11 | 10:J:71:LEU:HB2  | 2.00                     | 0.43              |
| 18:R:36:ASN:OD1  | 18:R:39:VAL:HG12 | 2.17                     | 0.43              |
| 20:T:67:ALA:HA   | 20:T:73:HIS:N    | 2.32                     | 0.43              |
| 1:A:149:A:H2'    | 1:A:150:C:C6     | 2.52                     | 0.43              |
| 1:A:436:C:H2'    | 1:A:437:U:C6     | 2.53                     | 0.43              |
| 1:A:1257:U:OP2   | 3:C:27:LYS:NZ    | 2.50                     | 0.43              |
| 1:A:1265:G:H2'   | 1:A:1266:G:O4'   | 2.18                     | 0.43              |
| 8:H:69:ARG:HG3   | 8:H:76:PRO:HA    | 1.99                     | 0.43              |
| 18:R:53:ARG:HG2  | 18:R:63:GLN:OE1  | 2.18                     | 0.43              |
| 1:A:563:A:H2'    | 1:A:567:G:C8     | 2.54                     | 0.43              |
| 1:A:986:A:H1'    | 19:S:54:GLY:O    | 2.17                     | 0.43              |
| 1:A:1286:A:C8    | 1:A:1287:A:H4'   | 2.53                     | 0.43              |
| 1:A:1374:A:OP1   | 7:G:36:LYS:NZ    | 2.51                     | 0.43              |
| 1:A:1465:C:H2'   | 1:A:1466:C:O4'   | 2.18                     | 0.43              |
| 4:D:187:ARG:NH2  | 4:D:188:LEU:HB2  | 2.33                     | 0.43              |
| 7:G:87:VAL:HA    | 7:G:88:PRO:HD3   | 1.75                     | 0.43              |
| 20:T:91:LEU:HD13 | 20:T:91:LEU:HA   | 1.80                     | 0.43              |
| 1:A:62:U:OP1     | 1:A:385:C:O2'    | 2.34                     | 0.43              |
| 1:A:757:U:H2'    | 1:A:758:G:O4'    | 2.18                     | 0.43              |
| 1:A:860:A:H2'    | 1:A:861:G:O4'    | 2.19                     | 0.43              |
| 1:A:1163:C:H2'   | 1:A:1164:G:H8    | 1.83                     | 0.43              |
| 2:B:131:PRO:HD2  | 2:B:134:GLU:OE2  | 2.18                     | 0.43              |
| 2:B:166:ASP:HB3  | 2:B:169:LYS:HB3  | 1.99                     | 0.43              |
| 4:D:50:ARG:NH2   | 5:E:10:MET:H     | 2.17                     | 0.43              |
| 5:E:78:HIS:O     | 5:E:78:HIS:ND1   | 2.51                     | 0.43              |
| 10:J:45:ARG:HD3  | 10:J:65:LEU:HD22 | 2.01                     | 0.43              |
| 11:K:54:ARG:HB3  | 11:K:54:ARG:HH11 | 1.84                     | 0.43              |
| 18:R:21:LYS:HE3  | 18:R:24:ALA:HB2  | 2.00                     | 0.43              |
| 1:A:129:U:O3'    | 1:A:129(A):G:H3' | 2.18                     | 0.43              |
| 1:A:166:G:H2'    | 1:A:167:G:H8     | 1.84                     | 0.43              |
| 1:A:976:G:OP2    | 1:A:1358:U:H1'   | 2.19                     | 0.43              |
| 1:A:1280:A:O4'   | 10:J:41:PRO:HG3  | 2.17                     | 0.43              |
| 1:A:1347:G:O6    | 9:I:10:ARG:NH2   | 2.50                     | 0.43              |
| 4:D:159:ARG:O    | 4:D:163:GLU:HB2  | 2.18                     | 0.43              |
| 5:E:65:ASN:ND2   | 5:E:65:ASN:O     | 2.51                     | 0.43              |
| 13:M:36:LYS:HD2  | 13:M:59:TYR:OH   | 2.19                     | 0.43              |
| 14:N:53:LEU:HB3  | 14:N:56:VAL:HG21 | 2.01                     | 0.43              |
| 18:R:44:LEU:HD21 | 18:R:70:ILE:HD13 | 2.00                     | 0.43              |
| 1:A:1030:C:H2'   | 1:A:1030(A):G:C8 | 2.54                     | 0.43              |
| 1:A:1425:U:H2'   | 1:A:1426:C:H6    | 1.82                     | 0.43              |
| 1:A:1278:U:H5''  | 1:A:1279:A:OP1   | 2.19                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1287:A:H2'   | 1:A:1288:A:C8     | 2.54                     | 0.43              |
| 2:B:179:LYS:HA   | 8:H:72:PRO:HD3    | 2.00                     | 0.43              |
| 5:E:45:PHE:CE2   | 5:E:47:LYS:HD2    | 2.54                     | 0.43              |
| 12:L:75:HIS:CD2  | 12:L:77:LEU:H     | 2.37                     | 0.43              |
| 13:M:49:THR:HG22 | 13:M:51:ALA:H     | 1.83                     | 0.43              |
| 13:M:64:TRP:HB2  | 13:M:66:LEU:HD21  | 2.00                     | 0.43              |
| 1:A:260:G:H2'    | 1:A:261:U:C6      | 2.53                     | 0.43              |
| 1:A:992:U:H1'    | 1:A:993:G:OP2     | 2.19                     | 0.43              |
| 1:A:1092:A:H1'   | 1:A:1183:A:N6     | 2.34                     | 0.43              |
| 8:H:108:GLY:HA3  | 8:H:138:TRP:HB3   | 2.01                     | 0.43              |
| 10:J:24:VAL:HG13 | 10:J:34:VAL:HG11  | 2.01                     | 0.43              |
| 1:A:129(A):G:H1' | 1:A:190(E):U:H2'  | 2.00                     | 0.43              |
| 1:A:528:C:H41    | 12:L:49:ASN:ND2   | 2.16                     | 0.43              |
| 1:A:1296:C:H4'   | 1:A:1302:U:H5     | 1.82                     | 0.43              |
| 15:O:85:LEU:HD23 | 15:O:85:LEU:HA    | 1.77                     | 0.43              |
| 20:T:11:SER:HA   | 20:T:13:LEU:HD22  | 2.01                     | 0.43              |
| 1:A:436:C:H2'    | 1:A:437:U:H6      | 1.83                     | 0.43              |
| 1:A:767:A:H2'    | 1:A:768:A:O4'     | 2.19                     | 0.43              |
| 5:E:102:ALA:O    | 5:E:107:ARG:NH1   | 2.52                     | 0.43              |
| 17:Q:22:LEU:HD13 | 17:Q:41:LYS:HG3   | 2.01                     | 0.43              |
| 1:A:105:G:OP1    | 20:T:22:ARG:NH2   | 2.51                     | 0.42              |
| 1:A:1227:A:N3    | 13:M:117:VAL:HG21 | 2.34                     | 0.42              |
| 2:B:106:LYS:HA   | 2:B:109:SER:HB3   | 2.01                     | 0.42              |
| 2:B:220:ASP:CG   | 2:B:230:VAL:HG21  | 2.44                     | 0.42              |
| 5:E:137:GLU:O    | 5:E:141:GLN:HG3   | 2.19                     | 0.42              |
| 13:M:96:LEU:HB3  | 13:M:97:PRO:HD2   | 2.01                     | 0.42              |
| 1:A:1168:A:H2'   | 1:A:1169:A:C8     | 2.54                     | 0.42              |
| 2:B:96:ARG:NH1   | 2:B:97:TRP:H      | 2.18                     | 0.42              |
| 20:T:56:MET:HG2  | 20:T:84:LEU:HD13  | 2.02                     | 0.42              |
| 1:A:10:A:OP2     | 5:E:126:ARG:HD2   | 2.19                     | 0.42              |
| 1:A:359:U:H2'    | 1:A:360:A:H8      | 1.83                     | 0.42              |
| 1:A:380:G:N2     | 1:A:382:A:H3'     | 2.34                     | 0.42              |
| 1:A:1139:G:H1'   | 1:A:1140:C:C5     | 2.55                     | 0.42              |
| 2:B:92:TYR:CE1   | 2:B:94:ASN:HB2    | 2.54                     | 0.42              |
| 11:K:95:ILE:HD13 | 11:K:108:ILE:HG21 | 2.01                     | 0.42              |
| 1:A:811:C:O2'    | 1:A:901:A:N1      | 2.48                     | 0.42              |
| 3:C:36:ASP:OD2   | 3:C:59:ARG:NH2    | 2.51                     | 0.42              |
| 9:I:48:GLU:N     | 9:I:49:PRO:HD2    | 2.34                     | 0.42              |
| 17:Q:56:VAL:CG2  | 17:Q:81:ARG:HG3   | 2.50                     | 0.42              |
| 1:A:325:A:H2'    | 1:A:326:G:O4'     | 2.19                     | 0.42              |
| 1:A:370:C:H2'    | 1:A:371:G:C8      | 2.55                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:412:A:H1'     | 4:D:35:ARG:HH22  | 1.85                     | 0.42              |
| 1:A:750:G:N3      | 15:O:23:GLY:HA3  | 2.35                     | 0.42              |
| 1:A:895:G:H2'     | 1:A:896:C:C6     | 2.54                     | 0.42              |
| 1:A:932:C:H5'     | 7:G:4:ARG:HG2    | 2.01                     | 0.42              |
| 4:D:35:ARG:C      | 4:D:36:ARG:HG2   | 2.44                     | 0.42              |
| 1:A:186:C:H2'     | 1:A:187:C:C6     | 2.54                     | 0.42              |
| 1:A:263:A:OP2     | 20:T:79:ARG:NH1  | 2.52                     | 0.42              |
| 1:A:877:C:O2'     | 8:H:3:THR:HG23   | 2.20                     | 0.42              |
| 1:A:1003(A):G:N2  | 1:A:1038:C:O2'   | 2.53                     | 0.42              |
| 1:A:1190:G:H5'    | 3:C:176:HIS:CE1  | 2.54                     | 0.42              |
| 1:A:1299:A:C8     | 1:A:1301:U:H1'   | 2.53                     | 0.42              |
| 2:B:21:ARG:HA     | 2:B:39:ILE:HG23  | 2.00                     | 0.42              |
| 10:J:32:ALA:HB3   | 10:J:75:ILE:O    | 2.18                     | 0.42              |
| 17:Q:40:LYS:HG2   | 17:Q:42:TYR:CE1  | 2.54                     | 0.42              |
| 17:Q:59:ILE:HA    | 17:Q:59:ILE:HD12 | 1.81                     | 0.42              |
| 1:A:839:U:H5'     | 1:A:840:C:C5     | 2.55                     | 0.42              |
| 3:C:50:ALA:HB2    | 3:C:75:VAL:HB    | 2.02                     | 0.42              |
| 4:D:24:GLU:O      | 4:D:25:ARG:HB3   | 2.19                     | 0.42              |
| 7:G:155:ARG:HA    | 7:G:155:ARG:HD3  | 1.78                     | 0.42              |
| 8:H:54:ASP:O      | 8:H:56:LYS:HG2   | 2.18                     | 0.42              |
| 9:I:48:GLU:OE2    | 9:I:51:ARG:NH1   | 2.48                     | 0.42              |
| 9:I:93:ARG:HH22   | 9:I:97:LYS:NZ    | 2.16                     | 0.42              |
| 11:K:18:ARG:HB3   | 11:K:20:TYR:HE1  | 1.84                     | 0.42              |
| 19:S:41:VAL:HG22  | 19:S:44:MET:HE3  | 2.02                     | 0.42              |
| 20:T:83:ARG:O     | 20:T:87:LYS:HB2  | 2.19                     | 0.42              |
| 1:A:532:A:O2'     | 1:A:533:A:OP1    | 2.23                     | 0.42              |
| 22:A:1601:SRY:CH2 | 12:L:48:PRO:HG3  | 2.49                     | 0.42              |
| 10:J:38:ILE:H     | 10:J:38:ILE:HG13 | 1.55                     | 0.42              |
| 19:S:16:LEU:O     | 19:S:20:LEU:HG   | 2.20                     | 0.42              |
| 1:A:47:C:C6       | 1:A:365:U:H2'    | 2.55                     | 0.42              |
| 1:A:949:A:OP2     | 13:M:106:ASN:ND2 | 2.53                     | 0.42              |
| 1:A:1070:U:H2'    | 1:A:1071:C:H6    | 1.85                     | 0.42              |
| 1:A:1135:U:H4'    | 1:A:1136:U:C5    | 2.47                     | 0.42              |
| 1:A:1241:G:H2'    | 1:A:1242:C:H6    | 1.82                     | 0.42              |
| 3:C:91:LEU:HD21   | 3:C:99:VAL:HG22  | 2.01                     | 0.42              |
| 6:F:2:ARG:O       | 6:F:66:GLU:HA    | 2.19                     | 0.42              |
| 1:A:142:G:O2'     | 1:A:196:A:N1     | 2.46                     | 0.42              |
| 1:A:989:C:N4      | 1:A:1216:G:H1    | 2.16                     | 0.42              |
| 1:A:1118:C:H2'    | 1:A:1119:C:H6    | 1.84                     | 0.42              |
| 3:C:72:LYS:HE2    | 3:C:72:LYS:HB3   | 1.94                     | 0.42              |
| 3:C:79:ARG:HG3    | 3:C:82:GLU:HB2   | 2.02                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:176:LEU:HD12 | 4:D:182:LYS:O     | 2.20                     | 0.42              |
| 5:E:71:LEU:HD21  | 5:E:115:VAL:HG22  | 2.01                     | 0.42              |
| 16:P:3:LYS:HB3   | 16:P:3:LYS:HE2    | 1.63                     | 0.42              |
| 17:Q:12:SER:HB3  | 17:Q:20:THR:CB    | 2.48                     | 0.42              |
| 17:Q:27:PHE:CE1  | 17:Q:36:ILE:HD11  | 2.55                     | 0.42              |
| 19:S:5:LEU:H     | 19:S:5:LEU:HG     | 1.71                     | 0.42              |
| 1:A:779:C:H2'    | 1:A:780:A:O4'     | 2.20                     | 0.41              |
| 1:A:858:G:N7     | 25:A:2098:HOH:O   | 2.37                     | 0.41              |
| 1:A:1000:U:H2'   | 1:A:1001:A:C8     | 2.55                     | 0.41              |
| 1:A:1148:U:C4    | 1:A:1149:C:C2     | 3.08                     | 0.41              |
| 1:A:1229:A:N6    | 13:M:105:THR:HG22 | 2.35                     | 0.41              |
| 2:B:83:MET:HB2   | 2:B:235:SER:OG    | 2.20                     | 0.41              |
| 4:D:105:VAL:HG13 | 4:D:110:PHE:HB2   | 2.01                     | 0.41              |
| 7:G:78:ARG:NH1   | 7:G:154:TYR:O     | 2.53                     | 0.41              |
| 13:M:27:LYS:HA   | 13:M:27:LYS:HD2   | 1.85                     | 0.41              |
| 17:Q:52:LYS:N    | 17:Q:55:ASP:OD2   | 2.50                     | 0.41              |
| 2:B:221:LEU:HD23 | 2:B:221:LEU:HA    | 1.93                     | 0.41              |
| 8:H:90:GLY:O     | 17:Q:34:LYS:HE2   | 2.20                     | 0.41              |
| 9:I:89:ASN:HB3   | 9:I:92:TYR:CD1    | 2.55                     | 0.41              |
| 11:K:92:GLU:HB3  | 11:K:96:ARG:HH22  | 1.84                     | 0.41              |
| 1:A:335:C:H2'    | 1:A:336:C:H6      | 1.86                     | 0.41              |
| 1:A:1203:C:HO2'  | 1:A:1204:A:P      | 2.43                     | 0.41              |
| 1:A:1361(A):C:O2 | 1:A:1362:C:H5     | 2.03                     | 0.41              |
| 2:B:210:SER:O    | 2:B:214:ILE:HG12  | 2.21                     | 0.41              |
| 3:C:56:ASP:O     | 3:C:66:VAL:HA     | 2.19                     | 0.41              |
| 1:A:341:C:H2'    | 1:A:342:C:H6      | 1.85                     | 0.41              |
| 1:A:344:A:H5''   | 1:A:345:C:H5      | 1.85                     | 0.41              |
| 1:A:1126:U:H6    | 1:A:1126:U:O5'    | 2.03                     | 0.41              |
| 2:B:102:LEU:HD21 | 2:B:162:ILE:HD11  | 2.01                     | 0.41              |
| 5:E:75:THR:HG23  | 5:E:76:ILE:O      | 2.20                     | 0.41              |
| 6:F:4:TYR:CZ     | 6:F:72:VAL:HG21   | 2.56                     | 0.41              |
| 9:I:60:ASP:OD1   | 9:I:61:ALA:N      | 2.53                     | 0.41              |
| 10:J:81:THR:O    | 10:J:85:LEU:HB2   | 2.20                     | 0.41              |
| 1:A:45:U:H2'     | 1:A:46:G:C8       | 2.55                     | 0.41              |
| 1:A:216:G:H2'    | 1:A:217:C:H6      | 1.85                     | 0.41              |
| 1:A:522:C:N4     | 12:L:53:ARG:HH22  | 2.19                     | 0.41              |
| 1:A:1321:C:H2'   | 1:A:1322:C:C5     | 2.56                     | 0.41              |
| 2:B:185:ILE:HA   | 2:B:199:TYR:O     | 2.21                     | 0.41              |
| 7:G:31:MET:SD    | 7:G:36:LYS:HB2    | 2.61                     | 0.41              |
| 7:G:122:HIS:HA   | 7:G:125:MET:HG2   | 2.03                     | 0.41              |
| 8:H:53:VAL:HB    | 8:H:58:TYR:CD1    | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:K:38:ASN:HA   | 11:K:39:PRO:HD3  | 1.88                     | 0.41              |
| 13:M:90:LEU:HD12 | 13:M:93:ARG:HH21 | 1.85                     | 0.41              |
| 16:P:11:SER:H    | 16:P:14:ASN:HB3  | 1.85                     | 0.41              |
| 17:Q:18:THR:HG23 | 17:Q:69:LYS:HE3  | 2.03                     | 0.41              |
| 20:T:14:LYS:O    | 20:T:18:GLN:HG3  | 2.20                     | 0.41              |
| 1:A:232:G:H1'    | 1:A:262:A:N1     | 2.36                     | 0.41              |
| 1:A:235:C:C5'    | 17:Q:70:ARG:HG3  | 2.50                     | 0.41              |
| 1:A:619:U:H3     | 4:D:134:ASP:CG   | 2.28                     | 0.41              |
| 1:A:826:C:H2'    | 1:A:827:U:C6     | 2.56                     | 0.41              |
| 1:A:938:A:N6     | 1:A:939:G:C6     | 2.88                     | 0.41              |
| 10:J:32:ALA:HB2  | 10:J:76:ASN:HB2  | 2.01                     | 0.41              |
| 10:J:64:GLU:HB3  | 14:N:59:ALA:HB2  | 2.02                     | 0.41              |
| 17:Q:3:LYS:H     | 17:Q:3:LYS:HG2   | 1.72                     | 0.41              |
| 1:A:448:A:P      | 1:A:485:G:H22    | 2.44                     | 0.41              |
| 1:A:998:G:H2'    | 1:A:999:C:C6     | 2.56                     | 0.41              |
| 1:A:1305:G:H22   | 1:A:1331:G:H1'   | 1.84                     | 0.41              |
| 1:A:1406:U:O2'   | 1:A:1517:G:N2    | 2.53                     | 0.41              |
| 5:E:78:HIS:HD1   | 5:E:78:HIS:C     | 2.29                     | 0.41              |
| 8:H:17:THR:HA    | 8:H:65:TYR:OH    | 2.21                     | 0.41              |
| 16:P:40:ASP:HA   | 16:P:41:PRO:HD2  | 1.89                     | 0.41              |
| 1:A:78:G:C2      | 1:A:92:C:C2      | 3.09                     | 0.41              |
| 1:A:1281:U:H3'   | 1:A:1282:C:H6    | 1.86                     | 0.41              |
| 1:A:1366:C:H2'   | 1:A:1367:C:H6    | 1.84                     | 0.41              |
| 2:B:25:ASN:O     | 2:B:27:LYS:N     | 2.53                     | 0.41              |
| 2:B:195:ASP:O    | 8:H:74:PRO:HG3   | 2.20                     | 0.41              |
| 7:G:46:ALA:O     | 7:G:50:ILE:HG13  | 2.20                     | 0.41              |
| 7:G:88:PRO:HG3   | 7:G:148:ASN:CB   | 2.51                     | 0.41              |
| 7:G:145:ALA:C    | 7:G:147:ALA:H    | 2.29                     | 0.41              |
| 12:L:126:LYS:HD3 | 12:L:126:LYS:HA  | 1.82                     | 0.41              |
| 13:M:69:GLU:H    | 13:M:69:GLU:CD   | 2.28                     | 0.41              |
| 17:Q:63:ARG:O    | 17:Q:65:ILE:HD12 | 2.21                     | 0.41              |
| 20:T:73:HIS:HB3  | 20:T:74:LYS:H    | 1.67                     | 0.41              |
| 1:A:567:G:H2'    | 1:A:568:G:O4'    | 2.21                     | 0.41              |
| 1:A:651:C:O2'    | 1:A:652:U:H5'    | 2.21                     | 0.41              |
| 1:A:1106:G:H5''  | 3:C:172:ARG:HD2  | 2.03                     | 0.41              |
| 1:A:1291:G:H2'   | 1:A:1292:U:C6    | 2.56                     | 0.41              |
| 1:A:1349:A:OP1   | 9:I:118:LYS:HD2  | 2.21                     | 0.41              |
| 2:B:24:TRP:CH2   | 2:B:26:PRO:HA    | 2.55                     | 0.41              |
| 2:B:208:ILE:H    | 2:B:208:ILE:HG13 | 1.56                     | 0.41              |
| 5:E:18:ARG:HG2   | 5:E:19:MET:N     | 2.32                     | 0.41              |
| 5:E:31:LEU:HD23  | 5:E:31:LEU:HA    | 1.78                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:65:ASN:O     | 5:E:65:ASN:CG    | 2.63                     | 0.41              |
| 5:E:76:ILE:HA    | 5:E:77:PRO:HD3   | 1.90                     | 0.41              |
| 8:H:122:ARG:NH1  | 8:H:122:ARG:HB2  | 2.36                     | 0.41              |
| 16:P:22:THR:HA   | 16:P:33:ILE:HD12 | 2.03                     | 0.41              |
| 18:R:52:PRO:HG3  | 18:R:54:ARG:HH21 | 1.86                     | 0.41              |
| 1:A:485:G:O2'    | 1:A:486:U:P      | 2.77                     | 0.41              |
| 1:A:507:C:OP2    | 1:A:508:C:O2'    | 2.36                     | 0.41              |
| 1:A:620:C:H2'    | 1:A:621:A:O4'    | 2.21                     | 0.41              |
| 1:A:971:G:H1'    | 1:A:1365:G:O2'   | 2.21                     | 0.41              |
| 2:B:74:LYS:HB2   | 2:B:77:ALA:HB3   | 2.03                     | 0.41              |
| 4:D:79:PHE:CE1   | 4:D:204:ILE:HD13 | 2.55                     | 0.41              |
| 4:D:162:LEU:HD23 | 4:D:162:LEU:HA   | 1.86                     | 0.41              |
| 7:G:89:MET:HE2   | 7:G:89:MET:HB3   | 1.88                     | 0.41              |
| 8:H:20:TYR:HA    | 8:H:65:TYR:CE2   | 2.56                     | 0.41              |
| 8:H:87:SER:HA    | 8:H:93:VAL:HG13  | 2.02                     | 0.41              |
| 8:H:105:ARG:HD3  | 8:H:105:ARG:HA   | 1.83                     | 0.41              |
| 1:A:838:G:N2     | 1:A:849:C:C2     | 2.89                     | 0.40              |
| 1:A:1003(A):G:C5 | 1:A:1004:A:H1'   | 2.55                     | 0.40              |
| 1:A:1300:G:HO2'  | 1:A:1301:U:P     | 2.41                     | 0.40              |
| 1:A:1321:C:H4'   | 13:M:87:TYR:CZ   | 2.56                     | 0.40              |
| 4:D:98:GLU:O     | 4:D:103:ASN:ND2  | 2.54                     | 0.40              |
| 10:J:48:THR:OG1  | 10:J:62:HIS:ND1  | 2.51                     | 0.40              |
| 16:P:60:LEU:HA   | 16:P:60:LEU:HD23 | 1.75                     | 0.40              |
| 17:Q:75:ARG:NH2  | 17:Q:77:VAL:HG13 | 2.36                     | 0.40              |
| 18:R:26:LEU:HD12 | 18:R:26:LEU:HA   | 1.77                     | 0.40              |
| 20:T:10:LEU:HD13 | 20:T:12:ALA:H    | 1.86                     | 0.40              |
| 1:A:51:A:H4'     | 1:A:52:G:C5'     | 2.51                     | 0.40              |
| 1:A:204:U:H4'    | 1:A:216:G:O4'    | 2.21                     | 0.40              |
| 1:A:217:C:H2'    | 1:A:218:C:H6     | 1.86                     | 0.40              |
| 1:A:411:A:N7     | 1:A:413:G:N3     | 2.69                     | 0.40              |
| 1:A:1145:C:O2'   | 1:A:1146:A:H8    | 2.04                     | 0.40              |
| 2:B:100:GLY:N    | 2:B:176:GLU:OE2  | 2.50                     | 0.40              |
| 3:C:111:LEU:HD21 | 3:C:144:SER:O    | 2.21                     | 0.40              |
| 3:C:113:ALA:N    | 3:C:114:PRO:HD2  | 2.37                     | 0.40              |
| 5:E:72:GLN:O     | 5:E:75:THR:HG22  | 2.21                     | 0.40              |
| 20:T:87:LYS:HB2  | 20:T:87:LYS:HE3  | 1.74                     | 0.40              |
| 1:A:783:C:H2'    | 1:A:784:C:H6     | 1.85                     | 0.40              |
| 1:A:1118:C:H5'   | 9:I:104:ARG:HG3  | 2.03                     | 0.40              |
| 1:A:1276:G:H2'   | 1:A:1277:C:C6    | 2.56                     | 0.40              |
| 2:B:145:LEU:HD23 | 2:B:145:LEU:HA   | 1.92                     | 0.40              |
| 4:D:108:LEU:HD23 | 4:D:174:LEU:HD13 | 2.04                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:63:LYS:HB2   | 7:G:63:LYS:HE3   | 1.83                     | 0.40              |
| 9:I:3:GLN:HG3    | 9:I:20:ARG:HG2   | 2.02                     | 0.40              |
| 15:O:26:GLU:OE1  | 15:O:77:ARG:HD2  | 2.21                     | 0.40              |
| 15:O:53:HIS:O    | 15:O:56:LEU:HB3  | 2.21                     | 0.40              |
| 1:A:6:G:H4'      | 1:A:298:A:H4'    | 2.03                     | 0.40              |
| 1:A:926:G:H3'    | 1:A:1505:G:H21   | 1.86                     | 0.40              |
| 1:A:1139:G:HO2'  | 1:A:1140:C:P     | 2.44                     | 0.40              |
| 1:A:1321:C:O2'   | 19:S:78:ARG:NH1  | 2.54                     | 0.40              |
| 2:B:127:ILE:H    | 2:B:127:ILE:HG13 | 1.54                     | 0.40              |
| 2:B:177:ALA:HB1  | 2:B:182:ILE:HB   | 2.02                     | 0.40              |
| 6:F:33:TYR:HD2   | 6:F:71:ARG:HE    | 1.69                     | 0.40              |
| 6:F:95:GLU:HA    | 6:F:96:PRO:HD3   | 1.90                     | 0.40              |
| 13:M:114:ARG:H   | 13:M:114:ARG:HG2 | 1.51                     | 0.40              |
| 17:Q:31:LEU:HD12 | 17:Q:31:LEU:HA   | 1.89                     | 0.40              |
| 1:A:445:G:H2'    | 1:A:446:G:C8     | 2.56                     | 0.40              |
| 1:A:579:G:H4'    | 15:O:54:ARG:HH21 | 1.87                     | 0.40              |
| 1:A:1250:A:N1    | 1:A:1353:G:N2    | 2.64                     | 0.40              |
| 5:E:79:GLU:HB3   | 5:E:92:LYS:HG2   | 2.04                     | 0.40              |
| 7:G:125:MET:HE3  | 7:G:125:MET:HB2  | 1.96                     | 0.40              |
| 11:K:19:ALA:HB3  | 11:K:82:VAL:HG22 | 2.03                     | 0.40              |
| 11:K:54:ARG:O    | 11:K:57:THR:HG22 | 2.21                     | 0.40              |
| 20:T:74:LYS:HB3  | 20:T:75:ASN:H    | 1.57                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2   | B     | 232/256 (91%) | 210 (90%) | 19 (8%)  | 3 (1%)   | 9           | 32  |
| 3   | C     | 204/239 (85%) | 182 (89%) | 21 (10%) | 1 (0%)   | 24          | 52  |
| 4   | D     | 206/209 (99%) | 198 (96%) | 8 (4%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 5   | E     | 148/162 (91%)   | 141 (95%)  | 6 (4%)   | 1 (1%)   | 18          | 46  |
| 6   | F     | 99/101 (98%)    | 97 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 7   | G     | 153/156 (98%)   | 145 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 8   | H     | 136/138 (99%)   | 133 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 9   | I     | 125/128 (98%)   | 113 (90%)  | 12 (10%) | 0        | 100         | 100 |
| 10  | J     | 96/105 (91%)    | 82 (85%)   | 13 (14%) | 1 (1%)   | 12          | 38  |
| 11  | K     | 114/129 (88%)   | 105 (92%)  | 9 (8%)   | 0        | 100         | 100 |
| 12  | L     | 122/135 (90%)   | 109 (89%)  | 13 (11%) | 0        | 100         | 100 |
| 13  | M     | 116/126 (92%)   | 104 (90%)  | 12 (10%) | 0        | 100         | 100 |
| 14  | N     | 58/61 (95%)     | 54 (93%)   | 3 (5%)   | 1 (2%)   | 7           | 27  |
| 15  | O     | 85/89 (96%)     | 82 (96%)   | 2 (2%)   | 1 (1%)   | 10          | 33  |
| 16  | P     | 81/88 (92%)     | 77 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 17  | Q     | 97/105 (92%)    | 93 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 18  | R     | 68/88 (77%)     | 64 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 19  | S     | 78/93 (84%)     | 72 (92%)   | 5 (6%)   | 1 (1%)   | 9           | 32  |
| 20  | T     | 97/106 (92%)    | 88 (91%)   | 9 (9%)   | 0        | 100         | 100 |
| 21  | U     | 22/27 (82%)     | 20 (91%)   | 2 (9%)   | 0        | 100         | 100 |
| All | All   | 2337/2541 (92%) | 2169 (93%) | 159 (7%) | 9 (0%)   | 30          | 58  |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | S     | 31  | ILE  |
| 2   | B     | 21  | ARG  |
| 2   | B     | 24  | TRP  |
| 5   | E     | 16  | THR  |
| 14  | N     | 23  | ARG  |
| 10  | J     | 34  | VAL  |
| 2   | B     | 229 | VAL  |
| 3   | C     | 66  | VAL  |
| 15  | O     | 45  | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

resolution.

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 2   | B     | 202/220 (92%)   | 174 (86%)  | 28 (14%)  | 3           | 14 |
| 3   | C     | 160/188 (85%)   | 137 (86%)  | 23 (14%)  | 3           | 13 |
| 4   | D     | 180/181 (99%)   | 156 (87%)  | 24 (13%)  | 4           | 15 |
| 5   | E     | 115/123 (94%)   | 98 (85%)   | 17 (15%)  | 3           | 12 |
| 6   | F     | 90/90 (100%)    | 78 (87%)   | 12 (13%)  | 4           | 15 |
| 7   | G     | 126/127 (99%)   | 117 (93%)  | 9 (7%)    | 13          | 39 |
| 8   | H     | 119/119 (100%)  | 109 (92%)  | 10 (8%)   | 10          | 34 |
| 9   | I     | 98/99 (99%)     | 83 (85%)   | 15 (15%)  | 3           | 10 |
| 10  | J     | 87/92 (95%)     | 74 (85%)   | 13 (15%)  | 3           | 12 |
| 11  | K     | 88/99 (89%)     | 77 (88%)   | 11 (12%)  | 4           | 17 |
| 12  | L     | 104/111 (94%)   | 85 (82%)   | 19 (18%)  | 2           | 7  |
| 13  | M     | 94/101 (93%)    | 76 (81%)   | 18 (19%)  | 1           | 6  |
| 14  | N     | 49/50 (98%)     | 38 (78%)   | 11 (22%)  | 1           | 3  |
| 15  | O     | 79/80 (99%)     | 63 (80%)   | 16 (20%)  | 1           | 4  |
| 16  | P     | 72/74 (97%)     | 66 (92%)   | 6 (8%)    | 10          | 35 |
| 17  | Q     | 94/97 (97%)     | 84 (89%)   | 10 (11%)  | 6           | 23 |
| 18  | R     | 61/77 (79%)     | 54 (88%)   | 7 (12%)   | 5           | 20 |
| 19  | S     | 71/80 (89%)     | 62 (87%)   | 9 (13%)   | 4           | 17 |
| 20  | T     | 76/82 (93%)     | 64 (84%)   | 12 (16%)  | 2           | 10 |
| 21  | U     | 19/22 (86%)     | 16 (84%)   | 3 (16%)   | 2           | 10 |
| All | All   | 1984/2112 (94%) | 1711 (86%) | 273 (14%) | 3           | 14 |

All (273) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 7   | VAL  |
| 2   | B     | 11  | LEU  |
| 2   | B     | 12  | GLU  |
| 2   | B     | 30  | ARG  |
| 2   | B     | 44  | LEU  |
| 2   | B     | 60  | ASP  |
| 2   | B     | 61  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 74  | LYS  |
| 2   | B     | 79  | ASP  |
| 2   | B     | 96  | ARG  |
| 2   | B     | 102 | LEU  |
| 2   | B     | 107 | THR  |
| 2   | B     | 108 | ILE  |
| 2   | B     | 119 | GLU  |
| 2   | B     | 126 | GLU  |
| 2   | B     | 127 | ILE  |
| 2   | B     | 142 | LEU  |
| 2   | B     | 150 | SER  |
| 2   | B     | 153 | ARG  |
| 2   | B     | 157 | ARG  |
| 2   | B     | 162 | ILE  |
| 2   | B     | 168 | THR  |
| 2   | B     | 170 | GLU  |
| 2   | B     | 187 | LEU  |
| 2   | B     | 190 | THR  |
| 2   | B     | 208 | ILE  |
| 2   | B     | 221 | LEU  |
| 2   | B     | 231 | GLU  |
| 3   | C     | 3   | ASN  |
| 3   | C     | 5   | ILE  |
| 3   | C     | 19  | GLU  |
| 3   | C     | 34  | LEU  |
| 3   | C     | 58  | GLU  |
| 3   | C     | 64  | VAL  |
| 3   | C     | 75  | VAL  |
| 3   | C     | 91  | LEU  |
| 3   | C     | 94  | LEU  |
| 3   | C     | 95  | THR  |
| 3   | C     | 99  | VAL  |
| 3   | C     | 111 | LEU  |
| 3   | C     | 119 | ARG  |
| 3   | C     | 143 | GLU  |
| 3   | C     | 147 | LYS  |
| 3   | C     | 153 | VAL  |
| 3   | C     | 167 | TRP  |
| 3   | C     | 175 | LEU  |
| 3   | C     | 178 | LEU  |
| 3   | C     | 188 | LEU  |
| 3   | C     | 195 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 196 | LEU  |
| 3   | C     | 207 | VAL  |
| 4   | D     | 8   | VAL  |
| 4   | D     | 10  | ARG  |
| 4   | D     | 19  | LEU  |
| 4   | D     | 28  | SER  |
| 4   | D     | 35  | ARG  |
| 4   | D     | 53  | ASP  |
| 4   | D     | 64  | LEU  |
| 4   | D     | 76  | ARG  |
| 4   | D     | 78  | LEU  |
| 4   | D     | 86  | LYS  |
| 4   | D     | 96  | LEU  |
| 4   | D     | 108 | LEU  |
| 4   | D     | 121 | VAL  |
| 4   | D     | 122 | ARG  |
| 4   | D     | 127 | THR  |
| 4   | D     | 141 | ARG  |
| 4   | D     | 151 | LYS  |
| 4   | D     | 152 | SER  |
| 4   | D     | 160 | GLN  |
| 4   | D     | 178 | VAL  |
| 4   | D     | 187 | ARG  |
| 4   | D     | 191 | ARG  |
| 4   | D     | 194 | LEU  |
| 4   | D     | 201 | GLN  |
| 5   | E     | 12  | LEU  |
| 5   | E     | 14  | ARG  |
| 5   | E     | 15  | ARG  |
| 5   | E     | 18  | ARG  |
| 5   | E     | 31  | LEU  |
| 5   | E     | 41  | VAL  |
| 5   | E     | 43  | LEU  |
| 5   | E     | 63  | ARG  |
| 5   | E     | 64  | ARG  |
| 5   | E     | 76  | ILE  |
| 5   | E     | 79  | GLU  |
| 5   | E     | 80  | ILE  |
| 5   | E     | 82  | VAL  |
| 5   | E     | 125 | SER  |
| 5   | E     | 131 | ILE  |
| 5   | E     | 147 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 151 | LEU  |
| 6   | F     | 3   | ARG  |
| 6   | F     | 10  | LEU  |
| 6   | F     | 14  | LEU  |
| 6   | F     | 15  | ASP  |
| 6   | F     | 19  | LEU  |
| 6   | F     | 24  | GLU  |
| 6   | F     | 26  | ILE  |
| 6   | F     | 32  | ASN  |
| 6   | F     | 43  | LEU  |
| 6   | F     | 70  | ASP  |
| 6   | F     | 75  | LEU  |
| 6   | F     | 95  | GLU  |
| 7   | G     | 4   | ARG  |
| 7   | G     | 12  | LEU  |
| 7   | G     | 41  | ARG  |
| 7   | G     | 51  | GLN  |
| 7   | G     | 56  | GLN  |
| 7   | G     | 80  | VAL  |
| 7   | G     | 84  | ASN  |
| 7   | G     | 90  | GLU  |
| 7   | G     | 113 | GLU  |
| 8   | H     | 11  | THR  |
| 8   | H     | 23  | SER  |
| 8   | H     | 26  | VAL  |
| 8   | H     | 63  | LEU  |
| 8   | H     | 85  | ARG  |
| 8   | H     | 91  | ARG  |
| 8   | H     | 93  | VAL  |
| 8   | H     | 98  | LYS  |
| 8   | H     | 129 | VAL  |
| 8   | H     | 133 | LEU  |
| 9   | I     | 12  | GLU  |
| 9   | I     | 18  | PHE  |
| 9   | I     | 26  | VAL  |
| 9   | I     | 27  | THR  |
| 9   | I     | 29  | ASN  |
| 9   | I     | 40  | LEU  |
| 9   | I     | 41  | VAL  |
| 9   | I     | 53  | VAL  |
| 9   | I     | 59  | PHE  |
| 9   | I     | 79  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | I     | 86  | VAL  |
| 9   | I     | 95  | LYS  |
| 9   | I     | 118 | LYS  |
| 9   | I     | 127 | LYS  |
| 9   | I     | 128 | ARG  |
| 10  | J     | 5   | ARG  |
| 10  | J     | 8   | LEU  |
| 10  | J     | 15  | THR  |
| 10  | J     | 24  | VAL  |
| 10  | J     | 28  | ARG  |
| 10  | J     | 38  | ILE  |
| 10  | J     | 40  | LEU  |
| 10  | J     | 62  | HIS  |
| 10  | J     | 74  | ILE  |
| 10  | J     | 82  | ILE  |
| 10  | J     | 96  | ILE  |
| 10  | J     | 97  | GLU  |
| 10  | J     | 98  | ILE  |
| 11  | K     | 12  | ARG  |
| 11  | K     | 13  | GLN  |
| 11  | K     | 14  | VAL  |
| 11  | K     | 18  | ARG  |
| 11  | K     | 29  | ILE  |
| 11  | K     | 40  | ILE  |
| 11  | K     | 41  | THR  |
| 11  | K     | 54  | ARG  |
| 11  | K     | 75  | TYR  |
| 11  | K     | 98  | LEU  |
| 11  | K     | 109 | VAL  |
| 12  | L     | 6   | THR  |
| 12  | L     | 7   | ILE  |
| 12  | L     | 18  | VAL  |
| 12  | L     | 20  | LYS  |
| 12  | L     | 33  | ARG  |
| 12  | L     | 43  | VAL  |
| 12  | L     | 44  | THR  |
| 12  | L     | 47  | LYS  |
| 12  | L     | 58  | VAL  |
| 12  | L     | 67  | THR  |
| 12  | L     | 75  | HIS  |
| 12  | L     | 79  | GLU  |
| 12  | L     | 80  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | L     | 82  | VAL  |
| 12  | L     | 91  | LYS  |
| 12  | L     | 104 | VAL  |
| 12  | L     | 119 | LYS  |
| 12  | L     | 122 | THR  |
| 12  | L     | 126 | LYS  |
| 13  | M     | 8   | GLU  |
| 13  | M     | 12  | ASN  |
| 13  | M     | 19  | LEU  |
| 13  | M     | 27  | LYS  |
| 13  | M     | 34  | LEU  |
| 13  | M     | 45  | VAL  |
| 13  | M     | 53  | VAL  |
| 13  | M     | 54  | VAL  |
| 13  | M     | 56  | LEU  |
| 13  | M     | 70  | LEU  |
| 13  | M     | 79  | LYS  |
| 13  | M     | 84  | ILE  |
| 13  | M     | 106 | ASN  |
| 13  | M     | 109 | THR  |
| 13  | M     | 110 | ARG  |
| 13  | M     | 114 | ARG  |
| 13  | M     | 115 | LYS  |
| 13  | M     | 117 | VAL  |
| 14  | N     | 6   | LEU  |
| 14  | N     | 8   | GLU  |
| 14  | N     | 15  | LYS  |
| 14  | N     | 22  | THR  |
| 14  | N     | 24  | CYS  |
| 14  | N     | 25  | VAL  |
| 14  | N     | 31  | ARG  |
| 14  | N     | 39  | LEU  |
| 14  | N     | 42  | ILE  |
| 14  | N     | 49  | HIS  |
| 14  | N     | 53  | LEU  |
| 15  | O     | 4   | THR  |
| 15  | O     | 5   | LYS  |
| 15  | O     | 24  | SER  |
| 15  | O     | 31  | LEU  |
| 15  | O     | 32  | LEU  |
| 15  | O     | 34  | LEU  |
| 15  | O     | 35  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | O     | 39  | LEU  |
| 15  | O     | 45  | VAL  |
| 15  | O     | 47  | LYS  |
| 15  | O     | 48  | LYS  |
| 15  | O     | 60  | VAL  |
| 15  | O     | 65  | ARG  |
| 15  | O     | 70  | LEU  |
| 15  | O     | 81  | LEU  |
| 15  | O     | 83  | GLU  |
| 16  | P     | 1   | MET  |
| 16  | P     | 2   | VAL  |
| 16  | P     | 51  | VAL  |
| 16  | P     | 61  | SER  |
| 16  | P     | 68  | ASP  |
| 16  | P     | 82  | GLN  |
| 17  | Q     | 3   | LYS  |
| 17  | Q     | 4   | LYS  |
| 17  | Q     | 38  | ARG  |
| 17  | Q     | 59  | ILE  |
| 17  | Q     | 60  | ILE  |
| 17  | Q     | 68  | ARG  |
| 17  | Q     | 75  | ARG  |
| 17  | Q     | 77  | VAL  |
| 17  | Q     | 85  | VAL  |
| 17  | Q     | 92  | ARG  |
| 18  | R     | 21  | LYS  |
| 18  | R     | 28  | GLU  |
| 18  | R     | 47  | THR  |
| 18  | R     | 68  | LYS  |
| 18  | R     | 69  | THR  |
| 18  | R     | 84  | LYS  |
| 18  | R     | 86  | VAL  |
| 19  | S     | 5   | LEU  |
| 19  | S     | 7   | LYS  |
| 19  | S     | 15  | LEU  |
| 19  | S     | 43  | GLU  |
| 19  | S     | 48  | THR  |
| 19  | S     | 58  | VAL  |
| 19  | S     | 60  | VAL  |
| 19  | S     | 62  | ILE  |
| 19  | S     | 71  | LEU  |
| 20  | T     | 13  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | T     | 35  | THR  |
| 20  | T     | 36  | LEU  |
| 20  | T     | 43  | LEU  |
| 20  | T     | 56  | MET  |
| 20  | T     | 62  | LEU  |
| 20  | T     | 68  | LYS  |
| 20  | T     | 72  | LEU  |
| 20  | T     | 73  | HIS  |
| 20  | T     | 84  | LEU  |
| 20  | T     | 91  | LEU  |
| 20  | T     | 100 | ILE  |
| 21  | U     | 8   | THR  |
| 21  | U     | 9   | ARG  |
| 21  | U     | 15  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 204 | ASN  |
| 2   | B     | 224 | GLN  |
| 3   | C     | 63  | ASN  |
| 3   | C     | 139 | GLN  |
| 4   | D     | 119 | GLN  |
| 4   | D     | 125 | HIS  |
| 6   | F     | 64  | GLN  |
| 6   | F     | 100 | ASN  |
| 9   | I     | 31  | GLN  |
| 9   | I     | 73  | GLN  |
| 9   | I     | 124 | GLN  |
| 11  | K     | 26  | ASN  |
| 12  | L     | 75  | HIS  |
| 15  | O     | 13  | GLN  |
| 16  | P     | 16  | HIS  |
| 17  | Q     | 29  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1510/1522 (99%) | 259 (17%)         | 38 (2%)         |

All (259) RNA backbone outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 6      | G    |
| 1   | A     | 9      | G    |
| 1   | A     | 31     | G    |
| 1   | A     | 32     | A    |
| 1   | A     | 39     | G    |
| 1   | A     | 47     | C    |
| 1   | A     | 48     | C    |
| 1   | A     | 50     | A    |
| 1   | A     | 51     | A    |
| 1   | A     | 81     | U    |
| 1   | A     | 88     | A    |
| 1   | A     | 91     | C    |
| 1   | A     | 101    | A    |
| 1   | A     | 115    | G    |
| 1   | A     | 116    | A    |
| 1   | A     | 117    | G    |
| 1   | A     | 121    | C    |
| 1   | A     | 129(A) | G    |
| 1   | A     | 130    | A    |
| 1   | A     | 131    | C    |
| 1   | A     | 145    | G    |
| 1   | A     | 163    | C    |
| 1   | A     | 182    | U    |
| 1   | A     | 183    | G    |
| 1   | A     | 190(D) | U    |
| 1   | A     | 195    | A    |
| 1   | A     | 197    | A    |
| 1   | A     | 202    | U    |
| 1   | A     | 203    | U    |
| 1   | A     | 204    | U    |
| 1   | A     | 216    | G    |
| 1   | A     | 231    | G    |
| 1   | A     | 247    | G    |
| 1   | A     | 251    | G    |
| 1   | A     | 266    | G    |
| 1   | A     | 267    | C    |
| 1   | A     | 289    | G    |
| 1   | A     | 321    | A    |
| 1   | A     | 328    | C    |
| 1   | A     | 329    | A    |
| 1   | A     | 332    | G    |
| 1   | A     | 345    | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 348 | G    |
| 1   | A     | 351 | G    |
| 1   | A     | 352 | C    |
| 1   | A     | 353 | A    |
| 1   | A     | 354 | G    |
| 1   | A     | 367 | U    |
| 1   | A     | 371 | G    |
| 1   | A     | 372 | C    |
| 1   | A     | 373 | A    |
| 1   | A     | 384 | G    |
| 1   | A     | 392 | G    |
| 1   | A     | 397 | A    |
| 1   | A     | 398 | C    |
| 1   | A     | 406 | G    |
| 1   | A     | 413 | G    |
| 1   | A     | 414 | A    |
| 1   | A     | 421 | U    |
| 1   | A     | 422 | C    |
| 1   | A     | 424 | G    |
| 1   | A     | 429 | U    |
| 1   | A     | 439 | A    |
| 1   | A     | 460 | A    |
| 1   | A     | 461 | C    |
| 1   | A     | 481 | G    |
| 1   | A     | 485 | G    |
| 1   | A     | 486 | U    |
| 1   | A     | 496 | A    |
| 1   | A     | 497 | A    |
| 1   | A     | 498 | U    |
| 1   | A     | 504 | C    |
| 1   | A     | 509 | A    |
| 1   | A     | 510 | A    |
| 1   | A     | 511 | C    |
| 1   | A     | 518 | C    |
| 1   | A     | 527 | 7MG  |
| 1   | A     | 532 | A    |
| 1   | A     | 533 | A    |
| 1   | A     | 547 | A    |
| 1   | A     | 559 | A    |
| 1   | A     | 560 | U    |
| 1   | A     | 562 | C    |
| 1   | A     | 563 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 564 | C    |
| 1   | A     | 568 | G    |
| 1   | A     | 572 | A    |
| 1   | A     | 573 | A    |
| 1   | A     | 576 | G    |
| 1   | A     | 577 | G    |
| 1   | A     | 579 | G    |
| 1   | A     | 581 | G    |
| 1   | A     | 588 | G    |
| 1   | A     | 596 | C    |
| 1   | A     | 616 | G    |
| 1   | A     | 618 | C    |
| 1   | A     | 653 | A    |
| 1   | A     | 665 | A    |
| 1   | A     | 686 | U    |
| 1   | A     | 687 | A    |
| 1   | A     | 688 | G    |
| 1   | A     | 701 | C    |
| 1   | A     | 702 | A    |
| 1   | A     | 721 | G    |
| 1   | A     | 723 | U    |
| 1   | A     | 731 | G    |
| 1   | A     | 749 | C    |
| 1   | A     | 755 | G    |
| 1   | A     | 773 | G    |
| 1   | A     | 774 | G    |
| 1   | A     | 777 | A    |
| 1   | A     | 781 | A    |
| 1   | A     | 782 | A    |
| 1   | A     | 792 | A    |
| 1   | A     | 793 | U    |
| 1   | A     | 794 | A    |
| 1   | A     | 799 | G    |
| 1   | A     | 810 | C    |
| 1   | A     | 813 | U    |
| 1   | A     | 817 | C    |
| 1   | A     | 828 | A    |
| 1   | A     | 839 | U    |
| 1   | A     | 840 | C    |
| 1   | A     | 841 | U    |
| 1   | A     | 848 | C    |
| 1   | A     | 855 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | A     | 858     | G    |
| 1   | A     | 859     | A    |
| 1   | A     | 874     | G    |
| 1   | A     | 887     | G    |
| 1   | A     | 902     | G    |
| 1   | A     | 913     | A    |
| 1   | A     | 914     | A    |
| 1   | A     | 922     | G    |
| 1   | A     | 926     | G    |
| 1   | A     | 927     | G    |
| 1   | A     | 934     | C    |
| 1   | A     | 935     | A    |
| 1   | A     | 960     | U    |
| 1   | A     | 961     | U    |
| 1   | A     | 969     | A    |
| 1   | A     | 971     | G    |
| 1   | A     | 974     | A    |
| 1   | A     | 976     | G    |
| 1   | A     | 977     | A    |
| 1   | A     | 982     | U    |
| 1   | A     | 984     | C    |
| 1   | A     | 989     | C    |
| 1   | A     | 991     | U    |
| 1   | A     | 992     | U    |
| 1   | A     | 993     | G    |
| 1   | A     | 1003(A) | G    |
| 1   | A     | 1004    | A    |
| 1   | A     | 1005    | A    |
| 1   | A     | 1008    | C    |
| 1   | A     | 1009    | G    |
| 1   | A     | 1022    | G    |
| 1   | A     | 1023    | G    |
| 1   | A     | 1024    | G    |
| 1   | A     | 1026    | G    |
| 1   | A     | 1045    | C    |
| 1   | A     | 1050    | G    |
| 1   | A     | 1054    | C    |
| 1   | A     | 1060    | C    |
| 1   | A     | 1061    | G    |
| 1   | A     | 1065    | U    |
| 1   | A     | 1066    | C    |
| 1   | A     | 1067    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1068 | G    |
| 1   | A     | 1094 | G    |
| 1   | A     | 1095 | U    |
| 1   | A     | 1101 | A    |
| 1   | A     | 1124 | G    |
| 1   | A     | 1125 | U    |
| 1   | A     | 1126 | U    |
| 1   | A     | 1127 | G    |
| 1   | A     | 1128 | C    |
| 1   | A     | 1129 | C    |
| 1   | A     | 1130 | A    |
| 1   | A     | 1131 | G    |
| 1   | A     | 1136 | U    |
| 1   | A     | 1137 | C    |
| 1   | A     | 1138 | G    |
| 1   | A     | 1139 | G    |
| 1   | A     | 1140 | C    |
| 1   | A     | 1145 | C    |
| 1   | A     | 1146 | A    |
| 1   | A     | 1152 | A    |
| 1   | A     | 1159 | U    |
| 1   | A     | 1160 | G    |
| 1   | A     | 1162 | C    |
| 1   | A     | 1164 | G    |
| 1   | A     | 1171 | G    |
| 1   | A     | 1182 | G    |
| 1   | A     | 1183 | A    |
| 1   | A     | 1184 | G    |
| 1   | A     | 1191 | A    |
| 1   | A     | 1196 | U    |
| 1   | A     | 1197 | G    |
| 1   | A     | 1198 | G    |
| 1   | A     | 1201 | A    |
| 1   | A     | 1202 | G    |
| 1   | A     | 1204 | A    |
| 1   | A     | 1212 | U    |
| 1   | A     | 1213 | A    |
| 1   | A     | 1225 | A    |
| 1   | A     | 1238 | A    |
| 1   | A     | 1243 | C    |
| 1   | A     | 1257 | U    |
| 1   | A     | 1258 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1278 | U    |
| 1   | A     | 1279 | A    |
| 1   | A     | 1280 | A    |
| 1   | A     | 1281 | U    |
| 1   | A     | 1286 | A    |
| 1   | A     | 1287 | A    |
| 1   | A     | 1288 | A    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1301 | U    |
| 1   | A     | 1302 | U    |
| 1   | A     | 1303 | C    |
| 1   | A     | 1304 | G    |
| 1   | A     | 1305 | G    |
| 1   | A     | 1310 | G    |
| 1   | A     | 1319 | A    |
| 1   | A     | 1320 | C    |
| 1   | A     | 1335 | C    |
| 1   | A     | 1336 | C    |
| 1   | A     | 1346 | A    |
| 1   | A     | 1347 | G    |
| 1   | A     | 1348 | U    |
| 1   | A     | 1353 | G    |
| 1   | A     | 1358 | U    |
| 1   | A     | 1362 | C    |
| 1   | A     | 1368 | G    |
| 1   | A     | 1381 | U    |
| 1   | A     | 1394 | A    |
| 1   | A     | 1398 | A    |
| 1   | A     | 1443 | G    |
| 1   | A     | 1446 | A    |
| 1   | A     | 1447 | G    |
| 1   | A     | 1452 | C    |
| 1   | A     | 1453 | G    |
| 1   | A     | 1454 | G    |
| 1   | A     | 1487 | G    |
| 1   | A     | 1490 | C    |
| 1   | A     | 1491 | G    |
| 1   | A     | 1497 | G    |
| 1   | A     | 1498 | UR3  |
| 1   | A     | 1499 | A    |
| 1   | A     | 1502 | A    |
| 1   | A     | 1504 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1505 | G    |
| 1   | A     | 1506 | U    |
| 1   | A     | 1507 | A    |
| 1   | A     | 1520 | G    |
| 1   | A     | 1529 | G    |
| 1   | A     | 1530 | G    |
| 1   | A     | 1532 | U    |

All (38) RNA pucker outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 5      | U    |
| 1   | A     | 115    | G    |
| 1   | A     | 129(A) | G    |
| 1   | A     | 181    | G    |
| 1   | A     | 250    | A    |
| 1   | A     | 328    | C    |
| 1   | A     | 372    | C    |
| 1   | A     | 428    | G    |
| 1   | A     | 484    | G    |
| 1   | A     | 485    | G    |
| 1   | A     | 496    | A    |
| 1   | A     | 509    | A    |
| 1   | A     | 532    | A    |
| 1   | A     | 559    | A    |
| 1   | A     | 575    | G    |
| 1   | A     | 687    | A    |
| 1   | A     | 701    | C    |
| 1   | A     | 748    | C    |
| 1   | A     | 792    | A    |
| 1   | A     | 812    | C    |
| 1   | A     | 840    | C    |
| 1   | A     | 913    | A    |
| 1   | A     | 960    | U    |
| 1   | A     | 992    | U    |
| 1   | A     | 1065   | U    |
| 1   | A     | 1067   | A    |
| 1   | A     | 1139   | G    |
| 1   | A     | 1145   | C    |
| 1   | A     | 1182   | G    |
| 1   | A     | 1190   | G    |
| 1   | A     | 1201   | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1203 | C    |
| 1   | A     | 1285 | A    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1346 | A    |
| 1   | A     | 1347 | G    |
| 1   | A     | 1380 | U    |
| 1   | A     | 1505 | G    |

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

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

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 1   | 5MC  | A     | 1400 | 1    | 19,22,23     | 1.15 | 3 (15%)     | 26,32,35    | 1.05 | 2 (7%)      |
| 1   | 5MC  | A     | 967  | 1    | 19,22,23     | 0.86 | 1 (5%)      | 26,32,35    | 0.86 | 2 (7%)      |
| 1   | 5MC  | A     | 1404 | 1    | 19,22,23     | 0.94 | 2 (10%)     | 26,32,35    | 0.95 | 2 (7%)      |
| 1   | 5MC  | A     | 1407 | 1    | 19,22,23     | 1.33 | 3 (15%)     | 26,32,35    | 1.16 | 3 (11%)     |
| 1   | PSU  | A     | 516  | 1,23 | 18,21,22     | 1.08 | 1 (5%)      | 21,30,33    | 1.98 | 6 (28%)     |
| 1   | MA6  | A     | 1519 | 1    | 23,26,27     | 1.44 | 5 (21%)     | 33,38,41    | 0.96 | 3 (9%)      |
| 1   | PSU  | A     | 1541 | 1    | 18,21,22     | 1.15 | 1 (5%)      | 21,30,33    | 1.80 | 4 (19%)     |
| 1   | 7MG  | A     | 527  | 1    | 23,26,27     | 4.17 | 4 (17%)     | 27,39,42    | 2.23 | 9 (33%)     |
| 1   | 2MG  | A     | 1207 | 1    | 23,26,27     | 1.48 | 6 (26%)     | 33,38,41    | 1.14 | 4 (12%)     |
| 1   | M2G  | A     | 966  | 1    | 24,27,28     | 1.07 | 2 (8%)      | 33,40,43    | 0.78 | 1 (3%)      |
| 1   | PSU  | A     | 1540 | 1    | 18,21,22     | 1.16 | 1 (5%)      | 21,30,33    | 1.83 | 5 (23%)     |
| 1   | MA6  | A     | 1518 | 1    | 23,26,27     | 1.54 | 5 (21%)     | 33,38,41    | 1.10 | 2 (6%)      |
| 1   | 4OC  | A     | 1402 | 1    | 20,23,24     | 0.87 | 1 (5%)      | 25,32,35    | 0.85 | 0           |
| 1   | UR3  | A     | 1498 | 1    | 19,22,23     | 0.79 | 1 (5%)      | 26,32,35    | 1.04 | 1 (3%)      |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 1   | 5MC  | A     | 1400 | 1    | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | A     | 967  | 1    | -       | 1/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | A     | 1404 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | A     | 1407 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | A     | 516  | 1,23 | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | MA6  | A     | 1519 | 1    | -       | 3/11/29/30 | 0/3/3/3 |
| 1   | PSU  | A     | 1541 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 7MG  | A     | 527  | 1    | -       | 2/7/37/38  | 0/3/3/3 |
| 1   | 2MG  | A     | 1207 | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | M2G  | A     | 966  | 1    | -       | 4/11/29/30 | 0/3/3/3 |
| 1   | PSU  | A     | 1540 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | MA6  | A     | 1518 | 1    | -       | 0/11/29/30 | 0/3/3/3 |
| 1   | 4OC  | A     | 1402 | 1    | -       | 1/9/29/30  | 0/2/2/2 |
| 1   | UR3  | A     | 1498 | 1    | -       | 0/7/25/26  | 0/2/2/2 |

All (36) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 1   | A     | 527  | 7MG  | C8-N9 | -18.67 | 1.33        | 1.45     |
| 1   | A     | 527  | 7MG  | C2-N2 | 4.35   | 1.44        | 1.34     |
| 1   | A     | 527  | 7MG  | C5-N7 | 3.97   | 1.40        | 1.35     |
| 1   | A     | 1541 | PSU  | C6-C5 | 3.91   | 1.39        | 1.35     |
| 1   | A     | 1540 | PSU  | C6-C5 | 3.84   | 1.39        | 1.35     |
| 1   | A     | 1518 | MA6  | C8-N9 | 3.33   | 1.43        | 1.37     |
| 1   | A     | 1207 | 2MG  | C2-N1 | 3.27   | 1.41        | 1.36     |
| 1   | A     | 516  | PSU  | C6-C5 | 3.26   | 1.38        | 1.35     |
| 1   | A     | 1407 | 5MC  | C2-N1 | 3.23   | 1.46        | 1.40     |
| 1   | A     | 1518 | MA6  | C5-C4 | 3.16   | 1.44        | 1.39     |
| 1   | A     | 1207 | 2MG  | C2-N2 | 3.10   | 1.39        | 1.33     |
| 1   | A     | 1519 | MA6  | C5-C4 | 2.98   | 1.44        | 1.39     |
| 1   | A     | 1407 | 5MC  | C5-C4 | 2.97   | 1.46        | 1.44     |
| 1   | A     | 1402 | 4OC  | C2-N3 | 2.92   | 1.42        | 1.36     |
| 1   | A     | 1518 | MA6  | C5-N7 | 2.90   | 1.44        | 1.39     |
| 1   | A     | 1519 | MA6  | C8-N9 | 2.87   | 1.42        | 1.37     |
| 1   | A     | 1400 | 5MC  | C6-C5 | 2.78   | 1.39        | 1.34     |
| 1   | A     | 1207 | 2MG  | C6-N1 | 2.68   | 1.43        | 1.38     |
| 1   | A     | 1207 | 2MG  | C8-N9 | 2.68   | 1.43        | 1.37     |
| 1   | A     | 1518 | MA6  | C2-N1 | 2.63   | 1.38        | 1.33     |
| 1   | A     | 967  | 5MC  | C2-N3 | 2.62   | 1.41        | 1.36     |
| 1   | A     | 527  | 7MG  | C4-N3 | 2.52   | 1.40        | 1.34     |
| 1   | A     | 1404 | 5MC  | C2-N3 | 2.43   | 1.41        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | A     | 1400 | 5MC  | C2-N1 | 2.43 | 1.45        | 1.40     |
| 1   | A     | 966  | M2G  | C8-N9 | 2.40 | 1.42        | 1.37     |
| 1   | A     | 1519 | MA6  | C4-N3 | 2.39 | 1.38        | 1.34     |
| 1   | A     | 966  | M2G  | C4-N3 | 2.36 | 1.39        | 1.34     |
| 1   | A     | 1519 | MA6  | C2-N1 | 2.34 | 1.38        | 1.33     |
| 1   | A     | 1400 | 5MC  | C2-N3 | 2.30 | 1.40        | 1.36     |
| 1   | A     | 1207 | 2MG  | C4-N3 | 2.29 | 1.39        | 1.34     |
| 1   | A     | 1518 | MA6  | C6-N1 | 2.23 | 1.38        | 1.34     |
| 1   | A     | 1519 | MA6  | C6-N1 | 2.20 | 1.38        | 1.34     |
| 1   | A     | 1498 | UR3  | C2-N1 | 2.16 | 1.41        | 1.38     |
| 1   | A     | 1407 | 5MC  | C2-N3 | 2.13 | 1.40        | 1.36     |
| 1   | A     | 1404 | 5MC  | C2-N1 | 2.09 | 1.44        | 1.40     |
| 1   | A     | 1207 | 2MG  | C2-N3 | 2.02 | 1.35        | 1.32     |

All (44) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 527  | 7MG  | C5-C6-N1 | 5.03  | 119.79      | 110.94   |
| 1   | A     | 527  | 7MG  | N9-C4-N3 | 4.96  | 132.73      | 125.46   |
| 1   | A     | 516  | PSU  | C4-N3-C2 | -4.91 | 119.61      | 126.37   |
| 1   | A     | 516  | PSU  | N1-C2-N3 | 4.76  | 120.19      | 115.17   |
| 1   | A     | 1541 | PSU  | C4-N3-C2 | -4.67 | 119.94      | 126.37   |
| 1   | A     | 1540 | PSU  | C4-N3-C2 | -4.60 | 120.04      | 126.37   |
| 1   | A     | 1540 | PSU  | N1-C2-N3 | 4.54  | 119.96      | 115.17   |
| 1   | A     | 527  | 7MG  | C2-N3-C4 | 4.47  | 119.99      | 112.30   |
| 1   | A     | 1541 | PSU  | N1-C2-N3 | 4.45  | 119.86      | 115.17   |
| 1   | A     | 527  | 7MG  | C5-C4-N3 | -4.26 | 120.13      | 128.13   |
| 1   | A     | 527  | 7MG  | N9-C8-N7 | 3.53  | 108.37      | 103.37   |
| 1   | A     | 527  | 7MG  | C2-N1-C6 | -3.05 | 119.58      | 125.11   |
| 1   | A     | 1407 | 5MC  | N4-C4-N3 | -2.92 | 113.23      | 118.51   |
| 1   | A     | 516  | PSU  | C6-C5-C4 | 2.83  | 120.08      | 118.17   |
| 1   | A     | 1540 | PSU  | O2-C2-N1 | -2.67 | 120.03      | 122.79   |
| 1   | A     | 516  | PSU  | O2-C2-N1 | -2.65 | 120.06      | 122.79   |
| 1   | A     | 527  | 7MG  | C6-C5-C4 | -2.56 | 117.91      | 122.40   |
| 1   | A     | 527  | 7MG  | O6-C6-C5 | -2.56 | 121.35      | 127.62   |
| 1   | A     | 1207 | 2MG  | C5-C4-N3 | -2.55 | 124.34      | 128.39   |
| 1   | A     | 1540 | PSU  | C6-N1-C2 | -2.54 | 120.33      | 122.69   |
| 1   | A     | 1541 | PSU  | O2-C2-N1 | -2.52 | 120.19      | 122.79   |
| 1   | A     | 1498 | UR3  | C6-N1-C2 | -2.48 | 119.77      | 121.80   |
| 1   | A     | 527  | 7MG  | C6-C5-N7 | 2.42  | 135.68      | 131.93   |
| 1   | A     | 1207 | 2MG  | C2-N1-C6 | -2.41 | 121.63      | 124.55   |
| 1   | A     | 1400 | 5MC  | C5-C4-N3 | 2.40  | 124.22      | 121.75   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1518 | MA6  | C4-N9-C1'   | -2.40 | 121.03      | 126.63   |
| 1   | A     | 1207 | 2MG  | O6-C6-N1    | -2.38 | 115.63      | 120.11   |
| 1   | A     | 1404 | 5MC  | N4-C4-N3    | -2.33 | 114.28      | 118.51   |
| 1   | A     | 1400 | 5MC  | N4-C4-N3    | -2.31 | 114.33      | 118.51   |
| 1   | A     | 516  | PSU  | C6-N1-C2    | -2.29 | 120.57      | 122.69   |
| 1   | A     | 967  | 5MC  | N4-C4-N3    | -2.27 | 114.40      | 118.51   |
| 1   | A     | 1407 | 5MC  | C5-C4-N3    | 2.23  | 124.05      | 121.75   |
| 1   | A     | 1404 | 5MC  | C5-C4-N3    | 2.20  | 124.01      | 121.75   |
| 1   | A     | 1541 | PSU  | C6-N1-C2    | -2.18 | 120.67      | 122.69   |
| 1   | A     | 1207 | 2MG  | N9-C4-N3    | 2.18  | 130.30      | 125.95   |
| 1   | A     | 1407 | 5MC  | O2-C2-N3    | -2.17 | 118.91      | 122.33   |
| 1   | A     | 1519 | MA6  | C5-C6-N6    | -2.17 | 121.90      | 125.33   |
| 1   | A     | 1519 | MA6  | C5-C4-N3    | -2.14 | 123.77      | 126.72   |
| 1   | A     | 1518 | MA6  | C2-N1-C6    | 2.07  | 116.88      | 111.83   |
| 1   | A     | 516  | PSU  | O4'-C1'-C2' | 2.06  | 108.00      | 105.15   |
| 1   | A     | 967  | 5MC  | C5-C4-N3    | 2.04  | 123.84      | 121.75   |
| 1   | A     | 966  | M2G  | O6-C6-N1    | -2.02 | 116.31      | 120.11   |
| 1   | A     | 1540 | PSU  | O4'-C1'-C2' | 2.01  | 107.93      | 105.15   |
| 1   | A     | 1519 | MA6  | C4-C5-C6    | 2.00  | 117.98      | 115.91   |

There are no chirality outliers.

All (13) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | A     | 527  | 7MG  | O4'-C4'-C5'-O5' |
| 1   | A     | 527  | 7MG  | C3'-C4'-C5'-O5' |
| 1   | A     | 966  | M2G  | N1-C2-N2-CM1    |
| 1   | A     | 966  | M2G  | N3-C2-N2-CM1    |
| 1   | A     | 1519 | MA6  | C5-C6-N6-C9     |
| 1   | A     | 1519 | MA6  | N1-C6-N6-C9     |
| 1   | A     | 1400 | 5MC  | O4'-C4'-C5'-O5' |
| 1   | A     | 1400 | 5MC  | C3'-C4'-C5'-O5' |
| 1   | A     | 966  | M2G  | N3-C2-N2-CM2    |
| 1   | A     | 966  | M2G  | N1-C2-N2-CM2    |
| 1   | A     | 1519 | MA6  | C5-C6-N6-C10    |
| 1   | A     | 1402 | 4OC  | O4'-C4'-C5'-O5' |
| 1   | A     | 967  | 5MC  | O4'-C4'-C5'-O5' |

There are no ring outliers.

4 monomers are involved in 5 short contacts:



| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | A     | 1400 | 5MC  | 1       | 0            |
| 1   | A     | 1407 | 5MC  | 1       | 0            |
| 1   | A     | 527  | 7MG  | 2       | 0            |
| 1   | A     | 1207 | 2MG  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 249 ligands modelled in this entry, 248 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | SRY  | A     | 1601 | -    | 40,42,42     | 2.35 | 10 (25%) | 49,63,63    | 1.69 | 8 (16%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 22  | SRY  | A     | 1601 | -    | -       | 4/20/87/87 | 0/3/3/3 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | A     | 1601 | SRY  | CD1-N31 | 9.34  | 1.49        | 1.33     |
| 22  | A     | 1601 | SRY  | CA1-N11 | 7.09  | 1.45        | 1.33     |
| 22  | A     | 1601 | SRY  | O53-C53 | -3.47 | 1.35        | 1.44     |
| 22  | A     | 1601 | SRY  | CA1-NB1 | 2.93  | 1.45        | 1.34     |
| 22  | A     | 1601 | SRY  | CD1-NE1 | 2.87  | 1.44        | 1.34     |
| 22  | A     | 1601 | SRY  | O32-C32 | -2.48 | 1.40        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | A     | 1601 | SR   | C23-N23 | -2.44 | 1.43        | 1.47     |
| 22  | A     | 1601 | SR   | O51-C51 | -2.43 | 1.36        | 1.43     |
| 22  | A     | 1601 | SR   | O43-C43 | -2.03 | 1.37        | 1.43     |
| 22  | A     | 1601 | SR   | C61-C11 | -2.02 | 1.49        | 1.53     |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1601 | SR   | C12-O42-C42 | -5.26 | 99.99       | 108.48   |
| 22  | A     | 1601 | SR   | C61-C11-N11 | -4.66 | 102.04      | 110.62   |
| 22  | A     | 1601 | SR   | C13-O13-C22 | -3.62 | 110.10      | 116.26   |
| 22  | A     | 1601 | SR   | O41-C12-O42 | -3.39 | 107.90      | 111.37   |
| 22  | A     | 1601 | SR   | C13-O53-C53 | -3.27 | 107.34      | 113.72   |
| 22  | A     | 1601 | SR   | O13-C13-C23 | 2.95  | 112.86      | 108.07   |
| 22  | A     | 1601 | SR   | O13-C22-C32 | 2.08  | 116.39      | 111.79   |
| 22  | A     | 1601 | SR   | O42-C12-C22 | -2.08 | 105.08      | 107.31   |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1601 | SR   | C61-C11-N11-CA1 |
| 22  | A     | 1601 | SR   | C13-C23-N23-CI3 |
| 22  | A     | 1601 | SR   | C21-C11-N11-CA1 |
| 22  | A     | 1601 | SR   | C21-C31-N31-CD1 |

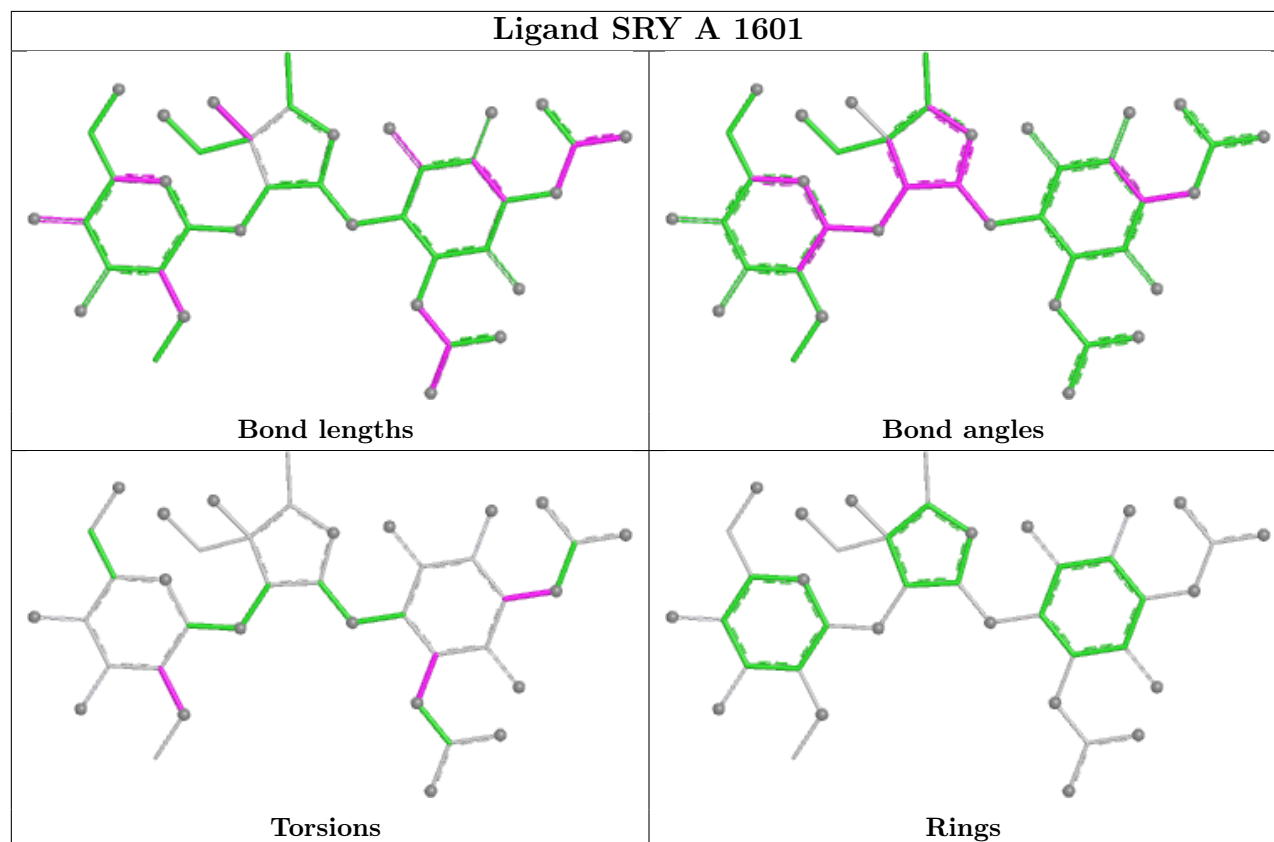
There are no ring outliers.

1 monomer is involved in 4 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22  | A     | 1601 | SR   | 4       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 1497/1522 (98%) | -0.56  | 10 (0%) 84 73 | 75, 126, 254, 372     | 0     |
| 2   | B     | 234/256 (91%)   | -0.34  | 0 100 100     | 102, 148, 210, 229    | 0     |
| 3   | C     | 206/239 (86%)   | -0.10  | 3 (1%) 72 57  | 130, 188, 244, 266    | 0     |
| 4   | D     | 208/209 (99%)   | -0.16  | 8 (3%) 44 31  | 90, 129, 167, 202     | 0     |
| 5   | E     | 150/162 (92%)   | -0.51  | 0 100 100     | 79, 107, 143, 204     | 0     |
| 6   | F     | 101/101 (100%)  | -0.38  | 0 100 100     | 111, 155, 184, 234    | 0     |
| 7   | G     | 155/156 (99%)   | -0.15  | 4 (2%) 57 42  | 120, 170, 221, 244    | 0     |
| 8   | H     | 138/138 (100%)  | -0.43  | 0 100 100     | 73, 99, 132, 167      | 0     |
| 9   | I     | 127/128 (99%)   | 0.17   | 4 (3%) 51 38  | 132, 195, 242, 259    | 0     |
| 10  | J     | 98/105 (93%)    | 0.28   | 4 (4%) 41 29  | 126, 214, 306, 335    | 0     |
| 11  | K     | 116/129 (89%)   | -0.33  | 1 (0%) 81 69  | 98, 130, 174, 208     | 0     |
| 12  | L     | 124/135 (91%)   | -0.13  | 2 (1%) 70 55  | 74, 122, 159, 213     | 0     |
| 13  | M     | 118/126 (93%)   | 0.01   | 5 (4%) 40 28  | 119, 153, 193, 258    | 0     |
| 14  | N     | 60/61 (98%)     | 0.31   | 2 (3%) 49 35  | 149, 175, 240, 282    | 0     |
| 15  | O     | 87/89 (97%)     | -0.47  | 1 (1%) 78 65  | 82, 117, 154, 175     | 0     |
| 16  | P     | 83/88 (94%)     | -0.43  | 0 100 100     | 92, 121, 150, 183     | 0     |
| 17  | Q     | 99/105 (94%)    | -0.42  | 0 100 100     | 80, 108, 144, 168     | 0     |
| 18  | R     | 70/88 (79%)     | -0.40  | 0 100 100     | 100, 131, 181, 209    | 0     |
| 19  | S     | 80/93 (86%)     | 0.24   | 5 (6%) 26 19  | 149, 204, 249, 280    | 0     |
| 20  | T     | 99/106 (93%)    | -0.11  | 4 (4%) 42 29  | 96, 127, 179, 211     | 0     |
| 21  | U     | 24/27 (88%)     | 0.38   | 1 (4%) 40 28  | 131, 162, 193, 205    | 0     |
| All | All   | 3874/4063 (95%) | -0.33  | 54 (1%) 73 59 | 73, 137, 230, 372     | 0     |

All (54) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | D     | 31   | CYS  | 6.0  |
| 4   | D     | 2    | GLY  | 5.6  |
| 1   | A     | 1129 | C    | 4.7  |
| 19  | S     | 2    | PRO  | 4.4  |
| 20  | T     | 106  | ALA  | 4.2  |
| 4   | D     | 9    | CYS  | 4.1  |
| 4   | D     | 26   | CYS  | 4.1  |
| 10  | J     | 37   | PRO  | 3.6  |
| 3   | C     | 65   | ALA  | 3.6  |
| 1   | A     | 985  | C    | 3.6  |
| 20  | T     | 12   | ALA  | 3.5  |
| 1   | A     | 78   | G    | 3.5  |
| 9   | I     | 128  | ARG  | 3.4  |
| 12  | L     | 73   | GLU  | 3.3  |
| 13  | M     | 116  | THR  | 3.1  |
| 19  | S     | 4    | SER  | 3.1  |
| 1   | A     | 793  | U    | 3.0  |
| 21  | U     | 6    | ARG  | 3.0  |
| 4   | D     | 21   | LEU  | 3.0  |
| 19  | S     | 34   | TRP  | 2.9  |
| 7   | G     | 125  | MET  | 2.9  |
| 13  | M     | 7    | VAL  | 2.8  |
| 7   | G     | 62   | PHE  | 2.8  |
| 3   | C     | 5    | ILE  | 2.7  |
| 7   | G     | 150  | ALA  | 2.7  |
| 9   | I     | 127  | LYS  | 2.7  |
| 1   | A     | 413  | G    | 2.6  |
| 10  | J     | 38   | ILE  | 2.6  |
| 13  | M     | 119  | GLY  | 2.6  |
| 14  | N     | 3    | ARG  | 2.6  |
| 14  | N     | 31   | ARG  | 2.5  |
| 4   | D     | 12   | CYS  | 2.5  |
| 1   | A     | 77   | G    | 2.4  |
| 13  | M     | 98   | VAL  | 2.4  |
| 1   | A     | 984  | C    | 2.4  |
| 20  | T     | 60   | GLU  | 2.4  |
| 19  | S     | 35   | SER  | 2.4  |
| 9   | I     | 108  | VAL  | 2.4  |
| 11  | K     | 118  | GLY  | 2.3  |
| 4   | D     | 116  | GLN  | 2.3  |
| 1   | A     | 1124 | G    | 2.3  |
| 7   | G     | 33   | ASP  | 2.2  |
| 1   | A     | 79   | G    | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 15  | O     | 23   | GLY  | 2.2  |
| 13  | M     | 117  | VAL  | 2.2  |
| 9   | I     | 9    | ARG  | 2.2  |
| 19  | S     | 3    | ARG  | 2.2  |
| 4   | D     | 20   | TYR  | 2.1  |
| 3   | C     | 66   | VAL  | 2.1  |
| 12  | L     | 26   | ALA  | 2.1  |
| 20  | T     | 11   | SER  | 2.0  |
| 10  | J     | 3    | LYS  | 2.0  |
| 10  | J     | 34   | VAL  | 2.0  |
| 1   | A     | 1126 | U    | 2.0  |

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

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. 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 | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 1   | PSU  | A     | 1541 | 20/21 | 0.76 | 0.18 | 307,319,331,332            | 0     |
| 1   | PSU  | A     | 1540 | 20/21 | 0.83 | 0.16 | 293,304,328,333            | 0     |
| 1   | MA6  | A     | 1518 | 24/25 | 0.92 | 0.10 | 114,128,149,156            | 0     |
| 1   | 5MC  | A     | 1407 | 21/22 | 0.94 | 0.09 | 143,156,168,170            | 0     |
| 1   | UR3  | A     | 1498 | 21/22 | 0.94 | 0.14 | 107,119,127,139            | 0     |
| 1   | PSU  | A     | 516  | 20/21 | 0.94 | 0.10 | 114,120,134,135            | 0     |
| 1   | 7MG  | A     | 527  | 24/25 | 0.94 | 0.10 | 102,107,117,124            | 0     |
| 1   | 5MC  | A     | 1400 | 21/22 | 0.94 | 0.08 | 96,119,128,133             | 0     |
| 1   | MA6  | A     | 1519 | 24/25 | 0.95 | 0.11 | 109,131,137,140            | 0     |
| 1   | M2G  | A     | 966  | 25/26 | 0.96 | 0.07 | 128,130,135,137            | 0     |
| 1   | 5MC  | A     | 1404 | 21/22 | 0.96 | 0.09 | 112,125,133,135            | 0     |
| 1   | 5MC  | A     | 967  | 21/22 | 0.97 | 0.07 | 117,134,142,143            | 0     |
| 1   | 2MG  | A     | 1207 | 24/25 | 0.97 | 0.11 | 166,200,208,210            | 0     |
| 1   | 4OC  | A     | 1402 | 22/23 | 0.98 | 0.08 | 105,113,122,124            | 0     |

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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 | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 23  | MG   | A     | 1757 | 1/1   | 0.60 | 0.33 | 123,123,123,123            | 0     |
| 23  | MG   | A     | 1805 | 1/1   | 0.62 | 0.51 | 123,123,123,123            | 0     |
| 23  | MG   | A     | 1809 | 1/1   | 0.64 | 0.27 | 132,132,132,132            | 0     |
| 23  | MG   | A     | 1823 | 1/1   | 0.64 | 1.19 | 143,143,143,143            | 0     |
| 23  | MG   | A     | 1628 | 1/1   | 0.66 | 0.19 | 165,165,165,165            | 0     |
| 23  | MG   | A     | 1801 | 1/1   | 0.67 | 0.57 | 114,114,114,114            | 0     |
| 23  | MG   | A     | 1755 | 1/1   | 0.70 | 0.25 | 116,116,116,116            | 0     |
| 23  | MG   | A     | 1767 | 1/1   | 0.71 | 0.36 | 119,119,119,119            | 0     |
| 23  | MG   | A     | 1771 | 1/1   | 0.76 | 0.46 | 111,111,111,111            | 0     |
| 23  | MG   | A     | 1799 | 1/1   | 0.76 | 0.10 | 361,361,361,361            | 0     |
| 23  | MG   | A     | 1674 | 1/1   | 0.77 | 0.29 | 128,128,128,128            | 0     |
| 23  | MG   | A     | 1794 | 1/1   | 0.78 | 0.24 | 120,120,120,120            | 0     |
| 23  | MG   | A     | 1800 | 1/1   | 0.78 | 0.86 | 128,128,128,128            | 0     |
| 23  | MG   | A     | 1720 | 1/1   | 0.79 | 0.29 | 165,165,165,165            | 0     |
| 23  | MG   | A     | 1683 | 1/1   | 0.79 | 0.67 | 117,117,117,117            | 0     |
| 23  | MG   | A     | 1829 | 1/1   | 0.79 | 0.54 | 114,114,114,114            | 0     |
| 23  | MG   | A     | 1782 | 1/1   | 0.80 | 0.14 | 264,264,264,264            | 0     |
| 23  | MG   | A     | 1791 | 1/1   | 0.80 | 0.33 | 155,155,155,155            | 0     |
| 23  | MG   | A     | 1719 | 1/1   | 0.80 | 0.24 | 117,117,117,117            | 0     |
| 23  | MG   | A     | 1768 | 1/1   | 0.80 | 0.32 | 149,149,149,149            | 0     |
| 23  | MG   | A     | 1763 | 1/1   | 0.80 | 0.23 | 146,146,146,146            | 0     |
| 23  | MG   | A     | 1743 | 1/1   | 0.81 | 0.43 | 110,110,110,110            | 0     |
| 23  | MG   | A     | 1660 | 1/1   | 0.82 | 0.21 | 154,154,154,154            | 0     |
| 23  | MG   | A     | 1723 | 1/1   | 0.82 | 0.41 | 111,111,111,111            | 0     |
| 23  | MG   | A     | 1724 | 1/1   | 0.82 | 0.28 | 140,140,140,140            | 0     |
| 23  | MG   | A     | 1697 | 1/1   | 0.82 | 0.14 | 166,166,166,166            | 0     |
| 23  | MG   | A     | 1633 | 1/1   | 0.82 | 0.43 | 122,122,122,122            | 0     |
| 23  | MG   | A     | 1760 | 1/1   | 0.83 | 0.33 | 116,116,116,116            | 0     |
| 23  | MG   | A     | 1659 | 1/1   | 0.83 | 0.11 | 158,158,158,158            | 0     |
| 23  | MG   | A     | 1807 | 1/1   | 0.83 | 0.48 | 120,120,120,120            | 0     |
| 23  | MG   | A     | 1754 | 1/1   | 0.83 | 0.30 | 118,118,118,118            | 0     |
| 23  | MG   | A     | 1813 | 1/1   | 0.83 | 0.24 | 130,130,130,130            | 0     |
| 23  | MG   | A     | 1709 | 1/1   | 0.83 | 0.29 | 253,253,253,253            | 0     |
| 23  | MG   | A     | 1695 | 1/1   | 0.83 | 0.10 | 144,144,144,144            | 0     |
| 23  | MG   | N     | 102  | 1/1   | 0.83 | 0.22 | 130,130,130,130            | 0     |
| 23  | MG   | Q     | 201  | 1/1   | 0.83 | 0.15 | 119,119,119,119            | 0     |
| 23  | MG   | A     | 1682 | 1/1   | 0.84 | 0.35 | 106,106,106,106            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 23  | MG   | A     | 1673 | 1/1   | 0.84 | 0.20 | 148,148,148,148             | 0     |
| 23  | MG   | A     | 1806 | 1/1   | 0.84 | 0.31 | 96,96,96,96                 | 0     |
| 23  | MG   | A     | 1642 | 1/1   | 0.84 | 0.30 | 113,113,113,113             | 0     |
| 23  | MG   | A     | 1764 | 1/1   | 0.84 | 0.26 | 123,123,123,123             | 0     |
| 23  | MG   | A     | 1619 | 1/1   | 0.85 | 0.23 | 117,117,117,117             | 0     |
| 23  | MG   | A     | 1776 | 1/1   | 0.85 | 0.30 | 137,137,137,137             | 0     |
| 23  | MG   | A     | 1718 | 1/1   | 0.85 | 0.19 | 144,144,144,144             | 0     |
| 23  | MG   | A     | 1736 | 1/1   | 0.85 | 0.37 | 114,114,114,114             | 0     |
| 23  | MG   | A     | 1810 | 1/1   | 0.85 | 0.23 | 106,106,106,106             | 0     |
| 23  | MG   | A     | 1678 | 1/1   | 0.86 | 0.39 | 104,104,104,104             | 0     |
| 23  | MG   | A     | 1797 | 1/1   | 0.86 | 0.41 | 126,126,126,126             | 0     |
| 23  | MG   | A     | 1825 | 1/1   | 0.86 | 0.49 | 126,126,126,126             | 0     |
| 23  | MG   | A     | 1777 | 1/1   | 0.86 | 0.10 | 135,135,135,135             | 0     |
| 23  | MG   | A     | 1733 | 1/1   | 0.86 | 0.08 | 120,120,120,120             | 0     |
| 23  | MG   | A     | 1748 | 1/1   | 0.86 | 0.28 | 117,117,117,117             | 0     |
| 23  | MG   | A     | 1775 | 1/1   | 0.87 | 0.08 | 108,108,108,108             | 0     |
| 23  | MG   | A     | 1725 | 1/1   | 0.87 | 0.24 | 120,120,120,120             | 0     |
| 23  | MG   | A     | 1770 | 1/1   | 0.87 | 0.41 | 114,114,114,114             | 0     |
| 23  | MG   | A     | 1672 | 1/1   | 0.87 | 0.21 | 134,134,134,134             | 0     |
| 23  | MG   | A     | 1821 | 1/1   | 0.87 | 0.28 | 135,135,135,135             | 0     |
| 23  | MG   | A     | 1604 | 1/1   | 0.88 | 0.17 | 107,107,107,107             | 0     |
| 23  | MG   | A     | 1728 | 1/1   | 0.88 | 0.19 | 120,120,120,120             | 0     |
| 23  | MG   | A     | 1730 | 1/1   | 0.88 | 0.18 | 92,92,92,92                 | 0     |
| 23  | MG   | A     | 1778 | 1/1   | 0.88 | 0.21 | 90,90,90,90                 | 0     |
| 23  | MG   | A     | 1804 | 1/1   | 0.88 | 0.14 | 116,116,116,116             | 0     |
| 23  | MG   | A     | 1666 | 1/1   | 0.88 | 0.34 | 133,133,133,133             | 0     |
| 23  | MG   | A     | 1707 | 1/1   | 0.88 | 0.18 | 131,131,131,131             | 0     |
| 23  | MG   | A     | 1739 | 1/1   | 0.88 | 0.15 | 106,106,106,106             | 0     |
| 23  | MG   | A     | 1808 | 1/1   | 0.88 | 0.27 | 95,95,95,95                 | 0     |
| 23  | MG   | A     | 1762 | 1/1   | 0.89 | 0.38 | 119,119,119,119             | 0     |
| 23  | MG   | A     | 1731 | 1/1   | 0.89 | 0.41 | 126,126,126,126             | 0     |
| 23  | MG   | A     | 1749 | 1/1   | 0.89 | 0.23 | 127,127,127,127             | 0     |
| 23  | MG   | A     | 1761 | 1/1   | 0.89 | 0.16 | 117,117,117,117             | 0     |
| 23  | MG   | A     | 1790 | 1/1   | 0.89 | 0.32 | 142,142,142,142             | 0     |
| 23  | MG   | A     | 1740 | 1/1   | 0.90 | 0.20 | 126,126,126,126             | 0     |
| 23  | MG   | A     | 1706 | 1/1   | 0.90 | 0.24 | 159,159,159,159             | 0     |
| 23  | MG   | A     | 1630 | 1/1   | 0.90 | 0.32 | 102,102,102,102             | 0     |
| 23  | MG   | A     | 1766 | 1/1   | 0.90 | 0.40 | 73,73,73,73                 | 0     |
| 23  | MG   | A     | 1627 | 1/1   | 0.90 | 0.39 | 108,108,108,108             | 0     |
| 23  | MG   | A     | 1812 | 1/1   | 0.90 | 0.50 | 117,117,117,117             | 0     |
| 23  | MG   | A     | 1751 | 1/1   | 0.90 | 0.14 | 89,89,89,89                 | 0     |
| 23  | MG   | A     | 1688 | 1/1   | 0.90 | 0.27 | 120,120,120,120             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 23  | MG   | A     | 1662 | 1/1   | 0.90 | 0.23 | 126,126,126,126             | 0     |
| 23  | MG   | A     | 1696 | 1/1   | 0.90 | 0.21 | 104,104,104,104             | 0     |
| 23  | MG   | A     | 1802 | 1/1   | 0.90 | 0.24 | 125,125,125,125             | 0     |
| 23  | MG   | A     | 1831 | 1/1   | 0.90 | 0.45 | 130,130,130,130             | 0     |
| 23  | MG   | H     | 201  | 1/1   | 0.90 | 0.14 | 107,107,107,107             | 0     |
| 23  | MG   | A     | 1721 | 1/1   | 0.90 | 0.10 | 77,77,77,77                 | 0     |
| 23  | MG   | A     | 1605 | 1/1   | 0.90 | 0.37 | 118,118,118,118             | 0     |
| 23  | MG   | A     | 1621 | 1/1   | 0.91 | 0.10 | 127,127,127,127             | 0     |
| 23  | MG   | A     | 1815 | 1/1   | 0.91 | 0.20 | 113,113,113,113             | 0     |
| 23  | MG   | A     | 1832 | 1/1   | 0.91 | 0.26 | 132,132,132,132             | 0     |
| 23  | MG   | A     | 1631 | 1/1   | 0.91 | 0.44 | 107,107,107,107             | 0     |
| 23  | MG   | A     | 1734 | 1/1   | 0.91 | 0.25 | 112,112,112,112             | 0     |
| 23  | MG   | A     | 1700 | 1/1   | 0.91 | 0.14 | 226,226,226,226             | 0     |
| 23  | MG   | A     | 1629 | 1/1   | 0.92 | 0.08 | 103,103,103,103             | 0     |
| 23  | MG   | A     | 1708 | 1/1   | 0.92 | 0.15 | 325,325,325,325             | 0     |
| 23  | MG   | A     | 1786 | 1/1   | 0.92 | 0.24 | 115,115,115,115             | 0     |
| 23  | MG   | A     | 1828 | 1/1   | 0.92 | 0.40 | 122,122,122,122             | 0     |
| 23  | MG   | A     | 1650 | 1/1   | 0.92 | 0.14 | 107,107,107,107             | 0     |
| 23  | MG   | A     | 1705 | 1/1   | 0.92 | 0.09 | 82,82,82,82                 | 0     |
| 23  | MG   | A     | 1747 | 1/1   | 0.92 | 0.23 | 136,136,136,136             | 0     |
| 23  | MG   | A     | 1685 | 1/1   | 0.92 | 0.33 | 173,173,173,173             | 0     |
| 23  | MG   | A     | 1817 | 1/1   | 0.92 | 0.11 | 113,113,113,113             | 0     |
| 23  | MG   | A     | 1820 | 1/1   | 0.92 | 0.22 | 92,92,92,92                 | 0     |
| 23  | MG   | A     | 1780 | 1/1   | 0.93 | 0.08 | 122,122,122,122             | 0     |
| 23  | MG   | A     | 1818 | 1/1   | 0.93 | 0.36 | 134,134,134,134             | 0     |
| 23  | MG   | A     | 1623 | 1/1   | 0.93 | 0.20 | 120,120,120,120             | 0     |
| 23  | MG   | A     | 1726 | 1/1   | 0.93 | 0.24 | 120,120,120,120             | 0     |
| 23  | MG   | A     | 1742 | 1/1   | 0.93 | 0.27 | 94,94,94,94                 | 0     |
| 23  | MG   | A     | 1752 | 1/1   | 0.93 | 0.18 | 87,87,87,87                 | 0     |
| 23  | MG   | A     | 1772 | 1/1   | 0.93 | 0.20 | 101,101,101,101             | 0     |
| 23  | MG   | A     | 1795 | 1/1   | 0.93 | 0.31 | 79,79,79,79                 | 0     |
| 23  | MG   | A     | 1753 | 1/1   | 0.93 | 0.31 | 112,112,112,112             | 0     |
| 23  | MG   | A     | 1625 | 1/1   | 0.93 | 0.20 | 134,134,134,134             | 0     |
| 23  | MG   | D     | 303  | 1/1   | 0.93 | 0.18 | 104,104,104,104             | 0     |
| 23  | MG   | A     | 1765 | 1/1   | 0.93 | 0.17 | 126,126,126,126             | 0     |
| 23  | MG   | A     | 1689 | 1/1   | 0.93 | 0.16 | 202,202,202,202             | 0     |
| 23  | MG   | P     | 102  | 1/1   | 0.93 | 0.16 | 125,125,125,125             | 0     |
| 23  | MG   | A     | 1816 | 1/1   | 0.93 | 0.33 | 100,100,100,100             | 0     |
| 23  | MG   | A     | 1735 | 1/1   | 0.94 | 0.07 | 110,110,110,110             | 0     |
| 23  | MG   | A     | 1667 | 1/1   | 0.94 | 0.25 | 97,97,97,97                 | 0     |
| 23  | MG   | A     | 1779 | 1/1   | 0.94 | 0.09 | 122,122,122,122             | 0     |
| 23  | MG   | A     | 1811 | 1/1   | 0.94 | 0.28 | 105,105,105,105             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 23  | MG   | A     | 1737 | 1/1   | 0.94 | 0.28 | 128,128,128,128             | 0     |
| 23  | MG   | A     | 1669 | 1/1   | 0.94 | 0.16 | 133,133,133,133             | 0     |
| 23  | MG   | A     | 1784 | 1/1   | 0.94 | 0.08 | 119,119,119,119             | 0     |
| 23  | MG   | A     | 1648 | 1/1   | 0.94 | 0.15 | 117,117,117,117             | 0     |
| 23  | MG   | A     | 1787 | 1/1   | 0.94 | 0.35 | 122,122,122,122             | 0     |
| 23  | MG   | A     | 1788 | 1/1   | 0.94 | 0.19 | 124,124,124,124             | 0     |
| 23  | MG   | A     | 1741 | 1/1   | 0.94 | 0.13 | 125,125,125,125             | 0     |
| 23  | MG   | A     | 1607 | 1/1   | 0.94 | 0.25 | 111,111,111,111             | 0     |
| 23  | MG   | A     | 1822 | 1/1   | 0.94 | 0.21 | 97,97,97,97                 | 0     |
| 23  | MG   | A     | 1651 | 1/1   | 0.94 | 0.25 | 76,76,76,76                 | 0     |
| 23  | MG   | A     | 1744 | 1/1   | 0.94 | 0.16 | 99,99,99,99                 | 0     |
| 23  | MG   | A     | 1826 | 1/1   | 0.94 | 0.16 | 82,82,82,82                 | 0     |
| 23  | MG   | A     | 1620 | 1/1   | 0.94 | 0.20 | 128,128,128,128             | 0     |
| 23  | MG   | A     | 1681 | 1/1   | 0.94 | 0.34 | 146,146,146,146             | 0     |
| 23  | MG   | A     | 1612 | 1/1   | 0.94 | 0.12 | 127,127,127,127             | 0     |
| 23  | MG   | A     | 1639 | 1/1   | 0.94 | 0.09 | 160,160,160,160             | 0     |
| 23  | MG   | A     | 1665 | 1/1   | 0.94 | 0.10 | 117,117,117,117             | 0     |
| 23  | MG   | A     | 1773 | 1/1   | 0.94 | 0.06 | 109,109,109,109             | 0     |
| 23  | MG   | A     | 1774 | 1/1   | 0.94 | 0.14 | 106,106,106,106             | 0     |
| 23  | MG   | P     | 101  | 1/1   | 0.94 | 0.21 | 97,97,97,97                 | 0     |
| 23  | MG   | A     | 1710 | 1/1   | 0.94 | 0.23 | 115,115,115,115             | 0     |
| 23  | MG   | A     | 1618 | 1/1   | 0.94 | 0.21 | 109,109,109,109             | 0     |
| 23  | MG   | A     | 1641 | 1/1   | 0.95 | 0.10 | 101,101,101,101             | 0     |
| 23  | MG   | A     | 1819 | 1/1   | 0.95 | 0.32 | 123,123,123,123             | 0     |
| 23  | MG   | A     | 1680 | 1/1   | 0.95 | 0.09 | 125,125,125,125             | 0     |
| 23  | MG   | A     | 1687 | 1/1   | 0.95 | 0.41 | 179,179,179,179             | 0     |
| 23  | MG   | A     | 1664 | 1/1   | 0.95 | 0.50 | 96,96,96,96                 | 0     |
| 23  | MG   | A     | 1785 | 1/1   | 0.95 | 0.18 | 154,154,154,154             | 0     |
| 23  | MG   | A     | 1712 | 1/1   | 0.95 | 0.24 | 194,194,194,194             | 0     |
| 23  | MG   | A     | 1713 | 1/1   | 0.95 | 0.35 | 109,109,109,109             | 0     |
| 23  | MG   | A     | 1827 | 1/1   | 0.95 | 0.25 | 116,116,116,116             | 0     |
| 23  | MG   | A     | 1729 | 1/1   | 0.95 | 0.19 | 110,110,110,110             | 0     |
| 23  | MG   | A     | 1758 | 1/1   | 0.95 | 0.28 | 111,111,111,111             | 0     |
| 23  | MG   | A     | 1717 | 1/1   | 0.95 | 0.16 | 107,107,107,107             | 0     |
| 23  | MG   | A     | 1793 | 1/1   | 0.95 | 0.05 | 92,92,92,92                 | 0     |
| 23  | MG   | B     | 301  | 1/1   | 0.95 | 0.11 | 125,125,125,125             | 0     |
| 23  | MG   | B     | 302  | 1/1   | 0.95 | 0.07 | 168,168,168,168             | 0     |
| 23  | MG   | C     | 301  | 1/1   | 0.95 | 0.14 | 92,92,92,92                 | 0     |
| 23  | MG   | A     | 1701 | 1/1   | 0.95 | 0.10 | 113,113,113,113             | 0     |
| 23  | MG   | A     | 1746 | 1/1   | 0.95 | 0.16 | 85,85,85,85                 | 0     |
| 23  | MG   | A     | 1814 | 1/1   | 0.95 | 0.25 | 108,108,108,108             | 0     |
| 23  | MG   | A     | 1652 | 1/1   | 0.95 | 0.10 | 118,118,118,118             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 23  | MG   | A     | 1798 | 1/1   | 0.95 | 0.29 | 129,129,129,129             | 0     |
| 23  | MG   | A     | 1694 | 1/1   | 0.95 | 0.27 | 116,116,116,116             | 0     |
| 24  | ZN   | D     | 301  | 1/1   | 0.95 | 0.25 | 102,102,102,102             | 0     |
| 23  | MG   | A     | 1684 | 1/1   | 0.96 | 0.10 | 114,114,114,114             | 0     |
| 23  | MG   | A     | 1609 | 1/1   | 0.96 | 0.08 | 106,106,106,106             | 0     |
| 23  | MG   | A     | 1686 | 1/1   | 0.96 | 0.21 | 146,146,146,146             | 0     |
| 23  | MG   | A     | 1640 | 1/1   | 0.96 | 0.07 | 67,67,67,67                 | 0     |
| 23  | MG   | A     | 1614 | 1/1   | 0.96 | 0.07 | 98,98,98,98                 | 0     |
| 23  | MG   | A     | 1655 | 1/1   | 0.96 | 0.10 | 93,93,93,93                 | 0     |
| 23  | MG   | A     | 1693 | 1/1   | 0.96 | 0.20 | 108,108,108,108             | 0     |
| 23  | MG   | A     | 1658 | 1/1   | 0.96 | 0.07 | 98,98,98,98                 | 0     |
| 23  | MG   | A     | 1637 | 1/1   | 0.96 | 0.22 | 99,99,99,99                 | 0     |
| 23  | MG   | A     | 1769 | 1/1   | 0.96 | 0.07 | 115,115,115,115             | 0     |
| 23  | MG   | A     | 1745 | 1/1   | 0.96 | 0.34 | 100,100,100,100             | 0     |
| 23  | MG   | A     | 1675 | 1/1   | 0.96 | 0.20 | 129,129,129,129             | 0     |
| 23  | MG   | A     | 1676 | 1/1   | 0.96 | 0.15 | 106,106,106,106             | 0     |
| 23  | MG   | A     | 1699 | 1/1   | 0.96 | 0.10 | 108,108,108,108             | 0     |
| 23  | MG   | A     | 1830 | 1/1   | 0.96 | 0.15 | 107,107,107,107             | 0     |
| 23  | MG   | A     | 1803 | 1/1   | 0.96 | 0.12 | 110,110,110,110             | 0     |
| 23  | MG   | A     | 1677 | 1/1   | 0.96 | 0.21 | 244,244,244,244             | 0     |
| 23  | MG   | A     | 1727 | 1/1   | 0.96 | 0.30 | 91,91,91,91                 | 0     |
| 23  | MG   | A     | 1643 | 1/1   | 0.96 | 0.27 | 77,77,77,77                 | 0     |
| 23  | MG   | A     | 1702 | 1/1   | 0.96 | 0.14 | 138,138,138,138             | 0     |
| 23  | MG   | A     | 1661 | 1/1   | 0.96 | 0.29 | 110,110,110,110             | 0     |
| 23  | MG   | F     | 201  | 1/1   | 0.96 | 0.08 | 112,112,112,112             | 0     |
| 23  | MG   | A     | 1646 | 1/1   | 0.96 | 0.22 | 103,103,103,103             | 0     |
| 23  | MG   | K     | 201  | 1/1   | 0.96 | 0.18 | 100,100,100,100             | 0     |
| 23  | MG   | L     | 201  | 1/1   | 0.96 | 0.07 | 123,123,123,123             | 0     |
| 23  | MG   | A     | 1756 | 1/1   | 0.96 | 0.33 | 153,153,153,153             | 0     |
| 23  | MG   | A     | 1638 | 1/1   | 0.96 | 0.28 | 101,101,101,101             | 0     |
| 23  | MG   | A     | 1783 | 1/1   | 0.96 | 0.19 | 319,319,319,319             | 0     |
| 23  | MG   | A     | 1649 | 1/1   | 0.96 | 0.23 | 106,106,106,106             | 0     |
| 23  | MG   | A     | 1759 | 1/1   | 0.96 | 0.20 | 88,88,88,88                 | 0     |
| 23  | MG   | A     | 1602 | 1/1   | 0.97 | 0.11 | 109,109,109,109             | 0     |
| 23  | MG   | A     | 1613 | 1/1   | 0.97 | 0.11 | 105,105,105,105             | 0     |
| 23  | MG   | A     | 1671 | 1/1   | 0.97 | 0.22 | 115,115,115,115             | 0     |
| 23  | MG   | A     | 1654 | 1/1   | 0.97 | 0.11 | 71,71,71,71                 | 0     |
| 23  | MG   | A     | 1622 | 1/1   | 0.97 | 0.09 | 94,94,94,94                 | 0     |
| 23  | MG   | A     | 1750 | 1/1   | 0.97 | 0.37 | 120,120,120,120             | 0     |
| 23  | MG   | A     | 1657 | 1/1   | 0.97 | 0.09 | 88,88,88,88                 | 0     |
| 23  | MG   | A     | 1690 | 1/1   | 0.97 | 0.12 | 151,151,151,151             | 0     |
| 23  | MG   | A     | 1603 | 1/1   | 0.97 | 0.11 | 126,126,126,126             | 0     |

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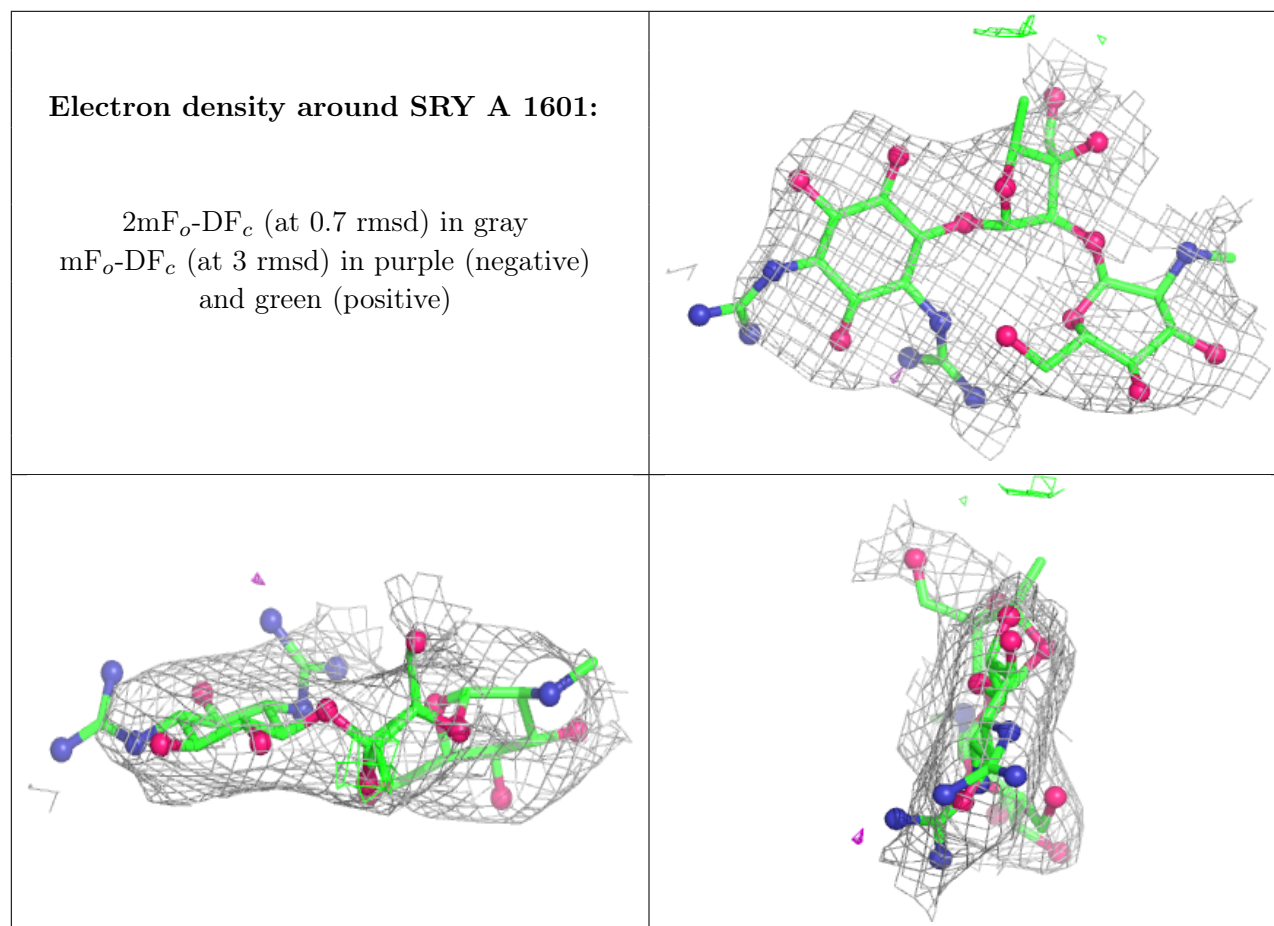
| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 23  | MG   | A     | 1792 | 1/1   | 0.97 | 0.27 | 120,120,120,120             | 0     |
| 23  | MG   | A     | 1716 | 1/1   | 0.97 | 0.06 | 102,102,102,102             | 0     |
| 23  | MG   | D     | 302  | 1/1   | 0.97 | 0.13 | 105,105,105,105             | 0     |
| 22  | SRY  | A     | 1601 | 40/40 | 0.97 | 0.08 | 93,111,127,129              | 0     |
| 23  | MG   | E     | 201  | 1/1   | 0.97 | 0.05 | 140,140,140,140             | 0     |
| 23  | MG   | A     | 1644 | 1/1   | 0.97 | 0.08 | 95,95,95,95                 | 0     |
| 23  | MG   | A     | 1645 | 1/1   | 0.97 | 0.12 | 88,88,88,88                 | 0     |
| 23  | MG   | A     | 1679 | 1/1   | 0.97 | 0.21 | 112,112,112,112             | 0     |
| 23  | MG   | A     | 1634 | 1/1   | 0.97 | 0.12 | 133,133,133,133             | 0     |
| 23  | MG   | A     | 1635 | 1/1   | 0.97 | 0.10 | 119,119,119,119             | 0     |
| 23  | MG   | A     | 1626 | 1/1   | 0.97 | 0.28 | 75,75,75,75                 | 0     |
| 23  | MG   | A     | 1610 | 1/1   | 0.97 | 0.07 | 85,85,85,85                 | 0     |
| 23  | MG   | A     | 1781 | 1/1   | 0.97 | 0.21 | 200,200,200,200             | 0     |
| 23  | MG   | Q     | 202  | 1/1   | 0.97 | 0.06 | 89,89,89,89                 | 0     |
| 23  | MG   | A     | 1824 | 1/1   | 0.97 | 0.32 | 118,118,118,118             | 0     |
| 23  | MG   | A     | 1698 | 1/1   | 0.98 | 0.04 | 136,136,136,136             | 0     |
| 23  | MG   | A     | 1796 | 1/1   | 0.98 | 0.26 | 98,98,98,98                 | 0     |
| 23  | MG   | A     | 1663 | 1/1   | 0.98 | 0.07 | 113,113,113,113             | 0     |
| 23  | MG   | A     | 1715 | 1/1   | 0.98 | 0.18 | 116,116,116,116             | 0     |
| 23  | MG   | A     | 1615 | 1/1   | 0.98 | 0.16 | 83,83,83,83                 | 0     |
| 23  | MG   | A     | 1617 | 1/1   | 0.98 | 0.08 | 112,112,112,112             | 0     |
| 23  | MG   | A     | 1691 | 1/1   | 0.98 | 0.13 | 136,136,136,136             | 0     |
| 23  | MG   | A     | 1703 | 1/1   | 0.98 | 0.06 | 141,141,141,141             | 0     |
| 23  | MG   | A     | 1704 | 1/1   | 0.98 | 0.08 | 112,112,112,112             | 0     |
| 23  | MG   | A     | 1738 | 1/1   | 0.98 | 0.04 | 91,91,91,91                 | 0     |
| 23  | MG   | A     | 1692 | 1/1   | 0.98 | 0.14 | 112,112,112,112             | 0     |
| 23  | MG   | A     | 1636 | 1/1   | 0.98 | 0.09 | 97,97,97,97                 | 0     |
| 23  | MG   | A     | 1789 | 1/1   | 0.98 | 0.27 | 125,125,125,125             | 0     |
| 23  | MG   | A     | 1611 | 1/1   | 0.98 | 0.06 | 179,179,179,179             | 0     |
| 23  | MG   | A     | 1668 | 1/1   | 0.98 | 0.09 | 116,116,116,116             | 0     |
| 23  | MG   | A     | 1608 | 1/1   | 0.98 | 0.04 | 114,114,114,114             | 0     |
| 23  | MG   | A     | 1656 | 1/1   | 0.98 | 0.17 | 174,174,174,174             | 0     |
| 23  | MG   | A     | 1711 | 1/1   | 0.98 | 0.09 | 103,103,103,103             | 0     |
| 24  | ZN   | N     | 101  | 1/1   | 0.98 | 0.05 | 166,166,166,166             | 0     |
| 23  | MG   | A     | 1647 | 1/1   | 0.99 | 0.04 | 143,143,143,143             | 0     |
| 23  | MG   | A     | 1722 | 1/1   | 0.99 | 0.11 | 106,106,106,106             | 0     |
| 23  | MG   | A     | 1732 | 1/1   | 0.99 | 0.08 | 87,87,87,87                 | 0     |
| 23  | MG   | A     | 1714 | 1/1   | 0.99 | 0.12 | 54,54,54,54                 | 0     |
| 23  | MG   | A     | 1653 | 1/1   | 0.99 | 0.04 | 99,99,99,99                 | 0     |
| 23  | MG   | A     | 1616 | 1/1   | 0.99 | 0.11 | 61,61,61,61                 | 0     |
| 23  | MG   | A     | 1632 | 1/1   | 0.99 | 0.04 | 85,85,85,85                 | 0     |
| 23  | MG   | A     | 1606 | 1/1   | 0.99 | 0.05 | 89,89,89,89                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 23  | MG   | A     | 1624 | 1/1   | 0.99 | 0.19 | 64,64,64,64                 | 0     |
| 23  | MG   | A     | 1670 | 1/1   | 0.99 | 0.12 | 105,105,105,105             | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.