



Full wwPDB X-ray Structure Validation Report

Nov 23, 2014 – 12:09 PM EST

PDB ID : 4W2A
Title : Crystal structure of the peptolide 12C bound to bacterial ribosome
Authors : Fagan, C.E.; Dunham, C.M.
Deposited on : 2014-03-24
Resolution : 3.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

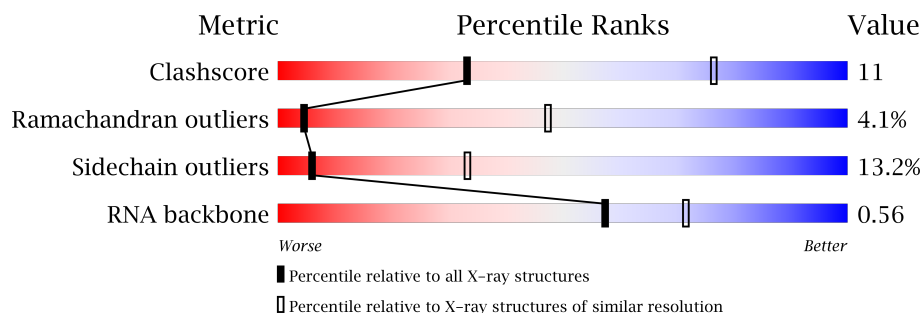
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24195

1 Overall quality at a glance

The reported resolution of this entry is 3.60 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 79885 | 1155 (3.80-3.40) |
| Ramachandran outliers | 78287 | 1109 (3.80-3.40) |
| Sidechain outliers | 78261 | 1108 (3.80-3.40) |
| RNA backbone | 1838 | 1012 (4.40-2.76) |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 1522 | |
| 2 | B | 256 | |
| 3 | C | 239 | |
| 4 | D | 209 | |
| 5 | E | 162 | |
| 6 | F | 101 | |
| 7 | H | 156 | |
| 8 | I | 138 | |
| 9 | J | 128 | |
| 10 | K | 105 | |
| 11 | L | 129 | |
| 12 | M | 132 | |
| 13 | N | 126 | |
| 14 | O | 61 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15 | P | 89 | |
| 16 | Q | 88 | |
| 17 | R | 105 | |
| 18 | S | 88 | |
| 19 | T | 93 | |
| 20 | U | 106 | |
| 21 | V | 27 | |
| 22 | W | 77 | |
| 23 | X | 76 | |
| 23 | Z | 76 | |
| 24 | Y | 24 | |

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 55431 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | A | 1500 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32247 | 14353 | 5981 | 10414 | 1499 | | | |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | B | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1924 | 1228 | 344 | 347 | 5 | | | |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | C | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 1011 | 313 | 280 | 1 | | | |

- Molecule 4 is a protein called 30S 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 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | E | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1155 | 729 | 218 | 204 | 4 | | | |

- Molecule 6 is a protein called 30S 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 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | K | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 801 | 504 | 157 | 139 | 1 | | | |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | L | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 549 | 168 | 165 | 3 | | | |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | M | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 975 | 614 | 196 | 164 | 1 | | | |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | N | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 597 | 199 | 166 | 2 | | | |

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | P | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | | |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | Q | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 705 | 446 | 140 | 118 | 1 | | | |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | R | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 534 | 155 | 143 | 2 | | | |

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | T | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 674 | 430 | 126 | 116 | 2 | | | |

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21 | V | 25 | Total | C | N | O | 0 | 0 | 0 |
| | | | 217 | 134 | 52 | 31 | | | |

- Molecule 22 is a RNA chain called tRNA-fMet.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22 | W | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1644 | 732 | 297 | 538 | 77 | | | |

- Molecule 23 is a RNA chain called E-Site tRNA-Phe or A-Site tRNA-Phe.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 23 | X | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1619 | 723 | 290 | 531 | 75 | | | |
| 23 | Z | 17 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 364 | 163 | 68 | 116 | 17 | | | |

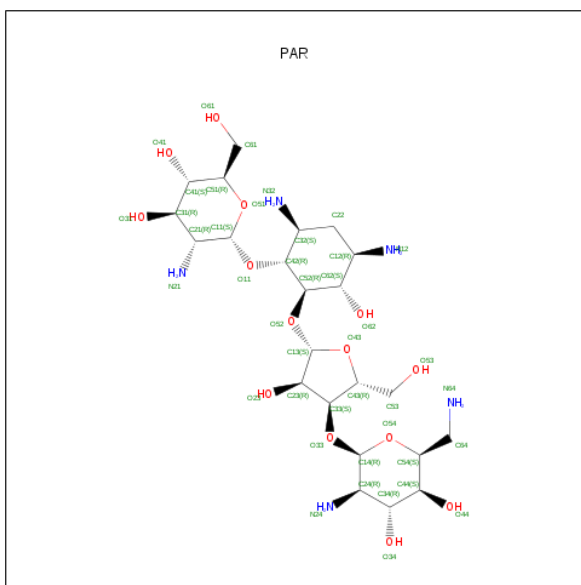
- Molecule 24 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 24 | Y | 10 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 210 | 96 | 39 | 66 | 9 | | | |

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 25 | I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 25 | W | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 25 | Z | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 25 | A | 66 | Total | Mg | 0 | 0 |
| | | | 66 | 66 | | |
| 25 | N | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 25 | F | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

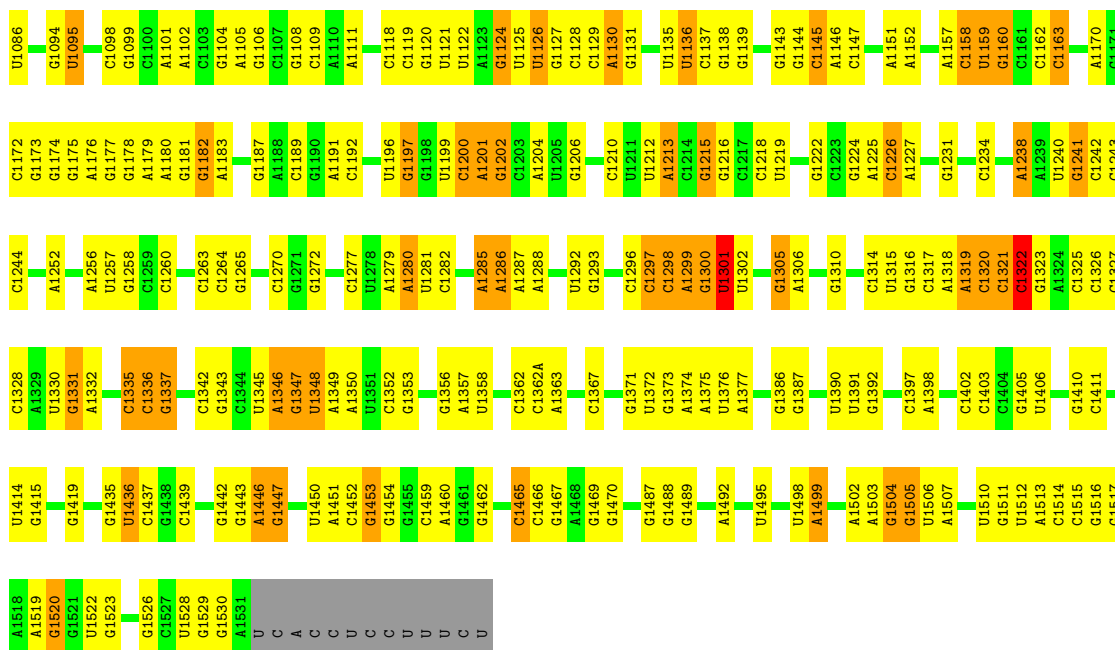
- Molecule 26 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 26 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 27 | O | 1 | Total Zn 1 1 | 0 | 0 |
| 27 | D | 1 | Total Zn 1 1 | 0 | 0 |



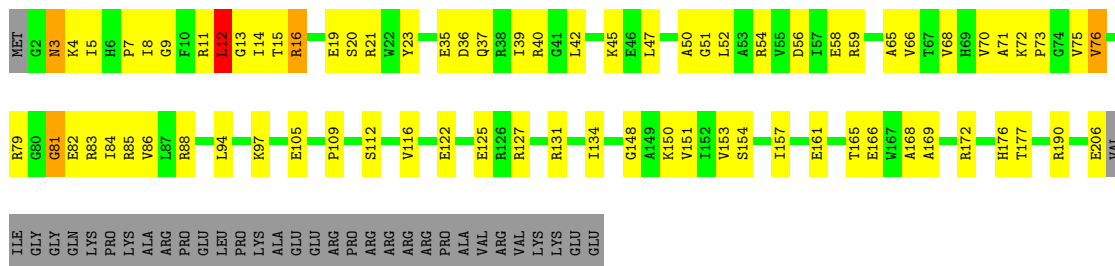
- Molecule 2: 30S ribosomal protein S2

Chain B:



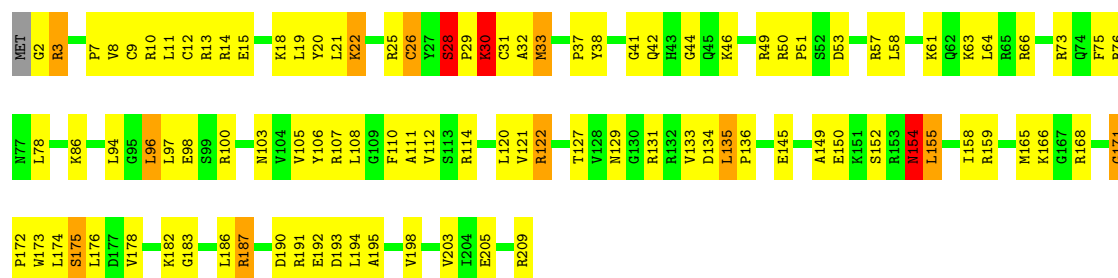
- Molecule 3: 30S ribosomal protein S3

Chain C:



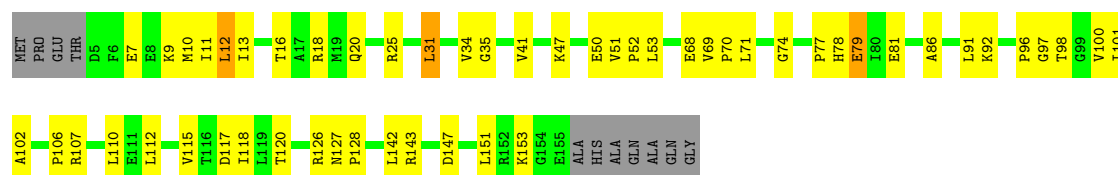
- Molecule 4: 30S ribosomal protein S4

Chain D:



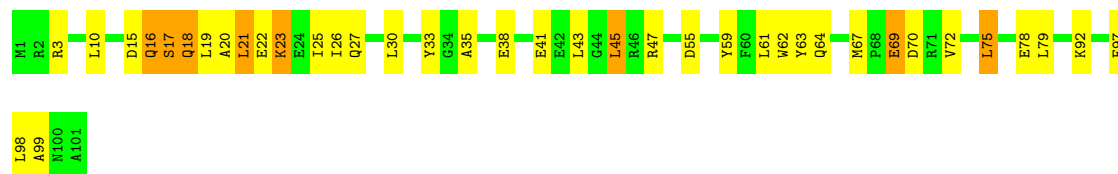
• Molecule 5: 30S ribosomal protein S5

Chain E:



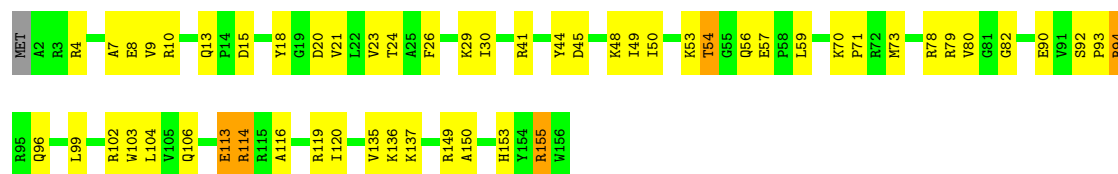
• Molecule 6: 30S ribosomal protein S6

Chain F:



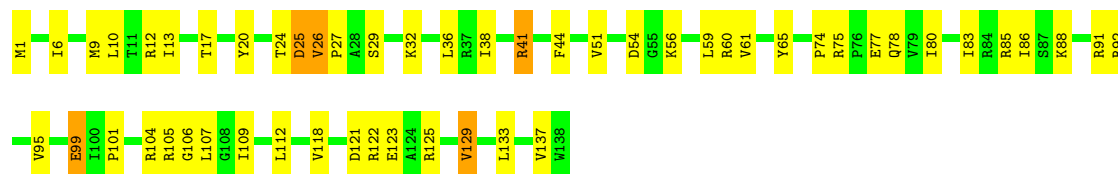
• Molecule 7: 30S ribosomal protein S7

Chain H:



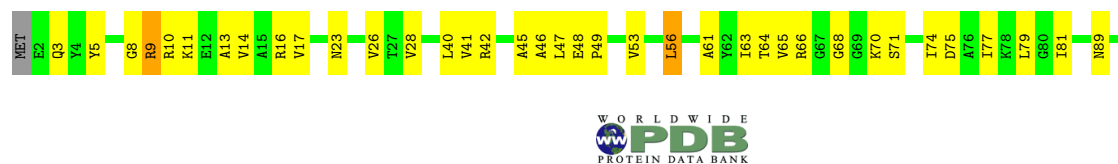
• Molecule 8: 30S ribosomal protein S8

Chain I:



• Molecule 9: 30S ribosomal protein S9

Chain J:





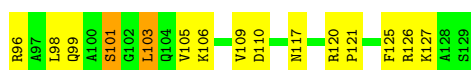
- Molecule 10: 30S ribosomal protein S10

Chain K:



- Molecule 11: 30S ribosomal protein S11

Chain L:



- Molecule 12: 30S ribosomal protein S12

Chain M:



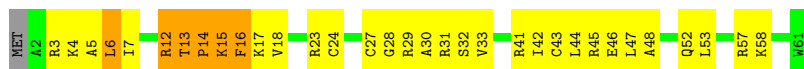
- Molecule 13: 30S ribosomal protein S13

Chain N:



- Molecule 14: 30S ribosomal protein S14 type Z

Chain O:



- Molecule 15: 30S ribosomal protein S15

Chain P:



- Molecule 16: 30S ribosomal protein S16

Chain Q:



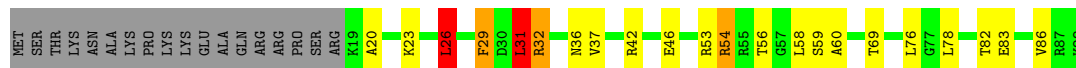
- Molecule 17: 30S ribosomal protein S17

Chain R:



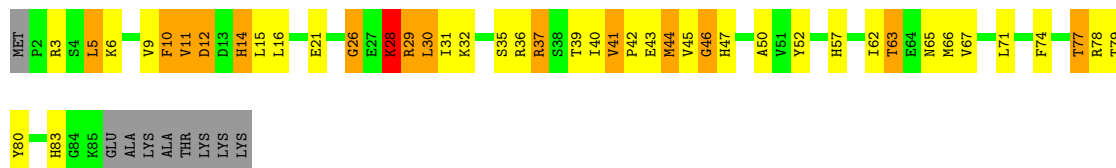
- Molecule 18: 30S ribosomal protein S18

Chain S:



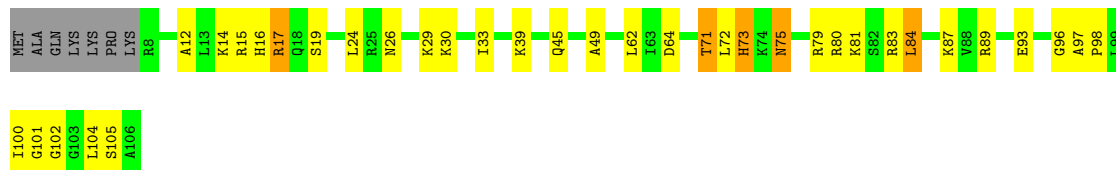
- Molecule 19: 30S ribosomal protein S19

Chain T:



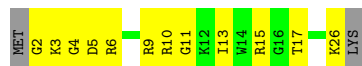
- Molecule 20: 30S ribosomal protein S20

Chain U:



- Molecule 21: 30S ribosomal protein Thx

Chain V:



- Molecule 22: tRNA-fMet

Chain W:





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 209.24Å 443.46Å 618.62Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.79 – 3.60 | Depositor |
| % Data completeness (in resolution range) | 98.1 (49.79-3.60) | Depositor |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | PHENIX (phenix.refine: 1.8.3_1479) | Depositor |
| R, R_{free} | 0.222 , 0.254 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 55431 | wwPDB-VP |
| Average B, all atoms (Å ²) | 132.0 | wwPDB-VP |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 | 0.23 | 0/36098 | 0.81 | 32/56341 (0.1%) |
| 2 | B | 0.31 | 0/1959 | 0.52 | 0/2642 |
| 3 | C | 0.32 | 0/1629 | 0.53 | 0/2195 |
| 4 | D | 0.45 | 0/1733 | 0.62 | 1/2318 (0.0%) |
| 5 | E | 0.35 | 0/1171 | 0.56 | 0/1576 |
| 6 | F | 0.39 | 0/856 | 0.57 | 0/1154 |
| 7 | H | 0.33 | 0/1276 | 0.50 | 0/1709 |
| 8 | I | 0.33 | 0/1136 | 0.55 | 0/1527 |
| 9 | J | 0.31 | 0/1029 | 0.55 | 0/1379 |
| 10 | K | 0.33 | 0/814 | 0.54 | 0/1095 |
| 11 | L | 0.37 | 0/900 | 0.57 | 0/1213 |
| 12 | M | 0.37 | 0/991 | 0.61 | 0/1327 |
| 13 | N | 0.32 | 0/974 | 0.59 | 0/1303 |
| 14 | O | 0.40 | 0/501 | 0.60 | 0/664 |
| 15 | P | 0.35 | 0/745 | 0.53 | 0/992 |
| 16 | Q | 0.36 | 0/721 | 0.57 | 0/970 |
| 17 | R | 0.35 | 0/847 | 0.53 | 0/1131 |
| 18 | S | 0.35 | 0/579 | 0.64 | 1/768 (0.1%) |
| 19 | T | 0.33 | 0/689 | 0.60 | 0/926 |
| 20 | U | 0.36 | 0/765 | 0.64 | 0/1007 |
| 21 | V | 0.31 | 0/221 | 0.53 | 0/288 |
| 22 | W | 0.32 | 1/1836 (0.1%) | 0.80 | 0/2859 |
| 23 | X | 0.19 | 0/1809 | 0.79 | 0/2819 |
| 23 | Z | 0.17 | 0/406 | 0.73 | 0/628 |
| 24 | Y | 0.19 | 0/235 | 0.71 | 0/364 |
| All | All | 0.28 | 1/59920 (0.0%) | 0.74 | 34/89195 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 12 | M | 0 | 1 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 22 | W | 0 | C | OP3-P | -10.61 | 1.48 | 1.61 |

All (34) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 1158 | C | C2-N1-C1' | 7.81 | 127.39 | 118.80 |
| 1 | A | 1495 | U | N1-C2-O2 | 7.48 | 128.04 | 122.80 |
| 1 | A | 1301 | U | C2-N1-C1' | 7.36 | 126.53 | 117.70 |
| 1 | A | 1158 | C | N1-C2-O2 | 7.23 | 123.24 | 118.90 |
| 1 | A | 993 | G | C4-N9-C1' | 7.11 | 135.74 | 126.50 |
| 1 | A | 1301 | U | N1-C2-O2 | 6.76 | 127.53 | 122.80 |
| 1 | A | 993 | G | N3-C4-N9 | 6.70 | 130.02 | 126.00 |
| 1 | A | 1301 | U | N3-C2-O2 | -6.64 | 117.55 | 122.20 |
| 1 | A | 993 | G | C8-N9-C1' | -6.61 | 118.41 | 127.00 |
| 4 | D | 28 | SER | C-N-CD | 6.58 | 142.23 | 128.40 |
| 1 | A | 754 | C | C2-N1-C1' | 6.35 | 125.78 | 118.80 |
| 1 | A | 1065 | U | P-O3'-C3' | 6.33 | 127.29 | 119.70 |
| 1 | A | 1465 | C | C2-N3-C4 | -6.07 | 116.86 | 119.90 |
| 1 | A | 365 | U | C5-C4-O4 | 5.76 | 129.36 | 125.90 |
| 1 | A | 49 | U | C5-C4-O4 | 5.69 | 129.31 | 125.90 |
| 1 | A | 1158 | C | N3-C2-O2 | -5.66 | 117.94 | 121.90 |
| 1 | A | 1065 | U | OP2-P-O3' | 5.62 | 117.56 | 105.20 |
| 1 | A | 1158 | C | C6-N1-C2 | -5.58 | 118.07 | 120.30 |
| 1 | A | 993 | G | C6-C5-N7 | -5.52 | 127.09 | 130.40 |
| 1 | A | 1046 | A | C5-C6-N1 | 5.50 | 120.45 | 117.70 |
| 1 | A | 993 | G | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 1 | A | 49 | U | N3-C4-O4 | -5.46 | 115.58 | 119.40 |
| 1 | A | 1027 | C | OP1-P-O3' | 5.44 | 117.18 | 105.20 |
| 1 | A | 701 | C | OP2-P-O3' | 5.32 | 116.90 | 105.20 |
| 18 | S | 31 | LEU | CA-CB-CG | 5.29 | 127.47 | 115.30 |
| 1 | A | 328 | C | P-O3'-C3' | 5.26 | 126.01 | 119.70 |
| 1 | A | 1158 | C | C6-N1-C1' | -5.25 | 114.50 | 120.80 |
| 1 | A | 1027 | C | P-O3'-C3' | 5.23 | 125.98 | 119.70 |
| 1 | A | 754 | C | N1-C2-O2 | 5.14 | 121.98 | 118.90 |
| 1 | A | 1436 | U | C2-N3-C4 | -5.14 | 123.92 | 127.00 |
| 1 | A | 1322 | C | C2-N1-C1' | 5.13 | 124.45 | 118.80 |
| 1 | A | 1297 | C | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 1 | A | 992 | U | P-O3'-C3' | 5.02 | 125.72 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | A | 1465 | C | C5-C4-N4 | -5.01 | 116.69 | 120.20 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 12 | M | 47 | LYS | Peptide |

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 32247 | 0 | 16278 | 465 | 0 |
| 2 | B | 1924 | 0 | 1975 | 62 | 0 |
| 3 | C | 1605 | 0 | 1668 | 43 | 0 |
| 4 | D | 1703 | 0 | 1763 | 68 | 0 |
| 5 | E | 1155 | 0 | 1213 | 28 | 0 |
| 6 | F | 843 | 0 | 857 | 29 | 0 |
| 7 | H | 1257 | 0 | 1296 | 46 | 0 |
| 8 | I | 1116 | 0 | 1175 | 38 | 0 |
| 9 | J | 1010 | 0 | 1037 | 37 | 0 |
| 10 | K | 801 | 0 | 849 | 50 | 0 |
| 11 | L | 885 | 0 | 904 | 36 | 0 |
| 12 | M | 975 | 0 | 1062 | 39 | 0 |
| 13 | N | 964 | 0 | 1034 | 38 | 0 |
| 14 | O | 492 | 0 | 529 | 27 | 0 |
| 15 | P | 734 | 0 | 771 | 20 | 0 |
| 16 | Q | 705 | 0 | 725 | 16 | 0 |
| 17 | R | 834 | 0 | 904 | 23 | 0 |
| 18 | S | 574 | 0 | 644 | 10 | 0 |
| 19 | T | 674 | 0 | 699 | 35 | 0 |
| 20 | U | 763 | 0 | 861 | 20 | 0 |
| 21 | V | 217 | 0 | 234 | 11 | 0 |
| 22 | W | 1644 | 0 | 835 | 13 | 0 |
| 23 | X | 1619 | 0 | 822 | 24 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 23 | Z | 364 | 0 | 186 | 1 | 0 |
| 24 | Y | 210 | 0 | 109 | 0 | 0 |
| 25 | A | 66 | 0 | 0 | 0 | 0 |
| 25 | F | 1 | 0 | 0 | 0 | 0 |
| 25 | I | 1 | 0 | 0 | 0 | 0 |
| 25 | N | 1 | 0 | 0 | 0 | 0 |
| 25 | W | 2 | 0 | 0 | 0 | 0 |
| 25 | Z | 1 | 0 | 0 | 0 | 0 |
| 26 | A | 42 | 0 | 45 | 1 | 0 |
| 27 | D | 1 | 0 | 0 | 0 | 0 |
| 27 | O | 1 | 0 | 0 | 0 | 0 |
| All | All | 55431 | 0 | 38475 | 1025 | 0 |

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

All (1025) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:D:166:LYS:HG3 | 4:D:178:VAL:HG11 | 1.32 | 1.10 |
| 4:D:28:SER:HB3 | 4:D:29:PRO:HD3 | 1.39 | 1.00 |
| 4:D:9:CYS:SG | 4:D:22:LYS:CE | 2.52 | 0.97 |
| 4:D:9:CYS:SG | 4:D:22:LYS:HE3 | 2.07 | 0.95 |
| 2:B:185:ILE:HG22 | 2:B:199:TYR:HB2 | 1.48 | 0.93 |
| 1:A:1002:G:H1 | 1:A:1038:C:H42 | 1.00 | 0.93 |
| 4:D:28:SER:HB3 | 4:D:29:PRO:CD | 1.96 | 0.90 |
| 1:A:49:U:C4 | 1:A:365:U:O4 | 2.26 | 0.88 |
| 1:A:963:G:H1 | 1:A:972:C:H42 | 1.22 | 0.88 |
| 1:A:49:U:C5 | 1:A:365:U:O4 | 2.27 | 0.87 |
| 1:A:1316:G:H22 | 1:A:1319:A:H5'' | 1.41 | 0.86 |
| 1:A:410:G:H3' | 4:D:25:ARG:HH21 | 1.41 | 0.85 |
| 5:E:50:GLU:HB3 | 5:E:53:LEU:HD13 | 1.59 | 0.85 |
| 1:A:1002:G:H1 | 1:A:1038:C:N4 | 1.75 | 0.84 |
| 2:B:80:ILE:HD11 | 2:B:208:ILE:HG23 | 1.58 | 0.83 |
| 6:F:17:SER:O | 6:F:20:ALA:N | 2.11 | 0.83 |
| 6:F:17:SER:O | 6:F:19:LEU:N | 2.12 | 0.82 |
| 13:N:14:ARG:H | 13:N:44:ARG:HD3 | 1.45 | 0.81 |
| 4:D:30:LYS:C | 4:D:32:ALA:H | 1.83 | 0.80 |
| 13:N:3:ARG:HA | 13:N:9:ILE:HG21 | 1.62 | 0.80 |
| 11:L:21:ILE:HB | 11:L:84:VAL:HG12 | 1.65 | 0.79 |
| 1:A:1392:G:H21 | 1:A:1502:A:H8 | 1.29 | 0.79 |
| 15:P:26:GLU:OE2 | 15:P:77:ARG:NH1 | 2.16 | 0.79 |
| 6:F:15:ASP:OD1 | 6:F:17:SER:HB2 | 1.83 | 0.79 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 8:I:91:ARG:HB2 | 12:M:7:ILE:HG13 | 1.65 | 0.78 |
| 20:U:100:ILE:HG13 | 20:U:102:GLY:H | 1.48 | 0.78 |
| 10:K:50:ILE:HA | 10:K:60:ARG:HG2 | 1.66 | 0.78 |
| 1:A:1502:A:H2 | 1:A:1505:G:H1 | 1.33 | 0.77 |
| 1:A:1243:C:OP2 | 21:V:10:ARG:NH2 | 2.18 | 0.77 |
| 23:X:12:U:H3 | 23:X:23:A:H61 | 1.33 | 0.76 |
| 1:A:31:G:O2' | 1:A:48:C:N4 | 2.18 | 0.76 |
| 1:A:1055:A:N7 | 1:A:1200:C:N4 | 2.34 | 0.75 |
| 5:E:102:ALA:HB1 | 5:E:106:PRO:HG2 | 1.69 | 0.75 |
| 8:I:29:SER:HB3 | 8:I:32:LYS:HG3 | 1.69 | 0.74 |
| 5:E:7:GLU:HG2 | 5:E:112:LEU:HD22 | 1.69 | 0.74 |
| 14:O:24:CYS:CB | 14:O:27:CYS:SG | 2.74 | 0.74 |
| 5:E:100:VAL:O | 5:E:107:ARG:NH2 | 2.20 | 0.74 |
| 1:A:658:G:OP1 | 15:P:8:LYS:NZ | 2.20 | 0.74 |
| 1:A:686:U:H1' | 11:L:42:TRP:HE1 | 1.51 | 0.73 |
| 4:D:175:SER:HB3 | 4:D:186:LEU:HD21 | 1.69 | 0.73 |
| 1:A:963:G:N3 | 10:K:55:LYS:NZ | 2.32 | 0.73 |
| 1:A:1086:U:H3 | 1:A:1099:G:H22 | 1.35 | 0.73 |
| 1:A:677:U:H3 | 1:A:713:G:H22 | 1.36 | 0.73 |
| 3:C:58:GLU:HB2 | 3:C:65:ALA:HB3 | 1.70 | 0.73 |
| 4:D:30:LYS:HD3 | 4:D:30:LYS:N | 2.03 | 0.73 |
| 1:A:261:U:OP2 | 20:U:79:ARG:NH2 | 2.22 | 0.72 |
| 7:H:9:VAL:HG13 | 7:H:94:ARG:HH21 | 1.54 | 0.72 |
| 3:C:20:SER:HB2 | 3:C:40:ARG:HH22 | 1.54 | 0.72 |
| 17:R:4:LYS:HE3 | 17:R:6:LEU:HD21 | 1.72 | 0.72 |
| 12:M:7:ILE:HG21 | 17:R:34:LYS:HB2 | 1.71 | 0.71 |
| 10:K:61:GLU:OE2 | 14:O:45:ARG:NH1 | 2.23 | 0.71 |
| 2:B:115:LEU:HB2 | 2:B:145:LEU:HD12 | 1.73 | 0.71 |
| 1:A:1204:A:OP1 | 14:O:3:ARG:NH2 | 2.24 | 0.70 |
| 13:N:59:TYR:O | 13:N:63:THR:OG1 | 2.07 | 0.70 |
| 19:T:41:VAL:HB | 19:T:42:PRO:HA | 1.74 | 0.70 |
| 19:T:40:ILE:HD11 | 19:T:62:ILE:HD12 | 1.74 | 0.70 |
| 1:A:259:G:H1 | 1:A:267:C:H42 | 1.38 | 0.70 |
| 1:A:589:C:H42 | 1:A:650:G:H1 | 1.40 | 0.70 |
| 1:A:953:G:H5' | 1:A:965:A:H61 | 1.55 | 0.70 |
| 10:K:48:THR:HA | 10:K:62:HIS:HB3 | 1.72 | 0.69 |
| 1:A:1263:C:H42 | 1:A:1272:G:H1 | 1.40 | 0.69 |
| 7:H:153:HIS:CE1 | 11:L:57:THR:HG23 | 2.28 | 0.69 |
| 1:A:49:U:O4 | 1:A:365:U:O4 | 2.10 | 0.69 |
| 1:A:954:G:H21 | 1:A:1227:A:H62 | 1.40 | 0.69 |
| 1:A:439:A:OP2 | 1:A:493:G:N1 | 2.26 | 0.68 |
| 1:A:501:C:OP1 | 12:M:117:ARG:NH2 | 2.24 | 0.68 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:E:79:GLU:OE2 | 8:I:104:ARG:HA | 1.94 | 0.68 |
| 3:C:3:ASN:N | 3:C:3:ASN:OD1 | 2.27 | 0.68 |
| 23:X:7:A:H61 | 23:X:66:U:H3 | 1.42 | 0.68 |
| 2:B:27:LYS:HD2 | 2:B:193:ASP:HB2 | 1.75 | 0.68 |
| 1:A:542:G:OP1 | 4:D:10:ARG:NH2 | 2.27 | 0.68 |
| 5:E:11:ILE:HG13 | 5:E:31:LEU:HB3 | 1.76 | 0.68 |
| 11:L:58:PRO:HB2 | 11:L:93:GLN:HG3 | 1.75 | 0.67 |
| 16:Q:4:ILE:HG12 | 16:Q:21:VAL:HG12 | 1.75 | 0.67 |
| 1:A:1346:A:H5'' | 9:J:120:ARG:HH12 | 1.58 | 0.67 |
| 6:F:15:ASP:OD2 | 6:F:18:GLN:CD | 2.33 | 0.67 |
| 19:T:29:ARG:HD3 | 19:T:30:LEU:HD13 | 1.77 | 0.67 |
| 1:A:78:G:O6 | 1:A:91:C:N4 | 2.27 | 0.67 |
| 1:A:1347:G:N2 | 1:A:1374:A:OP2 | 2.26 | 0.67 |
| 4:D:154:ASN:OD1 | 4:D:154:ASN:N | 2.26 | 0.66 |
| 1:A:1054:C:OP2 | 1:A:1197:G:OP2 | 2.14 | 0.66 |
| 1:A:8:A:N6 | 4:D:205:GLU:O | 2.28 | 0.66 |
| 3:C:70:VAL:HG12 | 3:C:72:LYS:H | 1.60 | 0.66 |
| 19:T:39:THR:HG22 | 19:T:40:ILE:H | 1.61 | 0.66 |
| 1:A:1002:G:H2' | 1:A:1003:G:C8 | 2.30 | 0.66 |
| 1:A:1055:A:O2' | 3:C:161:GLU:OE2 | 2.12 | 0.66 |
| 1:A:1175:G:H2' | 1:A:1176:A:C8 | 2.30 | 0.66 |
| 1:A:1296:C:OP1 | 13:N:44:ARG:NH2 | 2.29 | 0.65 |
| 1:A:1298:C:OP2 | 7:H:114:ARG:NH2 | 2.30 | 0.65 |
| 1:A:191:G:H1' | 20:U:105:SER:HB3 | 1.77 | 0.65 |
| 2:B:82:ARG:HA | 2:B:92:TYR:CE2 | 2.31 | 0.65 |
| 3:C:9:GLY:HA2 | 3:C:12:LEU:HD23 | 1.78 | 0.65 |
| 16:Q:53:VAL:HG12 | 16:Q:79:VAL:HG22 | 1.77 | 0.65 |
| 13:N:3:ARG:HD2 | 13:N:9:ILE:HG12 | 1.79 | 0.65 |
| 19:T:28:LYS:HB2 | 19:T:47:HIS:CE1 | 2.32 | 0.64 |
| 1:A:1227:A:OP1 | 19:T:80:TYR:OH | 2.12 | 0.64 |
| 5:E:11:ILE:HD11 | 5:E:31:LEU:HD12 | 1.80 | 0.64 |
| 10:K:53:PRO:HA | 14:O:42:ILE:HD12 | 1.79 | 0.64 |
| 13:N:121:LYS:NZ | 23:Z:40:C:O2' | 2.29 | 0.64 |
| 1:A:664:G:H22 | 1:A:741:G:H1 | 1.45 | 0.64 |
| 1:A:963:G:H1 | 1:A:972:C:N4 | 1.92 | 0.64 |
| 2:B:5:ILE:HG21 | 2:B:221:LEU:HD23 | 1.78 | 0.64 |
| 1:A:1128:C:OP1 | 9:J:66:ARG:NH2 | 2.26 | 0.64 |
| 1:A:963:G:N2 | 1:A:972:C:N3 | 2.40 | 0.64 |
| 10:K:77:PRO:O | 10:K:79:ARG:NH1 | 2.30 | 0.64 |
| 10:K:4:ILE:HB | 10:K:74:ILE:HG13 | 1.80 | 0.63 |
| 6:F:15:ASP:OD2 | 6:F:18:GLN:OE1 | 2.16 | 0.63 |
| 1:A:1224:G:C6 | 1:A:1322:C:H1' | 2.33 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:243:A:H4' | 1:A:244:U:O5' | 1.98 | 0.63 |
| 1:A:1080:A:H5'' | 5:E:16:THR:HG21 | 1.81 | 0.63 |
| 1:A:1002:G:H2' | 1:A:1003:G:H8 | 1.61 | 0.63 |
| 4:D:166:LYS:CG | 4:D:178:VAL:HG11 | 2.20 | 0.63 |
| 1:A:1446:A:O2' | 1:A:1447:G:O5' | 2.16 | 0.63 |
| 1:A:937:A:N6 | 1:A:1345:U:O4 | 2.30 | 0.63 |
| 2:B:24:TRP:H | 2:B:24:TRP:HD1 | 1.46 | 0.63 |
| 8:I:10:LEU:HD22 | 8:I:83:ILE:HD11 | 1.80 | 0.63 |
| 1:A:789:U:H1' | 1:A:792:A:H2 | 1.64 | 0.62 |
| 7:H:155:ARG:H | 7:H:155:ARG:HD3 | 1.64 | 0.62 |
| 11:L:98:LEU:O | 11:L:101:SER:OG | 2.14 | 0.62 |
| 1:A:1064:G:O2' | 1:A:1065:U:O5' | 2.17 | 0.62 |
| 4:D:7:PRO:HB2 | 4:D:10:ARG:HD2 | 1.81 | 0.62 |
| 19:T:40:ILE:HG23 | 19:T:41:VAL:HG22 | 1.79 | 0.62 |
| 1:A:1135:U:H4' | 1:A:1136:U:H5 | 1.64 | 0.62 |
| 17:R:66:SER:O | 17:R:70:ARG:NH1 | 2.33 | 0.62 |
| 1:A:1163:C:H42 | 1:A:1173:G:H1 | 1.47 | 0.62 |
| 6:F:17:SER:O | 6:F:18:GLN:C | 2.34 | 0.62 |
| 1:A:532:A:H2 | 1:A:1206:G:H21 | 1.46 | 0.62 |
| 8:I:6:ILE:HB | 8:I:85:ARG:NH1 | 2.15 | 0.62 |
| 11:L:121:PRO:HD2 | 11:L:126:ARG:HD3 | 1.80 | 0.62 |
| 1:A:27:G:H4' | 4:D:209:ARG:HG3 | 1.79 | 0.62 |
| 1:A:448:A:OP2 | 1:A:485:G:N2 | 2.30 | 0.62 |
| 7:H:149:ARG:HD3 | 11:L:59:TYR:OH | 1.99 | 0.62 |
| 22:W:53:G:H4' | 22:W:54:U:OP1 | 1.99 | 0.62 |
| 12:M:57:LYS:HG2 | 12:M:67:THR:HG22 | 1.81 | 0.61 |
| 1:A:1077:G:N2 | 1:A:1080:A:OP2 | 2.29 | 0.61 |
| 10:K:40:LEU:HB2 | 10:K:69:ASN:HB3 | 1.82 | 0.61 |
| 14:O:13:THR:N | 14:O:14:PRO:HD2 | 2.15 | 0.61 |
| 1:A:754:C:H5' | 15:P:72:ARG:HH22 | 1.65 | 0.61 |
| 3:C:14:ILE:O | 3:C:16:ARG:N | 2.33 | 0.61 |
| 4:D:30:LYS:C | 4:D:32:ALA:N | 2.52 | 0.61 |
| 1:A:973:G:OP1 | 10:K:57:LYS:NZ | 2.34 | 0.61 |
| 11:L:22:HIS:HB3 | 11:L:29:ILE:HG23 | 1.83 | 0.61 |
| 1:A:890:G:O2' | 1:A:906:G:O6 | 2.16 | 0.61 |
| 1:A:110:C:O2' | 16:Q:25:ARG:O | 2.17 | 0.61 |
| 21:V:6:ARG:HE | 21:V:15:ARG:NH2 | 1.99 | 0.61 |
| 2:B:178:ARG:HH21 | 8:I:74:PRO:HG3 | 1.66 | 0.61 |
| 4:D:105:VAL:HG13 | 4:D:110:PHE:HB2 | 1.83 | 0.61 |
| 15:P:82:ILE:O | 15:P:86:GLY:N | 2.33 | 0.61 |
| 1:A:1292:U:OP1 | 7:H:41:ARG:NH2 | 2.33 | 0.61 |
| 14:O:6:LEU:HD23 | 14:O:23:ARG:HH22 | 1.64 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:501:C:H2' | 1:A:502:G:C8 | 2.35 | 0.61 |
| 3:C:11:ARG:O | 3:C:13:GLY:N | 2.34 | 0.60 |
| 3:C:8:ILE:HG23 | 3:C:16:ARG:HG2 | 1.83 | 0.60 |
| 23:X:48:C:H2' | 23:X:59:U:H4' | 1.83 | 0.60 |
| 9:J:13:ALA:HB2 | 9:J:68:GLY:HA3 | 1.82 | 0.60 |
| 1:A:864:A:H5' | 5:E:86:ALA:HB2 | 1.83 | 0.60 |
| 15:P:39:LEU:HD13 | 15:P:56:LEU:HB2 | 1.83 | 0.60 |
| 1:A:1305:G:H22 | 1:A:1331:G:H2' | 1.66 | 0.60 |
| 2:B:15:VAL:H | 2:B:16:HIS:CE1 | 2.20 | 0.60 |
| 1:A:1106:G:H5'' | 3:C:172:ARG:HG2 | 1.84 | 0.60 |
| 12:M:84:LEU:HD22 | 12:M:104:VAL:HG11 | 1.84 | 0.60 |
| 1:A:344:A:O2' | 1:A:346:G:O6 | 2.18 | 0.60 |
| 7:H:26:PHE:O | 7:H:30:ILE:HG12 | 2.01 | 0.60 |
| 9:J:9:ARG:HB3 | 9:J:14:VAL:HG13 | 1.84 | 0.60 |
| 10:K:42:THR:HG23 | 10:K:68:HIS:HA | 1.83 | 0.60 |
| 7:H:149:ARG:NE | 11:L:59:TYR:CE1 | 2.70 | 0.60 |
| 1:A:1061:G:OP1 | 10:K:59:SER:OG | 2.21 | 0.59 |
| 1:A:1352:C:OP1 | 21:V:3:LYS:NZ | 2.29 | 0.59 |
| 1:A:1172:C:H2' | 1:A:1173:G:C8 | 2.38 | 0.59 |
| 3:C:50:ALA:HB2 | 3:C:75:VAL:HB | 1.85 | 0.59 |
| 13:N:49:THR:HB | 13:N:52:GLU:HG3 | 1.85 | 0.59 |
| 1:A:1023:G:H3' | 1:A:1024:G:H5'' | 1.83 | 0.59 |
| 4:D:166:LYS:HG3 | 4:D:178:VAL:CG1 | 2.20 | 0.59 |
| 7:H:73:MET:HG2 | 7:H:90:GLU:HA | 1.83 | 0.59 |
| 16:Q:21:VAL:O | 16:Q:33:ILE:HG12 | 2.02 | 0.59 |
| 4:D:64:LEU:HB2 | 4:D:198:VAL:HG11 | 1.83 | 0.59 |
| 7:H:149:ARG:HD3 | 11:L:59:TYR:CZ | 2.38 | 0.59 |
| 1:A:56:U:H2' | 1:A:57:G:C8 | 2.38 | 0.58 |
| 8:I:121:ASP:N | 8:I:121:ASP:OD1 | 2.34 | 0.58 |
| 1:A:119:A:H4' | 1:A:120:A:O5' | 2.02 | 0.58 |
| 4:D:111:ALA:HB2 | 4:D:120:LEU:HD12 | 1.85 | 0.58 |
| 10:K:49:VAL:HG13 | 14:O:41:ARG:HB2 | 1.86 | 0.58 |
| 1:A:352:C:O2' | 1:A:354:G:OP1 | 2.16 | 0.58 |
| 1:A:1201:A:HO2' | 1:A:1202:G:P | 2.27 | 0.58 |
| 4:D:29:PRO:HD2 | 4:D:30:LYS:HD3 | 1.84 | 0.58 |
| 12:M:53:ARG:HD3 | 12:M:93:LEU:HD21 | 1.86 | 0.58 |
| 2:B:77:ALA:HB2 | 2:B:211:ILE:HD13 | 1.86 | 0.58 |
| 1:A:427:U:OP1 | 4:D:13:ARG:NH2 | 2.36 | 0.58 |
| 1:A:382:A:H2' | 1:A:383:A:C8 | 2.39 | 0.58 |
| 1:A:181:G:O2' | 1:A:182:U:O5' | 2.20 | 0.58 |
| 14:O:24:CYS:HB3 | 14:O:27:CYS:SG | 2.40 | 0.58 |
| 1:A:927:G:H1 | 1:A:1390:U:H3 | 1.52 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 13:N:58:GLU:O | 13:N:62:ASN:ND2 | 2.31 | 0.57 |
| 1:A:559:A:H4' | 1:A:560:U:H3' | 1.85 | 0.57 |
| 3:C:134:ILE:HG23 | 3:C:151:VAL:HB | 1.85 | 0.57 |
| 7:H:26:PHE:CE2 | 7:H:30:ILE:HD11 | 2.38 | 0.57 |
| 1:A:1002:G:N2 | 1:A:1038:C:N3 | 2.46 | 0.57 |
| 3:C:134:ILE:HG22 | 3:C:168:ALA:HB3 | 1.86 | 0.57 |
| 7:H:79:ARG:HH12 | 7:H:82:GLY:HA2 | 1.69 | 0.57 |
| 1:A:953:G:N7 | 13:N:104:ARG:NH2 | 2.52 | 0.57 |
| 5:E:143:ARG:HH21 | 8:I:77:GLU:CD | 2.07 | 0.57 |
| 1:A:564:C:P | 12:M:15:ARG:HH21 | 2.26 | 0.57 |
| 13:N:14:ARG:N | 13:N:44:ARG:HD3 | 2.17 | 0.57 |
| 1:A:1376:U:P | 7:H:94:ARG:HH12 | 2.28 | 0.57 |
| 7:H:15:ASP:OD1 | 7:H:44:TYR:OH | 2.22 | 0.57 |
| 12:M:10:LEU:HB3 | 17:R:32:TYR:CE2 | 2.40 | 0.57 |
| 1:A:1163:C:N4 | 1:A:1173:G:H1 | 2.02 | 0.57 |
| 1:A:816:A:OP1 | 1:A:1526:G:O2' | 2.20 | 0.57 |
| 1:A:1286:A:H5'' | 21:V:26:LYS:HD2 | 1.85 | 0.57 |
| 1:A:765:G:N2 | 1:A:813:U:OP2 | 2.38 | 0.57 |
| 2:B:51:LEU:HD23 | 2:B:201:ILE:HD12 | 1.86 | 0.57 |
| 6:F:3:ARG:NH1 | 6:F:38:GLU:OE2 | 2.37 | 0.57 |
| 13:N:23:TYR:HB3 | 13:N:67:GLU:HG2 | 1.87 | 0.57 |
| 1:A:973:G:O6 | 1:A:974:A:N6 | 2.38 | 0.56 |
| 3:C:73:PRO:HG3 | 3:C:105:GLU:HG3 | 1.88 | 0.56 |
| 1:A:501:C:H2' | 1:A:502:G:H8 | 1.69 | 0.56 |
| 12:M:117:ARG:HB3 | 12:M:122:THR:HB | 1.86 | 0.56 |
| 19:T:41:VAL:HB | 19:T:42:PRO:CA | 2.35 | 0.56 |
| 1:A:1004:A:O5' | 1:A:1025:U:N3 | 2.38 | 0.56 |
| 1:A:613:C:H42 | 1:A:627:G:H1 | 1.53 | 0.56 |
| 17:R:90:ILE:O | 17:R:94:ASN:ND2 | 2.38 | 0.56 |
| 1:A:6:G:H4' | 1:A:298:A:H4' | 1.87 | 0.56 |
| 1:A:376:G:H5'' | 16:Q:5:ARG:HD2 | 1.87 | 0.56 |
| 1:A:942:G:N2 | 9:J:124:GLN:OE1 | 2.31 | 0.56 |
| 23:X:18:G:H22 | 23:X:55:U:H1' | 1.71 | 0.56 |
| 2:B:82:ARG:HA | 2:B:92:TYR:HE2 | 1.71 | 0.56 |
| 8:I:106:GLY:O | 8:I:122:ARG:NH2 | 2.36 | 0.56 |
| 10:K:5:ARG:HG3 | 10:K:71:LEU:HD11 | 1.87 | 0.56 |
| 12:M:45:PRO:HB3 | 12:M:92:ASP:HB3 | 1.87 | 0.56 |
| 1:A:620:C:C2 | 4:D:135:LEU:HG | 2.40 | 0.56 |
| 1:A:974:A:H1' | 14:O:31:ARG:HE | 1.70 | 0.56 |
| 4:D:165:MET:SD | 4:D:168:ARG:HD2 | 2.46 | 0.56 |
| 12:M:89:ARG:HB3 | 12:M:97:ARG:HA | 1.88 | 0.55 |
| 4:D:187:ARG:NH2 | 4:D:193:ASP:OD2 | 2.38 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 23:X:12:U:H3 | 23:X:23:A:N6 | 2.02 | 0.55 |
| 1:A:411:A:H62 | 1:A:413:G:H21 | 1.53 | 0.55 |
| 2:B:5:ILE:HD12 | 2:B:224:GLN:HG2 | 1.88 | 0.55 |
| 2:B:71:VAL:HG12 | 2:B:93:VAL:HB | 1.88 | 0.55 |
| 10:K:16:LEU:HD23 | 10:K:94:VAL:HG13 | 1.89 | 0.55 |
| 1:A:1118:C:H1' | 1:A:1179:A:C4 | 2.41 | 0.55 |
| 10:K:78:ASN:O | 10:K:81:THR:OG1 | 2.24 | 0.55 |
| 1:A:437:U:H2' | 1:A:438:G:O4' | 2.06 | 0.55 |
| 8:I:86:ILE:HG13 | 8:I:133:LEU:HD22 | 1.89 | 0.55 |
| 4:D:30:LYS:HG2 | 4:D:30:LYS:O | 2.07 | 0.55 |
| 9:J:77:ILE:O | 9:J:81:ILE:HG12 | 2.06 | 0.55 |
| 1:A:1047:G:H1 | 1:A:1210:C:H42 | 1.55 | 0.55 |
| 1:A:1159:U:O2' | 1:A:1160:G:N7 | 2.39 | 0.55 |
| 1:A:115:G:H4' | 1:A:116:A:O5' | 2.07 | 0.55 |
| 1:A:1162:C:H2' | 1:A:1163:C:O4' | 2.07 | 0.55 |
| 1:A:1405:G:OP2 | 26:A:1667:PAR:O34 | 2.25 | 0.55 |
| 1:A:976:G:OP2 | 1:A:1358:U:O2' | 2.25 | 0.55 |
| 10:K:8:LEU:HB3 | 10:K:16:LEU:HD21 | 1.87 | 0.55 |
| 14:O:48:ALA:HB2 | 14:O:53:LEU:HD12 | 1.89 | 0.55 |
| 5:E:78:HIS:CE1 | 5:E:142:LEU:HD23 | 2.42 | 0.54 |
| 10:K:13:HIS:CE1 | 10:K:14:LYS:HE3 | 2.42 | 0.54 |
| 14:O:24:CYS:HB3 | 14:O:28:GLY:H | 1.71 | 0.54 |
| 1:A:1321:C:H3' | 1:A:1322:C:H5'' | 1.88 | 0.54 |
| 5:E:7:GLU:N | 5:E:35:GLY:O | 2.36 | 0.54 |
| 9:J:26:VAL:HG22 | 9:J:61:ALA:HB3 | 1.89 | 0.54 |
| 22:W:21:A:H61 | 22:W:46:G:H2' | 1.73 | 0.54 |
| 1:A:352:C:N3 | 1:A:356:A:N6 | 2.55 | 0.54 |
| 4:D:149:ALA:HB3 | 4:D:152:SER:HB2 | 1.89 | 0.54 |
| 1:A:1126:U:H1' | 1:A:1280:A:N7 | 2.23 | 0.54 |
| 1:A:983:A:N1 | 1:A:1222:G:N2 | 2.56 | 0.54 |
| 9:J:121:ARG:NH1 | 9:J:122:ALA:O | 2.40 | 0.54 |
| 1:A:1453:G:H8 | 20:U:39:LYS:HZ1 | 1.55 | 0.54 |
| 1:A:1499:A:OP1 | 1:A:1505:G:OP2 | 2.26 | 0.54 |
| 1:A:1305:G:N2 | 1:A:1331:G:H2' | 2.22 | 0.54 |
| 1:A:1436:U:H2' | 1:A:1437:C:O4' | 2.07 | 0.54 |
| 13:N:22:ILE:HB | 13:N:25:ILE:HD12 | 1.89 | 0.54 |
| 23:X:68:C:H2' | 23:X:69:G:H8 | 1.71 | 0.54 |
| 1:A:412:A:H4' | 1:A:413:G:O5' | 2.08 | 0.54 |
| 2:B:204:ASN:HD22 | 2:B:206:ASP:H | 1.56 | 0.54 |
| 2:B:235:SER:O | 2:B:237:ALA:N | 2.41 | 0.54 |
| 19:T:10:PHE:HE1 | 19:T:16:LEU:HD22 | 1.73 | 0.54 |
| 3:C:84:ILE:HD11 | 3:C:88:ARG:HH21 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1175:G:H2' | 1:A:1176:A:H8 | 1.74 | 0.53 |
| 2:B:84:GLU:HB3 | 2:B:219:VAL:HG21 | 1.89 | 0.53 |
| 12:M:55:VAL:HG12 | 12:M:69:TYR:HA | 1.90 | 0.53 |
| 1:A:1318:A:H4' | 19:T:11:VAL:HG11 | 1.89 | 0.53 |
| 1:A:1004:A:P | 1:A:1025:U:H3 | 2.30 | 0.53 |
| 1:A:1367:C:H4' | 10:K:48:THR:HG21 | 1.90 | 0.53 |
| 3:C:35:GLU:HG2 | 3:C:59:ARG:NH2 | 2.23 | 0.53 |
| 1:A:1128:C:H4' | 9:J:16:ARG:HH12 | 1.74 | 0.53 |
| 1:A:957:U:H4' | 19:T:79:THR:HB | 1.89 | 0.53 |
| 4:D:78:LEU:HD22 | 4:D:96:LEU:HB3 | 1.89 | 0.53 |
| 8:I:51:VAL:HG11 | 8:I:60:ARG:HG3 | 1.90 | 0.53 |
| 1:A:1014:A:H4' | 19:T:14:HIS:CD2 | 2.44 | 0.53 |
| 1:A:51:A:N7 | 1:A:114:U:O2' | 2.40 | 0.53 |
| 1:A:673:G:H2' | 1:A:674:G:C8 | 2.43 | 0.53 |
| 9:J:71:SER:HA | 9:J:74:ILE:HD12 | 1.90 | 0.53 |
| 1:A:1263:C:N4 | 1:A:1272:G:H1 | 2.07 | 0.53 |
| 1:A:411:A:C5 | 1:A:413:G:H1' | 2.44 | 0.53 |
| 4:D:194:LEU:HD12 | 4:D:195:ALA:H | 1.73 | 0.53 |
| 6:F:10:LEU:HD13 | 6:F:61:LEU:HD13 | 1.90 | 0.53 |
| 1:A:1310:G:OP1 | 13:N:77:ASN:ND2 | 2.42 | 0.53 |
| 1:A:1095:U:P | 1:A:1108:G:H1 | 2.31 | 0.53 |
| 1:A:259:G:H1 | 1:A:267:C:N4 | 2.07 | 0.53 |
| 15:P:6:GLU:N | 15:P:6:GLU:OE2 | 2.35 | 0.53 |
| 1:A:1105:A:H2' | 1:A:1106:G:H8 | 1.74 | 0.53 |
| 1:A:1189:C:OP1 | 10:K:51:ARG:NH2 | 2.41 | 0.52 |
| 1:A:346:G:H1' | 1:A:347:G:H5' | 1.90 | 0.52 |
| 13:N:66:LEU:HA | 13:N:70:LEU:HB2 | 1.91 | 0.52 |
| 4:D:98:GLU:OE2 | 4:D:107:ARG:NE | 2.43 | 0.52 |
| 1:A:1316:G:H5'' | 14:O:17:LYS:HE3 | 1.91 | 0.52 |
| 19:T:44:MET:O | 19:T:46:GLY:N | 2.40 | 0.52 |
| 7:H:153:HIS:HE1 | 11:L:57:THR:HG23 | 1.75 | 0.52 |
| 1:A:690:G:H22 | 11:L:55:LYS:NZ | 2.08 | 0.52 |
| 1:A:1128:C:H4' | 9:J:16:ARG:HH22 | 1.73 | 0.52 |
| 1:A:103:C:P | 20:U:17:ARG:HH21 | 2.33 | 0.52 |
| 2:B:134:GLU:HA | 2:B:137:ARG:HB3 | 1.92 | 0.52 |
| 1:A:1126:U:H5 | 1:A:1127:G:C4 | 2.27 | 0.52 |
| 1:A:662:G:H2' | 1:A:663:A:C8 | 2.45 | 0.52 |
| 8:I:77:GLU:HG2 | 8:I:78:GLN:H | 1.74 | 0.52 |
| 1:A:971:G:N2 | 1:A:1363:A:OP2 | 2.28 | 0.52 |
| 23:X:33:U:H2' | 23:X:35:A:OP2 | 2.09 | 0.52 |
| 1:A:401:C:O2' | 1:A:621:A:N3 | 2.39 | 0.52 |
| 11:L:32:ILE:HG13 | 11:L:72:ALA:HB2 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 18:S:32:ARG:HA | 18:S:69:THR:HG21 | 1.91 | 0.52 |
| 1:A:1151:A:H2' | 1:A:1152:A:C8 | 2.45 | 0.51 |
| 1:A:359:U:H2' | 1:A:360:A:C8 | 2.44 | 0.51 |
| 20:U:14:LYS:HA | 20:U:17:ARG:HG3 | 1.91 | 0.51 |
| 1:A:49:U:O4 | 1:A:365:U:C4 | 2.63 | 0.51 |
| 12:M:54:LYS:H | 12:M:54:LYS:HD2 | 1.74 | 0.51 |
| 23:X:49:C:H42 | 23:X:65:G:H1 | 1.58 | 0.51 |
| 4:D:12:CYS:HA | 4:D:19:LEU:HD23 | 1.92 | 0.51 |
| 5:E:91:LEU:HD12 | 5:E:120:THR:HG22 | 1.93 | 0.51 |
| 11:L:96:ARG:HA | 11:L:99:GLN:HE21 | 1.76 | 0.51 |
| 3:C:37:GLN:NE2 | 14:O:52:GLN:OE1 | 2.32 | 0.51 |
| 1:A:1305:G:H1' | 1:A:1332:A:N6 | 2.25 | 0.51 |
| 22:W:23:C:H2' | 22:W:24:U:C6 | 2.45 | 0.51 |
| 1:A:539:A:H2' | 1:A:540:G:C8 | 2.46 | 0.51 |
| 1:A:947:G:O3' | 13:N:109:THR:OG1 | 2.28 | 0.51 |
| 1:A:963:G:H21 | 10:K:55:LYS:HE2 | 1.75 | 0.51 |
| 4:D:61:LYS:HB2 | 4:D:203:VAL:HG13 | 1.93 | 0.51 |
| 10:K:31:GLY:HA3 | 10:K:78:ASN:ND2 | 2.26 | 0.51 |
| 1:A:1043:C:H2' | 1:A:1044:A:H8 | 1.76 | 0.51 |
| 1:A:1326:C:OP1 | 21:V:17:THR:OG1 | 2.17 | 0.51 |
| 1:A:833:U:H3 | 1:A:853:G:H1 | 1.56 | 0.51 |
| 1:A:390:C:H2' | 1:A:391:G:C8 | 2.46 | 0.51 |
| 1:A:718:G:H5' | 11:L:117:ASN:ND2 | 2.24 | 0.51 |
| 11:L:33:THR:HG22 | 11:L:39:PRO:HA | 1.92 | 0.51 |
| 21:V:6:ARG:HE | 21:V:15:ARG:HH21 | 1.58 | 0.51 |
| 12:M:69:TYR:CG | 12:M:90:VAL:HG21 | 2.46 | 0.51 |
| 6:F:69:GLU:CD | 6:F:69:GLU:H | 2.15 | 0.51 |
| 8:I:20:TYR:HE2 | 8:I:75:ARG:HD2 | 1.76 | 0.51 |
| 1:A:1147:C:HO2' | 9:J:5:TYR:HH | 1.59 | 0.51 |
| 1:A:1152:A:OP1 | 10:K:68:HIS:NE2 | 2.43 | 0.51 |
| 12:M:38:THR:HG23 | 12:M:57:LYS:HB3 | 1.93 | 0.51 |
| 1:A:7:G:H5' | 1:A:298:A:O4' | 2.11 | 0.50 |
| 1:A:446:G:H1 | 1:A:488:C:H42 | 1.59 | 0.50 |
| 9:J:8:GLY:HA2 | 9:J:79:LEU:HD12 | 1.92 | 0.50 |
| 16:Q:3:LYS:HG3 | 16:Q:24:ALA:HB2 | 1.92 | 0.50 |
| 9:J:118:LYS:O | 9:J:120:ARG:N | 2.40 | 0.50 |
| 10:K:22:LYS:HZ2 | 10:K:23:ILE:HA | 1.77 | 0.50 |
| 13:N:33:ALA:HA | 13:N:59:TYR:HE2 | 1.76 | 0.50 |
| 1:A:752:G:H1' | 1:A:754:C:H41 | 1.75 | 0.50 |
| 13:N:40:ASN:HD22 | 13:N:43:THR:HG23 | 1.76 | 0.50 |
| 1:A:20:U:H2' | 1:A:21:G:C8 | 2.46 | 0.50 |
| 1:A:362:G:N2 | 1:A:365:U:OP2 | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:963:G:H21 | 10:K:55:LYS:CE | 2.25 | 0.50 |
| 23:X:16:U:H3' | 23:X:17:C:H5' | 1.93 | 0.50 |
| 1:A:1064:G:HO2' | 1:A:1065:U:P | 2.35 | 0.50 |
| 1:A:413:G:OP2 | 1:A:413:G:H8 | 1.95 | 0.50 |
| 7:H:116:ALA:O | 7:H:120:ILE:HG12 | 2.11 | 0.50 |
| 10:K:47:PHE:CE1 | 10:K:63:PHE:HB2 | 2.47 | 0.50 |
| 9:J:95:LYS:NZ | 9:J:96:LEU:HD13 | 2.26 | 0.50 |
| 2:B:231:GLU:HG3 | 2:B:233:SER:H | 1.77 | 0.50 |
| 9:J:53:VAL:HB | 9:J:95:LYS:HE3 | 1.93 | 0.50 |
| 13:N:40:ASN:ND2 | 13:N:43:THR:HG23 | 2.27 | 0.50 |
| 11:L:17:GLY:N | 11:L:79:SER:O | 2.44 | 0.50 |
| 1:A:485:G:H1' | 1:A:486:U:H5 | 1.77 | 0.50 |
| 1:A:757:U:O2' | 1:A:879:C:O2 | 2.29 | 0.50 |
| 4:D:33:MET:CE | 4:D:37:PRO:HA | 2.41 | 0.50 |
| 13:N:92:HIS:HD2 | 13:N:110:ARG:HH21 | 1.58 | 0.50 |
| 23:X:19:G:P | 23:X:60:U:H3 | 2.33 | 0.50 |
| 1:A:164:U:H2' | 1:A:165:C:C6 | 2.47 | 0.49 |
| 1:A:56:U:H2' | 1:A:57:G:H8 | 1.76 | 0.49 |
| 6:F:17:SER:C | 6:F:19:LEU:N | 2.64 | 0.49 |
| 12:M:24:VAL:HG13 | 12:M:98:TYR:HE1 | 1.76 | 0.49 |
| 1:A:1065:U:O2' | 1:A:1066:C:OP2 | 2.24 | 0.49 |
| 1:A:1218:C:H2' | 1:A:1219:U:C6 | 2.47 | 0.49 |
| 1:A:589:C:N4 | 1:A:650:G:H1 | 2.06 | 0.49 |
| 2:B:162:ILE:HD11 | 2:B:184:VAL:HG22 | 1.93 | 0.49 |
| 2:B:235:SER:OG | 2:B:236:TYR:N | 2.46 | 0.49 |
| 3:C:157:ILE:HD11 | 3:C:166:GLU:HB2 | 1.94 | 0.49 |
| 8:I:9:MET:HG3 | 8:I:26:VAL:HG21 | 1.94 | 0.49 |
| 9:J:46:ALA:HB2 | 9:J:74:ILE:HG23 | 1.94 | 0.49 |
| 1:A:1201:A:O2' | 1:A:1202:G:O5' | 2.29 | 0.49 |
| 1:A:946:A:H61 | 1:A:1234:C:H42 | 1.60 | 0.49 |
| 2:B:96:ARG:H | 2:B:96:ARG:HD2 | 1.76 | 0.49 |
| 3:C:14:ILE:HG12 | 3:C:15:THR:N | 2.27 | 0.49 |
| 1:A:1226:C:O2' | 13:N:103:THR:O | 2.25 | 0.49 |
| 14:O:15:LYS:HD2 | 14:O:16:PHE:CE2 | 2.47 | 0.49 |
| 14:O:24:CYS:HB3 | 14:O:29:ARG:H | 1.78 | 0.49 |
| 20:U:79:ARG:O | 20:U:83:ARG:HG3 | 2.12 | 0.49 |
| 1:A:1288:A:N1 | 1:A:1371:G:H1' | 2.27 | 0.49 |
| 3:C:14:ILE:HG12 | 3:C:15:THR:H | 1.76 | 0.49 |
| 3:C:73:PRO:O | 3:C:76:VAL:HG22 | 2.12 | 0.49 |
| 4:D:29:PRO:O | 4:D:30:LYS:HB3 | 2.11 | 0.49 |
| 18:S:26:LEU:HD22 | 18:S:42:ARG:HD2 | 1.94 | 0.49 |
| 22:W:3:G:HO2' | 22:W:4:G:H8 | 1.58 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1336:C:O2' | 1:A:1337:G:O5' | 2.30 | 0.49 |
| 4:D:129:ASN:HA | 4:D:145:GLU:HB2 | 1.94 | 0.49 |
| 7:H:20:ASP:HB3 | 7:H:23:VAL:HG23 | 1.94 | 0.49 |
| 1:A:1104:G:H4' | 2:B:111:ARG:NH1 | 2.28 | 0.49 |
| 2:B:204:ASN:ND2 | 2:B:206:ASP:O | 2.45 | 0.49 |
| 1:A:255:G:H1' | 17:R:16:GLN:NE2 | 2.28 | 0.49 |
| 17:R:18:THR:HG23 | 17:R:69:LYS:HE3 | 1.94 | 0.49 |
| 6:F:97:PHE:O | 18:S:31:LEU:HD23 | 2.12 | 0.49 |
| 19:T:41:VAL:HA | 19:T:44:MET:HG3 | 1.93 | 0.49 |
| 1:A:1152:A:H5'' | 10:K:13:HIS:CD2 | 2.48 | 0.49 |
| 1:A:1213:A:C6 | 1:A:1215:G:H1' | 2.48 | 0.49 |
| 1:A:570:G:O6 | 1:A:865:A:N6 | 2.44 | 0.49 |
| 3:C:47:LEU:HD23 | 3:C:68:VAL:HG11 | 1.94 | 0.49 |
| 8:I:95:VAL:HB | 8:I:99:GLU:O | 2.13 | 0.49 |
| 1:A:1015:A:H2' | 1:A:1016:A:C8 | 2.48 | 0.49 |
| 1:A:191:G:O2' | 20:U:101:GLY:O | 2.30 | 0.49 |
| 2:B:178:ARG:NH2 | 8:I:74:PRO:HG3 | 2.28 | 0.49 |
| 13:N:23:TYR:HE1 | 13:N:70:LEU:HD12 | 1.77 | 0.49 |
| 1:A:1004:A:H1' | 1:A:1036:G:N2 | 2.27 | 0.49 |
| 1:A:1356:G:H2' | 1:A:1357:A:C8 | 2.47 | 0.49 |
| 1:A:148:G:H1 | 1:A:174:C:H42 | 1.61 | 0.49 |
| 2:B:21:ARG:O | 2:B:23:ARG:N | 2.46 | 0.49 |
| 15:P:87:ILE:HG22 | 15:P:88:ARG:H | 1.78 | 0.49 |
| 1:A:1466:C:H2' | 1:A:1467:G:O4' | 2.12 | 0.49 |
| 1:A:64:G:H4' | 1:A:65:U:H5' | 1.95 | 0.49 |
| 1:A:769:G:H4' | 1:A:1513:A:H4' | 1.95 | 0.49 |
| 1:A:950:U:H2' | 1:A:951:G:C8 | 2.48 | 0.49 |
| 10:K:24:VAL:HG21 | 10:K:37:PRO:HD3 | 1.95 | 0.49 |
| 12:M:58:VAL:O | 12:M:65:GLU:HA | 2.13 | 0.49 |
| 19:T:77:THR:HG22 | 19:T:78:ARG:HD3 | 1.95 | 0.49 |
| 1:A:1159:U:C6 | 1:A:1182:G:H1' | 2.47 | 0.48 |
| 1:A:474:G:H5' | 16:Q:81:ARG:HG3 | 1.94 | 0.48 |
| 21:V:5:ASP:O | 21:V:11:GLY:HA3 | 2.13 | 0.48 |
| 23:X:7:A:N6 | 23:X:66:U:H3 | 2.10 | 0.48 |
| 1:A:510:A:OP2 | 4:D:49:ARG:NH2 | 2.45 | 0.48 |
| 1:A:35:G:O2' | 12:M:118:SER:O | 2.31 | 0.48 |
| 15:P:16:ALA:HB1 | 15:P:21:ASP:HB3 | 1.94 | 0.48 |
| 1:A:1392:G:N2 | 1:A:1502:A:H8 | 2.05 | 0.48 |
| 2:B:80:ILE:HG21 | 2:B:212:GLN:HA | 1.95 | 0.48 |
| 7:H:155:ARG:O | 7:H:155:ARG:NH2 | 2.46 | 0.48 |
| 7:H:57:GLU:N | 7:H:57:GLU:OE1 | 2.41 | 0.48 |
| 12:M:38:THR:O | 12:M:79:GLU:HG3 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:A:715:A:H2' | 1:A:716:A:C8 | 2.49 | 0.48 |
| 1:A:753:A:H4' | 1:A:754:C:O5' | 2.12 | 0.48 |
| 10:K:32:ALA:HB3 | 10:K:76:ASN:HB2 | 1.95 | 0.48 |
| 13:N:49:THR:HG22 | 13:N:51:ALA:H | 1.79 | 0.48 |
| 1:A:1465:C:H2' | 1:A:1466:C:O4' | 2.14 | 0.48 |
| 3:C:150:LYS:HG3 | 3:C:169:ALA:HB2 | 1.96 | 0.48 |
| 16:Q:43:LYS:HA | 16:Q:48:TRP:HB3 | 1.95 | 0.48 |
| 4:D:100:ARG:NH2 | 4:D:136:PRO:O | 2.46 | 0.48 |
| 7:H:149:ARG:CD | 11:L:59:TYR:CZ | 2.97 | 0.48 |
| 9:J:17:VAL:HG11 | 9:J:81:ILE:HA | 1.95 | 0.48 |
| 11:L:48:ILE:HD11 | 11:L:64:ALA:HA | 1.95 | 0.48 |
| 1:A:238:G:OP1 | 17:R:25:ARG:NH2 | 2.46 | 0.48 |
| 20:U:12:ALA:O | 20:U:15:ARG:HB2 | 2.14 | 0.48 |
| 11:L:54:ARG:NH1 | 23:X:39:U:O2' | 2.41 | 0.48 |
| 1:A:1310:G:OP2 | 13:N:88:ARG:NH2 | 2.46 | 0.48 |
| 1:A:745:C:OP1 | 1:A:851:G:O2' | 2.31 | 0.48 |
| 2:B:163:PHE:HD1 | 2:B:185:ILE:HG13 | 1.78 | 0.48 |
| 4:D:106:TYR:HE1 | 4:D:112:VAL:O | 1.97 | 0.48 |
| 1:A:877:C:H5'' | 8:I:88:LYS:HD3 | 1.95 | 0.48 |
| 9:J:40:LEU:O | 9:J:42:ARG:N | 2.46 | 0.48 |
| 1:A:1032(A):G:H2' | 1:A:1032(B):G:C8 | 2.49 | 0.48 |
| 1:A:1124:G:H3' | 1:A:1145:C:N4 | 2.29 | 0.48 |
| 1:A:703:G:H4' | 1:A:704:A:O5' | 2.14 | 0.48 |
| 7:H:113:GLU:HG3 | 7:H:119:ARG:HG2 | 1.94 | 0.48 |
| 13:N:57:ARG:HH11 | 13:N:57:ARG:HB2 | 1.79 | 0.48 |
| 22:W:15:C:H5'' | 22:W:16:C:H5 | 1.79 | 0.48 |
| 1:A:692:U:N3 | 1:A:695:A:OP2 | 2.39 | 0.48 |
| 1:A:757:U:H2' | 1:A:758:G:O4' | 2.13 | 0.48 |
| 12:M:17:LYS:HG2 | 12:M:19:ARG:HG2 | 1.94 | 0.48 |
| 1:A:134:A:H61 | 16:Q:25:ARG:NH1 | 2.12 | 0.48 |
| 19:T:26:GLY:O | 19:T:28:LYS:N | 2.41 | 0.48 |
| 23:X:30:G:H2' | 23:X:31:A:H8 | 1.77 | 0.48 |
| 5:E:69:VAL:O | 5:E:71:LEU:N | 2.47 | 0.47 |
| 10:K:78:ASN:O | 10:K:82:ILE:HG12 | 2.14 | 0.47 |
| 1:A:1391:U:H2' | 1:A:1392:G:C8 | 2.48 | 0.47 |
| 1:A:143:A:H2 | 1:A:220:G:H1 | 1.62 | 0.47 |
| 2:B:97:TRP:CH2 | 2:B:173:ALA:HA | 2.49 | 0.47 |
| 2:B:85:ALA:HB3 | 2:B:92:TYR:HD2 | 1.79 | 0.47 |
| 20:U:75:ASN:N | 20:U:75:ASN:OD1 | 2.40 | 0.47 |
| 23:X:38:A:H2' | 23:X:39:U:H5' | 1.96 | 0.47 |
| 2:B:70:PHE:O | 2:B:93:VAL:N | 2.48 | 0.47 |
| 4:D:12:CYS:HA | 4:D:19:LEU:CD2 | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 6:F:41:GLU:HB2 | 6:F:62:TRP:CE3 | 2.50 | 0.47 |
| 12:M:102:ARG:HE | 12:M:102:ARG:HB3 | 1.39 | 0.47 |
| 17:R:100:LYS:O | 17:R:101:ARG:NE | 2.47 | 0.47 |
| 20:U:30:LYS:O | 20:U:33:ILE:HB | 2.14 | 0.47 |
| 1:A:1213:A:N1 | 1:A:1215:G:H1' | 2.30 | 0.47 |
| 1:A:1226:C:H2' | 13:N:103:THR:HB | 1.95 | 0.47 |
| 1:A:321:A:N6 | 1:A:329:A:OP2 | 2.48 | 0.47 |
| 4:D:26:CYS:HA | 4:D:31:CYS:HA | 1.96 | 0.47 |
| 17:R:76:LEU:HD21 | 17:R:79:SER:HB2 | 1.97 | 0.47 |
| 22:W:53:G:HO2' | 22:W:54:U:H5 | 1.62 | 0.47 |
| 1:A:1321:C:H5'' | 1:A:1322:C:H5'' | 1.97 | 0.47 |
| 1:A:1443:G:H5' | 1:A:1446:A:OP2 | 2.15 | 0.47 |
| 1:A:1513:A:H2' | 1:A:1514:C:C6 | 2.50 | 0.47 |
| 1:A:377:G:H1 | 1:A:386:C:H42 | 1.61 | 0.47 |
| 2:B:211:ILE:O | 2:B:215:LEU:HB2 | 2.14 | 0.47 |
| 2:B:25:ASN:O | 2:B:27:LYS:N | 2.47 | 0.47 |
| 12:M:51:ALA:HB3 | 12:M:53:ARG:HE | 1.80 | 0.47 |
| 14:O:41:ARG:CZ | 14:O:42:ILE:HD11 | 2.44 | 0.47 |
| 22:W:16:C:N4 | 22:W:17:U:O4 | 2.48 | 0.47 |
| 1:A:1414:U:H2' | 1:A:1415:G:H8 | 1.80 | 0.47 |
| 9:J:28:VAL:HG22 | 9:J:63:ILE:HB | 1.95 | 0.47 |
| 12:M:27:LEU:O | 12:M:29:GLY:N | 2.47 | 0.47 |
| 10:K:61:GLU:HG3 | 14:O:58:LYS:HZ1 | 1.79 | 0.47 |
| 1:A:1084:G:H5' | 1:A:1102:A:OP2 | 2.14 | 0.47 |
| 1:A:1126:U:H1' | 1:A:1280:A:C5 | 2.49 | 0.47 |
| 1:A:273:A:H1' | 17:R:16:GLN:OE1 | 2.15 | 0.47 |
| 1:A:713:G:H2' | 1:A:714:G:C8 | 2.49 | 0.47 |
| 1:A:1128:C:C4' | 9:J:16:ARG:HH22 | 2.28 | 0.47 |
| 12:M:17:LYS:HG3 | 12:M:18:VAL:N | 2.30 | 0.47 |
| 13:N:78:ILE:HG23 | 13:N:92:HIS:ND1 | 2.29 | 0.47 |
| 22:W:21:A:N6 | 22:W:46:G:H2' | 2.30 | 0.47 |
| 1:A:265:G:H2' | 1:A:266:G:H5'' | 1.97 | 0.47 |
| 4:D:30:LYS:CD | 4:D:30:LYS:N | 2.77 | 0.47 |
| 6:F:61:LEU:HB3 | 6:F:63:TYR:HE1 | 1.80 | 0.47 |
| 1:A:1301:U:H2' | 1:A:1301:U:O2 | 2.13 | 0.47 |
| 1:A:1515:C:H2' | 1:A:1516:G:C8 | 2.50 | 0.47 |
| 1:A:34:C:H2' | 1:A:35:G:C8 | 2.50 | 0.47 |
| 1:A:736:C:H2' | 1:A:737:A:C8 | 2.49 | 0.47 |
| 2:B:8:LYS:H | 2:B:8:LYS:HD3 | 1.79 | 0.47 |
| 7:H:99:LEU:HD22 | 7:H:103:TRP:CZ2 | 2.49 | 0.47 |
| 1:A:690:G:H22 | 11:L:55:LYS:HZ2 | 1.62 | 0.47 |
| 1:A:1200:C:H4' | 1:A:1201:A:H5' | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:671:G:H1 | 1:A:735:C:H42 | 1.62 | 0.47 |
| 7:H:18:TYR:HD2 | 7:H:59:LEU:HD22 | 1.79 | 0.47 |
| 19:T:15:LEU:H | 19:T:15:LEU:HD23 | 1.79 | 0.47 |
| 23:X:30:G:H2' | 23:X:31:A:C8 | 2.49 | 0.47 |
| 1:A:452:A:O2' | 1:A:453:A:O4' | 2.30 | 0.47 |
| 1:A:962:C:H42 | 1:A:974:A:H61 | 1.62 | 0.47 |
| 2:B:32:ILE:HD13 | 2:B:40:HIS:HB3 | 1.95 | 0.47 |
| 5:E:9:LYS:HB3 | 5:E:112:LEU:HD11 | 1.97 | 0.47 |
| 19:T:35:SER:O | 19:T:71:LEU:HD12 | 2.15 | 0.47 |
| 1:A:606:G:H22 | 1:A:631:G:H5' | 1.80 | 0.46 |
| 1:A:953:G:C5' | 1:A:965:A:H61 | 2.27 | 0.46 |
| 3:C:82:GLU:O | 3:C:86:VAL:HG13 | 2.14 | 0.46 |
| 10:K:84:GLN:H | 10:K:84:GLN:HG3 | 1.49 | 0.46 |
| 1:A:1305:G:HO2' | 1:A:1306:A:H8 | 1.60 | 0.46 |
| 1:A:1306:A:N6 | 1:A:1331:G:H1' | 2.31 | 0.46 |
| 1:A:318:G:H2' | 1:A:319:G:H8 | 1.78 | 0.46 |
| 7:H:78:ARG:HG3 | 7:H:79:ARG:N | 2.30 | 0.46 |
| 11:L:16:SER:OG | 11:L:106:LYS:NZ | 2.48 | 0.46 |
| 1:A:1376:U:H2' | 1:A:1377:A:C8 | 2.50 | 0.46 |
| 1:A:224:C:H2' | 1:A:225:C:C6 | 2.51 | 0.46 |
| 1:A:403:C:H2' | 1:A:404:U:H6 | 1.81 | 0.46 |
| 1:A:932:C:H4' | 7:H:4:ARG:NH2 | 2.30 | 0.46 |
| 1:A:22:G:H2' | 1:A:23:C:C6 | 2.50 | 0.46 |
| 1:A:405:U:O4 | 4:D:2:GLY:N | 2.49 | 0.46 |
| 2:B:166:ASP:OD2 | 2:B:169:LYS:HB2 | 2.15 | 0.46 |
| 19:T:63:THR:HG23 | 19:T:65:ASN:OD1 | 2.15 | 0.46 |
| 1:A:1225:A:H5'' | 1:A:1226:C:OP2 | 2.16 | 0.46 |
| 1:A:1298:C:H4' | 1:A:1299:A:C8 | 2.50 | 0.46 |
| 1:A:381:C:H2' | 1:A:382:A:O4' | 2.14 | 0.46 |
| 1:A:411:A:C4 | 1:A:413:G:H1' | 2.50 | 0.46 |
| 1:A:64:G:H4' | 1:A:65:U:C5' | 2.46 | 0.46 |
| 6:F:10:LEU:N | 6:F:59:TYR:O | 2.46 | 0.46 |
| 16:Q:3:LYS:O | 16:Q:21:VAL:HA | 2.15 | 0.46 |
| 17:R:74:LEU:HB3 | 17:R:75:ARG:H | 1.63 | 0.46 |
| 20:U:33:ILE:HD13 | 20:U:62:LEU:HB3 | 1.97 | 0.46 |
| 1:A:1402:C:H2' | 1:A:1403:C:O4' | 2.16 | 0.46 |
| 1:A:701:C:H1' | 1:A:703:G:N1 | 2.30 | 0.46 |
| 1:A:751:U:H2' | 1:A:752:G:O4' | 2.16 | 0.46 |
| 12:M:54:LYS:HD2 | 12:M:54:LYS:N | 2.30 | 0.46 |
| 1:A:1109:C:OP2 | 3:C:176:HIS:ND1 | 2.46 | 0.46 |
| 1:A:1330:U:H4' | 13:N:23:TYR:CE2 | 2.50 | 0.46 |
| 1:A:137:C:O4' | 16:Q:63:GLY:HA2 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:A:243:A:H4' | 1:A:244:U:H3' | 1.98 | 0.46 |
| 2:B:165:VAL:HG23 | 2:B:166:ASP:H | 1.81 | 0.46 |
| 4:D:8:VAL:HG13 | 4:D:21:LEU:HD12 | 1.97 | 0.46 |
| 4:D:75:PHE:HE1 | 4:D:97:LEU:HD11 | 1.81 | 0.46 |
| 20:U:29:LYS:O | 20:U:33:ILE:HG12 | 2.16 | 0.46 |
| 11:L:54:ARG:NH2 | 23:X:39:U:O3' | 2.48 | 0.46 |
| 1:A:544:G:OP2 | 4:D:66:ARG:NH2 | 2.49 | 0.46 |
| 1:A:579:G:H5' | 1:A:728:A:H1' | 1.98 | 0.46 |
| 7:H:150:ALA:O | 11:L:57:THR:HG21 | 2.16 | 0.46 |
| 7:H:20:ASP:OD1 | 7:H:21:VAL:N | 2.48 | 0.46 |
| 22:W:6:G:O2' | 22:W:49:G:H5' | 2.16 | 0.46 |
| 1:A:1238:A:OP1 | 1:A:1335:C:O2' | 2.22 | 0.46 |
| 1:A:1410:G:H2' | 1:A:1411:C:C6 | 2.51 | 0.46 |
| 1:A:67:C:H2' | 1:A:68:G:C8 | 2.51 | 0.46 |
| 4:D:18:LYS:HD3 | 4:D:20:TYR:CZ | 2.51 | 0.46 |
| 4:D:15:GLU:HG2 | 4:D:63:LYS:HG3 | 1.97 | 0.46 |
| 13:N:89:GLY:O | 13:N:92:HIS:HB2 | 2.15 | 0.46 |
| 1:A:1014:A:H4' | 19:T:14:HIS:NE2 | 2.31 | 0.46 |
| 20:U:89:ARG:NH2 | 20:U:105:SER:O | 2.37 | 0.46 |
| 1:A:1001:G:H2' | 1:A:1002:G:O4' | 2.16 | 0.45 |
| 1:A:1012:U:H2' | 1:A:1013:G:C8 | 2.51 | 0.45 |
| 4:D:121:VAL:O | 4:D:134:ASP:HA | 2.16 | 0.45 |
| 4:D:53:ASP:O | 4:D:57:ARG:HD2 | 2.16 | 0.45 |
| 8:I:20:TYR:HA | 8:I:65:TYR:CZ | 2.51 | 0.45 |
| 1:A:1349:A:P | 9:J:118:LYS:HZ3 | 2.39 | 0.45 |
| 13:N:84:ILE:HD12 | 13:N:84:ILE:HA | 1.75 | 0.45 |
| 1:A:1342:C:H2' | 1:A:1343:G:C8 | 2.51 | 0.45 |
| 1:A:407:G:OP1 | 4:D:3:ARG:NH1 | 2.49 | 0.45 |
| 1:A:743:U:H2' | 1:A:744:C:C6 | 2.50 | 0.45 |
| 3:C:19:GLU:HA | 3:C:54:ARG:HH12 | 1.81 | 0.45 |
| 9:J:126:SER:O | 9:J:128:ARG:N | 2.45 | 0.45 |
| 9:J:45:ALA:O | 9:J:48:GLU:HG2 | 2.15 | 0.45 |
| 19:T:32:LYS:HA | 19:T:50:ALA:HB3 | 1.98 | 0.45 |
| 1:A:1129:C:H4' | 1:A:1130:A:H5' | 1.98 | 0.45 |
| 6:F:99:ALA:HB1 | 18:S:23:LYS:NZ | 2.31 | 0.45 |
| 12:M:113:ARG:HH21 | 12:M:116:SER:HB2 | 1.81 | 0.45 |
| 1:A:1375:A:H4' | 7:H:29:LYS:HE3 | 1.97 | 0.45 |
| 4:D:103:ASN:OD1 | 4:D:114:ARG:NE | 2.49 | 0.45 |
| 3:C:23:TYR:CD1 | 10:K:10:GLY:HA2 | 2.51 | 0.45 |
| 14:O:32:SER:O | 14:O:32:SER:OG | 2.26 | 0.45 |
| 20:U:26:ASN:HB2 | 20:U:71:THR:HG23 | 1.97 | 0.45 |
| 1:A:1172:C:H2' | 1:A:1173:G:H8 | 1.79 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:1298:C:H4' | 1:A:1299:A:C4 | 2.51 | 0.45 |
| 1:A:1435:G:H2' | 1:A:1436:U:C6 | 2.51 | 0.45 |
| 1:A:266:G:O2' | 1:A:268:C:OP2 | 2.35 | 0.45 |
| 1:A:939:G:H5'' | 7:H:102:ARG:NH2 | 2.32 | 0.45 |
| 8:I:104:ARG:O | 8:I:107:LEU:HB2 | 2.16 | 0.45 |
| 1:A:1227:A:OP2 | 13:N:111:LYS:HE3 | 2.16 | 0.45 |
| 10:K:51:ARG:NH2 | 14:O:58:LYS:HZ1 | 2.15 | 0.45 |
| 1:A:946:A:N6 | 1:A:1234:C:H42 | 2.14 | 0.45 |
| 1:A:1252:A:H61 | 1:A:1285:A:H61 | 1.64 | 0.45 |
| 1:A:129(A):G:N2 | 1:A:188:U:O2' | 2.50 | 0.45 |
| 1:A:518:C:H2' | 1:A:530:G:N3 | 2.32 | 0.45 |
| 1:A:565:U:H5'' | 1:A:566:G:H2' | 1.98 | 0.45 |
| 6:F:45:LEU:HD12 | 6:F:59:TYR:HD2 | 1.82 | 0.45 |
| 20:U:64:ASP:CG | 20:U:81:LYS:HZ2 | 2.20 | 0.45 |
| 1:A:481:G:O2' | 1:A:482:A:O5' | 2.35 | 0.45 |
| 2:B:76:GLN:O | 2:B:208:ILE:HG12 | 2.17 | 0.45 |
| 11:L:41:THR:HG21 | 11:L:71:LYS:HB2 | 1.99 | 0.45 |
| 12:M:109:GLY:HA3 | 12:M:121:GLY:O | 2.17 | 0.45 |
| 1:A:1016:A:H2' | 1:A:1017:G:O4' | 2.17 | 0.45 |
| 1:A:1504:G:OP1 | 1:A:1507:A:H4' | 2.17 | 0.45 |
| 1:A:244:U:H4' | 1:A:245:C:O5' | 2.16 | 0.45 |
| 1:A:696:A:H2' | 1:A:697:U:C6 | 2.52 | 0.45 |
| 7:H:113:GLU:CG | 7:H:119:ARG:HG2 | 2.47 | 0.45 |
| 7:H:49:ILE:O | 7:H:53:LYS:HB3 | 2.16 | 0.45 |
| 1:A:64:G:H4' | 1:A:65:U:O5' | 2.16 | 0.45 |
| 7:H:45:ASP:O | 7:H:49:ILE:HG12 | 2.16 | 0.45 |
| 8:I:92:ARG:HA | 8:I:92:ARG:HD3 | 1.77 | 0.45 |
| 1:A:1060:C:O2' | 10:K:56:HIS:ND1 | 2.46 | 0.45 |
| 11:L:91:ARG:NH1 | 11:L:110:ASP:OD2 | 2.47 | 0.45 |
| 12:M:71:PRO:HG3 | 12:M:99:HIS:HD2 | 1.82 | 0.45 |
| 1:A:1176:A:H2' | 1:A:1177:G:H5' | 1.98 | 0.45 |
| 1:A:1348:U:H4' | 9:J:120:ARG:HD2 | 1.98 | 0.45 |
| 1:A:892:A:O2' | 1:A:1415:G:H4' | 2.17 | 0.45 |
| 1:A:299:G:H2' | 1:A:300:A:C8 | 2.52 | 0.45 |
| 1:A:429:U:H1' | 1:A:430:A:H5'' | 1.98 | 0.45 |
| 8:I:6:ILE:HB | 8:I:85:ARG:HH11 | 1.82 | 0.45 |
| 8:I:6:ILE:O | 8:I:10:LEU:HG | 2.17 | 0.45 |
| 12:M:11:VAL:HG13 | 17:R:29:HIS:HD2 | 1.82 | 0.45 |
| 1:A:880:C:OP2 | 12:M:9:GLN:HG3 | 2.17 | 0.45 |
| 13:N:92:HIS:CD2 | 13:N:110:ARG:HH21 | 2.35 | 0.45 |
| 1:A:224:C:H2' | 1:A:225:C:H6 | 1.82 | 0.44 |
| 1:A:318:G:H2' | 1:A:319:G:C8 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:584:G:H2' | 1:A:585:G:H8 | 1.82 | 0.44 |
| 2:B:51:LEU:HD22 | 2:B:55:PHE:HE2 | 1.82 | 0.44 |
| 6:F:41:GLU:HB3 | 6:F:62:TRP:HB3 | 1.99 | 0.44 |
| 10:K:40:LEU:HB2 | 10:K:69:ASN:CB | 2.47 | 0.44 |
| 19:T:10:PHE:HB2 | 19:T:39:THR:H | 1.82 | 0.44 |
| 1:A:1105:A:H2' | 1:A:1106:G:C8 | 2.51 | 0.44 |
| 1:A:1152:A:H5'' | 10:K:13:HIS:HD2 | 1.82 | 0.44 |
| 1:A:1222:G:OP1 | 19:T:77:THR:HG21 | 2.17 | 0.44 |
| 1:A:1336:C:H1' | 1:A:1337:G:C2 | 2.53 | 0.44 |
| 1:A:620:C:H2' | 1:A:621:A:O4' | 2.18 | 0.44 |
| 1:A:992:U:H1' | 1:A:993:G:OP2 | 2.17 | 0.44 |
| 2:B:163:PHE:HA | 2:B:185:ILE:HG13 | 1.99 | 0.44 |
| 2:B:30:ARG:HH21 | 2:B:194:PRO:HG2 | 1.81 | 0.44 |
| 6:F:23:LYS:O | 6:F:27:GLN:HG2 | 2.17 | 0.44 |
| 19:T:66:MET:HB2 | 19:T:74:PHE:CZ | 2.51 | 0.44 |
| 1:A:1053:G:O6 | 1:A:1199:U:H2' | 2.17 | 0.44 |
| 1:A:1350:A:OP2 | 9:J:118:LYS:NZ | 2.47 | 0.44 |
| 1:A:1372:U:H2' | 1:A:1373:G:O4' | 2.18 | 0.44 |
| 1:A:20:U:O2 | 1:A:916:G:C2 | 2.70 | 0.44 |
| 1:A:1439:C:H42 | 1:A:1462:G:H1 | 1.63 | 0.44 |
| 1:A:601:C:H2' | 1:A:602:A:C8 | 2.53 | 0.44 |
| 1:A:974:A:H1' | 14:O:31:ARG:NE | 2.31 | 0.44 |
| 1:A:1191:A:P | 3:C:3:ASN:HD22 | 2.41 | 0.44 |
| 10:K:33:GLN:O | 10:K:75:ILE:HG12 | 2.17 | 0.44 |
| 20:U:16:HIS:O | 20:U:19:SER:HB3 | 2.17 | 0.44 |
| 1:A:1305:G:H5' | 21:V:4:GLY:HA3 | 1.99 | 0.44 |
| 4:D:150:GLU:OE1 | 4:D:150:GLU:N | 2.51 | 0.44 |
| 5:E:97:GLY:N | 5:E:117:ASP:OD2 | 2.40 | 0.44 |
| 16:Q:23:ASP:O | 16:Q:26:ARG:HB2 | 2.17 | 0.44 |
| 1:A:1111:A:N1 | 3:C:177:THR:OG1 | 2.43 | 0.44 |
| 1:A:1277:C:O2' | 1:A:1279:A:H8 | 2.01 | 0.44 |
| 1:A:966:G:O2' | 9:J:127:LYS:O | 2.35 | 0.44 |
| 20:U:87:LYS:HA | 20:U:87:LYS:HD2 | 1.68 | 0.44 |
| 22:W:15:C:O2' | 22:W:61:C:OP1 | 2.36 | 0.44 |
| 1:A:1244:C:H42 | 1:A:1293:G:H1 | 1.65 | 0.44 |
| 1:A:297:G:N2 | 1:A:300:A:OP2 | 2.48 | 0.44 |
| 1:A:484:G:H4' | 1:A:485:G:O5' | 2.16 | 0.44 |
| 3:C:70:VAL:HG21 | 3:C:76:VAL:HG11 | 2.00 | 0.44 |
| 7:H:113:GLU:H | 7:H:113:GLU:HG2 | 1.39 | 0.44 |
| 10:K:51:ARG:NE | 10:K:60:ARG:O | 2.45 | 0.44 |
| 10:K:47:PHE:HE1 | 10:K:63:PHE:HB2 | 1.83 | 0.44 |
| 15:P:50:HIS:O | 15:P:53:HIS:HB3 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 22:W:43:A:H2' | 22:W:44:A:C8 | 2.53 | 0.44 |
| 1:A:584:G:H2' | 1:A:585:G:C8 | 2.53 | 0.44 |
| 1:A:991:U:O2 | 1:A:993:G:H8 | 2.01 | 0.44 |
| 2:B:71:VAL:HA | 2:B:93:VAL:HB | 2.00 | 0.44 |
| 7:H:116:ALA:HA | 7:H:119:ARG:HE | 1.83 | 0.44 |
| 11:L:92:GLU:HB3 | 11:L:96:ARG:NH1 | 2.33 | 0.44 |
| 23:X:19:G:H22 | 23:X:56:C:N4 | 2.16 | 0.44 |
| 1:A:1015:A:H1' | 1:A:1219:U:H5' | 2.00 | 0.44 |
| 1:A:1231:G:O3' | 9:J:126:SER:OG | 2.22 | 0.44 |
| 1:A:17:U:H2' | 1:A:18:C:C6 | 2.53 | 0.44 |
| 1:A:280:C:H3' | 1:A:281:G:H5' | 1.99 | 0.44 |
| 1:A:489:C:H2' | 1:A:490:G:H8 | 1.83 | 0.44 |
| 1:A:738:C:OP2 | 6:F:92:LYS:NZ | 2.50 | 0.44 |
| 1:A:900:A:H2' | 1:A:901:A:C8 | 2.53 | 0.44 |
| 1:A:936:C:H2' | 1:A:937:A:O4' | 2.18 | 0.44 |
| 1:A:97:U:H2' | 1:A:99:C:C6 | 2.53 | 0.44 |
| 2:B:228:GLY:O | 2:B:230:VAL:N | 2.50 | 0.44 |
| 12:M:44:THR:HA | 12:M:45:PRO:HD3 | 1.74 | 0.44 |
| 15:P:39:LEU:HA | 15:P:39:LEU:HD23 | 1.68 | 0.44 |
| 1:A:838:G:C6 | 1:A:842:C:H1' | 2.53 | 0.43 |
| 2:B:74:LYS:O | 2:B:78:GLN:HG3 | 2.18 | 0.43 |
| 17:R:60:ILE:HB | 17:R:74:LEU:HD23 | 2.00 | 0.43 |
| 1:A:1124:G:H5'' | 1:A:1145:C:H41 | 1.81 | 0.43 |
| 1:A:1200:C:O2' | 1:A:1201:A:OP2 | 2.29 | 0.43 |
| 1:A:1317:C:N3 | 19:T:37:ARG:NH2 | 2.66 | 0.43 |
| 1:A:1488:G:H2' | 1:A:1489:G:H8 | 1.81 | 0.43 |
| 1:A:952:U:H2' | 1:A:953:G:H8 | 1.82 | 0.43 |
| 3:C:81:GLY:O | 3:C:85:ARG:HB2 | 2.18 | 0.43 |
| 7:H:9:VAL:HG13 | 7:H:94:ARG:NH2 | 2.27 | 0.43 |
| 9:J:16:ARG:O | 9:J:63:ILE:HA | 2.17 | 0.43 |
| 12:M:70:ILE:HD13 | 12:M:77:LEU:HD12 | 1.99 | 0.43 |
| 15:P:17:ARG:HD3 | 15:P:26:GLU:HG3 | 1.99 | 0.43 |
| 1:A:1510:U:H2' | 1:A:1511:G:C8 | 2.52 | 0.43 |
| 1:A:585:G:O3' | 17:R:34:LYS:NZ | 2.51 | 0.43 |
| 5:E:100:VAL:HG22 | 5:E:118:ILE:HG22 | 1.99 | 0.43 |
| 4:D:171:GLY:HA2 | 4:D:172:PRO:HD3 | 1.87 | 0.43 |
| 9:J:116:LYS:HE2 | 9:J:122:ALA:HB2 | 2.01 | 0.43 |
| 11:L:19:ALA:HB2 | 11:L:32:ILE:HG22 | 2.00 | 0.43 |
| 11:L:38:ASN:HA | 11:L:39:PRO:HD3 | 1.88 | 0.43 |
| 17:R:63:ARG:HG2 | 17:R:64:PRO:HD2 | 2.00 | 0.43 |
| 18:S:37:VAL:HG22 | 18:S:78:LEU:HB3 | 2.00 | 0.43 |
| 22:W:28:C:H2' | 22:W:29:G:H8 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1299:A:C6 | 1:A:1301:U:C2 | 3.06 | 0.43 |
| 1:A:452:A:O2' | 1:A:453:A:O5' | 2.36 | 0.43 |
| 1:A:767:A:H2' | 1:A:768:A:O4' | 2.18 | 0.43 |
| 8:I:105:ARG:HD3 | 8:I:105:ARG:HA | 1.78 | 0.43 |
| 16:Q:20:VAL:HG21 | 16:Q:32:TYR:CE2 | 2.54 | 0.43 |
| 1:A:1321:C:H4' | 13:N:87:TYR:CZ | 2.54 | 0.43 |
| 1:A:1511:G:H2' | 1:A:1512:U:O4' | 2.19 | 0.43 |
| 1:A:157:G:H1 | 1:A:164:U:H3 | 1.66 | 0.43 |
| 1:A:842:C:O2' | 1:A:848:C:N4 | 2.51 | 0.43 |
| 1:A:857:C:H2' | 1:A:858:G:O4' | 2.19 | 0.43 |
| 4:D:133:VAL:HG12 | 4:D:135:LEU:H | 1.83 | 0.43 |
| 8:I:13:ILE:O | 8:I:17:THR:HG23 | 2.19 | 0.43 |
| 9:J:112:LYS:HD3 | 9:J:113:LYS:O | 2.18 | 0.43 |
| 14:O:47:LEU:HA | 14:O:47:LEU:HD23 | 1.74 | 0.43 |
| 6:F:99:ALA:HB1 | 18:S:23:LYS:HZ2 | 1.83 | 0.43 |
| 1:A:601:C:H2' | 1:A:602:A:H8 | 1.83 | 0.43 |
| 2:B:8:LYS:HE3 | 2:B:11:LEU:HB3 | 2.01 | 0.43 |
| 2:B:167:PRO:HG3 | 2:B:188:ALA:HB2 | 2.01 | 0.43 |
| 12:M:85:ILE:HA | 12:M:85:ILE:HD12 | 1.75 | 0.43 |
| 13:N:44:ARG:HB2 | 13:N:47:ASP:OD2 | 2.19 | 0.43 |
| 17:R:45:HIS:NE2 | 17:R:47:PRO:HG3 | 2.34 | 0.43 |
| 23:X:16:U:H5' | 23:X:17:C:OP2 | 2.18 | 0.43 |
| 1:A:1179:A:H2' | 1:A:1180:A:O4' | 2.19 | 0.43 |
| 1:A:1488:G:H2' | 1:A:1489:G:C8 | 2.53 | 0.43 |
| 1:A:24:U:H2' | 1:A:25:C:H6 | 1.84 | 0.43 |
| 1:A:266:G:O2' | 1:A:267:C:OP2 | 2.32 | 0.43 |
| 1:A:383:A:O5' | 1:A:383:A:H8 | 2.02 | 0.43 |
| 4:D:155:LEU:O | 4:D:159:ARG:HG2 | 2.19 | 0.43 |
| 5:E:18:ARG:HB3 | 5:E:18:ARG:HE | 1.52 | 0.43 |
| 1:A:1346:A:H2' | 7:H:10:ARG:HH22 | 1.83 | 0.43 |
| 8:I:101:PRO:HG2 | 8:I:133:LEU:HD11 | 2.01 | 0.43 |
| 9:J:17:VAL:HG11 | 9:J:81:ILE:HD13 | 2.00 | 0.43 |
| 1:A:999:U:H2' | 1:A:1000:A:C8 | 2.54 | 0.43 |
| 1:A:398:C:H2' | 1:A:399:G:H8 | 1.84 | 0.43 |
| 1:A:579:G:H2' | 1:A:580:U:C6 | 2.54 | 0.43 |
| 3:C:11:ARG:HB3 | 3:C:15:THR:HB | 2.01 | 0.43 |
| 1:A:384:G:H2' | 1:A:385:C:C6 | 2.54 | 0.42 |
| 1:A:580:U:H2' | 1:A:581:G:O4' | 2.18 | 0.42 |
| 1:A:612:C:O2 | 1:A:629:G:N2 | 2.52 | 0.42 |
| 1:A:901:A:H8 | 1:A:901:A:O5' | 2.02 | 0.42 |
| 4:D:158:ILE:HD13 | 4:D:158:ILE:HA | 1.82 | 0.42 |
| 6:F:62:TRP:CH2 | 6:F:64:GLN:HB2 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 7:H:102:ARG:HG2 | 7:H:106:GLN:OE1 | 2.19 | 0.42 |
| 8:I:25:ASP:N | 8:I:25:ASP:OD1 | 2.50 | 0.42 |
| 13:N:4:ILE:H | 13:N:9:ILE:HG22 | 1.84 | 0.42 |
| 18:S:53:ARG:HH21 | 18:S:60:ALA:N | 2.17 | 0.42 |
| 23:X:37:A:H2' | 23:X:38:A:O4' | 2.19 | 0.42 |
| 1:A:1192:C:O2 | 5:E:25:ARG:NH2 | 2.50 | 0.42 |
| 1:A:701:C:H1' | 1:A:703:G:C6 | 2.54 | 0.42 |
| 1:A:986:A:N3 | 19:T:52:TYR:OH | 2.46 | 0.42 |
| 4:D:108:LEU:HD21 | 4:D:183:GLY:HA3 | 2.01 | 0.42 |
| 9:J:48:GLU:N | 9:J:49:PRO:HD2 | 2.34 | 0.42 |
| 15:P:25:THR:HG21 | 15:P:70:LEU:HB2 | 2.00 | 0.42 |
| 18:S:29:PHE:CD1 | 18:S:29:PHE:N | 2.87 | 0.42 |
| 19:T:41:VAL:HG12 | 19:T:44:MET:HB2 | 2.02 | 0.42 |
| 1:A:1499:A:H1' | 1:A:1520:G:H5' | 2.01 | 0.42 |
| 1:A:24:U:H2' | 1:A:25:C:C6 | 2.54 | 0.42 |
| 1:A:296:U:H2' | 1:A:297:G:C8 | 2.54 | 0.42 |
| 2:B:130:ARG:HA | 2:B:131:PRO:HD3 | 1.81 | 0.42 |
| 1:A:542:G:H5' | 4:D:41:GLY:HA3 | 2.00 | 0.42 |
| 1:A:1367:C:H5' | 10:K:60:ARG:NH2 | 2.35 | 0.42 |
| 11:L:120:ARG:HA | 11:L:121:PRO:HD3 | 1.87 | 0.42 |
| 7:H:153:HIS:HB3 | 11:L:58:PRO:HG2 | 2.01 | 0.42 |
| 17:R:29:HIS:CG | 17:R:30:PRO:HD2 | 2.54 | 0.42 |
| 1:A:1226:C:H4' | 19:T:80:TYR:OH | 2.20 | 0.42 |
| 1:A:1306:A:H1' | 1:A:1332:A:C2 | 2.55 | 0.42 |
| 1:A:812:C:H1' | 1:A:813:U:OP2 | 2.19 | 0.42 |
| 2:B:217:ARG:HB2 | 2:B:217:ARG:HE | 1.29 | 0.42 |
| 2:B:21:ARG:HG3 | 2:B:38:GLY:O | 2.19 | 0.42 |
| 2:B:44:LEU:H | 2:B:44:LEU:HD12 | 1.83 | 0.42 |
| 3:C:148:GLY:HA3 | 3:C:172:ARG:O | 2.18 | 0.42 |
| 3:C:59:ARG:HH12 | 3:C:97:LYS:HE3 | 1.84 | 0.42 |
| 4:D:120:LEU:HA | 4:D:120:LEU:HD23 | 1.86 | 0.42 |
| 4:D:165:MET:O | 4:D:166:LYS:C | 2.54 | 0.42 |
| 4:D:29:PRO:C | 4:D:30:LYS:HD3 | 2.39 | 0.42 |
| 4:D:11:LEU:HD22 | 4:D:66:ARG:HD3 | 2.02 | 0.42 |
| 6:F:15:ASP:OD2 | 6:F:18:GLN:CG | 2.66 | 0.42 |
| 10:K:54:PHE:HB3 | 10:K:55:LYS:H | 1.69 | 0.42 |
| 10:K:79:ARG:HA | 10:K:79:ARG:HD3 | 1.78 | 0.42 |
| 14:O:41:ARG:NH2 | 14:O:42:ILE:HD11 | 2.35 | 0.42 |
| 19:T:10:PHE:CG | 19:T:11:VAL:N | 2.88 | 0.42 |
| 23:X:67:C:H2' | 23:X:68:C:C6 | 2.54 | 0.42 |
| 1:A:1170:A:O5' | 1:A:1170:A:H8 | 2.02 | 0.42 |
| 1:A:1162:C:H42 | 1:A:1174:G:H1 | 1.68 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1292:U:H2' | 1:A:1293:G:C8 | 2.54 | 0.42 |
| 1:A:464:G:C6 | 1:A:466:C:H5' | 2.54 | 0.42 |
| 1:A:514:C:H2' | 1:A:515:G:C8 | 2.54 | 0.42 |
| 1:A:707:C:H2' | 1:A:708:C:C6 | 2.55 | 0.42 |
| 2:B:92:TYR:CD1 | 2:B:151:GLY:HA3 | 2.55 | 0.42 |
| 6:F:22:GLU:O | 6:F:26:ILE:HG13 | 2.19 | 0.42 |
| 11:L:41:THR:HG22 | 11:L:42:TRP:N | 2.34 | 0.42 |
| 15:P:48:LYS:HA | 15:P:48:LYS:HD3 | 1.76 | 0.42 |
| 1:A:1386:G:H2' | 1:A:1387:G:H8 | 1.83 | 0.42 |
| 1:A:836:G:C6 | 1:A:851:G:C6 | 3.08 | 0.42 |
| 3:C:112:SER:O | 3:C:116:VAL:HG23 | 2.20 | 0.42 |
| 5:E:47:LYS:HB2 | 5:E:47:LYS:HE2 | 1.82 | 0.42 |
| 12:M:38:THR:HG21 | 12:M:65:GLU:OE2 | 2.19 | 0.42 |
| 1:A:1036:G:H5' | 1:A:1037:C:OP2 | 2.18 | 0.42 |
| 1:A:1264:C:H2' | 1:A:1265:G:C8 | 2.54 | 0.42 |
| 1:A:630:G:O3' | 1:A:631:G:H4' | 2.19 | 0.42 |
| 1:A:648:A:H2' | 1:A:649:G:C8 | 2.55 | 0.42 |
| 1:A:662:G:H2' | 1:A:663:A:H8 | 1.84 | 0.42 |
| 1:A:728:A:H2' | 1:A:729:A:C8 | 2.55 | 0.42 |
| 1:A:828:A:H2' | 1:A:829:G:O4' | 2.20 | 0.42 |
| 2:B:27:LYS:HD2 | 2:B:193:ASP:CB | 2.46 | 0.42 |
| 5:E:79:GLU:HB3 | 5:E:92:LYS:HA | 2.02 | 0.42 |
| 10:K:22:LYS:HB3 | 10:K:22:LYS:HE3 | 1.68 | 0.42 |
| 10:K:76:ASN:HA | 10:K:77:PRO:HD2 | 1.85 | 0.42 |
| 15:P:43:LEU:HD23 | 15:P:43:LEU:HA | 1.74 | 0.42 |
| 17:R:10:VAL:HG13 | 17:R:19:VAL:HB | 2.01 | 0.42 |
| 1:A:1216:G:H5'' | 14:O:5:ALA:HB2 | 2.02 | 0.42 |
| 1:A:389:A:H2' | 1:A:390:C:O4' | 2.20 | 0.42 |
| 1:A:518:C:H5' | 1:A:530:G:O4' | 2.20 | 0.42 |
| 1:A:939:G:H2' | 1:A:940:C:C6 | 2.55 | 0.42 |
| 2:B:219:VAL:O | 2:B:223:ILE:HG13 | 2.19 | 0.42 |
| 2:B:60:ASP:O | 2:B:64:ARG:HG2 | 2.19 | 0.42 |
| 3:C:134:ILE:HD11 | 3:C:153:VAL:HG21 | 2.02 | 0.42 |
| 3:C:56:ASP:O | 3:C:66:VAL:HA | 2.20 | 0.42 |
| 10:K:81:THR:C | 10:K:83:GLU:H | 2.23 | 0.42 |
| 15:P:87:ILE:HG22 | 15:P:88:ARG:N | 2.35 | 0.42 |
| 1:A:1320:C:N4 | 19:T:36:ARG:HG3 | 2.35 | 0.42 |
| 22:W:28:C:H2' | 22:W:29:G:C8 | 2.54 | 0.42 |
| 23:X:57:G:H2' | 23:X:58:A:H5' | 2.01 | 0.42 |
| 1:A:1285:A:H1' | 1:A:1286:A:OP2 | 2.20 | 0.42 |
| 1:A:1314:C:H2' | 1:A:1315:U:C6 | 2.55 | 0.42 |
| 1:A:328:C:H4' | 1:A:329:A:O5' | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:596:C:H2' | 1:A:597:G:H8 | 1.84 | 0.42 |
| 2:B:88:ALA:HB2 | 2:B:219:VAL:HG13 | 2.02 | 0.42 |
| 4:D:122:ARG:HD3 | 4:D:122:ARG:O | 2.20 | 0.42 |
| 6:F:15:ASP:O | 6:F:17:SER:N | 2.53 | 0.42 |
| 7:H:13:GLN:O | 7:H:24:THR:HG21 | 2.20 | 0.42 |
| 8:I:54:ASP:O | 8:I:56:LYS:HG3 | 2.20 | 0.42 |
| 11:L:48:ILE:HG23 | 11:L:63:LEU:HD22 | 2.01 | 0.42 |
| 12:M:11:VAL:HG11 | 17:R:36:ILE:HG21 | 2.00 | 0.42 |
| 18:S:53:ARG:HE | 18:S:59:SER:C | 2.22 | 0.42 |
| 1:A:1024:G:H4' | 1:A:1024:G:OP1 | 2.20 | 0.42 |
| 1:A:1347:G:O2' | 1:A:1348:U:P | 2.78 | 0.42 |
| 1:A:9:G:H5'' | 5:E:126:ARG:HE | 1.84 | 0.42 |
| 2:B:184:VAL:N | 2:B:198:ASP:OD2 | 2.44 | 0.42 |
| 3:C:36:ASP:HA | 3:C:39:ILE:HD12 | 2.02 | 0.42 |
| 3:C:42:LEU:HD12 | 3:C:42:LEU:HA | 1.79 | 0.42 |
| 8:I:12:ARG:NH1 | 8:I:27:PRO:HD2 | 2.35 | 0.42 |
| 8:I:20:TYR:CE2 | 8:I:75:ARG:HD2 | 2.54 | 0.42 |
| 9:J:95:LYS:HZ1 | 9:J:96:LEU:HD13 | 1.85 | 0.42 |
| 15:P:31:LEU:O | 15:P:35:ARG:HG3 | 2.20 | 0.42 |
| 18:S:56:THR:HB | 18:S:58:LEU:CD1 | 2.50 | 0.42 |
| 19:T:50:ALA:HB1 | 19:T:57:HIS:HB3 | 2.02 | 0.42 |
| 1:A:222:U:H2' | 1:A:223:U:C6 | 2.55 | 0.41 |
| 2:B:69:LEU:O | 2:B:162:ILE:HA | 2.19 | 0.41 |
| 1:A:1240:U:OP1 | 7:H:119:ARG:NH2 | 2.53 | 0.41 |
| 14:O:23:ARG:NH1 | 14:O:30:ALA:HB2 | 2.35 | 0.41 |
| 21:V:2:GLY:O | 21:V:5:ASP:N | 2.47 | 0.41 |
| 1:A:514:C:H2' | 1:A:515:G:H8 | 1.85 | 0.41 |
| 1:A:826:C:H2' | 1:A:827:U:O2 | 2.20 | 0.41 |
| 1:A:992:U:O2 | 1:A:993:G:N2 | 2.53 | 0.41 |
| 2:B:104:ASN:OD1 | 2:B:107:THR:OG1 | 2.30 | 0.41 |
| 8:I:38:ILE:HD12 | 8:I:118:VAL:HG12 | 2.02 | 0.41 |
| 8:I:36:LEU:HD12 | 8:I:59:LEU:HD13 | 2.02 | 0.41 |
| 8:I:59:LEU:O | 8:I:61:VAL:HG23 | 2.21 | 0.41 |
| 20:U:84:LEU:HD23 | 20:U:84:LEU:HA | 1.86 | 0.41 |
| 1:A:1241:G:H2' | 1:A:1242:C:C6 | 2.55 | 0.41 |
| 1:A:414:A:OP2 | 1:A:428:G:N2 | 2.33 | 0.41 |
| 2:B:120:ALA:C | 2:B:122:PHE:H | 2.23 | 0.41 |
| 2:B:208:ILE:HA | 2:B:211:ILE:HD12 | 2.02 | 0.41 |
| 2:B:210:SER:O | 2:B:214:ILE:HG12 | 2.21 | 0.41 |
| 4:D:173:TRP:CD1 | 4:D:174:LEU:HG | 2.55 | 0.41 |
| 8:I:51:VAL:HG21 | 8:I:60:ARG:HG2 | 2.02 | 0.41 |
| 12:M:103:GLY:N | 12:M:107:ALA:O | 2.49 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 17:R:83:ASP:O | 17:R:87:LYS:HG2 | 2.20 | 0.41 |
| 1:A:1367:C:OP2 | 9:J:112:LYS:NZ | 2.51 | 0.41 |
| 1:A:156:G:H2' | 1:A:157:G:H8 | 1.85 | 0.41 |
| 1:A:300:A:H8 | 1:A:300:A:O5' | 2.03 | 0.41 |
| 1:A:973:G:H3' | 1:A:974:A:H5'' | 2.02 | 0.41 |
| 1:A:1298:C:H41 | 7:H:114:ARG:HB3 | 1.85 | 0.41 |
| 8:I:54:ASP:OD1 | 8:I:54:ASP:N | 2.53 | 0.41 |
| 11:L:99:GLN:HG2 | 11:L:105:VAL:HG21 | 2.03 | 0.41 |
| 14:O:4:LYS:O | 14:O:7:ILE:HG12 | 2.20 | 0.41 |
| 16:Q:53:VAL:O | 16:Q:57:ARG:HG2 | 2.21 | 0.41 |
| 1:A:105:G:H2' | 1:A:106:C:C6 | 2.55 | 0.41 |
| 1:A:1119:C:H2' | 1:A:1120:G:C8 | 2.56 | 0.41 |
| 1:A:1130:A:O2' | 9:J:3:GLN:NE2 | 2.41 | 0.41 |
| 1:A:1151:A:H2' | 1:A:1152:A:H8 | 1.85 | 0.41 |
| 1:A:162:A:C5 | 1:A:163:C:H1' | 2.55 | 0.41 |
| 1:A:181:G:O2' | 1:A:182:U:P | 2.79 | 0.41 |
| 1:A:779:C:H2' | 1:A:780:A:O4' | 2.21 | 0.41 |
| 1:A:838:G:C5 | 1:A:842:C:H1' | 2.54 | 0.41 |
| 1:A:859:A:H2' | 1:A:860:A:O4' | 2.20 | 0.41 |
| 14:O:29:ARG:HG2 | 14:O:31:ARG:O | 2.20 | 0.41 |
| 15:P:4:THR:HB | 15:P:6:GLU:CD | 2.41 | 0.41 |
| 19:T:28:LYS:HA | 19:T:47:HIS:HE1 | 1.86 | 0.41 |
| 20:U:89:ARG:HH21 | 20:U:104:LEU:HG | 1.85 | 0.41 |
| 1:A:1227:A:O3' | 13:N:115:LYS:HE3 | 2.20 | 0.41 |
| 1:A:1459:C:H2' | 1:A:1460:A:C8 | 2.55 | 0.41 |
| 1:A:74:C:H42 | 1:A:96:G:H1 | 1.69 | 0.41 |
| 2:B:47:THR:HA | 2:B:202:PRO:HG2 | 2.00 | 0.41 |
| 3:C:122:GLU:HA | 3:C:125:GLU:OE1 | 2.21 | 0.41 |
| 7:H:45:ASP:O | 7:H:48:LYS:HB3 | 2.21 | 0.41 |
| 12:M:11:VAL:HG13 | 17:R:29:HIS:CD2 | 2.55 | 0.41 |
| 13:N:91:ARG:HB2 | 13:N:98:VAL:HG13 | 2.03 | 0.41 |
| 23:X:35:A:N6 | 23:X:36:A:N1 | 2.68 | 0.41 |
| 1:A:1043:C:H2' | 1:A:1044:A:C8 | 2.56 | 0.41 |
| 1:A:1053:G:N7 | 1:A:1200:C:H5'' | 2.36 | 0.41 |
| 1:A:1327:C:H2' | 1:A:1328:C:C6 | 2.56 | 0.41 |
| 1:A:1450:U:O2' | 1:A:1451:A:N7 | 2.53 | 0.41 |
| 1:A:1522:U:H2' | 1:A:1523:G:H8 | 1.86 | 0.41 |
| 1:A:662:G:O2' | 1:A:836:G:OP1 | 2.35 | 0.41 |
| 5:E:110:LEU:HD13 | 5:E:118:ILE:HG12 | 2.01 | 0.41 |
| 9:J:40:LEU:HD11 | 9:J:70:LYS:HG2 | 2.02 | 0.41 |
| 16:Q:20:VAL:HG21 | 16:Q:32:TYR:CD2 | 2.56 | 0.41 |
| 1:A:1120:G:H2' | 1:A:1121:U:C6 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:179:A:H2' | 1:A:180:U:C6 | 2.55 | 0.41 |
| 1:A:661:G:H1 | 1:A:744:C:H42 | 1.68 | 0.41 |
| 4:D:38:TYR:HB2 | 4:D:44:GLY:O | 2.21 | 0.41 |
| 5:E:12:LEU:O | 5:E:13:ILE:HD12 | 2.21 | 0.41 |
| 7:H:70:LYS:HA | 7:H:71:PRO:HD2 | 1.89 | 0.41 |
| 7:H:93:PRO:O | 7:H:96:GLN:HB2 | 2.21 | 0.41 |
| 19:T:36:ARG:HA | 19:T:71:LEU:HB2 | 2.02 | 0.41 |
| 1:A:1314:C:P | 19:T:6:LYS:HD2 | 2.61 | 0.41 |
| 1:A:149:A:H4' | 1:A:1450:U:C4 | 2.55 | 0.41 |
| 1:A:618:C:H5' | 1:A:619:U:H5'' | 2.03 | 0.41 |
| 8:I:44:PHE:HD1 | 8:I:80:ILE:HG12 | 1.86 | 0.41 |
| 17:R:92:ARG:HD3 | 17:R:92:ARG:HA | 1.91 | 0.41 |
| 1:A:1095:U:OP1 | 1:A:1108:G:N2 | 2.54 | 0.41 |
| 3:C:83:ARG:O | 3:C:86:VAL:HG22 | 2.21 | 0.41 |
| 5:E:127:ASN:HA | 5:E:128:PRO:HD3 | 1.89 | 0.41 |
| 5:E:147:ASP:O | 5:E:151:LEU:HG | 2.21 | 0.41 |
| 6:F:30:LEU:HD23 | 6:F:75:LEU:HD11 | 2.02 | 0.41 |
| 11:L:25:TYR:CZ | 11:L:87:THR:HB | 2.55 | 0.41 |
| 15:P:2:PRO:HB2 | 15:P:3:ILE:H | 1.56 | 0.41 |
| 21:V:10:ARG:HA | 21:V:13:ILE:HB | 2.01 | 0.41 |
| 1:A:1035:A:N6 | 1:A:1036:G:N3 | 2.69 | 0.41 |
| 1:A:1143:G:H2' | 1:A:1144:G:C8 | 2.55 | 0.41 |
| 1:A:34:C:H2' | 1:A:35:G:H8 | 1.86 | 0.41 |
| 4:D:63:LYS:HB2 | 4:D:63:LYS:HE3 | 1.77 | 0.41 |
| 7:H:150:ALA:O | 11:L:57:THR:CG2 | 2.69 | 0.41 |
| 8:I:41:ARG:NH2 | 8:I:123:GLU:OE2 | 2.54 | 0.41 |
| 15:P:32:LEU:HA | 15:P:32:LEU:HD23 | 1.76 | 0.41 |
| 1:A:1098:C:H2' | 1:A:1099:G:O4' | 2.20 | 0.40 |
| 1:A:1122:U:H3 | 1:A:1151:A:H2 | 1.66 | 0.40 |
| 1:A:1199:U:H4' | 10:K:54:PHE:CZ | 2.56 | 0.40 |
| 1:A:452:A:HO2' | 1:A:453:A:C4' | 2.33 | 0.40 |
| 1:A:452:A:H2' | 1:A:453:A:C8 | 2.56 | 0.40 |
| 1:A:754:C:H1' | 15:P:69:TYR:CD2 | 2.57 | 0.40 |
| 1:A:977:A:O2' | 1:A:979:C:OP2 | 2.31 | 0.40 |
| 1:A:985:C:H2' | 1:A:986:A:H8 | 1.84 | 0.40 |
| 1:A:922:G:H4' | 5:E:20:GLN:HA | 2.03 | 0.40 |
| 7:H:54:THR:O | 7:H:56:GLN:N | 2.52 | 0.40 |
| 8:I:83:ILE:HB | 8:I:137:VAL:HG13 | 2.03 | 0.40 |
| 12:M:27:LEU:HG | 12:M:62:SER:HB3 | 2.02 | 0.40 |
| 19:T:5:LEU:HA | 19:T:5:LEU:HD12 | 1.93 | 0.40 |
| 23:X:61:C:H2' | 23:X:62:C:C6 | 2.56 | 0.40 |
| 1:A:109:A:C6 | 1:A:326:G:C6 | 3.09 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:10:A:H2' | 1:A:11:G:H8 | 1.86 | 0.40 |
| 1:A:271:C:H2' | 1:A:272:C:C6 | 2.56 | 0.40 |
| 1:A:509:A:O2' | 1:A:510:A:OP1 | 2.35 | 0.40 |
| 1:A:664:G:N2 | 1:A:741:G:H1 | 2.15 | 0.40 |
| 6:F:35:ALA:HA | 6:F:67:MET:HB3 | 2.02 | 0.40 |
| 6:F:79:LEU:HD23 | 6:F:79:LEU:HA | 1.93 | 0.40 |
| 1:A:1367:C:H5' | 10:K:60:ARG:CZ | 2.51 | 0.40 |
| 10:K:31:GLY:HA3 | 10:K:78:ASN:CG | 2.41 | 0.40 |
| 1:A:1325:C:OP2 | 21:V:6:ARG:NH2 | 2.49 | 0.40 |
| 1:A:337:C:H2' | 1:A:338:A:C8 | 2.57 | 0.40 |
| 6:F:33:TYR:CE1 | 6:F:78:GLU:HG2 | 2.56 | 0.40 |
| 10:K:4:ILE:HA | 10:K:100:THR:HG22 | 2.02 | 0.40 |
| 1:A:1300:G:N1 | 1:A:1335:C:O4' | 2.55 | 0.40 |
| 1:A:976:G:N2 | 1:A:1362:C:H2' | 2.36 | 0.40 |
| 1:A:298:A:H2' | 1:A:299:G:O4' | 2.22 | 0.40 |
| 1:A:422:C:O2' | 1:A:423:G:H5'' | 2.22 | 0.40 |
| 1:A:766:A:H2' | 1:A:767:A:O4' | 2.21 | 0.40 |
| 1:A:985:C:H2' | 1:A:986:A:C8 | 2.57 | 0.40 |
| 3:C:71:ALA:HB2 | 3:C:109:PRO:HB3 | 2.04 | 0.40 |
| 4:D:176:LEU:HD12 | 4:D:182:LYS:O | 2.21 | 0.40 |
| 10:K:61:GLU:OE1 | 14:O:58:LYS:HE2 | 2.21 | 0.40 |
| 8:I:91:ARG:CB | 12:M:7:ILE:HG13 | 2.44 | 0.40 |
| 13:N:40:ASN:HA | 13:N:41:PRO:HD3 | 1.89 | 0.40 |
| 13:N:4:ILE:H | 13:N:9:ILE:CG2 | 2.35 | 0.40 |
| 23:X:16:U:H3' | 23:X:17:C:C5' | 2.51 | 0.40 |
| 1:A:1469:G:H2' | 1:A:1470:G:C8 | 2.57 | 0.40 |
| 1:A:148:G:H2' | 1:A:149:A:C8 | 2.55 | 0.40 |
| 1:A:181:G:HO2' | 1:A:182:U:P | 2.45 | 0.40 |
| 1:A:410:G:H4' | 1:A:411:A:OP1 | 2.21 | 0.40 |
| 1:A:486:U:H2' | 1:A:487:A:H8 | 1.87 | 0.40 |
| 3:C:7:PRO:O | 3:C:11:ARG:NH1 | 2.54 | 0.40 |
| 4:D:46:LYS:HD3 | 4:D:46:LYS:HA | 1.78 | 0.40 |
| 5:E:50:GLU:HG3 | 5:E:52:PRO:HD2 | 2.04 | 0.40 |
| 6:F:21:LEU:O | 6:F:25:ILE:HG12 | 2.20 | 0.40 |
| 1:A:376:G:H5'' | 16:Q:5:ARG:HB2 | 2.02 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 2 | B | 235/256 (92%) | 173 (74%) | 45 (19%) | 17 (7%) | 2 | 29 |
| 3 | C | 203/239 (85%) | 163 (80%) | 34 (17%) | 6 (3%) | 7 | 57 |
| 4 | D | 206/209 (99%) | 177 (86%) | 22 (11%) | 7 (3%) | 6 | 54 |
| 5 | E | 149/162 (92%) | 136 (91%) | 8 (5%) | 5 (3%) | 6 | 54 |
| 6 | F | 99/101 (98%) | 93 (94%) | 3 (3%) | 3 (3%) | 7 | 57 |
| 7 | H | 153/156 (98%) | 135 (88%) | 16 (10%) | 2 (1%) | 18 | 75 |
| 8 | I | 136/138 (99%) | 121 (89%) | 14 (10%) | 1 (1%) | 30 | 84 |
| 9 | J | 125/128 (98%) | 103 (82%) | 17 (14%) | 5 (4%) | 5 | 48 |
| 10 | K | 97/105 (92%) | 75 (77%) | 19 (20%) | 3 (3%) | 7 | 57 |
| 11 | L | 117/129 (91%) | 100 (86%) | 14 (12%) | 3 (3%) | 8 | 60 |
| 12 | M | 123/132 (93%) | 98 (80%) | 18 (15%) | 7 (6%) | 3 | 36 |
| 13 | N | 119/126 (94%) | 95 (80%) | 15 (13%) | 9 (8%) | 2 | 26 |
| 14 | O | 58/61 (95%) | 49 (84%) | 5 (9%) | 4 (7%) | 2 | 30 |
| 15 | P | 86/89 (97%) | 80 (93%) | 5 (6%) | 1 (1%) | 19 | 77 |
| 16 | Q | 82/88 (93%) | 73 (89%) | 8 (10%) | 1 (1%) | 19 | 77 |
| 17 | R | 98/105 (93%) | 91 (93%) | 5 (5%) | 2 (2%) | 11 | 66 |
| 18 | S | 68/88 (77%) | 56 (82%) | 9 (13%) | 3 (4%) | 4 | 45 |
| 19 | T | 82/93 (88%) | 55 (67%) | 16 (20%) | 11 (13%) | 0 | 10 |
| 20 | U | 97/106 (92%) | 76 (78%) | 15 (16%) | 6 (6%) | 2 | 34 |
| 21 | V | 23/27 (85%) | 19 (83%) | 3 (13%) | 1 (4%) | 4 | 46 |
| All | All | 2356/2538 (93%) | 1968 (84%) | 291 (12%) | 97 (4%) | 4 | 47 |

All (97) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 236 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 12 | LEU |
| 3 | C | 190 | ARG |
| 4 | D | 28 | SER |
| 6 | F | 16 | GLN |
| 6 | F | 17 | SER |
| 6 | F | 18 | GLN |
| 13 | N | 67 | GLU |
| 13 | N | 106 | ASN |
| 13 | N | 118 | ALA |
| 14 | O | 16 | PHE |
| 19 | T | 12 | ASP |
| 19 | T | 45 | VAL |
| 20 | U | 49 | ALA |
| 2 | B | 15 | VAL |
| 2 | B | 96 | ARG |
| 2 | B | 229 | VAL |
| 2 | B | 230 | VAL |
| 2 | B | 237 | ALA |
| 3 | C | 79 | ARG |
| 4 | D | 51 | PRO |
| 4 | D | 154 | ASN |
| 5 | E | 115 | VAL |
| 8 | I | 129 | VAL |
| 9 | J | 41 | VAL |
| 9 | J | 117 | HIS |
| 11 | L | 101 | SER |
| 12 | M | 47 | LYS |
| 12 | M | 91 | LYS |
| 13 | N | 12 | ASN |
| 14 | O | 12 | ARG |
| 17 | R | 74 | LEU |
| 17 | R | 81 | ARG |
| 19 | T | 3 | ARG |
| 19 | T | 11 | VAL |
| 19 | T | 26 | GLY |
| 19 | T | 31 | ILE |
| 19 | T | 41 | VAL |
| 2 | B | 26 | PRO |
| 2 | B | 87 | ARG |
| 2 | B | 204 | ASN |
| 2 | B | 207 | ALA |
| 3 | C | 4 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 51 | GLY |
| 4 | D | 155 | LEU |
| 5 | E | 77 | PRO |
| 10 | K | 30 | SER |
| 11 | L | 103 | LEU |
| 11 | L | 125 | PHE |
| 12 | M | 28 | LYS |
| 13 | N | 120 | LYS |
| 14 | O | 14 | PRO |
| 15 | P | 23 | GLY |
| 19 | T | 9 | VAL |
| 19 | T | 14 | HIS |
| 19 | T | 28 | LYS |
| 20 | U | 96 | GLY |
| 2 | B | 22 | LYS |
| 2 | B | 126 | GLU |
| 2 | B | 209 | ARG |
| 4 | D | 171 | GLY |
| 9 | J | 56 | LEU |
| 12 | M | 27 | LEU |
| 12 | M | 48 | PRO |
| 13 | N | 6 | GLY |
| 13 | N | 13 | LYS |
| 18 | S | 20 | ALA |
| 18 | S | 54 | ARG |
| 20 | U | 71 | THR |
| 21 | V | 9 | ARG |
| 2 | B | 234 | PRO |
| 4 | D | 30 | LYS |
| 4 | D | 42 | GLN |
| 5 | E | 70 | PRO |
| 5 | E | 96 | PRO |
| 7 | H | 7 | ALA |
| 9 | J | 121 | ARG |
| 12 | M | 19 | ARG |
| 12 | M | 121 | GLY |
| 13 | N | 4 | ILE |
| 18 | S | 26 | LEU |
| 20 | U | 73 | HIS |
| 20 | U | 97 | ALA |
| 2 | B | 155 | LEU |
| 10 | K | 82 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | N | 10 | PRO |
| 14 | O | 15 | LYS |
| 20 | U | 98 | PRO |
| 2 | B | 5 | ILE |
| 16 | Q | 46 | PRO |
| 3 | C | 81 | GLY |
| 5 | E | 74 | GLY |
| 19 | T | 46 | GLY |
| 7 | H | 50 | ILE |
| 9 | J | 89 | ASN |
| 10 | K | 37 | PRO |
| 2 | B | 227 | GLY |

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 | 205/220 (93%) | 171 (83%) | 34 (17%) | 3 | 21 |
| 3 | C | 159/188 (85%) | 145 (91%) | 14 (9%) | 14 | 58 |
| 4 | D | 180/181 (99%) | 157 (87%) | 23 (13%) | 6 | 35 |
| 5 | E | 116/123 (94%) | 104 (90%) | 12 (10%) | 10 | 48 |
| 6 | F | 90/90 (100%) | 78 (87%) | 12 (13%) | 6 | 33 |
| 7 | H | 126/127 (99%) | 114 (90%) | 12 (10%) | 12 | 52 |
| 8 | I | 119/119 (100%) | 109 (92%) | 10 (8%) | 16 | 61 |
| 9 | J | 98/99 (99%) | 81 (83%) | 17 (17%) | 3 | 19 |
| 10 | K | 89/92 (97%) | 77 (86%) | 12 (14%) | 6 | 32 |
| 11 | L | 90/99 (91%) | 81 (90%) | 9 (10%) | 11 | 50 |
| 12 | M | 104/109 (95%) | 87 (84%) | 17 (16%) | 3 | 22 |
| 13 | N | 97/101 (96%) | 73 (75%) | 24 (25%) | 1 | 7 |
| 14 | O | 49/50 (98%) | 40 (82%) | 9 (18%) | 2 | 15 |
| 15 | P | 79/80 (99%) | 72 (91%) | 7 (9%) | 14 | 58 |
| 16 | Q | 72/74 (97%) | 63 (88%) | 9 (12%) | 7 | 36 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|-----|
| 17 | R | 95/97 (98%) | 87 (92%) | 8 (8%) | 16 | 61 |
| 18 | S | 61/77 (79%) | 50 (82%) | 11 (18%) | 2 | 16 |
| 19 | T | 73/80 (91%) | 59 (81%) | 14 (19%) | 2 | 13 |
| 20 | U | 76/82 (93%) | 67 (88%) | 9 (12%) | 8 | 39 |
| 21 | V | 20/22 (91%) | 20 (100%) | 0 | 100 | 100 |
| All | All | 1998/2110 (95%) | 1735 (87%) | 263 (13%) | 6 | 33 |

All (263) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 5 | ILE |
| 2 | B | 6 | THR |
| 2 | B | 7 | VAL |
| 2 | B | 8 | LYS |
| 2 | B | 15 | VAL |
| 2 | B | 23 | ARG |
| 2 | B | 24 | TRP |
| 2 | B | 32 | ILE |
| 2 | B | 33 | TYR |
| 2 | B | 36 | ARG |
| 2 | B | 53 | ARG |
| 2 | B | 60 | ASP |
| 2 | B | 67 | THR |
| 2 | B | 82 | ARG |
| 2 | B | 87 | ARG |
| 2 | B | 92 | TYR |
| 2 | B | 94 | ASN |
| 2 | B | 101 | MET |
| 2 | B | 109 | SER |
| 2 | B | 119 | GLU |
| 2 | B | 121 | LEU |
| 2 | B | 150 | SER |
| 2 | B | 155 | LEU |
| 2 | B | 158 | LEU |
| 2 | B | 163 | PHE |
| 2 | B | 165 | VAL |
| 2 | B | 168 | THR |
| 2 | B | 172 | ILE |
| 2 | B | 175 | ARG |
| 2 | B | 187 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 196 | LEU |
| 2 | B | 204 | ASN |
| 2 | B | 215 | LEU |
| 2 | B | 217 | ARG |
| 3 | C | 3 | ASN |
| 3 | C | 5 | ILE |
| 3 | C | 12 | LEU |
| 3 | C | 16 | ARG |
| 3 | C | 21 | ARG |
| 3 | C | 45 | LYS |
| 3 | C | 52 | LEU |
| 3 | C | 76 | VAL |
| 3 | C | 94 | LEU |
| 3 | C | 127 | ARG |
| 3 | C | 131 | ARG |
| 3 | C | 154 | SER |
| 3 | C | 165 | THR |
| 3 | C | 206 | GLU |
| 4 | D | 3 | ARG |
| 4 | D | 14 | ARG |
| 4 | D | 22 | LYS |
| 4 | D | 26 | CYS |
| 4 | D | 30 | LYS |
| 4 | D | 33 | MET |
| 4 | D | 50 | ARG |
| 4 | D | 58 | LEU |
| 4 | D | 73 | ARG |
| 4 | D | 76 | ARG |
| 4 | D | 86 | LYS |
| 4 | D | 94 | LEU |
| 4 | D | 96 | LEU |
| 4 | D | 122 | ARG |
| 4 | D | 127 | THR |
| 4 | D | 131 | ARG |
| 4 | D | 135 | LEU |
| 4 | D | 154 | ASN |
| 4 | D | 175 | SER |
| 4 | D | 187 | ARG |
| 4 | D | 190 | ASP |
| 4 | D | 191 | ARG |
| 4 | D | 192 | GLU |
| 5 | E | 10 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 12 | LEU |
| 5 | E | 31 | LEU |
| 5 | E | 34 | VAL |
| 5 | E | 41 | VAL |
| 5 | E | 51 | VAL |
| 5 | E | 68 | GLU |
| 5 | E | 79 | GLU |
| 5 | E | 81 | GLU |
| 5 | E | 98 | THR |
| 5 | E | 101 | ILE |
| 5 | E | 153 | LYS |
| 6 | F | 16 | GLN |
| 6 | F | 21 | LEU |
| 6 | F | 23 | LYS |
| 6 | F | 43 | LEU |
| 6 | F | 45 | LEU |
| 6 | F | 47 | ARG |
| 6 | F | 55 | ASP |
| 6 | F | 69 | GLU |
| 6 | F | 70 | ASP |
| 6 | F | 72 | VAL |
| 6 | F | 75 | LEU |
| 6 | F | 98 | LEU |
| 7 | H | 8 | GLU |
| 7 | H | 54 | THR |
| 7 | H | 80 | VAL |
| 7 | H | 92 | SER |
| 7 | H | 94 | ARG |
| 7 | H | 104 | LEU |
| 7 | H | 113 | GLU |
| 7 | H | 114 | ARG |
| 7 | H | 135 | VAL |
| 7 | H | 136 | LYS |
| 7 | H | 137 | LYS |
| 7 | H | 155 | ARG |
| 8 | I | 1 | MET |
| 8 | I | 24 | THR |
| 8 | I | 25 | ASP |
| 8 | I | 26 | VAL |
| 8 | I | 41 | ARG |
| 8 | I | 99 | GLU |
| 8 | I | 109 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | I | 112 | LEU |
| 8 | I | 125 | ARG |
| 8 | I | 129 | VAL |
| 9 | J | 9 | ARG |
| 9 | J | 10 | ARG |
| 9 | J | 11 | LYS |
| 9 | J | 23 | ASN |
| 9 | J | 47 | LEU |
| 9 | J | 56 | LEU |
| 9 | J | 64 | THR |
| 9 | J | 65 | VAL |
| 9 | J | 75 | ASP |
| 9 | J | 95 | LYS |
| 9 | J | 104 | ARG |
| 9 | J | 105 | ASP |
| 9 | J | 113 | LYS |
| 9 | J | 114 | TYR |
| 9 | J | 121 | ARG |
| 9 | J | 125 | TYR |
| 9 | J | 128 | ARG |
| 10 | K | 22 | LYS |
| 10 | K | 47 | PHE |
| 10 | K | 54 | PHE |
| 10 | K | 57 | LYS |
| 10 | K | 58 | ASP |
| 10 | K | 62 | HIS |
| 10 | K | 73 | ASP |
| 10 | K | 74 | ILE |
| 10 | K | 80 | LYS |
| 10 | K | 84 | GLN |
| 10 | K | 92 | THR |
| 10 | K | 96 | ILE |
| 11 | L | 26 | ASN |
| 11 | L | 29 | ILE |
| 11 | L | 32 | ILE |
| 11 | L | 34 | ASP |
| 11 | L | 63 | LEU |
| 11 | L | 92 | GLU |
| 11 | L | 103 | LEU |
| 11 | L | 109 | VAL |
| 11 | L | 127 | LYS |
| 12 | M | 17 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | M | 18 | VAL |
| 12 | M | 20 | LYS |
| 12 | M | 27 | LEU |
| 12 | M | 33 | ARG |
| 12 | M | 38 | THR |
| 12 | M | 42 | THR |
| 12 | M | 50 | SER |
| 12 | M | 54 | LYS |
| 12 | M | 59 | ARG |
| 12 | M | 60 | LEU |
| 12 | M | 73 | GLU |
| 12 | M | 83 | VAL |
| 12 | M | 85 | ILE |
| 12 | M | 89 | ARG |
| 12 | M | 102 | ARG |
| 12 | M | 113 | ARG |
| 13 | N | 8 | GLU |
| 13 | N | 11 | ARG |
| 13 | N | 13 | LYS |
| 13 | N | 17 | VAL |
| 13 | N | 19 | LEU |
| 13 | N | 45 | VAL |
| 13 | N | 47 | ASP |
| 13 | N | 48 | LEU |
| 13 | N | 56 | LEU |
| 13 | N | 57 | ARG |
| 13 | N | 64 | TRP |
| 13 | N | 66 | LEU |
| 13 | N | 70 | LEU |
| 13 | N | 77 | ASN |
| 13 | N | 84 | ILE |
| 13 | N | 88 | ARG |
| 13 | N | 90 | LEU |
| 13 | N | 98 | VAL |
| 13 | N | 108 | ARG |
| 13 | N | 111 | LYS |
| 13 | N | 114 | ARG |
| 13 | N | 115 | LYS |
| 13 | N | 117 | VAL |
| 13 | N | 122 | LYS |
| 14 | O | 6 | LEU |
| 14 | O | 12 | ARG |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | O | 13 | THR |
| 14 | O | 18 | VAL |
| 14 | O | 33 | VAL |
| 14 | O | 43 | CYS |
| 14 | O | 44 | LEU |
| 14 | O | 46 | GLU |
| 14 | O | 57 | ARG |
| 15 | P | 3 | ILE |
| 15 | P | 4 | THR |
| 15 | P | 26 | GLU |
| 15 | P | 31 | LEU |
| 15 | P | 39 | LEU |
| 15 | P | 64 | ARG |
| 15 | P | 84 | LYS |
| 16 | Q | 2 | VAL |
| 16 | Q | 20 | VAL |
| 16 | Q | 26 | ARG |
| 16 | Q | 28 | ARG |
| 16 | Q | 33 | ILE |
| 16 | Q | 53 | VAL |
| 16 | Q | 67 | THR |
| 16 | Q | 69 | THR |
| 16 | Q | 71 | ARG |
| 17 | R | 37 | LYS |
| 17 | R | 38 | ARG |
| 17 | R | 52 | LYS |
| 17 | R | 59 | ILE |
| 17 | R | 62 | SER |
| 17 | R | 68 | ARG |
| 17 | R | 74 | LEU |
| 17 | R | 101 | ARG |
| 18 | S | 26 | LEU |
| 18 | S | 29 | PHE |
| 18 | S | 31 | LEU |
| 18 | S | 32 | ARG |
| 18 | S | 36 | ASN |
| 18 | S | 46 | GLU |
| 18 | S | 54 | ARG |
| 18 | S | 76 | LEU |
| 18 | S | 82 | THR |
| 18 | S | 83 | GLU |
| 18 | S | 86 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | T | 5 | LEU |
| 19 | T | 10 | PHE |
| 19 | T | 12 | ASP |
| 19 | T | 21 | GLU |
| 19 | T | 28 | LYS |
| 19 | T | 29 | ARG |
| 19 | T | 30 | LEU |
| 19 | T | 37 | ARG |
| 19 | T | 43 | GLU |
| 19 | T | 44 | MET |
| 19 | T | 63 | THR |
| 19 | T | 67 | VAL |
| 19 | T | 77 | THR |
| 19 | T | 83 | HIS |
| 20 | U | 17 | ARG |
| 20 | U | 24 | LEU |
| 20 | U | 45 | GLN |
| 20 | U | 72 | LEU |
| 20 | U | 73 | HIS |
| 20 | U | 75 | ASN |
| 20 | U | 80 | ARG |
| 20 | U | 84 | LEU |
| 20 | U | 93 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 19 | HIS |
| 2 | B | 204 | ASN |
| 2 | B | 212 | GLN |
| 10 | K | 13 | HIS |
| 10 | K | 78 | ASN |
| 13 | N | 77 | ASN |
| 13 | N | 92 | HIS |
| 19 | T | 47 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 1499/1522 (98%) | 267 (17%) | 43 (2%) |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 22 | W | 76/77 (98%) | 19 (25%) | 1 (1%) |
| 23 | X | 75/76 (98%) | 16 (21%) | 0 |
| 23 | Z | 15/76 (19%) | 3 (20%) | 0 |
| 24 | Y | 9/24 (37%) | 0 | 0 |
| All | All | 1674/1775 (94%) | 305 (18%) | 44 (2%) |

All (305) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 6 | G |
| 1 | A | 7 | G |
| 1 | A | 22 | G |
| 1 | A | 32 | A |
| 1 | A | 39 | G |
| 1 | A | 47 | C |
| 1 | A | 48 | C |
| 1 | A | 51 | A |
| 1 | A | 64 | G |
| 1 | A | 65 | U |
| 1 | A | 66 | G |
| 1 | A | 76 | G |
| 1 | A | 79 | G |
| 1 | A | 80 | G |
| 1 | A | 90 | C |
| 1 | A | 91 | C |
| 1 | A | 95 | G |
| 1 | A | 101 | A |
| 1 | A | 116 | A |
| 1 | A | 120 | A |
| 1 | A | 121 | C |
| 1 | A | 129(A) | G |
| 1 | A | 144 | G |
| 1 | A | 146 | G |
| 1 | A | 147 | G |
| 1 | A | 163 | C |
| 1 | A | 169 | C |
| 1 | A | 171 | A |
| 1 | A | 173 | U |
| 1 | A | 174 | C |
| 1 | A | 182 | U |
| 1 | A | 190 | G |
| 1 | A | 191(A) | G |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 195 | A |
| 1 | A | 197 | A |
| 1 | A | 209 | U |
| 1 | A | 210 | U |
| 1 | A | 216 | G |
| 1 | A | 244 | U |
| 1 | A | 245 | C |
| 1 | A | 247 | G |
| 1 | A | 251 | G |
| 1 | A | 267 | C |
| 1 | A | 270 | A |
| 1 | A | 281 | G |
| 1 | A | 289 | G |
| 1 | A | 321 | A |
| 1 | A | 328 | C |
| 1 | A | 329 | A |
| 1 | A | 332 | G |
| 1 | A | 344 | A |
| 1 | A | 346 | G |
| 1 | A | 347 | G |
| 1 | A | 351 | G |
| 1 | A | 352 | C |
| 1 | A | 353 | A |
| 1 | A | 354 | G |
| 1 | A | 356 | A |
| 1 | A | 367 | U |
| 1 | A | 372 | C |
| 1 | A | 373 | A |
| 1 | A | 390 | C |
| 1 | A | 397 | A |
| 1 | A | 398 | C |
| 1 | A | 406 | G |
| 1 | A | 411 | A |
| 1 | A | 412 | A |
| 1 | A | 413 | G |
| 1 | A | 414 | A |
| 1 | A | 421 | U |
| 1 | A | 422 | C |
| 1 | A | 423 | G |
| 1 | A | 424 | G |
| 1 | A | 429 | U |
| 1 | A | 430 | A |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 442 | C |
| 1 | A | 452 | A |
| 1 | A | 465 | A |
| 1 | A | 466 | C |
| 1 | A | 482 | A |
| 1 | A | 485 | G |
| 1 | A | 486 | U |
| 1 | A | 496 | A |
| 1 | A | 497 | U |
| 1 | A | 505 | G |
| 1 | A | 509 | A |
| 1 | A | 510 | A |
| 1 | A | 511 | C |
| 1 | A | 518 | C |
| 1 | A | 527 | G |
| 1 | A | 531 | U |
| 1 | A | 532 | A |
| 1 | A | 533 | A |
| 1 | A | 534 | U |
| 1 | A | 545 | C |
| 1 | A | 547 | A |
| 1 | A | 559 | A |
| 1 | A | 561 | U |
| 1 | A | 562 | C |
| 1 | A | 564 | C |
| 1 | A | 566 | G |
| 1 | A | 568 | G |
| 1 | A | 572 | A |
| 1 | A | 573 | A |
| 1 | A | 576 | G |
| 1 | A | 577 | G |
| 1 | A | 596 | C |
| 1 | A | 618 | C |
| 1 | A | 630 | G |
| 1 | A | 631 | G |
| 1 | A | 632 | A |
| 1 | A | 653 | A |
| 1 | A | 665 | A |
| 1 | A | 666 | G |
| 1 | A | 688 | G |
| 1 | A | 701 | C |
| 1 | A | 702 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 703 | G |
| 1 | A | 704 | A |
| 1 | A | 723 | U |
| 1 | A | 731 | G |
| 1 | A | 748 | C |
| 1 | A | 754 | C |
| 1 | A | 755 | G |
| 1 | A | 777 | A |
| 1 | A | 786 | G |
| 1 | A | 792 | A |
| 1 | A | 793 | U |
| 1 | A | 794 | A |
| 1 | A | 813 | U |
| 1 | A | 817 | C |
| 1 | A | 819 | A |
| 1 | A | 821 | G |
| 1 | A | 828 | A |
| 1 | A | 841 | U |
| 1 | A | 843 | U |
| 1 | A | 848 | C |
| 1 | A | 859 | A |
| 1 | A | 871 | U |
| 1 | A | 872 | A |
| 1 | A | 902 | G |
| 1 | A | 914 | A |
| 1 | A | 927 | G |
| 1 | A | 934 | C |
| 1 | A | 935 | A |
| 1 | A | 960 | U |
| 1 | A | 961 | U |
| 1 | A | 968 | A |
| 1 | A | 969 | A |
| 1 | A | 971 | G |
| 1 | A | 974 | A |
| 1 | A | 975 | A |
| 1 | A | 976 | G |
| 1 | A | 977 | A |
| 1 | A | 980 | C |
| 1 | A | 983 | A |
| 1 | A | 991 | U |
| 1 | A | 992 | U |
| 1 | A | 993 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | A | 994 | A |
| 1 | A | 1001 | G |
| 1 | A | 1004 | A |
| 1 | A | 1006 | C |
| 1 | A | 1009 | G |
| 1 | A | 1021 | G |
| 1 | A | 1024 | G |
| 1 | A | 1025 | U |
| 1 | A | 1028 | C |
| 1 | A | 1029 | G |
| 1 | A | 1032(A) | G |
| 1 | A | 1036 | G |
| 1 | A | 1040 | U |
| 1 | A | 1046 | A |
| 1 | A | 1053 | G |
| 1 | A | 1054 | C |
| 1 | A | 1055 | A |
| 1 | A | 1064 | G |
| 1 | A | 1065 | U |
| 1 | A | 1066 | C |
| 1 | A | 1081 | 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 | 1130 | A |
| 1 | A | 1131 | G |
| 1 | A | 1136 | U |
| 1 | A | 1137 | C |
| 1 | A | 1138 | G |
| 1 | A | 1139 | G |
| 1 | A | 1145 | C |
| 1 | A | 1146 | A |
| 1 | A | 1157 | A |
| 1 | A | 1158 | C |
| 1 | A | 1159 | U |
| 1 | A | 1160 | G |
| 1 | A | 1163 | C |
| 1 | A | 1178 | G |
| 1 | A | 1181 | G |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1182 | G |
| 1 | A | 1183 | A |
| 1 | A | 1187 | G |
| 1 | A | 1196 | U |
| 1 | A | 1197 | G |
| 1 | A | 1200 | C |
| 1 | A | 1201 | A |
| 1 | A | 1202 | G |
| 1 | A | 1212 | U |
| 1 | A | 1213 | A |
| 1 | A | 1215 | G |
| 1 | A | 1226 | C |
| 1 | A | 1238 | A |
| 1 | A | 1241 | G |
| 1 | A | 1256 | A |
| 1 | A | 1257 | U |
| 1 | A | 1258 | G |
| 1 | A | 1260 | C |
| 1 | A | 1270 | C |
| 1 | A | 1280 | A |
| 1 | A | 1281 | U |
| 1 | A | 1282 | C |
| 1 | A | 1286 | A |
| 1 | A | 1287 | A |
| 1 | A | 1297 | C |
| 1 | A | 1298 | C |
| 1 | A | 1299 | A |
| 1 | A | 1300 | G |
| 1 | A | 1301 | U |
| 1 | A | 1302 | U |
| 1 | A | 1305 | G |
| 1 | A | 1319 | A |
| 1 | A | 1320 | C |
| 1 | A | 1321 | C |
| 1 | A | 1322 | C |
| 1 | A | 1323 | G |
| 1 | A | 1331 | G |
| 1 | A | 1335 | C |
| 1 | A | 1336 | C |
| 1 | A | 1337 | G |
| 1 | A | 1346 | A |
| 1 | A | 1347 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | A | 1348 | U |
| 1 | A | 1353 | G |
| 1 | A | 1362(A) | C |
| 1 | A | 1397 | C |
| 1 | A | 1398 | A |
| 1 | A | 1406 | U |
| 1 | A | 1419 | G |
| 1 | A | 1442 | 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 | 1492 | A |
| 1 | A | 1499 | A |
| 1 | A | 1504 | G |
| 1 | A | 1505 | G |
| 1 | A | 1506 | U |
| 1 | A | 1517 | G |
| 1 | A | 1519 | A |
| 1 | A | 1520 | G |
| 1 | A | 1529 | G |
| 1 | A | 1530 | G |
| 22 | W | 3 | G |
| 22 | W | 4 | G |
| 22 | W | 7 | U |
| 22 | W | 15 | C |
| 22 | W | 17 | U |
| 22 | W | 18 | G |
| 22 | W | 19 | G |
| 22 | W | 21 | A |
| 22 | W | 22 | G |
| 22 | W | 31 | G |
| 22 | W | 47 | U |
| 22 | W | 48 | C |
| 22 | W | 52 | G |
| 22 | W | 53 | G |
| 22 | W | 54 | U |
| 22 | W | 64 | G |
| 22 | W | 67 | C |
| 22 | W | 75 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | W | 76 | A |
| 23 | X | 6 | G |
| 23 | X | 14 | A |
| 23 | X | 16 | U |
| 23 | X | 17 | C |
| 23 | X | 18 | G |
| 23 | X | 19 | G |
| 23 | X | 21 | A |
| 23 | X | 37 | A |
| 23 | X | 41 | C |
| 23 | X | 43 | C |
| 23 | X | 45 | U |
| 23 | X | 47 | U |
| 23 | X | 48 | C |
| 23 | X | 57 | G |
| 23 | X | 59 | U |
| 23 | X | 71 | G |
| 23 | Z | 29 | G |
| 23 | Z | 36 | A |
| 23 | Z | 37 | A |

All (44) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 5 | U |
| 1 | A | 31 | G |
| 1 | A | 64 | G |
| 1 | A | 115 | G |
| 1 | A | 119 | A |
| 1 | A | 181 | G |
| 1 | A | 243 | A |
| 1 | A | 244 | U |
| 1 | A | 250 | A |
| 1 | A | 266 | G |
| 1 | A | 328 | C |
| 1 | A | 410 | G |
| 1 | A | 412 | A |
| 1 | A | 429 | U |
| 1 | A | 481 | G |
| 1 | A | 484 | G |
| 1 | A | 485 | G |
| 1 | A | 509 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 533 | A |
| 1 | A | 687 | A |
| 1 | A | 701 | C |
| 1 | A | 703 | G |
| 1 | A | 753 | A |
| 1 | A | 792 | A |
| 1 | A | 812 | C |
| 1 | A | 913 | A |
| 1 | A | 934 | C |
| 1 | A | 960 | U |
| 1 | A | 992 | U |
| 1 | A | 1027 | C |
| 1 | A | 1064 | G |
| 1 | A | 1065 | U |
| 1 | A | 1200 | C |
| 1 | A | 1201 | A |
| 1 | A | 1285 | A |
| 1 | A | 1297 | C |
| 1 | A | 1336 | C |
| 1 | A | 1346 | A |
| 1 | A | 1347 | G |
| 1 | A | 1446 | A |
| 1 | A | 1498 | U |
| 1 | A | 1503 | A |
| 1 | A | 1528 | U |
| 22 | W | 53 | G |

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 75 ligands modelled in this entry, 74 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 |
| 26 | PAR | A | 1667 | - | 45,45,45 | 1.40 | 7 (15%) | 67,67,67 | 1.19 | 5 (7%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 26 | PAR | A | 1667 | - | - | 0/18/94/94 | 0/4/4/4 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 26 | A | 1667 | PAR | C52-C42 | 3.24 | 1.58 | 1.52 |
| 26 | A | 1667 | PAR | O54-C14 | 2.93 | 1.49 | 1.41 |
| 26 | A | 1667 | PAR | C64-C54 | 2.87 | 1.59 | 1.51 |
| 26 | A | 1667 | PAR | C11-C21 | 2.64 | 1.57 | 1.52 |
| 26 | A | 1667 | PAR | O51-C11 | 2.55 | 1.48 | 1.41 |
| 26 | A | 1667 | PAR | C31-C21 | 2.15 | 1.56 | 1.53 |
| 26 | A | 1667 | PAR | C14-C24 | 2.11 | 1.56 | 1.52 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 26 | A | 1667 | PAR | O52-C13-C23 | 4.40 | 115.35 | 107.50 |
| 26 | A | 1667 | PAR | C14-O54-C54 | 4.08 | 121.62 | 113.73 |
| 26 | A | 1667 | PAR | O54-C54-C64 | 3.14 | 111.95 | 105.97 |
| 26 | A | 1667 | PAR | O33-C14-C24 | 3.11 | 114.23 | 108.08 |
| 26 | A | 1667 | PAR | C11-O51-C51 | 2.04 | 117.67 | 113.73 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.