



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:40 PM BST

PDB ID : 4V7F
EMDB ID: : EMD-2528
Title : Arx1 pre-60S particle.
Authors : Leidig, C.; Thoms, M.; Holdermann, I.; Bradatsch, B.; Berninghausen, O.;
Bange, G.; Sinning, I.; Hurt, E.; Beckmann, R.
Deposited on : 2013-12-10
Resolution : 8.70 Å(reported)
Based on PDB ID : 3U5D

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

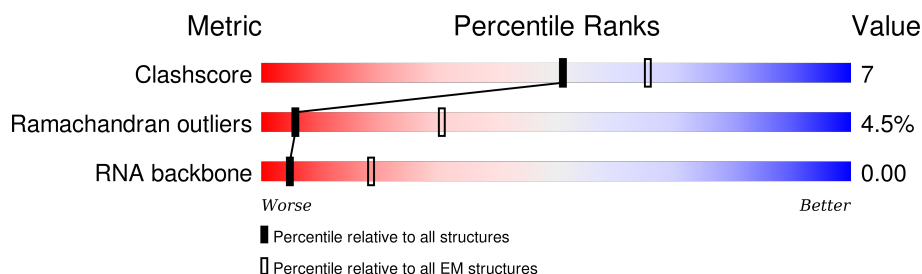
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.70 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.






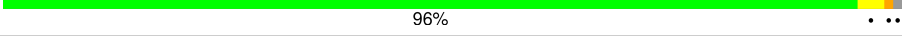

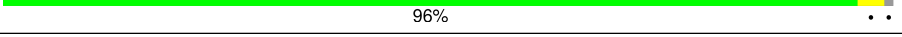


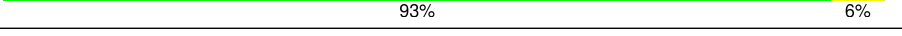

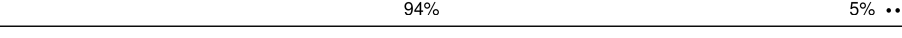
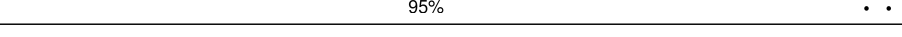
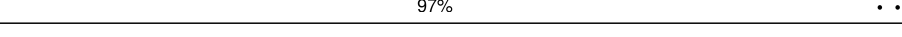
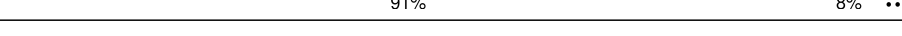
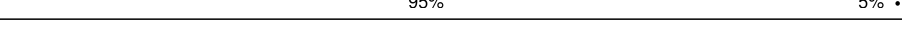

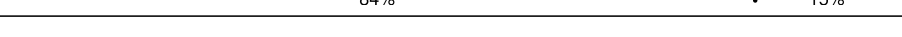
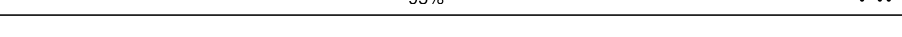
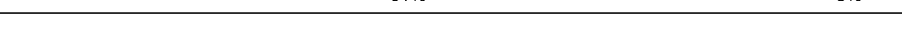






| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| RNA backbone | 3027 | 244 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 1 | 3396 | 87% 12% |
| 2 | 2 | 158 | 97% . |
| 3 | 3 | 121 | 87% 13% |
| 4 | A | 217 | 94% 6% |
| 5 | B | 254 | 96% . . |
| 6 | C | 387 | 95% 5% |
| 7 | D | 362 | 92% 7% . |
| 8 | E | 174 | 78% 18% . . |
| 9 | F | 191 | 94% 6% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 10 | G | 176 |  |
| 11 | H | 256 |  |
| 12 | I | 165 |  |
| 13 | J | 199 |  |
| 14 | K | 199 |  |
| 15 | L | 137 |  |
| 16 | M | 138 |  |
| 17 | N | 149 |  |
| 18 | O | 204 |  |
| 19 | P | 297 |  |
| 20 | Q | 186 |  |
| 21 | R | 189 |  |
| 22 | S | 172 |  |
| 23 | T | 160 |  |
| 24 | U | 184 |  |
| 25 | V | 121 |  |
| 26 | W | 142 |  |
| 27 | X | 127 |  |
| 28 | Y | 136 |  |
| 29 | Z | 120 |  |
| 30 | a | 244 |  |
| 31 | b | 105 |  |
| 32 | c | 113 |  |
| 33 | d | 130 |  |
| 34 | e | 107 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 35 | f | 121 |  89% 7% |
| 36 | g | 100 |  87% 12% |
| 37 | h | 88 |  95% |
| 38 | i | 78 |  97% |
| 39 | j | 51 |  98% |
| 40 | k | 92 |  96% |
| 41 | l | 593 |  63% 36% |
| 42 | m | 245 |  91% 9% |
| 43 | n | 236 |  97% |
| 44 | o | 647 |  53% 46% |
| 45 | p | 199 |  29% 68% |
| 46 | q | 515 |  80% 5% 14% |
| 47 | r | 322 |  93% 7% |
| 47 | s | 322 |  93% 7% |

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 47221 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|---------|-------|
| 1 | 1 | 3394 | Total | C | O | P | 0 | 0 |
| | | | 20363 | 10182 | 6788 | 3393 | | |

- Molecule 2 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 2 | 2 | 158 | Total | C | O | P | 0 | 0 |
| | | | 948 | 474 | 316 | 158 | | |

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 3 | 3 | 121 | Total | C | O | P | 0 | 0 |
| | | | 725 | 363 | 242 | 120 | | |

- Molecule 4 is a protein called 60S ribosomal protein L1.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 4 | A | 217 | Total | C | N | 0 | 0 |
| | | | 651 | 434 | 217 | | |

- Molecule 5 is a protein called 60S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 5 | B | 252 | Total | C | N | 0 | 0 |
| | | | 756 | 504 | 252 | | |

- Molecule 6 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 6 | C | 386 | Total | C | N | 0 | 0 |
| | | | 1158 | 772 | 386 | | |

- Molecule 7 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 7 | D | 361 | Total | C | N | 0 | 0 |
| | | | 1083 | 722 | 361 | | |

- Molecule 8 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 8 | E | 169 | Total | C | N | 0 | 0 |
| | | | 507 | 338 | 169 | | |

- Molecule 9 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 9 | F | 191 | Total | C | N | 0 | 0 |
| | | | 573 | 382 | 191 | | |

- Molecule 10 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 10 | G | 175 | Total | C | N | 0 | 0 |
| | | | 525 | 350 | 175 | | |

- Molecule 11 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 11 | H | 233 | Total | C | N | 0 | 0 |
| | | | 699 | 466 | 233 | | |

- Molecule 12 is a protein called 60S ribosomal protein L12.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 12 | I | 127 | Total | C | N | 0 | 0 |
| | | | 381 | 254 | 127 | | |

- Molecule 13 is a protein called 60S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 13 | J | 197 | Total | C | N | 0 | 0 |
| | | | 591 | 394 | 197 | | |

- Molecule 14 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 14 | K | 193 | Total | C | N | 0 | 0 |
| | | | 579 | 386 | 193 | | |

- Molecule 15 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 15 | L | 136 | Total | C | N | 0 | 0 |
| | | | 408 | 272 | 136 | | |

- Molecule 16 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 16 | M | 136 | Total | C | N | 0 | 0 |
| | | | 408 | 272 | 136 | | |

- Molecule 17 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 17 | N | 148 | Total | C | N | 0 | 0 |
| | | | 444 | 296 | 148 | | |

- Molecule 18 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 18 | O | 203 | Total | C | N | 0 | 0 |
| | | | 609 | 406 | 203 | | |

- Molecule 19 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 19 | P | 269 | Total | C | N | 0 | 0 |
| | | | 807 | 538 | 269 | | |

- Molecule 20 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 20 | Q | 185 | Total | C | N | 0 | 0 |
| | | | 555 | 370 | 185 | | |

- Molecule 21 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 21 | R | 188 | Total | C | N | 0 | 0 |
| | | | 564 | 376 | 188 | | |

- Molecule 22 is a protein called 60S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 22 | S | 172 | Total | C | N | 0 | 0 |
| | | | 516 | 344 | 172 | | |

- Molecule 23 is a protein called 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 23 | T | 159 | Total | C | N | 0 | 0 |
| | | | 477 | 318 | 159 | | |

- Molecule 24 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 24 | U | 183 | Total | C | N | 0 | 0 |
| | | | 549 | 366 | 183 | | |

- Molecule 25 is a protein called 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 25 | V | 100 | Total | C | N | 0 | 0 |
| | | | 300 | 200 | 100 | | |

- Molecule 26 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 26 | W | 121 | Total | C | N | 0 | 0 |
| | | | 363 | 242 | 121 | | |

- Molecule 27 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 27 | X | 126 | Total | C | N | 0 | 0 |
| | | | 378 | 252 | 126 | | |

- Molecule 28 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 28 | Y | 135 | Total | C | N | 0 | 0 |
| | | | 405 | 270 | 135 | | |

- Molecule 29 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 29 | Z | 119 | Total | C | N | 0 | 0 |
| | | | 357 | 238 | 119 | | |

- Molecule 30 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 30 | a | 222 | Total | C | N | 0 | 0 |
| | | | 666 | 444 | 222 | | |

- Molecule 31 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|---------|-------|
| 31 | b | 97 | Total | C | N | 0 | 0 |
| | | | 291 | 194 | 97 | | |

- Molecule 32 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 32 | c | 109 | Total | C | N | 0 | 0 |
| | | | 327 | 218 | 109 | | |

- Molecule 33 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 33 | d | 127 | Total | C | N | 0 | 0 |
| | | | 381 | 254 | 127 | | |

- Molecule 34 is a protein called 60S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 34 | e | 106 | Total | C | N | 0 | 0 |
| | | | 318 | 212 | 106 | | |

- Molecule 35 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 35 | f | 112 | Total | C | N | 0 | 0 |
| | | | 336 | 224 | 112 | | |

- Molecule 36 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|---------|-------|
| 36 | g | 99 | Total | C | N | 0 | 0 |
| | | | 297 | 198 | 99 | | |

- Molecule 37 is a protein called 60S ribosomal protein L37.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|---------|-------|
| 37 | h | 87 | Total | C | N | 0 | 0 |
| | | | 261 | 174 | 87 | | |

- Molecule 38 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|---------|-------|
| 38 | i | 77 | Total | C | N | 0 | 0 |
| | | | 231 | 154 | 77 | | |

- Molecule 39 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|---------|-------|
| 39 | j | 50 | Total | C | N | 0 | 0 |
| | | | 150 | 100 | 50 | | |

- Molecule 40 is a protein called 60S ribosomal protein L43.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|---------|-------|
| 40 | k | 91 | Total | C | N | 0 | 0 |
| | | | 273 | 182 | 91 | | |

- Molecule 41 is a protein called metalloprotease ARX1.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 41 | l | 380 | Total | C | N | 0 | 0 |
| | | | 1140 | 760 | 380 | | |

- Molecule 42 is a protein called Eukaryotic translation initiation factor 6.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 42 | m | 224 | Total | C | N | 0 | 0 |
| | | | 672 | 448 | 224 | | |

- Molecule 43 is a protein called mRNA turnover protein 4.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 43 | n | 236 | Total | C | N | 0 | 0 |
| | | | 708 | 472 | 236 | | |

- Molecule 44 is a protein called Nucleolar GTP-binding protein 1.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 44 | o | 347 | Total | C | N | 0 | 0 |
| | | | 1041 | 694 | 347 | | |

- Molecule 45 is a protein called Ribosome biogenesis protein RLP24.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|---------|-------|
| 45 | p | 63 | Total | C | N | 0 | 0 |
| | | | 189 | 126 | 63 | | |

- Molecule 46 is a protein called Ribosome assembly protein 4.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 46 | q | 443 | Total | C | N | 0 | 0 |
| | | | 1329 | 886 | 443 | | |

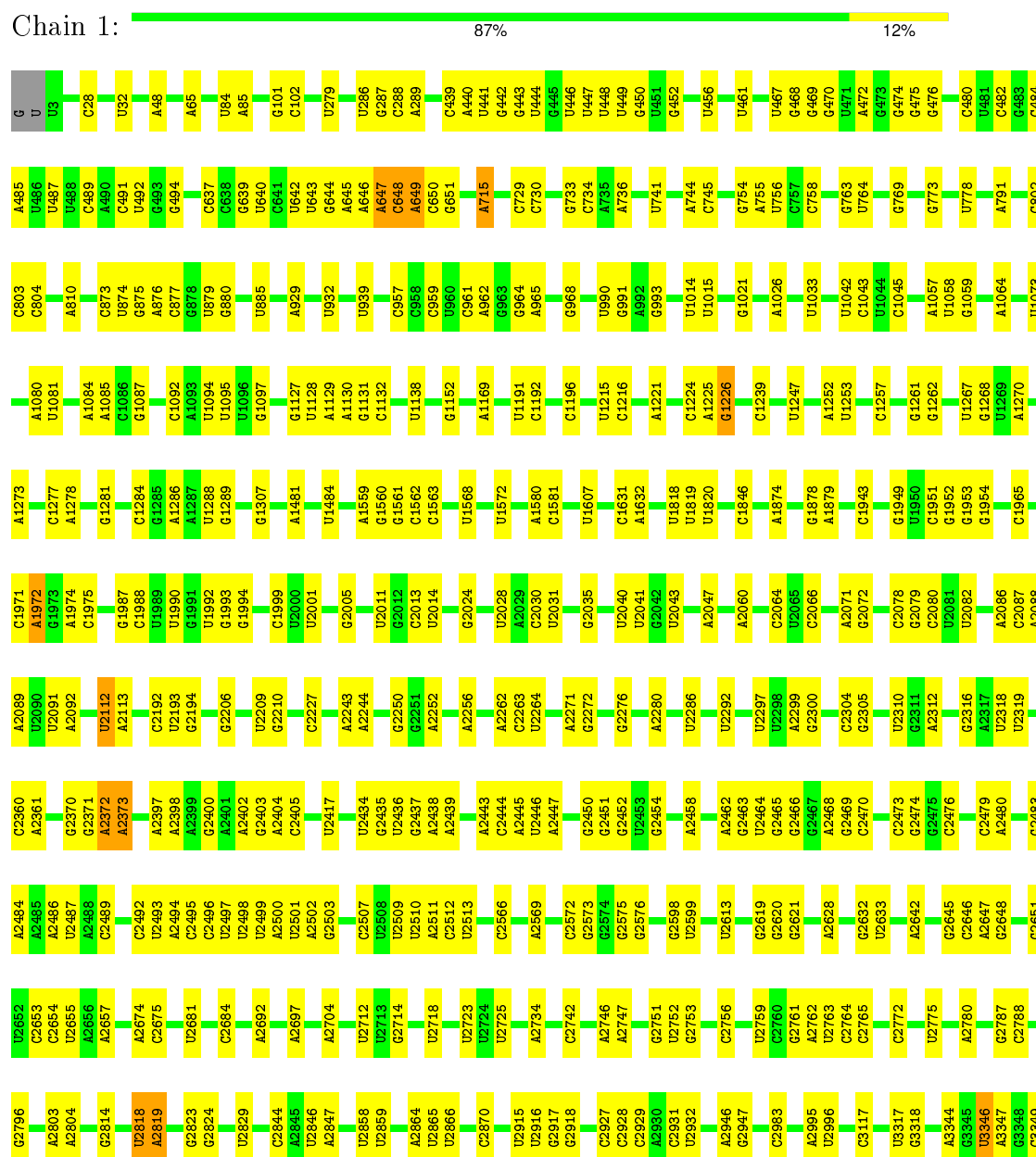
- Molecule 47 is a protein called Ribosome biogenesis protein RLP7.

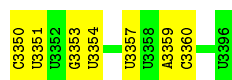
| Mol | Chain | Residues | Atoms | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|-------|
| 47 | r | 322 | Total | C | N | 0 | 0 |
| | | | 966 | 644 | 322 | | |
| 47 | s | 322 | Total | C | N | 0 | 0 |
| | | | 966 | 644 | 322 | | |

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

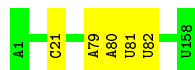
• Molecule 1: 25S ribosomal RNA





- Molecule 2: 5.8S ribosomal RNA

Chain 2: 97%



- Molecule 3: 5S ribosomal RNA

Chain 3: 87% 13%



- Molecule 4: 60S ribosomal protein L1

Chain A: 94% 6%



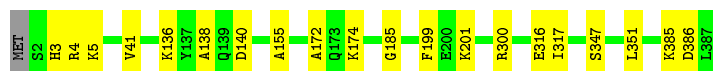
- Molecule 5: 60S ribosomal protein L2

Chain B: 96%



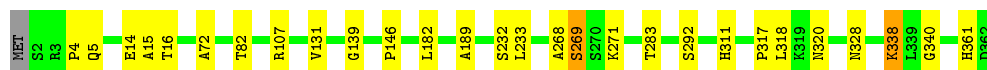
- Molecule 6: 60S ribosomal protein L3

Chain C: 95% 5%



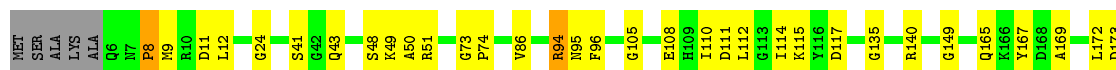
- Molecule 7: 60S ribosomal protein L4

Chain D: 92% 7%



- Molecule 8: 60S ribosomal protein L11

Chain E: 78% 18%



K174

- Molecule 9: 60S ribosomal protein L9

Chain F: 94% 6%

- Molecule 10: 60S ribosomal protein L6

Chain G: 92% 7% ..

- Molecule 11: 60S ribosomal protein L8

Chain H: 82% 9% 9%

- Molecule 12: 60S ribosomal protein L12

Chain I: 68% 7% .. 23%

- Molecule 13: 60S ribosomal protein L16

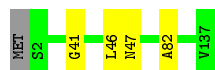
Chain J: 96% ..

- Molecule 14: 60S ribosomal protein L13

Chain K: 89% 7% ..

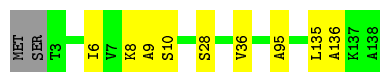
- Molecule 15: 60S ribosomal protein L23

Chain L:  96% ..



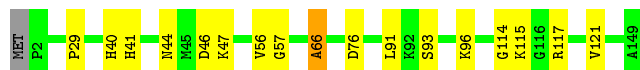
- Molecule 16: 60S ribosomal protein L14

Chain M:  92% 7% .



- Molecule 17: 60S ribosomal protein L28

Chain N:  88% 11% ..




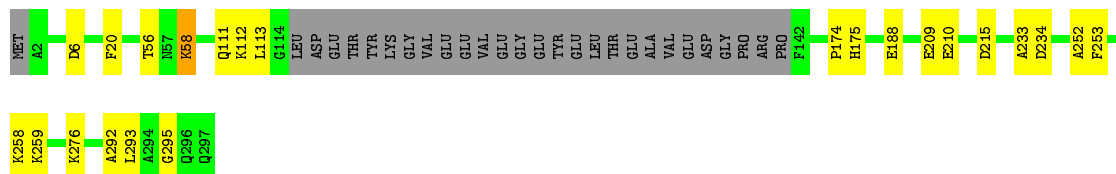
- Molecule 18: 60S ribosomal protein L15

Chain O:  93% 6%



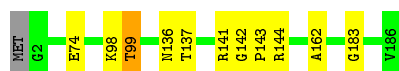
- Molecule 19: 60S ribosomal protein L5

Chain P:  83% 7% 9%



- Molecule 20: 60S ribosomal protein L18

Chain Q:  94% 5% ..




- Molecule 21: 60S ribosomal protein L19

Chain R:  95% ..




- Molecule 22: 60S ribosomal protein L20

Chain S:  97% ..



- Molecule 23: 60S ribosomal protein L21

Chain T:  91% 8% ..



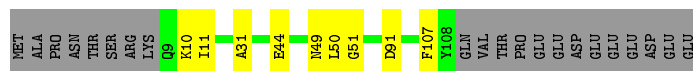
- Molecule 24: 60S ribosomal protein L17

Chain U:  95% 5% .




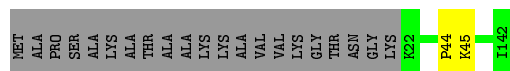
- Molecule 25: 60S ribosomal protein L22

Chain V:  75% 7% 17%



- Molecule 26: 60S ribosomal protein L25

Chain W:  84% . 15%



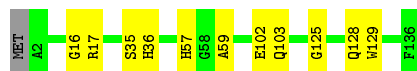
- Molecule 27: 60S ribosomal protein L26

Chain X:  95% ..



- Molecule 28: 60S ribosomal protein L27

Chain Y:  91% 8% .



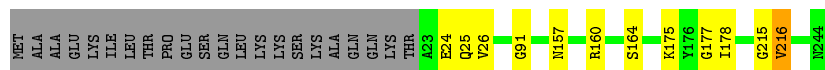
- Molecule 29: 60S ribosomal protein L35

Chain Z:  91% 8% .



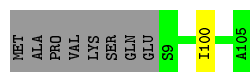
- Molecule 30: 60S ribosomal protein L7

Chain a: 86% 5% 9%



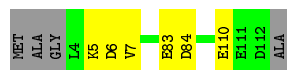
- Molecule 31: 60S ribosomal protein L30

Chain b: 91% 8%



- Molecule 32: 60S ribosomal protein L31

Chain c: 91% 5%



- Molecule 33: 60S ribosomal protein L32

Chain d: 95%



- Molecule 34: 60S ribosomal protein L33

Chain e: 97%



- Molecule 35: 60S ribosomal protein L34

Chain f: 89% 7%

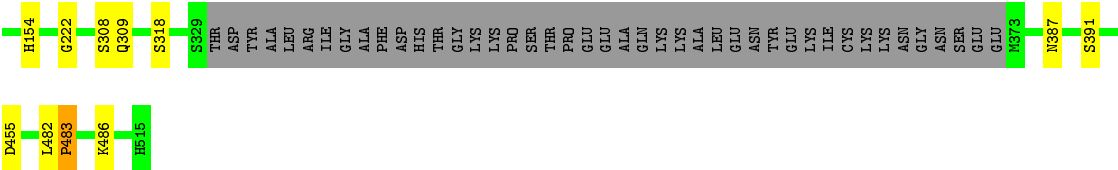


- Molecule 36: 60S ribosomal protein L36

Chain g: 87% 12%



- Chain m: 91% 9%



- Molecule 47: Ribosome biogenesis protein RLP7

Chain r:

93%

7%



- Molecule 47: Ribosome biogenesis protein RLP7

Chain s:

93%

7%



4 Experimental information ⓘ

| Property | Value | Source |
|--------------------------------------|---------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of images | Not provided | Depositor |
| Resolution determination method | Not provided | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | Not provided | Depositor |
| Voltage (kV) | Not provided | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | Not provided | Depositor |
| Minimum defocus (nm) | Not provided | Depositor |
| Maximum defocus (nm) | Not provided | Depositor |
| Magnification | Not provided | Depositor |
| Image detector | Not provided | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|------------------|
| | | RMSZ | $\# Z > 2$ | RMSZ | $\# Z > 2$ |
| 1 | 1 | 1.65 | 185/20361 (0.9%) | 1.81 | 364/20359 (1.8%) |
| 10 | G | 0.69 | 0/524 | 1.13 | 1/523 (0.2%) |
| 11 | H | 0.49 | 0/698 | 0.92 | 1/697 (0.1%) |
| 12 | I | 1.82 | 5/380 (1.3%) | 2.01 | 5/379 (1.3%) |
| 13 | J | 0.48 | 0/590 | 0.76 | 0/589 |
| 14 | K | 0.66 | 0/578 | 1.07 | 2/577 (0.3%) |
| 15 | L | 0.63 | 0/407 | 0.98 | 0/406 |
| 16 | M | 0.66 | 0/407 | 0.97 | 0/406 |
| 17 | N | 0.77 | 0/443 | 1.25 | 3/442 (0.7%) |
| 18 | O | 0.68 | 0/608 | 1.03 | 0/607 |
| 19 | P | 0.54 | 0/805 | 0.91 | 0/803 |
| 2 | 2 | 1.24 | 2/947 (0.2%) | 0.67 | 0/946 |
| 20 | Q | 0.73 | 0/554 | 1.07 | 1/553 (0.2%) |
| 21 | R | 0.56 | 0/563 | 0.91 | 0/562 |
| 22 | S | 0.73 | 0/515 | 1.03 | 1/514 (0.2%) |
| 23 | T | 0.66 | 0/476 | 0.98 | 0/475 |
| 24 | U | 0.66 | 0/548 | 1.01 | 0/547 |
| 25 | V | 0.42 | 0/299 | 0.82 | 0/298 |
| 26 | W | 0.56 | 0/362 | 0.89 | 0/361 |
| 27 | X | 0.61 | 0/377 | 1.00 | 0/376 |
| 28 | Y | 0.46 | 0/404 | 0.94 | 0/403 |
| 29 | Z | 0.60 | 0/356 | 0.94 | 0/355 |
| 3 | 3 | 1.97 | 7/724 (1.0%) | 1.58 | 5/723 (0.7%) |
| 30 | a | 0.69 | 0/665 | 1.09 | 3/664 (0.5%) |
| 31 | b | 0.42 | 0/290 | 0.79 | 0/289 |
| 32 | c | 0.59 | 0/326 | 0.92 | 0/325 |
| 33 | d | 0.70 | 0/380 | 1.01 | 0/379 |
| 34 | e | 0.76 | 0/317 | 1.01 | 0/316 |
| 35 | f | 0.57 | 0/335 | 0.92 | 0/334 |
| 36 | g | 0.62 | 0/296 | 1.05 | 1/295 (0.3%) |
| 37 | h | 0.74 | 0/260 | 1.12 | 0/259 |
| 38 | i | 0.46 | 0/230 | 0.81 | 0/229 |
| 39 | j | 0.62 | 0/149 | 1.08 | 0/148 |
| 4 | A | 1.38 | 1/650 (0.2%) | 1.56 | 1/649 (0.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|------------------|
| | | RMSZ | # Z >2 | RMSZ | # Z >2 |
| 40 | k | 0.60 | 0/272 | 0.97 | 0/271 |
| 41 | l | 0.54 | 1/1138 (0.1%) | 0.74 | 0/1136 |
| 42 | m | 0.29 | 0/671 | 0.84 | 1/670 (0.1%) |
| 43 | n | 1.15 | 0/707 | 1.35 | 0/706 |
| 44 | o | 1.11 | 0/1040 | 1.20 | 0/1039 |
| 45 | p | 1.66 | 2/188 (1.1%) | 1.86 | 4/187 (2.1%) |
| 46 | q | 1.19 | 1/1327 (0.1%) | 1.35 | 6/1325 (0.5%) |
| 47 | r | 1.14 | 0/965 | 1.33 | 2/964 (0.2%) |
| 47 | s | 1.14 | 0/965 | 1.33 | 2/964 (0.2%) |
| 5 | B | 0.63 | 0/755 | 1.00 | 0/754 |
| 6 | C | 0.68 | 0/1157 | 1.04 | 1/1156 (0.1%) |
| 7 | D | 0.70 | 0/1082 | 1.14 | 4/1081 (0.4%) |
| 8 | E | 0.55 | 0/506 | 0.93 | 0/505 |
| 9 | F | 0.56 | 0/572 | 0.91 | 0/571 |
| All | All | 1.28 | 204/47169 (0.4%) | 1.45 | 408/47117 (0.9%) |

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 |
|-----|-------|---------------------|---------------------|
| 10 | G | 0 | 1 |
| 11 | H | 0 | 3 |
| 12 | I | 0 | 5 |
| 13 | J | 0 | 1 |
| 23 | T | 0 | 1 |
| 30 | a | 0 | 1 |
| 32 | c | 0 | 1 |
| 4 | A | 0 | 2 |
| 43 | n | 0 | 2 |
| 45 | p | 0 | 1 |
| 46 | q | 0 | 7 |
| 47 | r | 0 | 1 |
| 47 | s | 0 | 1 |
| 6 | C | 0 | 1 |
| 7 | D | 0 | 1 |
| 8 | E | 0 | 1 |
| 9 | F | 0 | 1 |
| All | All | 0 | 31 |

All (204) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1 | 1 | 648 | C | O5'-C5' | 38.19 | 2.05 | 1.44 |
| 1 | 1 | 648 | C | P-O5' | -26.01 | 1.33 | 1.59 |
| 1 | 1 | 2819 | A | C5'-C4' | 25.95 | 1.82 | 1.51 |
| 1 | 1 | 651 | G | C5'-C4' | 17.76 | 1.72 | 1.51 |
| 1 | 1 | 651 | G | C4'-C3' | 16.66 | 1.71 | 1.53 |
| 1 | 1 | 650 | C | C4'-C3' | 14.56 | 1.69 | 1.53 |
| 1 | 1 | 2818 | U | O3'-P | -14.40 | 1.43 | 1.61 |
| 1 | 1 | 2372 | A | P-O5' | -14.19 | 1.45 | 1.59 |
| 45 | p | 61 | LYS | C-N | 13.98 | 1.66 | 1.34 |
| 1 | 1 | 648 | C | O3'-P | -13.39 | 1.45 | 1.61 |
| 1 | 1 | 644 | G | C4'-C3' | -13.25 | 1.38 | 1.53 |
| 1 | 1 | 439 | C | O3'-P | 13.07 | 1.76 | 1.61 |
| 1 | 1 | 643 | U | P-O5' | -12.55 | 1.47 | 1.59 |
| 1 | 1 | 2370 | G | O3'-P | -11.66 | 1.47 | 1.61 |
| 1 | 1 | 642 | U | C4'-C3' | -11.64 | 1.40 | 1.53 |
| 1 | 1 | 2373 | A | O3'-P | -10.96 | 1.48 | 1.61 |
| 1 | 1 | 642 | U | O3'-P | -10.79 | 1.48 | 1.61 |
| 1 | 1 | 2819 | A | O5'-C5' | 10.73 | 1.61 | 1.44 |
| 1 | 1 | 440 | A | C5'-C4' | 9.85 | 1.63 | 1.51 |
| 1 | 1 | 650 | C | C5'-C4' | 9.60 | 1.62 | 1.51 |
| 1 | 1 | 651 | G | P-O5' | 9.58 | 1.69 | 1.59 |
| 46 | q | 482 | LEU | C-N | 9.05 | 1.51 | 1.34 |
| 1 | 1 | 640 | U | C5'-C4' | 8.85 | 1.61 | 1.51 |
| 12 | I | 76 | SER | N-CA | 8.82 | 1.64 | 1.46 |
| 1 | 1 | 2319 | U | P-O5' | -8.65 | 1.51 | 1.59 |
| 1 | 1 | 645 | A | P-O5' | -8.62 | 1.51 | 1.59 |
| 1 | 1 | 639 | G | C4'-C3' | 8.60 | 1.62 | 1.53 |
| 1 | 1 | 440 | A | C4'-C3' | 8.16 | 1.62 | 1.53 |
| 1 | 1 | 644 | G | O3'-P | -7.99 | 1.51 | 1.61 |
| 1 | 1 | 2417 | U | O3'-P | -7.73 | 1.51 | 1.61 |
| 1 | 1 | 2264 | U | P-O5' | -7.73 | 1.52 | 1.59 |
| 1 | 1 | 1129 | A | C5'-C4' | 7.70 | 1.60 | 1.51 |
| 1 | 1 | 1268 | G | C5'-C4' | 7.69 | 1.60 | 1.51 |
| 1 | 1 | 1267 | U | P-O5' | -7.61 | 1.52 | 1.59 |
| 1 | 1 | 2371 | G | P-O5' | -7.51 | 1.52 | 1.59 |
| 1 | 1 | 756 | U | P-O5' | -7.29 | 1.52 | 1.59 |
| 1 | 1 | 2503 | G | O3'-P | -7.28 | 1.52 | 1.61 |
| 1 | 1 | 1026 | A | C5'-C4' | 7.19 | 1.59 | 1.51 |
| 1 | 1 | 1988 | C | O3'-P | -7.18 | 1.52 | 1.61 |
| 1 | 1 | 1021 | G | C5'-C4' | 7.14 | 1.59 | 1.51 |
| 1 | 1 | 1073 | U | C5'-C4' | 7.11 | 1.59 | 1.51 |
| 1 | 1 | 644 | G | C5'-C4' | 7.11 | 1.59 | 1.51 |
| 1 | 1 | 1278 | A | C4'-C3' | 7.11 | 1.60 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | 1 | 2372 | A | C4'-C3' | 7.09 | 1.60 | 1.53 |
| 3 | 3 | 75 | G | P-O5' | -7.07 | 1.52 | 1.59 |
| 1 | 1 | 646 | A | P-O5' | -7.01 | 1.52 | 1.59 |
| 1 | 1 | 2497 | U | O3'-P | -6.93 | 1.52 | 1.61 |
| 1 | 1 | 494 | G | C5'-C4' | 6.92 | 1.59 | 1.51 |
| 1 | 1 | 2493 | U | P-O5' | -6.86 | 1.52 | 1.59 |
| 1 | 1 | 1581 | C | C4'-C3' | 6.85 | 1.60 | 1.53 |
| 1 | 1 | 1993 | G | C5'-C4' | 6.85 | 1.59 | 1.51 |
| 1 | 1 | 2305 | G | O3'-P | -6.74 | 1.53 | 1.61 |
| 1 | 1 | 648 | C | C4'-C3' | -6.73 | 1.45 | 1.53 |
| 1 | 1 | 1560 | G | P-O5' | -6.73 | 1.53 | 1.59 |
| 1 | 1 | 2271 | A | O3'-P | -6.73 | 1.53 | 1.61 |
| 1 | 1 | 778 | U | C3'-O3' | 6.72 | 1.51 | 1.42 |
| 1 | 1 | 2299 | A | O3'-P | -6.64 | 1.53 | 1.61 |
| 1 | 1 | 1128 | U | C4'-C3' | 6.64 | 1.60 | 1.53 |
| 3 | 3 | 7 | G | P-O5' | -6.63 | 1.53 | 1.59 |
| 3 | 3 | 36 | C | C5'-C4' | 6.62 | 1.59 | 1.51 |
| 1 | 1 | 2404 | A | C5'-C4' | 6.61 | 1.59 | 1.51 |
| 1 | 1 | 651 | G | C3'-O3' | 6.54 | 1.51 | 1.42 |
| 1 | 1 | 2734 | A | C5'-C4' | 6.53 | 1.59 | 1.51 |
| 1 | 1 | 2858 | U | P-O5' | -6.50 | 1.53 | 1.59 |
| 1 | 1 | 2014 | U | P-O5' | -6.46 | 1.53 | 1.59 |
| 3 | 3 | 111 | U | O3'-P | -6.39 | 1.53 | 1.61 |
| 1 | 1 | 2653 | C | C5'-C4' | 6.39 | 1.59 | 1.51 |
| 1 | 1 | 1152 | G | P-O5' | -6.38 | 1.53 | 1.59 |
| 1 | 1 | 650 | C | C3'-O3' | 6.35 | 1.51 | 1.42 |
| 1 | 1 | 468 | G | O3'-P | -6.33 | 1.53 | 1.61 |
| 1 | 1 | 2509 | U | O3'-P | -6.30 | 1.53 | 1.61 |
| 1 | 1 | 639 | G | C5'-C4' | 6.29 | 1.58 | 1.51 |
| 1 | 1 | 85 | A | O3'-P | -6.27 | 1.53 | 1.61 |
| 1 | 1 | 2276 | G | C5'-C4' | 6.26 | 1.58 | 1.51 |
| 1 | 1 | 2078 | C | P-O5' | -6.23 | 1.53 | 1.59 |
| 1 | 1 | 1846 | C | P-O5' | -6.21 | 1.53 | 1.59 |
| 1 | 1 | 2297 | U | O3'-P | -6.21 | 1.53 | 1.61 |
| 1 | 1 | 715 | A | C5'-C4' | 6.20 | 1.58 | 1.51 |
| 1 | 1 | 2915 | U | P-O5' | -6.18 | 1.53 | 1.59 |
| 2 | 2 | 82 | U | P-O5' | 6.17 | 1.66 | 1.59 |
| 1 | 1 | 1307 | G | C3'-O3' | 6.15 | 1.50 | 1.42 |
| 1 | 1 | 1042 | U | P-O5' | -6.15 | 1.53 | 1.59 |
| 1 | 1 | 482 | C | C5'-C4' | 6.14 | 1.58 | 1.51 |
| 1 | 1 | 2451 | G | P-O5' | -6.14 | 1.53 | 1.59 |
| 1 | 1 | 2436 | U | O3'-P | -6.11 | 1.53 | 1.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | 1 | 1563 | C | C5'-C4' | 6.10 | 1.58 | 1.51 |
| 1 | 1 | 476 | G | O3'-P | -6.10 | 1.53 | 1.61 |
| 1 | 1 | 2300 | G | C4'-C3' | 6.07 | 1.59 | 1.53 |
| 1 | 1 | 3347 | A | C5'-C4' | 6.06 | 1.58 | 1.51 |
| 3 | 3 | 48 | U | O3'-P | -6.06 | 1.53 | 1.61 |
| 1 | 1 | 102 | C | C5'-C4' | 6.05 | 1.58 | 1.51 |
| 1 | 1 | 2788 | C | C5'-C4' | 6.02 | 1.58 | 1.51 |
| 3 | 3 | 8 | G | C5'-C4' | 5.99 | 1.58 | 1.51 |
| 1 | 1 | 449 | U | C4'-C3' | 5.91 | 1.59 | 1.53 |
| 1 | 1 | 1561 | G | C5'-C4' | 5.91 | 1.58 | 1.51 |
| 12 | I | 77 | ALA | N-CA | 5.91 | 1.58 | 1.46 |
| 1 | 1 | 2746 | A | O3'-P | -5.90 | 1.54 | 1.61 |
| 1 | 1 | 1057 | A | P-O5' | -5.90 | 1.53 | 1.59 |
| 1 | 1 | 1987 | G | C5'-C4' | 5.89 | 1.58 | 1.51 |
| 1 | 1 | 754 | G | O3'-P | -5.89 | 1.54 | 1.61 |
| 1 | 1 | 1286 | A | P-O5' | -5.89 | 1.53 | 1.59 |
| 1 | 1 | 1951 | C | O3'-P | -5.88 | 1.54 | 1.61 |
| 1 | 1 | 2865 | U | C5'-C4' | 5.87 | 1.58 | 1.51 |
| 1 | 1 | 1033 | U | P-O5' | -5.86 | 1.53 | 1.59 |
| 1 | 1 | 2492 | C | P-O5' | 5.86 | 1.65 | 1.59 |
| 1 | 1 | 1014 | U | C4'-C3' | -5.85 | 1.46 | 1.52 |
| 12 | I | 75 | PRO | N-CA | 5.85 | 1.57 | 1.47 |
| 1 | 1 | 1138 | U | O3'-P | -5.82 | 1.54 | 1.61 |
| 1 | 1 | 2001 | U | C5'-C4' | 5.81 | 1.58 | 1.51 |
| 1 | 1 | 2796 | G | C5'-C4' | 5.80 | 1.58 | 1.51 |
| 12 | I | 97 | ASN | N-CA | -5.79 | 1.34 | 1.46 |
| 1 | 1 | 440 | A | P-O5' | 5.78 | 1.65 | 1.59 |
| 1 | 1 | 2454 | G | C5'-C4' | 5.77 | 1.58 | 1.51 |
| 1 | 1 | 1281 | G | P-O5' | -5.77 | 1.53 | 1.59 |
| 1 | 1 | 2013 | C | C5'-C4' | 5.74 | 1.58 | 1.51 |
| 1 | 1 | 2746 | A | P-O5' | -5.74 | 1.54 | 1.59 |
| 1 | 1 | 1994 | G | O3'-P | -5.73 | 1.54 | 1.61 |
| 1 | 1 | 2507 | C | O3'-P | -5.71 | 1.54 | 1.61 |
| 1 | 1 | 2697 | A | C5'-C4' | 5.70 | 1.58 | 1.51 |
| 1 | 1 | 491 | C | O3'-P | -5.70 | 1.54 | 1.61 |
| 1 | 1 | 480 | C | C5'-C4' | 5.69 | 1.58 | 1.51 |
| 1 | 1 | 929 | A | C5'-C4' | 5.68 | 1.58 | 1.51 |
| 1 | 1 | 2272 | G | C5'-C4' | 5.67 | 1.58 | 1.51 |
| 1 | 1 | 962 | A | P-O5' | 5.67 | 1.65 | 1.59 |
| 1 | 1 | 286 | U | O3'-P | -5.64 | 1.54 | 1.61 |
| 1 | 1 | 803 | C | C5'-C4' | 5.64 | 1.58 | 1.51 |
| 1 | 1 | 2772 | C | O3'-P | -5.63 | 1.54 | 1.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | 1 | 48 | A | O3'-P | -5.61 | 1.54 | 1.61 |
| 1 | 1 | 3349 | C | C5'-C4' | 5.61 | 1.58 | 1.51 |
| 1 | 1 | 968 | G | C5'-C4' | 5.59 | 1.58 | 1.51 |
| 1 | 1 | 2657 | A | C4'-C3' | 5.56 | 1.59 | 1.53 |
| 1 | 1 | 1252 | A | O3'-P | -5.54 | 1.54 | 1.61 |
| 1 | 1 | 2718 | U | C5'-C4' | 5.54 | 1.57 | 1.51 |
| 1 | 1 | 804 | C | C5'-C4' | 5.54 | 1.57 | 1.51 |
| 1 | 1 | 3351 | U | C4'-C3' | 5.53 | 1.59 | 1.53 |
| 1 | 1 | 2647 | A | P-O5' | -5.52 | 1.54 | 1.59 |
| 1 | 1 | 2866 | U | C5'-C4' | 5.52 | 1.57 | 1.51 |
| 1 | 1 | 957 | C | C4'-C3' | 5.51 | 1.59 | 1.53 |
| 1 | 1 | 484 | C | P-O5' | -5.43 | 1.54 | 1.59 |
| 1 | 1 | 2572 | C | C5'-C4' | 5.43 | 1.57 | 1.51 |
| 1 | 1 | 469 | G | O3'-P | -5.43 | 1.54 | 1.61 |
| 1 | 1 | 485 | A | C5'-C4' | 5.43 | 1.57 | 1.51 |
| 1 | 1 | 1169 | A | P-O5' | -5.42 | 1.54 | 1.59 |
| 1 | 1 | 2041 | U | O3'-P | -5.42 | 1.54 | 1.61 |
| 1 | 1 | 2648 | G | C5'-C4' | 5.41 | 1.57 | 1.51 |
| 1 | 1 | 1288 | U | O3'-P | -5.41 | 1.54 | 1.61 |
| 1 | 1 | 470 | G | C4'-C3' | -5.40 | 1.47 | 1.52 |
| 1 | 1 | 2087 | C | C4'-C3' | 5.40 | 1.59 | 1.53 |
| 1 | 1 | 1257 | C | O3'-P | -5.39 | 1.54 | 1.61 |
| 1 | 1 | 650 | C | O3'-P | 5.38 | 1.67 | 1.61 |
| 1 | 1 | 932 | U | C5'-C4' | 5.36 | 1.57 | 1.51 |
| 1 | 1 | 2280 | A | C4'-C3' | 5.36 | 1.59 | 1.53 |
| 1 | 1 | 651 | G | O3'-P | 5.35 | 1.67 | 1.61 |
| 1 | 1 | 2028 | U | P-O5' | -5.35 | 1.54 | 1.59 |
| 45 | p | 62 | GLU | N-CA | 5.35 | 1.57 | 1.46 |
| 1 | 1 | 2576 | G | C5'-C4' | 5.33 | 1.57 | 1.51 |
| 1 | 1 | 2632 | G | O3'-P | -5.32 | 1.54 | 1.61 |
| 1 | 1 | 2031 | U | O3'-P | -5.31 | 1.54 | 1.61 |
| 1 | 1 | 791 | A | P-O5' | -5.30 | 1.54 | 1.59 |
| 1 | 1 | 2064 | C | C4'-C3' | 5.30 | 1.58 | 1.53 |
| 1 | 1 | 2983 | C | P-O5' | -5.28 | 1.54 | 1.59 |
| 1 | 1 | 2858 | U | O3'-P | -5.28 | 1.54 | 1.61 |
| 1 | 1 | 647 | A | C4'-C3' | 5.26 | 1.58 | 1.53 |
| 3 | 3 | 33 | U | C5'-C4' | 5.26 | 1.57 | 1.51 |
| 1 | 1 | 1196 | C | C5'-C4' | 5.25 | 1.57 | 1.51 |
| 1 | 1 | 2927 | C | C3'-O3' | 5.24 | 1.49 | 1.42 |
| 1 | 1 | 449 | U | C5'-C4' | 5.24 | 1.57 | 1.51 |
| 1 | 1 | 2642 | A | P-O5' | 5.23 | 1.65 | 1.59 |
| 1 | 1 | 2043 | U | C5'-C4' | 5.23 | 1.57 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | 1 | 2714 | G | C5'-C4' | 5.23 | 1.57 | 1.51 |
| 1 | 1 | 2864 | A | P-O5' | -5.22 | 1.54 | 1.59 |
| 1 | 1 | 993 | G | P-O5' | -5.22 | 1.54 | 1.59 |
| 41 | 1 | 388 | TYR | C-N | 5.21 | 1.44 | 1.34 |
| 2 | 2 | 21 | C | P-O5' | -5.21 | 1.54 | 1.59 |
| 12 | I | 57 | LYS | CA-C | -5.20 | 1.39 | 1.52 |
| 1 | 1 | 2400 | G | C5'-C4' | 5.20 | 1.57 | 1.51 |
| 1 | 1 | 758 | C | O3'-P | -5.18 | 1.54 | 1.61 |
| 1 | 1 | 1045 | C | P-O5' | -5.18 | 1.54 | 1.59 |
| 1 | 1 | 2082 | U | P-O5' | -5.17 | 1.54 | 1.59 |
| 1 | 1 | 2692 | A | C5'-C4' | 5.17 | 1.57 | 1.51 |
| 4 | A | 43 | PRO | N-CA | -5.17 | 1.38 | 1.47 |
| 1 | 1 | 1999 | C | C5'-C4' | 5.16 | 1.57 | 1.51 |
| 1 | 1 | 2227 | C | O3'-P | -5.13 | 1.54 | 1.61 |
| 1 | 1 | 1247 | U | C4'-C3' | 5.10 | 1.58 | 1.53 |
| 1 | 1 | 2312 | A | C4'-C3' | 5.09 | 1.58 | 1.53 |
| 1 | 1 | 443 | G | P-O5' | -5.09 | 1.54 | 1.59 |
| 1 | 1 | 736 | A | P-O5' | -5.09 | 1.54 | 1.59 |
| 1 | 1 | 1261 | G | O3'-P | -5.08 | 1.55 | 1.61 |
| 1 | 1 | 1572 | U | C3'-O3' | 5.07 | 1.49 | 1.42 |
| 1 | 1 | 2439 | A | O3'-P | -5.07 | 1.55 | 1.61 |
| 1 | 1 | 646 | A | O3'-P | -5.06 | 1.55 | 1.61 |
| 1 | 1 | 1481 | A | P-O5' | -5.06 | 1.54 | 1.59 |
| 1 | 1 | 1043 | C | P-O5' | -5.06 | 1.54 | 1.59 |
| 1 | 1 | 1273 | A | P-O5' | -5.06 | 1.54 | 1.59 |
| 1 | 1 | 1129 | A | O3'-P | -5.06 | 1.55 | 1.61 |
| 1 | 1 | 287 | G | C5'-C4' | 5.06 | 1.57 | 1.51 |
| 1 | 1 | 734 | C | C5'-C4' | 5.04 | 1.57 | 1.51 |
| 1 | 1 | 773 | G | C4'-C3' | 5.03 | 1.58 | 1.53 |
| 1 | 1 | 2464 | U | O3'-P | -5.03 | 1.55 | 1.61 |
| 1 | 1 | 2804 | A | C5'-C4' | 5.03 | 1.57 | 1.51 |
| 1 | 1 | 2193 | U | C5'-C4' | 5.02 | 1.57 | 1.51 |
| 1 | 1 | 2112 | U | C3'-O3' | 5.01 | 1.49 | 1.42 |
| 1 | 1 | 2761 | G | C5'-C4' | 5.01 | 1.57 | 1.51 |
| 1 | 1 | 2263 | C | O3'-P | -5.00 | 1.55 | 1.61 |

All (408) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | 1 | 885 | U | P-O3'-C3' | 44.33 | 172.90 | 119.70 |
| 1 | 1 | 649 | A | P-O5'-C5' | 31.07 | 170.61 | 120.90 |
| 1 | 1 | 648 | C | P-O5'-C5' | -29.22 | 74.15 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1 | 1 | 2370 | G | P-O3'-C3' | 27.58 | 152.80 | 119.70 |
| 1 | 1 | 2509 | U | P-O3'-C3' | 27.15 | 152.28 | 119.70 |
| 1 | 1 | 2497 | U | P-O3'-C3' | 26.29 | 151.24 | 119.70 |
| 1 | 1 | 2819 | A | O5'-C5'-C4' | 25.63 | 160.39 | 111.70 |
| 1 | 1 | 2507 | C | P-O3'-C3' | 25.18 | 149.92 | 119.70 |
| 1 | 1 | 2503 | G | P-O3'-C3' | 22.24 | 146.39 | 119.70 |
| 1 | 1 | 2462 | A | P-O3'-C3' | 21.73 | 145.78 | 119.70 |
| 1 | 1 | 1138 | U | P-O3'-C3' | 21.21 | 145.16 | 119.70 |
| 1 | 1 | 2041 | U | P-O3'-C3' | 21.02 | 144.93 | 119.70 |
| 1 | 1 | 2500 | A | P-O3'-C3' | 21.00 | 144.90 | 119.70 |
| 1 | 1 | 647 | A | O3'-P-O5' | -19.54 | 66.87 | 104.00 |
| 1 | 1 | 2030 | C | P-O3'-C3' | 19.48 | 143.08 | 119.70 |
| 1 | 1 | 440 | A | C5'-C4'-C3' | 19.34 | 146.95 | 116.00 |
| 1 | 1 | 651 | G | C5'-C4'-C3' | 19.26 | 146.82 | 116.00 |
| 1 | 1 | 2310 | U | P-O3'-C3' | 19.00 | 142.50 | 119.70 |
| 1 | 1 | 2489 | C | P-O3'-C3' | 18.96 | 142.46 | 119.70 |
| 1 | 1 | 2818 | U | P-O3'-C3' | 18.41 | 141.80 | 119.70 |
| 1 | 1 | 1288 | U | P-O3'-C3' | 18.39 | 141.76 | 119.70 |
| 1 | 1 | 1965 | C | P-O3'-C3' | 18.29 | 141.64 | 119.70 |
| 1 | 1 | 2439 | A | P-O3'-C3' | 18.00 | 141.30 | 119.70 |
| 1 | 1 | 456 | U | P-O3'-C3' | 17.98 | 141.28 | 119.70 |
| 1 | 1 | 2468 | A | P-O3'-C3' | 17.98 | 141.28 | 119.70 |
| 1 | 1 | 2194 | G | P-O3'-C3' | 17.98 | 141.27 | 119.70 |
| 1 | 1 | 2372 | A | P-O5'-C5' | 17.91 | 149.56 | 120.90 |
| 1 | 1 | 991 | G | P-O5'-C5' | 17.84 | 149.45 | 120.90 |
| 1 | 1 | 2697 | A | P-O3'-C3' | 17.74 | 140.99 | 119.70 |
| 1 | 1 | 2079 | G | P-O3'-C3' | 17.57 | 140.79 | 119.70 |
| 1 | 1 | 468 | G | P-O3'-C3' | 17.57 | 140.78 | 119.70 |
| 1 | 1 | 647 | A | C5'-C4'-C3' | -17.36 | 88.22 | 116.00 |
| 1 | 1 | 648 | C | O3'-P-O5' | -17.02 | 71.66 | 104.00 |
| 1 | 1 | 2080 | C | P-O3'-C3' | 16.72 | 139.76 | 119.70 |
| 1 | 1 | 2192 | C | P-O3'-C3' | 16.59 | 139.61 | 119.70 |
| 1 | 1 | 2483 | G | P-O3'-C3' | 16.16 | 139.09 | 119.70 |
| 1 | 1 | 880 | G | P-O3'-C3' | 16.01 | 138.91 | 119.70 |
| 1 | 1 | 876 | A | C5'-C4'-C3' | 15.77 | 141.24 | 116.00 |
| 1 | 1 | 2480 | A | P-O3'-C3' | 15.52 | 138.33 | 119.70 |
| 1 | 1 | 1580 | A | P-O3'-C3' | 15.51 | 138.31 | 119.70 |
| 1 | 1 | 494 | G | P-O3'-C3' | 15.48 | 138.28 | 119.70 |
| 1 | 1 | 2446 | U | P-O3'-C3' | 15.46 | 138.25 | 119.70 |
| 1 | 1 | 879 | U | P-O3'-C3' | 15.35 | 138.12 | 119.70 |
| 1 | 1 | 2499 | U | P-O5'-C5' | 15.23 | 145.26 | 120.90 |
| 1 | 1 | 2086 | A | P-O3'-C3' | 15.19 | 137.92 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1 | 1 | 2434 | U | P-O3'-C3' | 15.16 | 137.89 | 119.70 |
| 1 | 1 | 2450 | G | P-O3'-C3' | 15.05 | 137.76 | 119.70 |
| 1 | 1 | 1064 | A | P-O3'-C3' | 14.92 | 137.61 | 119.70 |
| 1 | 1 | 2297 | U | P-O3'-C3' | 14.86 | 137.53 | 119.70 |
| 1 | 1 | 2031 | U | P-O3'-C3' | 14.81 | 137.47 | 119.70 |
| 1 | 1 | 2654 | C | P-O3'-C3' | 14.81 | 137.47 | 119.70 |
| 1 | 1 | 2043 | U | P-O3'-C3' | 14.69 | 137.32 | 119.70 |
| 1 | 1 | 651 | G | P-O5'-C5' | 14.60 | 144.25 | 120.90 |
| 1 | 1 | 2803 | A | P-O3'-C3' | 14.49 | 137.09 | 119.70 |
| 1 | 1 | 491 | C | P-O3'-C3' | 14.09 | 136.61 | 119.70 |
| 1 | 1 | 2316 | G | P-O3'-C3' | 13.97 | 136.46 | 119.70 |
| 1 | 1 | 2445 | A | P-O3'-C3' | 13.94 | 136.42 | 119.70 |
| 10 | G | 128 | LYS | CA-C-N | 13.92 | 147.82 | 117.20 |
| 1 | 1 | 2463 | G | P-O3'-C3' | 13.92 | 136.40 | 119.70 |
| 1 | 1 | 959 | C | P-O3'-C3' | 13.88 | 136.36 | 119.70 |
| 1 | 1 | 2510 | U | P-O5'-C5' | 13.76 | 142.92 | 120.90 |
| 1 | 1 | 2501 | U | P-O3'-C3' | 13.72 | 136.16 | 119.70 |
| 1 | 1 | 472 | A | P-O3'-C3' | 13.61 | 136.03 | 119.70 |
| 1 | 1 | 2492 | C | P-O3'-C3' | 13.60 | 136.02 | 119.70 |
| 1 | 1 | 1058 | U | P-O3'-C3' | 13.58 | 136.00 | 119.70 |
| 1 | 1 | 2655 | U | P-O3'-C3' | 13.56 | 135.97 | 119.70 |
| 1 | 1 | 650 | C | C5'-C4'-C3' | 13.41 | 137.46 | 116.00 |
| 1 | 1 | 2403 | G | P-O3'-C3' | 13.35 | 135.72 | 119.70 |
| 1 | 1 | 2751 | G | P-O3'-C3' | 13.21 | 135.55 | 119.70 |
| 1 | 1 | 3350 | C | P-O3'-C3' | 13.08 | 135.40 | 119.70 |
| 1 | 1 | 2060 | A | P-O3'-C3' | 13.04 | 135.34 | 119.70 |
| 1 | 1 | 2071 | A | P-O3'-C3' | 13.02 | 135.33 | 119.70 |
| 1 | 1 | 2484 | A | P-O3'-C3' | 12.95 | 135.24 | 119.70 |
| 1 | 1 | 1221 | A | P-O3'-C3' | 12.94 | 135.22 | 119.70 |
| 1 | 1 | 2819 | A | P-O5'-C5' | 12.92 | 141.58 | 120.90 |
| 1 | 1 | 2437 | G | P-O3'-C3' | 12.70 | 134.93 | 119.70 |
| 1 | 1 | 442 | G | P-O3'-C3' | 12.69 | 134.92 | 119.70 |
| 1 | 1 | 763 | G | P-O3'-C3' | 12.65 | 134.88 | 119.70 |
| 1 | 1 | 2495 | C | P-O3'-C3' | 12.62 | 134.84 | 119.70 |
| 12 | I | 76 | SER | N-CA-C | -12.61 | 76.96 | 111.00 |
| 1 | 1 | 1972 | A | P-O3'-C3' | 12.58 | 134.79 | 119.70 |
| 1 | 1 | 2373 | A | P-O3'-C3' | 12.48 | 134.68 | 119.70 |
| 1 | 1 | 715 | A | P-O3'-C3' | 12.45 | 134.64 | 119.70 |
| 1 | 1 | 2633 | U | P-O3'-C3' | 12.45 | 134.64 | 119.70 |
| 1 | 1 | 640 | U | P-O5'-C5' | 12.44 | 140.81 | 120.90 |
| 1 | 1 | 1094 | U | P-O3'-C3' | 12.15 | 134.28 | 119.70 |
| 1 | 1 | 2927 | C | P-O3'-C3' | -12.10 | 105.18 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1 | 1 | 645 | A | O3'-P-O5' | -12.08 | 81.05 | 104.00 |
| 1 | 1 | 2829 | U | P-O3'-C3' | 11.98 | 134.08 | 119.70 |
| 1 | 1 | 448 | U | P-O3'-C3' | 11.92 | 134.00 | 119.70 |
| 1 | 1 | 1059 | G | P-O3'-C3' | 11.67 | 133.70 | 119.70 |
| 1 | 1 | 2494 | A | P-O3'-C3' | 11.54 | 133.55 | 119.70 |
| 1 | 1 | 2823 | G | P-O3'-C3' | 11.49 | 133.49 | 119.70 |
| 1 | 1 | 764 | U | P-O3'-C3' | 11.41 | 133.40 | 119.70 |
| 1 | 1 | 961 | C | P-O3'-C3' | 11.39 | 133.36 | 119.70 |
| 1 | 1 | 2040 | U | P-O3'-C3' | 11.38 | 133.36 | 119.70 |
| 1 | 1 | 439 | C | P-O3'-C3' | -11.38 | 106.05 | 119.70 |
| 1 | 1 | 1988 | C | P-O3'-C3' | 11.30 | 133.27 | 119.70 |
| 1 | 1 | 1273 | A | P-O3'-C3' | 11.21 | 133.15 | 119.70 |
| 1 | 1 | 646 | A | P-O3'-C3' | 11.14 | 133.07 | 119.70 |
| 1 | 1 | 1562 | C | P-O3'-C3' | 11.13 | 133.06 | 119.70 |
| 1 | 1 | 474 | G | P-O3'-C3' | 10.96 | 132.85 | 119.70 |
| 1 | 1 | 650 | C | O3'-P-O5' | 10.95 | 124.80 | 104.00 |
| 1 | 1 | 1095 | U | P-O3'-C3' | 10.94 | 132.83 | 119.70 |
| 1 | 1 | 2072 | G | P-O3'-C3' | 10.81 | 132.67 | 119.70 |
| 1 | 1 | 2493 | U | P-O3'-C3' | 10.80 | 132.66 | 119.70 |
| 1 | 1 | 2511 | A | P-O5'-C5' | 10.69 | 138.01 | 120.90 |
| 1 | 1 | 2227 | C | P-O3'-C3' | 10.64 | 132.47 | 119.70 |
| 1 | 1 | 2753 | G | P-O3'-C3' | 10.62 | 132.44 | 119.70 |
| 1 | 1 | 2445 | A | P-O5'-C5' | 10.58 | 137.83 | 120.90 |
| 1 | 1 | 2066 | C | P-O3'-C3' | 10.48 | 132.28 | 119.70 |
| 46 | q | 123 | PRO | C-N-CA | 10.37 | 147.62 | 121.70 |
| 1 | 1 | 2870 | C | P-O3'-C3' | 10.30 | 132.06 | 119.70 |
| 1 | 1 | 2763 | U | P-O3'-C3' | 10.30 | 132.06 | 119.70 |
| 1 | 1 | 639 | G | C5'-C4'-C3' | 10.27 | 132.44 | 116.00 |
| 1 | 1 | 2404 | A | P-O3'-C3' | 10.15 | 131.88 | 119.70 |
| 1 | 1 | 2372 | A | P-O3'-C3' | -10.01 | 107.69 | 119.70 |
| 1 | 1 | 651 | G | O5'-C5'-C4' | 9.95 | 130.61 | 111.70 |
| 1 | 1 | 2436 | U | O3'-P-O5' | -9.94 | 85.11 | 104.00 |
| 1 | 1 | 649 | A | O5'-C5'-C4' | 9.93 | 130.57 | 111.70 |
| 1 | 1 | 1953 | G | P-O3'-C3' | 9.86 | 131.53 | 119.70 |
| 1 | 1 | 1277 | C | P-O3'-C3' | 9.78 | 131.44 | 119.70 |
| 1 | 1 | 1132 | C | C5'-C4'-C3' | 9.78 | 131.64 | 116.00 |
| 1 | 1 | 877 | C | P-O5'-C5' | -9.76 | 105.29 | 120.90 |
| 1 | 1 | 1216 | C | P-O3'-C3' | 9.73 | 131.38 | 119.70 |
| 1 | 1 | 1994 | G | P-O3'-C3' | 9.68 | 131.31 | 119.70 |
| 1 | 1 | 645 | A | P-O3'-C3' | 9.67 | 131.30 | 119.70 |
| 1 | 1 | 2513 | U | P-O3'-C3' | 9.57 | 131.18 | 119.70 |
| 1 | 1 | 2451 | G | P-O5'-C5' | 9.54 | 136.17 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 45 | p | 61 | LYS | C-N-CA | -9.54 | 97.86 | 121.70 |
| 1 | 1 | 2447 | A | P-O3'-C3' | 9.46 | 131.05 | 119.70 |
| 3 | 3 | 52 | G | P-O3'-C3' | 9.42 | 131.01 | 119.70 |
| 1 | 1 | 494 | G | O3'-P-O5' | 9.38 | 121.82 | 104.00 |
| 1 | 1 | 1128 | U | C5'-C4'-C3' | 9.33 | 130.93 | 116.00 |
| 45 | p | 62 | GLU | N-CA-C | 9.33 | 136.19 | 111.00 |
| 1 | 1 | 2493 | U | P-O5'-C5' | 9.28 | 135.75 | 120.90 |
| 1 | 1 | 1097 | G | P-O3'-C3' | 9.25 | 130.80 | 119.70 |
| 1 | 1 | 2469 | G | C5'-C4'-C3' | 9.12 | 130.60 | 116.00 |
| 1 | 1 | 2928 | C | P-O3'-C3' | -9.07 | 108.82 | 119.70 |
| 1 | 1 | 2446 | U | P-O5'-C5' | 9.01 | 135.31 | 120.90 |
| 1 | 1 | 645 | A | C5'-C4'-C3' | -8.98 | 101.62 | 116.00 |
| 1 | 1 | 441 | U | P-O5'-C5' | 8.98 | 135.27 | 120.90 |
| 1 | 1 | 2435 | G | P-O3'-C3' | 8.97 | 130.47 | 119.70 |
| 1 | 1 | 2613 | U | P-O3'-C3' | 8.97 | 130.46 | 119.70 |
| 1 | 1 | 1952 | G | P-O3'-C3' | 8.94 | 130.43 | 119.70 |
| 1 | 1 | 2509 | U | O3'-P-O5' | -8.93 | 87.03 | 104.00 |
| 1 | 1 | 1215 | U | P-O3'-C3' | 8.89 | 130.38 | 119.70 |
| 1 | 1 | 2486 | A | P-O3'-C3' | 8.77 | 130.23 | 119.70 |
| 1 | 1 | 643 | U | C5'-C4'-C3' | -8.64 | 102.18 | 116.00 |
| 1 | 1 | 2444 | C | P-O3'-C3' | -8.62 | 109.36 | 119.70 |
| 1 | 1 | 2772 | C | P-O3'-C3' | 8.60 | 130.02 | 119.70 |
| 1 | 1 | 2819 | A | C5'-C4'-C3' | 8.52 | 129.63 | 116.00 |
| 47 | r | 308 | PRO | N-CA-C | 8.48 | 134.15 | 112.10 |
| 47 | s | 308 | PRO | N-CA-C | 8.47 | 134.13 | 112.10 |
| 1 | 1 | 2402 | A | P-O3'-C3' | 8.40 | 129.78 | 119.70 |
| 1 | 1 | 1581 | C | P-O3'-C3' | 8.38 | 129.76 | 119.70 |
| 1 | 1 | 3351 | U | P-O3'-C3' | 8.33 | 129.70 | 119.70 |
| 46 | q | 146 | ILE | C-N-CA | 8.32 | 142.50 | 121.70 |
| 1 | 1 | 640 | U | C5'-C4'-C3' | 8.32 | 129.31 | 116.00 |
| 1 | 1 | 1975 | C | P-O5'-C5' | 8.32 | 134.21 | 120.90 |
| 1 | 1 | 450 | G | P-O3'-C3' | 8.27 | 129.63 | 119.70 |
| 1 | 1 | 2292 | U | P-O3'-C3' | 8.22 | 129.57 | 119.70 |
| 1 | 1 | 2250 | G | P-O5'-C5' | 8.22 | 134.05 | 120.90 |
| 1 | 1 | 2370 | G | O3'-P-O5' | -8.21 | 88.40 | 104.00 |
| 1 | 1 | 2372 | A | O5'-C5'-C4' | -8.15 | 96.22 | 111.70 |
| 1 | 1 | 475 | G | P-O3'-C3' | 8.11 | 129.44 | 119.70 |
| 12 | I | 75 | PRO | CA-C-N | 7.97 | 134.74 | 117.20 |
| 1 | 1 | 2451 | G | P-O3'-C3' | 7.93 | 129.22 | 119.70 |
| 1 | 1 | 644 | G | P-O3'-C3' | -7.91 | 110.21 | 119.70 |
| 1 | 1 | 2047 | A | P-O3'-C3' | 7.85 | 129.12 | 119.70 |
| 1 | 1 | 2866 | U | P-O3'-C3' | 7.81 | 129.08 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 1 | 1972 | A | C5'-C4'-C3' | 7.77 | 128.44 | 116.00 |
| 46 | q | 147 | LEU | N-CA-C | 7.72 | 131.84 | 111.00 |
| 1 | 1 | 2859 | U | P-O3'-C3' | 7.67 | 128.90 | 119.70 |
| 1 | 1 | 639 | G | O3'-P-O5' | 7.65 | 118.54 | 104.00 |
| 1 | 1 | 2752 | U | P-O3'-C3' | 7.56 | 128.78 | 119.70 |
| 1 | 1 | 447 | U | P-O3'-C3' | 7.54 | 128.75 | 119.70 |
| 45 | p | 15 | PRO | N-CA-C | 7.54 | 131.71 | 112.10 |
| 1 | 1 | 650 | C | P-O3'-C3' | 7.53 | 128.74 | 119.70 |
| 1 | 1 | 2438 | A | C5'-C4'-C3' | 7.52 | 128.03 | 116.00 |
| 1 | 1 | 2299 | A | P-O3'-C3' | 7.50 | 128.70 | 119.70 |
| 12 | I | 77 | ALA | C-N-CA | 7.50 | 140.46 | 121.70 |
| 1 | 1 | 492 | U | P-O3'-C3' | 7.40 | 128.58 | 119.70 |
| 1 | 1 | 991 | G | P-O3'-C3' | -7.37 | 110.86 | 119.70 |
| 1 | 1 | 1951 | C | P-O3'-C3' | 7.36 | 128.53 | 119.70 |
| 1 | 1 | 3344 | A | P-O3'-C3' | 7.36 | 128.53 | 119.70 |
| 1 | 1 | 2764 | C | P-O3'-C3' | -7.30 | 110.94 | 119.70 |
| 1 | 1 | 990 | U | O3'-P-O5' | -7.28 | 90.17 | 104.00 |
| 1 | 1 | 2089 | A | P-O3'-C3' | 7.28 | 128.44 | 119.70 |
| 1 | 1 | 1132 | C | P-O3'-C3' | 7.27 | 128.43 | 119.70 |
| 1 | 1 | 2684 | C | P-O3'-C3' | -7.27 | 110.98 | 119.70 |
| 1 | 1 | 485 | A | P-O3'-C3' | 7.24 | 128.39 | 119.70 |
| 1 | 1 | 2575 | G | P-O5'-C5' | 7.23 | 132.47 | 120.90 |
| 1 | 1 | 646 | A | O5'-C5'-C4' | -7.23 | 97.97 | 111.70 |
| 1 | 1 | 2469 | G | P-O3'-C3' | 7.22 | 128.36 | 119.70 |
| 1 | 1 | 1015 | U | P-O5'-C5' | 7.19 | 132.41 | 120.90 |
| 1 | 1 | 1131 | G | C5'-C4'-C3' | 7.19 | 127.50 | 116.00 |
| 1 | 1 | 2286 | U | P-O3'-C3' | 7.18 | 128.32 | 119.70 |
| 1 | 1 | 3360 | C | P-O3'-C3' | 7.14 | 128.27 | 119.70 |
| 1 | 1 | 2846 | U | P-O3'-C3' | -7.12 | 111.15 | 119.70 |
| 1 | 1 | 1559 | A | P-O3'-C3' | 7.09 | 128.21 | 119.70 |
| 1 | 1 | 487 | U | P-O5'-C5' | 7.07 | 132.21 | 120.90 |
| 1 | 1 | 2452 | G | P-O3'-C3' | 7.06 | 128.18 | 119.70 |
| 1 | 1 | 1974 | A | P-O3'-C3' | 7.00 | 128.11 | 119.70 |
| 1 | 1 | 1130 | A | P-O3'-C3' | 6.96 | 128.05 | 119.70 |
| 1 | 1 | 2088 | A | C5'-C4'-C3' | 6.95 | 127.12 | 116.00 |
| 1 | 1 | 442 | G | P-O5'-C5' | -6.87 | 109.91 | 120.90 |
| 1 | 1 | 3359 | A | P-O3'-C3' | -6.86 | 111.47 | 119.70 |
| 1 | 1 | 1131 | G | P-O5'-C5' | 6.86 | 131.87 | 120.90 |
| 1 | 1 | 3353 | G | P-O3'-C3' | 6.83 | 127.90 | 119.70 |
| 1 | 1 | 2759 | U | P-O3'-C3' | 6.83 | 127.89 | 119.70 |
| 1 | 1 | 2210 | G | P-O5'-C5' | 6.81 | 131.80 | 120.90 |
| 1 | 1 | 1975 | C | P-O3'-C3' | 6.80 | 127.87 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 1 | 2458 | A | P-O3'-C3' | 6.80 | 127.86 | 119.70 |
| 1 | 1 | 644 | G | O3'-P-O5' | -6.79 | 91.09 | 104.00 |
| 1 | 1 | 1058 | U | C5'-C4'-C3' | 6.77 | 126.83 | 116.00 |
| 1 | 1 | 2469 | G | O3'-P-O5' | -6.75 | 91.18 | 104.00 |
| 1 | 1 | 1560 | G | P-O5'-C5' | 6.71 | 131.63 | 120.90 |
| 1 | 1 | 1057 | A | P-O5'-C5' | 6.70 | 131.62 | 120.90 |
| 1 | 1 | 642 | U | C5'-C4'-C3' | -6.68 | 105.31 | 116.00 |
| 1 | 1 | 2918 | G | P-O3'-C3' | -6.64 | 111.73 | 119.70 |
| 1 | 1 | 2474 | G | P-O3'-C3' | 6.64 | 127.67 | 119.70 |
| 1 | 1 | 2931 | C | P-O5'-C5' | 6.64 | 131.53 | 120.90 |
| 1 | 1 | 1262 | G | P-O3'-C3' | 6.61 | 127.63 | 119.70 |
| 1 | 1 | 2502 | A | P-O3'-C3' | 6.60 | 127.62 | 119.70 |
| 30 | a | 216 | VAL | N-CA-C | 6.60 | 128.82 | 111.00 |
| 1 | 1 | 440 | A | P-O5'-C5' | 6.57 | 131.41 | 120.90 |
| 1 | 1 | 1129 | A | P-O5'-C5' | -6.57 | 110.39 | 120.90 |
| 1 | 1 | 2492 | C | O5'-C5'-C4' | 6.57 | 124.18 | 111.70 |
| 1 | 1 | 2621 | G | P-O3'-C3' | 6.56 | 127.57 | 119.70 |
| 1 | 1 | 452 | G | P-O3'-C3' | 6.55 | 127.56 | 119.70 |
| 1 | 1 | 2479 | C | P-O3'-C3' | -6.52 | 111.87 | 119.70 |
| 1 | 1 | 2759 | U | C5'-C4'-C3' | 6.50 | 126.40 | 116.00 |
| 1 | 1 | 1286 | A | P-O3'-C3' | 6.42 | 127.40 | 119.70 |
| 1 | 1 | 2470 | C | P-O3'-C3' | 6.39 | 127.37 | 119.70 |
| 1 | 1 | 2078 | C | P-O3'-C3' | 6.37 | 127.34 | 119.70 |
| 1 | 1 | 2466 | G | P-O3'-C3' | 6.36 | 127.33 | 119.70 |
| 1 | 1 | 2645 | G | C5'-C4'-C3' | -6.36 | 105.83 | 116.00 |
| 3 | 3 | 111 | U | P-O3'-C3' | 6.33 | 127.29 | 119.70 |
| 1 | 1 | 2487 | U | P-O3'-C3' | -6.31 | 112.12 | 119.70 |
| 1 | 1 | 2756 | C | P-O3'-C3' | 6.31 | 127.27 | 119.70 |
| 1 | 1 | 2464 | U | P-O5'-C5' | -6.28 | 110.85 | 120.90 |
| 1 | 1 | 645 | A | C4'-C3'-O3' | 6.28 | 125.55 | 113.00 |
| 17 | N | 46 | ASP | N-CA-C | -6.28 | 94.06 | 111.00 |
| 1 | 1 | 647 | A | C4'-C3'-O3' | 6.27 | 125.54 | 113.00 |
| 1 | 1 | 647 | A | O5'-C5'-C4' | 6.22 | 123.52 | 111.70 |
| 20 | Q | 99 | THR | N-CA-C | 6.21 | 127.76 | 111.00 |
| 1 | 1 | 2646 | C | P-O3'-C3' | -6.20 | 112.26 | 119.70 |
| 1 | 1 | 1289 | G | P-O3'-C3' | 6.19 | 127.12 | 119.70 |
| 1 | 1 | 28 | C | P-O3'-C3' | 6.19 | 127.12 | 119.70 |
| 1 | 1 | 2628 | A | C5'-C4'-C3' | 6.18 | 125.89 | 116.00 |
| 1 | 1 | 84 | U | P-O3'-C3' | 6.17 | 127.11 | 119.70 |
| 1 | 1 | 2462 | A | O3'-P-O5' | -6.17 | 92.27 | 104.00 |
| 1 | 1 | 2206 | G | P-O5'-C5' | 6.16 | 130.75 | 120.90 |
| 1 | 1 | 2927 | C | P-O5'-C5' | 6.16 | 130.75 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4 | A | 22 | GLU | N-CA-C | 6.15 | 127.60 | 111.00 |
| 1 | 1 | 2024 | G | P-O3'-C3' | 6.15 | 127.08 | 119.70 |
| 1 | 1 | 2499 | U | P-O3'-C3' | 6.13 | 127.05 | 119.70 |
| 1 | 1 | 2818 | U | O3'-P-O5' | 6.12 | 115.63 | 104.00 |
| 11 | H | 158 | ASP | N-CA-C | 6.12 | 127.53 | 111.00 |
| 1 | 1 | 2371 | G | P-O5'-C5' | 6.10 | 130.66 | 120.90 |
| 1 | 1 | 2263 | C | C5'-C4'-C3' | 6.06 | 125.70 | 116.00 |
| 1 | 1 | 1820 | U | P-O3'-C3' | 6.05 | 126.96 | 119.70 |
| 1 | 1 | 1992 | U | C5'-C4'-C3' | 6.04 | 125.67 | 116.00 |
| 17 | N | 66 | ALA | N-CA-C | -6.03 | 94.71 | 111.00 |
| 1 | 1 | 2262 | A | O3'-P-O5' | -6.02 | 92.56 | 104.00 |
| 1 | 1 | 1092 | C | P-O3'-C3' | 6.01 | 126.91 | 119.70 |
| 1 | 1 | 644 | G | O5'-C5'-C4' | 6.00 | 123.11 | 111.70 |
| 1 | 1 | 1484 | U | P-O3'-C3' | 6.00 | 126.89 | 119.70 |
| 1 | 1 | 1239 | C | P-O3'-C3' | -5.98 | 112.53 | 119.70 |
| 1 | 1 | 2035 | G | P-O3'-C3' | 5.97 | 126.86 | 119.70 |
| 1 | 1 | 1284 | C | P-O3'-C3' | 5.96 | 126.85 | 119.70 |
| 1 | 1 | 2443 | A | P-O3'-C3' | 5.96 | 126.85 | 119.70 |
| 1 | 1 | 2566 | C | P-O3'-C3' | -5.96 | 112.55 | 119.70 |
| 1 | 1 | 2620 | G | P-O3'-C3' | 5.94 | 126.83 | 119.70 |
| 1 | 1 | 2373 | A | P-O5'-C5' | -5.93 | 111.41 | 120.90 |
| 1 | 1 | 1278 | A | P-O3'-C3' | 5.93 | 126.81 | 119.70 |
| 7 | D | 189 | ALA | C-N-CA | -5.92 | 109.87 | 122.30 |
| 1 | 1 | 2476 | C | P-O3'-C3' | 5.91 | 126.80 | 119.70 |
| 14 | K | 141 | ALA | N-CA-C | -5.91 | 95.04 | 111.00 |
| 1 | 1 | 755 | A | P-O5'-C5' | -5.90 | 111.46 | 120.90 |
| 1 | 1 | 1129 | A | O5'-C5'-C4' | 5.90 | 122.91 | 111.70 |
| 1 | 1 | 2465 | G | P-O5'-C5' | -5.89 | 111.47 | 120.90 |
| 1 | 1 | 885 | U | O3'-P-O5' | -5.88 | 92.83 | 104.00 |
| 1 | 1 | 1226 | G | P-O5'-C5' | 5.87 | 130.30 | 120.90 |
| 1 | 1 | 3357 | U | P-O3'-C3' | -5.86 | 112.67 | 119.70 |
| 1 | 1 | 480 | C | P-O3'-C3' | 5.85 | 126.72 | 119.70 |
| 1 | 1 | 2438 | A | P-O5'-C5' | -5.84 | 111.55 | 120.90 |
| 1 | 1 | 2280 | A | P-O5'-C5' | -5.84 | 111.56 | 120.90 |
| 17 | N | 115 | LYS | C-N-CA | -5.83 | 110.05 | 122.30 |
| 1 | 1 | 2192 | C | P-O5'-C5' | 5.81 | 130.19 | 120.90 |
| 30 | a | 215 | GLY | N-CA-C | -5.80 | 98.61 | 113.10 |
| 1 | 1 | 2927 | C | O3'-P-O5' | -5.79 | 92.99 | 104.00 |
| 1 | 1 | 2507 | C | C5'-C4'-C3' | -5.79 | 106.74 | 116.00 |
| 7 | D | 139 | GLY | N-CA-C | -5.78 | 98.66 | 113.10 |
| 1 | 1 | 650 | C | C4'-C3'-O3' | 5.77 | 124.54 | 113.00 |
| 1 | 1 | 876 | A | O3'-P-O5' | -5.77 | 93.04 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 1 | 2028 | U | P-O5'-C5' | 5.77 | 130.13 | 120.90 |
| 1 | 1 | 2765 | C | P-O5'-C5' | 5.77 | 130.12 | 120.90 |
| 1 | 1 | 443 | G | C5'-C4'-C3' | -5.76 | 106.79 | 116.00 |
| 1 | 1 | 467 | U | P-O3'-C3' | 5.73 | 126.57 | 119.70 |
| 12 | I | 73 | VAL | N-CA-C | -5.72 | 95.55 | 111.00 |
| 1 | 1 | 2438 | A | P-O3'-C3' | 5.72 | 126.56 | 119.70 |
| 1 | 1 | 444 | U | P-O3'-C3' | 5.70 | 126.54 | 119.70 |
| 1 | 1 | 1129 | A | P-O3'-C3' | 5.70 | 126.54 | 119.70 |
| 1 | 1 | 2675 | C | P-O3'-C3' | 5.70 | 126.54 | 119.70 |
| 1 | 1 | 2209 | U | P-O3'-C3' | 5.68 | 126.52 | 119.70 |
| 1 | 1 | 279 | U | P-O5'-C5' | -5.67 | 111.83 | 120.90 |
| 1 | 1 | 2492 | C | P-O5'-C5' | -5.66 | 111.84 | 120.90 |
| 1 | 1 | 875 | G | P-O3'-C3' | 5.64 | 126.47 | 119.70 |
| 1 | 1 | 2569 | A | P-O3'-C3' | 5.64 | 126.46 | 119.70 |
| 45 | p | 32 | CYS | CA-C-N | 5.63 | 129.59 | 117.20 |
| 1 | 1 | 1954 | G | P-O3'-C3' | 5.61 | 126.43 | 119.70 |
| 1 | 1 | 3354 | U | P-O3'-C3' | -5.61 | 112.97 | 119.70 |
| 1 | 1 | 1081 | U | P-O3'-C3' | 5.61 | 126.43 | 119.70 |
| 1 | 1 | 2503 | G | O3'-P-O5' | -5.60 | 93.35 | 104.00 |
| 1 | 1 | 991 | G | C5'-C4'-C3' | 5.58 | 124.93 | 116.00 |
| 1 | 1 | 1580 | A | C5'-C4'-C3' | -5.58 | 107.07 | 116.00 |
| 6 | C | 316 | GLU | N-CA-C | 5.58 | 126.06 | 111.00 |
| 1 | 1 | 2493 | U | C5'-C4'-C3' | 5.56 | 124.90 | 116.00 |
| 1 | 1 | 65 | A | P-O3'-C3' | 5.56 | 126.37 | 119.70 |
| 1 | 1 | 802 | C | P-O3'-C3' | 5.56 | 126.37 | 119.70 |
| 1 | 1 | 2454 | G | P-O3'-C3' | 5.55 | 126.37 | 119.70 |
| 1 | 1 | 2371 | G | P-O3'-C3' | -5.55 | 113.04 | 119.70 |
| 36 | g | 27 | SER | N-CA-C | -5.53 | 96.06 | 111.00 |
| 46 | q | 222 | GLY | N-CA-C | -5.53 | 99.27 | 113.10 |
| 1 | 1 | 2653 | C | P-O3'-C3' | 5.53 | 126.33 | 119.70 |
| 1 | 1 | 1949 | G | P-O3'-C3' | 5.52 | 126.32 | 119.70 |
| 1 | 1 | 2405 | C | P-O3'-C3' | 5.52 | 126.32 | 119.70 |
| 12 | I | 88 | PRO | CA-C-N | 5.51 | 132.54 | 117.10 |
| 1 | 1 | 446 | U | P-O5'-C5' | 5.51 | 129.72 | 120.90 |
| 1 | 1 | 2091 | U | P-O5'-C5' | 5.51 | 129.72 | 120.90 |
| 1 | 1 | 2473 | C | P-O3'-C3' | 5.50 | 126.31 | 119.70 |
| 47 | r | 266 | PHE | N-CA-C | -5.50 | 96.14 | 111.00 |
| 47 | s | 266 | PHE | N-CA-C | -5.50 | 96.14 | 111.00 |
| 1 | 1 | 2723 | U | P-O3'-C3' | -5.49 | 113.11 | 119.70 |
| 1 | 1 | 990 | U | P-O3'-C3' | -5.48 | 113.12 | 119.70 |
| 1 | 1 | 2243 | A | P-O5'-C5' | -5.47 | 112.14 | 120.90 |
| 1 | 1 | 2498 | U | C5'-C4'-C3' | -5.47 | 107.25 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 1 | 2450 | G | O3'-P-O5' | -5.47 | 93.61 | 104.00 |
| 1 | 1 | 1080 | A | P-O5'-C5' | -5.45 | 112.18 | 120.90 |
| 1 | 1 | 1270 | A | P-O3'-C3' | 5.45 | 126.24 | 119.70 |
| 1 | 1 | 2512 | C | P-O3'-C3' | 5.45 | 126.24 | 119.70 |
| 1 | 1 | 1128 | U | O3'-P-O5' | 5.45 | 114.35 | 104.00 |
| 1 | 1 | 645 | A | O5'-C5'-C4' | -5.44 | 101.36 | 111.70 |
| 3 | 3 | 93 | C | P-O3'-C3' | -5.44 | 113.17 | 119.70 |
| 1 | 1 | 644 | G | P-O5'-C5' | -5.43 | 112.21 | 120.90 |
| 1 | 1 | 2304 | C | P-O3'-C3' | 5.40 | 126.18 | 119.70 |
| 1 | 1 | 2479 | C | C5'-C4'-C3' | 5.40 | 124.63 | 116.00 |
| 1 | 1 | 1130 | A | P-O5'-C5' | -5.39 | 112.28 | 120.90 |
| 1 | 1 | 2787 | G | P-O3'-C3' | 5.39 | 126.17 | 119.70 |
| 1 | 1 | 1990 | U | P-O5'-C5' | 5.38 | 129.51 | 120.90 |
| 1 | 1 | 2847 | A | P-O5'-C5' | -5.38 | 112.29 | 120.90 |
| 46 | q | 147 | LEU | CA-C-N | 5.37 | 129.02 | 117.20 |
| 14 | K | 57 | VAL | N-CA-C | -5.36 | 96.54 | 111.00 |
| 1 | 1 | 2256 | A | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 1 | 1 | 2466 | G | C5'-C4'-C3' | 5.35 | 124.56 | 116.00 |
| 3 | 3 | 63 | A | P-O5'-C5' | -5.35 | 112.34 | 120.90 |
| 1 | 1 | 440 | A | P-O3'-C3' | 5.34 | 126.11 | 119.70 |
| 1 | 1 | 1607 | U | P-O3'-C3' | 5.33 | 126.10 | 119.70 |
| 1 | 1 | 2742 | C | C5'-C4'-C3' | -5.32 | 107.49 | 116.00 |
| 1 | 1 | 461 | U | P-O3'-C3' | -5.30 | 113.33 | 119.70 |
| 1 | 1 | 2496 | C | O3'-P-O5' | -5.29 | 93.95 | 104.00 |
| 1 | 1 | 2858 | U | P-O3'-C3' | 5.29 | 126.05 | 119.70 |
| 1 | 1 | 1087 | G | P-O3'-C3' | -5.28 | 113.37 | 119.70 |
| 1 | 1 | 101 | G | P-O3'-C3' | 5.27 | 126.03 | 119.70 |
| 1 | 1 | 643 | U | P-O3'-C3' | -5.26 | 113.39 | 119.70 |
| 1 | 1 | 2011 | U | P-O5'-C5' | -5.26 | 112.48 | 120.90 |
| 1 | 1 | 1127 | G | P-O5'-C5' | -5.24 | 112.51 | 120.90 |
| 1 | 1 | 2762 | A | P-O3'-C3' | 5.24 | 125.99 | 119.70 |
| 1 | 1 | 733 | G | P-O5'-C5' | 5.23 | 129.26 | 120.90 |
| 1 | 1 | 1224 | C | P-O5'-C5' | 5.22 | 129.26 | 120.90 |
| 1 | 1 | 639 | G | C4'-C3'-O3' | 5.22 | 123.44 | 113.00 |
| 1 | 1 | 3346 | U | P-O5'-C5' | 5.21 | 129.24 | 120.90 |
| 1 | 1 | 2718 | U | P-O5'-C5' | 5.19 | 129.21 | 120.90 |
| 1 | 1 | 2276 | G | P-O5'-C5' | -5.18 | 112.61 | 120.90 |
| 46 | q | 483 | PRO | N-CA-C | 5.18 | 125.56 | 112.10 |
| 1 | 1 | 1224 | C | P-O3'-C3' | -5.17 | 113.49 | 119.70 |
| 1 | 1 | 2252 | A | P-O5'-C5' | -5.17 | 112.63 | 120.90 |
| 1 | 1 | 2657 | A | P-O3'-C3' | 5.17 | 125.90 | 119.70 |
| 1 | 1 | 1225 | A | P-O3'-C3' | 5.17 | 125.90 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 1 | 2476 | C | C5'-C4'-C3' | 5.15 | 124.23 | 116.00 |
| 1 | 1 | 1568 | U | P-O3'-C3' | 5.14 | 125.87 | 119.70 |
| 7 | D | 82 | THR | C-N-CA | -5.14 | 111.51 | 122.30 |
| 1 | 1 | 2318 | U | P-O5'-C5' | -5.14 | 112.68 | 120.90 |
| 1 | 1 | 2263 | C | P-O5'-C5' | -5.12 | 112.70 | 120.90 |
| 3 | 3 | 10 | C | P-O5'-C5' | 5.10 | 129.06 | 120.90 |
| 1 | 1 | 2775 | U | P-O3'-C3' | -5.10 | 113.58 | 119.70 |
| 42 | m | 7 | PHE | N-CA-C | -5.10 | 97.24 | 111.00 |
| 1 | 1 | 2373 | A | C5'-C4'-C3' | 5.09 | 124.15 | 116.00 |
| 1 | 1 | 2929 | C | P-O3'-C3' | -5.08 | 113.60 | 119.70 |
| 1 | 1 | 2619 | G | P-O3'-C3' | 5.08 | 125.80 | 119.70 |
| 1 | 1 | 2507 | C | P-O5'-C5' | -5.08 | 112.77 | 120.90 |
| 1 | 1 | 2824 | G | P-O5'-C5' | -5.07 | 112.78 | 120.90 |
| 7 | D | 328 | ASN | N-CA-C | 5.07 | 124.70 | 111.00 |
| 22 | S | 12 | ARG | N-CA-C | 5.07 | 124.69 | 111.00 |
| 1 | 1 | 2725 | U | P-O3'-C3' | -5.07 | 113.62 | 119.70 |
| 1 | 1 | 2417 | U | P-O5'-C5' | -5.07 | 112.80 | 120.90 |
| 1 | 1 | 2500 | A | O3'-P-O5' | -5.06 | 94.39 | 104.00 |
| 30 | a | 177 | GLY | N-CA-C | -5.05 | 100.48 | 113.10 |
| 1 | 1 | 1131 | G | O5'-C5'-C4' | -5.05 | 102.11 | 111.70 |
| 1 | 1 | 2492 | C | C5'-C4'-C3' | 5.05 | 124.08 | 116.00 |
| 1 | 1 | 2704 | A | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 1 | 1 | 2005 | G | P-O5'-C5' | -5.02 | 112.86 | 120.90 |
| 1 | 1 | 637 | C | P-O3'-C3' | 5.01 | 125.71 | 119.70 |
| 1 | 1 | 489 | C | P-O5'-C5' | 5.01 | 128.91 | 120.90 |
| 1 | 1 | 2712 | U | P-O3'-C3' | 5.01 | 125.71 | 119.70 |
| 1 | 1 | 1289 | G | P-O5'-C5' | 5.00 | 128.90 | 120.90 |

There are no chirality outliers.

All (31) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 4 | A | 19 | TYR | Peptide |
| 4 | A | 210 | MET | Peptide |
| 6 | C | 172 | ALA | Peptide |
| 7 | D | 318 | LEU | Peptide |
| 8 | E | 8 | PRO | Peptide |
| 9 | F | 21 | LYS | Peptide |
| 10 | G | 51 | ARG | Peptide |
| 11 | H | 158 | ASP | Peptide |
| 11 | H | 30 | THR | Peptide |
| 11 | H | 74 | THR | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 12 | I | 121 | PHE | Peptide |
| 12 | I | 59 | THR | Peptide |
| 12 | I | 74 | VAL | Peptide |
| 12 | I | 75 | PRO | Peptide |
| 12 | I | 76 | SER | Peptide |
| 13 | J | 110 | PRO | Peptide |
| 23 | T | 16 | GLN | Peptide |
| 30 | a | 157 | ASN | Peptide |
| 32 | c | 110 | GLU | Peptide |
| 43 | n | 231 | THR | Peptide |
| 43 | n | 26 | ILE | Peptide |
| 45 | p | 32 | CYS | Peptide |
| 46 | q | 123 | PRO | Peptide |
| 46 | q | 124 | ARG | Peptide |
| 46 | q | 133 | THR | Peptide |
| 46 | q | 146 | ILE | Peptide |
| 46 | q | 81 | CYS | Peptide |
| 46 | q | 85 | GLY | Peptide |
| 46 | q | 94 | THR | Peptide |
| 47 | r | 307 | ALA | Peptide |
| 47 | s | 307 | ALA | Peptide |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 1 | 20363 | 0 | 6792 | 139 | 0 |
| 2 | 2 | 948 | 0 | 317 | 2 | 0 |
| 3 | 3 | 725 | 0 | 244 | 7 | 0 |
| 4 | A | 651 | 0 | 230 | 0 | 0 |
| 5 | B | 756 | 0 | 310 | 3 | 0 |
| 6 | C | 1158 | 0 | 433 | 2 | 0 |
| 7 | D | 1083 | 0 | 399 | 2 | 0 |
| 8 | E | 507 | 0 | 193 | 24 | 0 |
| 9 | F | 573 | 0 | 215 | 2 | 0 |
| 10 | G | 525 | 0 | 179 | 2 | 0 |
| 11 | H | 699 | 0 | 242 | 2 | 0 |
| 12 | I | 381 | 0 | 140 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 13 | J | 591 | 0 | 214 | 1 | 0 |
| 14 | K | 579 | 0 | 199 | 3 | 0 |
| 15 | L | 408 | 0 | 162 | 9 | 0 |
| 16 | M | 408 | 0 | 145 | 0 | 0 |
| 17 | N | 444 | 0 | 176 | 10 | 0 |
| 18 | O | 609 | 0 | 221 | 11 | 0 |
| 19 | P | 807 | 0 | 293 | 6 | 0 |
| 20 | Q | 555 | 0 | 204 | 22 | 0 |
| 21 | R | 564 | 0 | 202 | 7 | 0 |
| 22 | S | 516 | 0 | 175 | 2 | 0 |
| 23 | T | 477 | 0 | 175 | 9 | 0 |
| 24 | U | 549 | 0 | 196 | 0 | 0 |
| 25 | V | 300 | 0 | 109 | 0 | 0 |
| 26 | W | 363 | 0 | 121 | 0 | 0 |
| 27 | X | 378 | 0 | 134 | 2 | 0 |
| 28 | Y | 405 | 0 | 142 | 1 | 0 |
| 29 | Z | 357 | 0 | 118 | 1 | 0 |
| 30 | a | 666 | 0 | 241 | 0 | 0 |
| 31 | b | 291 | 0 | 113 | 0 | 0 |
| 32 | c | 327 | 0 | 114 | 0 | 0 |
| 33 | d | 381 | 0 | 135 | 0 | 0 |
| 34 | e | 318 | 0 | 117 | 0 | 0 |
| 35 | f | 336 | 0 | 121 | 0 | 0 |
| 36 | g | 297 | 0 | 109 | 0 | 0 |
| 37 | h | 261 | 0 | 104 | 0 | 0 |
| 38 | i | 231 | 0 | 79 | 0 | 0 |
| 39 | j | 150 | 0 | 47 | 0 | 0 |
| 40 | k | 273 | 0 | 108 | 0 | 0 |
| 41 | l | 1140 | 0 | 410 | 0 | 0 |
| 42 | m | 672 | 0 | 257 | 0 | 0 |
| 43 | n | 708 | 0 | 251 | 0 | 0 |
| 44 | o | 1041 | 0 | 359 | 0 | 0 |
| 45 | p | 189 | 0 | 68 | 0 | 0 |
| 46 | q | 1329 | 0 | 491 | 0 | 0 |
| 47 | r | 966 | 0 | 321 | 0 | 0 |
| 47 | s | 966 | 0 | 316 | 0 | 0 |
| All | All | 47221 | 0 | 16441 | 171 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:1:2819:A:C5' | 1:1:2819:A:C4' | 1.82 | 1.51 |
| 1:1:648:C:C5' | 1:1:648:C:P | 2.12 | 1.37 |
| 1:1:730:C:P | 20:Q:136:ASN:N | 2.04 | 1.30 |
| 1:1:715:A:P | 17:N:114:GLY:H | 1.54 | 1.29 |
| 1:1:1943:C:C5' | 1:1:3346:U:H5' | 1.64 | 1.26 |
| 1:1:1943:C:C4' | 1:1:3346:U:H5' | 1.65 | 1.23 |
| 1:1:2573:G:P | 28:Y:57:HIS:CA | 2.28 | 1.21 |
| 1:1:1226:G:C4' | 1:1:3117:C:C4' | 2.26 | 1.13 |
| 1:1:965:A:H5' | 17:N:41:HIS:CA | 1.81 | 1.10 |
| 1:1:648:C:C5' | 1:1:648:C:O5' | 2.05 | 1.03 |
| 1:1:647:A:O3' | 1:1:648:C:C5' | 2.09 | 1.01 |
| 1:1:2681:U:H5'' | 8:E:49:LYS:N | 1.76 | 1.01 |
| 1:1:2599:U:P | 18:O:70:ASN:H | 1.86 | 0.99 |
| 1:1:1943:C:H5' | 1:1:3346:U:H5' | 1.41 | 0.98 |
| 1:1:2092:A:O5' | 21:R:144:GLN:N | 1.86 | 0.97 |
| 1:1:715:A:P | 17:N:114:GLY:N | 2.37 | 0.97 |
| 1:1:2844:C:H5'' | 23:T:159:PHE:C | 1.86 | 0.96 |
| 1:1:1943:C:C5' | 1:1:3346:U:C5' | 2.43 | 0.95 |
| 1:1:729:C:O3' | 20:Q:136:ASN:N | 2.00 | 0.94 |
| 1:1:2092:A:P | 21:R:140:GLU:C | 2.47 | 0.93 |
| 1:1:1943:C:H5' | 1:1:3346:U:C5' | 1.98 | 0.92 |
| 1:1:2747:A:H5' | 19:P:175:HIS:CA | 2.00 | 0.92 |
| 1:1:2681:U:H5'' | 8:E:48:SER:C | 1.90 | 0.91 |
| 1:1:744:A:C4' | 20:Q:142:GLY:C | 2.39 | 0.91 |
| 1:1:729:C:C4' | 20:Q:137:THR:C | 2.41 | 0.89 |
| 1:1:729:C:O3' | 20:Q:136:ASN:CA | 2.23 | 0.87 |
| 1:1:2844:C:C4' | 23:T:159:PHE:C | 2.43 | 0.87 |
| 1:1:2651:G:H5'' | 23:T:23:GLY:HA2 | 1.57 | 0.85 |
| 1:1:964:G:C4' | 17:N:40:HIS:CA | 2.54 | 0.85 |
| 1:1:648:C:H5'' | 1:1:648:C:P | 2.17 | 0.84 |
| 1:1:288:C:H5'' | 18:O:171:SER:CA | 2.08 | 0.84 |
| 1:1:2917:G:H5'' | 15:L:47:ASN:N | 1.93 | 0.84 |
| 1:1:2917:G:H5'' | 15:L:47:ASN:H | 1.44 | 0.83 |
| 1:1:1226:G:C5' | 1:1:3117:C:C4' | 2.56 | 0.83 |
| 1:1:2844:C:C5' | 23:T:159:PHE:C | 2.49 | 0.81 |
| 1:1:730:C:P | 20:Q:136:ASN:CA | 2.68 | 0.80 |
| 1:1:964:G:C3' | 17:N:40:HIS:C | 2.50 | 0.79 |
| 1:1:965:A:C5' | 17:N:41:HIS:CA | 2.61 | 0.79 |
| 1:1:769:G:H5'' | 14:K:172:LEU:CA | 2.14 | 0.76 |
| 1:1:2916:U:O3' | 15:L:46:LEU:CA | 2.33 | 0.76 |
| 1:1:1226:G:H5'' | 1:1:3117:C:C4' | 2.17 | 0.74 |
| 1:1:744:A:C4' | 20:Q:142:GLY:CA | 2.65 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:1:2917:G:C5' | 15:L:47:ASN:H | 2.01 | 0.74 |
| 3:3:56:A:O3' | 8:E:149:GLY:N | 2.22 | 0.72 |
| 1:1:1943:C:O5' | 1:1:3346:U:C4' | 2.38 | 0.72 |
| 6:C:41:VAL:CA | 6:C:185:GLY:HA3 | 2.21 | 0.70 |
| 1:1:2932:U:P | 15:L:41:GLY:H | 2.14 | 0.70 |
| 1:1:647:A:O3' | 1:1:648:C:H5' | 1.89 | 0.70 |
| 1:1:1943:C:C5' | 1:1:3346:U:C4' | 2.70 | 0.69 |
| 1:1:2681:U:C5' | 8:E:48:SER:C | 2.59 | 0.69 |
| 1:1:729:C:C4' | 20:Q:137:THR:N | 2.55 | 0.69 |
| 1:1:1943:C:H5' | 1:1:3346:U:C4' | 2.23 | 0.69 |
| 1:1:2819:A:H5' | 1:1:2819:A:C4' | 2.15 | 0.68 |
| 1:1:1084:A:O3' | 23:T:35:LYS:CA | 2.42 | 0.68 |
| 1:1:2917:G:P | 15:L:47:ASN:H | 2.17 | 0.67 |
| 1:1:2946:A:H5'' | 1:1:2947:G:H5' | 1.75 | 0.67 |
| 1:1:2397:A:O5' | 1:1:2398:A:H5' | 1.95 | 0.66 |
| 1:1:1943:C:C4' | 1:1:3346:U:C5' | 2.60 | 0.65 |
| 1:1:964:G:C3' | 17:N:40:HIS:CA | 2.75 | 0.65 |
| 1:1:2917:G:H5'' | 15:L:47:ASN:CA | 2.27 | 0.65 |
| 1:1:648:C:H5'' | 1:1:649:A:H5'' | 1.77 | 0.65 |
| 1:1:741:U:C4' | 20:Q:74:GLU:CA | 2.75 | 0.65 |
| 1:1:744:A:C4' | 20:Q:142:GLY:HA2 | 2.28 | 0.63 |
| 1:1:2681:U:C5' | 8:E:49:LYS:C | 2.68 | 0.62 |
| 1:1:2819:A:C4' | 1:1:2819:A:H5'' | 2.15 | 0.62 |
| 1:1:1818:U:C3' | 1:1:1819:U:H5'' | 2.30 | 0.62 |
| 1:1:744:A:C3' | 20:Q:142:GLY:C | 2.68 | 0.62 |
| 1:1:965:A:O3' | 17:N:44:ASN:N | 2.32 | 0.61 |
| 1:1:2372:A:C3' | 1:1:2373:A:H5' | 2.29 | 0.61 |
| 1:1:2818:U:C4' | 1:1:2819:A:H5' | 2.32 | 0.60 |
| 1:1:2674:A:P | 8:E:105:GLY:N | 2.75 | 0.59 |
| 1:1:741:U:C4' | 20:Q:74:GLU:C | 2.71 | 0.59 |
| 1:1:2244:A:P | 5:B:244:GLY:HA2 | 2.43 | 0.58 |
| 1:1:2780:A:O3' | 14:K:181:GLY:HA3 | 2.02 | 0.58 |
| 21:R:46:LYS:C | 22:S:61:ILE:C | 159.71 | 0.58 |
| 1:1:729:C:C4' | 20:Q:137:THR:H | 2.16 | 0.58 |
| 3:3:28:C:C4' | 8:E:135:GLY:HA2 | 2.33 | 0.58 |
| 1:1:729:C:C4' | 20:Q:137:THR:CA | 2.83 | 0.57 |
| 3:3:56:A:O3' | 8:E:149:GLY:CA | 2.53 | 0.57 |
| 1:1:2244:A:P | 5:B:244:GLY:CA | 2.94 | 0.56 |
| 1:1:2681:U:O3' | 8:E:48:SER:CA | 2.55 | 0.55 |
| 1:1:741:U:O3' | 20:Q:74:GLU:N | 2.40 | 0.55 |
| 8:E:94:ARG:C | 8:E:96:PHE:H | 2.09 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:1:741:U:C4' | 20:Q:74:GLU:N | 2.69 | 0.55 |
| 1:1:1226:G:C4' | 1:1:3117:C:C5' | 2.85 | 0.54 |
| 13:J:62:THR:H | 13:J:69:GLY:HA3 | 1.72 | 0.54 |
| 1:1:2995:A:C3' | 1:1:2996:U:H5'' | 2.37 | 0.54 |
| 1:1:1191:U:C4' | 1:1:1192:C:H5' | 2.38 | 0.54 |
| 1:1:965:A:C4' | 17:N:41:HIS:CA | 2.87 | 0.53 |
| 1:1:810:A:H5'' | 18:O:81:TYR:C | 2.28 | 0.53 |
| 1:1:1631:C:H5'' | 1:1:1632:A:H5'' | 1.91 | 0.52 |
| 1:1:1253:U:P | 12:I:94:LYS:C | 2.88 | 0.52 |
| 1:1:2598:G:O3' | 18:O:69:GLY:HA3 | 2.09 | 0.52 |
| 1:1:2747:A:H5' | 19:P:175:HIS:N | 2.25 | 0.52 |
| 19:P:111:GLN:C | 19:P:113:LEU:H | 2.12 | 0.52 |
| 1:1:2747:A:C4' | 19:P:174:PRO:C | 2.78 | 0.52 |
| 1:1:2818:U:C4' | 1:1:2819:A:C5' | 2.88 | 0.52 |
| 1:1:2917:G:C5' | 15:L:47:ASN:N | 2.64 | 0.51 |
| 29:Z:68:GLN:C | 29:Z:70:TYR:H | 2.13 | 0.51 |
| 3:3:56:A:O3' | 8:E:149:GLY:HA3 | 2.09 | 0.51 |
| 1:1:2681:U:H5' | 8:E:49:LYS:C | 2.31 | 0.51 |
| 1:1:2372:A:H5'' | 1:1:2373:A:H5'' | 1.92 | 0.51 |
| 10:G:120:ASN:C | 10:G:122:PHE:H | 2.15 | 0.50 |
| 1:1:965:A:C3' | 17:N:44:ASN:H | 2.25 | 0.50 |
| 1:1:2598:G:O3' | 18:O:69:GLY:CA | 2.60 | 0.49 |
| 1:1:2681:U:C4' | 8:E:48:SER:CA | 2.91 | 0.49 |
| 1:1:2651:G:H5'' | 23:T:23:GLY:CA | 2.37 | 0.49 |
| 1:1:744:A:C4' | 20:Q:143:PRO:N | 2.75 | 0.49 |
| 7:D:338:LYS:C | 7:D:340:GLY:H | 2.16 | 0.48 |
| 1:1:1085:A:H5' | 23:T:36:VAL:N | 2.28 | 0.48 |
| 1:1:873:C:H5'' | 1:1:874:U:O5' | 2.13 | 0.48 |
| 1:1:1874:A:H5'' | 21:R:18:GLY:HA3 | 1.95 | 0.48 |
| 1:1:1191:U:C5' | 1:1:1192:C:H5' | 2.43 | 0.48 |
| 1:1:289:A:H5' | 18:O:95:GLN:C | 2.34 | 0.48 |
| 1:1:730:C:C5' | 20:Q:136:ASN:CA | 2.92 | 0.47 |
| 1:1:741:U:C5' | 20:Q:74:GLU:CA | 2.93 | 0.47 |
| 27:X:90:VAL:C | 27:X:92:GLY:H | 2.18 | 0.47 |
| 1:1:2917:G:P | 15:L:46:LEU:CA | 3.03 | 0.47 |
| 1:1:2681:U:P | 8:E:51:ARG:N | 2.88 | 0.46 |
| 1:1:2946:A:C5' | 1:1:2947:G:H5' | 2.44 | 0.46 |
| 1:1:2747:A:C5' | 19:P:174:PRO:C | 2.84 | 0.46 |
| 9:F:49:ASN:C | 9:F:51:GLN:H | 2.19 | 0.46 |
| 1:1:2674:A:P | 8:E:105:GLY:CA | 3.04 | 0.46 |
| 6:C:199:PHE:C | 6:C:201:LYS:H | 2.19 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 11:H:78:PHE:C | 11:H:80:TYR:H | 2.20 | 0.45 |
| 2:2:80:A:H5' | 2:2:81:U:P | 2.57 | 0.45 |
| 1:1:648:C:C5' | 1:1:649:A:H5'' | 2.44 | 0.44 |
| 1:1:288:C:C5' | 18:O:171:SER:CA | 2.88 | 0.44 |
| 1:1:288:C:C5' | 18:O:171:SER:C | 2.86 | 0.44 |
| 7:D:269:SER:C | 7:D:271:LYS:H | 2.20 | 0.44 |
| 8:E:110:ILE:C | 8:E:112:LEU:H | 2.21 | 0.44 |
| 1:1:32:U:P | 18:O:95:GLN:H | 2.41 | 0.44 |
| 1:1:1878:G:C3' | 1:1:1879:A:H5' | 2.48 | 0.43 |
| 9:F:189:GLU:C | 9:F:191:LEU:H | 2.21 | 0.43 |
| 1:1:2681:U:H5'' | 8:E:49:LYS:C | 2.38 | 0.43 |
| 1:1:769:G:C5' | 14:K:172:LEU:CA | 2.90 | 0.43 |
| 1:1:2674:A:C4' | 8:E:105:GLY:HA3 | 2.49 | 0.43 |
| 1:1:2397:A:P | 1:1:2398:A:H5' | 2.59 | 0.43 |
| 1:1:730:C:H5' | 20:Q:136:ASN:CA | 2.49 | 0.43 |
| 27:X:91:ASN:C | 27:X:93:ALA:H | 2.22 | 0.43 |
| 19:P:56:THR:C | 19:P:58:LYS:H | 2.22 | 0.43 |
| 1:1:2112:U:C4' | 1:1:2113:A:H5' | 2.49 | 0.43 |
| 1:1:288:C:H5'' | 18:O:171:SER:C | 2.39 | 0.42 |
| 1:1:1191:U:H5'' | 1:1:1192:C:H5' | 2.00 | 0.42 |
| 23:T:100:LYS:C | 23:T:102:ARG:H | 2.22 | 0.42 |
| 1:1:939:U:H5' | 1:1:2814:G:O3' | 2.19 | 0.42 |
| 3:3:13:A:C3' | 3:3:14:U:H5' | 2.50 | 0.42 |
| 21:R:46:LYS:N | 22:S:60:SER:CA | 160.47 | 0.42 |
| 1:1:2092:A:H5'' | 21:R:140:GLU:C | 2.39 | 0.42 |
| 1:1:1971:C:C3' | 1:1:1972:A:H5' | 2.50 | 0.42 |
| 1:1:2244:A:P | 5:B:244:GLY:HA3 | 2.59 | 0.42 |
| 11:H:118:GLU:C | 11:H:120:LYS:H | 2.22 | 0.42 |
| 1:1:1226:G:O3' | 1:1:3117:C:C4' | 2.68 | 0.41 |
| 1:1:2681:U:P | 8:E:50:ALA:CA | 3.08 | 0.41 |
| 3:3:57:G:P | 8:E:149:GLY:HA3 | 2.61 | 0.41 |
| 1:1:1226:G:H5'' | 1:1:3117:C:C3' | 2.49 | 0.41 |
| 1:1:1943:C:C3' | 1:1:3346:U:H5' | 2.40 | 0.41 |
| 1:1:2674:A:P | 8:E:105:GLY:HA3 | 2.60 | 0.41 |
| 10:G:120:ASN:C | 10:G:122:PHE:N | 2.74 | 0.41 |
| 1:1:1253:U:P | 12:I:94:LYS:CA | 3.08 | 0.41 |
| 8:E:41:SER:C | 8:E:43:GLN:H | 2.24 | 0.41 |
| 18:O:184:LYS:H | 18:O:186:GLY:H | 1.68 | 0.41 |
| 1:1:2092:A:C5' | 21:R:144:GLN:N | 2.80 | 0.41 |
| 1:1:744:A:C4' | 20:Q:141:ARG:C | 2.89 | 0.41 |
| 3:3:28:C:O3' | 8:E:135:GLY:HA2 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:1:1085:A:H5' | 23:T:36:VAL:CA | 2.51 | 0.40 |
| 1:1:745:C:H5' | 20:Q:144:ARG:H | 1.86 | 0.40 |
| 1:1:2360:C:H5'' | 1:1:2361:A:P | 2.61 | 0.40 |
| 1:1:3317:U:C4' | 1:1:3318:G:O5' | 2.69 | 0.40 |
| 1:1:2681:U:C4' | 8:E:48:SER:C | 2.90 | 0.40 |
| 2:2:79:A:O3' | 2:2:80:A:C4' | 2.70 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 4 | A | 215/217 (99%) | 194 (90%) | 11 (5%) | 10 (5%) | 3 | 32 |
| 5 | B | 250/254 (98%) | 230 (92%) | 14 (6%) | 6 (2%) | 7 | 47 |
| 6 | C | 384/387 (99%) | 333 (87%) | 37 (10%) | 14 (4%) | 4 | 38 |
| 7 | D | 359/362 (99%) | 304 (85%) | 34 (10%) | 21 (6%) | 2 | 27 |
| 8 | E | 167/174 (96%) | 120 (72%) | 26 (16%) | 21 (13%) | 0 | 8 |
| 9 | F | 189/191 (99%) | 166 (88%) | 17 (9%) | 6 (3%) | 5 | 41 |
| 10 | G | 173/176 (98%) | 147 (85%) | 16 (9%) | 10 (6%) | 2 | 27 |
| 11 | H | 231/256 (90%) | 186 (80%) | 26 (11%) | 19 (8%) | 1 | 18 |
| 12 | I | 125/165 (76%) | 107 (86%) | 11 (9%) | 7 (6%) | 2 | 28 |
| 13 | J | 195/199 (98%) | 180 (92%) | 11 (6%) | 4 (2%) | 9 | 50 |
| 14 | K | 191/199 (96%) | 161 (84%) | 18 (9%) | 12 (6%) | 2 | 25 |
| 15 | L | 134/137 (98%) | 124 (92%) | 9 (7%) | 1 (1%) | 26 | 71 |
| 16 | M | 134/138 (97%) | 117 (87%) | 8 (6%) | 9 (7%) | 1 | 24 |
| 17 | N | 146/149 (98%) | 120 (82%) | 15 (10%) | 11 (8%) | 1 | 21 |
| 18 | O | 201/204 (98%) | 184 (92%) | 10 (5%) | 7 (4%) | 4 | 39 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 19 | P | 265/297 (89%) | 220 (83%) | 27 (10%) | 18 (7%) | 1 | 23 |
| 20 | Q | 183/186 (98%) | 163 (89%) | 16 (9%) | 4 (2%) | 8 | 49 |
| 21 | R | 186/189 (98%) | 170 (91%) | 12 (6%) | 4 (2%) | 8 | 49 |
| 22 | S | 170/172 (99%) | 154 (91%) | 12 (7%) | 4 (2%) | 7 | 47 |
| 23 | T | 157/160 (98%) | 140 (89%) | 10 (6%) | 7 (4%) | 3 | 33 |
| 24 | U | 181/184 (98%) | 155 (86%) | 17 (9%) | 9 (5%) | 3 | 31 |
| 25 | V | 98/121 (81%) | 75 (76%) | 14 (14%) | 9 (9%) | 1 | 17 |
| 26 | W | 119/142 (84%) | 106 (89%) | 11 (9%) | 2 (2%) | 11 | 55 |
| 27 | X | 124/127 (98%) | 107 (86%) | 15 (12%) | 2 (2%) | 12 | 56 |
| 28 | Y | 133/136 (98%) | 114 (86%) | 9 (7%) | 10 (8%) | 1 | 21 |
| 29 | Z | 117/120 (98%) | 99 (85%) | 10 (8%) | 8 (7%) | 1 | 23 |
| 30 | a | 220/244 (90%) | 200 (91%) | 11 (5%) | 9 (4%) | 3 | 35 |
| 31 | b | 95/105 (90%) | 86 (90%) | 8 (8%) | 1 (1%) | 17 | 63 |
| 32 | c | 107/113 (95%) | 94 (88%) | 8 (8%) | 5 (5%) | 3 | 32 |
| 33 | d | 125/130 (96%) | 111 (89%) | 10 (8%) | 4 (3%) | 5 | 41 |
| 34 | e | 104/107 (97%) | 100 (96%) | 2 (2%) | 2 (2%) | 10 | 52 |
| 35 | f | 110/121 (91%) | 97 (88%) | 9 (8%) | 4 (4%) | 4 | 38 |
| 36 | g | 97/100 (97%) | 75 (77%) | 11 (11%) | 11 (11%) | 0 | 10 |
| 37 | h | 85/88 (97%) | 71 (84%) | 11 (13%) | 3 (4%) | 4 | 39 |
| 38 | i | 75/78 (96%) | 66 (88%) | 8 (11%) | 1 (1%) | 15 | 60 |
| 39 | j | 48/51 (94%) | 44 (92%) | 4 (8%) | 0 | 100 | 100 |
| 40 | k | 89/92 (97%) | 77 (86%) | 9 (10%) | 3 (3%) | 5 | 40 |
| 41 | l | 376/593 (63%) | 354 (94%) | 14 (4%) | 8 (2%) | 9 | 50 |
| 42 | m | 222/245 (91%) | 208 (94%) | 13 (6%) | 1 (0%) | 34 | 77 |
| 43 | n | 234/236 (99%) | 219 (94%) | 9 (4%) | 6 (3%) | 7 | 45 |
| 44 | o | 345/647 (53%) | 330 (96%) | 9 (3%) | 6 (2%) | 11 | 55 |
| 45 | p | 61/199 (31%) | 53 (87%) | 4 (7%) | 4 (7%) | 1 | 24 |
| 46 | q | 439/515 (85%) | 377 (86%) | 40 (9%) | 22 (5%) | 3 | 31 |
| 47 | r | 320/322 (99%) | 266 (83%) | 31 (10%) | 23 (7%) | 1 | 22 |
| 47 | s | 320/322 (99%) | 266 (83%) | 31 (10%) | 23 (7%) | 1 | 22 |
| All | All | 8299/9350 (89%) | 7270 (88%) | 658 (8%) | 371 (4%) | 6 | 33 |

All (371) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | A | 21 | ASN |
| 4 | A | 74 | VAL |
| 4 | A | 135 | PRO |
| 4 | A | 151 | VAL |
| 5 | B | 144 | ASN |
| 6 | C | 3 | HIS |
| 6 | C | 5 | LYS |
| 6 | C | 140 | ASP |
| 6 | C | 174 | LYS |
| 6 | C | 300 | ARG |
| 6 | C | 347 | SER |
| 6 | C | 351 | LEU |
| 6 | C | 385 | LYS |
| 7 | D | 4 | PRO |
| 7 | D | 268 | ALA |
| 7 | D | 269 | SER |
| 7 | D | 283 | THR |
| 7 | D | 292 | SER |
| 7 | D | 320 | ASN |
| 7 | D | 338 | LYS |
| 7 | D | 361 | HIS |
| 8 | E | 8 | PRO |
| 8 | E | 11 | ASP |
| 8 | E | 12 | LEU |
| 8 | E | 74 | PRO |
| 8 | E | 94 | ARG |
| 8 | E | 165 | GLN |
| 9 | F | 50 | ASN |
| 9 | F | 109 | ALA |
| 10 | G | 6 | ALA |
| 10 | G | 98 | VAL |
| 10 | G | 121 | LEU |
| 10 | G | 122 | PHE |
| 11 | H | 25 | PRO |
| 11 | H | 31 | PRO |
| 11 | H | 36 | ILE |
| 11 | H | 37 | GLY |
| 11 | H | 156 | ASP |
| 12 | I | 37 | LEU |
| 12 | I | 51 | LYS |
| 12 | I | 75 | PRO |
| 12 | I | 76 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | J | 110 | PRO |
| 13 | J | 111 | PRO |
| 13 | J | 182 | ASN |
| 14 | K | 5 | LYS |
| 14 | K | 47 | ALA |
| 14 | K | 50 | PRO |
| 14 | K | 129 | ASN |
| 14 | K | 131 | LYS |
| 14 | K | 193 | ALA |
| 16 | M | 8 | LYS |
| 16 | M | 9 | ALA |
| 16 | M | 135 | LEU |
| 16 | M | 136 | ALA |
| 17 | N | 66 | ALA |
| 17 | N | 76 | ASP |
| 18 | O | 74 | PRO |
| 18 | O | 75 | VAL |
| 19 | P | 20 | PHE |
| 19 | P | 58 | LYS |
| 19 | P | 210 | GLU |
| 19 | P | 233 | ALA |
| 19 | P | 234 | ASP |
| 19 | P | 258 | LYS |
| 19 | P | 276 | LYS |
| 19 | P | 293 | LEU |
| 19 | P | 295 | GLY |
| 20 | Q | 99 | THR |
| 21 | R | 5 | ARG |
| 21 | R | 47 | ASN |
| 22 | S | 167 | ARG |
| 23 | T | 124 | VAL |
| 23 | T | 159 | PHE |
| 24 | U | 157 | VAL |
| 24 | U | 182 | ILE |
| 25 | V | 107 | PHE |
| 26 | W | 44 | PRO |
| 27 | X | 84 | LYS |
| 28 | Y | 17 | ARG |
| 28 | Y | 59 | ALA |
| 28 | Y | 125 | GLY |
| 28 | Y | 128 | GLN |
| 28 | Y | 129 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | Z | 97 | ALA |
| 29 | Z | 119 | LYS |
| 30 | a | 25 | GLN |
| 30 | a | 26 | VAL |
| 30 | a | 216 | VAL |
| 31 | b | 100 | ILE |
| 32 | c | 5 | LYS |
| 32 | c | 6 | ASP |
| 32 | c | 7 | VAL |
| 32 | c | 83 | GLU |
| 32 | c | 84 | ASP |
| 33 | d | 12 | LYS |
| 33 | d | 27 | ARG |
| 33 | d | 123 | LYS |
| 36 | g | 13 | LYS |
| 36 | g | 33 | ALA |
| 37 | h | 85 | LYS |
| 41 | l | 62 | PRO |
| 41 | l | 169 | ILE |
| 43 | n | 18 | LYS |
| 43 | n | 25 | ARG |
| 43 | n | 133 | LEU |
| 44 | o | 203 | SER |
| 45 | p | 15 | PRO |
| 45 | p | 33 | ARG |
| 46 | q | 77 | TYR |
| 46 | q | 83 | ILE |
| 46 | q | 84 | GLN |
| 46 | q | 91 | PRO |
| 46 | q | 107 | LYS |
| 46 | q | 124 | ARG |
| 46 | q | 132 | VAL |
| 46 | q | 133 | THR |
| 46 | q | 391 | SER |
| 46 | q | 455 | ASP |
| 47 | r | 81 | LEU |
| 47 | r | 107 | ALA |
| 47 | r | 133 | THR |
| 47 | r | 134 | THR |
| 47 | r | 153 | VAL |
| 47 | r | 194 | VAL |
| 47 | r | 216 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | r | 227 | ILE |
| 47 | r | 238 | GLN |
| 47 | r | 269 | GLN |
| 47 | r | 294 | ALA |
| 47 | r | 296 | SER |
| 47 | r | 308 | PRO |
| 47 | s | 81 | LEU |
| 47 | s | 107 | ALA |
| 47 | s | 133 | THR |
| 47 | s | 134 | THR |
| 47 | s | 153 | VAL |
| 47 | s | 194 | VAL |
| 47 | s | 216 | TYR |
| 47 | s | 227 | ILE |
| 47 | s | 238 | GLN |
| 47 | s | 269 | GLN |
| 47 | s | 294 | ALA |
| 47 | s | 296 | SER |
| 47 | s | 308 | PRO |
| 4 | A | 99 | LEU |
| 4 | A | 168 | ALA |
| 4 | A | 198 | TRP |
| 4 | A | 199 | GLN |
| 5 | B | 13 | GLY |
| 5 | B | 70 | ARG |
| 6 | C | 136 | LYS |
| 6 | C | 138 | ALA |
| 7 | D | 15 | ALA |
| 7 | D | 107 | ARG |
| 7 | D | 182 | LEU |
| 7 | D | 232 | SER |
| 7 | D | 311 | HIS |
| 7 | D | 317 | PRO |
| 8 | E | 9 | MET |
| 8 | E | 73 | GLY |
| 8 | E | 86 | VAL |
| 8 | E | 115 | LYS |
| 8 | E | 167 | TYR |
| 10 | G | 97 | ASN |
| 10 | G | 123 | PRO |
| 11 | H | 39 | ALA |
| 11 | H | 115 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | H | 159 | PRO |
| 11 | H | 254 | ASP |
| 12 | I | 32 | ILE |
| 12 | I | 77 | ALA |
| 14 | K | 136 | GLU |
| 14 | K | 141 | ALA |
| 15 | L | 82 | ALA |
| 16 | M | 10 | SER |
| 17 | N | 47 | LYS |
| 17 | N | 57 | GLY |
| 17 | N | 121 | VAL |
| 18 | O | 144 | ARG |
| 18 | O | 184 | LYS |
| 19 | P | 188 | GLU |
| 19 | P | 209 | GLU |
| 19 | P | 215 | ASP |
| 19 | P | 292 | ALA |
| 20 | Q | 98 | LYS |
| 20 | Q | 183 | GLY |
| 22 | S | 2 | ALA |
| 22 | S | 12 | ARG |
| 22 | S | 13 | ARG |
| 23 | T | 125 | ALA |
| 24 | U | 164 | LYS |
| 25 | V | 11 | ILE |
| 25 | V | 50 | LEU |
| 25 | V | 51 | GLY |
| 25 | V | 91 | ASP |
| 26 | W | 45 | LYS |
| 27 | X | 92 | GLY |
| 29 | Z | 90 | ARG |
| 29 | Z | 95 | PHE |
| 29 | Z | 96 | GLU |
| 30 | a | 24 | GLU |
| 30 | a | 175 | LYS |
| 35 | f | 74 | ARG |
| 35 | f | 77 | GLY |
| 36 | g | 28 | TYR |
| 36 | g | 49 | GLY |
| 36 | g | 50 | LEU |
| 37 | h | 65 | ARG |
| 40 | k | 60 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | l | 61 | VAL |
| 41 | l | 354 | ILE |
| 43 | n | 170 | GLU |
| 44 | o | 87 | GLU |
| 45 | p | 62 | GLU |
| 46 | q | 106 | ILE |
| 46 | q | 129 | VAL |
| 46 | q | 146 | ILE |
| 46 | q | 154 | HIS |
| 46 | q | 308 | SER |
| 46 | q | 309 | GLN |
| 46 | q | 318 | SER |
| 47 | r | 45 | ILE |
| 47 | r | 108 | ASN |
| 47 | r | 230 | ASN |
| 47 | r | 276 | GLU |
| 47 | s | 45 | ILE |
| 47 | s | 108 | ASN |
| 47 | s | 230 | ASN |
| 47 | s | 276 | GLU |
| 4 | A | 137 | PRO |
| 5 | B | 250 | GLN |
| 6 | C | 4 | ARG |
| 7 | D | 14 | GLU |
| 7 | D | 16 | THR |
| 8 | E | 140 | ARG |
| 8 | E | 169 | ALA |
| 8 | E | 173 | ASP |
| 9 | F | 42 | ASP |
| 11 | H | 78 | PHE |
| 11 | H | 122 | LYS |
| 14 | K | 134 | GLU |
| 14 | K | 166 | ALA |
| 16 | M | 28 | SER |
| 16 | M | 95 | ALA |
| 17 | N | 93 | SER |
| 18 | O | 145 | ASP |
| 19 | P | 112 | LYS |
| 21 | R | 53 | LYS |
| 21 | R | 64 | ARG |
| 23 | T | 114 | ALA |
| 24 | U | 160 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | V | 10 | LYS |
| 25 | V | 44 | GLU |
| 28 | Y | 16 | GLY |
| 28 | Y | 35 | SER |
| 28 | Y | 102 | GLU |
| 29 | Z | 4 | VAL |
| 29 | Z | 91 | ALA |
| 35 | f | 46 | ASP |
| 35 | f | 98 | GLN |
| 36 | g | 34 | SER |
| 36 | g | 95 | ALA |
| 36 | g | 98 | ARG |
| 40 | k | 58 | SER |
| 41 | l | 173 | THR |
| 41 | l | 175 | PRO |
| 43 | n | 5 | LYS |
| 43 | n | 23 | LYS |
| 44 | o | 311 | GLU |
| 44 | o | 342 | SER |
| 45 | p | 61 | LYS |
| 46 | q | 486 | LYS |
| 47 | r | 259 | GLU |
| 47 | s | 259 | GLU |
| 6 | C | 386 | ASP |
| 7 | D | 146 | PRO |
| 7 | D | 233 | LEU |
| 8 | E | 95 | ASN |
| 8 | E | 108 | GLU |
| 8 | E | 114 | ILE |
| 8 | E | 117 | ASP |
| 9 | F | 13 | PRO |
| 10 | G | 95 | GLY |
| 10 | G | 129 | GLU |
| 11 | H | 157 | VAL |
| 11 | H | 253 | SER |
| 13 | J | 181 | ALA |
| 17 | N | 96 | LYS |
| 18 | O | 94 | TYR |
| 18 | O | 149 | ASN |
| 19 | P | 6 | ASP |
| 19 | P | 252 | ALA |
| 19 | P | 253 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | Q | 162 | ALA |
| 23 | T | 12 | ARG |
| 24 | U | 158 | ALA |
| 24 | U | 161 | ALA |
| 24 | U | 163 | LYS |
| 25 | V | 31 | ALA |
| 25 | V | 49 | ASN |
| 28 | Y | 103 | GLN |
| 29 | Z | 27 | GLU |
| 30 | a | 160 | ARG |
| 33 | d | 40 | SER |
| 37 | h | 25 | ARG |
| 38 | i | 33 | LYS |
| 40 | k | 51 | ALA |
| 46 | q | 49 | LEU |
| 47 | r | 87 | LYS |
| 47 | r | 307 | ALA |
| 47 | r | 310 | ILE |
| 47 | s | 87 | LYS |
| 47 | s | 307 | ALA |
| 47 | s | 310 | ILE |
| 5 | B | 35 | ALA |
| 5 | B | 251 | LYS |
| 7 | D | 5 | GLN |
| 8 | E | 24 | GLY |
| 8 | E | 111 | ASP |
| 8 | E | 172 | LEU |
| 9 | F | 2 | LYS |
| 9 | F | 107 | ASP |
| 10 | G | 108 | LYS |
| 11 | H | 47 | SER |
| 12 | I | 95 | ASP |
| 14 | K | 130 | GLY |
| 14 | K | 133 | PRO |
| 16 | M | 6 | ILE |
| 16 | M | 36 | VAL |
| 17 | N | 56 | VAL |
| 17 | N | 117 | ARG |
| 23 | T | 18 | ASP |
| 30 | a | 178 | ILE |
| 34 | e | 59 | VAL |
| 36 | g | 3 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | r | 167 | ARG |
| 47 | r | 295 | GLU |
| 47 | s | 167 | ARG |
| 47 | s | 295 | GLU |
| 4 | A | 134 | PHE |
| 6 | C | 155 | ALA |
| 6 | C | 317 | ILE |
| 7 | D | 72 | ALA |
| 10 | G | 130 | ILE |
| 11 | H | 75 | ILE |
| 17 | N | 91 | LEU |
| 19 | P | 259 | LYS |
| 24 | U | 162 | GLU |
| 30 | a | 164 | SER |
| 34 | e | 91 | ALA |
| 36 | g | 21 | THR |
| 36 | g | 94 | ILE |
| 44 | o | 221 | THR |
| 17 | N | 29 | PRO |
| 41 | l | 389 | PRO |
| 11 | H | 158 | ASP |
| 30 | a | 91 | GLY |
| 41 | l | 550 | VAL |
| 44 | o | 344 | ILE |
| 46 | q | 73 | ASP |
| 11 | H | 116 | VAL |
| 11 | H | 119 | GLY |
| 11 | H | 135 | GLY |
| 28 | Y | 36 | HIS |
| 7 | D | 131 | VAL |
| 24 | U | 84 | PRO |
| 42 | m | 58 | ILE |
| 46 | q | 387 | ASN |
| 46 | q | 483 | PRO |
| 23 | T | 123 | GLY |

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|----------|-------------------|-----------------|
| 1 | 1 | 0/3396 | - | - |
| 2 | 2 | 0/158 | - | - |
| 3 | 3 | 0/121 | - | - |
| All | All | 0/3675 | - | - |

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 ⓘ

There are no ligands in this entry.

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.