



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 10:40 AM EDT

PDB ID : 5LMN
EMDB ID: : EMD-4073
Title : Structure of bacterial 30S-IF1-IF3-mRNA translation pre-initiation complex (state-1A)
Authors : Hussain, T.; Llacer, J.L.; Wimberly, B.T.; Ramakrishnan, V.
Deposited on : 2016-08-01
Resolution : 3.55 Å(reported)

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) : rb-20027939

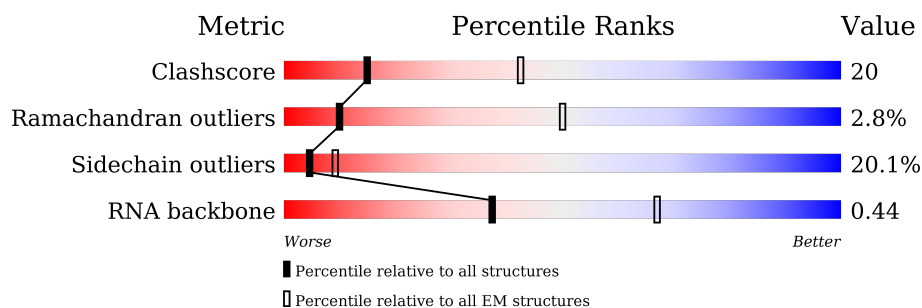
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.55 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 |
| Sidechain outliers | 111093 | 686 |
| 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 | A | 1522 | 23% 57% 17% .. |
| 2 | B | 256 | 45% 32% 13% . 9% |
| 3 | C | 239 | 55% 27% 5% 14% |
| 4 | D | 209 | 56% 35% 9% |
| 5 | E | 162 | 60% 27% 6% 7% |
| 6 | F | 101 | 59% 38% .. |
| 7 | G | 156 | 66% 31% . |
| 8 | H | 138 | 56% 34% 10% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 9 | I | 128 |  |
| 10 | J | 105 |  |
| 11 | K | 129 |  |
| 12 | L | 132 |  |
| 13 | M | 126 |  |
| 14 | N | 61 |  |
| 15 | O | 89 |  |
| 16 | P | 88 |  |
| 17 | Q | 105 |  |
| 18 | R | 88 |  |
| 19 | S | 93 |  |
| 20 | T | 106 |  |
| 21 | V | 27 |  |
| 22 | W | 72 |  |
| 23 | X | 171 |  |
| 24 | Y | 42 |  |

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 54149 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 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1 | A | 1514 | Total | C | N | O | P | 0 | 0 |
| | | | 32527 | 14481 | 6019 | 10515 | 1512 | | |

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

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

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

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 9 | I | 127 | Total | C | N | O | 0 | 0 |
| | | | 999 | 633 | 193 | 173 | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | K | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 892 | 554 | 169 | 166 | 3 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | L | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 970 | 611 | 195 | 163 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | M | 117 | Total | C | N | O | S | 0 | 0 |
| | | | 933 | 577 | 192 | 162 | 2 | | |

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 18 | R | 73 | Total | C | N | O | 0 | 0 |
| | | | 598 | 381 | 118 | 99 | | |

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

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

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

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

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

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

- Molecule 22 is a protein called Translation initiation factor IF-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | W | 71 | Total | C | N | O | S | 0 | 0 |
| | | | 570 | 362 | 103 | 103 | 2 | | |

- Molecule 23 is a protein called Translation initiation factor IF-3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | X | 168 | Total | C | N | O | S | 0 | 0 |
| | | | 1356 | 853 | 249 | 245 | 9 | | |

- Molecule 24 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 24 | Y | 20 | Total | C | N | O | P | 0 | 0 |
| | | | 439 | 196 | 89 | 134 | 20 | | |

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

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|-----|---------|
| 25 | A | 126 | Total | Mg | 0 |
| | | | 126 | 126 | |
| 25 | N | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

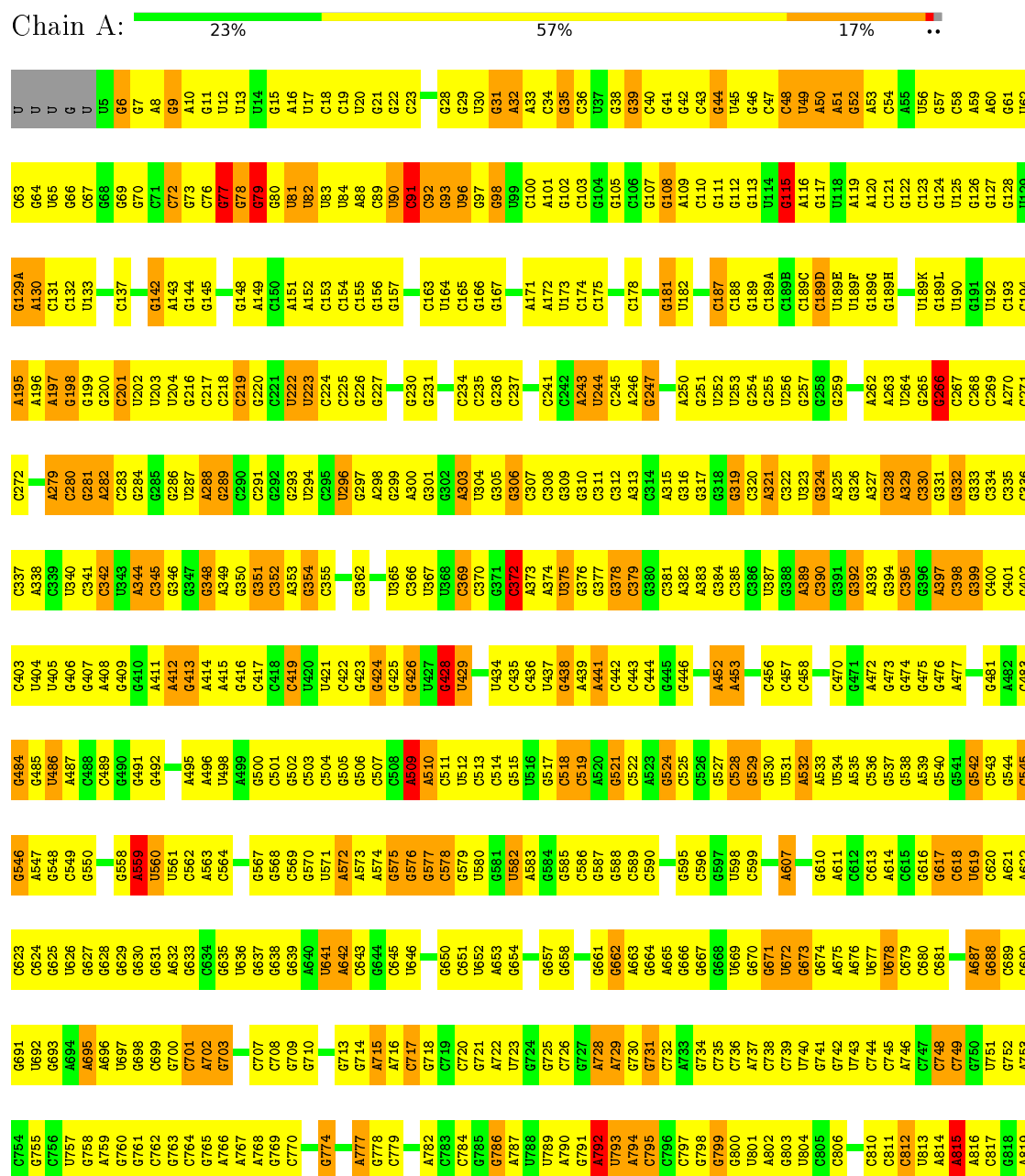
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

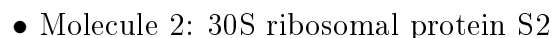
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 26 | D | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 26 | N | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

3 Residue-property plots

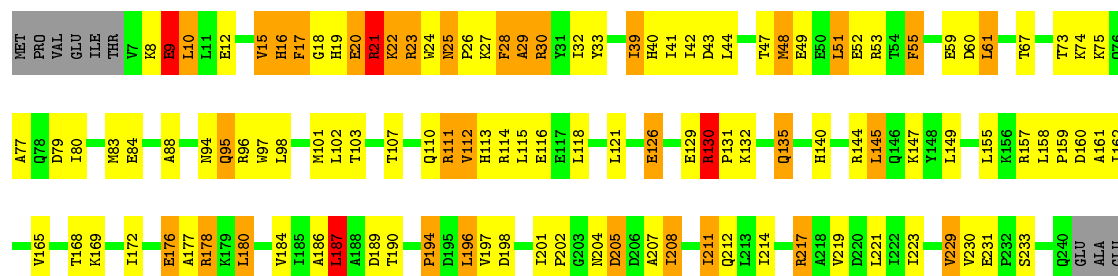
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: 16S ribosomal RNA






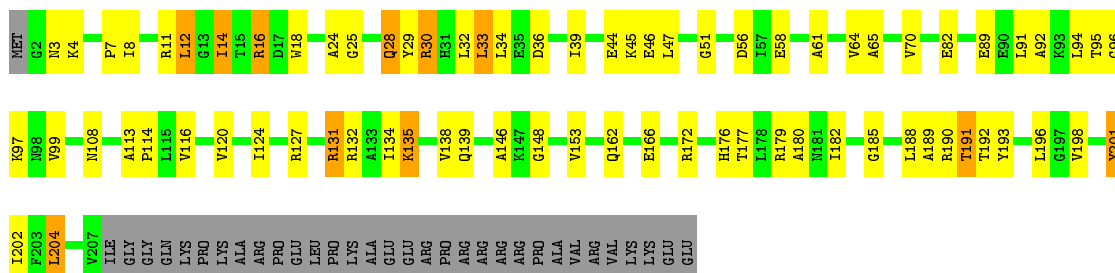
Chain B:  45% 32% 13% 2% 8%



ALA
THR
GLU
THR
PRO
GLU
GLY
GLU
SER
GLU
VAL
GLU
ALA

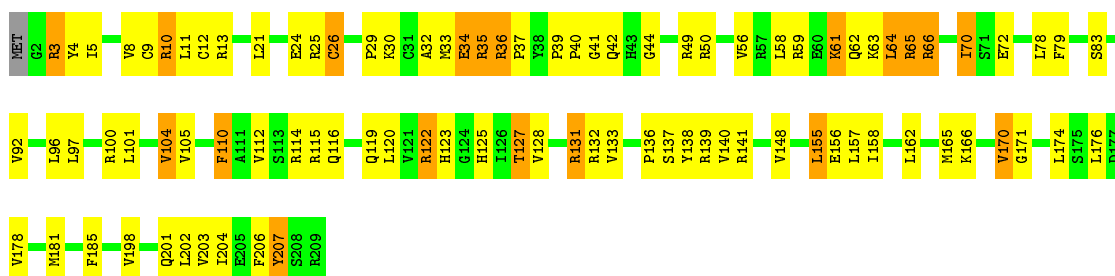
- Molecule 3: 30S ribosomal protein S3

Chain C:  55% 27% 5% 14%



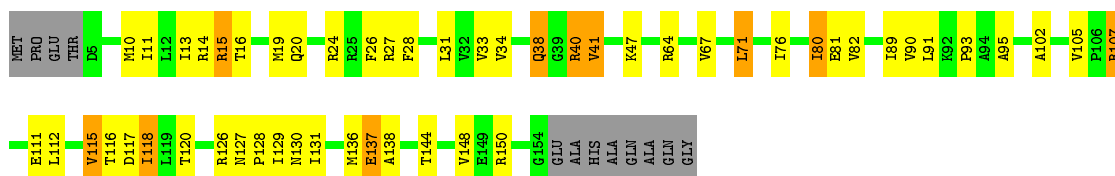
- Molecule 4: 30S ribosomal protein S4

Chain D:  56% 35% 9%



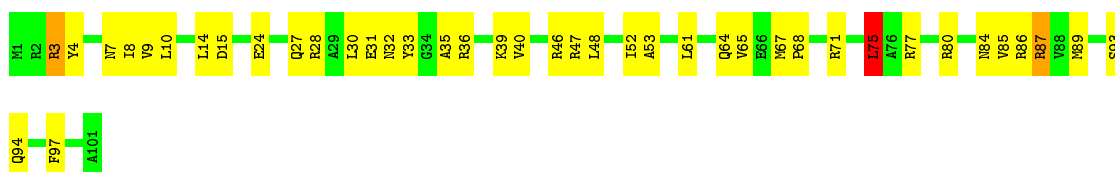
- Molecule 5: 30S ribosomal protein S5

Chain E:  60% 27% 6% 7%



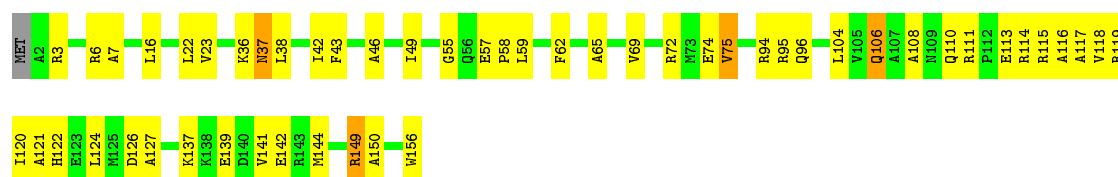
- Molecule 6: 30S ribosomal protein S6

Chain F:  59% 38% 2% 1%



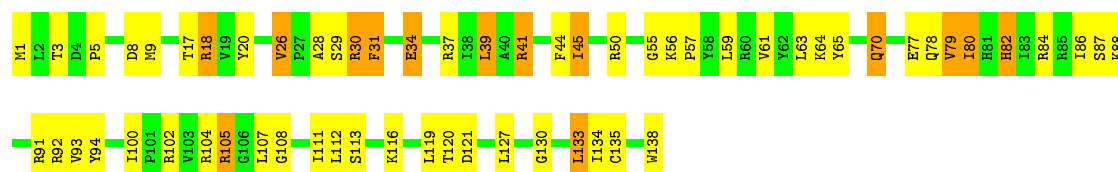
- Molecule 7: 30S ribosomal protein S7

Chain G:  66% 31% 2% 1%



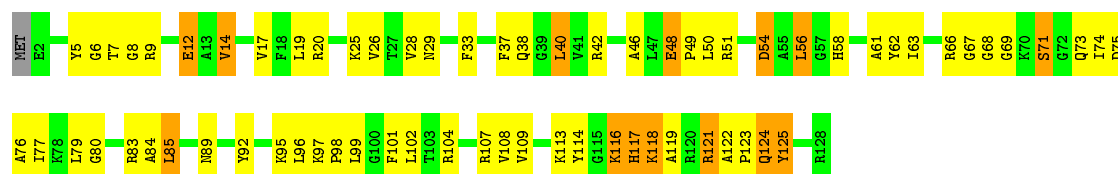
- Molecule 8: 30S ribosomal protein S8

Chain H: 56% 34% 10%



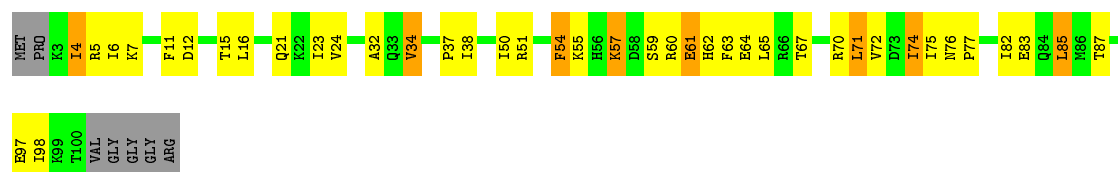
- Molecule 9: 30S ribosomal protein S9

Chain I: 45% 43% 11%



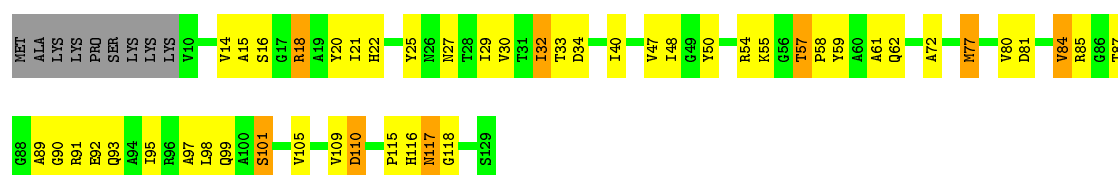
- Molecule 10: 30S ribosomal protein S10

Chain J: 54% 31% 8% 7%



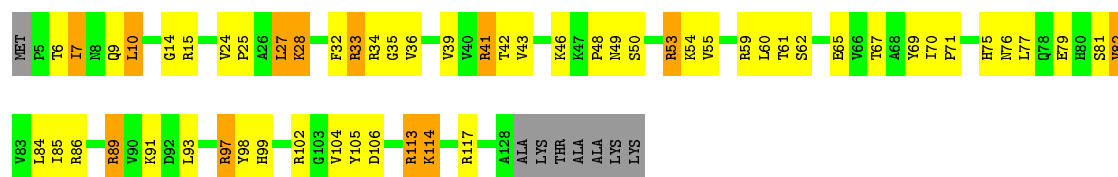
- Molecule 11: 30S ribosomal protein S11

Chain K: 55% 32% 6% 7%



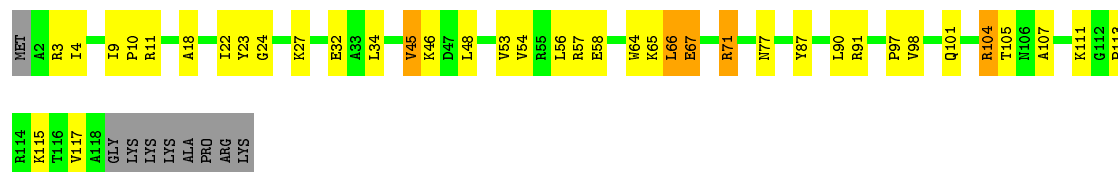
- Molecule 12: 30S ribosomal protein S12

Chain L: 51% 34% 9% 6%



- Molecule 13: 30S ribosomal protein S13

Chain M: 62% 27% 7%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain N: 39% 48% 11%



- Molecule 15: 30S ribosomal protein S15

Chain O: 69% 25%



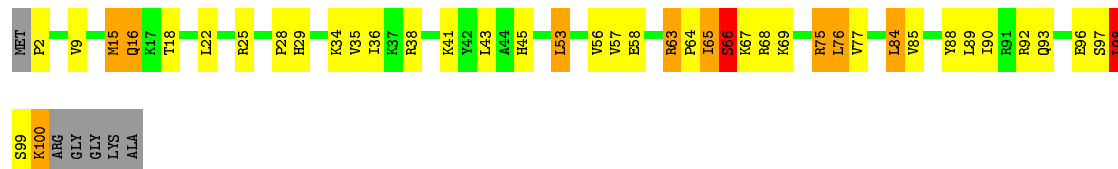
- Molecule 16: 30S ribosomal protein S16

Chain P: 64% 24% 6% 6%



- Molecule 17: 30S ribosomal protein S17

Chain Q: 54% 30% 9% 6%



- Molecule 18: 30S ribosomal protein S18

Chain R: 47% 31% 6% 17%



- | | P1 | P2 | P3 | P4 | P5 | P6 | P7 | P8 | P9 | P10 | P11 | P12 | P13 | P14 | P15 | P16 | P17 | P18 | P19 | P20 | P21 | P22 | P23 | P24 | P25 | P26 | P27 | P28 | P29 | P30 | P31 | P32 | P33 | P34 | P35 | P36 | P37 | P38 | P39 | P40 | P41 | P42 | P43 | P44 | P45 | P46 | P47 | P48 | P49 | P50 | P51 | P52 | P53 | P54 | P55 | P56 | P57 | P58 | P59 | P60 | P61 | P62 | P63 | P64 | P65 | P66 | P67 | P68 | P69 | P70 | P71 | P72 | P73 | P74 | P75 | P76 | P77 | P78 | P79 | P80 | P81 | P82 | P83 | P84 | P85 | P86 | P87 | P88 | P89 | P90 | P91 | P92 | P93 | P94 | P95 | P96 | P97 | P98 | P99 | P100 | P101 | P102 | P103 | P104 | P105 | P106 | P107 | P108 | P109 | P110 | P111 | P112 | P113 | P114 | P115 | P116 | P117 | P118 | P119 | P120 | P121 | P122 | P123 | P124 | P125 | P126 | P127 | P128 | P129 | P130 | P131 | P132 | P133 | P134 | P135 | P136 | P137 | P138 | P139 | P140 | P141 | P142 | P143 | P144 | P145 | P146 | P147 | P148 | P149 | P150 | P151 | P152 | P153 | P154 | P155 | P156 | P157 | P158 | P159 | P160 | P161 | P162 | P163 | P164 | P165 | P166 | P167 | P168 | P169 | P170 | P171 | P172 | P173 | P174 | P175 | P176 | P177 | P178 | P179 | P180 | P181 | P182 | P183 | P184 | P185 | P186 | P187 | P188 | P189 | P190 | P191 | P192 | P193 | P194 | P195 | P196 | P197 | P198 | P199 | P200 | P201 | P202 | P203 | P204 | P205 | P206 | P207 | P208 | P209 | P210 | P211 | P212 | P213 | P214 | P215 | P216 | P217 | P218 | P219 | P220 | P221 | P222 | P223 | P224 | P225 | P226 | P227 | P228 | P229 | P230 | P231 | P232 | P233 | P234 | P235 | P236 | P237 | P238 | P239 | P240 | P241 | P242 | P243 | P244 | P245 | P246 | P247 | P248 | P249 | P250 | P251 | P252 | P253 | P254 | P255 | P256 | P257 | P258 | P259 | P260 | P261 | P262 | P263 | P264 | P265 | P266 | P267 | P268 | P269 | P270 | P271 | P272 | P273 | P274 | P275 | P276 | P277 | P278 | P279 | P280 | P281 | P282 | P283 | P284 | P285 | P286 | P287 | P288 | P289 | P290 | P291 | P292 | P293 | P294 | P295 | P296 | P297 | P298 | P299 | P300 | P301 | P302 | P303 | P304 | P305 | P306 | P307 | P308 | P309 | P310 | P311 | P312 | P313 | P314 | P315 | P316 | P317 | P318 | P319 | P320 | P321 | P322 | P323 | P324 | P325 | P326 | P327 | P328 | P329 | P330 | P331 | P332 | P333 | P334 | P335 | P336 | P337 | P338 | P339 | P340 | P341 | P342 | P343 | P344 | P345 | P346 | P347 | P348 | P349 | P350 | P351 | P352 | P353 | P354 | P355 | P356 | P357 | P358 | P359 | P360 | P361 | P362 | P363 | P364 | P365 | P366 | P367 | P368 | P369 | P370 | P371 | P372 | P373 | P374 | P375 | P376 | P377 | P378 | P379 | P380 | P381 | P382 | P383 | P384 | P385 | P386 | P387 | P388 | P389 | P390 | P391 | P392 | P393 | P394 | P395 | P396 | P397 | P398 | P399 | P400 | P401 | P402 | P403 | P404 | P405 | P406 | P407 | P408 | P409 | P410 | P411 | P412 | P413 | P414 | P415 | P416 | P417 | P418 | P419 | P420 | P421 | P422 | P423 | P424 | P425 | P426 | P427 | P428 | P429 | P430 | P431 | P432 | P433 | P434 | P435 | P436 | P437 | P438 | P439 | P440 | P441 | P442 | P443 | P444 | P445 | P446 | P447 | P448 | P449 | P450 | P451 | P452 | P453 | P454 | P455 | P456 | P457 | P458 | P459 | P460 | P461 | P462 | P463 | P464 | P465 | P466 | P467 | P468 | P469 | P470 | P471 | P472 | P473 | P474 | P475 | P476 | P477 | P478 | P479 | P480 | P481 | P482 | P483 | P484 | P485 | P486 | P487 | P488 | P489 | P490 | P491 | P492 | P493 | P494 | P495 | P496 | P497 | P498 | P499 | P500 | P501 | P502 | P503 | P504 | P505 | P506 | P507 | P508 | P509 | P510 | P511 | P512 | P513 | P514 | P515 | P516 | P517 | P518 | P519 | P520 | P521 | P522 | P523 | P52 |
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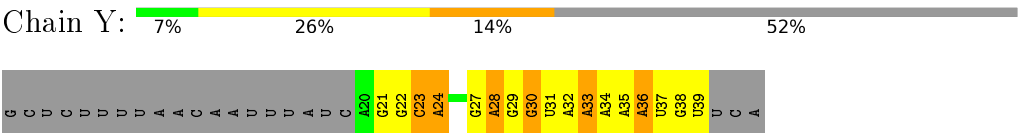
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| MET | G2 | K3 | G4 | D5 | R6 | R7 | T8 | R9 | R10 | G11 | K12 | I13 | W14 | R15 | | K20 | Y21 | R22 | | K25 | LYS | LYS |
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- | Mutation Type | Count |
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| MET | 1 |
| A1 | 1 |
| K2 | 1 |
| V12 | 1 |
| V13 | 1 |
| T14 | 1 |
| E15 | 1 |
| A16 | 1 |
| L17 | 1 |
| P18 | 1 |
| P19 | 1 |
| A20 | 1 |
| T21 | 1 |
| F22 | 1 |
| R23 | 1 |
| V24 | 1 |
| T32 | 1 |
| L33 | 1 |
| M40 | 1 |
| I45 | 1 |
| R46 | 1 |
| I47 | 1 |
| L48 | 1 |
| D51 | 1 |
| R52 | 1 |
| V53 | 1 |
| T58 | 1 |
| T63 | 1 |
| V68 | 1 |
| Y69 | 1 |
| R70 | 1 |
| K71 | 1 |

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| Ti19 | Ti20 | M11 | F122 | Ri23 | Pi30 | Ei31 | L132 | G133 | Ei34 | Ri35 | I136 | L137 | L147 | I148 | V149 | M152 | M156 | D160 | M161 | M162 | M163 | L164 | V168 | K169 | V170 | SER | ALA |
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4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of particles used | 86892 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | FEI POLARA 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | Not provided | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 3500 | Depositor |
| Magnification | 78000 | Depositor |
| Image detector | Not provided | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 | A | 0.38 | 5/36403 (0.0%) | 0.76 | 22/56800 (0.0%) |
| 10 | J | 0.44 | 0/805 | 0.73 | 0/1082 |
| 11 | K | 0.43 | 0/907 | 0.71 | 0/1223 |
| 12 | L | 0.47 | 0/986 | 0.86 | 0/1320 |
| 13 | M | 0.43 | 0/943 | 0.76 | 0/1265 |
| 14 | N | 0.43 | 0/501 | 0.82 | 0/664 |
| 15 | O | 0.46 | 0/745 | 0.90 | 1/992 (0.1%) |
| 16 | P | 0.55 | 0/716 | 0.85 | 1/963 (0.1%) |
| 17 | Q | 0.46 | 0/836 | 0.82 | 0/1117 |
| 18 | R | 0.44 | 0/604 | 0.83 | 0/801 |
| 19 | S | 0.41 | 0/661 | 0.70 | 0/890 |
| 2 | B | 0.43 | 0/1935 | 0.77 | 2/2609 (0.1%) |
| 20 | T | 0.46 | 0/765 | 0.90 | 0/1007 |
| 21 | V | 0.47 | 0/212 | 0.79 | 0/277 |
| 22 | W | 0.44 | 0/580 | 0.76 | 0/782 |
| 23 | X | 0.42 | 0/1375 | 0.77 | 0/1844 |
| 24 | Y | 0.33 | 0/494 | 0.79 | 0/770 |
| 3 | C | 0.45 | 0/1636 | 0.79 | 0/2205 |
| 4 | D | 0.45 | 0/1733 | 0.84 | 1/2318 (0.0%) |
| 5 | E | 0.50 | 0/1162 | 0.86 | 0/1564 |
| 6 | F | 0.42 | 0/856 | 0.81 | 1/1154 (0.1%) |
| 7 | G | 0.43 | 0/1276 | 0.79 | 0/1709 |
| 8 | H | 0.47 | 0/1136 | 0.89 | 2/1527 (0.1%) |
| 9 | I | 0.43 | 0/1018 | 0.73 | 0/1368 |
| All | All | 0.41 | 5/58285 (0.0%) | 0.78 | 30/86251 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 8 | H | 0 | 1 |
| All | All | 0 | 2 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | A | 1459 | C | O3'-P | -8.53 | 1.50 | 1.61 |
| 1 | A | 1458 | G | O3'-P | 7.51 | 1.70 | 1.61 |
| 1 | A | 999 | C | O3'-P | -5.64 | 1.54 | 1.61 |
| 1 | A | 559 | A | O3'-P | 5.30 | 1.67 | 1.61 |
| 1 | A | 79 | G | O3'-P | -5.17 | 1.54 | 1.61 |

All (30) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1 | A | 93 | G | O3'-P-O5' | -26.72 | 53.24 | 104.00 |
| 1 | A | 93 | G | OP1-P-O3' | -22.17 | 56.43 | 105.20 |
| 1 | A | 93 | G | P-O3'-C3' | -10.18 | 107.49 | 119.70 |
| 1 | A | 93 | G | OP2-P-O3' | 8.72 | 124.37 | 105.20 |
| 1 | A | 266 | G | C2'-C3'-O3' | 8.44 | 128.07 | 109.50 |
| 1 | A | 1001 | A | C4'-C3'-O3' | -8.17 | 92.25 | 109.40 |
| 1 | A | 1498 | U | C2'-C3'-O3' | 7.46 | 125.91 | 109.50 |
| 1 | A | 1301 | U | C2'-C3'-O3' | 7.32 | 125.60 | 109.50 |
| 1 | A | 288 | A | C2'-C3'-O3' | 7.04 | 125.00 | 109.50 |
| 1 | A | 509 | A | C4'-C3'-O3' | 6.87 | 126.74 | 113.00 |
| 6 | F | 75 | LEU | CA-CB-CG | 6.83 | 131.02 | 115.30 |
| 1 | A | 792 | A | C2'-C3'-O3' | 6.59 | 124.25 | 113.70 |
| 1 | A | 115 | G | C2'-C3'-O3' | 6.50 | 124.11 | 113.70 |
| 2 | B | 221 | LEU | CA-CB-CG | 6.45 | 130.13 | 115.30 |
| 4 | D | 12 | CYS | CA-CB-SG | 6.23 | 125.21 | 114.00 |
| 1 | A | 815 | A | C4'-C3'-O3' | -6.19 | 96.39 | 109.40 |
| 1 | A | 77 | G | C2'-C3'-O3' | 5.80 | 122.98 | 113.70 |
| 15 | O | 65 | ARG | NE-CZ-NH1 | 5.62 | 123.11 | 120.30 |
| 1 | A | 91 | C | N1-C1'-C2' | -5.60 | 105.84 | 112.00 |
| 2 | B | 187 | LEU | CA-CB-CG | 5.47 | 127.89 | 115.30 |
| 1 | A | 181 | G | C2'-C3'-O3' | 5.47 | 122.45 | 113.70 |
| 1 | A | 1101 | A | C2'-C3'-O3' | 5.44 | 122.40 | 113.70 |
| 1 | A | 484 | G | C2'-C3'-O3' | 5.43 | 122.39 | 113.70 |
| 1 | A | 428 | G | C2'-C3'-O3' | 5.39 | 122.32 | 113.70 |
| 8 | H | 133 | LEU | CB-CG-CD1 | -5.39 | 101.84 | 111.00 |
| 16 | P | 73 | LEU | CA-CB-CG | -5.28 | 103.16 | 115.30 |
| 8 | H | 55 | GLY | N-CA-C | 5.26 | 126.26 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 372 | C | C2'-C3'-O3' | 5.14 | 121.93 | 113.70 |
| 1 | A | 77 | G | N9-C1'-C2' | -5.10 | 106.39 | 112.00 |
| 1 | A | 1145 | C | C2'-C3'-O3' | 5.07 | 121.81 | 113.70 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | A | 1458 | G | Sidechain |
| 8 | H | 3 | THR | Peptide |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 32527 | 0 | 16428 | 1136 | 0 |
| 2 | B | 1900 | 0 | 1951 | 112 | 0 |
| 3 | C | 1612 | 0 | 1677 | 58 | 0 |
| 4 | D | 1703 | 0 | 1766 | 65 | 0 |
| 5 | E | 1146 | 0 | 1207 | 50 | 0 |
| 6 | F | 843 | 0 | 857 | 18 | 0 |
| 7 | G | 1257 | 0 | 1296 | 29 | 0 |
| 8 | H | 1116 | 0 | 1177 | 33 | 0 |
| 9 | I | 999 | 0 | 1015 | 79 | 0 |
| 10 | J | 792 | 0 | 829 | 37 | 0 |
| 11 | K | 892 | 0 | 913 | 38 | 0 |
| 12 | L | 970 | 0 | 1057 | 43 | 0 |
| 13 | M | 933 | 0 | 992 | 19 | 0 |
| 14 | N | 492 | 0 | 527 | 52 | 0 |
| 15 | O | 734 | 0 | 771 | 17 | 0 |
| 16 | P | 700 | 0 | 720 | 14 | 0 |
| 17 | Q | 823 | 0 | 891 | 29 | 0 |
| 18 | R | 598 | 0 | 670 | 34 | 0 |
| 19 | S | 647 | 0 | 673 | 27 | 0 |
| 20 | T | 763 | 0 | 861 | 31 | 0 |
| 21 | V | 208 | 0 | 221 | 11 | 0 |
| 22 | W | 570 | 0 | 599 | 37 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 23 | X | 1356 | 0 | 1401 | 40 | 0 |
| 24 | Y | 439 | 0 | 218 | 17 | 0 |
| 25 | A | 126 | 0 | 0 | 0 | 0 |
| 25 | N | 1 | 0 | 0 | 0 | 0 |
| 26 | D | 1 | 0 | 0 | 1 | 0 |
| 26 | N | 1 | 0 | 0 | 0 | 0 |
| All | All | 54149 | 0 | 38717 | 1806 | 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 20.

All (1806) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:563:A:N6 | 1:A:884:U:H3 | 1.13 | 1.44 |
| 23:X:91:ARG:N | 23:X:94:ILE:HD11 | 1.33 | 1.41 |
| 5:E:15:ARG:CG | 5:E:28:PHE:CE1 | 2.06 | 1.38 |
| 23:X:91:ARG:H | 23:X:94:ILE:CD1 | 1.39 | 1.35 |
| 1:A:89:C:C2' | 1:A:90:U:H5' | 1.57 | 1.32 |
| 11:K:91:ARG:NH1 | 18:R:88:LYS:NZ | 1.73 | 1.32 |
| 1:A:1358:U:N3 | 1:A:1363(A):A:N6 | 1.80 | 1.29 |
| 1:A:1081:G:OP1 | 5:E:16:THR:HG23 | 1.32 | 1.29 |
| 9:I:12:GLU:O | 9:I:68:GLY:N | 1.62 | 1.29 |
| 11:K:91:ARG:NH1 | 18:R:88:LYS:HZ2 | 1.26 | 1.28 |
| 1:A:1371:G:OP1 | 9:I:12:GLU:HB2 | 1.10 | 1.26 |
| 1:A:1371:G:OP1 | 9:I:12:GLU:CB | 1.85 | 1.25 |
| 1:A:961:U:N3 | 1:A:1201:A:N6 | 1.84 | 1.23 |
| 9:I:12:GLU:O | 9:I:68:GLY:CA | 1.84 | 1.23 |
| 2:B:28:PHE:O | 2:B:30:ARG:N | 1.69 | 1.22 |
| 5:E:15:ARG:NH2 | 5:E:26:PHE:CD1 | 2.06 | 1.22 |
| 1:A:961:U:H3 | 1:A:1201:A:N6 | 1.37 | 1.22 |
| 22:W:23:ARG:NE | 22:W:33:LEU:CD2 | 2.02 | 1.22 |
| 1:A:93:G:H2' | 1:A:96:U:O4' | 1.06 | 1.20 |
| 22:W:22:PHE:CE2 | 22:W:47:ILE:HD12 | 1.77 | 1.18 |
| 7:G:37:ASN:ND2 | 9:I:40:LEU:O | 1.77 | 1.17 |
| 1:A:93:G:H5'' | 1:A:96:U:OP2 | 1.44 | 1.17 |
| 1:A:93:G:C2' | 1:A:96:U:O4' | 1.92 | 1.17 |
| 5:E:15:ARG:HG3 | 5:E:28:PHE:CE1 | 1.75 | 1.16 |
| 5:E:15:ARG:HG2 | 5:E:28:PHE:CE1 | 1.76 | 1.11 |
| 5:E:15:ARG:HG3 | 5:E:28:PHE:HE1 | 0.96 | 1.11 |
| 1:A:1358:U:H3 | 1:A:1363(A):A:N6 | 1.38 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 22:W:23:ARG:HE | 22:W:33:LEU:HD21 | 1.08 | 1.10 |
| 1:A:1219:U:H2' | 1:A:1220:G:C8 | 1.88 | 1.09 |
| 1:A:793:U:H3' | 1:A:794:A:H5'' | 1.27 | 1.08 |
| 9:I:12:GLU:HB3 | 9:I:68:GLY:HA2 | 1.17 | 1.08 |
| 1:A:1370:G:O3' | 9:I:12:GLU:HG2 | 1.52 | 1.08 |
| 5:E:15:ARG:NH2 | 5:E:26:PHE:CE1 | 2.17 | 1.08 |
| 1:A:89:C:H2' | 1:A:90:U:H5' | 1.31 | 1.07 |
| 1:A:89:C:O2' | 1:A:90:U:H5' | 1.57 | 1.05 |
| 1:A:1080:A:H4' | 5:E:16:THR:OG1 | 1.56 | 1.04 |
| 22:W:13:VAL:HA | 22:W:24:VAL:HG22 | 1.37 | 1.04 |
| 5:E:15:ARG:HG2 | 5:E:28:PHE:CD1 | 1.91 | 1.04 |
| 1:A:829:G:O4' | 2:B:26:PRO:HG2 | 1.58 | 1.03 |
| 22:W:23:ARG:NH2 | 22:W:33:LEU:HD23 | 1.72 | 1.03 |
| 22:W:23:ARG:HE | 22:W:33:LEU:CD2 | 1.68 | 1.02 |
| 2:B:17:PHE:HD1 | 2:B:18:GLY:N | 1.57 | 1.02 |
| 1:A:1081:G:P | 5:E:16:THR:HG23 | 2.00 | 1.02 |
| 5:E:15:ARG:CG | 5:E:28:PHE:HE1 | 1.54 | 1.02 |
| 10:J:38:ILE:HG23 | 10:J:71:LEU:O | 1.60 | 1.01 |
| 22:W:21:THR:O | 22:W:22:PHE:HD1 | 1.42 | 1.01 |
| 22:W:23:ARG:CZ | 22:W:33:LEU:HD23 | 1.90 | 1.00 |
| 1:A:79:G:H2' | 1:A:80:G:H8 | 1.24 | 1.00 |
| 1:A:664:G:H22 | 1:A:741:G:H1 | 1.08 | 1.00 |
| 1:A:1349:A:OP2 | 9:I:118:LYS:HD3 | 1.63 | 0.99 |
| 17:Q:63:ARG:HH11 | 17:Q:63:ARG:HG3 | 1.28 | 0.99 |
| 22:W:22:PHE:HE2 | 22:W:47:ILE:HD12 | 0.85 | 0.98 |
| 1:A:1371:G:P | 9:I:12:GLU:HB2 | 2.04 | 0.98 |
| 2:B:24:TRP:CD1 | 2:B:40:HIS:CE1 | 2.53 | 0.96 |
| 1:A:1370:G:O3' | 9:I:12:GLU:CG | 2.13 | 0.96 |
| 1:A:80:G:H3' | 1:A:81:U:H5'' | 1.46 | 0.96 |
| 2:B:21:ARG:HA | 2:B:39:ILE:HA | 1.47 | 0.96 |
| 4:D:29:PRO:O | 4:D:35:ARG:HD3 | 1.64 | 0.96 |
| 19:S:72:GLY:O | 19:S:75:ALA:N | 1.99 | 0.96 |
| 7:G:37:ASN:ND2 | 9:I:40:LEU:HD12 | 1.81 | 0.96 |
| 1:A:1219:U:H2' | 1:A:1220:G:H8 | 1.20 | 0.96 |
| 11:K:91:ARG:HH12 | 18:R:88:LYS:CE | 1.78 | 0.95 |
| 22:W:32:ILE:HD13 | 22:W:32:ILE:H | 1.32 | 0.95 |
| 12:L:53:ARG:HH11 | 12:L:53:ARG:HG2 | 1.29 | 0.94 |
| 1:A:1458:G:OP1 | 20:T:35:THR:OG1 | 1.87 | 0.93 |
| 10:J:38:ILE:CG2 | 10:J:71:LEU:O | 2.16 | 0.92 |
| 7:G:37:ASN:HD21 | 9:I:40:LEU:HD12 | 1.33 | 0.92 |
| 1:A:981:U:H4' | 14:N:21:TYR:HE2 | 1.31 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:222:U:H2' | 1:A:223:U:C6 | 2.05 | 0.91 |
| 23:X:130:PRO:O | 23:X:134:GLU:HB2 | 1.71 | 0.91 |
| 1:A:973:G:H3' | 1:A:974:A:H5'' | 1.52 | 0.90 |
| 4:D:26:CYS:SG | 26:D:300:ZN:ZN | 1.59 | 0.90 |
| 9:I:12:GLU:O | 9:I:68:GLY:HA3 | 1.69 | 0.90 |
| 1:A:93:G:H2' | 1:A:96:U:C1' | 2.01 | 0.90 |
| 1:A:1081:G:P | 5:E:16:THR:CG2 | 2.59 | 0.90 |
| 1:A:426:G:OP1 | 4:D:36:ARG:NH2 | 2.04 | 0.90 |
| 22:W:23:ARG:CZ | 22:W:33:LEU:CD2 | 2.49 | 0.89 |
| 22:W:23:ARG:NE | 22:W:33:LEU:HD21 | 1.73 | 0.89 |
| 1:A:1350:A:N7 | 9:I:118:LYS:NZ | 2.21 | 0.88 |
| 11:K:91:ARG:HH12 | 18:R:88:LYS:NZ | 1.50 | 0.88 |
| 3:C:12:LEU:HD21 | 3:C:18:TRP:CD1 | 2.08 | 0.88 |
| 22:W:21:THR:C | 22:W:22:PHE:CD1 | 2.47 | 0.88 |
| 1:A:981:U:H4' | 14:N:21:TYR:CE2 | 2.09 | 0.88 |
| 2:B:17:PHE:HD1 | 2:B:18:GLY:H | 0.93 | 0.88 |
| 1:A:1327:C:H5'' | 21:V:20:LYS:HB2 | 1.55 | 0.87 |
| 1:A:961:U:O4 | 1:A:1201:A:N1 | 2.08 | 0.87 |
| 3:C:12:LEU:HD11 | 14:N:51:GLY:CA | 2.05 | 0.87 |
| 1:A:1128:C:H1' | 1:A:1146:A:H61 | 1.40 | 0.87 |
| 22:W:22:PHE:HE2 | 22:W:47:ILE:CD1 | 1.81 | 0.87 |
| 4:D:34:GLU:OE1 | 4:D:34:GLU:N | 2.08 | 0.86 |
| 1:A:1025:U:H2' | 1:A:1026:G:C8 | 2.11 | 0.86 |
| 3:C:92:ALA:O | 3:C:95:THR:O | 1.93 | 0.86 |
| 20:T:15:ARG:HH11 | 20:T:15:ARG:HG2 | 1.39 | 0.86 |
| 1:A:1495:U:H5'' | 23:X:93:LYS:O | 1.75 | 0.85 |
| 23:X:94:ILE:HG23 | 23:X:98:ASP:OD2 | 1.75 | 0.85 |
| 1:A:792:A:H4' | 1:A:793:U:H5'' | 1.57 | 0.85 |
| 1:A:829:G:O4' | 2:B:26:PRO:CG | 2.24 | 0.85 |
| 9:I:12:GLU:HB3 | 9:I:68:GLY:CA | 2.05 | 0.85 |
| 2:B:129:GLU:C | 2:B:130:ARG:HD2 | 1.96 | 0.85 |
| 2:B:17:PHE:CD1 | 2:B:18:GLY:N | 2.44 | 0.85 |
| 14:N:23:ARG:NH1 | 14:N:30:ALA:HB2 | 1.92 | 0.85 |
| 1:A:793:U:H3' | 1:A:794:A:C5' | 2.06 | 0.84 |
| 22:W:14:THR:HB | 22:W:23:ARG:O | 1.78 | 0.84 |
| 1:A:89:C:O2' | 1:A:90:U:C5' | 2.24 | 0.84 |
| 1:A:224:C:OP1 | 20:T:74:LYS:CE | 2.26 | 0.84 |
| 1:A:1081:G:OP1 | 5:E:16:THR:CG2 | 2.24 | 0.84 |
| 1:A:1232:U:H5'' | 9:I:124:GLN:NE2 | 1.93 | 0.84 |
| 11:K:91:ARG:NH1 | 18:R:88:LYS:HZ1 | 1.71 | 0.84 |
| 2:B:129:GLU:O | 2:B:130:ARG:HB2 | 1.75 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1314:C:OP2 | 19:S:6:LYS:HB3 | 1.76 | 0.83 |
| 1:A:946:A:H2' | 1:A:947:G:C8 | 2.14 | 0.83 |
| 18:R:53:ARG:HH21 | 18:R:60:ALA:HB2 | 1.42 | 0.83 |
| 1:A:1513:A:H2' | 1:A:1514:C:C6 | 2.14 | 0.82 |
| 15:O:65:ARG:HH11 | 15:O:65:ARG:HG2 | 1.43 | 0.82 |
| 1:A:829:G:H4' | 2:B:26:PRO:HG3 | 1.61 | 0.82 |
| 1:A:829:G:C4' | 2:B:26:PRO:HG3 | 2.10 | 0.82 |
| 1:A:563:A:N1 | 1:A:884:U:O4 | 2.13 | 0.82 |
| 1:A:1218:C:H2' | 1:A:1219:U:C6 | 2.15 | 0.82 |
| 1:A:1358:U:C2 | 1:A:1363(A):A:N6 | 2.48 | 0.82 |
| 2:B:28:PHE:O | 2:B:30:ARG:HG3 | 1.80 | 0.81 |
| 22:W:21:THR:O | 22:W:22:PHE:CD1 | 2.32 | 0.81 |
| 3:C:14:ILE:H | 3:C:14:ILE:HD13 | 1.45 | 0.81 |
| 1:A:981:U:C4' | 14:N:21:TYR:HE2 | 1.93 | 0.81 |
| 2:B:8:LYS:O | 2:B:9:GLU:HB2 | 1.79 | 0.80 |
| 9:I:42:ARG:NH2 | 9:I:71:SER:CB | 2.44 | 0.80 |
| 3:C:12:LEU:CD2 | 3:C:18:TRP:NE1 | 2.45 | 0.80 |
| 11:K:91:ARG:HH12 | 18:R:88:LYS:HZ2 | 1.07 | 0.80 |
| 1:A:1232:U:H5'' | 9:I:124:GLN:HE21 | 1.46 | 0.80 |
| 1:A:1152:A:OP1 | 10:J:70:ARG:NH2 | 2.14 | 0.79 |
| 3:C:64:VAL:HB | 3:C:99:VAL:HG23 | 1.63 | 0.79 |
| 2:B:24:TRP:HB2 | 2:B:190:THR:OG1 | 1.81 | 0.79 |
| 1:A:814:A:O2' | 1:A:815:A:H3' | 1.82 | 0.79 |
| 1:A:79:G:H2' | 1:A:80:G:C8 | 2.13 | 0.79 |
| 4:D:35:ARG:HH11 | 4:D:35:ARG:CB | 1.95 | 0.79 |
| 4:D:35:ARG:HH11 | 4:D:35:ARG:HB3 | 1.47 | 0.79 |
| 9:I:42:ARG:HH21 | 9:I:71:SER:HB2 | 1.47 | 0.78 |
| 1:A:224:C:OP1 | 20:T:74:LYS:HE3 | 1.82 | 0.78 |
| 22:W:21:THR:C | 22:W:22:PHE:HD1 | 1.87 | 0.78 |
| 1:A:961:U:H3 | 1:A:1201:A:H61 | 0.79 | 0.77 |
| 1:A:745:C:H2' | 1:A:746:A:C8 | 2.19 | 0.77 |
| 1:A:674:G:H2' | 1:A:675:A:H8 | 1.48 | 0.77 |
| 2:B:25:ASN:HD21 | 2:B:27:LYS:HB3 | 1.50 | 0.77 |
| 1:A:1287:A:H2' | 1:A:1288:A:C8 | 2.20 | 0.77 |
| 1:A:658:G:C2 | 1:A:749:C:N3 | 2.53 | 0.77 |
| 2:B:16:HIS:NE2 | 2:B:214:ILE:HD11 | 1.99 | 0.77 |
| 1:A:972:C:O3' | 10:J:57:LYS:HG3 | 1.83 | 0.77 |
| 5:E:40:ARG:HH11 | 5:E:40:ARG:HG2 | 1.50 | 0.77 |
| 23:X:88:ILE:HD13 | 23:X:106:ILE:HG12 | 1.65 | 0.77 |
| 11:K:91:ARG:NH1 | 18:R:88:LYS:CE | 2.43 | 0.77 |
| 11:K:91:ARG:HH11 | 18:R:88:LYS:NZ | 1.76 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1391:U:H2' | 1:A:1392:G:C8 | 2.20 | 0.76 |
| 1:A:563:A:N6 | 1:A:884:U:N3 | 1.91 | 0.76 |
| 1:A:1111:A:N1 | 3:C:177:THR:HG22 | 2.01 | 0.76 |
| 10:J:38:ILE:O | 10:J:71:LEU:N | 2.15 | 0.76 |
| 5:E:127:ASN:HB3 | 5:E:130:ASN:HB2 | 1.65 | 0.76 |
| 10:J:6:ILE:HD11 | 10:J:23:ILE:HG21 | 1.68 | 0.76 |
| 5:E:15:ARG:CG | 5:E:28:PHE:CD1 | 2.59 | 0.75 |
| 11:K:91:ARG:HH11 | 18:R:88:LYS:HZ1 | 1.30 | 0.75 |
| 1:A:1151:A:O2' | 1:A:1152:A:H8 | 1.68 | 0.75 |
| 1:A:1399:C:C2 | 1:A:1502:A:N6 | 2.54 | 0.75 |
| 1:A:370:C:C2 | 1:A:392:G:N2 | 2.54 | 0.75 |
| 1:A:1189:C:OP1 | 10:J:51:ARG:NH2 | 2.20 | 0.75 |
| 3:C:30:ARG:NH1 | 14:N:35:ARG:O | 2.20 | 0.75 |
| 9:I:117:HIS:HE1 | 9:I:123:PRO:HB3 | 1.49 | 0.75 |
| 11:K:91:ARG:HH12 | 18:R:88:LYS:HE3 | 1.50 | 0.75 |
| 1:A:253:U:H2' | 1:A:254:G:C8 | 2.21 | 0.75 |
| 1:A:89:C:C2 | 1:A:90:U:C6 | 2.74 | 0.75 |
| 22:W:23:ARG:HH21 | 22:W:33:LEU:HD23 | 1.51 | 0.75 |
| 1:A:715:A:H2' | 1:A:716:A:C8 | 2.21 | 0.74 |
| 3:C:8:ILE:HG23 | 3:C:16:ARG:HE | 1.51 | 0.74 |
| 1:A:677:U:H3 | 1:A:713:G:H22 | 1.33 | 0.74 |
| 2:B:21:ARG:HD3 | 2:B:21:ARG:H | 1.52 | 0.74 |
| 1:A:528:C:H3' | 1:A:529:G:H5'' | 1.69 | 0.74 |
| 5:E:15:ARG:CD | 5:E:28:PHE:CE1 | 2.70 | 0.74 |
| 1:A:1349:A:P | 9:I:118:LYS:HD3 | 2.27 | 0.74 |
| 3:C:12:LEU:CD2 | 3:C:18:TRP:CD1 | 2.71 | 0.74 |
| 9:I:42:ARG:NH2 | 9:I:71:SER:HA | 2.01 | 0.74 |
| 2:B:25:ASN:HD21 | 2:B:27:LYS:CB | 2.01 | 0.74 |
| 12:L:60:LEU:HD11 | 12:L:85:ILE:HD12 | 1.70 | 0.74 |
| 1:A:568:G:N2 | 1:A:883:C:C2 | 2.56 | 0.74 |
| 3:C:14:ILE:HD13 | 3:C:14:ILE:N | 2.02 | 0.73 |
| 2:B:28:PHE:C | 2:B:30:ARG:H | 1.92 | 0.73 |
| 1:A:1099:G:C6 | 1:A:1100:C:N3 | 2.57 | 0.73 |
| 7:G:75:VAL:HG21 | 7:G:144:MET:HB3 | 1.69 | 0.73 |
| 3:C:189:ALA:HB3 | 3:C:196:LEU:HB2 | 1.68 | 0.73 |
| 22:W:53:VAL:HG12 | 22:W:71:LYS:HA | 1.69 | 0.73 |
| 1:A:1225:A:H2' | 1:A:1226:C:C6 | 2.23 | 0.73 |
| 17:Q:98:LEU:HD23 | 17:Q:98:LEU:H | 1.53 | 0.73 |
| 1:A:30:U:H3' | 1:A:31:G:H5'' | 1.68 | 0.73 |
| 23:X:102:LYS:O | 23:X:106:ILE:HG13 | 1.87 | 0.73 |
| 1:A:312:C:H2' | 1:A:313:A:C8 | 2.24 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:40:LEU:HD12 | 9:I:40:LEU:O | 1.88 | 0.72 |
| 1:A:1391:U:H2' | 1:A:1392:G:H8 | 1.54 | 0.72 |
| 1:A:765:G:C6 | 1:A:812:C:N3 | 2.57 | 0.72 |
| 14:N:24:CYS:HB3 | 14:N:29:ARG:H | 1.54 | 0.72 |
| 18:R:37:VAL:HG21 | 18:R:78:LEU:HB3 | 1.70 | 0.72 |
| 1:A:1080:A:C4' | 5:E:16:THR:OG1 | 2.35 | 0.72 |
| 3:C:58:GLU:HB2 | 3:C:65:ALA:HB3 | 1.71 | 0.72 |
| 10:J:50:ILE:HD11 | 10:J:60:ARG:NH1 | 2.04 | 0.72 |
| 22:W:32:ILE:HB | 22:W:63:THR:O | 1.88 | 0.72 |
| 1:A:19:C:H2' | 1:A:20:U:H6 | 1.54 | 0.72 |
| 1:A:559:A:H4' | 1:A:560:U:O5' | 1.88 | 0.72 |
| 1:A:73:G:H1 | 1:A:96:U:H3 | 1.38 | 0.72 |
| 11:K:62:GLN:HG2 | 11:K:97:ALA:HB2 | 1.71 | 0.72 |
| 1:A:222:U:H2' | 1:A:223:U:H6 | 1.52 | 0.72 |
| 1:A:195:A:H4' | 20:T:68:LYS:HD3 | 1.72 | 0.72 |
| 1:A:113:G:H1' | 1:A:354:G:H5' | 1.71 | 0.72 |
| 11:K:25:TYR:HE1 | 24:Y:29:G:H5'' | 1.53 | 0.72 |
| 14:N:23:ARG:HG3 | 14:N:30:ALA:HA | 1.72 | 0.72 |
| 22:W:45:ILE:HD13 | 22:W:70:ARG:HB3 | 1.70 | 0.72 |
| 1:A:1264:C:H2' | 1:A:1265:G:H8 | 1.55 | 0.71 |
| 1:A:91:C:C6 | 1:A:91:C:H3' | 2.25 | 0.71 |
| 5:E:76:ILE:HD12 | 5:E:118:ILE:HG21 | 1.71 | 0.71 |
| 23:X:106:ILE:HG23 | 23:X:116:VAL:HG11 | 1.73 | 0.71 |
| 9:I:117:HIS:CE1 | 9:I:123:PRO:HB3 | 2.24 | 0.71 |
| 23:X:94:ILE:CG2 | 23:X:98:ASP:OD2 | 2.39 | 0.71 |
| 2:B:223:ILE:HG21 | 2:B:230:VAL:HB | 1.73 | 0.71 |
| 1:A:1305:G:HO2' | 1:A:1306:A:H8 | 1.37 | 0.71 |
| 1:A:1349:A:H5'' | 9:I:121:ARG:HB2 | 1.73 | 0.71 |
| 10:J:38:ILE:HG23 | 10:J:71:LEU:HB3 | 1.73 | 0.71 |
| 1:A:961:U:O2 | 1:A:983:A:H2' | 1.90 | 0.70 |
| 4:D:8:VAL:HG11 | 4:D:21:LEU:HB2 | 1.73 | 0.70 |
| 1:A:1281:U:H4' | 1:A:1282:C:OP2 | 1.91 | 0.70 |
| 1:A:486:U:H2' | 1:A:487:A:H8 | 1.55 | 0.70 |
| 1:A:253:U:H2' | 1:A:254:G:H8 | 1.56 | 0.70 |
| 1:A:501:C:H2' | 1:A:502:G:H8 | 1.55 | 0.70 |
| 3:C:12:LEU:HD11 | 14:N:51:GLY:HA3 | 1.73 | 0.70 |
| 8:H:17:THR:HG21 | 8:H:80:ILE:HD13 | 1.72 | 0.70 |
| 1:A:89:C:H2' | 1:A:90:U:C5' | 2.15 | 0.70 |
| 9:I:116:LYS:HB3 | 9:I:122:ALA:HA | 1.73 | 0.70 |
| 1:A:1192:C:H2' | 1:A:1193:G:O4' | 1.92 | 0.70 |
| 23:X:130:PRO:O | 23:X:134:GLU:CB | 2.39 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:398:C:H2' | 1:A:399:G:H8 | 1.55 | 0.70 |
| 16:P:38:TYR:CE2 | 16:P:50:LYS:HB3 | 2.27 | 0.70 |
| 1:A:434:U:H2' | 1:A:435:C:C6 | 2.26 | 0.69 |
| 19:S:72:GLY:O | 19:S:74:PHE:N | 2.25 | 0.69 |
| 1:A:1244:C:H2' | 1:A:1245:A:H8 | 1.57 | 0.69 |
| 1:A:38:G:H22 | 1:A:397:A:H5' | 1.56 | 0.69 |
| 3:C:28:GLN:OE1 | 3:C:28:GLN:N | 2.24 | 0.69 |
| 9:I:42:ARG:HH21 | 9:I:71:SER:CB | 2.03 | 0.69 |
| 1:A:528:C:H41 | 12:L:49:ASN:HD22 | 1.39 | 0.69 |
| 2:B:112:VAL:HG23 | 2:B:149:LEU:HD13 | 1.74 | 0.69 |
| 22:W:32:ILE:HD13 | 22:W:32:ILE:N | 2.06 | 0.69 |
| 1:A:501:C:H2' | 1:A:502:G:C8 | 2.28 | 0.69 |
| 3:C:131:ARG:HH11 | 3:C:131:ARG:HG2 | 1.57 | 0.69 |
| 10:J:61:GLU:OE1 | 14:N:49:HIS:CE1 | 2.45 | 0.69 |
| 23:X:94:ILE:HG23 | 23:X:98:ASP:CG | 2.13 | 0.69 |
| 12:L:53:ARG:NH1 | 12:L:53:ARG:HG2 | 2.05 | 0.69 |
| 2:B:129:GLU:O | 2:B:130:ARG:CB | 2.41 | 0.69 |
| 10:J:61:GLU:OE1 | 14:N:49:HIS:NE2 | 2.26 | 0.69 |
| 14:N:9:LYS:HE3 | 14:N:21:TYR:O | 1.92 | 0.69 |
| 3:C:7:PRO:CA | 3:C:11:ARG:HH21 | 2.06 | 0.69 |
| 1:A:872:A:O2' | 1:A:873:A:H3' | 1.93 | 0.68 |
| 2:B:16:HIS:HE2 | 2:B:214:ILE:HD11 | 1.57 | 0.68 |
| 3:C:12:LEU:HD11 | 14:N:51:GLY:HA2 | 1.74 | 0.68 |
| 1:A:1373:G:H5'' | 7:G:36:LYS:HB2 | 1.76 | 0.68 |
| 9:I:42:ARG:NH2 | 9:I:71:SER:CA | 2.56 | 0.68 |
| 7:G:65:ALA:HB1 | 7:G:127:ALA:HB3 | 1.75 | 0.68 |
| 1:A:678:U:H2' | 1:A:679:C:C6 | 2.28 | 0.68 |
| 1:A:917:G:H2' | 1:A:918:A:C8 | 2.29 | 0.68 |
| 1:A:924:C:H4' | 1:A:1399:C:OP2 | 1.93 | 0.68 |
| 3:C:12:LEU:HD23 | 3:C:18:TRP:CE2 | 2.27 | 0.68 |
| 5:E:80:ILE:HD13 | 5:E:138:ALA:HB1 | 1.76 | 0.68 |
| 1:A:335:C:H2' | 1:A:336:C:C6 | 2.29 | 0.68 |
| 1:A:961:U:C2 | 1:A:1201:A:N6 | 2.55 | 0.68 |
| 7:G:37:ASN:ND2 | 9:I:40:LEU:CD1 | 2.55 | 0.68 |
| 17:Q:63:ARG:HG3 | 17:Q:63:ARG:NH1 | 2.01 | 0.67 |
| 19:S:71:LEU:HD23 | 19:S:71:LEU:C | 2.14 | 0.67 |
| 1:A:955:U:H2' | 1:A:956:U:H6 | 1.59 | 0.67 |
| 3:C:7:PRO:HA | 3:C:11:ARG:NH2 | 2.09 | 0.67 |
| 1:A:1127:G:N2 | 1:A:1145:C:C2 | 2.62 | 0.67 |
| 1:A:992:U:H4' | 1:A:993:G:O5' | 1.95 | 0.67 |
| 1:A:1347:G:C8 | 9:I:107:ARG:HB3 | 2.29 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1392:G:N2 | 1:A:1502:A:H8 | 1.93 | 0.67 |
| 1:A:870:U:H4' | 1:A:871:U:H5'' | 1.77 | 0.67 |
| 1:A:891:U:H2' | 1:A:892:A:H8 | 1.60 | 0.67 |
| 1:A:227:G:N2 | 16:P:62:VAL:O | 2.24 | 0.67 |
| 1:A:674:G:H2' | 1:A:675:A:C8 | 2.29 | 0.66 |
| 1:A:1314:C:H2' | 1:A:1315:U:C6 | 2.31 | 0.66 |
| 1:A:618:C:H5'' | 1:A:619:U:H5'' | 1.76 | 0.66 |
| 17:Q:65:ILE:O | 17:Q:66:SER:HB2 | 1.95 | 0.66 |
| 1:A:946:A:H5' | 1:A:946:A:H8 | 1.59 | 0.66 |
| 2:B:74:LYS:HD2 | 2:B:169:LYS:HD2 | 1.76 | 0.66 |
| 18:R:40:LEU:HB3 | 18:R:79:LEU:HD11 | 1.78 | 0.66 |
| 20:T:15:ARG:HG2 | 20:T:15:ARG:NH1 | 2.11 | 0.66 |
| 1:A:829:G:C4' | 2:B:26:PRO:CG | 2.73 | 0.66 |
| 21:V:3:LYS:O | 21:V:11:GLY:HA2 | 1.95 | 0.66 |
| 1:A:1249:C:H4' | 9:I:73:GLN:HE22 | 1.61 | 0.66 |
| 1:A:312:C:H2' | 1:A:313:A:H8 | 1.58 | 0.66 |
| 1:A:636:U:H5' | 17:Q:2:PRO:HG3 | 1.78 | 0.65 |
| 1:A:1227:A:H1' | 13:M:117:VAL:HB | 1.77 | 0.65 |
| 1:A:20:U:H2' | 1:A:21:G:O4' | 1.96 | 0.65 |
| 1:A:247:G:OP2 | 17:Q:100:LYS:HB2 | 1.96 | 0.65 |
| 1:A:123:C:H5'' | 1:A:311:C:O2' | 1.96 | 0.65 |
| 5:E:33:VAL:HG13 | 5:E:112:LEU:HD22 | 1.78 | 0.65 |
| 6:F:48:LEU:HD22 | 6:F:52:ILE:HD12 | 1.78 | 0.65 |
| 7:G:49:ILE:HD13 | 7:G:118:VAL:HA | 1.77 | 0.65 |
| 9:I:17:VAL:HG22 | 9:I:63:ILE:HG12 | 1.78 | 0.65 |
| 1:A:1349:A:OP1 | 9:I:118:LYS:HB3 | 1.96 | 0.65 |
| 1:A:792:A:H4' | 1:A:793:U:C5' | 2.26 | 0.65 |
| 1:A:89:C:C3' | 1:A:90:U:H5' | 2.26 | 0.65 |
| 2:B:15:VAL:O | 2:B:204:ASN:OD1 | 2.14 | 0.65 |
| 22:W:40:MET:HA | 22:W:45:ILE:HD12 | 1.78 | 0.65 |
| 1:A:1187:G:H21 | 14:N:60:SER:HB3 | 1.61 | 0.65 |
| 1:A:575:G:H4' | 1:A:576:G:H5'' | 1.78 | 0.65 |
| 1:A:1196:U:H5' | 1:A:1197:G:H5' | 1.79 | 0.65 |
| 1:A:333:G:N2 | 1:A:334:C:C2 | 2.64 | 0.65 |
| 1:A:757:U:H2' | 1:A:758:G:O4' | 1.95 | 0.65 |
| 1:A:829:G:C1' | 2:B:26:PRO:HG2 | 2.26 | 0.65 |
| 1:A:1371:G:P | 9:I:12:GLU:CB | 2.77 | 0.65 |
| 1:A:1126:U:O2 | 1:A:1126:U:H2' | 1.96 | 0.65 |
| 9:I:42:ARG:HH22 | 9:I:71:SER:HA | 1.60 | 0.65 |
| 16:P:20:VAL:HG23 | 16:P:35:LYS:HA | 1.78 | 0.65 |
| 22:W:14:THR:CB | 22:W:23:ARG:O | 2.44 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:405:U:H3' | 4:D:5:ILE:HD11 | 1.79 | 0.65 |
| 1:A:524:G:C6 | 1:A:525:C:N4 | 2.65 | 0.65 |
| 4:D:8:VAL:CG1 | 4:D:21:LEU:HB2 | 2.27 | 0.65 |
| 4:D:78:LEU:HG | 4:D:96:LEU:HD23 | 1.79 | 0.65 |
| 1:A:570:G:C6 | 1:A:873:A:C2 | 2.86 | 0.64 |
| 13:M:23:TYR:HB3 | 13:M:67:GLU:HA | 1.80 | 0.64 |
| 1:A:765:G:N2 | 1:A:813:U:OP2 | 2.30 | 0.64 |
| 2:B:162:ILE:HD12 | 2:B:177:ALA:HB2 | 1.79 | 0.64 |
| 2:B:24:TRP:CD1 | 2:B:40:HIS:HE1 | 2.11 | 0.64 |
| 10:J:37:PRO:HA | 10:J:72:VAL:CG2 | 2.27 | 0.64 |
| 1:A:827:U:O4 | 1:A:872:A:N1 | 2.30 | 0.64 |
| 1:A:877:C:OP1 | 8:H:88:LYS:HD3 | 1.97 | 0.64 |
| 1:A:148:G:H2' | 1:A:149:A:C8 | 2.32 | 0.64 |
| 1:A:344:A:H4' | 1:A:345:C:OP2 | 1.96 | 0.64 |
| 1:A:617:G:N1 | 1:A:618:C:C4 | 2.65 | 0.64 |
| 1:A:676:A:H2' | 1:A:677:U:C6 | 2.32 | 0.64 |
| 3:C:153:VAL:HG22 | 3:C:198:VAL:HG13 | 1.78 | 0.64 |
| 1:A:532:A:N6 | 3:C:193:TYR:HB3 | 2.12 | 0.64 |
| 8:H:9:MET:HG3 | 8:H:26:VAL:HG21 | 1.79 | 0.64 |
| 1:A:576:G:H3' | 1:A:577:G:H5'' | 1.80 | 0.64 |
| 1:A:46:G:H2' | 1:A:366:C:C5 | 2.32 | 0.64 |
| 1:A:658:G:C2 | 1:A:749:C:C2 | 2.86 | 0.64 |
| 1:A:1458:G:OP1 | 20:T:35:THR:CB | 2.46 | 0.63 |
| 1:A:93:G:C5' | 1:A:96:U:OP2 | 2.36 | 0.63 |
| 3:C:7:PRO:HA | 3:C:11:ARG:HH21 | 1.63 | 0.63 |
| 1:A:1081:G:P | 5:E:16:THR:HG21 | 2.36 | 0.63 |
| 1:A:61:G:H2' | 1:A:62:U:O4' | 1.98 | 0.63 |
| 3:C:124:ILE:HG21 | 3:C:196:LEU:HD22 | 1.79 | 0.63 |
| 4:D:170:VAL:HG22 | 4:D:171:GLY:H | 1.64 | 0.63 |
| 10:J:34:VAL:HG22 | 10:J:74:ILE:HG23 | 1.80 | 0.63 |
| 12:L:32:PHE:HB3 | 12:L:84:LEU:HD11 | 1.81 | 0.63 |
| 1:A:1049:U:H4' | 1:A:1050:G:OP2 | 1.99 | 0.63 |
| 1:A:293:G:C4 | 1:A:305:G:N2 | 2.67 | 0.63 |
| 1:A:56:U:H2' | 1:A:57:G:C8 | 2.33 | 0.63 |
| 4:D:101:LEU:O | 4:D:104:VAL:HG12 | 1.98 | 0.63 |
| 1:A:398:C:H2' | 1:A:399:G:C8 | 2.33 | 0.63 |
| 1:A:296:U:H2' | 1:A:297:G:C8 | 2.33 | 0.63 |
| 10:J:37:PRO:HA | 10:J:72:VAL:HG23 | 1.79 | 0.63 |
| 11:K:115:PRO:HB2 | 11:K:118:GLY:H | 1.63 | 0.63 |
| 1:A:1358:U:O4 | 1:A:1363(A):A:N1 | 2.32 | 0.63 |
| 1:A:651:C:H2' | 1:A:652:U:C6 | 2.34 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:669:U:H2' | 1:A:670:G:C8 | 2.34 | 0.63 |
| 2:B:130:ARG:HA | 2:B:130:ARG:HE | 1.64 | 0.63 |
| 23:X:47:LEU:HD12 | 23:X:57:ALA:HB2 | 1.80 | 0.63 |
| 1:A:928:G:H1 | 1:A:1389:C:H42 | 1.45 | 0.63 |
| 2:B:24:TRP:NE1 | 2:B:40:HIS:CE1 | 2.66 | 0.63 |
| 12:L:54:LYS:HG2 | 12:L:75:HIS:HE1 | 1.64 | 0.63 |
| 14:N:9:LYS:HG3 | 14:N:21:TYR:CD1 | 2.34 | 0.63 |
| 1:A:1278:U:H5'' | 1:A:1279:A:O4' | 1.99 | 0.63 |
| 2:B:8:LYS:O | 2:B:9:GLU:CB | 2.47 | 0.63 |
| 4:D:162:LEU:HD12 | 4:D:178:VAL:HG23 | 1.79 | 0.63 |
| 1:A:10:A:H2' | 1:A:11:G:H8 | 1.63 | 0.62 |
| 1:A:1116:C:H2' | 1:A:1117:G:H5'' | 1.82 | 0.62 |
| 1:A:513:C:H2' | 1:A:514:C:C6 | 2.35 | 0.62 |
| 2:B:187:LEU:HD13 | 2:B:205:ASP:HA | 1.81 | 0.62 |
| 9:I:42:ARG:HH22 | 9:I:71:SER:CA | 2.12 | 0.62 |
| 3:C:116:VAL:O | 3:C:120:VAL:HG23 | 2.00 | 0.62 |
| 1:A:1251:A:H2' | 1:A:1252:A:O4' | 1.99 | 0.62 |
| 1:A:501:C:OP1 | 12:L:117:ARG:NH2 | 2.31 | 0.62 |
| 1:A:613:C:H2' | 1:A:614:A:C8 | 2.35 | 0.62 |
| 9:I:116:LYS:HA | 9:I:123:PRO:HD3 | 1.82 | 0.62 |
| 1:A:1001:A:OP2 | 1:A:1001:A:H8 | 1.81 | 0.62 |
| 1:A:1477:C:H2' | 1:A:1478:C:C6 | 2.35 | 0.62 |
| 1:A:354:G:N2 | 1:A:355:C:C2 | 2.68 | 0.62 |
| 15:O:65:ARG:HH11 | 15:O:65:ARG:CG | 2.12 | 0.62 |
| 1:A:1015:A:H2' | 1:A:1016:A:C8 | 2.35 | 0.62 |
| 1:A:56:U:H2' | 1:A:57:G:H8 | 1.65 | 0.62 |
| 1:A:955:U:H1' | 1:A:1227:A:N6 | 2.15 | 0.62 |
| 1:A:1312:G:C2 | 1:A:1326:C:C2 | 2.88 | 0.62 |
| 1:A:324:G:N2 | 1:A:326:G:H3' | 2.14 | 0.61 |
| 1:A:89:C:H2' | 1:A:90:U:H6 | 1.65 | 0.61 |
| 2:B:61:LEU:HD23 | 2:B:161:ALA:HB2 | 1.82 | 0.61 |
| 1:A:528:C:H41 | 12:L:49:ASN:ND2 | 1.98 | 0.61 |
| 1:A:1394:A:H8 | 1:A:1394:A:OP1 | 1.83 | 0.61 |
| 1:A:568:G:C2 | 1:A:883:C:N3 | 2.68 | 0.61 |
| 4:D:70:ILE:HD11 | 4:D:97:LEU:HD21 | 1.81 | 0.61 |
| 17:Q:45:HIS:HB2 | 17:Q:65:ILE:HD13 | 1.81 | 0.61 |
| 18:R:53:ARG:HH21 | 18:R:60:ALA:CB | 2.13 | 0.61 |
| 2:B:12:GLU:CD | 2:B:12:GLU:H | 1.98 | 0.61 |
| 1:A:1263:C:H2' | 1:A:1264:C:C6 | 2.35 | 0.61 |
| 4:D:3:ARG:CZ | 4:D:3:ARG:HA | 2.30 | 0.61 |
| 16:P:39:TYR:CD1 | 16:P:73:LEU:HD21 | 2.35 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:132:C:H5'' | 20:T:75:ASN:HD22 | 1.66 | 0.61 |
| 1:A:1521:G:H2' | 1:A:1522:U:C6 | 2.34 | 0.61 |
| 1:A:322:C:H2' | 1:A:323:U:H6 | 1.64 | 0.61 |
| 1:A:80:G:H3' | 1:A:81:U:C5' | 2.26 | 0.61 |
| 1:A:891:U:H2' | 1:A:892:A:C8 | 2.36 | 0.61 |
| 2:B:158:LEU:HD23 | 2:B:159:PRO:HD2 | 1.82 | 0.61 |
| 12:L:113:ARG:HH11 | 12:L:113:ARG:HB3 | 1.65 | 0.61 |
| 1:A:1323:G:H2' | 1:A:1324:A:C8 | 2.36 | 0.61 |
| 1:A:1431:C:C2 | 1:A:1470:G:N2 | 2.69 | 0.61 |
| 1:A:1493:A:H4' | 1:A:1494:G:OP1 | 2.01 | 0.61 |
| 1:A:728:A:H2' | 1:A:729:A:C8 | 2.36 | 0.61 |
| 1:A:923:A:H2' | 1:A:924:C:O4' | 2.00 | 0.61 |
| 1:A:630:G:H2' | 1:A:631:G:O4' | 2.00 | 0.60 |
| 1:A:765:G:C2 | 1:A:812:C:O2 | 2.54 | 0.60 |
| 1:A:1371:G:OP1 | 9:I:12:GLU:HB3 | 1.92 | 0.60 |
| 2:B:25:ASN:ND2 | 2:B:27:LYS:HB3 | 2.15 | 0.60 |
| 19:S:49:ILE:CG2 | 19:S:71:LEU:HD11 | 2.31 | 0.60 |
| 1:A:1264:C:H2' | 1:A:1265:G:C8 | 2.36 | 0.60 |
| 1:A:321:A:H2' | 1:A:322:C:C6 | 2.36 | 0.60 |
| 1:A:769:G:H4' | 1:A:1513:A:H4' | 1.83 | 0.60 |
| 2:B:130:ARG:CA | 2:B:130:ARG:HE | 2.14 | 0.60 |
| 2:B:130:ARG:HB3 | 2:B:131:PRO:HD2 | 1.82 | 0.60 |
| 5:E:11:ILE:HG21 | 5:E:105:VAL:HG13 | 1.81 | 0.60 |
| 22:W:12:VAL:O | 22:W:24:VAL:HG13 | 2.01 | 0.60 |
| 1:A:1081:G:OP2 | 5:E:16:THR:HG21 | 2.01 | 0.60 |
| 8:H:34:GLU:HG2 | 8:H:37:ARG:HH21 | 1.65 | 0.60 |
| 22:W:23:ARG:CG | 22:W:23:ARG:HH11 | 2.14 | 0.60 |
| 1:A:404:U:H5' | 4:D:122:ARG:HD2 | 1.82 | 0.60 |
| 20:T:44:ALA:HB1 | 20:T:91:LEU:HB2 | 1.83 | 0.60 |
| 1:A:235:C:O2' | 1:A:236:G:H5' | 2.01 | 0.60 |
| 1:A:446:G:N2 | 1:A:489:C:C2 | 2.70 | 0.60 |
| 10:J:38:ILE:HG22 | 10:J:71:LEU:O | 1.98 | 0.60 |
| 1:A:518:C:H2' | 1:A:530:G:C8 | 2.36 | 0.60 |
| 1:A:736:C:H2' | 1:A:737:A:C8 | 2.37 | 0.60 |
| 9:I:113:LYS:NZ | 9:I:119:ALA:O | 2.28 | 0.60 |
| 18:R:53:ARG:NH2 | 18:R:60:ALA:HB2 | 2.13 | 0.60 |
| 23:X:115:LYS:HB3 | 23:X:164:LEU:HD21 | 1.83 | 0.60 |
| 3:C:96:GLY:C | 3:C:97:LYS:HG2 | 2.23 | 0.60 |
| 1:A:1128:C:H1' | 1:A:1146:A:N6 | 2.15 | 0.59 |
| 4:D:166:LYS:HG3 | 4:D:178:VAL:HG21 | 1.84 | 0.59 |
| 8:H:41:ARG:HH11 | 8:H:41:ARG:HB3 | 1.66 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1437:C:H2' | 1:A:1438:G:H8 | 1.67 | 0.59 |
| 20:T:67:ALA:HB1 | 20:T:74:LYS:HG2 | 1.85 | 0.59 |
| 24:Y:27:G:H2' | 24:Y:28:A:O4' | 2.02 | 0.59 |
| 1:A:1346:A:C8 | 1:A:1348:U:C2 | 2.91 | 0.59 |
| 1:A:1502:A:H2' | 1:A:1504:G:C8 | 2.37 | 0.59 |
| 1:A:975:A:H5' | 1:A:975:A:C8 | 2.37 | 0.59 |
| 2:B:28:PHE:HA | 2:B:194:PRO:HG3 | 1.83 | 0.59 |
| 1:A:1542:U:H5' | 18:R:19:LYS:HB3 | 1.84 | 0.59 |
| 1:A:524:G:H2' | 1:A:525:C:C6 | 2.37 | 0.59 |
| 1:A:1182:G:H4' | 1:A:1183:A:H5'' | 1.85 | 0.59 |
| 1:A:296:U:H2' | 1:A:297:G:H8 | 1.67 | 0.59 |
| 1:A:588:G:N2 | 1:A:589:C:C2 | 2.69 | 0.59 |
| 1:A:91:C:C6 | 1:A:91:C:C3' | 2.86 | 0.59 |
| 2:B:28:PHE:C | 2:B:30:ARG:N | 2.49 | 0.59 |
| 23:X:94:ILE:HG23 | 23:X:98:ASP:OD1 | 2.01 | 0.59 |
| 1:A:392:G:H2' | 1:A:393:A:H8 | 1.66 | 0.59 |
| 1:A:444:C:C2 | 1:A:491:G:N2 | 2.71 | 0.59 |
| 1:A:1000:U:C6 | 1:A:1000:U:H3' | 2.38 | 0.59 |
| 1:A:1225:A:H2' | 1:A:1226:C:C5 | 2.38 | 0.59 |
| 1:A:1536:C:H42 | 24:Y:29:G:H1 | 1.51 | 0.59 |
| 1:A:1082:G:H2' | 1:A:1083:U:O4' | 2.02 | 0.59 |
| 1:A:328:C:H4' | 1:A:329:A:C5' | 2.33 | 0.59 |
| 1:A:78:G:H8 | 1:A:78:G:OP2 | 1.86 | 0.59 |
| 4:D:61:LYS:HD3 | 4:D:206:PHE:CE2 | 2.37 | 0.59 |
| 17:Q:85:VAL:HG12 | 17:Q:89:LEU:HD12 | 1.82 | 0.59 |
| 20:T:73:HIS:O | 20:T:77:ALA:N | 2.22 | 0.59 |
| 1:A:518:C:H5'' | 1:A:519:C:C6 | 2.38 | 0.59 |
| 7:G:37:ASN:CG | 9:I:40:LEU:O | 2.40 | 0.59 |
| 1:A:224:C:OP1 | 20:T:74:LYS:HE2 | 2.00 | 0.59 |
| 1:A:1372:U:H5'' | 9:I:71:SER:HB3 | 1.83 | 0.58 |
| 4:D:8:VAL:HG11 | 4:D:21:LEU:CB | 2.32 | 0.58 |
| 11:K:99:GLN:HG2 | 11:K:105:VAL:HG21 | 1.85 | 0.58 |
| 1:A:216:G:C6 | 1:A:217:C:N4 | 2.72 | 0.58 |
| 1:A:688:G:H2' | 1:A:689:C:O4' | 2.02 | 0.58 |
| 8:H:111:ILE:HG22 | 8:H:134:ILE:HD12 | 1.85 | 0.58 |
| 1:A:1507:A:H5'' | 1:A:1507:A:H8 | 1.69 | 0.58 |
| 1:A:658:G:N2 | 1:A:749:C:C2 | 2.71 | 0.58 |
| 1:A:916:G:H2' | 1:A:917:G:H8 | 1.67 | 0.58 |
| 18:R:34:TYR:HB3 | 18:R:69:THR:HG22 | 1.85 | 0.58 |
| 1:A:1065:U:H4' | 1:A:1066:C:O5' | 2.03 | 0.58 |
| 1:A:1443:G:C6 | 1:A:1444:C:N4 | 2.72 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:153:VAL:CG1 | 3:C:196:LEU:HD23 | 2.34 | 0.58 |
| 2:B:25:ASN:ND2 | 2:B:27:LYS:N | 2.51 | 0.58 |
| 9:I:51:ARG:HG2 | 9:I:56:LEU:HD11 | 1.85 | 0.58 |
| 1:A:309:G:H2' | 1:A:310:G:H8 | 1.67 | 0.58 |
| 1:A:645:C:H2' | 1:A:646:U:O4' | 2.04 | 0.58 |
| 1:A:715:A:H2' | 1:A:716:A:H8 | 1.65 | 0.58 |
| 1:A:664:G:N2 | 1:A:741:G:H1 | 1.89 | 0.58 |
| 10:J:7:LYS:HB3 | 10:J:97:GLU:HB2 | 1.84 | 0.58 |
| 1:A:718:G:H5' | 11:K:117:ASN:HB2 | 1.86 | 0.58 |
| 1:A:1305:G:H5' | 21:V:4:GLY:C | 2.24 | 0.58 |
| 1:A:1164:G:H1 | 1:A:1172:C:H42 | 1.51 | 0.58 |
| 1:A:446:G:C2 | 1:A:489:C:N3 | 2.72 | 0.58 |
| 12:L:36:VAL:HG22 | 12:L:82:VAL:HG23 | 1.86 | 0.58 |
| 1:A:1091:U:O2 | 1:A:1093:A:C8 | 2.57 | 0.58 |
| 1:A:1308:U:H2' | 1:A:1309:G:C8 | 2.39 | 0.58 |
| 4:D:105:VAL:HG13 | 4:D:110:PHE:HB2 | 1.86 | 0.58 |
| 5:E:127:ASN:O | 5:E:131:ILE:HB | 2.04 | 0.58 |
| 5:E:15:ARG:HD3 | 5:E:28:PHE:CE1 | 2.39 | 0.58 |
| 9:I:5:TYR:CE2 | 9:I:7:THR:OG1 | 2.57 | 0.58 |
| 14:N:9:LYS:HG3 | 14:N:21:TYR:O | 2.03 | 0.58 |
| 1:A:1161:C:H2' | 1:A:1162:C:C6 | 2.39 | 0.57 |
| 1:A:262:A:H5'' | 20:T:76:ALA:HB2 | 1.85 | 0.57 |
| 1:A:93:G:H5'' | 1:A:96:U:P | 2.42 | 0.57 |
| 2:B:84:GLU:HB3 | 2:B:219:VAL:HG21 | 1.86 | 0.57 |
| 3:C:39:ILE:HG23 | 3:C:91:LEU:HD11 | 1.86 | 0.57 |
| 1:A:1217:C:N4 | 1:A:1218:C:N4 | 2.53 | 0.57 |
| 1:A:474:G:H2' | 1:A:475:G:C8 | 2.40 | 0.57 |
| 1:A:737:A:H2' | 1:A:738:C:C6 | 2.39 | 0.57 |
| 1:A:977:A:H1' | 1:A:982:U:O4 | 2.03 | 0.57 |
| 19:S:71:LEU:HD23 | 19:S:71:LEU:O | 2.04 | 0.57 |
| 1:A:1119:C:H42 | 1:A:1154:G:H1 | 1.53 | 0.57 |
| 1:A:97:G:H2' | 1:A:98:G:O4' | 2.05 | 0.57 |
| 1:A:172:A:H2' | 1:A:174:C:H5 | 1.69 | 0.57 |
| 1:A:794:A:H2' | 1:A:795:C:C6 | 2.39 | 0.57 |
| 12:L:89:ARG:HA | 12:L:97:ARG:HA | 1.85 | 0.57 |
| 1:A:1365:G:C6 | 1:A:1366:C:C4 | 2.93 | 0.57 |
| 1:A:1497:G:OP2 | 23:X:91:ARG:NH1 | 2.37 | 0.57 |
| 1:A:142:G:O2' | 1:A:196:A:N1 | 2.37 | 0.57 |
| 1:A:828:A:H4' | 1:A:828:A:OP1 | 2.03 | 0.57 |
| 2:B:24:TRP:CG | 2:B:40:HIS:CE1 | 2.92 | 0.57 |
| 10:J:23:ILE:HG23 | 10:J:85:LEU:HD22 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 14:N:21:TYR:HD1 | 14:N:21:TYR:H | 1.53 | 0.57 |
| 1:A:1536:C:N4 | 24:Y:29:G:H1 | 2.02 | 0.57 |
| 1:A:624:C:H2' | 1:A:625:G:H8 | 1.70 | 0.57 |
| 1:A:998:G:N2 | 1:A:999:C:C2 | 2.72 | 0.57 |
| 2:B:51:LEU:HA | 2:B:201:ILE:HG12 | 1.87 | 0.57 |
| 12:L:85:ILE:HG23 | 12:L:98:TYR:HB3 | 1.85 | 0.57 |
| 14:N:9:LYS:CE | 14:N:21:TYR:O | 2.52 | 0.57 |
| 4:D:56:VAL:HG12 | 4:D:202:LEU:HD21 | 1.86 | 0.57 |
| 13:M:22:ILE:HG22 | 13:M:24:GLY:H | 1.69 | 0.57 |
| 1:A:443:C:C2 | 1:A:492:G:C2 | 2.92 | 0.57 |
| 1:A:491:G:C4 | 1:A:492:G:C8 | 2.93 | 0.57 |
| 1:A:701:C:H4' | 1:A:702:A:O5' | 2.04 | 0.57 |
| 1:A:765:G:C5 | 1:A:812:C:N3 | 2.73 | 0.57 |
| 1:A:1244:C:H2' | 1:A:1245:A:C8 | 2.40 | 0.57 |
| 1:A:864:A:H2' | 1:A:865:A:C8 | 2.39 | 0.57 |
| 2:B:12:GLU:HG3 | 2:B:16:HIS:CB | 2.34 | 0.57 |
| 10:J:32:ALA:HB2 | 10:J:76:ASN:HB2 | 1.87 | 0.57 |
| 1:A:981:U:C5' | 14:N:21:TYR:HE2 | 2.17 | 0.57 |
| 1:A:1048:G:H1 | 1:A:1209:C:H42 | 1.53 | 0.56 |
| 1:A:1384:C:H2' | 1:A:1385:G:C8 | 2.40 | 0.56 |
| 6:F:9:VAL:HB | 6:F:87:ARG:HB3 | 1.87 | 0.56 |
| 1:A:988:G:N1 | 1:A:989:C:C2 | 2.73 | 0.56 |
| 17:Q:28:PRO:HA | 17:Q:35:VAL:HA | 1.87 | 0.56 |
| 11:K:91:ARG:CZ | 18:R:88:LYS:HZ2 | 2.10 | 0.56 |
| 1:A:1488:G:H2' | 1:A:1489:G:H8 | 1.70 | 0.56 |
| 1:A:1509:C:H2' | 1:A:1510:U:O4' | 2.06 | 0.56 |
| 1:A:392:G:H2' | 1:A:393:A:C8 | 2.40 | 0.56 |
| 1:A:939:G:H2' | 1:A:940:C:C6 | 2.41 | 0.56 |
| 4:D:64:LEU:HD12 | 4:D:203:VAL:HG21 | 1.87 | 0.56 |
| 22:W:23:ARG:NH1 | 22:W:23:ARG:HG3 | 2.20 | 0.56 |
| 1:A:1232:U:C5' | 9:I:124:GLN:NE2 | 2.68 | 0.56 |
| 1:A:428:G:H4' | 1:A:429:U:O5' | 2.05 | 0.56 |
| 1:A:751:U:C5 | 1:A:752:G:C5 | 2.93 | 0.56 |
| 1:A:1232:U:P | 9:I:124:GLN:HE22 | 2.28 | 0.56 |
| 9:I:19:LEU:HD12 | 9:I:84:ALA:HB3 | 1.88 | 0.56 |
| 1:A:1402:C:H2' | 1:A:1403:C:O4' | 2.06 | 0.56 |
| 1:A:291:C:O2 | 1:A:310:G:C2 | 2.59 | 0.56 |
| 1:A:945:G:H2' | 1:A:945:G:N3 | 2.20 | 0.56 |
| 4:D:29:PRO:O | 4:D:35:ARG:CD | 2.48 | 0.56 |
| 12:L:33:ARG:HB3 | 12:L:60:LEU:HD12 | 1.86 | 0.56 |
| 14:N:21:TYR:CD1 | 14:N:21:TYR:N | 2.72 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:171:A:H2' | 1:A:172:A:C8 | 2.41 | 0.56 |
| 1:A:80:G:N2 | 1:A:90:U:H1' | 2.21 | 0.56 |
| 1:A:89:C:C4 | 1:A:90:U:C5 | 2.94 | 0.56 |
| 3:C:8:ILE:O | 3:C:12:LEU:N | 2.38 | 0.56 |
| 1:A:30:U:H3' | 1:A:31:G:C5' | 2.36 | 0.56 |
| 1:A:1466:C:H2' | 1:A:1467:G:O4' | 2.06 | 0.56 |
| 1:A:621:A:H2' | 1:A:622:A:C8 | 2.41 | 0.56 |
| 1:A:76:C:H2' | 1:A:77:G:C8 | 2.41 | 0.56 |
| 1:A:946:A:H5' | 1:A:946:A:C8 | 2.39 | 0.56 |
| 3:C:12:LEU:CD2 | 3:C:18:TRP:CE2 | 2.87 | 0.56 |
| 20:T:44:ALA:HB1 | 20:T:91:LEU:CB | 2.36 | 0.56 |
| 1:A:424:G:O5' | 1:A:424:G:H8 | 1.89 | 0.56 |
| 1:A:82:U:H2' | 1:A:83:U:O4' | 2.05 | 0.56 |
| 9:I:8:GLY:HA3 | 9:I:76:ALA:O | 2.05 | 0.56 |
| 1:A:745:C:H2' | 1:A:746:A:H8 | 1.69 | 0.56 |
| 22:W:23:ARG:NE | 22:W:33:LEU:HD22 | 2.11 | 0.56 |
| 5:E:76:ILE:CD1 | 5:E:118:ILE:HG21 | 2.36 | 0.56 |
| 15:O:41:GLU:O | 15:O:44:LYS:HB2 | 2.05 | 0.56 |
| 1:A:1382:C:H2' | 1:A:1383:C:H6 | 1.71 | 0.55 |
| 1:A:1434:A:H2' | 1:A:1435:G:O4' | 2.06 | 0.55 |
| 1:A:174:C:H2' | 1:A:175:C:C6 | 2.40 | 0.55 |
| 1:A:266:G:H5'' | 1:A:266:G:H8 | 1.71 | 0.55 |
| 3:C:8:ILE:HG23 | 3:C:16:ARG:NE | 2.21 | 0.55 |
| 1:A:707:C:H4' | 11:K:20:TYR:CD2 | 2.41 | 0.55 |
| 1:A:1239:A:H62 | 1:A:1299:A:N6 | 2.05 | 0.55 |
| 4:D:62:GLN:O | 4:D:66:ARG:HD2 | 2.07 | 0.55 |
| 14:N:9:LYS:CD | 14:N:21:TYR:O | 2.55 | 0.55 |
| 1:A:107:G:C2 | 1:A:108:G:H1' | 2.41 | 0.55 |
| 1:A:269:C:H2' | 1:A:270:A:H8 | 1.70 | 0.55 |
| 5:E:82:VAL:HG11 | 5:E:137:GLU:HB3 | 1.89 | 0.55 |
| 19:S:22:LEU:HD13 | 19:S:28:LYS:HB3 | 1.88 | 0.55 |
| 1:A:323:U:H5' | 20:T:23:ARG:HB2 | 1.87 | 0.55 |
| 1:A:321:A:H2' | 1:A:322:C:H6 | 1.70 | 0.55 |
| 1:A:657:G:H1 | 1:A:749:C:N4 | 2.04 | 0.55 |
| 1:A:1103:C:H5' | 2:B:98:LEU:HD22 | 1.89 | 0.55 |
| 1:A:1459:C:H2' | 1:A:1460:A:O4' | 2.07 | 0.55 |
| 10:J:21:GLN:HA | 10:J:24:VAL:HB | 1.88 | 0.55 |
| 1:A:1292:U:H2' | 1:A:1293:G:C8 | 2.40 | 0.55 |
| 1:A:636:U:H2' | 1:A:637:G:C8 | 2.42 | 0.55 |
| 9:I:9:ARG:HG2 | 9:I:14:VAL:HG12 | 1.88 | 0.55 |
| 12:L:85:ILE:HA | 12:L:99:HIS:O | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:8:ILE:HG22 | 3:C:12:LEU:HD12 | 1.89 | 0.55 |
| 1:A:1144:G:N2 | 1:A:1146:A:H62 | 2.04 | 0.55 |
| 1:A:1386:G:H2' | 1:A:1387:G:H8 | 1.72 | 0.55 |
| 1:A:589:C:O2 | 1:A:651:C:O2 | 2.25 | 0.55 |
| 2:B:24:TRP:CB | 2:B:190:THR:OG1 | 2.53 | 0.55 |
| 6:F:3:ARG:HB3 | 6:F:93:SER:HB2 | 1.89 | 0.55 |
| 11:K:84:VAL:HG11 | 11:K:95:ILE:HD11 | 1.87 | 0.55 |
| 12:L:60:LEU:HB3 | 12:L:62:SER:H | 1.71 | 0.55 |
| 1:A:790:A:C4 | 24:Y:36:A:N6 | 2.75 | 0.55 |
| 1:A:1151:A:O2' | 1:A:1152:A:C8 | 2.44 | 0.54 |
| 1:A:1464:G:N2 | 1:A:1465:C:C2 | 2.75 | 0.54 |
| 1:A:1513:A:H2' | 1:A:1514:C:H6 | 1.67 | 0.54 |
| 1:A:734:G:C2 | 1:A:735:C:C2 | 2.94 | 0.54 |
| 1:A:1093:A:O2' | 1:A:1094:G:H3' | 2.06 | 0.54 |
| 1:A:269:C:H2' | 1:A:270:A:C8 | 2.41 | 0.54 |
| 1:A:70:G:C2 | 1:A:100:C:C2 | 2.95 | 0.54 |
| 1:A:568:G:C2 | 1:A:883:C:C2 | 2.95 | 0.54 |
| 2:B:111:ARG:HD3 | 2:B:145:LEU:HD21 | 1.88 | 0.54 |
| 2:B:24:TRP:HZ3 | 2:B:29:ALA:HB2 | 1.73 | 0.54 |
| 2:B:77:ALA:HB2 | 2:B:211:ILE:HD13 | 1.90 | 0.54 |
| 5:E:129:ILE:HD12 | 5:E:129:ILE:H | 1.71 | 0.54 |
| 1:A:111:G:O6 | 1:A:330:C:N4 | 2.39 | 0.54 |
| 1:A:1326:C:H2' | 1:A:1327:C:C6 | 2.42 | 0.54 |
| 1:A:148:G:C2 | 1:A:175:C:C2 | 2.95 | 0.54 |
| 1:A:1354:C:H2' | 1:A:1355:G:C8 | 2.43 | 0.54 |
| 1:A:1428:A:H2' | 1:A:1429:C:C6 | 2.42 | 0.54 |
| 1:A:19:C:H2' | 1:A:20:U:C6 | 2.38 | 0.54 |
| 13:M:10:PRO:HB2 | 13:M:18:ALA:HB1 | 1.88 | 0.54 |
| 1:A:419:C:H42 | 1:A:424:G:H1 | 1.55 | 0.54 |
| 1:A:777:A:H2' | 1:A:778:G:C8 | 2.42 | 0.54 |
| 1:A:826:C:H2' | 1:A:827:U:C6 | 2.43 | 0.54 |
| 1:A:1475:G:H2' | 1:A:1476:G:H8 | 1.72 | 0.54 |
| 1:A:243:A:H4' | 1:A:244:U:O5' | 2.07 | 0.54 |
| 1:A:89:C:C2' | 1:A:90:U:C5' | 2.54 | 0.54 |
| 2:B:129:GLU:O | 2:B:130:ARG:HD2 | 2.08 | 0.54 |
| 1:A:1349:A:P | 9:I:118:LYS:CD | 2.94 | 0.54 |
| 11:K:32:ILE:HG21 | 11:K:72:ALA:HB2 | 1.90 | 0.54 |
| 1:A:1320:C:N3 | 19:S:36:ARG:HD3 | 2.22 | 0.54 |
| 1:A:109:A:C6 | 1:A:326:G:C6 | 2.96 | 0.54 |
| 1:A:452:A:HO2' | 1:A:453:A:H8 | 1.54 | 0.54 |
| 1:A:624:C:H2' | 1:A:625:G:C8 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:O:26:GLU:HA | 15:O:81:LEU:HD21 | 1.89 | 0.54 |
| 11:K:110:ASP:HB3 | 18:R:85:LEU:HB3 | 1.89 | 0.54 |
| 23:X:17:ARG:HH22 | 23:X:25:GLN:HA | 1.73 | 0.54 |
| 1:A:1367:C:H2' | 1:A:1368:G:O4' | 2.08 | 0.54 |
| 1:A:437:U:H2' | 1:A:438:G:O4' | 2.07 | 0.54 |
| 5:E:15:ARG:NH2 | 5:E:26:PHE:CG | 2.62 | 0.54 |
| 9:I:26:VAL:HG22 | 9:I:61:ALA:HB3 | 1.90 | 0.54 |
| 14:N:24:CYS:HB2 | 14:N:40:CYS:HB3 | 1.90 | 0.54 |
| 1:A:580:U:H5'' | 15:O:58:MET:HG3 | 1.89 | 0.54 |
| 20:T:33:ILE:HG13 | 20:T:62:LEU:HB3 | 1.89 | 0.54 |
| 1:A:1161:C:H2' | 1:A:1162:C:H6 | 1.72 | 0.54 |
| 1:A:1411:C:H2' | 1:A:1412:C:O4' | 2.08 | 0.54 |
| 5:E:76:ILE:O | 5:E:93:PRO:HB3 | 2.07 | 0.54 |
| 12:L:27:LEU:HG | 12:L:28:LYS:H | 1.73 | 0.54 |
| 1:A:193:C:H2' | 1:A:194:C:C6 | 2.43 | 0.54 |
| 1:A:568:G:N1 | 1:A:883:C:C4 | 2.76 | 0.54 |
| 2:B:24:TRP:CZ3 | 2:B:26:PRO:HA | 2.43 | 0.54 |
| 24:Y:21:G:H2' | 24:Y:22:G:H8 | 1.72 | 0.54 |
| 1:A:1328:C:H2' | 1:A:1329:A:O4' | 2.07 | 0.53 |
| 1:A:1438:G:N2 | 1:A:1439:C:C2 | 2.76 | 0.53 |
| 1:A:312:C:C2' | 1:A:313:A:H8 | 2.20 | 0.53 |
| 1:A:337:C:H2' | 1:A:338:A:C8 | 2.43 | 0.53 |
| 1:A:953:G:H2' | 1:A:954:G:O4' | 2.08 | 0.53 |
| 2:B:17:PHE:O | 2:B:42:ILE:N | 2.37 | 0.53 |
| 2:B:102:LEU:HB3 | 2:B:180:LEU:HD11 | 1.89 | 0.53 |
| 1:A:1004:A:H5'' | 1:A:1025:U:C5 | 2.43 | 0.53 |
| 1:A:1162:C:C2 | 1:A:1175:G:N2 | 2.77 | 0.53 |
| 1:A:236:G:C6 | 1:A:237:C:N3 | 2.76 | 0.53 |
| 1:A:514:C:H2' | 1:A:515:G:H8 | 1.73 | 0.53 |
| 1:A:567:G:H5' | 1:A:567:G:H8 | 1.73 | 0.53 |
| 1:A:962:C:H1' | 1:A:1201:A:N6 | 2.24 | 0.53 |
| 23:X:85:VAL:HA | 23:X:115:LYS:O | 2.08 | 0.53 |
| 1:A:1352:C:H2' | 1:A:1353:G:C8 | 2.43 | 0.53 |
| 1:A:225:C:H2' | 1:A:226:G:H8 | 1.73 | 0.53 |
| 1:A:370:C:N3 | 1:A:392:G:C2 | 2.76 | 0.53 |
| 1:A:524:G:C2 | 1:A:525:C:N3 | 2.76 | 0.53 |
| 1:A:92:C:H2' | 1:A:93:G:C8 | 2.43 | 0.53 |
| 7:G:62:PHE:HD1 | 7:G:124:LEU:HD21 | 1.72 | 0.53 |
| 17:Q:41:LYS:HE2 | 17:Q:88:TYR:HE1 | 1.74 | 0.53 |
| 1:A:1239:A:H62 | 1:A:1299:A:H62 | 1.54 | 0.53 |
| 1:A:1241:G:N2 | 1:A:1242:C:C2 | 2.77 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:865:A:H2' | 1:A:866:C:C6 | 2.43 | 0.53 |
| 4:D:33:MET:HB2 | 4:D:34:GLU:OE1 | 2.09 | 0.53 |
| 2:B:12:GLU:HG3 | 2:B:16:HIS:HB2 | 1.90 | 0.53 |
| 6:F:4:TYR:HB2 | 6:F:65:VAL:HG22 | 1.89 | 0.53 |
| 1:A:1038:C:H2' | 1:A:1039:C:H6 | 1.74 | 0.53 |
| 1:A:1172:C:H2' | 1:A:1173:G:C8 | 2.44 | 0.53 |
| 1:A:1404:C:H2' | 1:A:1405:G:C8 | 2.43 | 0.53 |
| 1:A:172:A:H2' | 1:A:174:C:C5 | 2.42 | 0.53 |
| 2:B:94:ASN:HD22 | 2:B:95:GLN:HG2 | 1.73 | 0.53 |
| 1:A:1308:U:H2' | 1:A:1309:G:H8 | 1.72 | 0.53 |
| 1:A:669:U:H2' | 1:A:670:G:H8 | 1.73 | 0.53 |
| 4:D:65:ARG:HH11 | 4:D:65:ARG:HB3 | 1.73 | 0.53 |
| 9:I:42:ARG:O | 9:I:42:ARG:HG2 | 2.08 | 0.53 |
| 9:I:69:GLY:O | 9:I:73:GLN:HG3 | 2.09 | 0.53 |
| 23:X:17:ARG:HH21 | 23:X:19:VAL:HG22 | 1.73 | 0.53 |
| 23:X:34:ALA:HB1 | 23:X:45:LEU:HD13 | 1.91 | 0.53 |
| 1:A:1258:G:C6 | 1:A:1259:C:N4 | 2.77 | 0.53 |
| 1:A:582:U:H2' | 1:A:583:A:C8 | 2.44 | 0.53 |
| 3:C:114:PRO:HA | 3:C:185:GLY:HA3 | 1.89 | 0.53 |
| 13:M:64:TRP:HE3 | 13:M:66:LEU:HD11 | 1.74 | 0.53 |
| 1:A:1172:C:H2' | 1:A:1173:G:H8 | 1.74 | 0.53 |
| 1:A:1298:C:C4 | 7:G:114:ARG:HD2 | 2.44 | 0.53 |
| 2:B:28:PHE:CD2 | 2:B:190:THR:HA | 2.44 | 0.53 |
| 11:K:15:ALA:HA | 11:K:77:MET:HA | 1.91 | 0.53 |
| 22:W:22:PHE:N | 22:W:22:PHE:CD1 | 2.73 | 0.53 |
| 1:A:512:U:H2' | 1:A:513:C:C6 | 2.44 | 0.53 |
| 1:A:575:G:H4' | 1:A:576:G:C5' | 2.38 | 0.53 |
| 1:A:908:A:H2' | 1:A:909:A:C8 | 2.44 | 0.53 |
| 1:A:97:G:H2' | 1:A:98:G:C8 | 2.44 | 0.53 |
| 1:A:998:G:N1 | 1:A:999:C:C4 | 2.77 | 0.53 |
| 1:A:1182:G:H4' | 1:A:1183:A:C5' | 2.39 | 0.52 |
| 1:A:617:G:N2 | 1:A:618:C:C2 | 2.77 | 0.52 |
| 1:A:774:G:N2 | 1:A:806:C:C2 | 2.78 | 0.52 |
| 23:X:46:VAL:HG21 | 23:X:62:TYR:HB2 | 1.90 | 0.52 |
| 1:A:1292:U:H2' | 1:A:1293:G:H8 | 1.74 | 0.52 |
| 1:A:678:U:H2' | 1:A:679:C:H6 | 1.72 | 0.52 |
| 1:A:79:G:N1 | 1:A:91:C:C2 | 2.74 | 0.52 |
| 2:B:55:PHE:CZ | 2:B:217:ARG:HB3 | 2.44 | 0.52 |
| 1:A:1396:A:H4' | 1:A:1397:C:H5'' | 1.92 | 0.52 |
| 1:A:1416:G:H2' | 1:A:1417:G:O4' | 2.09 | 0.52 |
| 1:A:344:A:H5'' | 1:A:345:C:H5 | 1.73 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:975:A:O5' | 1:A:976:G:H5' | 2.09 | 0.52 |
| 19:S:49:ILE:HG21 | 19:S:71:LEU:CD1 | 2.39 | 0.52 |
| 1:A:1148:U:H2' | 1:A:1149:C:O4' | 2.09 | 0.52 |
| 1:A:216:G:C2 | 1:A:217:C:N3 | 2.77 | 0.52 |
| 1:A:939:G:C6 | 1:A:940:C:N4 | 2.78 | 0.52 |
| 1:A:1104:G:O5' | 2:B:111:ARG:HD2 | 2.08 | 0.52 |
| 1:A:1164:G:N2 | 1:A:1165:C:C2 | 2.76 | 0.52 |
| 1:A:1435:G:H2' | 1:A:1436:U:C6 | 2.44 | 0.52 |
| 1:A:299:G:H2' | 1:A:300:A:C8 | 2.45 | 0.52 |
| 3:C:14:ILE:CD1 | 3:C:14:ILE:N | 2.73 | 0.52 |
| 15:O:33:THR:HA | 15:O:63:ARG:HH11 | 1.73 | 0.52 |
| 23:X:61:ASP:HB3 | 23:X:64:LYS:HB3 | 1.92 | 0.52 |
| 1:A:128:G:C2 | 1:A:234:C:C2 | 2.97 | 0.52 |
| 1:A:521:G:N2 | 1:A:522:C:C2 | 2.78 | 0.52 |
| 1:A:974:A:C8 | 14:N:31:ARG:HG2 | 2.44 | 0.52 |
| 9:I:14:VAL:HG23 | 9:I:66:ARG:HB3 | 1.91 | 0.52 |
| 19:S:72:GLY:O | 19:S:73:GLU:C | 2.45 | 0.52 |
| 1:A:1060:C:OP1 | 14:N:45:ARG:NH2 | 2.43 | 0.52 |
| 1:A:1133:G:H1 | 1:A:1141:C:H42 | 1.58 | 0.52 |
| 1:A:542:G:N2 | 1:A:543:C:C2 | 2.78 | 0.52 |
| 1:A:928:G:H1 | 1:A:1389:C:N4 | 2.06 | 0.52 |
| 2:B:184:VAL:HG13 | 2:B:197:VAL:HA | 1.92 | 0.52 |
| 1:A:673:G:H5'' | 6:F:87:ARG:CZ | 2.40 | 0.52 |
| 14:N:14:PRO:C | 14:N:16:PHE:H | 2.13 | 0.52 |
| 1:A:1475:G:H2' | 1:A:1476:G:C8 | 2.44 | 0.52 |
| 1:A:949:A:H2' | 1:A:950:U:O4' | 2.10 | 0.52 |
| 21:V:3:LYS:H | 21:V:10:ARG:HG2 | 1.74 | 0.52 |
| 23:X:149:VAL:HG13 | 23:X:168:VAL:HG22 | 1.91 | 0.52 |
| 1:A:1129:C:P | 1:A:1130:A:H5' | 2.50 | 0.52 |
| 1:A:351:G:OP2 | 1:A:351:G:H8 | 1.93 | 0.52 |
| 1:A:793:U:C3' | 1:A:794:A:H5'' | 2.20 | 0.52 |
| 1:A:955:U:H2' | 1:A:956:U:C6 | 2.43 | 0.52 |
| 2:B:49:GLU:O | 2:B:52:GLU:HG2 | 2.09 | 0.52 |
| 10:J:62:HIS:HB2 | 14:N:59:ALA:HB3 | 1.91 | 0.52 |
| 1:A:1064:G:H1' | 1:A:1190:G:H21 | 1.75 | 0.51 |
| 1:A:129(A):G:H4' | 1:A:130:A:O5' | 2.09 | 0.51 |
| 1:A:1365:G:C2 | 1:A:1366:C:C2 | 2.98 | 0.51 |
| 1:A:16:A:O2' | 5:E:16:THR:OG1 | 2.19 | 0.51 |
| 1:A:352:C:H4' | 1:A:354:G:OP1 | 2.10 | 0.51 |
| 1:A:491:G:H2' | 1:A:492:G:O4' | 2.10 | 0.51 |
| 1:A:999:C:N3 | 1:A:1043:C:N3 | 2.58 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:725:G:N2 | 1:A:726:C:C2 | 2.78 | 0.51 |
| 4:D:9:CYS:SG | 4:D:26:CYS:SG | 3.08 | 0.51 |
| 10:J:5:ARG:HG2 | 10:J:71:LEU:HD21 | 1.91 | 0.51 |
| 4:D:100:ARG:NH1 | 4:D:137:SER:HA | 2.25 | 0.51 |
| 7:G:113:GLU:HG2 | 7:G:119:ARG:HG2 | 1.93 | 0.51 |
| 1:A:522:C:OP2 | 12:L:69:TYR:OH | 2.27 | 0.51 |
| 1:A:362:G:H5'' | 12:L:61:THR:HB | 1.92 | 0.51 |
| 1:A:673:G:H2' | 1:A:674:G:C8 | 2.45 | 0.51 |
| 1:A:662:G:C2 | 1:A:744:C:O2 | 2.64 | 0.51 |
| 1:A:1030:C:H42 | 1:A:1031:G:H1 | 1.59 | 0.51 |
| 1:A:174:C:H2' | 1:A:175:C:H6 | 1.75 | 0.51 |
| 5:E:40:ARG:CG | 5:E:40:ARG:HH11 | 2.21 | 0.51 |
| 9:I:46:ALA:HB2 | 9:I:74:ILE:HG23 | 1.91 | 0.51 |
| 19:S:49:ILE:HG22 | 19:S:71:LEU:HD11 | 1.91 | 0.51 |
| 1:A:320:C:H2' | 1:A:321:A:C8 | 2.46 | 0.51 |
| 1:A:884:U:H4' | 1:A:885:G:H5'' | 1.93 | 0.51 |
| 4:D:110:PHE:H | 4:D:110:PHE:HD1 | 1.57 | 0.51 |
| 11:K:18:ARG:HG3 | 11:K:81:ASP:HB3 | 1.92 | 0.51 |
| 1:A:1001(A):G:N1 | 1:A:1002:G:C6 | 2.78 | 0.51 |
| 1:A:1405:G:H2' | 1:A:1406:U:H6 | 1.75 | 0.51 |
| 1:A:1506:U:O2' | 1:A:1507:A:O5' | 2.27 | 0.51 |
| 2:B:130:ARG:N | 2:B:130:ARG:CD | 2.73 | 0.51 |
| 12:L:32:PHE:HE1 | 12:L:86:ARG:HG3 | 1.76 | 0.51 |
| 1:A:1364:U:C6 | 21:V:14:TRP:HH2 | 2.29 | 0.51 |
| 1:A:49:U:H3' | 1:A:50:A:H5'' | 1.93 | 0.51 |
| 1:A:77:G:C8 | 1:A:77:G:H3' | 2.46 | 0.51 |
| 4:D:120:LEU:HD12 | 4:D:125:HIS:HD2 | 1.76 | 0.51 |
| 5:E:81:GLU:HG2 | 5:E:90:VAL:HG22 | 1.91 | 0.51 |
| 1:A:981:U:C4' | 14:N:21:TYR:CE2 | 2.81 | 0.51 |
| 19:S:45:VAL:HA | 19:S:62:ILE:HG22 | 1.93 | 0.51 |
| 1:A:1272:G:H2' | 1:A:1273:G:C8 | 2.46 | 0.51 |
| 1:A:1502:A:H2 | 1:A:1505:G:H1 | 1.57 | 0.51 |
| 1:A:374:A:C6 | 1:A:375:U:C4 | 2.99 | 0.51 |
| 1:A:441:A:H3' | 1:A:442:C:C6 | 2.46 | 0.51 |
| 1:A:582:U:H2' | 1:A:583:A:H8 | 1.75 | 0.51 |
| 1:A:613:C:H2' | 1:A:614:A:H8 | 1.74 | 0.51 |
| 1:A:563:A:N6 | 1:A:884:U:C2 | 2.72 | 0.50 |
| 1:A:59:A:H5'' | 1:A:387:U:H5'' | 1.93 | 0.50 |
| 10:J:6:ILE:HG13 | 10:J:72:VAL:O | 2.11 | 0.50 |
| 23:X:130:PRO:HD2 | 23:X:131:GLU:OE2 | 2.11 | 0.50 |
| 1:A:123:C:H2' | 1:A:124:G:H8 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:31:G:OP1 | 1:A:31:G:H2' | 2.10 | 0.50 |
| 1:A:698:G:C6 | 1:A:699:C:N4 | 2.79 | 0.50 |
| 1:A:108:G:C6 | 20:T:15:ARG:HG3 | 2.46 | 0.50 |
| 23:X:91:ARG:H | 23:X:94:ILE:HD11 | 0.49 | 0.50 |
| 1:A:1495:U:OP1 | 23:X:93:LYS:HE3 | 2.10 | 0.50 |
| 1:A:1537:U:H3 | 24:Y:28:A:H61 | 1.59 | 0.50 |
| 1:A:1216:G:H5'' | 14:N:5:ALA:HB2 | 1.92 | 0.50 |
| 1:A:1422:G:N2 | 1:A:1479:C:C2 | 2.80 | 0.50 |
| 1:A:578:C:H5'' | 1:A:578:C:H6 | 1.76 | 0.50 |
| 1:A:884:U:H4' | 1:A:885:G:C5' | 2.40 | 0.50 |
| 1:A:895:G:H1 | 1:A:904:C:H42 | 1.58 | 0.50 |
| 12:L:84:LEU:HB2 | 12:L:105:TYR:HE2 | 1.75 | 0.50 |
| 1:A:254:G:H21 | 17:Q:16:GLN:HE22 | 1.58 | 0.50 |
| 20:T:45:GLN:HA | 20:T:91:LEU:HD22 | 1.92 | 0.50 |
| 1:A:1368:G:N2 | 1:A:1369:C:C2 | 2.80 | 0.50 |
| 1:A:657:G:H4' | 15:O:28:GLN:HG3 | 1.93 | 0.50 |
| 1:A:713:G:H2' | 1:A:714:G:C8 | 2.46 | 0.50 |
| 1:A:975:A:H4' | 1:A:976:G:O5' | 2.12 | 0.50 |
| 3:C:131:ARG:NH1 | 3:C:131:ARG:HG2 | 2.26 | 0.50 |
| 4:D:8:VAL:O | 4:D:11:LEU:N | 2.43 | 0.50 |
| 1:A:266:G:O3' | 17:Q:67:LYS:HB2 | 2.10 | 0.50 |
| 24:Y:23:C:H2' | 24:Y:24:A:O4' | 2.12 | 0.50 |
| 1:A:1129:C:OP1 | 1:A:1130:A:H5' | 2.12 | 0.50 |
| 1:A:1216:G:N2 | 1:A:1217:C:C2 | 2.79 | 0.50 |
| 1:A:1258:G:C2 | 1:A:1259:C:N3 | 2.79 | 0.50 |
| 1:A:1409:C:H2' | 1:A:1410:G:C8 | 2.47 | 0.50 |
| 1:A:156:G:H1 | 1:A:165:C:H42 | 1.60 | 0.50 |
| 3:C:113:ALA:HA | 3:C:202:ILE:HD13 | 1.93 | 0.50 |
| 1:A:544:G:OP1 | 4:D:62:GLN:HG3 | 2.11 | 0.50 |
| 12:L:84:LEU:HB2 | 12:L:105:TYR:CE2 | 2.46 | 0.50 |
| 1:A:1272:G:H2' | 1:A:1273:G:H8 | 1.75 | 0.50 |
| 1:A:70:G:C2 | 1:A:100:C:O2 | 2.65 | 0.50 |
| 1:A:794:A:H2' | 1:A:795:C:H6 | 1.77 | 0.50 |
| 2:B:130:ARG:N | 2:B:130:ARG:HE | 2.10 | 0.50 |
| 5:E:11:ILE:HD12 | 5:E:31:LEU:CD1 | 2.42 | 0.50 |
| 12:L:32:PHE:CB | 12:L:84:LEU:HD11 | 2.42 | 0.50 |
| 1:A:1310:G:N2 | 1:A:1328:C:C2 | 2.80 | 0.50 |
| 1:A:671:G:N2 | 1:A:736:C:C2 | 2.80 | 0.50 |
| 1:A:945:G:H2' | 1:A:946:A:H5'' | 1.93 | 0.50 |
| 1:A:985:C:C2 | 1:A:1221:G:C2 | 3.00 | 0.50 |
| 18:R:26:LEU:HD21 | 18:R:39:VAL:HG22 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 19:S:72:GLY:C | 19:S:74:PHE:N | 2.58 | 0.50 |
| 1:A:11:G:H2' | 1:A:12:U:O4' | 2.11 | 0.50 |
| 1:A:247:G:OP2 | 17:Q:100:LYS:N | 2.45 | 0.50 |
| 1:A:34:C:H2' | 1:A:35:G:C8 | 2.47 | 0.50 |
| 2:B:24:TRP:NE1 | 2:B:40:HIS:HE1 | 2.06 | 0.50 |
| 3:C:46:GLU:HB2 | 3:C:47:LEU:HD12 | 1.93 | 0.50 |
| 14:N:23:ARG:HG3 | 14:N:30:ALA:CA | 2.38 | 0.50 |
| 19:S:15:LEU:HD23 | 19:S:33:THR:HG21 | 1.94 | 0.50 |
| 1:A:1000:U:C3' | 1:A:1000:U:C6 | 2.94 | 0.50 |
| 1:A:1248:A:H2' | 1:A:1249:C:C6 | 2.47 | 0.50 |
| 1:A:1355:G:H1 | 1:A:1367:C:H42 | 1.60 | 0.50 |
| 1:A:17:U:H2' | 1:A:18:C:C6 | 2.46 | 0.50 |
| 1:A:189(K):U:H2' | 1:A:189(L):G:C8 | 2.46 | 0.50 |
| 1:A:331:G:OP1 | 1:A:332:G:H5' | 2.11 | 0.50 |
| 1:A:474:G:H2' | 1:A:475:G:H8 | 1.76 | 0.50 |
| 1:A:662:G:C6 | 1:A:744:C:N3 | 2.80 | 0.50 |
| 1:A:1190:G:H5' | 3:C:176:HIS:CE1 | 2.47 | 0.50 |
| 3:C:29:TYR:C | 3:C:29:TYR:CD1 | 2.85 | 0.50 |
| 4:D:8:VAL:HG21 | 4:D:115:ARG:HE | 1.76 | 0.50 |
| 9:I:79:LEU:O | 9:I:83:ARG:HG3 | 2.12 | 0.50 |
| 2:B:130:ARG:CA | 2:B:130:ARG:NE | 2.73 | 0.49 |
| 2:B:25:ASN:ND2 | 2:B:27:LYS:H | 2.10 | 0.49 |
| 2:B:28:PHE:O | 2:B:30:ARG:CA | 2.57 | 0.49 |
| 23:X:131:GLU:O | 23:X:135:ARG:HB2 | 2.11 | 0.49 |
| 1:A:407:G:C2 | 1:A:436:C:C2 | 3.00 | 0.49 |
| 1:A:44:G:C2 | 1:A:45:U:H1' | 2.47 | 0.49 |
| 1:A:44:G:H2' | 1:A:45:U:O4' | 2.12 | 0.49 |
| 1:A:51:A:H4' | 1:A:52:G:C5' | 2.42 | 0.49 |
| 1:A:824:C:H2' | 1:A:825:G:H8 | 1.77 | 0.49 |
| 1:A:897:C:O2 | 1:A:903:G:C2 | 2.65 | 0.49 |
| 1:A:132:C:C5' | 20:T:75:ASN:HD22 | 2.24 | 0.49 |
| 1:A:1095:U:P | 1:A:1108:G:H1 | 2.35 | 0.49 |
| 1:A:925:G:H1 | 1:A:1391:U:H3 | 1.61 | 0.49 |
| 1:A:765:G:C6 | 1:A:812:C:C4 | 3.00 | 0.49 |
| 1:A:84:U:H2' | 1:A:88:A:O4' | 2.12 | 0.49 |
| 4:D:56:VAL:HG12 | 4:D:202:LEU:CD2 | 2.42 | 0.49 |
| 1:A:1348:U:H2' | 1:A:1349:A:H8 | 1.77 | 0.49 |
| 1:A:403:C:H5'' | 4:D:136:PRO:HD2 | 1.94 | 0.49 |
| 1:A:778:G:N1 | 1:A:779:C:C2 | 2.81 | 0.49 |
| 1:A:825:G:C6 | 1:A:826:C:C4 | 3.00 | 0.49 |
| 1:A:975:A:H5' | 1:A:975:A:H8 | 1.76 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C:131:ARG:HA | 3:C:134:ILE:HD12 | 1.94 | 0.49 |
| 23:X:94:ILE:CG2 | 23:X:98:ASP:OD1 | 2.61 | 0.49 |
| 1:A:1158:C:O2 | 1:A:1158:C:H3' | 2.12 | 0.49 |
| 1:A:201:C:H42 | 1:A:216:G:H1 | 1.59 | 0.49 |
| 1:A:354:G:N1 | 1:A:355:C:C4 | 2.80 | 0.49 |
| 1:A:438:G:OP1 | 4:D:125:HIS:HE1 | 1.95 | 0.49 |
| 2:B:178:ARG:HD3 | 2:B:196:LEU:HD23 | 1.94 | 0.49 |
| 12:L:71:PRO:O | 12:L:102:ARG:HD2 | 2.12 | 0.49 |
| 1:A:1431:C:H2' | 1:A:1432:G:O4' | 2.13 | 0.49 |
| 1:A:77:G:OP2 | 1:A:77:G:H8 | 1.96 | 0.49 |
| 5:E:15:ARG:HD3 | 5:E:28:PHE:CZ | 2.47 | 0.49 |
| 6:F:52:ILE:HD11 | 18:R:77:GLY:HA3 | 1.95 | 0.49 |
| 1:A:1017:G:C2 | 1:A:1018:C:C2 | 3.01 | 0.49 |
| 1:A:1125:U:H5' | 1:A:1126:U:O4 | 2.13 | 0.49 |
| 1:A:1128:C:H2' | 1:A:1139:G:N7 | 2.26 | 0.49 |
| 1:A:1363(A):A:H1' | 1:A:1365:G:N7 | 2.27 | 0.49 |
| 1:A:370:C:C2 | 1:A:392:G:C2 | 3.01 | 0.49 |
| 2:B:88:ALA:HB2 | 2:B:219:VAL:HG13 | 1.93 | 0.49 |
| 10:J:38:ILE:CG2 | 10:J:71:LEU:HD13 | 2.43 | 0.49 |
| 1:A:1128:C:H42 | 1:A:1143:G:H1 | 1.60 | 0.49 |
| 1:A:1315:U:H2' | 1:A:1316:G:C8 | 2.48 | 0.49 |
| 1:A:264:U:H2' | 1:A:265:G:O4' | 2.12 | 0.49 |
| 1:A:424:G:H2' | 1:A:425:G:C8 | 2.47 | 0.49 |
| 1:A:51:A:H4' | 1:A:52:G:H5' | 1.94 | 0.49 |
| 1:A:911:U:H2' | 1:A:912:C:C6 | 2.47 | 0.49 |
| 2:B:19:HIS:CD2 | 2:B:20:GLU:HG2 | 2.48 | 0.49 |
| 1:A:1124:G:H1 | 1:A:1149:C:H42 | 1.61 | 0.49 |
| 1:A:286:G:H2' | 1:A:287:U:O4' | 2.13 | 0.49 |
| 1:A:456:C:C2 | 1:A:476:G:C2 | 3.01 | 0.49 |
| 1:A:658:G:C6 | 1:A:749:C:N4 | 2.81 | 0.49 |
| 1:A:93:G:C3' | 1:A:96:U:O4' | 2.60 | 0.49 |
| 3:C:113:ALA:N | 3:C:114:PRO:CD | 2.76 | 0.49 |
| 1:A:1495:U:C5' | 23:X:93:LYS:O | 2.54 | 0.49 |
| 1:A:1300:G:H1' | 1:A:1301:U:H5 | 1.77 | 0.49 |
| 1:A:837:G:H1 | 1:A:849:C:H42 | 1.59 | 0.49 |
| 1:A:945:G:C2 | 1:A:946:A:C8 | 3.01 | 0.49 |
| 2:B:33:TYR:HB2 | 2:B:43:ASP:HA | 1.95 | 0.49 |
| 10:J:11:PHE:HB3 | 14:N:55:GLY:HA3 | 1.95 | 0.49 |
| 24:Y:22:G:C6 | 24:Y:23:C:N4 | 2.80 | 0.49 |
| 1:A:124:G:H2' | 1:A:125:U:O4' | 2.13 | 0.48 |
| 1:A:411:A:H2' | 1:A:412:A:H4' | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:456:C:C2 | 1:A:476:G:N2 | 2.81 | 0.48 |
| 1:A:486:U:H2' | 1:A:487:A:C8 | 2.41 | 0.48 |
| 1:A:707:C:H2' | 1:A:708:C:C6 | 2.48 | 0.48 |
| 2:B:10:LEU:CA | 2:B:48:MET:HE2 | 2.42 | 0.48 |
| 4:D:10:ARG:HG3 | 4:D:10:ARG:HH11 | 1.78 | 0.48 |
| 4:D:174:LEU:HD23 | 4:D:185:PHE:HA | 1.95 | 0.48 |
| 1:A:1251:A:H5' | 9:I:12:GLU:OE1 | 2.13 | 0.48 |
| 14:N:22:THR:HB | 14:N:33:VAL:HG11 | 1.95 | 0.48 |
| 24:Y:21:G:H2' | 24:Y:22:G:C8 | 2.48 | 0.48 |
| 1:A:1094:G:O2' | 1:A:1095:U:P | 2.71 | 0.48 |
| 1:A:187:C:H2' | 1:A:188:C:C6 | 2.49 | 0.48 |
| 1:A:457:C:H2' | 1:A:458:C:C6 | 2.48 | 0.48 |
| 1:A:457:C:H2' | 1:A:458:C:H6 | 1.77 | 0.48 |
| 1:A:73:G:C6 | 1:A:97:G:C6 | 3.01 | 0.48 |
| 3:C:201:TYR:N | 3:C:201:TYR:CD1 | 2.82 | 0.48 |
| 1:A:441:A:H3' | 1:A:442:C:H6 | 1.78 | 0.48 |
| 2:B:129:GLU:C | 2:B:130:ARG:CD | 2.75 | 0.48 |
| 5:E:71:LEU:HD11 | 5:E:115:VAL:HG23 | 1.94 | 0.48 |
| 23:X:7:THR:HG22 | 23:X:46:VAL:HG13 | 1.94 | 0.48 |
| 1:A:1164:G:N1 | 1:A:1165:C:C4 | 2.80 | 0.48 |
| 1:A:1326:C:H5'' | 21:V:12:LYS:NZ | 2.28 | 0.48 |
| 1:A:382:A:H2' | 1:A:383:A:C8 | 2.48 | 0.48 |
| 1:A:1308:U:OP1 | 13:M:98:VAL:N | 2.45 | 0.48 |
| 1:A:333:G:N1 | 1:A:334:C:C4 | 2.82 | 0.48 |
| 1:A:393:A:C2 | 1:A:394:G:C8 | 3.01 | 0.48 |
| 1:A:623:C:H2' | 1:A:624:C:O4' | 2.13 | 0.48 |
| 1:A:952:U:H2' | 1:A:953:G:H8 | 1.79 | 0.48 |
| 1:A:986:A:H2' | 1:A:987:G:O4' | 2.13 | 0.48 |
| 2:B:103:THR:H | 2:B:176:GLU:CD | 2.16 | 0.48 |
| 6:F:68:PRO:HG2 | 6:F:71:ARG:HH21 | 1.78 | 0.48 |
| 7:G:150:ALA:HB1 | 11:K:57:THR:HG21 | 1.96 | 0.48 |
| 12:L:35:GLY:HA3 | 12:L:60:LEU:HD13 | 1.96 | 0.48 |
| 12:L:75:HIS:C | 12:L:77:LEU:H | 2.15 | 0.48 |
| 12:L:93:LEU:HD12 | 12:L:93:LEU:H | 1.77 | 0.48 |
| 1:A:1320:C:C5' | 19:S:73:GLU:OE2 | 2.61 | 0.48 |
| 1:A:1299:A:O2' | 1:A:1301:U:C6 | 2.64 | 0.48 |
| 1:A:563:A:H2 | 12:L:15:ARG:CZ | 2.26 | 0.48 |
| 1:A:570:G:C5 | 1:A:873:A:C2 | 3.01 | 0.48 |
| 1:A:679:C:H2' | 1:A:680:C:C6 | 2.48 | 0.48 |
| 1:A:784:C:C2 | 1:A:799:G:N2 | 2.81 | 0.48 |
| 1:A:90:U:H2' | 1:A:91:C:C6 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 9:I:50:LEU:HD23 | 9:I:85:LEU:HD11 | 1.95 | 0.48 |
| 14:N:24:CYS:O | 14:N:28:GLY:HA2 | 2.13 | 0.48 |
| 23:X:94:ILE:CG2 | 23:X:98:ASP:CG | 2.80 | 0.48 |
| 1:A:1464:G:N1 | 1:A:1465:C:C4 | 2.81 | 0.48 |
| 1:A:802:A:H2' | 1:A:803:G:O4' | 2.14 | 0.48 |
| 4:D:39:PRO:O | 4:D:44:GLY:HA2 | 2.14 | 0.48 |
| 4:D:64:LEU:HG | 4:D:198:VAL:HG21 | 1.95 | 0.48 |
| 7:G:62:PHE:HA | 7:G:124:LEU:HD22 | 1.96 | 0.48 |
| 9:I:96:LEU:HG | 9:I:101:PHE:HB2 | 1.95 | 0.48 |
| 9:I:6:GLY:HA3 | 9:I:80:GLY:O | 2.12 | 0.48 |
| 13:M:10:PRO:HG2 | 13:M:45:VAL:HG11 | 1.96 | 0.48 |
| 1:A:1134:G:N2 | 1:A:1141:C:C2 | 2.81 | 0.48 |
| 1:A:1367:C:H5'' | 9:I:114:TYR:HB3 | 1.95 | 0.48 |
| 1:A:246:A:N6 | 1:A:281:G:H1' | 2.29 | 0.48 |
| 1:A:545:C:H5' | 4:D:72:GLU:HB2 | 1.95 | 0.48 |
| 1:A:80:G:C2 | 1:A:90:U:H1' | 2.49 | 0.48 |
| 2:B:103:THR:N | 2:B:176:GLU:OE1 | 2.47 | 0.48 |
| 2:B:24:TRP:CZ3 | 2:B:29:ALA:HB2 | 2.49 | 0.48 |
| 1:A:590:C:C2 | 1:A:650:G:C2 | 3.02 | 0.48 |
| 1:A:734:G:C6 | 1:A:735:C:C4 | 3.01 | 0.48 |
| 1:A:580:U:H3 | 1:A:761:G:H1 | 1.61 | 0.48 |
| 1:A:834:C:C2 | 1:A:853:G:C2 | 3.02 | 0.48 |
| 1:A:918:A:H2' | 1:A:919:A:O4' | 2.14 | 0.48 |
| 1:A:1041:A:H2' | 1:A:1042:G:C8 | 2.49 | 0.48 |
| 1:A:1129:C:O5' | 1:A:1130:A:H5' | 2.13 | 0.48 |
| 1:A:1361:G:C6 | 1:A:1362:C:N3 | 2.82 | 0.48 |
| 1:A:1419:G:C6 | 1:A:1420:C:C4 | 3.02 | 0.48 |
| 1:A:424:G:H2' | 1:A:425:G:H8 | 1.76 | 0.48 |
| 1:A:722:A:H3' | 1:A:722:A:N3 | 2.28 | 0.48 |
| 1:A:728:A:OP1 | 1:A:742:G:O2' | 2.31 | 0.48 |
| 1:A:825:G:C2 | 1:A:826:C:C2 | 3.02 | 0.48 |
| 2:B:130:ARG:N | 2:B:130:ARG:NE | 2.62 | 0.48 |
| 14:N:9:LYS:CG | 14:N:21:TYR:O | 2.61 | 0.48 |
| 22:W:32:ILE:N | 22:W:32:ILE:CD1 | 2.73 | 0.48 |
| 1:A:1354:C:H2' | 1:A:1355:G:H8 | 1.79 | 0.47 |
| 1:A:1489:G:C2 | 1:A:1490:C:C2 | 3.02 | 0.47 |
| 1:A:1507:A:H2' | 1:A:1508:G:C8 | 2.49 | 0.47 |
| 1:A:434:U:H2' | 1:A:435:C:H6 | 1.78 | 0.47 |
| 1:A:778:G:C6 | 1:A:779:C:N3 | 2.82 | 0.47 |
| 1:A:829:G:C1' | 2:B:26:PRO:CG | 2.89 | 0.47 |
| 5:E:102:ALA:O | 5:E:107:ARG:NH1 | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 11:K:61:ALA:CB | 11:K:90:GLY:HA3 | 2.44 | 0.47 |
| 23:X:137:LEU:HD22 | 23:X:163:MET:SD | 2.53 | 0.47 |
| 1:A:1232:U:OP1 | 9:I:124:GLN:NE2 | 2.44 | 0.47 |
| 1:A:1250:A:H2' | 1:A:1251:A:C8 | 2.49 | 0.47 |
| 1:A:1255:G:O2' | 1:A:1258:G:H1' | 2.14 | 0.47 |
| 1:A:1326:C:H5'' | 21:V:12:LYS:HZ1 | 1.79 | 0.47 |
| 1:A:145:G:N2 | 1:A:178:C:C2 | 2.82 | 0.47 |
| 1:A:563:A:N1 | 1:A:884:U:C4 | 2.82 | 0.47 |
| 1:A:632:A:H2' | 1:A:633:G:O4' | 2.14 | 0.47 |
| 1:A:69:G:H1 | 1:A:100:C:H42 | 1.62 | 0.47 |
| 1:A:778:G:C6 | 1:A:779:C:C4 | 3.02 | 0.47 |
| 1:A:932:C:H42 | 1:A:1385:G:H1 | 1.62 | 0.47 |
| 2:B:19:HIS:O | 2:B:190:THR:HG22 | 2.14 | 0.47 |
| 1:A:626:U:H5'' | 16:P:38:TYR:CG | 2.48 | 0.47 |
| 1:A:1112:C:H1' | 3:C:179:ARG:HE | 1.79 | 0.47 |
| 1:A:18:C:H2' | 1:A:19:C:O4' | 2.14 | 0.47 |
| 1:A:778:G:H2' | 1:A:779:C:O4' | 2.14 | 0.47 |
| 1:A:802:A:H3' | 1:A:803:G:H8 | 1.79 | 0.47 |
| 3:C:12:LEU:HD22 | 3:C:18:TRP:NE1 | 2.27 | 0.47 |
| 7:G:106:GLN:O | 7:G:110:GLN:HG2 | 2.14 | 0.47 |
| 8:H:30:ARG:HA | 8:H:30:ARG:HD3 | 1.63 | 0.47 |
| 1:A:1371:G:P | 9:I:12:GLU:CG | 3.01 | 0.47 |
| 1:A:1069:C:H2' | 1:A:1070:U:O4' | 2.14 | 0.47 |
| 1:A:1489:G:C6 | 1:A:1490:C:C4 | 3.02 | 0.47 |
| 1:A:585:G:C6 | 1:A:586:C:C4 | 3.01 | 0.47 |
| 8:H:113:SER:HB2 | 8:H:134:ILE:HD11 | 1.96 | 0.47 |
| 13:M:87:TYR:O | 13:M:91:ARG:HG2 | 2.14 | 0.47 |
| 1:A:652:U:C2 | 1:A:752:G:N2 | 2.83 | 0.47 |
| 1:A:769:G:N2 | 1:A:770:C:C2 | 2.82 | 0.47 |
| 1:A:225:C:H2' | 1:A:226:G:C8 | 2.50 | 0.47 |
| 1:A:351:G:H4' | 1:A:352:C:OP1 | 2.15 | 0.47 |
| 1:A:512:U:H2' | 1:A:513:C:H6 | 1.79 | 0.47 |
| 1:A:546:G:H4' | 1:A:548:G:H4' | 1.96 | 0.47 |
| 2:B:55:PHE:HZ | 2:B:217:ARG:HB3 | 1.79 | 0.47 |
| 13:M:54:VAL:O | 13:M:58:GLU:HG2 | 2.14 | 0.47 |
| 1:A:834:C:H5'' | 18:R:60:ALA:CB | 2.44 | 0.47 |
| 1:A:1356:G:H2' | 1:A:1357:A:C8 | 2.49 | 0.47 |
| 1:A:189(K):U:H2' | 1:A:189(L):G:H8 | 1.79 | 0.47 |
| 1:A:317:G:C2 | 1:A:337:C:O2 | 2.68 | 0.47 |
| 1:A:330:C:H5'' | 1:A:330:C:C6 | 2.50 | 0.47 |
| 1:A:340:U:H2' | 1:A:341:C:H6 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:30:LEU:HD23 | 6:F:75:LEU:HD21 | 1.97 | 0.47 |
| 9:I:92:TYR:O | 9:I:96:LEU:HB2 | 2.13 | 0.47 |
| 13:M:67:GLU:O | 13:M:71:ARG:HG3 | 2.14 | 0.47 |
| 19:S:72:GLY:C | 19:S:74:PHE:H | 2.16 | 0.47 |
| 1:A:100:C:H2' | 1:A:101:A:C8 | 2.49 | 0.47 |
| 1:A:1117:G:C5' | 1:A:1117:G:H8 | 2.28 | 0.47 |
| 1:A:1233:G:C2 | 1:A:1234:C:C2 | 3.03 | 0.47 |
| 1:A:130:A:H8 | 1:A:130:A:OP1 | 1.98 | 0.47 |
| 1:A:370:C:C4 | 1:A:392:G:N1 | 2.83 | 0.47 |
| 1:A:834:C:O2 | 1:A:853:G:C2 | 2.68 | 0.47 |
| 17:Q:41:LYS:HE2 | 17:Q:88:TYR:CE1 | 2.49 | 0.47 |
| 22:W:17:LEU:HB3 | 22:W:18:PRO:CD | 2.45 | 0.47 |
| 1:A:1033:G:H2' | 1:A:1034:G:C8 | 2.50 | 0.47 |
| 1:A:1122:U:H2' | 1:A:1123:A:O4' | 2.14 | 0.47 |
| 1:A:1255:G:H2' | 1:A:1279:A:N6 | 2.29 | 0.47 |
| 1:A:1362:C:HO2' | 1:A:1363:C:H6 | 1.60 | 0.47 |
| 1:A:1443:G:N2 | 1:A:1444:C:C2 | 2.83 | 0.47 |
| 1:A:372:C:H42 | 1:A:389:A:H62 | 1.63 | 0.47 |
| 1:A:502:G:C2 | 1:A:503:C:C2 | 3.03 | 0.47 |
| 1:A:73:G:N3 | 1:A:73:G:H2' | 2.30 | 0.47 |
| 2:B:18:GLY:HA3 | 2:B:41:ILE:HA | 1.97 | 0.47 |
| 4:D:79:PHE:CZ | 4:D:204:ILE:HA | 2.50 | 0.47 |
| 1:A:1279:A:H5'' | 10:J:7:LYS:HE2 | 1.96 | 0.47 |
| 20:T:10:LEU:HG | 20:T:12:ALA:H | 1.79 | 0.47 |
| 1:A:28:G:H2' | 1:A:29:G:O4' | 2.14 | 0.47 |
| 1:A:492:G:N3 | 1:A:492:G:H2' | 2.29 | 0.47 |
| 9:I:117:HIS:N | 9:I:117:HIS:ND1 | 2.63 | 0.47 |
| 19:S:49:ILE:HG21 | 19:S:71:LEU:HD11 | 1.96 | 0.47 |
| 20:T:56:MET:HG2 | 20:T:84:LEU:HD21 | 1.96 | 0.47 |
| 22:W:23:ARG:HH11 | 22:W:23:ARG:HG3 | 1.77 | 0.47 |
| 1:A:1058:G:H2' | 1:A:1059:C:O4' | 2.14 | 0.47 |
| 1:A:10:A:H2' | 1:A:11:G:C8 | 2.48 | 0.47 |
| 1:A:1507:A:H8 | 1:A:1507:A:C5' | 2.27 | 0.47 |
| 1:A:337:C:H2' | 1:A:338:A:H8 | 1.80 | 0.47 |
| 1:A:536:C:H2' | 1:A:537:G:H8 | 1.79 | 0.47 |
| 1:A:588:G:N1 | 1:A:589:C:C4 | 2.83 | 0.47 |
| 5:E:16:THR:HG22 | 5:E:27:ARG:O | 2.14 | 0.47 |
| 1:A:189:G:C2 | 1:A:189(A):C:C2 | 3.03 | 0.46 |
| 1:A:881:G:C2 | 1:A:882:C:C2 | 3.04 | 0.46 |
| 2:B:10:LEU:HB2 | 2:B:48:MET:HE3 | 1.40 | 0.46 |
| 17:Q:43:LEU:HD13 | 17:Q:68:ARG:HH12 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:153:C:N4 | 1:A:154:C:N4 | 2.63 | 0.46 |
| 1:A:199:G:N2 | 1:A:219:C:C2 | 2.83 | 0.46 |
| 1:A:408:A:H2' | 1:A:409:G:O4' | 2.14 | 0.46 |
| 1:A:426:G:P | 4:D:36:ARG:NH2 | 2.87 | 0.46 |
| 1:A:66:G:N2 | 1:A:67:C:C2 | 2.83 | 0.46 |
| 1:A:865:A:H2' | 1:A:866:C:H6 | 1.78 | 0.46 |
| 5:E:115:VAL:CG1 | 5:E:118:ILE:HG23 | 2.45 | 0.46 |
| 11:K:33:THR:HA | 11:K:40:ILE:H | 1.80 | 0.46 |
| 12:L:6:THR:O | 12:L:9:GLN:HB2 | 2.16 | 0.46 |
| 1:A:247:G:P | 17:Q:99:SER:HG | 2.38 | 0.46 |
| 18:R:48:GLY:N | 18:R:83:GLU:HB2 | 2.30 | 0.46 |
| 1:A:1010:G:H2' | 1:A:1011:G:C8 | 2.51 | 0.46 |
| 1:A:1062:U:H2' | 1:A:1063:C:C6 | 2.50 | 0.46 |
| 1:A:961:U:C4 | 1:A:1201:A:N1 | 2.81 | 0.46 |
| 1:A:122:G:C2 | 1:A:123:C:C2 | 3.03 | 0.46 |
| 1:A:389:A:H3' | 1:A:390:C:C6 | 2.51 | 0.46 |
| 1:A:44:G:OP2 | 16:P:12:LYS:HE3 | 2.15 | 0.46 |
| 1:A:585:G:C2 | 1:A:586:C:C2 | 3.04 | 0.46 |
| 1:A:663:A:H2' | 1:A:664:G:O4' | 2.15 | 0.46 |
| 1:A:902:G:H2' | 1:A:903:G:H8 | 1.79 | 0.46 |
| 1:A:910:C:H4' | 1:A:1413:A:H4' | 1.98 | 0.46 |
| 1:A:1226:C:P | 13:M:91:ARG:HH12 | 2.39 | 0.46 |
| 1:A:1268:A:H2' | 1:A:1269:A:C8 | 2.50 | 0.46 |
| 1:A:1430:C:C2 | 1:A:1471:G:N2 | 2.83 | 0.46 |
| 1:A:255:G:H2' | 1:A:256:U:C6 | 2.50 | 0.46 |
| 1:A:688:G:C2 | 1:A:689:C:C2 | 3.03 | 0.46 |
| 1:A:743:U:H2' | 1:A:744:C:C6 | 2.51 | 0.46 |
| 1:A:89:C:H2' | 1:A:90:U:O4' | 2.14 | 0.46 |
| 2:B:187:LEU:HD12 | 2:B:211:ILE:HG23 | 1.98 | 0.46 |
| 4:D:10:ARG:NH1 | 4:D:10:ARG:HG3 | 2.30 | 0.46 |
| 3:C:33:LEU:HD11 | 14:N:53:LEU:HD23 | 1.97 | 0.46 |
| 15:O:25:THR:HG23 | 15:O:66:LEU:HD23 | 1.97 | 0.46 |
| 1:A:1042:G:N2 | 1:A:1043:C:C2 | 2.84 | 0.46 |
| 1:A:31:G:C6 | 1:A:48:C:O4' | 2.68 | 0.46 |
| 1:A:538:G:H5'' | 12:L:114:LYS:HB2 | 1.97 | 0.46 |
| 1:A:539:A:H2' | 1:A:540:G:C8 | 2.51 | 0.46 |
| 1:A:108:G:H5' | 1:A:109:A:H5'' | 1.97 | 0.46 |
| 1:A:1163:C:C2 | 1:A:1174:G:N2 | 2.84 | 0.46 |
| 1:A:1266:G:N2 | 1:A:1270:C:C2 | 2.83 | 0.46 |
| 1:A:1287:A:H2' | 1:A:1288:A:H8 | 1.76 | 0.46 |
| 1:A:1502:A:H2' | 1:A:1504:G:N7 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:193:C:H2' | 1:A:194:C:H6 | 1.81 | 0.46 |
| 1:A:457:C:C2 | 1:A:475:G:N2 | 2.83 | 0.46 |
| 3:C:146:ALA:C | 3:C:148:GLY:H | 2.19 | 0.46 |
| 8:H:20:TYR:HA | 8:H:65:TYR:CZ | 2.51 | 0.46 |
| 17:Q:43:LEU:HD13 | 17:Q:68:ARG:HH22 | 1.80 | 0.46 |
| 23:X:48:VAL:HG23 | 23:X:56:VAL:HG12 | 1.98 | 0.46 |
| 1:A:15:G:H2' | 1:A:16:A:H8 | 1.80 | 0.46 |
| 1:A:542:G:H5' | 4:D:41:GLY:HA3 | 1.97 | 0.46 |
| 1:A:638:G:H2' | 1:A:639:G:O4' | 2.15 | 0.46 |
| 2:B:77:ALA:HA | 2:B:80:ILE:HD12 | 1.97 | 0.46 |
| 1:A:1099:G:C2 | 1:A:1100:C:O2 | 2.68 | 0.46 |
| 1:A:1127:G:H21 | 1:A:1147:C:H41 | 1.64 | 0.46 |
| 1:A:1362:C:O2' | 1:A:1363:C:O4' | 2.34 | 0.46 |
| 1:A:1381:U:H2' | 1:A:1382:C:H6 | 1.80 | 0.46 |
| 1:A:256:U:H2' | 1:A:257:G:H8 | 1.81 | 0.46 |
| 1:A:369:C:H2' | 1:A:370:C:H6 | 1.80 | 0.46 |
| 1:A:425:G:H2' | 1:A:426:G:O4' | 2.16 | 0.46 |
| 1:A:786:G:C2 | 1:A:797:C:C2 | 3.04 | 0.46 |
| 3:C:96:GLY:O | 3:C:97:LYS:HG2 | 2.15 | 0.46 |
| 1:A:1504:G:O2' | 1:A:1505:G:OP2 | 2.25 | 0.46 |
| 1:A:245:C:C2 | 1:A:284:G:C2 | 3.03 | 0.46 |
| 1:A:812:C:O2' | 1:A:813:U:O4' | 2.34 | 0.46 |
| 9:I:63:ILE:HG21 | 9:I:77:ILE:HG12 | 1.98 | 0.46 |
| 14:N:27:CYS:SG | 14:N:28:GLY:N | 2.89 | 0.46 |
| 15:O:67:LEU:HA | 15:O:67:LEU:HD23 | 1.64 | 0.46 |
| 24:Y:33:A:N3 | 24:Y:33:A:H2' | 2.31 | 0.46 |
| 1:A:1144:G:H21 | 1:A:1146:A:H62 | 1.62 | 0.46 |
| 1:A:1048:G:H1 | 1:A:1209:C:N4 | 2.14 | 0.46 |
| 1:A:1355:G:H1 | 1:A:1367:C:N4 | 2.14 | 0.46 |
| 1:A:1423:G:C6 | 1:A:1424:C:C4 | 3.04 | 0.46 |
| 1:A:342:C:C2 | 1:A:348:G:N2 | 2.84 | 0.46 |
| 1:A:35:G:H2' | 1:A:36:C:C6 | 2.50 | 0.46 |
| 1:A:419:C:N4 | 1:A:424:G:H1 | 2.13 | 0.46 |
| 1:A:661:G:C2 | 1:A:745:C:N3 | 2.84 | 0.46 |
| 1:A:982:U:H4' | 1:A:983:A:O4' | 2.15 | 0.46 |
| 2:B:29:ALA:HA | 2:B:32:ILE:HD12 | 1.98 | 0.46 |
| 1:A:1080:A:O3' | 5:E:16:THR:OG1 | 2.34 | 0.46 |
| 8:H:100:ILE:HD11 | 8:H:130:GLY:HA2 | 1.99 | 0.46 |
| 1:A:1250:A:H4' | 9:I:67:GLY:HA2 | 1.98 | 0.46 |
| 1:A:1132:C:H2' | 1:A:1133:G:H8 | 1.82 | 0.45 |
| 1:A:1310:G:C2 | 1:A:1328:C:N3 | 2.84 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:211:ILE:H | 2:B:211:ILE:HG13 | 1.52 | 0.45 |
| 3:C:135:LYS:O | 3:C:139:GLN:HG2 | 2.15 | 0.45 |
| 3:C:16:ARG:NH1 | 3:C:16:ARG:HG2 | 2.31 | 0.45 |
| 1:A:1308:U:OP1 | 13:M:97:PRO:HA | 2.16 | 0.45 |
| 18:R:19:LYS:HG2 | 18:R:20:ALA:N | 2.31 | 0.45 |
| 1:A:1198:G:H2' | 1:A:1199:U:O4' | 2.15 | 0.45 |
| 1:A:1221:G:H2' | 1:A:1222:G:C8 | 2.51 | 0.45 |
| 1:A:1462:G:C6 | 1:A:1463:C:N4 | 2.84 | 0.45 |
| 1:A:1487:G:H2' | 1:A:1488:G:C8 | 2.51 | 0.45 |
| 1:A:157:G:C6 | 1:A:165:C:N3 | 2.84 | 0.45 |
| 1:A:317:G:C2 | 1:A:337:C:C2 | 3.04 | 0.45 |
| 1:A:70:G:C6 | 1:A:100:C:N3 | 2.85 | 0.45 |
| 1:A:774:G:C2 | 1:A:806:C:N3 | 2.84 | 0.45 |
| 2:B:80:ILE:HD11 | 2:B:208:ILE:HG23 | 1.97 | 0.45 |
| 6:F:35:ALA:HA | 6:F:67:MET:HB3 | 1.98 | 0.45 |
| 6:F:33:TYR:HD1 | 6:F:71:ARG:HD2 | 1.82 | 0.45 |
| 1:A:1401:G:H2' | 1:A:1402:C:O4' | 2.16 | 0.45 |
| 1:A:1458:G:H2' | 1:A:1459:C:C6 | 2.51 | 0.45 |
| 1:A:189:G:C6 | 1:A:189(A):C:C4 | 3.04 | 0.45 |
| 1:A:324:G:H22 | 1:A:327:A:P | 2.40 | 0.45 |
| 1:A:32:A:C2 | 1:A:33:A:C4 | 3.05 | 0.45 |
| 5:E:107:ARG:NH1 | 5:E:107:ARG:HB2 | 2.31 | 0.45 |
| 14:N:12:ARG:HH22 | 14:N:14:PRO:HG3 | 1.81 | 0.45 |
| 20:T:36:LEU:HB3 | 20:T:59:ALA:HB2 | 1.99 | 0.45 |
| 24:Y:30:G:H2' | 24:Y:31:U:C6 | 2.51 | 0.45 |
| 1:A:133:U:O2 | 1:A:230:G:C2 | 2.70 | 0.45 |
| 1:A:1502:A:H2 | 1:A:1505:G:N1 | 2.15 | 0.45 |
| 1:A:32:A:H2' | 1:A:33:A:C8 | 2.51 | 0.45 |
| 1:A:536:C:H2' | 1:A:537:G:C8 | 2.51 | 0.45 |
| 1:A:812:C:H4' | 1:A:812:C:OP1 | 2.15 | 0.45 |
| 8:H:17:THR:HG22 | 8:H:63:LEU:HG | 1.98 | 0.45 |
| 8:H:17:THR:OG1 | 8:H:18:ARG:NH1 | 2.49 | 0.45 |
| 14:N:23:ARG:HH12 | 14:N:30:ALA:HB2 | 1.77 | 0.45 |
| 1:A:1048:G:N2 | 1:A:1210:C:C2 | 2.85 | 0.45 |
| 1:A:166:G:H2' | 1:A:167:G:H8 | 1.81 | 0.45 |
| 1:A:166:G:H2' | 1:A:167:G:C8 | 2.51 | 0.45 |
| 1:A:563:A:N3 | 1:A:563:A:H2' | 2.30 | 0.45 |
| 8:H:91:ARG:HB2 | 12:L:7:ILE:HG13 | 1.99 | 0.45 |
| 14:N:24:CYS:HB3 | 14:N:28:GLY:H | 1.81 | 0.45 |
| 1:A:1366:C:H2' | 1:A:1367:C:C6 | 2.51 | 0.45 |
| 1:A:33:A:O5' | 1:A:33:A:H8 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:446:G:C2 | 1:A:489:C:C2 | 3.05 | 0.45 |
| 1:A:999:C:O2 | 1:A:1043:C:O2 | 2.33 | 0.45 |
| 21:V:2:GLY:O | 21:V:4:GLY:N | 2.50 | 0.45 |
| 1:A:1000:U:H6 | 1:A:1000:U:H3' | 1.81 | 0.45 |
| 1:A:1103:C:H2' | 1:A:1104:G:O4' | 2.16 | 0.45 |
| 1:A:15:G:H2' | 1:A:16:A:C8 | 2.52 | 0.45 |
| 1:A:243:A:N6 | 1:A:281:G:O2' | 2.49 | 0.45 |
| 1:A:836:G:H1 | 1:A:850:U:H3 | 1.65 | 0.45 |
| 3:C:12:LEU:CD1 | 14:N:51:GLY:HA2 | 2.43 | 0.45 |
| 15:O:26:GLU:HG2 | 15:O:81:LEU:HD11 | 1.98 | 0.45 |
| 1:A:1277:C:HO2' | 1:A:1279:A:H8 | 1.63 | 0.45 |
| 1:A:767:A:H2' | 1:A:768:A:C8 | 2.52 | 0.45 |
| 1:A:79:G:O2' | 1:A:80:G:H5' | 2.16 | 0.45 |
| 1:A:864:A:C2 | 1:A:865:A:C2 | 3.05 | 0.45 |
| 1:A:945:G:C2' | 1:A:946:A:H5'' | 2.47 | 0.45 |
| 2:B:30:ARG:HH21 | 2:B:194:PRO:HB2 | 1.81 | 0.45 |
| 4:D:127:THR:HG23 | 4:D:131:ARG:H | 1.82 | 0.45 |
| 6:F:14:LEU:HD11 | 6:F:84:ASN:HB3 | 1.98 | 0.45 |
| 8:H:39:LEU:HD23 | 8:H:44:PHE:HB2 | 1.98 | 0.45 |
| 1:A:1326:C:H2' | 1:A:1327:C:H6 | 1.82 | 0.45 |
| 1:A:585:G:N1 | 1:A:586:C:C2 | 2.85 | 0.45 |
| 1:A:672:U:H5' | 6:F:80:ARG:HD3 | 1.98 | 0.45 |
| 1:A:77:G:OP2 | 1:A:77:G:C8 | 2.70 | 0.45 |
| 1:A:765:G:N1 | 1:A:812:C:C2 | 2.85 | 0.45 |
| 7:G:42:ILE:HG23 | 7:G:117:ALA:HA | 1.99 | 0.45 |
| 7:G:23:VAL:HG13 | 7:G:43:PHE:CE2 | 2.52 | 0.45 |
| 9:I:48:GLU:N | 9:I:49:PRO:HD2 | 2.32 | 0.45 |
| 10:J:6:ILE:HG22 | 10:J:98:ILE:HA | 1.99 | 0.45 |
| 16:P:58:TYR:O | 16:P:62:VAL:HG13 | 2.16 | 0.45 |
| 17:Q:84:LEU:HA | 17:Q:84:LEU:HD12 | 1.88 | 0.45 |
| 19:S:63:THR:HG22 | 19:S:64:GLU:H | 1.81 | 0.45 |
| 1:A:1097:C:H2' | 1:A:1098:C:C6 | 2.52 | 0.45 |
| 1:A:1218:C:H2' | 1:A:1219:U:C5 | 2.50 | 0.45 |
| 1:A:1284:C:H2' | 1:A:1285:A:C8 | 2.51 | 0.45 |
| 1:A:256:U:H2' | 1:A:257:G:C8 | 2.52 | 0.45 |
| 1:A:376:G:H2' | 1:A:377:G:H8 | 1.82 | 0.45 |
| 1:A:502:G:C6 | 1:A:503:C:C4 | 3.05 | 0.45 |
| 1:A:691:G:H22 | 1:A:695:A:H5'' | 1.82 | 0.45 |
| 1:A:9:G:H5'' | 5:E:126:ARG:HD2 | 1.99 | 0.45 |
| 1:A:1240:U:O4' | 7:G:42:ILE:HD11 | 2.17 | 0.45 |
| 8:H:86:ILE:HB | 8:H:133:LEU:HD22 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:82:HIS:CD2 | 8:H:138:TRP:CE2 | 3.05 | 0.45 |
| 18:R:74:ARG:HB3 | 18:R:81:PHE:CZ | 2.52 | 0.45 |
| 1:A:790:A:N3 | 24:Y:36:A:N6 | 2.64 | 0.45 |
| 1:A:1004:A:C8 | 1:A:1038:C:N3 | 2.85 | 0.44 |
| 1:A:67:C:H42 | 1:A:102:G:H1 | 1.64 | 0.44 |
| 1:A:394:G:C2 | 1:A:395:C:C2 | 3.06 | 0.44 |
| 1:A:399:G:C2 | 1:A:400:C:C2 | 3.05 | 0.44 |
| 1:A:41:G:H2' | 1:A:42:G:H8 | 1.82 | 0.44 |
| 1:A:671:G:C2 | 1:A:736:C:N3 | 2.85 | 0.44 |
| 1:A:832:C:C2 | 1:A:855:G:C2 | 3.04 | 0.44 |
| 1:A:91:C:C6 | 1:A:91:C:OP2 | 2.70 | 0.44 |
| 1:A:946:A:H2' | 1:A:947:G:H8 | 1.75 | 0.44 |
| 1:A:518:C:HO2' | 12:L:50:SER:HB3 | 1.83 | 0.44 |
| 18:R:53:ARG:HE | 18:R:60:ALA:HA | 1.81 | 0.44 |
| 20:T:14:LYS:HA | 20:T:17:ARG:CZ | 2.47 | 0.44 |
| 1:A:1017:G:C6 | 1:A:1018:C:C4 | 3.05 | 0.44 |
| 1:A:1316:G:N2 | 1:A:1318:A:H3' | 2.33 | 0.44 |
| 1:A:416:G:C6 | 1:A:417:C:C4 | 3.05 | 0.44 |
| 1:A:509:A:H4' | 1:A:510:A:OP1 | 2.16 | 0.44 |
| 1:A:904:C:H2' | 1:A:905:U:O4' | 2.16 | 0.44 |
| 1:A:91:C:C5 | 1:A:91:C:OP2 | 2.70 | 0.44 |
| 1:A:1240:U:OP1 | 7:G:116:ALA:HB2 | 2.17 | 0.44 |
| 14:N:9:LYS:CG | 14:N:21:TYR:CD1 | 3.00 | 0.44 |
| 1:A:1086:U:H2' | 1:A:1087:G:H8 | 1.82 | 0.44 |
| 1:A:1126:U:C2' | 1:A:1126:U:O2 | 2.65 | 0.44 |
| 1:A:1237:C:H5'' | 1:A:1238:A:O4' | 2.18 | 0.44 |
| 1:A:1381:U:H2' | 1:A:1382:C:C6 | 2.53 | 0.44 |
| 1:A:1436:U:H2' | 1:A:1437:C:O4' | 2.17 | 0.44 |
| 1:A:763:G:C6 | 1:A:764:C:C4 | 3.06 | 0.44 |
| 1:A:793:U:C3' | 1:A:794:A:C5' | 2.87 | 0.44 |
| 1:A:861:G:C6 | 1:A:862:C:C4 | 3.05 | 0.44 |
| 3:C:7:PRO:CB | 3:C:11:ARG:HH21 | 2.30 | 0.44 |
| 1:A:428:G:O3' | 4:D:13:ARG:NH2 | 2.50 | 0.44 |
| 5:E:148:VAL:HG21 | 8:H:107:LEU:HD23 | 1.99 | 0.44 |
| 11:K:91:ARG:NH1 | 18:R:88:LYS:HE3 | 2.20 | 0.44 |
| 15:O:33:THR:HA | 15:O:63:ARG:NH1 | 2.32 | 0.44 |
| 1:A:1034:G:H2' | 1:A:1035:A:H8 | 1.82 | 0.44 |
| 1:A:1040:U:H2' | 1:A:1041:A:C8 | 2.52 | 0.44 |
| 1:A:1360:A:H2' | 1:A:1361:G:C8 | 2.52 | 0.44 |
| 1:A:35:G:C6 | 1:A:36:C:N4 | 2.86 | 0.44 |
| 1:A:375:U:C4 | 1:A:376:G:N7 | 2.86 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:414:A:H2' | 1:A:415:A:O4' | 2.18 | 0.44 |
| 1:A:444:C:N3 | 1:A:491:G:C2 | 2.85 | 0.44 |
| 1:A:443:C:C2 | 1:A:492:G:N2 | 2.86 | 0.44 |
| 1:A:626:U:H2' | 1:A:627:G:C8 | 2.53 | 0.44 |
| 1:A:800:G:H2' | 1:A:801:U:C6 | 2.53 | 0.44 |
| 6:F:46:ARG:HB3 | 6:F:46:ARG:HH11 | 1.83 | 0.44 |
| 9:I:97:LYS:N | 9:I:98:PRO:HD2 | 2.31 | 0.44 |
| 16:P:18:ARG:HA | 16:P:38:TYR:HA | 1.99 | 0.44 |
| 1:A:1480:G:H2' | 1:A:1481:U:O4' | 2.17 | 0.44 |
| 1:A:1495:U:H2' | 1:A:1496:C:C6 | 2.53 | 0.44 |
| 1:A:1504:G:H4' | 1:A:1505:G:O5' | 2.16 | 0.44 |
| 1:A:293:G:C5 | 1:A:305:G:N2 | 2.86 | 0.44 |
| 1:A:681:C:C2 | 1:A:710:G:N2 | 2.85 | 0.44 |
| 1:A:866:C:H4' | 1:A:919:A:H5' | 1.99 | 0.44 |
| 8:H:64:LYS:HB3 | 8:H:79:VAL:HG11 | 1.99 | 0.44 |
| 9:I:26:VAL:HB | 9:I:33:PHE:HB2 | 1.99 | 0.44 |
| 14:N:37:PHE:HB3 | 14:N:39:LEU:HD12 | 1.99 | 0.44 |
| 1:A:1061:G:H5'' | 10:J:59:SER:OG | 2.17 | 0.44 |
| 1:A:667:G:C2 | 1:A:740:U:O2 | 2.71 | 0.44 |
| 1:A:725:G:C6 | 1:A:726:C:N4 | 2.85 | 0.44 |
| 1:A:983:A:H5' | 1:A:984:C:OP2 | 2.17 | 0.44 |
| 7:G:150:ALA:HA | 11:K:59:TYR:HB3 | 2.00 | 0.44 |
| 1:A:1253:G:C6 | 1:A:1254:C:C4 | 3.06 | 0.44 |
| 1:A:41:G:H2' | 1:A:42:G:C8 | 2.52 | 0.44 |
| 1:A:563:A:N3 | 1:A:563:A:C2' | 2.81 | 0.44 |
| 1:A:577:G:C2 | 1:A:578:C:C2 | 3.05 | 0.44 |
| 1:A:916:G:H2' | 1:A:917:G:C8 | 2.49 | 0.44 |
| 1:A:973:G:C3' | 1:A:974:A:H5'' | 2.34 | 0.44 |
| 4:D:10:ARG:NH1 | 4:D:40:PRO:HG3 | 2.32 | 0.44 |
| 8:H:82:HIS:C | 8:H:82:HIS:CD2 | 2.91 | 0.44 |
| 11:K:58:PRO:HD3 | 11:K:89:ALA:HB1 | 1.99 | 0.44 |
| 1:A:1030:C:N4 | 1:A:1031:G:H1 | 2.16 | 0.44 |
| 1:A:132:C:C2 | 1:A:231:G:N2 | 2.86 | 0.44 |
| 1:A:1419:G:C2 | 1:A:1420:C:C2 | 3.06 | 0.44 |
| 1:A:416:G:C2 | 1:A:417:C:C2 | 3.05 | 0.44 |
| 1:A:748:C:H4' | 1:A:749:C:O5' | 2.18 | 0.44 |
| 1:A:988:G:C6 | 1:A:989:C:N3 | 2.86 | 0.44 |
| 17:Q:29:HIS:HB2 | 17:Q:36:ILE:HG13 | 2.00 | 0.44 |
| 1:A:109:A:C6 | 1:A:327:A:C6 | 3.06 | 0.44 |
| 1:A:1182:G:H4' | 1:A:1183:A:O5' | 2.18 | 0.44 |
| 1:A:860:A:H2' | 1:A:861:G:O4' | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:866:C:N3 | 1:A:867:G:H1' | 2.33 | 0.44 |
| 2:B:24:TRP:O | 2:B:24:TRP:CG | 2.71 | 0.44 |
| 6:F:53:ALA:HB3 | 6:F:86:ARG:HD3 | 1.99 | 0.44 |
| 1:A:1061:G:C5' | 10:J:59:SER:OG | 2.66 | 0.44 |
| 14:N:24:CYS:CB | 14:N:29:ARG:H | 2.28 | 0.44 |
| 16:P:13:HIS:C | 16:P:15:PRO:HD3 | 2.38 | 0.44 |
| 1:A:1018:C:H2' | 1:A:1019:C:C6 | 2.53 | 0.43 |
| 1:A:1164:G:H1 | 1:A:1172:C:N4 | 2.16 | 0.43 |
| 1:A:164:U:H2' | 1:A:165:C:C6 | 2.53 | 0.43 |
| 1:A:310:G:C6 | 1:A:311:C:C4 | 3.05 | 0.43 |
| 1:A:42:G:C6 | 1:A:43:C:C4 | 3.06 | 0.43 |
| 1:A:481:G:O2' | 1:A:483:C:N4 | 2.49 | 0.43 |
| 1:A:830:G:N2 | 1:A:857:C:C2 | 2.86 | 0.43 |
| 1:A:947:G:C2 | 1:A:948:C:C2 | 3.06 | 0.43 |
| 2:B:47:THR:HG23 | 2:B:202:PRO:HD2 | 2.00 | 0.43 |
| 8:H:86:ILE:HG22 | 8:H:93:VAL:HG21 | 2.00 | 0.43 |
| 1:A:981:U:H5' | 14:N:21:TYR:HE2 | 1.82 | 0.43 |
| 1:A:112:G:OP2 | 16:P:27:LYS:HE2 | 2.18 | 0.43 |
| 1:A:1064:G:N2 | 1:A:1190:G:O2' | 2.51 | 0.43 |
| 1:A:1133:G:H1 | 1:A:1141:C:N4 | 2.16 | 0.43 |
| 1:A:1196:U:H5' | 1:A:1197:G:C5' | 2.48 | 0.43 |
| 1:A:1276:G:H2' | 1:A:1277:C:O4' | 2.18 | 0.43 |
| 1:A:413:G:N2 | 1:A:429:U:OP2 | 2.47 | 0.43 |
| 1:A:521:G:N1 | 1:A:522:C:C4 | 2.86 | 0.43 |
| 1:A:64:G:H4' | 1:A:65:U:H5'' | 1.99 | 0.43 |
| 1:A:690:G:OP2 | 11:K:27:ASN:HB3 | 2.18 | 0.43 |
| 1:A:717:C:H4' | 11:K:117:ASN:HB3 | 1.99 | 0.43 |
| 1:A:927:G:H1 | 1:A:1390:U:H3 | 1.65 | 0.43 |
| 2:B:23:ARG:O | 2:B:23:ARG:HG3 | 2.17 | 0.43 |
| 2:B:24:TRP:CD1 | 2:B:24:TRP:N | 2.86 | 0.43 |
| 4:D:35:ARG:CB | 4:D:35:ARG:NH1 | 2.73 | 0.43 |
| 15:O:65:ARG:HG2 | 15:O:65:ARG:NH1 | 2.21 | 0.43 |
| 22:W:45:ILE:HG21 | 22:W:70:ARG:CB | 2.48 | 0.43 |
| 23:X:91:ARG:NH1 | 24:Y:36:A:H2 | 2.16 | 0.43 |
| 1:A:1030(C):G:H2' | 1:A:1030(D):A:C8 | 2.52 | 0.43 |
| 1:A:1060:C:O2 | 1:A:1198:G:C2 | 2.71 | 0.43 |
| 1:A:1423:G:C2 | 1:A:1424:C:C2 | 3.06 | 0.43 |
| 1:A:598:U:H2' | 1:A:599:C:C6 | 2.53 | 0.43 |
| 1:A:829:G:H4' | 2:B:26:PRO:CG | 2.38 | 0.43 |
| 1:A:855:G:C6 | 1:A:856:C:C4 | 3.06 | 0.43 |
| 1:A:933:G:OP2 | 7:G:3:ARG:HB2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:155:LEU:HD23 | 4:D:156:GLU:H | 1.83 | 0.43 |
| 7:G:57:GLU:HA | 7:G:58:PRO:HD3 | 1.88 | 0.43 |
| 11:K:22:HIS:HB3 | 11:K:29:ILE:HG23 | 1.98 | 0.43 |
| 12:L:54:LYS:HG2 | 12:L:75:HIS:CE1 | 2.51 | 0.43 |
| 13:M:48:LEU:HD13 | 13:M:53:VAL:HG22 | 2.00 | 0.43 |
| 17:Q:58:GLU:HB2 | 17:Q:75:ARG:HG3 | 2.00 | 0.43 |
| 1:A:1163:C:H2' | 1:A:1164:G:H8 | 1.82 | 0.43 |
| 1:A:123:C:OP1 | 1:A:311:C:O2' | 2.36 | 0.43 |
| 1:A:1253:G:C2 | 1:A:1254:C:C2 | 3.07 | 0.43 |
| 1:A:1384:C:H2' | 1:A:1385:G:H8 | 1.81 | 0.43 |
| 1:A:1421:G:H1 | 1:A:1479:C:H42 | 1.67 | 0.43 |
| 1:A:198:G:H2' | 1:A:199:G:C8 | 2.53 | 0.43 |
| 1:A:217:C:H2' | 1:A:218:C:C6 | 2.53 | 0.43 |
| 1:A:378:G:H2' | 1:A:379:C:O4' | 2.19 | 0.43 |
| 1:A:616:G:H1 | 1:A:624:C:H42 | 1.66 | 0.43 |
| 1:A:728:A:N7 | 15:O:54:ARG:HD3 | 2.34 | 0.43 |
| 1:A:731:G:OP1 | 1:A:766:A:H1' | 2.19 | 0.43 |
| 2:B:130:ARG:N | 2:B:130:ARG:HD2 | 2.33 | 0.43 |
| 2:B:15:VAL:HB | 2:B:204:ASN:OD1 | 2.18 | 0.43 |
| 10:J:54:PHE:H | 14:N:41:ARG:NH2 | 2.16 | 0.43 |
| 20:T:29:LYS:NZ | 20:T:65:LYS:HB3 | 2.32 | 0.43 |
| 1:A:1266:G:C2 | 1:A:1270:C:N3 | 2.87 | 0.43 |
| 1:A:1508:G:C2 | 1:A:1509:C:C2 | 3.07 | 0.43 |
| 1:A:1524:C:H2' | 1:A:1525:G:C8 | 2.53 | 0.43 |
| 1:A:262:A:C6 | 1:A:263:A:C6 | 3.06 | 0.43 |
| 1:A:504:C:C2 | 1:A:542:G:C2 | 3.06 | 0.43 |
| 1:A:748:C:H1' | 1:A:749:C:H5 | 1.82 | 0.43 |
| 1:A:973:G:OP1 | 10:J:57:LYS:HD2 | 2.18 | 0.43 |
| 3:C:191:THR:O | 3:C:193:TYR:N | 2.52 | 0.43 |
| 4:D:29:PRO:C | 4:D:35:ARG:HD3 | 2.32 | 0.43 |
| 1:A:1320:C:H4' | 19:S:73:GLU:OE2 | 2.18 | 0.43 |
| 1:A:1225:A:H4' | 19:S:78:ARG:CD | 2.48 | 0.43 |
| 1:A:1074:G:C2 | 1:A:1075:C:C2 | 3.07 | 0.43 |
| 1:A:1119:C:N4 | 1:A:1154:G:H1 | 2.15 | 0.43 |
| 1:A:1162:C:C2 | 1:A:1175:G:C2 | 3.06 | 0.43 |
| 1:A:1203:C:H4' | 14:N:27:CYS:HB2 | 2.01 | 0.43 |
| 1:A:1050:G:C2 | 1:A:1209:C:O2 | 2.71 | 0.43 |
| 1:A:1438:G:N1 | 1:A:1439:C:C4 | 2.86 | 0.43 |
| 1:A:145:G:C2 | 1:A:178:C:C2 | 3.06 | 0.43 |
| 1:A:401:C:H2' | 1:A:402:G:H8 | 1.83 | 0.43 |
| 1:A:613:C:H42 | 1:A:627:G:H1 | 1.65 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:690:G:H2' | 1:A:691:G:O4' | 2.18 | 0.43 |
| 8:H:80:ILE:H | 8:H:80:ILE:HD12 | 1.83 | 0.43 |
| 9:I:28:VAL:HA | 9:I:63:ILE:O | 2.19 | 0.43 |
| 11:K:21:ILE:HG12 | 11:K:30:VAL:HG22 | 1.99 | 0.43 |
| 23:X:47:LEU:HD11 | 23:X:55:PRO:HB2 | 2.01 | 0.43 |
| 1:A:961:U:C4 | 1:A:1201:A:N6 | 2.69 | 0.43 |
| 1:A:1353:G:N2 | 1:A:1354:C:C2 | 2.87 | 0.43 |
| 1:A:1358:U:OP2 | 1:A:1359:C:H5 | 2.01 | 0.43 |
| 1:A:1444:C:H2' | 1:A:1445:C:C6 | 2.54 | 0.43 |
| 1:A:1422:G:C2 | 1:A:1479:C:C2 | 3.07 | 0.43 |
| 1:A:558:G:H3' | 1:A:559:A:H3' | 2.01 | 0.43 |
| 1:A:858:G:H5'' | 1:A:869:G:O6 | 2.19 | 0.43 |
| 1:A:861:G:H2' | 1:A:862:C:O4' | 2.18 | 0.43 |
| 2:B:186:ALA:HB3 | 2:B:197:VAL:HG11 | 2.01 | 0.43 |
| 4:D:128:VAL:HB | 4:D:133:VAL:HG21 | 2.01 | 0.43 |
| 7:G:108:ALA:HB1 | 7:G:120:ILE:HG13 | 2.00 | 0.43 |
| 23:X:103:LEU:HA | 23:X:106:ILE:HD12 | 2.00 | 0.43 |
| 1:A:1071:C:H2' | 1:A:1072:G:C8 | 2.54 | 0.43 |
| 1:A:1508:G:H2' | 1:A:1509:C:C6 | 2.54 | 0.43 |
| 1:A:1524:C:H2' | 1:A:1525:G:O4' | 2.18 | 0.43 |
| 1:A:197:A:H4' | 1:A:198:G:OP1 | 2.17 | 0.43 |
| 1:A:115:G:O2' | 1:A:289:G:H5'' | 2.19 | 0.43 |
| 1:A:349:A:H2' | 1:A:350:G:O4' | 2.19 | 0.43 |
| 1:A:407:G:C2 | 1:A:436:C:O2 | 2.71 | 0.43 |
| 1:A:44:G:N2 | 1:A:399:G:C4 | 2.87 | 0.43 |
| 1:A:542:G:C2 | 1:A:543:C:C2 | 3.07 | 0.43 |
| 1:A:763:G:C2 | 1:A:764:C:C2 | 3.06 | 0.43 |
| 8:H:111:ILE:HG22 | 8:H:134:ILE:CD1 | 2.48 | 0.43 |
| 11:K:91:ARG:O | 11:K:95:ILE:HG13 | 2.18 | 0.43 |
| 15:O:41:GLU:HA | 15:O:44:LYS:HD2 | 1.99 | 0.43 |
| 17:Q:9:VAL:HG11 | 17:Q:84:LEU:HD23 | 2.01 | 0.43 |
| 6:F:7:ASN:ND2 | 18:R:34:TYR:OH | 2.52 | 0.43 |
| 20:T:15:ARG:CG | 20:T:15:ARG:NH1 | 2.81 | 0.43 |
| 1:A:1001(A):G:C2 | 1:A:1002:G:C6 | 3.07 | 0.43 |
| 1:A:18:C:H4' | 1:A:1078:U:O2 | 2.18 | 0.43 |
| 1:A:1481:U:H2' | 1:A:1482:G:O4' | 2.18 | 0.43 |
| 1:A:270:A:H2' | 1:A:271:C:C6 | 2.54 | 0.43 |
| 1:A:636:U:H2' | 1:A:637:G:H8 | 1.84 | 0.43 |
| 3:C:24:ALA:HB2 | 3:C:32:LEU:HD12 | 2.00 | 0.43 |
| 4:D:112:VAL:N | 4:D:116:GLN:OE1 | 2.49 | 0.43 |
| 9:I:26:VAL:HA | 9:I:61:ALA:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:61:GLU:OE1 | 10:J:63:PHE:CZ | 2.72 | 0.43 |
| 13:M:4:ILE:HA | 13:M:57:ARG:HG3 | 2.00 | 0.43 |
| 6:F:97:PHE:HB2 | 18:R:32:ARG:HH11 | 1.84 | 0.43 |
| 20:T:22:ARG:O | 20:T:25:ARG:HG2 | 2.19 | 0.43 |
| 22:W:17:LEU:HB2 | 22:W:21:THR:HB | 2.01 | 0.43 |
| 1:A:1057:G:H2' | 1:A:1058:G:O4' | 2.19 | 0.43 |
| 1:A:1095:U:H2' | 1:A:1096:C:O4' | 2.18 | 0.43 |
| 1:A:126:G:H2' | 1:A:127:G:O4' | 2.19 | 0.43 |
| 1:A:306:G:C6 | 1:A:307:C:C4 | 3.07 | 0.43 |
| 1:A:319:G:C6 | 1:A:320:C:C4 | 3.07 | 0.43 |
| 1:A:369:C:H2' | 1:A:370:C:C6 | 2.54 | 0.43 |
| 1:A:48:C:H4' | 1:A:49:U:OP1 | 2.17 | 0.43 |
| 1:A:628:G:H2' | 1:A:629:G:O4' | 2.19 | 0.43 |
| 1:A:79:G:C4 | 1:A:80:G:C8 | 3.07 | 0.43 |
| 1:A:988:G:C6 | 1:A:989:C:C4 | 3.07 | 0.43 |
| 7:G:46:ALA:HA | 7:G:121:ALA:HB2 | 2.01 | 0.43 |
| 8:H:28:ALA:HB3 | 8:H:57:PRO:HB2 | 2.01 | 0.43 |
| 10:J:4:ILE:HD11 | 10:J:77:PRO:HA | 2.00 | 0.43 |
| 12:L:32:PHE:CE1 | 12:L:86:ARG:HG3 | 2.54 | 0.43 |
| 1:A:102:G:C2 | 1:A:103:C:C2 | 3.06 | 0.42 |
| 1:A:1074:G:C6 | 1:A:1075:C:N3 | 2.87 | 0.42 |
| 1:A:1462:G:N2 | 1:A:1463:C:C2 | 2.87 | 0.42 |
| 1:A:308:C:H2' | 1:A:309:G:H8 | 1.84 | 0.42 |
| 1:A:48:C:H5' | 1:A:365:U:O4 | 2.19 | 0.42 |
| 1:A:39:G:N2 | 1:A:40:C:C2 | 2.87 | 0.42 |
| 1:A:768:A:C5 | 1:A:769:G:C8 | 3.07 | 0.42 |
| 1:A:920:U:H2' | 1:A:921:U:C6 | 2.54 | 0.42 |
| 5:E:107:ARG:HH11 | 5:E:107:ARG:HB2 | 1.83 | 0.42 |
| 5:E:41:VAL:HG23 | 5:E:67:VAL:HB | 2.01 | 0.42 |
| 9:I:125:TYR:O | 9:I:125:TYR:CD2 | 2.70 | 0.42 |
| 1:A:124:G:C2 | 1:A:125:U:C2 | 3.07 | 0.42 |
| 1:A:1463:C:H2' | 1:A:1464:G:H8 | 1.84 | 0.42 |
| 1:A:294:U:O5' | 1:A:294:U:H6 | 2.03 | 0.42 |
| 1:A:518:C:O2' | 12:L:50:SER:HB3 | 2.18 | 0.42 |
| 1:A:545:C:O2' | 1:A:549:C:H5'' | 2.19 | 0.42 |
| 1:A:708:C:H2' | 1:A:709:G:H8 | 1.83 | 0.42 |
| 2:B:67:THR:H | 2:B:160:ASP:HB2 | 1.84 | 0.42 |
| 2:B:103:THR:HA | 2:B:180:LEU:HD21 | 2.01 | 0.42 |
| 8:H:87:SER:HA | 8:H:93:VAL:HG23 | 2.01 | 0.42 |
| 1:A:953:G:N7 | 13:M:104:ARG:NH2 | 2.67 | 0.42 |
| 1:A:986:A:H1' | 19:S:54:GLY:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 22:W:17:LEU:HB3 | 22:W:18:PRO:HD2 | 2.01 | 0.42 |
| 1:A:1347:G:HO2' | 1:A:1373:G:H1 | 1.66 | 0.42 |
| 1:A:173:U:H5' | 1:A:197:A:O4' | 2.19 | 0.42 |
| 1:A:279:A:O2' | 1:A:280:C:OP2 | 2.27 | 0.42 |
| 1:A:784:C:N3 | 1:A:799:G:C2 | 2.87 | 0.42 |
| 8:H:104:ARG:O | 8:H:105:ARG:C | 2.57 | 0.42 |
| 14:N:7:ILE:HG22 | 14:N:7:ILE:O | 2.18 | 0.42 |
| 1:A:1095:U:H2' | 1:A:1096:C:C6 | 2.54 | 0.42 |
| 1:A:1235:U:H2' | 1:A:1236:A:O4' | 2.20 | 0.42 |
| 1:A:1357:A:H2' | 1:A:1358:U:C6 | 2.54 | 0.42 |
| 1:A:34:C:H2' | 1:A:35:G:H8 | 1.84 | 0.42 |
| 1:A:598:U:H4' | 8:H:94:TYR:CG | 2.54 | 0.42 |
| 1:A:620:C:H2' | 1:A:621:A:O4' | 2.19 | 0.42 |
| 1:A:736:C:H2' | 1:A:737:A:H8 | 1.83 | 0.42 |
| 1:A:922:G:C2 | 1:A:923:A:C4 | 3.07 | 0.42 |
| 8:H:45:ILE:HG21 | 8:H:61:VAL:HG12 | 2.01 | 0.42 |
| 9:I:108:VAL:HG12 | 9:I:109:VAL:N | 2.34 | 0.42 |
| 9:I:37:PHE:CE1 | 9:I:74:ILE:HG13 | 2.54 | 0.42 |
| 14:N:14:PRO:C | 14:N:16:PHE:N | 2.73 | 0.42 |
| 15:O:39:LEU:HD13 | 15:O:56:LEU:HB2 | 2.01 | 0.42 |
| 23:X:64:LYS:O | 23:X:68:GLU:HG2 | 2.19 | 0.42 |
| 1:A:1345:U:C2 | 1:A:1377:A:C2 | 3.08 | 0.42 |
| 1:A:1495:U:H2' | 1:A:1496:C:H6 | 1.84 | 0.42 |
| 1:A:394:G:C6 | 1:A:395:C:C4 | 3.07 | 0.42 |
| 1:A:688:G:C6 | 1:A:689:C:C4 | 3.08 | 0.42 |
| 1:A:744:C:H2' | 1:A:745:C:C6 | 2.55 | 0.42 |
| 1:A:570:G:O6 | 1:A:873:A:C2 | 2.73 | 0.42 |
| 1:A:961:U:N3 | 1:A:1201:A:C6 | 2.72 | 0.42 |
| 7:G:111:ARG:CZ | 7:G:122:HIS:HB3 | 2.49 | 0.42 |
| 8:H:108:GLY:HA3 | 8:H:138:TRP:HB3 | 2.01 | 0.42 |
| 8:H:91:ARG:HD3 | 12:L:7:ILE:HG21 | 2.01 | 0.42 |
| 15:O:23:GLY:O | 15:O:28:GLN:NE2 | 2.52 | 0.42 |
| 24:Y:22:G:C2 | 24:Y:23:C:N3 | 2.88 | 0.42 |
| 1:A:1001(A):G:C6 | 1:A:1002:G:O6 | 2.73 | 0.42 |
| 1:A:1104:G:H8 | 1:A:1104:G:H5'' | 1.84 | 0.42 |
| 1:A:1132:C:H2' | 1:A:1133:G:C8 | 2.55 | 0.42 |
| 1:A:1233:G:C6 | 1:A:1234:C:C4 | 3.07 | 0.42 |
| 1:A:1125:U:O2' | 1:A:1281:U:O2 | 2.36 | 0.42 |
| 1:A:1283:G:H2' | 1:A:1283:G:N3 | 2.33 | 0.42 |
| 1:A:1349:A:H2' | 1:A:1350:A:O4' | 2.19 | 0.42 |
| 1:A:1347:G:C4 | 1:A:1373:G:C6 | 3.08 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1500:A:O2' | 1:A:1501:C:H5' | 2.20 | 0.42 |
| 1:A:192:U:H5'' | 20:T:57:ARG:HH21 | 1.84 | 0.42 |
| 1:A:419:C:C2 | 1:A:425:G:C2 | 3.08 | 0.42 |
| 2:B:21:ARG:HG2 | 2:B:22:LYS:H | 1.84 | 0.42 |
| 4:D:119:GLN:O | 4:D:123:HIS:HD2 | 2.02 | 0.42 |
| 1:A:1054:C:H2' | 1:A:1054:C:H6 | 1.65 | 0.42 |
| 1:A:1168:A:H2' | 1:A:1169:A:C8 | 2.55 | 0.42 |
| 1:A:1118:C:H1' | 1:A:1179:A:C5 | 2.55 | 0.42 |
| 1:A:1233:G:C6 | 1:A:1234:C:N4 | 2.87 | 0.42 |
| 1:A:1300:G:H1' | 1:A:1301:U:C5 | 2.53 | 0.42 |
| 1:A:1311:G:N2 | 1:A:1327:C:C2 | 2.88 | 0.42 |
| 1:A:1370:G:O3' | 9:I:12:GLU:HG3 | 2.12 | 0.42 |
| 1:A:1510:U:H2' | 1:A:1511:G:C8 | 2.54 | 0.42 |
| 1:A:200:G:N2 | 1:A:218:C:C2 | 2.87 | 0.42 |
| 1:A:778:G:C2 | 1:A:779:C:C2 | 3.07 | 0.42 |
| 2:B:73:THR:HG23 | 2:B:95:GLN:O | 2.20 | 0.42 |
| 3:C:202:ILE:HG22 | 3:C:204:LEU:HD23 | 2.01 | 0.42 |
| 19:S:51:VAL:HG11 | 19:S:71:LEU:HD23 | 1.71 | 0.42 |
| 1:A:1022:G:H2' | 1:A:1023:G:C8 | 2.54 | 0.42 |
| 1:A:1113:C:H2' | 1:A:1114:C:C6 | 2.55 | 0.42 |
| 1:A:1262:C:H42 | 1:A:1273:G:H1 | 1.67 | 0.42 |
| 1:A:1445:C:C2 | 1:A:1458:G:C2 | 3.08 | 0.42 |
| 1:A:42:G:C2 | 1:A:43:C:C2 | 3.08 | 0.42 |
| 1:A:62:U:H5'' | 1:A:385:C:O2' | 2.20 | 0.42 |
| 1:A:789:U:O4 | 23:X:86:LYS:NZ | 2.53 | 0.42 |
| 1:A:908:A:H2' | 1:A:909:A:H8 | 1.84 | 0.42 |
| 2:B:132:LYS:HA | 2:B:135:GLN:HG2 | 2.01 | 0.42 |
| 2:B:217:ARG:HD3 | 2:B:217:ARG:HA | 1.71 | 0.42 |
| 5:E:80:ILE:HG23 | 8:H:104:ARG:HH12 | 1.85 | 0.42 |
| 10:J:62:HIS:CD2 | 14:N:61:TRP:HH2 | 2.37 | 0.42 |
| 12:L:85:ILE:CG2 | 12:L:86:ARG:N | 2.81 | 0.42 |
| 16:P:39:TYR:OH | 16:P:41:PRO:HB3 | 2.19 | 0.42 |
| 17:Q:15:MET:HB2 | 17:Q:18:THR:HB | 2.02 | 0.42 |
| 18:R:19:LYS:HG2 | 18:R:20:ALA:H | 1.85 | 0.42 |
| 22:W:12:VAL:HA | 22:W:51:ASP:O | 2.20 | 0.42 |
| 23:X:152:MET:HB2 | 23:X:164:LEU:H | 1.84 | 0.42 |
| 1:A:1014:A:H2' | 1:A:1015:A:C8 | 2.55 | 0.42 |
| 1:A:110:C:H2' | 1:A:111:G:O4' | 2.19 | 0.42 |
| 1:A:1312:G:N2 | 1:A:1326:C:C2 | 2.88 | 0.42 |
| 1:A:1464:G:C2 | 1:A:1465:C:C4 | 3.08 | 0.42 |
| 1:A:244:U:H4' | 1:A:245:C:H5'' | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:409:G:H5' | 4:D:24:GLU:HB3 | 2.02 | 0.42 |
| 1:A:696:A:N3 | 1:A:786:G:O2' | 2.52 | 0.42 |
| 1:A:926:G:H2' | 1:A:1505:G:N3 | 2.35 | 0.42 |
| 2:B:25:ASN:HD21 | 2:B:27:LYS:N | 2.17 | 0.42 |
| 1:A:1240:U:H4' | 7:G:38:LEU:HD11 | 2.02 | 0.42 |
| 9:I:20:ARG:HH21 | 9:I:62:TYR:HB3 | 1.85 | 0.42 |
| 11:K:91:ARG:O | 11:K:95:ILE:HD12 | 2.20 | 0.42 |
| 12:L:24:VAL:HG13 | 12:L:98:TYR:HE1 | 1.85 | 0.42 |
| 16:P:1:MET:O | 16:P:2:VAL:C | 2.57 | 0.42 |
| 17:Q:66:SER:HB3 | 17:Q:69:LYS:HB3 | 2.01 | 0.42 |
| 17:Q:9:VAL:HG12 | 17:Q:56:VAL:HB | 2.00 | 0.42 |
| 1:A:1001:A:C8 | 1:A:1001:A:OP2 | 2.68 | 0.42 |
| 1:A:1074:G:C6 | 1:A:1075:C:C4 | 3.07 | 0.42 |
| 1:A:122:G:C6 | 1:A:123:C:C4 | 3.07 | 0.42 |
| 1:A:199:G:C2 | 1:A:219:C:N3 | 2.88 | 0.42 |
| 1:A:224:C:H2' | 1:A:225:C:C6 | 2.55 | 0.42 |
| 1:A:241:C:C2 | 1:A:286:G:C2 | 3.08 | 0.42 |
| 1:A:6:G:O6 | 5:E:95:ALA:N | 2.43 | 0.42 |
| 1:A:79:G:O6 | 1:A:91:C:N3 | 2.52 | 0.42 |
| 7:G:22:LEU:HG | 7:G:62:PHE:HE2 | 1.85 | 0.42 |
| 13:M:22:ILE:HG23 | 13:M:67:GLU:HG2 | 2.02 | 0.42 |
| 23:X:91:ARG:HH21 | 23:X:123:ARG:HH12 | 1.68 | 0.42 |
| 1:A:1101:A:N6 | 2:B:176:GLU:HG2 | 2.35 | 0.41 |
| 1:A:1243:C:H5'' | 21:V:8:THR:HG21 | 2.02 | 0.41 |
| 1:A:1350:A:C6 | 1:A:1351:U:N3 | 2.88 | 0.41 |
| 1:A:1410:G:H2' | 1:A:1411:C:C6 | 2.55 | 0.41 |
| 1:A:137:C:C2 | 1:A:227:G:C2 | 3.07 | 0.41 |
| 1:A:384:G:C2 | 1:A:385:C:C2 | 3.08 | 0.41 |
| 1:A:500:G:H2' | 1:A:501:C:C6 | 2.55 | 0.41 |
| 1:A:568:G:C6 | 1:A:883:C:N4 | 2.88 | 0.41 |
| 1:A:641:U:H1' | 1:A:642:A:N7 | 2.35 | 0.41 |
| 1:A:698:G:C2 | 1:A:699:C:N3 | 2.88 | 0.41 |
| 1:A:741:G:C5' | 15:O:39:LEU:HD11 | 2.49 | 0.41 |
| 1:A:829:G:O2' | 2:B:26:PRO:HD3 | 2.20 | 0.41 |
| 1:A:83:U:H2' | 1:A:84:U:O4' | 2.20 | 0.41 |
| 1:A:881:G:C6 | 1:A:882:C:C4 | 3.08 | 0.41 |
| 2:B:25:ASN:ND2 | 2:B:25:ASN:C | 2.73 | 0.41 |
| 3:C:180:ALA:HB1 | 3:C:182:ILE:HG13 | 2.02 | 0.41 |
| 5:E:90:VAL:O | 5:E:120:THR:HA | 2.21 | 0.41 |
| 1:A:1095:U:OP1 | 1:A:1108:G:N1 | 2.52 | 0.41 |
| 1:A:1134:G:C2 | 1:A:1141:C:N3 | 2.88 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1288:A:H2' | 1:A:1289:A:C8 | 2.55 | 0.41 |
| 1:A:1464:G:C6 | 1:A:1465:C:N4 | 2.88 | 0.41 |
| 1:A:201:C:N4 | 1:A:216:G:H1 | 2.18 | 0.41 |
| 1:A:473:G:H2' | 1:A:474:G:H8 | 1.85 | 0.41 |
| 1:A:687:A:N1 | 1:A:700:G:O2' | 2.47 | 0.41 |
| 1:A:765:G:C2 | 1:A:812:C:C2 | 3.08 | 0.41 |
| 1:A:16:A:C2 | 1:A:920:U:O2 | 2.73 | 0.41 |
| 1:A:955:U:H1' | 1:A:1227:A:H61 | 1.83 | 0.41 |
| 6:F:4:TYR:O | 6:F:64:GLN:HA | 2.20 | 0.41 |
| 9:I:89:ASN:O | 9:I:92:TYR:HB2 | 2.20 | 0.41 |
| 19:S:58:VAL:HA | 19:S:59:PRO:HD3 | 1.91 | 0.41 |
| 1:A:1144:G:C2 | 1:A:1145:C:N3 | 2.88 | 0.41 |
| 1:A:1311:G:C2 | 1:A:1327:C:C2 | 3.08 | 0.41 |
| 1:A:1513:A:C2 | 1:A:1523:G:C6 | 3.09 | 0.41 |
| 1:A:254:G:OP1 | 17:Q:67:LYS:O | 2.37 | 0.41 |
| 1:A:262:A:H2' | 1:A:263:A:C8 | 2.55 | 0.41 |
| 1:A:333:G:C6 | 1:A:334:C:N4 | 2.87 | 0.41 |
| 1:A:444:C:C2 | 1:A:491:G:C2 | 3.08 | 0.41 |
| 1:A:790:A:C6 | 1:A:791:G:C6 | 3.08 | 0.41 |
| 1:A:861:G:C2 | 1:A:862:C:C2 | 3.07 | 0.41 |
| 2:B:130:ARG:HA | 2:B:130:ARG:NE | 2.31 | 0.41 |
| 7:G:69:VAL:O | 7:G:69:VAL:HG12 | 2.21 | 0.41 |
| 11:K:91:ARG:O | 11:K:95:ILE:CD1 | 2.68 | 0.41 |
| 18:R:50:ILE:H | 18:R:50:ILE:HG13 | 1.74 | 0.41 |
| 1:A:1117:G:H21 | 1:A:1180:A:H1' | 1.85 | 0.41 |
| 1:A:1216:G:H5'' | 14:N:5:ALA:CB | 2.50 | 0.41 |
| 1:A:1392:G:N2 | 1:A:1502:A:C8 | 2.80 | 0.41 |
| 1:A:236:G:C6 | 1:A:237:C:C4 | 3.08 | 0.41 |
| 1:A:389:A:C2 | 1:A:390:C:H1' | 2.55 | 0.41 |
| 1:A:60:A:N7 | 1:A:110:C:N4 | 2.64 | 0.41 |
| 1:A:61:G:H5'' | 1:A:61:G:H8 | 1.84 | 0.41 |
| 1:A:701:C:H1' | 1:A:703:G:C6 | 2.54 | 0.41 |
| 4:D:30:LYS:C | 4:D:32:ALA:H | 2.24 | 0.41 |
| 10:J:37:PRO:HA | 10:J:72:VAL:HG22 | 2.00 | 0.41 |
| 14:N:26:ARG:HD3 | 14:N:47:LEU:HD11 | 2.02 | 0.41 |
| 1:A:1257:U:H4' | 1:A:1258:G:O5' | 2.21 | 0.41 |
| 1:A:1324:A:H2' | 1:A:1325:C:O4' | 2.20 | 0.41 |
| 1:A:1389:C:H2' | 1:A:1390:U:O4' | 2.20 | 0.41 |
| 1:A:610:G:C4 | 1:A:611:A:C8 | 3.08 | 0.41 |
| 1:A:725:G:N1 | 1:A:726:C:C4 | 2.87 | 0.41 |
| 2:B:80:ILE:HG21 | 2:B:212:GLN:HA | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:J:38:ILE:HG23 | 10:J:71:LEU:CB | 2.47 | 0.41 |
| 10:J:64:GLU:N | 14:N:59:ALA:HB2 | 2.36 | 0.41 |
| 1:A:188:C:H5' | 20:T:89:ARG:HD3 | 2.02 | 0.41 |
| 1:A:376:G:O2' | 1:A:377:G:H5' | 2.20 | 0.41 |
| 1:A:738:C:H2' | 1:A:739:C:C6 | 2.56 | 0.41 |
| 1:A:952:U:H2' | 1:A:953:G:C8 | 2.56 | 0.41 |
| 4:D:120:LEU:HD12 | 4:D:125:HIS:CD2 | 2.55 | 0.41 |
| 9:I:42:ARG:NH2 | 9:I:71:SER:OG | 2.52 | 0.41 |
| 17:Q:57:VAL:HG12 | 17:Q:76:LEU:HA | 2.03 | 0.41 |
| 23:X:92:VAL:CG1 | 23:X:132:LEU:HD13 | 2.50 | 0.41 |
| 1:A:1231:G:C6 | 1:A:1232:U:C4 | 3.09 | 0.41 |
| 1:A:1507:A:C5' | 1:A:1507:A:C8 | 3.04 | 0.41 |
| 1:A:435:C:H2' | 1:A:436:C:C6 | 2.55 | 0.41 |
| 1:A:582:U:C2 | 1:A:760:G:C6 | 3.09 | 0.41 |
| 1:A:860:A:H3' | 1:A:861:G:H8 | 1.86 | 0.41 |
| 1:A:874:G:C6 | 1:A:875:C:C4 | 3.08 | 0.41 |
| 1:A:545:C:H5' | 4:D:72:GLU:CB | 2.51 | 0.41 |
| 11:K:91:ARG:HG2 | 11:K:92:GLU:N | 2.35 | 0.41 |
| 1:A:981:U:H5' | 14:N:21:TYR:CE2 | 2.55 | 0.41 |
| 19:S:10:PHE:HE2 | 19:S:37:ARG:HB3 | 1.85 | 0.41 |
| 1:A:1114:C:C2 | 1:A:1187:G:C2 | 3.09 | 0.41 |
| 1:A:19:C:O2 | 1:A:917:G:C2 | 2.73 | 0.41 |
| 1:A:22:G:C6 | 1:A:23:C:C4 | 3.08 | 0.41 |
| 1:A:411:A:OP2 | 4:D:25:ARG:NH2 | 2.52 | 0.41 |
| 1:A:568:G:C6 | 1:A:569:C:N4 | 2.89 | 0.41 |
| 1:A:570:G:C4 | 1:A:571:U:C5 | 3.09 | 0.41 |
| 1:A:643:C:H4' | 8:H:31:PHE:CE2 | 2.55 | 0.41 |
| 1:A:66:G:C6 | 1:A:67:C:C4 | 3.09 | 0.41 |
| 1:A:810:C:H2' | 1:A:811:C:O4' | 2.20 | 0.41 |
| 1:A:895:G:C2 | 1:A:896:C:C2 | 3.08 | 0.41 |
| 1:A:903:G:C2 | 1:A:904:C:C2 | 3.08 | 0.41 |
| 3:C:28:GLN:CD | 3:C:28:GLN:H | 2.17 | 0.41 |
| 4:D:207:TYR:HD1 | 4:D:207:TYR:HA | 1.70 | 0.41 |
| 8:H:84:ARG:HH11 | 8:H:84:ARG:HG3 | 1.85 | 0.41 |
| 12:L:53:ARG:HG3 | 12:L:69:TYR:HE1 | 1.85 | 0.41 |
| 13:M:10:PRO:CB | 13:M:18:ALA:HB1 | 2.51 | 0.41 |
| 18:R:26:LEU:HD13 | 18:R:42:ARG:HG3 | 2.03 | 0.41 |
| 19:S:37:ARG:O | 19:S:70:LYS:HG3 | 2.21 | 0.41 |
| 20:T:68:LYS:HE3 | 20:T:68:LYS:HA | 2.03 | 0.41 |
| 1:A:1437:C:H2' | 1:A:1438:G:C8 | 2.52 | 0.41 |
| 1:A:1431:C:N3 | 1:A:1470:G:C2 | 2.89 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:189(L):G:C6 | 1:A:190:U:O4 | 2.74 | 0.41 |
| 1:A:21:G:N2 | 1:A:22:G:C2 | 2.89 | 0.41 |
| 1:A:264:U:O2 | 17:Q:64:PRO:HG2 | 2.21 | 0.41 |
| 1:A:376:G:H5'' | 16:P:5:ARG:HB2 | 2.02 | 0.41 |
| 1:A:542:G:N1 | 1:A:543:C:C4 | 2.88 | 0.41 |
| 1:A:826:C:H2' | 1:A:827:U:H6 | 1.83 | 0.41 |
| 1:A:855:G:C2 | 1:A:856:C:C2 | 3.08 | 0.41 |
| 1:A:883:C:O2' | 1:A:884:U:H5' | 2.21 | 0.41 |
| 10:J:12:ASP:HB3 | 10:J:15:THR:HG22 | 2.03 | 0.41 |
| 12:L:10:LEU:HD12 | 12:L:10:LEU:HA | 1.84 | 0.41 |
| 13:M:107:ALA:HB3 | 13:M:111:LYS:HE3 | 2.03 | 0.41 |
| 1:A:279:A:C4 | 17:Q:98:LEU:HD12 | 2.56 | 0.41 |
| 1:A:1255:G:H2' | 1:A:1279:A:H62 | 1.86 | 0.41 |
| 1:A:319:G:N1 | 1:A:320:C:C2 | 2.89 | 0.41 |
| 1:A:734:G:C5 | 1:A:735:C:C4 | 3.09 | 0.41 |
| 4:D:148:VAL:HG11 | 4:D:158:ILE:HG21 | 2.03 | 0.41 |
| 12:L:32:PHE:HB3 | 12:L:84:LEU:CD1 | 2.51 | 0.41 |
| 20:T:89:ARG:HD2 | 20:T:104:LEU:HD22 | 2.03 | 0.41 |
| 1:A:931:C:O2 | 1:A:1387:G:C2 | 2.74 | 0.41 |
| 1:A:1422:G:C2 | 1:A:1479:C:N3 | 2.88 | 0.41 |
| 1:A:1526:G:C2 | 1:A:1527:C:C2 | 3.09 | 0.41 |
| 1:A:155:C:H42 | 1:A:166:G:H1 | 1.68 | 0.41 |
| 1:A:259:G:C2 | 1:A:268:C:C2 | 3.09 | 0.41 |
| 1:A:502:G:H2' | 1:A:503:C:O4' | 2.21 | 0.41 |
| 1:A:671:G:C2 | 1:A:736:C:C2 | 3.08 | 0.41 |
| 1:A:803:G:H2' | 1:A:804:U:O4' | 2.20 | 0.41 |
| 1:A:874:G:C2 | 1:A:875:C:C2 | 3.09 | 0.41 |
| 1:A:925:G:O2' | 1:A:927:G:OP1 | 2.39 | 0.41 |
| 11:K:87:THR:HG21 | 24:Y:28:A:O2' | 2.20 | 0.41 |
| 12:L:41:ARG:HD2 | 12:L:43:VAL:HG23 | 2.03 | 0.41 |
| 1:A:1011:G:C6 | 1:A:1012:U:C4 | 3.09 | 0.40 |
| 1:A:113:G:N3 | 1:A:113:G:H2' | 2.35 | 0.40 |
| 1:A:1048:G:C2 | 1:A:1210:C:C2 | 3.10 | 0.40 |
| 1:A:1500:A:H5'' | 1:A:1508:G:H5'' | 2.03 | 0.40 |
| 1:A:148:G:N2 | 1:A:175:C:C2 | 2.90 | 0.40 |
| 1:A:266:G:C5' | 1:A:266:G:H8 | 2.34 | 0.40 |
| 1:A:399:G:C6 | 1:A:400:C:N4 | 2.89 | 0.40 |
| 1:A:768:A:H2' | 1:A:769:G:O4' | 2.21 | 0.40 |
| 1:A:881:G:H2' | 1:A:882:C:O4' | 2.22 | 0.40 |
| 1:A:929:G:C6 | 1:A:930:C:C4 | 3.09 | 0.40 |
| 1:A:977:A:O2' | 1:A:979:C:OP2 | 2.28 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:4:TYR:CE2 | 4:D:11:LEU:HD21 | 2.56 | 0.40 |
| 6:F:10:LEU:HA | 6:F:85:VAL:HA | 2.03 | 0.40 |
| 22:W:18:PRO:C | 22:W:20:ALA:H | 2.25 | 0.40 |
| 1:A:1106:G:C2 | 1:A:1107:C:C2 | 3.09 | 0.40 |
| 1:A:1295:G:C6 | 1:A:1296:C:C4 | 3.09 | 0.40 |
| 1:A:46:G:H2' | 1:A:366:C:H5 | 1.82 | 0.40 |
| 1:A:725:G:H1 | 1:A:732:C:H42 | 1.69 | 0.40 |
| 1:A:798:G:H2' | 1:A:799:G:O4' | 2.21 | 0.40 |
| 1:A:977:A:C3' | 1:A:978:A:H5'' | 2.51 | 0.40 |
| 2:B:126:GLU:HG2 | 2:B:129:GLU:HB3 | 2.03 | 0.40 |
| 2:B:95:GLN:HG3 | 2:B:147:LYS:HG2 | 2.03 | 0.40 |
| 3:C:177:THR:OG1 | 3:C:180:ALA:HB2 | 2.22 | 0.40 |
| 7:G:62:PHE:HD1 | 7:G:124:LEU:CD2 | 2.33 | 0.40 |
| 8:H:84:ARG:O | 8:H:135:CYS:HB2 | 2.20 | 0.40 |
| 12:L:10:LEU:O | 12:L:14:GLY:N | 2.53 | 0.40 |
| 12:L:85:ILE:HG22 | 12:L:86:ARG:N | 2.35 | 0.40 |
| 16:P:20:VAL:HG21 | 16:P:32:TYR:CD2 | 2.56 | 0.40 |
| 1:A:1320:C:H4' | 19:S:73:GLU:HG2 | 2.02 | 0.40 |
| 1:A:1541:U:H3 | 24:Y:24:A:H61 | 1.69 | 0.40 |
| 1:A:1320:C:C4' | 19:S:73:GLU:OE2 | 2.69 | 0.40 |
| 1:A:506:G:C2 | 1:A:507:C:C2 | 3.09 | 0.40 |
| 1:A:769:G:H2' | 1:A:769:G:N3 | 2.37 | 0.40 |
| 4:D:201:GLN:HA | 4:D:204:ILE:HD12 | 2.02 | 0.40 |
| 1:A:663:A:H5'' | 18:R:61:LYS:HE3 | 2.03 | 0.40 |
| 21:V:14:TRP:HE3 | 21:V:15:ARG:HG2 | 1.87 | 0.40 |
| 1:A:1216:G:C6 | 1:A:1217:C:N4 | 2.90 | 0.40 |
| 1:A:1405:G:H2' | 1:A:1406:U:C6 | 2.56 | 0.40 |
| 1:A:142:G:H2' | 1:A:143:A:C8 | 2.57 | 0.40 |
| 1:A:1476:G:C2 | 1:A:1477:C:C2 | 3.09 | 0.40 |
| 1:A:333:G:C2 | 1:A:334:C:C4 | 3.09 | 0.40 |
| 1:A:518:C:C5 | 1:A:529:G:H3' | 2.57 | 0.40 |
| 1:A:635:G:C6 | 1:A:636:U:C4 | 3.09 | 0.40 |
| 3:C:25:GLY:O | 3:C:29:TYR:HB2 | 2.22 | 0.40 |
| 5:E:107:ARG:O | 5:E:111:GLU:HB2 | 2.22 | 0.40 |
| 1:A:1371:G:P | 9:I:12:GLU:HG2 | 2.57 | 0.40 |
| 13:M:34:LEU:HD23 | 13:M:56:LEU:HD21 | 2.02 | 0.40 |
| 17:Q:53:LEU:HD23 | 17:Q:85:VAL:HG11 | 2.02 | 0.40 |
| 18:R:55:ARG:HA | 18:R:55:ARG:HD2 | 1.88 | 0.40 |
| 1:A:1457:G:H5'' | 20:T:35:THR:HG21 | 2.03 | 0.40 |
| 1:A:1010:G:H2' | 1:A:1011:G:H8 | 1.84 | 0.40 |
| 1:A:1343:G:C5 | 1:A:1344:C:C4 | 3.09 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:189(C):C:H2' | 1:A:189(D):C:O4' | 2.22 | 0.40 |
| 1:A:128:G:C2 | 1:A:234:C:O2 | 2.74 | 0.40 |
| 1:A:244:U:C6 | 1:A:894:G:N2 | 2.90 | 0.40 |
| 1:A:246:A:C4 | 1:A:282:A:N6 | 2.90 | 0.40 |
| 1:A:117:G:O6 | 1:A:289:G:H1' | 2.22 | 0.40 |
| 1:A:303:A:C4 | 1:A:304:U:C6 | 3.10 | 0.40 |
| 1:A:572:A:N1 | 1:A:864:A:C5 | 2.90 | 0.40 |
| 1:A:309:G:O2' | 1:A:607:A:N1 | 2.48 | 0.40 |
| 1:A:72:C:OP1 | 1:A:72:C:C4' | 2.69 | 0.40 |
| 1:A:730:G:C5 | 1:A:731:G:H1' | 2.56 | 0.40 |
| 1:A:657:G:N2 | 1:A:749:C:N3 | 2.60 | 0.40 |
| 1:A:917:G:C6 | 1:A:918:A:C6 | 3.09 | 0.40 |
| 4:D:33:MET:CA | 4:D:36:ARG:O | 2.69 | 0.40 |
| 4:D:63:LYS:HB2 | 4:D:63:LYS:HE3 | 1.83 | 0.40 |
| 11:K:62:GLN:CG | 11:K:97:ALA:HB2 | 2.46 | 0.40 |
| 21:V:9:ARG:HD2 | 21:V:22:ARG:HG3 | 2.02 | 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 | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2 | B | 232/256 (91%) | 194 (84%) | 28 (12%) | 10 (4%) | 3 | 33 |
| 3 | C | 204/239 (85%) | 176 (86%) | 23 (11%) | 5 (2%) | 7 | 48 |
| 4 | D | 206/209 (99%) | 180 (87%) | 23 (11%) | 3 (2%) | 13 | 58 |
| 5 | E | 148/162 (91%) | 135 (91%) | 10 (7%) | 3 (2%) | 9 | 53 |
| 6 | F | 99/101 (98%) | 91 (92%) | 8 (8%) | 0 | 100 | 100 |
| 7 | G | 153/156 (98%) | 142 (93%) | 8 (5%) | 3 (2%) | 9 | 53 |
| 8 | H | 136/138 (99%) | 127 (93%) | 7 (5%) | 2 (2%) | 13 | 58 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 9 | I | 125/128 (98%) | 108 (86%) | 13 (10%) | 4 (3%) | 5 | 42 |
| 10 | J | 96/105 (91%) | 76 (79%) | 16 (17%) | 4 (4%) | 3 | 34 |
| 11 | K | 118/129 (92%) | 98 (83%) | 16 (14%) | 4 (3%) | 5 | 41 |
| 12 | L | 122/132 (92%) | 103 (84%) | 15 (12%) | 4 (3%) | 5 | 41 |
| 13 | M | 115/126 (91%) | 97 (84%) | 15 (13%) | 3 (3%) | 7 | 46 |
| 14 | N | 58/61 (95%) | 44 (76%) | 10 (17%) | 4 (7%) | 1 | 20 |
| 15 | O | 86/89 (97%) | 80 (93%) | 5 (6%) | 1 (1%) | 16 | 63 |
| 16 | P | 81/88 (92%) | 73 (90%) | 6 (7%) | 2 (2%) | 7 | 48 |
| 17 | Q | 97/105 (92%) | 82 (84%) | 10 (10%) | 5 (5%) | 2 | 27 |
| 18 | R | 71/88 (81%) | 61 (86%) | 9 (13%) | 1 (1%) | 14 | 59 |
| 19 | S | 78/93 (84%) | 66 (85%) | 9 (12%) | 3 (4%) | 4 | 37 |
| 20 | T | 97/106 (92%) | 84 (87%) | 10 (10%) | 3 (3%) | 5 | 43 |
| 21 | V | 22/27 (82%) | 20 (91%) | 1 (4%) | 1 (4%) | 3 | 32 |
| 22 | W | 69/72 (96%) | 55 (80%) | 11 (16%) | 3 (4%) | 3 | 33 |
| 23 | X | 166/171 (97%) | 145 (87%) | 16 (10%) | 5 (3%) | 5 | 43 |
| All | All | 2579/2781 (93%) | 2237 (87%) | 269 (10%) | 73 (3%) | 10 | 45 |

All (73) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 9 | GLU |
| 2 | B | 29 | ALA |
| 3 | C | 192 | THR |
| 4 | D | 37 | PRO |
| 17 | Q | 66 | SER |
| 17 | Q | 98 | LEU |
| 19 | S | 6 | LYS |
| 21 | V | 3 | LYS |
| 22 | W | 20 | ALA |
| 23 | X | 54 | PRO |
| 2 | B | 21 | ARG |
| 2 | B | 130 | ARG |
| 2 | B | 207 | ALA |
| 2 | B | 229 | VAL |
| 4 | D | 170 | VAL |
| 7 | G | 55 | GLY |
| 9 | I | 56 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | J | 34 | VAL |
| 10 | J | 55 | LYS |
| 11 | K | 50 | TYR |
| 22 | W | 70 | ARG |
| 23 | X | 8 | ASN |
| 23 | X | 55 | PRO |
| 2 | B | 20 | GLU |
| 3 | C | 4 | LYS |
| 3 | C | 61 | ALA |
| 3 | C | 108 | ASN |
| 4 | D | 138 | TYR |
| 7 | G | 7 | ALA |
| 7 | G | 149 | ARG |
| 8 | H | 5 | PRO |
| 8 | H | 70 | GLN |
| 9 | I | 29 | ASN |
| 11 | K | 101 | SER |
| 12 | L | 28 | LYS |
| 12 | L | 76 | ASN |
| 14 | N | 14 | PRO |
| 15 | O | 5 | LYS |
| 16 | P | 2 | VAL |
| 16 | P | 31 | LYS |
| 17 | Q | 77 | VAL |
| 17 | Q | 96 | GLU |
| 17 | Q | 97 | SER |
| 19 | S | 35 | SER |
| 2 | B | 208 | ILE |
| 2 | B | 233 | SER |
| 9 | I | 54 | ASP |
| 9 | I | 58 | HIS |
| 14 | N | 17 | LYS |
| 14 | N | 32 | SER |
| 18 | R | 17 | SER |
| 19 | S | 30 | LEU |
| 20 | T | 49 | ALA |
| 20 | T | 95 | ALA |
| 22 | W | 2 | LYS |
| 23 | X | 23 | GLY |
| 23 | X | 81 | LYS |
| 5 | E | 38 | GLN |
| 10 | J | 54 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | J | 83 | GLU |
| 12 | L | 25 | PRO |
| 12 | L | 48 | PRO |
| 13 | M | 104 | ARG |
| 13 | M | 113 | PRO |
| 5 | E | 128 | PRO |
| 11 | K | 14 | VAL |
| 13 | M | 67 | GLU |
| 2 | B | 194 | PRO |
| 5 | E | 115 | VAL |
| 11 | K | 48 | ILE |
| 14 | N | 54 | PRO |
| 20 | T | 103 | GLY |
| 3 | C | 51 | GLY |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | B | 202/220 (92%) | 142 (70%) | 60 (30%) | 0 | 3 |
| 3 | C | 160/188 (85%) | 131 (82%) | 29 (18%) | 2 | 14 |
| 4 | D | 180/181 (99%) | 146 (81%) | 34 (19%) | 2 | 12 |
| 5 | E | 115/123 (94%) | 90 (78%) | 25 (22%) | 1 | 9 |
| 6 | F | 90/90 (100%) | 72 (80%) | 18 (20%) | 1 | 11 |
| 7 | G | 126/127 (99%) | 106 (84%) | 20 (16%) | 3 | 21 |
| 8 | H | 119/119 (100%) | 90 (76%) | 29 (24%) | 1 | 6 |
| 9 | I | 96/99 (97%) | 76 (79%) | 20 (21%) | 1 | 10 |
| 10 | J | 87/92 (95%) | 75 (86%) | 12 (14%) | 4 | 28 |
| 11 | K | 91/99 (92%) | 72 (79%) | 19 (21%) | 1 | 10 |
| 12 | L | 104/109 (95%) | 79 (76%) | 25 (24%) | 1 | 6 |
| 13 | M | 94/101 (93%) | 79 (84%) | 15 (16%) | 3 | 21 |
| 14 | N | 49/50 (98%) | 41 (84%) | 8 (16%) | 3 | 20 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 15 | O | 79/80 (99%) | 64 (81%) | 15 (19%) | 2 | 12 |
| 16 | P | 72/74 (97%) | 59 (82%) | 13 (18%) | 2 | 14 |
| 17 | Q | 94/97 (97%) | 76 (81%) | 18 (19%) | 2 | 12 |
| 18 | R | 64/77 (83%) | 52 (81%) | 12 (19%) | 2 | 13 |
| 19 | S | 71/80 (89%) | 59 (83%) | 12 (17%) | 2 | 18 |
| 20 | T | 76/82 (93%) | 55 (72%) | 21 (28%) | 0 | 4 |
| 21 | V | 19/22 (86%) | 15 (79%) | 4 (21%) | 1 | 10 |
| 22 | W | 62/63 (98%) | 51 (82%) | 11 (18%) | 2 | 15 |
| 23 | X | 145/150 (97%) | 123 (85%) | 22 (15%) | 3 | 23 |
| All | All | 2195/2323 (94%) | 1753 (80%) | 442 (20%) | 4 | 11 |

All (442) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 9 | GLU |
| 2 | B | 10 | LEU |
| 2 | B | 15 | VAL |
| 2 | B | 16 | HIS |
| 2 | B | 17 | PHE |
| 2 | B | 21 | ARG |
| 2 | B | 22 | LYS |
| 2 | B | 23 | ARG |
| 2 | B | 25 | ASN |
| 2 | B | 28 | PHE |
| 2 | B | 30 | ARG |
| 2 | B | 39 | ILE |
| 2 | B | 44 | LEU |
| 2 | B | 48 | MET |
| 2 | B | 51 | LEU |
| 2 | B | 53 | ARG |
| 2 | B | 55 | PHE |
| 2 | B | 59 | GLU |
| 2 | B | 60 | ASP |
| 2 | B | 61 | LEU |
| 2 | B | 75 | LYS |
| 2 | B | 79 | ASP |
| 2 | B | 83 | MET |
| 2 | B | 95 | GLN |
| 2 | B | 96 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 97 | TRP |
| 2 | B | 101 | MET |
| 2 | B | 107 | THR |
| 2 | B | 110 | GLN |
| 2 | B | 111 | ARG |
| 2 | B | 112 | VAL |
| 2 | B | 113 | HIS |
| 2 | B | 114 | ARG |
| 2 | B | 115 | LEU |
| 2 | B | 116 | GLU |
| 2 | B | 118 | LEU |
| 2 | B | 121 | LEU |
| 2 | B | 126 | GLU |
| 2 | B | 130 | ARG |
| 2 | B | 135 | GLN |
| 2 | B | 140 | HIS |
| 2 | B | 144 | ARG |
| 2 | B | 145 | LEU |
| 2 | B | 155 | LEU |
| 2 | B | 157 | ARG |
| 2 | B | 165 | VAL |
| 2 | B | 168 | THR |
| 2 | B | 172 | ILE |
| 2 | B | 176 | GLU |
| 2 | B | 178 | ARG |
| 2 | B | 180 | LEU |
| 2 | B | 187 | LEU |
| 2 | B | 189 | ASP |
| 2 | B | 196 | LEU |
| 2 | B | 198 | ASP |
| 2 | B | 205 | ASP |
| 2 | B | 211 | ILE |
| 2 | B | 217 | ARG |
| 2 | B | 229 | VAL |
| 2 | B | 231 | GLU |
| 3 | C | 3 | ASN |
| 3 | C | 12 | LEU |
| 3 | C | 14 | ILE |
| 3 | C | 16 | ARG |
| 3 | C | 28 | GLN |
| 3 | C | 30 | ARG |
| 3 | C | 33 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 34 | LEU |
| 3 | C | 36 | ASP |
| 3 | C | 44 | GLU |
| 3 | C | 45 | LYS |
| 3 | C | 56 | ASP |
| 3 | C | 70 | VAL |
| 3 | C | 82 | GLU |
| 3 | C | 89 | GLU |
| 3 | C | 94 | LEU |
| 3 | C | 127 | ARG |
| 3 | C | 131 | ARG |
| 3 | C | 132 | ARG |
| 3 | C | 135 | LYS |
| 3 | C | 138 | VAL |
| 3 | C | 162 | GLN |
| 3 | C | 166 | GLU |
| 3 | C | 172 | ARG |
| 3 | C | 188 | LEU |
| 3 | C | 190 | ARG |
| 3 | C | 191 | THR |
| 3 | C | 201 | TYR |
| 3 | C | 204 | LEU |
| 4 | D | 3 | ARG |
| 4 | D | 10 | ARG |
| 4 | D | 26 | CYS |
| 4 | D | 34 | GLU |
| 4 | D | 35 | ARG |
| 4 | D | 36 | ARG |
| 4 | D | 42 | GLN |
| 4 | D | 49 | ARG |
| 4 | D | 50 | ARG |
| 4 | D | 58 | LEU |
| 4 | D | 59 | ARG |
| 4 | D | 61 | LYS |
| 4 | D | 64 | LEU |
| 4 | D | 65 | ARG |
| 4 | D | 66 | ARG |
| 4 | D | 70 | ILE |
| 4 | D | 83 | SER |
| 4 | D | 92 | VAL |
| 4 | D | 104 | VAL |
| 4 | D | 110 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 114 | ARG |
| 4 | D | 122 | ARG |
| 4 | D | 127 | THR |
| 4 | D | 131 | ARG |
| 4 | D | 132 | ARG |
| 4 | D | 139 | ARG |
| 4 | D | 140 | VAL |
| 4 | D | 141 | ARG |
| 4 | D | 155 | LEU |
| 4 | D | 157 | LEU |
| 4 | D | 165 | MET |
| 4 | D | 176 | LEU |
| 4 | D | 181 | MET |
| 4 | D | 207 | TYR |
| 5 | E | 10 | MET |
| 5 | E | 13 | ILE |
| 5 | E | 14 | ARG |
| 5 | E | 15 | ARG |
| 5 | E | 19 | MET |
| 5 | E | 20 | GLN |
| 5 | E | 24 | ARG |
| 5 | E | 34 | VAL |
| 5 | E | 38 | GLN |
| 5 | E | 40 | ARG |
| 5 | E | 41 | VAL |
| 5 | E | 47 | LYS |
| 5 | E | 64 | ARG |
| 5 | E | 71 | LEU |
| 5 | E | 80 | ILE |
| 5 | E | 89 | ILE |
| 5 | E | 91 | LEU |
| 5 | E | 107 | ARG |
| 5 | E | 116 | THR |
| 5 | E | 117 | ASP |
| 5 | E | 118 | ILE |
| 5 | E | 136 | MET |
| 5 | E | 137 | GLU |
| 5 | E | 144 | THR |
| 5 | E | 150 | ARG |
| 6 | F | 3 | ARG |
| 6 | F | 8 | ILE |
| 6 | F | 15 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | F | 24 | GLU |
| 6 | F | 27 | GLN |
| 6 | F | 28 | ARG |
| 6 | F | 31 | GLU |
| 6 | F | 32 | ASN |
| 6 | F | 36 | ARG |
| 6 | F | 39 | LYS |
| 6 | F | 40 | VAL |
| 6 | F | 47 | ARG |
| 6 | F | 61 | LEU |
| 6 | F | 75 | LEU |
| 6 | F | 77 | ARG |
| 6 | F | 87 | ARG |
| 6 | F | 89 | MET |
| 6 | F | 94 | GLN |
| 7 | G | 6 | ARG |
| 7 | G | 16 | LEU |
| 7 | G | 37 | ASN |
| 7 | G | 59 | LEU |
| 7 | G | 72 | ARG |
| 7 | G | 74 | GLU |
| 7 | G | 75 | VAL |
| 7 | G | 94 | ARG |
| 7 | G | 95 | ARG |
| 7 | G | 96 | GLN |
| 7 | G | 104 | LEU |
| 7 | G | 106 | GLN |
| 7 | G | 115 | ARG |
| 7 | G | 126 | ASP |
| 7 | G | 137 | LYS |
| 7 | G | 139 | GLU |
| 7 | G | 141 | VAL |
| 7 | G | 142 | GLU |
| 7 | G | 149 | ARG |
| 7 | G | 156 | TRP |
| 8 | H | 1 | MET |
| 8 | H | 8 | ASP |
| 8 | H | 18 | ARG |
| 8 | H | 26 | VAL |
| 8 | H | 29 | SER |
| 8 | H | 30 | ARG |
| 8 | H | 31 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | H | 34 | GLU |
| 8 | H | 39 | LEU |
| 8 | H | 41 | ARG |
| 8 | H | 45 | ILE |
| 8 | H | 50 | ARG |
| 8 | H | 56 | LYS |
| 8 | H | 59 | LEU |
| 8 | H | 70 | GLN |
| 8 | H | 77 | GLU |
| 8 | H | 78 | GLN |
| 8 | H | 79 | VAL |
| 8 | H | 80 | ILE |
| 8 | H | 82 | HIS |
| 8 | H | 92 | ARG |
| 8 | H | 102 | ARG |
| 8 | H | 105 | ARG |
| 8 | H | 112 | LEU |
| 8 | H | 116 | LYS |
| 8 | H | 119 | LEU |
| 8 | H | 120 | THR |
| 8 | H | 121 | ASP |
| 8 | H | 127 | LEU |
| 9 | I | 12 | GLU |
| 9 | I | 14 | VAL |
| 9 | I | 25 | LYS |
| 9 | I | 38 | GLN |
| 9 | I | 40 | LEU |
| 9 | I | 48 | GLU |
| 9 | I | 54 | ASP |
| 9 | I | 71 | SER |
| 9 | I | 75 | ASP |
| 9 | I | 85 | LEU |
| 9 | I | 95 | LYS |
| 9 | I | 99 | LEU |
| 9 | I | 102 | LEU |
| 9 | I | 104 | ARG |
| 9 | I | 116 | LYS |
| 9 | I | 117 | HIS |
| 9 | I | 118 | LYS |
| 9 | I | 121 | ARG |
| 9 | I | 124 | GLN |
| 9 | I | 125 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | J | 4 | ILE |
| 10 | J | 16 | LEU |
| 10 | J | 57 | LYS |
| 10 | J | 61 | GLU |
| 10 | J | 65 | LEU |
| 10 | J | 67 | THR |
| 10 | J | 71 | LEU |
| 10 | J | 74 | ILE |
| 10 | J | 75 | ILE |
| 10 | J | 82 | ILE |
| 10 | J | 85 | LEU |
| 10 | J | 87 | THR |
| 11 | K | 16 | SER |
| 11 | K | 18 | ARG |
| 11 | K | 32 | ILE |
| 11 | K | 34 | ASP |
| 11 | K | 47 | VAL |
| 11 | K | 54 | ARG |
| 11 | K | 55 | LYS |
| 11 | K | 57 | THR |
| 11 | K | 77 | MET |
| 11 | K | 80 | VAL |
| 11 | K | 84 | VAL |
| 11 | K | 85 | ARG |
| 11 | K | 93 | GLN |
| 11 | K | 98 | LEU |
| 11 | K | 101 | SER |
| 11 | K | 109 | VAL |
| 11 | K | 110 | ASP |
| 11 | K | 116 | HIS |
| 11 | K | 117 | ASN |
| 12 | L | 7 | ILE |
| 12 | L | 10 | LEU |
| 12 | L | 27 | LEU |
| 12 | L | 33 | ARG |
| 12 | L | 34 | ARG |
| 12 | L | 39 | VAL |
| 12 | L | 41 | ARG |
| 12 | L | 42 | THR |
| 12 | L | 46 | LYS |
| 12 | L | 53 | ARG |
| 12 | L | 55 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | L | 59 | ARG |
| 12 | L | 65 | GLU |
| 12 | L | 67 | THR |
| 12 | L | 70 | ILE |
| 12 | L | 79 | GLU |
| 12 | L | 81 | SER |
| 12 | L | 82 | VAL |
| 12 | L | 89 | ARG |
| 12 | L | 91 | LYS |
| 12 | L | 97 | ARG |
| 12 | L | 104 | VAL |
| 12 | L | 106 | ASP |
| 12 | L | 113 | ARG |
| 12 | L | 114 | LYS |
| 13 | M | 3 | ARG |
| 13 | M | 9 | ILE |
| 13 | M | 11 | ARG |
| 13 | M | 27 | LYS |
| 13 | M | 32 | GLU |
| 13 | M | 45 | VAL |
| 13 | M | 46 | LYS |
| 13 | M | 65 | LYS |
| 13 | M | 66 | LEU |
| 13 | M | 71 | ARG |
| 13 | M | 77 | ASN |
| 13 | M | 90 | LEU |
| 13 | M | 101 | GLN |
| 13 | M | 105 | THR |
| 13 | M | 115 | LYS |
| 14 | N | 3 | ARG |
| 14 | N | 4 | LYS |
| 14 | N | 12 | ARG |
| 14 | N | 16 | PHE |
| 14 | N | 17 | LYS |
| 14 | N | 21 | TYR |
| 14 | N | 31 | ARG |
| 14 | N | 41 | ARG |
| 15 | O | 4 | THR |
| 15 | O | 10 | LYS |
| 15 | O | 17 | ARG |
| 15 | O | 22 | THR |
| 15 | O | 28 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | O | 34 | LEU |
| 15 | O | 35 | ARG |
| 15 | O | 56 | LEU |
| 15 | O | 58 | MET |
| 15 | O | 64 | ARG |
| 15 | O | 65 | ARG |
| 15 | O | 66 | LEU |
| 15 | O | 70 | LEU |
| 15 | O | 79 | ARG |
| 15 | O | 88 | ARG |
| 16 | P | 1 | MET |
| 16 | P | 8 | ARG |
| 16 | P | 12 | LYS |
| 16 | P | 20 | VAL |
| 16 | P | 22 | THR |
| 16 | P | 28 | ARG |
| 16 | P | 45 | THR |
| 16 | P | 49 | LEU |
| 16 | P | 50 | LYS |
| 16 | P | 71 | ARG |
| 16 | P | 72 | ARG |
| 16 | P | 73 | LEU |
| 16 | P | 81 | ARG |
| 17 | Q | 15 | MET |
| 17 | Q | 16 | GLN |
| 17 | Q | 22 | LEU |
| 17 | Q | 25 | ARG |
| 17 | Q | 34 | LYS |
| 17 | Q | 38 | ARG |
| 17 | Q | 53 | LEU |
| 17 | Q | 63 | ARG |
| 17 | Q | 65 | ILE |
| 17 | Q | 66 | SER |
| 17 | Q | 75 | ARG |
| 17 | Q | 76 | LEU |
| 17 | Q | 84 | LEU |
| 17 | Q | 90 | ILE |
| 17 | Q | 92 | ARG |
| 17 | Q | 93 | GLN |
| 17 | Q | 98 | LEU |
| 17 | Q | 100 | LYS |
| 18 | R | 19 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | R | 31 | LEU |
| 18 | R | 36 | ASN |
| 18 | R | 37 | VAL |
| 18 | R | 38 | GLU |
| 18 | R | 47 | THR |
| 18 | R | 53 | ARG |
| 18 | R | 54 | ARG |
| 18 | R | 68 | LYS |
| 18 | R | 69 | THR |
| 18 | R | 75 | ILE |
| 18 | R | 78 | LEU |
| 19 | S | 3 | ARG |
| 19 | S | 5 | LEU |
| 19 | S | 6 | LYS |
| 19 | S | 7 | LYS |
| 19 | S | 15 | LEU |
| 19 | S | 18 | LYS |
| 19 | S | 25 | LYS |
| 19 | S | 39 | THR |
| 19 | S | 41 | VAL |
| 19 | S | 63 | THR |
| 19 | S | 67 | VAL |
| 19 | S | 77 | THR |
| 20 | T | 8 | ARG |
| 20 | T | 11 | SER |
| 20 | T | 13 | LEU |
| 20 | T | 14 | LYS |
| 20 | T | 15 | ARG |
| 20 | T | 19 | SER |
| 20 | T | 22 | ARG |
| 20 | T | 23 | ARG |
| 20 | T | 46 | GLU |
| 20 | T | 51 | GLU |
| 20 | T | 54 | LYS |
| 20 | T | 55 | ILE |
| 20 | T | 57 | ARG |
| 20 | T | 62 | LEU |
| 20 | T | 64 | ASP |
| 20 | T | 68 | LYS |
| 20 | T | 74 | LYS |
| 20 | T | 75 | ASN |
| 20 | T | 83 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | T | 84 | LEU |
| 20 | T | 90 | GLN |
| 21 | V | 6 | ARG |
| 21 | V | 9 | ARG |
| 21 | V | 10 | ARG |
| 21 | V | 12 | LYS |
| 22 | W | 15 | GLU |
| 22 | W | 19 | ASN |
| 22 | W | 22 | PHE |
| 22 | W | 23 | ARG |
| 22 | W | 32 | ILE |
| 22 | W | 33 | LEU |
| 22 | W | 47 | ILE |
| 22 | W | 48 | LEU |
| 22 | W | 51 | ASP |
| 22 | W | 58 | THR |
| 22 | W | 68 | VAL |
| 23 | X | 22 | ASP |
| 23 | X | 35 | LEU |
| 23 | X | 69 | GLN |
| 23 | X | 87 | SER |
| 23 | X | 91 | ARG |
| 23 | X | 93 | LYS |
| 23 | X | 95 | ASP |
| 23 | X | 98 | ASP |
| 23 | X | 100 | GLN |
| 23 | X | 119 | THR |
| 23 | X | 120 | ILE |
| 23 | X | 121 | MET |
| 23 | X | 123 | ARG |
| 23 | X | 132 | LEU |
| 23 | X | 134 | GLU |
| 23 | X | 135 | ARG |
| 23 | X | 147 | LEU |
| 23 | X | 156 | MET |
| 23 | X | 160 | ASP |
| 23 | X | 162 | ASN |
| 23 | X | 163 | MET |
| 23 | X | 164 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 25 | ASN |
| 2 | B | 40 | HIS |
| 2 | B | 95 | GLN |
| 2 | B | 204 | ASN |
| 3 | C | 3 | ASN |
| 3 | C | 108 | ASN |
| 3 | C | 176 | HIS |
| 4 | D | 77 | ASN |
| 4 | D | 123 | HIS |
| 4 | D | 125 | HIS |
| 4 | D | 129 | ASN |
| 4 | D | 201 | GLN |
| 5 | E | 20 | GLN |
| 5 | E | 72 | GLN |
| 6 | F | 7 | ASN |
| 6 | F | 11 | ASN |
| 6 | F | 13 | ASN |
| 6 | F | 100 | ASN |
| 8 | H | 82 | HIS |
| 9 | I | 3 | GLN |
| 9 | I | 117 | HIS |
| 9 | I | 124 | GLN |
| 10 | J | 62 | HIS |
| 11 | K | 117 | ASN |
| 12 | L | 8 | ASN |
| 12 | L | 49 | ASN |
| 12 | L | 75 | HIS |
| 13 | M | 106 | ASN |
| 15 | O | 37 | ASN |
| 15 | O | 62 | GLN |
| 17 | Q | 16 | GLN |
| 20 | T | 26 | ASN |
| 20 | T | 75 | ASN |
| 23 | X | 69 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 1508/1522 (99%) | 447 (29%) | 99 (6%) |
| 24 | Y | 19/42 (45%) | 12 (63%) | 2 (10%) |
| All | All | 1527/1564 (97%) | 459 (30%) | 101 (6%) |

All (459) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 6 | G |
| 1 | A | 7 | G |
| 1 | A | 8 | A |
| 1 | A | 9 | G |
| 1 | A | 13 | U |
| 1 | A | 31 | G |
| 1 | A | 32 | A |
| 1 | A | 35 | G |
| 1 | A | 39 | G |
| 1 | A | 44 | G |
| 1 | A | 47 | C |
| 1 | A | 48 | C |
| 1 | A | 49 | U |
| 1 | A | 50 | A |
| 1 | A | 51 | A |
| 1 | A | 52 | G |
| 1 | A | 53 | A |
| 1 | A | 54 | C |
| 1 | A | 58 | C |
| 1 | A | 63 | C |
| 1 | A | 72 | C |
| 1 | A | 77 | G |
| 1 | A | 78 | G |
| 1 | A | 79 | G |
| 1 | A | 81 | U |
| 1 | A | 82 | U |
| 1 | A | 90 | U |
| 1 | A | 91 | C |
| 1 | A | 92 | C |
| 1 | A | 96 | U |
| 1 | A | 98 | G |
| 1 | A | 105 | G |
| 1 | A | 108 | G |
| 1 | A | 115 | G |
| 1 | A | 116 | A |
| 1 | A | 120 | A |
| 1 | A | 121 | C |
| 1 | A | 129(A) | G |
| 1 | A | 130 | A |
| 1 | A | 131 | C |
| 1 | A | 142 | G |
| 1 | A | 144 | G |
| 1 | A | 151 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 152 | A |
| 1 | A | 163 | C |
| 1 | A | 181 | G |
| 1 | A | 182 | U |
| 1 | A | 187 | C |
| 1 | A | 189(D) | C |
| 1 | A | 189(E) | U |
| 1 | A | 189(F) | U |
| 1 | A | 189(G) | G |
| 1 | A | 189(H) | G |
| 1 | A | 195 | A |
| 1 | A | 197 | A |
| 1 | A | 198 | G |
| 1 | A | 201 | C |
| 1 | A | 203 | U |
| 1 | A | 204 | U |
| 1 | A | 219 | C |
| 1 | A | 220 | G |
| 1 | A | 222 | U |
| 1 | A | 223 | U |
| 1 | A | 244 | U |
| 1 | A | 247 | G |
| 1 | A | 251 | G |
| 1 | A | 252 | U |
| 1 | A | 266 | G |
| 1 | A | 267 | C |
| 1 | A | 272 | C |
| 1 | A | 279 | A |
| 1 | A | 280 | C |
| 1 | A | 281 | G |
| 1 | A | 282 | A |
| 1 | A | 283 | C |
| 1 | A | 289 | G |
| 1 | A | 296 | U |
| 1 | A | 298 | A |
| 1 | A | 301 | G |
| 1 | A | 303 | A |
| 1 | A | 306 | G |
| 1 | A | 315 | A |
| 1 | A | 316 | G |
| 1 | A | 319 | G |
| 1 | A | 321 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 324 | G |
| 1 | A | 325 | A |
| 1 | A | 328 | C |
| 1 | A | 329 | A |
| 1 | A | 330 | C |
| 1 | A | 332 | G |
| 1 | A | 342 | C |
| 1 | A | 344 | A |
| 1 | A | 345 | C |
| 1 | A | 346 | G |
| 1 | A | 348 | G |
| 1 | A | 351 | G |
| 1 | A | 352 | C |
| 1 | A | 353 | A |
| 1 | A | 354 | G |
| 1 | A | 367 | U |
| 1 | A | 369 | C |
| 1 | A | 372 | C |
| 1 | A | 373 | A |
| 1 | A | 375 | U |
| 1 | A | 378 | G |
| 1 | A | 379 | C |
| 1 | A | 381 | C |
| 1 | A | 390 | C |
| 1 | A | 392 | G |
| 1 | A | 395 | C |
| 1 | A | 397 | A |
| 1 | A | 398 | C |
| 1 | A | 399 | G |
| 1 | A | 406 | G |
| 1 | A | 412 | A |
| 1 | A | 413 | G |
| 1 | A | 419 | C |
| 1 | A | 421 | U |
| 1 | A | 422 | C |
| 1 | A | 423 | G |
| 1 | A | 424 | G |
| 1 | A | 426 | G |
| 1 | A | 428 | G |
| 1 | A | 429 | U |
| 1 | A | 438 | G |
| 1 | A | 439 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 441 | A |
| 1 | A | 452 | A |
| 1 | A | 453 | A |
| 1 | A | 470 | C |
| 1 | A | 472 | A |
| 1 | A | 477 | A |
| 1 | A | 484 | G |
| 1 | A | 485 | G |
| 1 | A | 486 | U |
| 1 | A | 495 | A |
| 1 | A | 496 | A |
| 1 | A | 498 | U |
| 1 | A | 505 | G |
| 1 | A | 509 | A |
| 1 | A | 510 | A |
| 1 | A | 511 | C |
| 1 | A | 517 | G |
| 1 | A | 518 | C |
| 1 | A | 519 | C |
| 1 | A | 521 | G |
| 1 | A | 524 | G |
| 1 | A | 527 | G |
| 1 | A | 528 | C |
| 1 | A | 529 | G |
| 1 | A | 531 | U |
| 1 | A | 532 | A |
| 1 | A | 533 | A |
| 1 | A | 534 | U |
| 1 | A | 535 | A |
| 1 | A | 542 | G |
| 1 | A | 545 | C |
| 1 | A | 546 | G |
| 1 | A | 547 | A |
| 1 | A | 550 | G |
| 1 | A | 559 | A |
| 1 | A | 560 | U |
| 1 | A | 561 | U |
| 1 | A | 562 | C |
| 1 | A | 564 | C |
| 1 | A | 572 | A |
| 1 | A | 573 | A |
| 1 | A | 574 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 576 | G |
| 1 | A | 577 | G |
| 1 | A | 578 | C |
| 1 | A | 579 | G |
| 1 | A | 582 | U |
| 1 | A | 587 | G |
| 1 | A | 595 | G |
| 1 | A | 596 | C |
| 1 | A | 607 | A |
| 1 | A | 617 | G |
| 1 | A | 618 | C |
| 1 | A | 619 | U |
| 1 | A | 641 | U |
| 1 | A | 642 | A |
| 1 | A | 653 | A |
| 1 | A | 654 | G |
| 1 | A | 662 | G |
| 1 | A | 665 | A |
| 1 | A | 666 | G |
| 1 | A | 671 | G |
| 1 | A | 672 | U |
| 1 | A | 673 | G |
| 1 | A | 678 | U |
| 1 | A | 687 | A |
| 1 | A | 688 | G |
| 1 | A | 692 | U |
| 1 | A | 693 | G |
| 1 | A | 695 | A |
| 1 | A | 697 | U |
| 1 | A | 701 | C |
| 1 | A | 702 | A |
| 1 | A | 703 | G |
| 1 | A | 715 | A |
| 1 | A | 717 | C |
| 1 | A | 720 | C |
| 1 | A | 721 | G |
| 1 | A | 723 | U |
| 1 | A | 728 | A |
| 1 | A | 729 | A |
| 1 | A | 731 | G |
| 1 | A | 748 | C |
| 1 | A | 749 | C |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 753 | A |
| 1 | A | 755 | G |
| 1 | A | 759 | A |
| 1 | A | 762 | C |
| 1 | A | 774 | G |
| 1 | A | 777 | A |
| 1 | A | 782 | A |
| 1 | A | 786 | G |
| 1 | A | 787 | A |
| 1 | A | 792 | A |
| 1 | A | 793 | U |
| 1 | A | 794 | A |
| 1 | A | 795 | C |
| 1 | A | 799 | G |
| 1 | A | 812 | C |
| 1 | A | 815 | A |
| 1 | A | 816 | A |
| 1 | A | 817 | C |
| 1 | A | 819 | A |
| 1 | A | 821 | G |
| 1 | A | 828 | A |
| 1 | A | 835 | U |
| 1 | A | 839 | U |
| 1 | A | 840 | C |
| 1 | A | 841 | U |
| 1 | A | 849 | C |
| 1 | A | 851 | G |
| 1 | A | 867 | G |
| 1 | A | 871 | U |
| 1 | A | 873 | A |
| 1 | A | 876 | G |
| 1 | A | 883 | C |
| 1 | A | 884 | U |
| 1 | A | 885 | G |
| 1 | A | 888 | G |
| 1 | A | 889 | A |
| 1 | A | 891 | U |
| 1 | A | 900 | A |
| 1 | A | 911 | U |
| 1 | A | 914 | A |
| 1 | A | 922 | G |
| 1 | A | 926 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 927 | G |
| 1 | A | 931 | C |
| 1 | A | 932 | C |
| 1 | A | 933 | G |
| 1 | A | 934 | C |
| 1 | A | 935 | A |
| 1 | A | 938 | A |
| 1 | A | 942 | G |
| 1 | A | 945 | G |
| 1 | A | 946 | A |
| 1 | A | 947 | G |
| 1 | A | 960 | U |
| 1 | A | 961 | U |
| 1 | A | 966 | G |
| 1 | A | 968 | A |
| 1 | A | 969 | A |
| 1 | A | 971 | G |
| 1 | A | 974 | A |
| 1 | A | 975 | A |
| 1 | A | 976 | G |
| 1 | A | 977 | A |
| 1 | A | 984 | C |
| 1 | A | 989 | C |
| 1 | A | 991 | U |
| 1 | A | 992 | U |
| 1 | A | 993 | G |
| 1 | A | 994 | A |
| 1 | A | 1000 | U |
| 1 | A | 1001 | A |
| 1 | A | 1002 | G |
| 1 | A | 1003 | G |
| 1 | A | 1005 | A |
| 1 | A | 1007 | C |
| 1 | A | 1023 | G |
| 1 | A | 1024 | G |
| 1 | A | 1025 | U |
| 1 | A | 1026 | G |
| 1 | A | 1028 | C |
| 1 | A | 1029 | C |
| 1 | A | 1038 | C |
| 1 | A | 1042 | G |
| 1 | A | 1045 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1046 | A |
| 1 | A | 1050 | G |
| 1 | A | 1051 | C |
| 1 | A | 1053 | G |
| 1 | A | 1054 | C |
| 1 | A | 1055 | A |
| 1 | A | 1064 | G |
| 1 | A | 1065 | U |
| 1 | A | 1066 | C |
| 1 | A | 1070 | U |
| 1 | A | 1078 | U |
| 1 | A | 1086 | U |
| 1 | A | 1089 | G |
| 1 | A | 1092 | A |
| 1 | A | 1094 | G |
| 1 | A | 1095 | U |
| 1 | A | 1100 | C |
| 1 | A | 1101 | A |
| 1 | A | 1102 | A |
| 1 | A | 1103 | C |
| 1 | A | 1104 | G |
| 1 | A | 1108 | G |
| 1 | A | 1117 | G |
| 1 | A | 1124 | G |
| 1 | A | 1125 | U |
| 1 | A | 1126 | U |
| 1 | A | 1127 | G |
| 1 | A | 1128 | C |
| 1 | A | 1129 | C |
| 1 | A | 1130 | A |
| 1 | A | 1131 | G |
| 1 | A | 1137 | C |
| 1 | A | 1138 | G |
| 1 | A | 1139 | G |
| 1 | A | 1140 | C |
| 1 | A | 1145 | C |
| 1 | A | 1146 | A |
| 1 | A | 1151 | A |
| 1 | A | 1152 | A |
| 1 | A | 1157 | A |
| 1 | A | 1159 | U |
| 1 | A | 1169 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1177 | G |
| 1 | A | 1183 | A |
| 1 | A | 1184 | G |
| 1 | A | 1185 | G |
| 1 | A | 1191 | A |
| 1 | A | 1195 | C |
| 1 | A | 1196 | U |
| 1 | A | 1197 | G |
| 1 | A | 1200 | C |
| 1 | A | 1201 | A |
| 1 | A | 1202 | G |
| 1 | A | 1206 | G |
| 1 | A | 1209 | C |
| 1 | A | 1212 | U |
| 1 | A | 1213 | A |
| 1 | A | 1215 | G |
| 1 | A | 1221 | G |
| 1 | A | 1226 | C |
| 1 | A | 1227 | A |
| 1 | A | 1231 | G |
| 1 | A | 1236 | A |
| 1 | A | 1238 | A |
| 1 | A | 1239 | A |
| 1 | A | 1240 | U |
| 1 | A | 1249 | C |
| 1 | A | 1250 | A |
| 1 | A | 1256 | A |
| 1 | A | 1257 | U |
| 1 | A | 1258 | G |
| 1 | A | 1260 | C |
| 1 | A | 1266 | G |
| 1 | A | 1267 | C |
| 1 | A | 1270 | C |
| 1 | A | 1277 | C |
| 1 | A | 1278 | U |
| 1 | A | 1279 | A |
| 1 | A | 1281 | U |
| 1 | A | 1283 | G |
| 1 | A | 1285 | A |
| 1 | A | 1286 | A |
| 1 | A | 1287 | A |
| 1 | A | 1288 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | A | 1296 | C |
| 1 | A | 1297 | C |
| 1 | A | 1299 | A |
| 1 | A | 1300 | G |
| 1 | A | 1301 | U |
| 1 | A | 1302 | U |
| 1 | A | 1305 | G |
| 1 | A | 1315 | U |
| 1 | A | 1316 | G |
| 1 | A | 1318 | A |
| 1 | A | 1319 | A |
| 1 | A | 1320 | C |
| 1 | A | 1323 | G |
| 1 | A | 1331 | G |
| 1 | A | 1332 | A |
| 1 | A | 1335 | C |
| 1 | A | 1336 | C |
| 1 | A | 1337 | G |
| 1 | A | 1340 | A |
| 1 | A | 1346 | A |
| 1 | A | 1347 | G |
| 1 | A | 1348 | U |
| 1 | A | 1353 | G |
| 1 | A | 1357 | A |
| 1 | A | 1363 | C |
| 1 | A | 1363(A) | A |
| 1 | A | 1364 | U |
| 1 | A | 1368 | G |
| 1 | A | 1370 | G |
| 1 | A | 1378 | C |
| 1 | A | 1379 | G |
| 1 | A | 1380 | U |
| 1 | A | 1381 | U |
| 1 | A | 1388 | C |
| 1 | A | 1394 | A |
| 1 | A | 1397 | C |
| 1 | A | 1398 | A |
| 1 | A | 1399 | C |
| 1 | A | 1400 | C |
| 1 | A | 1415 | G |
| 1 | A | 1434 | A |
| 1 | A | 1442 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1443 | G |
| 1 | A | 1447 | A |
| 1 | A | 1452 | C |
| 1 | A | 1456 | G |
| 1 | A | 1457 | G |
| 1 | A | 1459 | C |
| 1 | A | 1486 | G |
| 1 | A | 1492 | A |
| 1 | A | 1493 | A |
| 1 | A | 1494 | G |
| 1 | A | 1497 | G |
| 1 | A | 1499 | A |
| 1 | A | 1502 | A |
| 1 | A | 1503 | A |
| 1 | A | 1504 | G |
| 1 | A | 1505 | G |
| 1 | A | 1506 | U |
| 1 | A | 1507 | A |
| 1 | A | 1517 | G |
| 1 | A | 1519 | A |
| 1 | A | 1520 | G |
| 1 | A | 1529 | G |
| 1 | A | 1530 | G |
| 1 | A | 1532 | U |
| 1 | A | 1536 | C |
| 1 | A | 1538 | C |
| 24 | Y | 23 | C |
| 24 | Y | 24 | A |
| 24 | Y | 28 | A |
| 24 | Y | 30 | G |
| 24 | Y | 32 | A |
| 24 | Y | 33 | A |
| 24 | Y | 34 | A |
| 24 | Y | 35 | A |
| 24 | Y | 36 | A |
| 24 | Y | 37 | U |
| 24 | Y | 38 | G |
| 24 | Y | 39 | U |

All (101) RNA pucker outliers are listed below:

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
|-----|-------|-----|------|

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 7 | G |
| 1 | A | 47 | C |
| 1 | A | 48 | C |
| 1 | A | 49 | U |
| 1 | A | 77 | G |
| 1 | A | 108 | G |
| 1 | A | 115 | G |
| 1 | A | 119 | A |
| 1 | A | 129(A) | G |
| 1 | A | 181 | G |
| 1 | A | 197 | A |
| 1 | A | 202 | U |
| 1 | A | 243 | A |
| 1 | A | 250 | A |
| 1 | A | 251 | G |
| 1 | A | 266 | G |
| 1 | A | 279 | A |
| 1 | A | 280 | C |
| 1 | A | 281 | G |
| 1 | A | 288 | A |
| 1 | A | 329 | A |
| 1 | A | 344 | A |
| 1 | A | 351 | G |
| 1 | A | 372 | C |
| 1 | A | 389 | A |
| 1 | A | 421 | U |
| 1 | A | 428 | G |
| 1 | A | 484 | G |
| 1 | A | 495 | A |
| 1 | A | 496 | A |
| 1 | A | 509 | A |
| 1 | A | 518 | C |
| 1 | A | 531 | U |
| 1 | A | 535 | A |
| 1 | A | 559 | A |
| 1 | A | 560 | U |
| 1 | A | 575 | G |
| 1 | A | 576 | G |
| 1 | A | 595 | G |
| 1 | A | 641 | U |
| 1 | A | 672 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 687 | A |
| 1 | A | 701 | C |
| 1 | A | 702 | A |
| 1 | A | 717 | C |
| 1 | A | 748 | C |
| 1 | A | 792 | A |
| 1 | A | 820 | U |
| 1 | A | 840 | C |
| 1 | A | 872 | A |
| 1 | A | 873 | A |
| 1 | A | 897 | C |
| 1 | A | 934 | C |
| 1 | A | 946 | A |
| 1 | A | 965 | A |
| 1 | A | 975 | A |
| 1 | A | 992 | U |
| 1 | A | 993 | G |
| 1 | A | 1000 | U |
| 1 | A | 1049 | U |
| 1 | A | 1054 | C |
| 1 | A | 1064 | G |
| 1 | A | 1065 | U |
| 1 | A | 1085 | U |
| 1 | A | 1101 | A |
| 1 | A | 1126 | U |
| 1 | A | 1128 | C |
| 1 | A | 1137 | C |
| 1 | A | 1145 | C |
| 1 | A | 1151 | A |
| 1 | A | 1182 | G |
| 1 | A | 1190 | G |
| 1 | A | 1196 | U |
| 1 | A | 1201 | A |
| 1 | A | 1211 | U |
| 1 | A | 1212 | U |
| 1 | A | 1214 | C |
| 1 | A | 1239 | A |
| 1 | A | 1257 | U |
| 1 | A | 1266 | G |
| 1 | A | 1278 | U |
| 1 | A | 1285 | A |
| 1 | A | 1299 | A |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | A | 1300 | G |
| 1 | A | 1301 | U |
| 1 | A | 1322 | C |
| 1 | A | 1331 | G |
| 1 | A | 1346 | A |
| 1 | A | 1363(A) | A |
| 1 | A | 1380 | U |
| 1 | A | 1399 | C |
| 1 | A | 1442(B) | A |
| 1 | A | 1447 | A |
| 1 | A | 1452 | C |
| 1 | A | 1493 | A |
| 1 | A | 1498 | U |
| 1 | A | 1503 | A |
| 1 | A | 1504 | G |
| 1 | A | 1507 | A |
| 24 | Y | 32 | A |
| 24 | Y | 33 | A |

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 129 ligands modelled in this entry, 129 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | A | 4 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | A | 84:U | O3' | 88:A | P | 5.75 |
| 1 | A | 1442(A):G | O3' | 1442(B):A | P | 5.10 |
| 1 | A | 841:U | O3' | 848:C | P | 4.14 |
| 1 | A | 204:U | O3' | 216:G | P | 3.78 |