# Full wwPDB EM Validation Report ⓘ

Apr 22, 2025 – 06:41 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 8VR8 / pdb_00008vr8 |
| EMDB ID | : | EMD-43477 |
| Title | : | Structure of Mycobacterium smegmatis 50S ribosomal subunit bound to HflX and chloramphenicol:50S-HflX-B-Clm |
| Authors | : | Majumdar, S.; Koripella, R.K.; Sharma, M.R.; Manjari, S.R.; Banavali, N.K.; Agrawal, R.K. |
| Deposited on | : | 2024-01-20 |
| Resolution | : | 3.25 Å(reported) |
| Based on initial models | : | 6DZI, 5O61 |

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

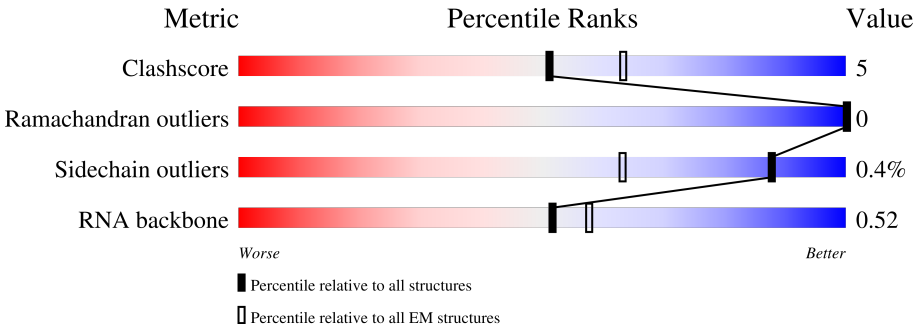
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev117 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.42 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.25 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 | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 2 | 61 | 84% 13% |
| 2 | 3 | 24 | 92% |
| 3 | 4 | 470 | 31% 69% 27% |
| 4 | B | 118 | 5% 58% 29% 13% |
| 5 | C | 278 | 88% 10% |
| 6 | D | 217 | 91% 7% |
| 7 | E | 215 | 86% 11% |

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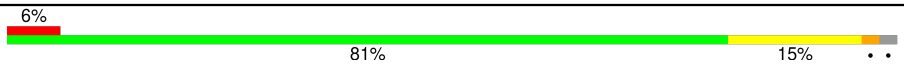
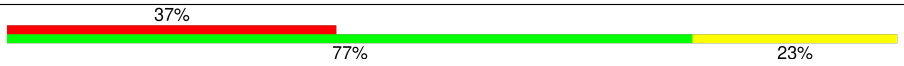
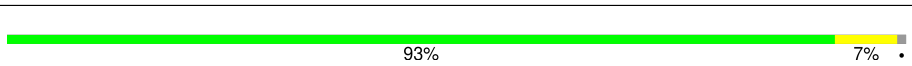
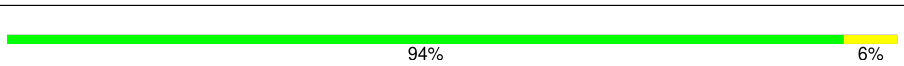
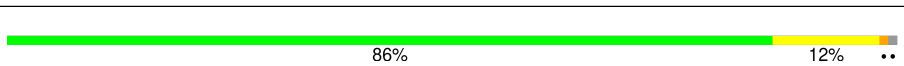
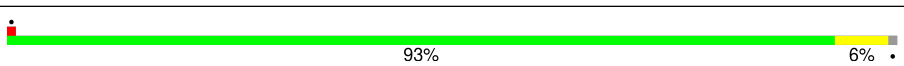
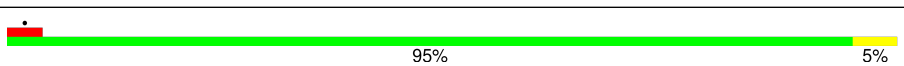
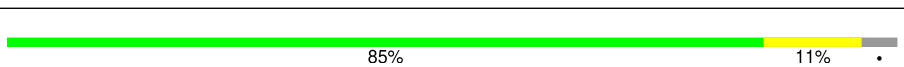
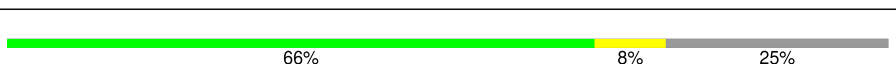
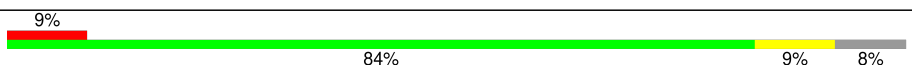
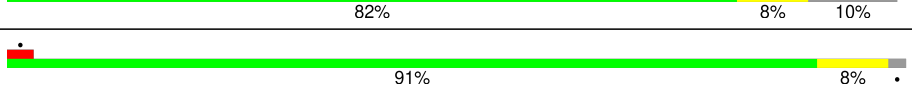
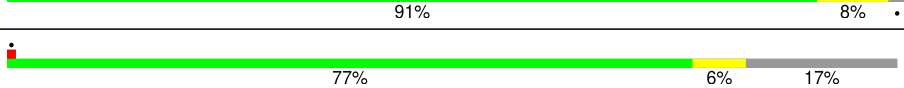
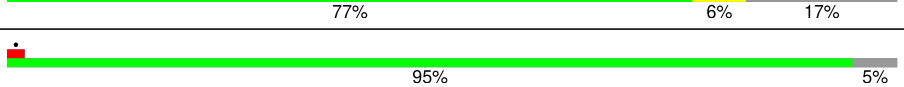
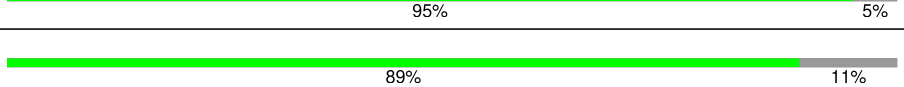
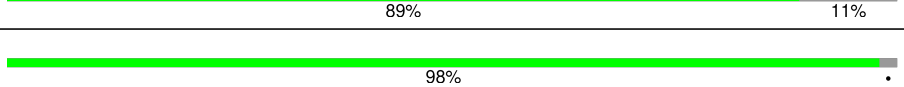
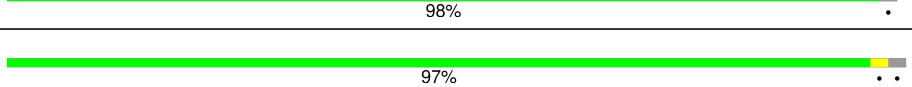
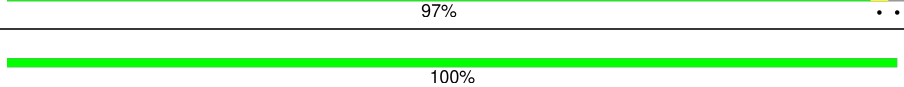
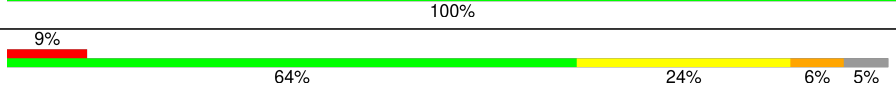
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 8 | G | 179 |   |
| 9 | H | 151 |   |
| 10 | I | 175 |   |
| 11 | K | 147 |   |
| 12 | L | 122 |   |
| 13 | M | 147 |   |
| 14 | N | 138 |   |
| 15 | O | 199 |   |
| 16 | Q | 113 |   |
| 17 | R | 129 |   |
| 18 | S | 103 |   |
| 19 | T | 153 |   |
| 20 | U | 100 |   |
| 21 | V | 105 |   |
| 22 | W | 215 |   |
| 23 | X | 88 |   |
| 24 | Y | 64 |   |
| 25 | Z | 77 |   |
| 26 | b | 57 |   |
| 27 | c | 55 |   |
| 28 | d | 47 |   |
| 29 | e | 64 |   |
| 30 | f | 37 |   |
| 31 | A | 3120 |   |

# 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 93099 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 protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 59 | Total | C | N | O | 0 | 0 |
| | | | 474 | 292 | 95 | 87 | | |

- Molecule 2 is a protein called 50S Ribosomal Protein L37.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 2 | 3 | 23 | Total | C | N | O | 0 | 0 |
| | | | 189 | 111 | 50 | 28 | | |

- Molecule 3 is a protein called GTPase HflX.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | 4 | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3444 | 2127 | 638 | 672 | 7 | | |

- Molecule 4 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | B | 118 | Total | C | N | O | P | 0 | 0 |
| | | | 2522 | 1126 | 468 | 810 | 118 | | |

- Molecule 5 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | C | 275 | Total | C | N | O | S | 0 | 0 |
| | | | 2110 | 1298 | 438 | 370 | 4 | | |

- Molecule 6 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | D | 214 | Total | C | N | O | S | 0 | 0 |
| | | | 1587 | 982 | 310 | 290 | 5 | | |

- Molecule 7 is a protein called 50S Ribosomal Protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | E | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1569 | 969 | 295 | 303 | 2 | | |

- Molecule 8 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | G | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1348 | 845 | 249 | 253 | 1 | | |

- Molecule 9 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | H | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1018 | 635 | 188 | 194 | 1 | | |

- Molecule 10 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | I | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 918 | 580 | 156 | 180 | 2 | | |

- Molecule 11 is a protein called 50S Ribosomal Protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | K | 146 | Total | C | N | O | S | 0 | 0 |
| | | | 1130 | 722 | 207 | 200 | 1 | | |

- Molecule 12 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | L | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 938 | 586 | 179 | 170 | 3 | | |

- Molecule 13 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | M | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1078 | 676 | 205 | 194 | 3 | | |

- Molecule 14 is a protein called Large ribosomal subunit protein uL16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | N | 136 | Total<br>1092 | C<br>690 | N<br>213 | O<br>187 | S<br>2 | 0 | 0 |

- Molecule 15 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | O | 118 | Total<br>928 | C<br>583 | N<br>180 | O<br>163 | S<br>2 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | Q | 113 | Total<br>907 | C<br>570 | N<br>171 | O<br>165 | S<br>1 | 0 | 0 |

- Molecule 17 is a protein called 50S Ribosomal Protein L20.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 17 | R | 124 | Total<br>988 | C<br>613 | N<br>203 | O<br>172 | 0 | 0 |

- Molecule 18 is a protein called 50S Ribosomal Protein L21.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 18 | S | 100 | Total<br>754 | C<br>478 | N<br>137 | O<br>139 | 0 | 0 |

- Molecule 19 is a protein called 50S Ribosomal Protein L22.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 19 | T | 114 | Total<br>873 | C<br>543 | N<br>171 | O<br>159 | 0 | 0 |

- Molecule 20 is a protein called 50S Ribosomal Protein L23.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 20 | U | 97 | Total<br>756 | C<br>479 | N<br>138 | O<br>139 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | V | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 732 | 456 | 137 | 137 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 22 | W | 95 | Total | C | N | O | 0 | 0 |
| | | | 735 | 452 | 149 | 134 | | |

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

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 23 | X | 79 | Total | C | N | O | 0 | 0 |
| | | | 586 | 361 | 123 | 102 | | |

- Molecule 24 is a protein called 50S Ribosomal Protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | Y | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 470 | 283 | 103 | 80 | 4 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | Z | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 531 | 324 | 103 | 103 | 1 | | |

- Molecule 26 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | b | 54 | Total | C | N | O | S | 0 | 0 |
| | | | 423 | 260 | 93 | 69 | 1 | | |

- Molecule 27 is a protein called 50S Ribosomal Protein L33.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | c | 49 | Total | C | N | O | S | 0 | 0 |
| | | | 405 | 248 | 82 | 71 | 4 | | |

- Molecule 28 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | d | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 377 | 225 | 97 | 54 | 1 | | |

- Molecule 29 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 29 | e | 63 | Total | C | N | O | 0 | 0 |
| | | | 502 | 302 | 115 | 85 | | |

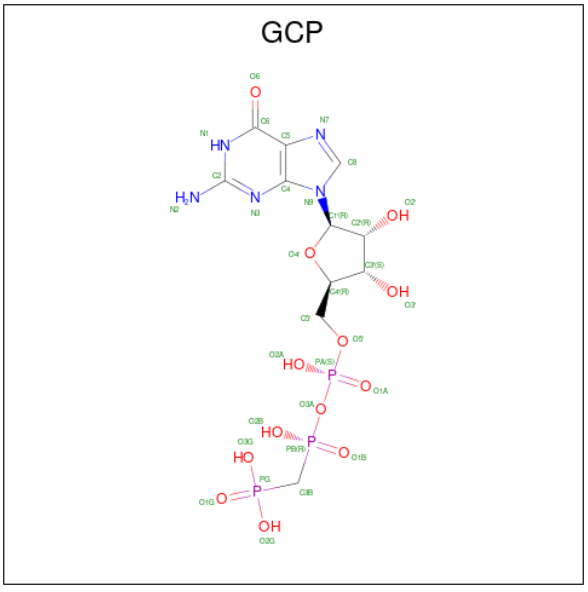
- Molecule 30 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | f | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 299 | 181 | 66 | 47 | 5 | | |

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

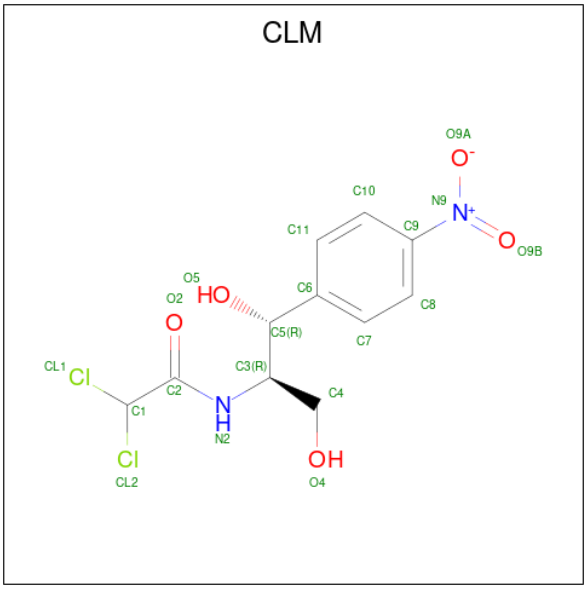
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | A | 2950 | Total | C | N | O | P | 0 | 0 |
| | | | 63364 | 28241 | 11658 | 20515 | 2950 | | |

- Molecule 32 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 32 | 4 | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 11 | 5 | 13 | 3 | |

- Molecule 33 is CHLORAMPHENICOL (CCD ID: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$) (labeled as "Ligand of Interest" by depositor).



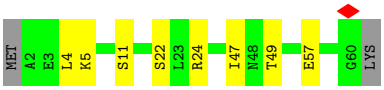

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 33 | A | 1 | Total | C | Cl | N | O | 0 |
| | | | 20 | 11 | 2 | 2 | 5 | |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

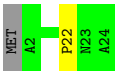
- Molecule 1: 50S ribosomal protein L30

Chain 2:

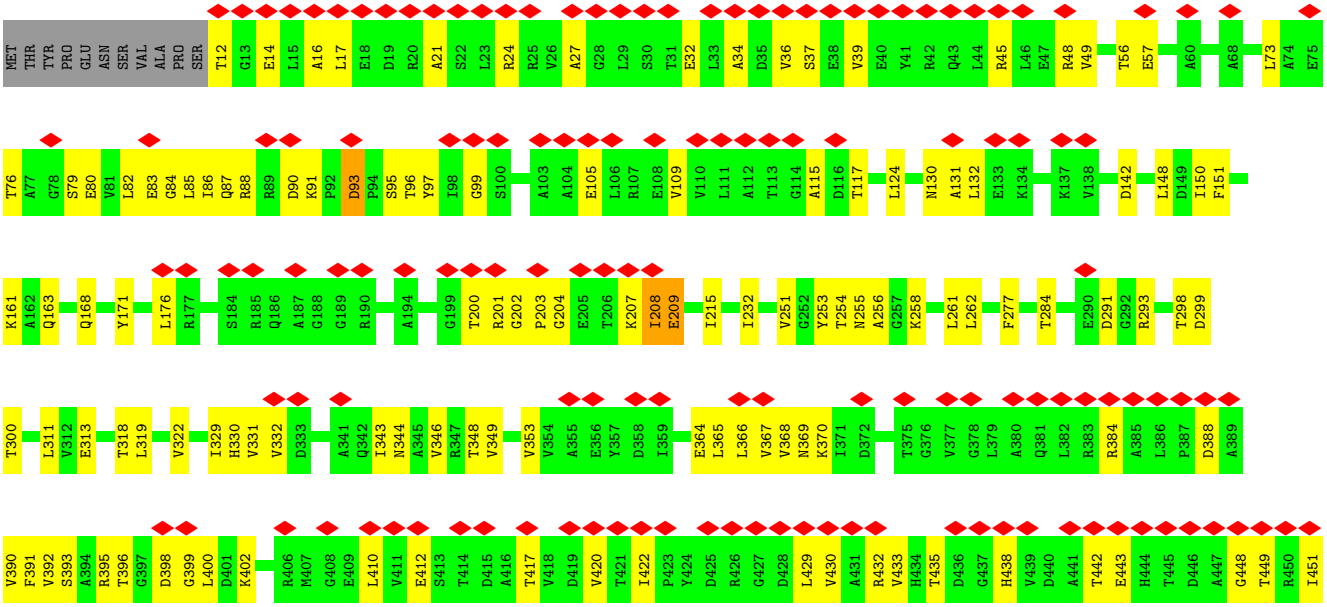

- Molecule 2: 50S Ribosomal Protein L37

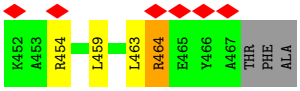
Chain 3:


- Molecule 3: GTPase HflX

Chain 4:




• Molecule 4: 5S ribosomal RNA

Chain B:



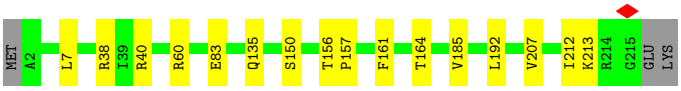
• Molecule 5: 50S ribosomal protein L2

Chain C:



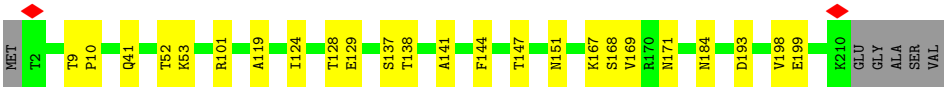
• Molecule 6: 50S ribosomal protein L3

Chain D:

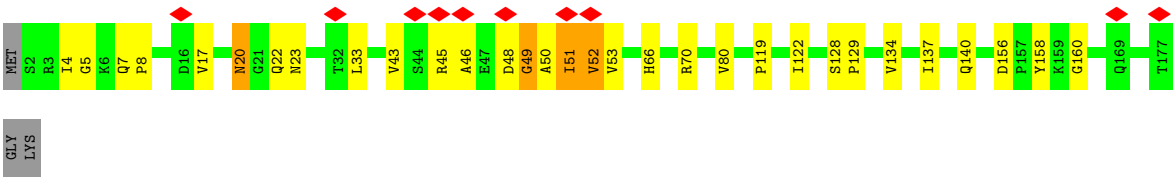

• Molecule 7: 50S Ribosomal Protein L4

Chain E:

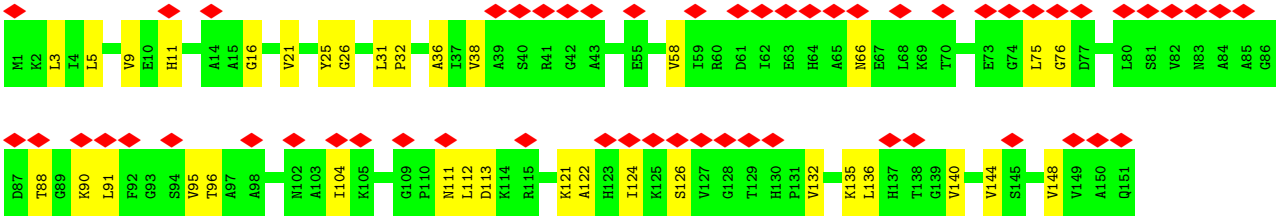

• Molecule 8: 50S ribosomal protein L6

Chain G:

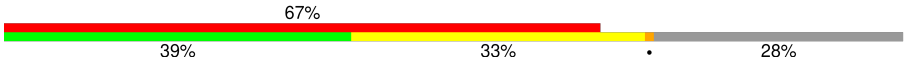

• Molecule 9: 50S ribosomal protein L9

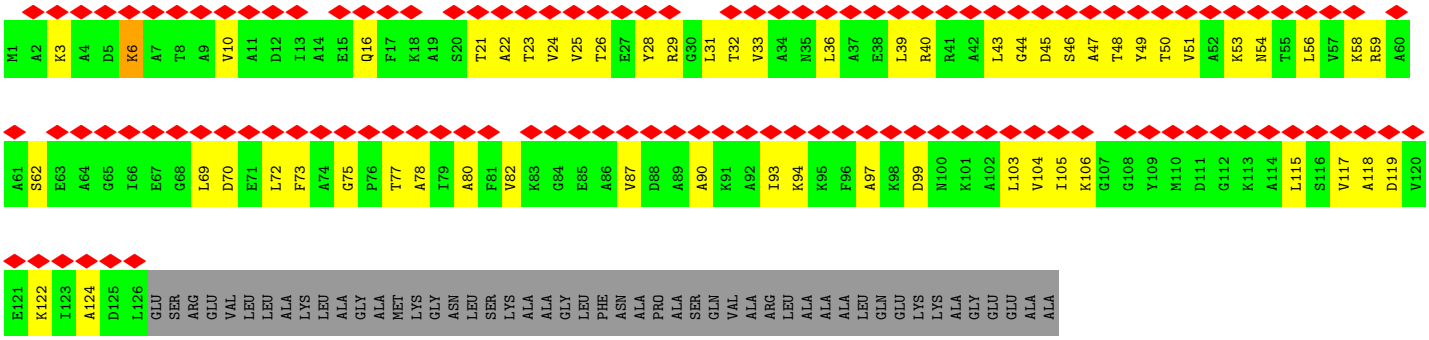
Chain H:




• Molecule 10: 50S ribosomal protein L10

Chain I:



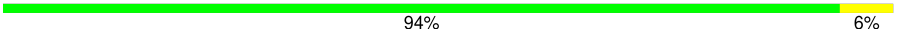

• Molecule 11: 50S Ribosomal Protein L13

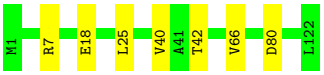
Chain K:



• Molecule 12: 50S ribosomal protein L14

Chain L:



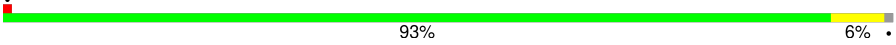

• Molecule 13: 50S ribosomal protein L15

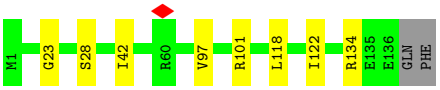
Chain M:



• Molecule 14: Large ribosomal subunit protein uL16

Chain N:



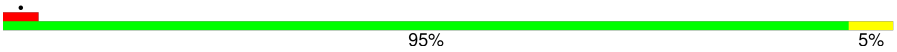
• Molecule 15: 50S ribosomal protein L17

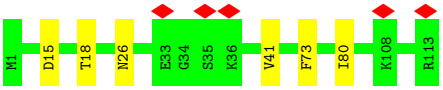
Chain O:




• Molecule 16: 50S ribosomal protein L19

Chain Q:



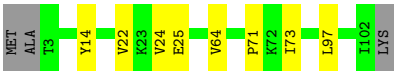

• Molecule 17: 50S Ribosomal Protein L20

Chain R:



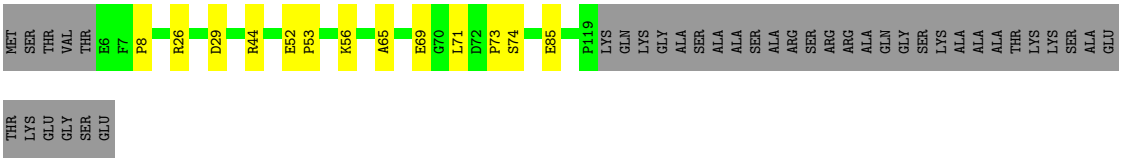
• Molecule 18: 50S Ribosomal Protein L21

Chain S:

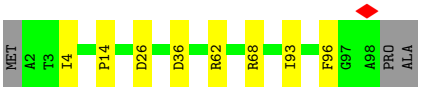

• Molecule 19: 50S Ribosomal Protein L22

Chain T:

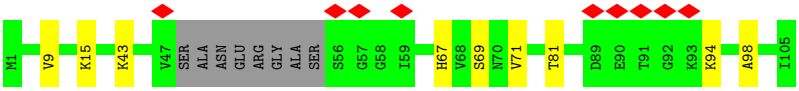

• Molecule 20: 50S Ribosomal Protein L23

Chain U:

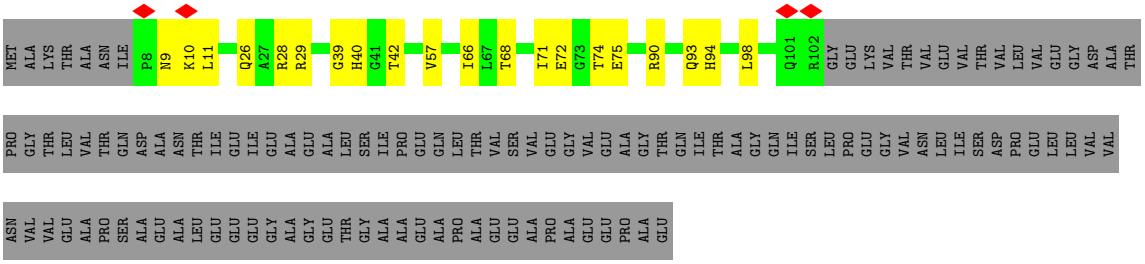

• Molecule 21: 50S ribosomal protein L24

Chain V:

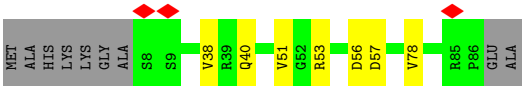

• Molecule 22: 50S ribosomal protein L25

Chain W:

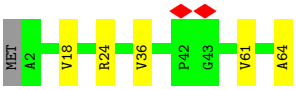

• Molecule 23: 50S ribosomal protein L27

Chain X:

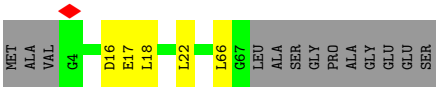

• Molecule 24: 50S Ribosomal Protein L28

Chain Y:

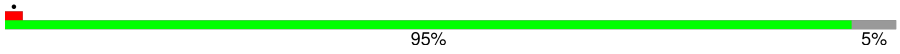

• Molecule 25: 50S ribosomal protein L29

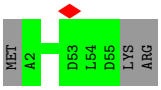
Chain Z:


• Molecule 26: 50S ribosomal protein L32

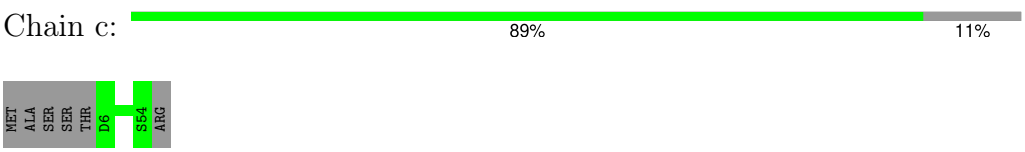
Chain b:



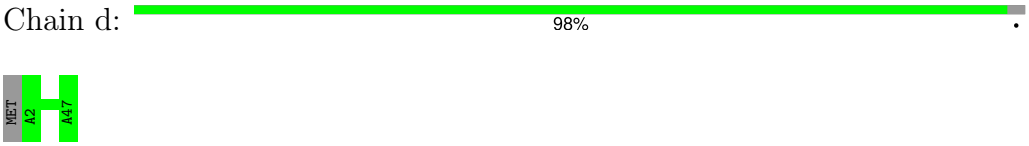

• Molecule 27: 50S Ribosomal Protein L33

Chain c:



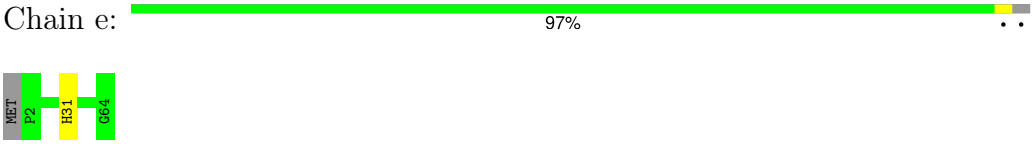

• Molecule 28: 50S ribosomal protein L34

Chain d:




• Molecule 29: 50S ribosomal protein L35

Chain e:



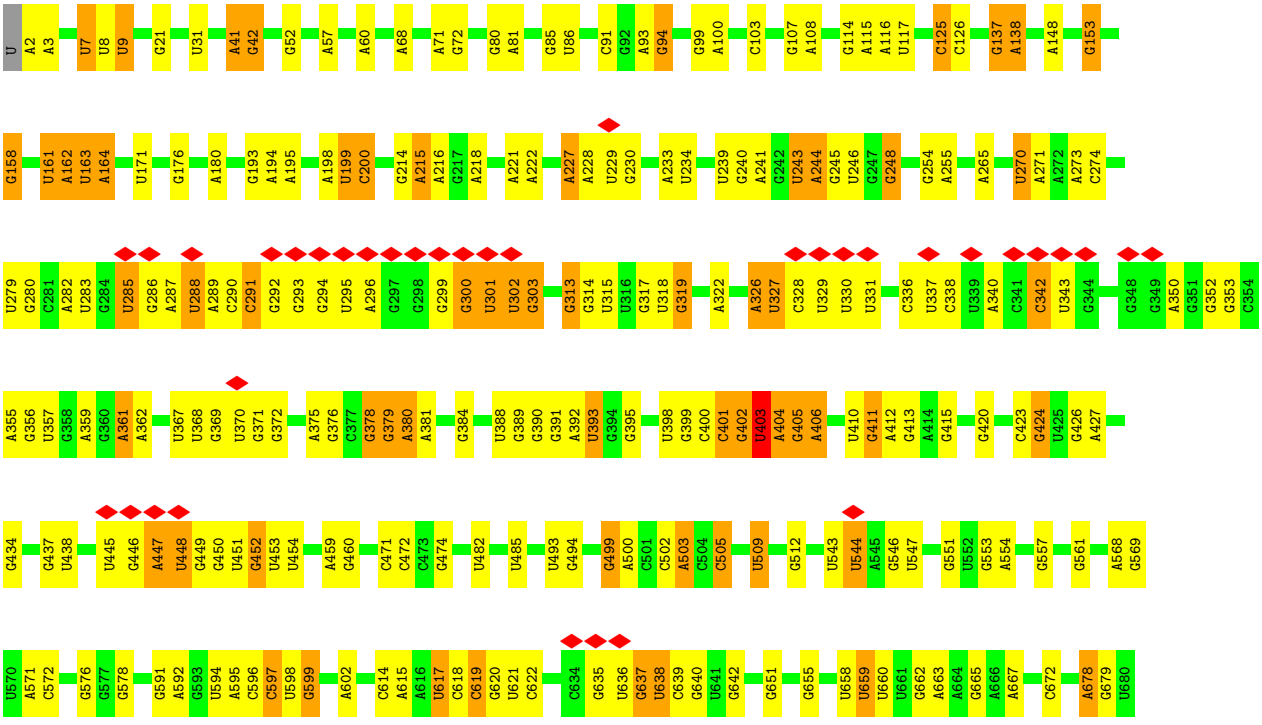

• Molecule 30: 50S ribosomal protein L36

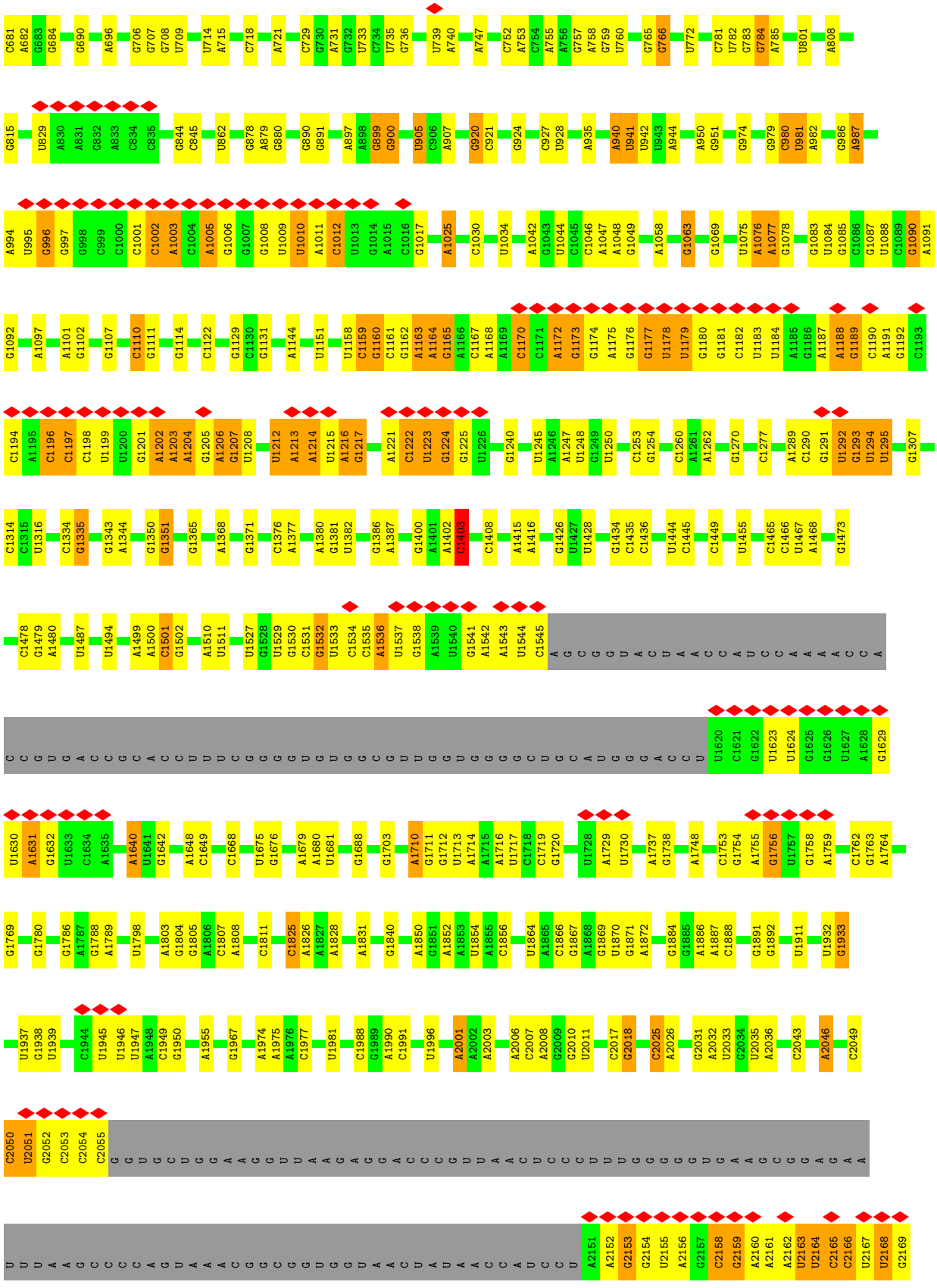
Chain f:

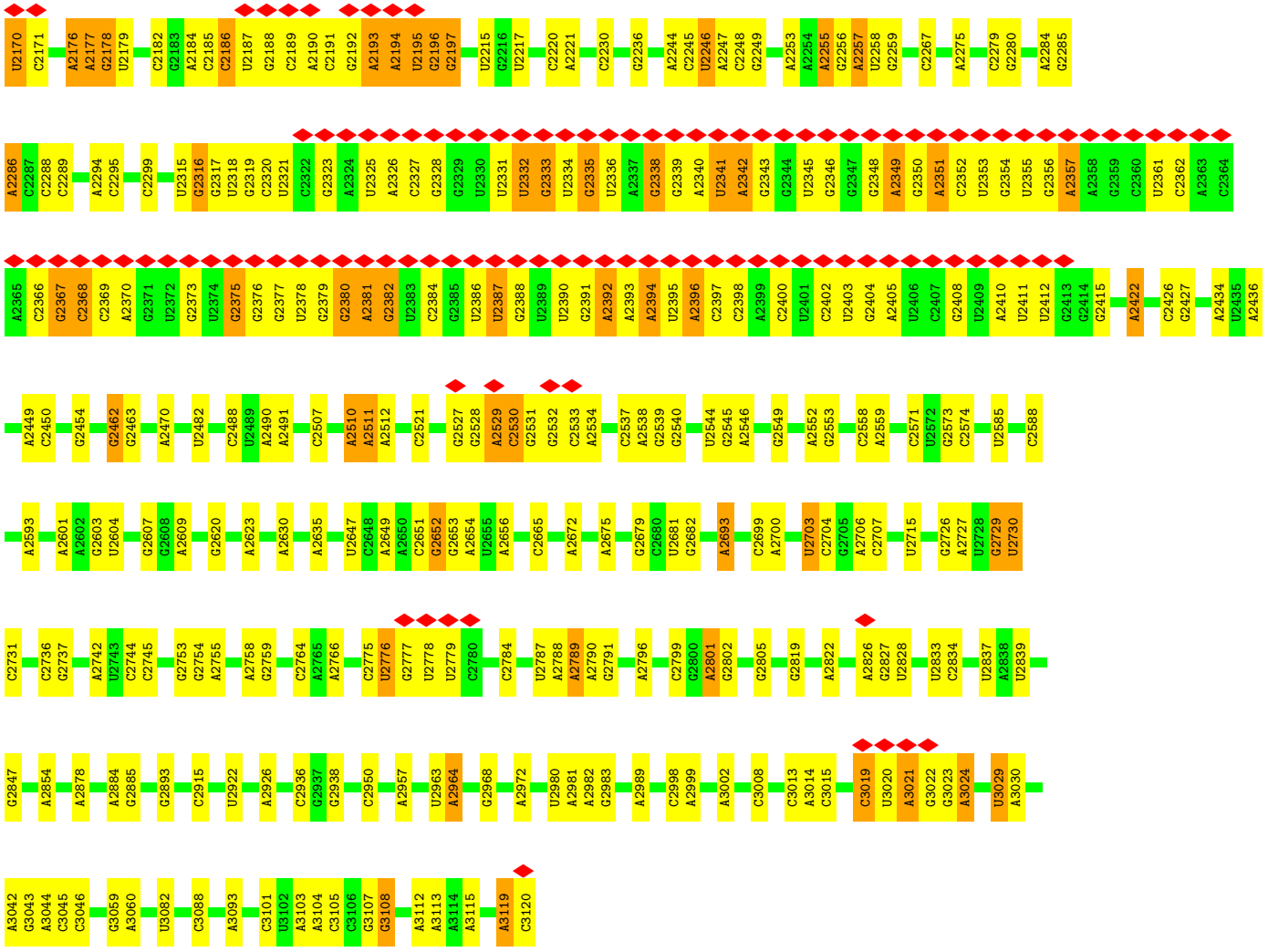

There are no outlier residues recorded for this chain.

• Molecule 31: 23S ribosomal RNA

Chain A:




U2170 C2171 A2176 A2177 G2178 U2179 C2182 G2183 A2184 C2185 C2186 U2187 G2188 C2189 A2190 C2191 G2192 A2193 A2194 U2195 G2196 G2197 U2215 G2216 U2217 C2220 A2221 C2230 G2236 A2244 C2245 U2246 A2247 C2248 G2249 A2253 A2254 A2255 G2256 A2257 U2258 G2259 C2267 A2275 C2279 G2280 A2284 G2285
A2286 C2287 C2288 C2289 A2294 C2295 C2299 U2315 G2316 G2317 U2318 G2319 C2320 U2321 C2322 G2323 A2324 U2325 A2326 C2327 G2328 G2329 U2330 U2331 U2332 G2333 U2334 G2335 U2336 A2337 G2338 G2339 A2340 U2341 A2342 G2343 G2344 U2345 G2346 G2347 G2348 A2349 G2350 A2351 C2352 U2353 G2354 U2355 G2356 A2357 A2358 G2359 C2360 U2361 C2362 A2363 C2364
A2365 C2366 G2367 C2368 C2369 A2370 G2371 U2372 G2373 U2374 G2375 G2376 G2377 U2378 G2379 G2380 A2381 G2382 U2383 C2384 G2385 U2386 U2387 G2388 U2389 U2390 G2391 A2392 A2393 A2394 U2395 A2396 C2397 C2398 A2399 C2400 U2401 C2402 U2403 G2404 A2405 U2406 C2407 G2408 U2409 A2410 U2411 U2412 C2413 G2414 G2415 A2422 C2426 G2427 A2434 U2435 A2436
A2449 C2450 G2454 G2462 G2463 A2470 U2482 C2488 U2489 A2490 A2491 C2507 A2510 A2511 A2512 C2521 G2527 G2528 A2529 C2530 G2531 G2532 C2533 A2534 C2537 A2538 G2539 G2540 U2544 G2545 A2546 G2549 A2552 G2553 C2558 A2559 C2571 U2572 G2573 C2574 U2585 C2588
A2593 A2601 A2602 G2603 U2604 G2607 G2608 A2609 G2620 A2623 A2630 A2635 U2647 C2648 A2649 A2650 C2651 G2652 G2653 A2654 U2655 A2656 C2665 A2672 A2675 G2679 C2680 U2681 G2682 A2693 C2699 A2700 U2703 C2704 G2705 A2706 C2707 U2715 G2726 A2727 U2728 G2729 U2730
C2731 C2736 G2737 A2742 U2743 C2744 C2745 G2753 G2754 A2755 A2758 G2759 C2764 A2765 A2766 C2775 U2776 G2777 U2778 U2779 C2780 C2784 U2787 A2788 A2789 A2790 C2791 A2796 C2799 G2800 A2801 G2802 G2805 G2819 A2822 A2826 G2827 U2828 U2833 C2834 U2837 A2838 U2839
G2847 A2854 A2878 A2884 G2885 G2893 C2915 U2922 A2926 C2936 G2937 G2938 C2950 A2957 U2963 A2964 G2968 A2972 U2980 A2981 A2982 G2983 A2989 C2998 A2999 A3002 C3008 C3013 A3014 C3015 C3019 U3020 A3021 G3022 G3023 A3024 U3029 A3030
A3042 G3043 A3044 C3045 C3046 G3059 A3060 U3082 C3088 A3093 C3101 U3102 A3103 A3104 C3105 C3106 G3107 G3108 A3112 A3113 A3114 A3115 A3119 C3120

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 116149 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 70.14 | Depositor |
| Minimum defocus (nm) | 800 | Depositor |
| Maximum defocus (nm) | 2500 | Depositor |
| Magnification | 105000 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 1.775 | Depositor |
| Minimum map value | -1.185 | Depositor |
| Average map value | 0.002 | Depositor |
| Map value standard deviation | 0.062 | Depositor |
| Recommended contour level | 0.2 | Depositor |
| Map size (Å) | 432.2816, 432.2816, 432.2816 | wwPDB |
| Map dimensions | 512, 512, 512 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.8443, 0.8443, 0.8443 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | 2 | 0.23 | 0/477 | 0.56 | 0/640 |
| 2 | 3 | 0.22 | 0/191 | 0.64 | 0/247 |
| 3 | 4 | 0.27 | 0/3484 | 0.57 | 0/4721 |
| 4 | B | 0.25 | 0/2821 | 0.85 | 0/4396 |
| 5 | C | 0.24 | 0/2153 | 0.58 | 0/2895 |
| 6 | D | 0.25 | 0/1609 | 0.55 | 0/2165 |
| 7 | E | 0.25 | 0/1592 | 0.50 | 0/2153 |
| 8 | G | 0.30 | 0/1369 | 0.61 | 1/1848 (0.1%) |
| 9 | H | 0.26 | 0/1027 | 0.49 | 0/1398 |
| 10 | I | 0.26 | 0/925 | 0.49 | 0/1246 |
| 11 | K | 0.25 | 0/1157 | 0.50 | 0/1567 |
| 12 | L | 0.25 | 0/946 | 0.58 | 0/1268 |
| 13 | M | 0.26 | 0/1091 | 0.55 | 0/1457 |
| 14 | N | 0.24 | 0/1118 | 0.53 | 0/1506 |
| 15 | O | 0.25 | 0/945 | 0.54 | 0/1267 |
| 16 | Q | 0.26 | 0/921 | 0.56 | 0/1236 |
| 17 | R | 0.25 | 0/1000 | 0.57 | 0/1341 |
| 18 | S | 0.24 | 0/764 | 0.50 | 0/1030 |
| 19 | T | 0.25 | 0/887 | 0.61 | 0/1204 |
| 20 | U | 0.27 | 0/766 | 0.55 | 0/1030 |
| 21 | V | 0.24 | 0/738 | 0.51 | 0/987 |
| 22 | W | 0.23 | 0/745 | 0.58 | 0/1008 |
| 23 | X | 0.25 | 0/595 | 0.59 | 0/798 |
| 24 | Y | 0.24 | 0/478 | 0.58 | 0/641 |
| 25 | Z | 0.26 | 0/534 | 0.59 | 0/713 |
| 26 | b | 0.22 | 0/427 | 0.61 | 0/572 |
| 27 | c | 0.25 | 0/413 | 0.56 | 0/553 |
| 28 | d | 0.24 | 0/380 | 0.75 | 0/500 |
| 29 | e | 0.25 | 0/507 | 0.66 | 0/672 |
| 30 | f | 0.26 | 0/303 | 0.59 | 0/401 |
| 31 | A | 0.25 | 1/70952 (0.0%) | 0.77 | 13/110707 (0.0%) |
| All | All | 0.25 | 1/101315 (0.0%) | 0.73 | 14/152167 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 31 | A | 2286 | A | O3'-P | -7.01 | 1.52 | 1.61 |

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 31 | A | 1719 | C | N3-C2-O2 | -7.03 | 116.98 | 121.90 |
| 31 | A | 1012 | C | N3-C2-O2 | -6.46 | 117.38 | 121.90 |
| 8 | G | 49 | GLY | N-CA-C | -6.31 | 97.34 | 113.10 |
| 31 | A | 1012 | C | N1-C2-O2 | 6.14 | 122.59 | 118.90 |
| 31 | A | 905 | U | C2-N1-C1' | 6.04 | 124.95 | 117.70 |
| 31 | A | 2245 | C | C2-N1-C1' | 5.99 | 125.38 | 118.80 |
| 31 | A | 1017 | G | N1-C6-O6 | -5.98 | 116.31 | 119.90 |
| 31 | A | 342 | C | N1-C2-O2 | 5.84 | 122.41 | 118.90 |
| 31 | A | 342 | C | N3-C2-O2 | -5.79 | 117.85 | 121.90 |
| 31 | A | 1403 | C | C2-N1-C1' | 5.77 | 125.15 | 118.80 |
| 31 | A | 403 | U | C2-N1-C1' | 5.33 | 124.09 | 117.70 |
| 31 | A | 3019 | C | N1-C2-O2 | 5.28 | 122.07 | 118.90 |
| 31 | A | 1428 | U | C2-N1-C1' | 5.14 | 123.86 | 117.70 |
| 31 | A | 1017 | G | C5-C6-O6 | 5.08 | 131.65 | 128.60 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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 | 2 | 474 | 0 | 500 | 7 | 0 |
| 2 | 3 | 189 | 0 | 205 | 1 | 0 |
| 3 | 4 | 3444 | 0 | 3500 | 118 | 0 |
| 4 | B | 2522 | 0 | 1285 | 21 | 0 |
| 5 | C | 2110 | 0 | 2165 | 22 | 0 |
| 6 | D | 1587 | 0 | 1630 | 13 | 0 |
| 7 | E | 1569 | 0 | 1607 | 16 | 0 |
| 8 | G | 1348 | 0 | 1399 | 49 | 0 |
| 9 | H | 1018 | 0 | 988 | 29 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 10 | I | 918 | 0 | 959 | 67 | 0 |
| 11 | K | 1130 | 0 | 1167 | 6 | 0 |
| 12 | L | 938 | 0 | 1000 | 6 | 0 |
| 13 | M | 1078 | 0 | 1151 | 16 | 0 |
| 14 | N | 1092 | 0 | 1128 | 5 | 0 |
| 15 | O | 928 | 0 | 972 | 7 | 0 |
| 16 | Q | 907 | 0 | 938 | 4 | 0 |
| 17 | R | 988 | 0 | 1038 | 14 | 0 |
| 18 | S | 754 | 0 | 802 | 6 | 0 |
| 19 | T | 873 | 0 | 909 | 7 | 0 |
| 20 | U | 756 | 0 | 802 | 7 | 0 |
| 21 | V | 732 | 0 | 782 | 7 | 0 |
| 22 | W | 735 | 0 | 756 | 13 | 0 |
| 23 | X | 586 | 0 | 601 | 5 | 0 |
| 24 | Y | 470 | 0 | 484 | 3 | 0 |
| 25 | Z | 531 | 0 | 541 | 4 | 0 |
| 26 | b | 423 | 0 | 463 | 0 | 0 |
| 27 | c | 405 | 0 | 411 | 0 | 0 |
| 28 | d | 377 | 0 | 411 | 0 | 0 |
| 29 | e | 502 | 0 | 541 | 0 | 0 |
| 30 | f | 299 | 0 | 324 | 0 | 0 |
| 31 | A | 63364 | 0 | 31879 | 384 | 0 |
| 32 | 4 | 32 | 0 | 14 | 3 | 0 |
| 33 | A | 20 | 0 | 11 | 4 | 0 |
| All | All | 93099 | 0 | 61363 | 777 | 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 5.

All (777) 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) |
|---|---|---|---|
| 8:G:7:GLN:O | 8:G:51:ILE:HD12 | 1.03 | 1.19 |
| 8:G:7:GLN:C | 8:G:51:ILE:HD12 | 1.64 | 1.16 |
| 8:G:7:GLN:O | 8:G:51:ILE:CD1 | 1.96 | 1.12 |
| 8:G:8:PRO:HA | 8:G:51:ILE:CD1 | 1.80 | 1.11 |
| 8:G:51:ILE:HB | 8:G:53:VAL:HG22 | 1.35 | 1.08 |
| 8:G:8:PRO:HA | 8:G:51:ILE:HD13 | 1.12 | 1.08 |
| 8:G:7:GLN:C | 8:G:51:ILE:CD1 | 2.28 | 1.00 |
| 17:R:77:ASN:OD1 | 31:A:1270:G:O2' | 1.80 | 1.00 |
| 8:G:8:PRO:CA | 8:G:51:ILE:CD1 | 2.41 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:A:163:U:O2' | 31:A:164:A:O4' | 1.82 | 0.97 |
| 21:V:94:LYS:NZ | 31:A:80:G:OP1 | 1.98 | 0.95 |
| 31:A:163:U:O2' | 31:A:164:A:O5' | 1.89 | 0.91 |
| 8:G:8:PRO:CA | 8:G:51:ILE:HD13 | 1.99 | 0.89 |
| 3:4:255:ASN:HA | 32:4:501:GCP:O1B | 1.71 | 0.89 |
| 17:R:33:ARG:NH2 | 31:A:672:C:OP1 | 2.05 | 0.89 |
| 13:M:84:ASN:ND2 | 13:M:117:LYS:O | 2.07 | 0.88 |
| 31:A:1710:A:N6 | 31:A:1716:A:OP2 | 2.06 | 0.88 |
| 21:V:94:LYS:NZ | 31:A:378:G:OP1 | 2.07 | 0.87 |
| 31:A:635:G:N2 | 31:A:635:G:OP2 | 2.07 | 0.86 |
| 1:2:4:LEU:HD21 | 1:2:47:ILE:HD11 | 1.56 | 0.86 |
| 3:4:56:THR:OG1 | 3:4:57:GLU:OE1 | 1.93 | 0.85 |
| 3:4:392:VAL:HG23 | 3:4:398:ASP:HB3 | 1.55 | 0.85 |
| 31:A:1203:A:O2' | 31:A:1204:A:O5' | 1.91 | 0.85 |
| 31:A:2255:A:N3 | 31:A:2679:G:O2' | 2.09 | 0.85 |
| 31:A:2257:A:O2' | 31:A:2259:G:OP2 | 1.95 | 0.84 |
| 31:A:1854:U:O2' | 31:A:1977:C:O2' | 1.95 | 0.84 |
| 9:H:58:VAL:O | 9:H:111:ASN:ND2 | 2.12 | 0.83 |
| 11:K:125:TYR:HH | 11:K:132:HIS:HE2 | 1.18 | 0.82 |
| 31:A:1996:U:OP2 | 31:A:2001:A:N6 | 2.11 | 0.82 |
| 10:I:58:LYS:O | 10:I:62:SER:OG | 1.96 | 0.82 |
| 31:A:980:C:O2' | 31:A:981:U:O5' | 1.96 | 0.81 |
| 31:A:1170:C:N4 | 31:A:1225:G:O6 | 2.11 | 0.81 |
| 10:I:49:TYR:OH | 31:A:1203:A:N6 | 2.14 | 0.81 |
| 31:A:291:C:N4 | 31:A:293:G:O6 | 2.13 | 0.80 |
| 31:A:2805:G:N2 | 31:A:2805:G:OP2 | 2.14 | 0.80 |
| 8:G:45:ARG:O | 8:G:52:VAL:HB | 1.82 | 0.80 |
| 8:G:8:PRO:N | 8:G:51:ILE:CD1 | 2.43 | 0.80 |
| 31:A:447:A:O2' | 31:A:448:U:O4' | 1.99 | 0.80 |
| 10:I:21:THR:HG22 | 10:I:22:ALA:H | 1.46 | 0.79 |
| 31:A:2366:C:O2' | 31:A:2368:C:N4 | 2.16 | 0.79 |
| 10:I:28:TYR:OH | 31:A:1225:G:O4' | 1.99 | 0.78 |
| 6:D:40:ARG:NH1 | 6:D:83:GLU:OE2 | 2.17 | 0.78 |
| 8:G:53:VAL:HG23 | 8:G:66:HIS:CE1 | 2.19 | 0.78 |
| 8:G:20:ASN:O | 8:G:20:ASN:ND2 | 2.13 | 0.77 |
| 3:4:201:ARG:O | 3:4:204:GLY:N | 2.17 | 0.77 |
| 31:A:499:G:OP2 | 31:A:2630:A:O2' | 2.02 | 0.77 |
| 10:I:93:ILE:HD12 | 10:I:105:ILE:HG21 | 1.67 | 0.76 |
| 31:A:218:A:N3 | 31:A:234:U:O2' | 2.17 | 0.76 |
| 31:A:1530:G:H21 | 31:A:1805:G:H22 | 1.34 | 0.76 |
| 31:A:103:C:HO2' | 31:A:375:A:HO2' | 1.33 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:A:1426:G:OP2 | 31:A:1426:G:N2 | 2.16 | 0.75 |
| 31:A:2482:U:O2' | 31:A:2651:C:OP2 | 2.04 | 0.75 |
| 3:4:384:ARG:HD3 | 3:4:391:PHE:HE2 | 1.51 | 0.74 |
| 31:A:1825:C:N4 | 31:A:1840:G:OP2 | 2.19 | 0.74 |
| 31:A:2527:G:C6 | 31:A:2538:A:N6 | 2.56 | 0.74 |
| 6:D:38:ARG:NH2 | 31:A:3008:C:O2' | 2.20 | 0.74 |
| 8:G:5:GLY:O | 8:G:51:ILE:HG21 | 1.88 | 0.74 |
| 10:I:72:LEU:HD22 | 10:I:115:LEU:HD21 | 1.70 | 0.73 |
| 3:4:203:PRO:O | 3:4:207:LYS:N | 2.22 | 0.73 |
| 17:R:8:LEU:HD23 | 17:R:8:LEU:O | 1.88 | 0.73 |
| 20:U:68:ARG:NH2 | 31:A:1449:C:OP1 | 2.21 | 0.73 |
| 31:A:1758:G:O2' | 31:A:1759:A:O4' | 2.06 | 0.73 |
| 13:M:84:ASN:OD1 | 13:M:85:LYS:N | 2.22 | 0.73 |
| 22:W:9:ASN:ND2 | 22:W:66:ILE:O | 2.21 | 0.73 |
| 8:G:51:ILE:O | 8:G:52:VAL:C | 2.27 | 0.73 |
| 31:A:1533:U:OP2 | 31:A:1536:A:N6 | 2.21 | 0.72 |
| 10:I:48:THR:HG23 | 10:I:49:TYR:H | 1.53 | 0.72 |
| 31:A:285:U:O2' | 31:A:287:A:OP1 | 2.06 | 0.72 |
| 7:E:128:THR:HG22 | 7:E:129:GLU:H | 1.53 | 0.72 |
| 31:A:815:G:O2' | 31:A:1850:A:N3 | 2.19 | 0.72 |
| 8:G:48:ASP:OD1 | 8:G:50:ALA:N | 2.22 | 0.72 |
| 8:G:51:ILE:HD13 | 8:G:51:ILE:H | 1.55 | 0.71 |
| 15:O:96:ARG:NH1 | 31:A:3103:A:OP1 | 2.22 | 0.71 |
| 10:I:10:VAL:HG22 | 10:I:56:LEU:HD11 | 1.72 | 0.71 |
| 31:A:2375:G:O2' | 31:A:2376:G:O4' | 2.04 | 0.71 |
| 31:A:544:U:O2 | 31:A:547:U:O2' | 2.09 | 0.71 |
| 31:A:980:C:HO2' | 31:A:981:U:P | 2.13 | 0.71 |
| 31:A:1196:C:O2' | 31:A:1197:C:O5' | 2.09 | 0.71 |
| 10:I:119:ASP:OD1 | 10:I:122:LYS:NZ | 2.24 | 0.70 |
| 15:O:106:ASP:OD2 | 31:A:1867:G:O2' | 2.10 | 0.70 |
| 3:4:384:ARG:HD3 | 3:4:391:PHE:CE2 | 2.25 | 0.70 |
| 8:G:8:PRO:N | 8:G:51:ILE:HD11 | 2.04 | 0.70 |
| 3:4:331:VAL:HG22 | 3:4:367:VAL:HB | 1.73 | 0.70 |
| 10:I:50:THR:HG22 | 10:I:50:THR:O | 1.92 | 0.70 |
| 1:2:11:SER:OG | 31:A:1107:G:OP2 | 2.09 | 0.69 |
| 31:A:2163:U:O2' | 31:A:2164:U:N3 | 2.25 | 0.69 |
| 7:E:137:SER:O | 7:E:168:SER:OG | 2.10 | 0.69 |
| 31:A:392:A:O2' | 31:A:393:U:OP2 | 2.06 | 0.69 |
| 31:A:1174:G:N2 | 31:A:1222:C:N3 | 2.40 | 0.69 |
| 31:A:378:G:O2' | 31:A:424:G:N1 | 2.25 | 0.69 |
| 31:A:1545:C:N4 | 31:A:1623:U:O2 | 2.26 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:4:17:LEU:O | 3:4:17:LEU:HD23 | 1.93 | 0.69 |
| 3:4:433:VAL:HG11 | 3:4:451:ILE:HD13 | 1.75 | 0.69 |
| 31:A:2754:G:OP2 | 31:A:2759:G:N2 | 2.26 | 0.69 |
| 31:A:1174:G:O2' | 31:A:1204:A:O2' | 2.04 | 0.68 |
| 7:E:41:GLN:NE2 | 7:E:184:ASN:OD1 | 2.26 | 0.68 |
| 10:I:59:ARG:NH1 | 31:A:1164:A:O4' | 2.27 | 0.68 |
| 31:A:1932:U:O2' | 31:A:1933:G:OP1 | 2.12 | 0.68 |
| 3:4:45:ARG:NH1 | 3:4:79:SER:O | 2.27 | 0.67 |
| 5:C:209:ALA:HB2 | 31:A:2007:C:O2' | 1.95 | 0.67 |
| 3:4:132:LEU:O | 3:4:132:LEU:HD23 | 1.94 | 0.67 |
| 4:B:35:G:O2' | 4:B:45:G:N7 | 2.24 | 0.67 |
| 31:A:2253:A:N6 | 31:A:2257:A:OP2 | 2.22 | 0.67 |
| 31:A:245:G:O2' | 31:A:246:U:H5' | 1.95 | 0.67 |
| 1:2:24:ARG:NH2 | 31:A:1044:U:O2 | 2.27 | 0.67 |
| 12:L:7:ARG:NE | 12:L:18:GLU:OE2 | 2.27 | 0.67 |
| 10:I:59:ARG:NH2 | 31:A:1164:A:OP1 | 2.28 | 0.66 |
| 31:A:1177:G:N2 | 31:A:1199:U:O4 | 2.29 | 0.66 |
| 8:G:140:GLN:OE1 | 31:A:2983:G:N2 | 2.28 | 0.66 |
| 1:2:4:LEU:HD21 | 1:2:47:ILE:CD1 | 2.24 | 0.65 |
| 3:4:93:ASP:OD1 | 3:4:96:THR:O | 2.14 | 0.65 |
| 31:A:283:U:O2 | 31:A:303:G:O6 | 2.13 | 0.65 |
| 6:D:7:LEU:HD23 | 6:D:207:VAL:HG22 | 1.77 | 0.65 |
| 31:A:3043:G:O2' | 31:A:3045:C:OP2 | 2.11 | 0.65 |
| 31:A:103:C:O2' | 31:A:375:A:O2' | 2.02 | 0.65 |
| 9:H:38:VAL:HG13 | 9:H:38:VAL:O | 1.97 | 0.65 |
| 10:I:40:ARG:NH2 | 10:I:48:THR:OG1 | 2.30 | 0.65 |
| 31:A:7:U:O2' | 31:A:8:U:O4' | 2.15 | 0.65 |
| 3:4:148:LEU:HD23 | 3:4:311:LEU:HD11 | 1.79 | 0.64 |
| 3:4:370:LYS:HA | 32:4:501:GCP:O6 | 1.97 | 0.64 |
| 22:W:26:GLN:OE1 | 22:W:29:ARG:NH2 | 2.30 | 0.64 |
| 22:W:28:ARG:NH1 | 22:W:93:GLN:O | 2.30 | 0.64 |
| 9:H:124:ILE:HG22 | 9:H:124:ILE:O | 1.97 | 0.64 |
| 10:I:54:ASN:ND2 | 10:I:77:THR:O | 2.29 | 0.64 |
| 3:4:208:ILE:O | 3:4:209:GLU:C | 2.36 | 0.64 |
| 10:I:31:LEU:HD12 | 10:I:31:LEU:O | 1.97 | 0.63 |
| 10:I:51:VAL:HG23 | 10:I:78:ALA:HB1 | 1.80 | 0.63 |
| 31:A:2801:A:H5' | 31:A:2802:G:C5' | 2.28 | 0.63 |
| 31:A:2529:A:O2' | 31:A:2530:C:O5' | 2.15 | 0.63 |
| 31:A:1198:C:N4 | 31:A:1206:A:OP1 | 2.31 | 0.63 |
| 17:R:77:ASN:ND2 | 31:A:1270:G:N3 | 2.47 | 0.63 |
| 3:4:90:ASP:OD1 | 3:4:91:LYS:N | 2.32 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:B:76:G:H21 | 22:W:94:HIS:CD2 | 2.17 | 0.62 |
| 8:G:51:ILE:HG12 | 8:G:52:VAL:H | 1.63 | 0.62 |
| 13:M:82:ASP:OD1 | 13:M:83:ILE:N | 2.32 | 0.62 |
| 31:A:2351:A:O2' | 31:A:2352:C:O5' | 2.14 | 0.62 |
| 31:A:287:A:OP2 | 31:A:299:G:N2 | 2.33 | 0.62 |
| 3:4:142:ASP:OD2 | 3:4:171:TYR:OH | 2.17 | 0.62 |
| 3:4:163:GLN:NE2 | 3:4:313:GLU:O | 2.32 | 0.62 |
| 31:A:1668:C:O2' | 31:A:1764:A:N3 | 2.32 | 0.62 |
| 31:A:1886:A:N3 | 31:A:1888:C:N4 | 2.47 | 0.61 |
| 21:V:9:VAL:HB | 21:V:71:VAL:HG13 | 1.82 | 0.61 |
| 31:A:2328:G:N1 | 31:A:2408:G:O6 | 2.33 | 0.61 |
| 8:G:51:ILE:CB | 8:G:53:VAL:HG22 | 2.20 | 0.61 |
| 10:I:21:THR:HG22 | 10:I:22:ALA:N | 2.15 | 0.61 |
| 31:A:153:G:O6 | 31:A:171:U:O2 | 2.18 | 0.61 |
| 31:A:2538:A:H2' | 31:A:2539:G:O4' | 2.01 | 0.61 |
| 3:4:432:ARG:HA | 3:4:435:THR:HG22 | 1.83 | 0.60 |
| 4:B:15:U:OP2 | 4:B:71:C:O2' | 2.19 | 0.60 |
| 3:4:392:VAL:CG2 | 3:4:398:ASP:HB3 | 2.31 | 0.60 |
| 31:A:2332:U:O4 | 31:A:2394:A:O2' | 2.16 | 0.60 |
| 5:C:158:SER:O | 5:C:196:VAL:HG11 | 2.00 | 0.60 |
| 20:U:62:ARG:NH2 | 31:A:1455:U:OP2 | 2.35 | 0.60 |
| 31:A:2727:A:O2' | 31:A:2729:G:OP2 | 2.19 | 0.60 |
| 31:A:176:G:N2 | 31:A:176:G:OP2 | 2.30 | 0.60 |
| 4:B:29:C:O2' | 4:B:60:G:N2 | 2.35 | 0.60 |
| 10:I:117:VAL:HG13 | 10:I:118:ALA:H | 1.65 | 0.60 |
| 31:A:2244:A:O2' | 31:A:2246:U:OP2 | 2.13 | 0.60 |
| 3:4:253:TYR:O | 3:4:258:LYS:NZ | 2.35 | 0.60 |
| 20:U:36:ASP:OD1 | 20:U:36:ASP:O | 2.20 | 0.60 |
| 3:4:32:GLU:HG2 | 3:4:80:GLU:OE2 | 2.02 | 0.59 |
| 8:G:53:VAL:HG23 | 8:G:66:HIS:HE1 | 1.64 | 0.59 |
| 12:L:42:THR:HG21 | 31:A:2176:A:OP1 | 2.01 | 0.59 |
| 19:T:73:PRO:O | 19:T:74:SER:OG | 2.12 | 0.59 |
| 3:4:161:LYS:NZ | 31:A:2707:C:OP1 | 2.34 | 0.59 |
| 4:B:111:C:H2' | 4:B:112:C:H5' | 1.84 | 0.59 |
| 3:4:84:GLY:O | 3:4:86:ILE:HD12 | 2.02 | 0.59 |
| 31:A:1478:C:O2' | 31:A:2026:A:N3 | 2.30 | 0.59 |
| 31:A:2422:A:N1 | 31:A:2450:C:N4 | 2.50 | 0.59 |
| 3:4:429:LEU:O | 3:4:433:VAL:HG23 | 2.03 | 0.59 |
| 6:D:135:GLN:HE21 | 31:A:2802:G:H21 | 1.49 | 0.59 |
| 10:I:21:THR:HG21 | 10:I:82:VAL:HG13 | 1.85 | 0.59 |
| 20:U:26:ASP:OD1 | 20:U:26:ASP:O | 2.21 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:4:393:SER:H | 3:4:398:ASP:CB | 2.16 | 0.59 |
| 10:I:16:GLN:O | 10:I:16:GLN:NE2 | 2.35 | 0.59 |
| 8:G:80:VAL:HG12 | 8:G:80:VAL:O | 2.03 | 0.59 |
| 8:G:119:PRO:O | 8:G:122:ILE:HG22 | 2.03 | 0.58 |
| 3:4:93:ASP:O | 3:4:95:SER:N | 2.35 | 0.58 |
| 3:4:366:LEU:HD23 | 3:4:388:ASP:O | 2.02 | 0.58 |
| 31:A:1076:A:O2' | 31:A:1077:A:O5' | 2.14 | 0.58 |
| 31:A:2335:G:O6 | 31:A:2392:A:N6 | 2.35 | 0.58 |
| 31:A:2179:U:O2' | 31:A:2776:U:OP1 | 2.21 | 0.58 |
| 31:A:3014:A:H62 | 31:A:3113:A:H2 | 1.50 | 0.58 |
| 11:K:24:VAL:HG12 | 11:K:27:ARG:HD2 | 1.84 | 0.58 |
| 8:G:7:GLN:C | 8:G:51:ILE:HD11 | 2.21 | 0.58 |
| 8:G:51:ILE:C | 8:G:53:VAL:N | 2.50 | 0.58 |
| 1:2:4:LEU:CD2 | 1:2:47:ILE:HD11 | 2.31 | 0.58 |
| 3:4:151:PHE:HE2 | 3:4:311:LEU:HD13 | 1.69 | 0.58 |
| 3:4:449:THR:HB | 3:4:451:ILE:HG23 | 1.86 | 0.58 |
| 3:4:151:PHE:CE2 | 3:4:311:LEU:HD13 | 2.39 | 0.58 |
| 10:I:10:VAL:CG2 | 10:I:56:LEU:HD11 | 2.34 | 0.57 |
| 8:G:122:ILE:HD11 | 8:G:134:VAL:CG1 | 2.34 | 0.57 |
| 15:O:10:LEU:HD21 | 15:O:40:LYS:HG2 | 1.85 | 0.57 |
| 23:X:53:ARG:NH1 | 23:X:57:ASP:OD1 | 2.36 | 0.57 |
| 31:A:2819:G:N2 | 31:A:2822:A:OP2 | 2.34 | 0.57 |
| 14:N:23:GLY:O | 14:N:101:ARG:NH2 | 2.37 | 0.57 |
| 3:4:393:SER:C | 3:4:395:ARG:H | 2.07 | 0.57 |
| 18:S:22:VAL:HG12 | 18:S:24:VAL:HG13 | 1.87 | 0.57 |
| 3:4:39:VAL:HG23 | 3:4:39:VAL:O | 2.05 | 0.57 |
| 3:4:87:GLN:NE2 | 3:4:88:ARG:O | 2.37 | 0.57 |
| 5:C:271:ARG:NH2 | 5:C:274:THR:HG21 | 2.19 | 0.57 |
| 8:G:20:ASN:HD22 | 8:G:20:ASN:C | 2.04 | 0.57 |
| 31:A:1530:G:N2 | 31:A:1805:G:H22 | 2.00 | 0.57 |
| 10:I:69:LEU:HD11 | 10:I:73:PHE:CZ | 2.40 | 0.56 |
| 3:4:329:ILE:HG23 | 3:4:367:VAL:HG23 | 1.85 | 0.56 |
| 4:B:78:U:OP1 | 22:W:28:ARG:NH2 | 2.38 | 0.56 |
| 8:G:8:PRO:CA | 8:G:51:ILE:HD11 | 2.28 | 0.56 |
| 31:A:161:U:O2' | 31:A:162:A:OP2 | 2.19 | 0.56 |
| 31:A:1063:G:O6 | 31:A:1090:G:N2 | 2.39 | 0.56 |
| 13:M:125:THR:HG23 | 13:M:125:THR:O | 2.05 | 0.56 |
| 31:A:2176:A:N3 | 31:A:2784:C:O2' | 2.36 | 0.56 |
| 31:A:2170:U:O2' | 31:A:2185:C:O2 | 2.18 | 0.56 |
| 13:M:22:VAL:HB | 13:M:33:ALA:HB1 | 1.88 | 0.56 |
| 5:C:273:ARG:O | 5:C:274:THR:OG1 | 2.18 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:4:83:GLU:OE2 | 3:4:85:LEU:HD21 | 2.07 | 0.55 |
| 9:H:11:HIS:NE2 | 31:A:2318:U:O3' | 2.39 | 0.55 |
| 12:L:66:VAL:HG22 | 12:L:66:VAL:O | 2.07 | 0.55 |
| 31:A:401:C:O2' | 31:A:415:G:N2 | 2.40 | 0.55 |
| 31:A:678:A:N1 | 31:A:924:G:O2' | 2.36 | 0.55 |
| 31:A:199:U:O2' | 31:A:200:C:OP1 | 2.20 | 0.55 |
| 31:A:3020:U:O2' | 31:A:3021:A:O5' | 2.24 | 0.55 |
| 31:A:2573:G:O6 | 31:A:2593:A:N6 | 2.40 | 0.55 |
| 31:A:2745:C:O2' | 31:A:2788:A:N3 | 2.37 | 0.55 |
| 9:H:135:LYS:O | 9:H:136:LEU:HD12 | 2.06 | 0.55 |
| 31:A:941:U:OP1 | 31:A:2652:G:H3' | 2.06 | 0.55 |
| 31:A:1172:A:N6 | 31:A:1224:G:O6 | 2.40 | 0.55 |
| 31:A:402:G:N3 | 31:A:405:G:N1 | 2.55 | 0.55 |
| 31:A:1756:G:O5' | 31:A:1758:G:N2 | 2.40 | 0.55 |
| 3:4:393:SER:H | 3:4:398:ASP:HB2 | 1.72 | 0.54 |
| 3:4:32:GLU:O | 3:4:82:LEU:HA | 2.08 | 0.54 |
| 9:H:21:VAL:HG21 | 9:H:25:TYR:CD2 | 2.42 | 0.54 |
| 31:A:287:A:O2' | 31:A:288:U:O4' | 2.24 | 0.54 |
| 3:4:168:GLN:HB3 | 3:4:208:ILE:HG13 | 1.89 | 0.54 |
| 31:A:2730:U:H3' | 31:A:2730:U:O2 | 2.08 | 0.54 |
| 31:A:114:G:OP2 | 31:A:116:A:O2' | 2.20 | 0.54 |
| 31:A:2333:G:OP1 | 31:A:2341:U:N3 | 2.40 | 0.54 |
| 9:H:135:LYS:C | 9:H:136:LEU:HD12 | 2.28 | 0.54 |
| 17:R:4:VAL:HG22 | 31:A:1314:C:H1' | 1.89 | 0.54 |
| 22:W:10:LYS:H | 22:W:68:THR:HG1 | 1.54 | 0.54 |
| 3:4:429:LEU:HD21 | 3:4:463:LEU:HD21 | 1.90 | 0.54 |
| 3:4:344:ASN:O | 3:4:348:THR:HG23 | 2.07 | 0.54 |
| 31:A:1381:G:O2' | 31:A:2236:G:O6 | 2.23 | 0.54 |
| 5:C:145:VAL:HG23 | 5:C:155:LEU:HD12 | 1.90 | 0.53 |
| 5:C:161:VAL:O | 5:C:196:VAL:HG12 | 2.09 | 0.53 |
| 8:G:45:ARG:HG3 | 8:G:46:ALA:H | 1.73 | 0.53 |
| 5:C:2:GLY:N | 5:C:20:ASP:OD1 | 2.41 | 0.53 |
| 11:K:116:ARG:NH2 | 31:A:615:A:OP2 | 2.41 | 0.53 |
| 23:X:51:VAL:HG21 | 23:X:78:VAL:O | 2.08 | 0.53 |
| 31:A:940:A:H2' | 31:A:941:U:O4' | 2.08 | 0.53 |
| 31:A:2338:G:N1 | 31:A:2342:A:OP1 | 2.42 | 0.53 |
| 3:4:262:LEU:HD22 | 3:4:299:ASP:OD2 | 2.09 | 0.53 |
| 31:A:597:C:O2' | 31:A:1351:G:OP1 | 2.21 | 0.53 |
| 31:A:1291:G:H2' | 31:A:1292:U:H4' | 1.90 | 0.53 |
| 31:A:1479:G:HO2' | 31:A:2025:C:H5 | 1.57 | 0.53 |
| 31:A:2801:A:H5' | 31:A:2802:G:H5' | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:R:83:LEU:HD22 | 17:R:88:VAL:HG11 | 1.91 | 0.53 |
| 31:A:2357:A:H8 | 31:A:2380:G:H21 | 1.56 | 0.53 |
| 9:H:122:ALA:HB3 | 9:H:124:ILE:HD11 | 1.90 | 0.53 |
| 7:E:52:THR:HG22 | 7:E:53:LYS:H | 1.74 | 0.52 |
| 8:G:17:VAL:O | 8:G:17:VAL:HG23 | 2.08 | 0.52 |
| 10:I:51:VAL:HG23 | 10:I:78:ALA:CB | 2.39 | 0.52 |
| 10:I:97:ALA:HB1 | 10:I:104:VAL:HA | 1.91 | 0.52 |
| 22:W:40:HIS:ND1 | 22:W:40:HIS:O | 2.43 | 0.52 |
| 31:A:1292:U:O2' | 31:A:1293:G:O5' | 2.23 | 0.52 |
| 6:D:156:THR:HB | 6:D:157:PRO:HD3 | 1.90 | 0.52 |
| 31:A:1188:A:H3' | 31:A:1189:G:H3' | 1.90 | 0.52 |
| 20:U:93:ILE:HG21 | 20:U:96:PHE:CE2 | 2.44 | 0.52 |
| 3:4:200:THR:O | 3:4:201:ARG:HG2 | 2.09 | 0.52 |
| 10:I:26:THR:HB | 10:I:103:LEU:HA | 1.90 | 0.52 |
| 31:A:808:A:O2' | 31:A:1468:A:N3 | 2.39 | 0.52 |
| 31:A:1402:A:O2' | 31:A:1403:C:O5' | 2.27 | 0.52 |
| 31:A:2528:G:N2 | 31:A:2537:C:O2 | 2.42 | 0.52 |
| 10:I:47:ALA:HB1 | 10:I:80:ALA:HB1 | 1.91 | 0.52 |
| 10:I:25:VAL:HB | 10:I:77:THR:HB | 1.91 | 0.52 |
| 10:I:56:LEU:HD13 | 31:A:1164:A:H1' | 1.92 | 0.52 |
| 31:A:2799:C:H6 | 31:A:2799:C:O5' | 1.93 | 0.52 |
| 31:A:1991:C:H2' | 31:A:1991:C:O2 | 2.09 | 0.52 |
| 3:4:27:ALA:HA | 3:4:85:LEU:HD23 | 1.91 | 0.51 |
| 3:4:365:LEU:HD12 | 3:4:388:ASP:HB2 | 1.92 | 0.51 |
| 10:I:117:VAL:HG13 | 10:I:118:ALA:N | 2.25 | 0.51 |
| 10:I:24:VAL:HG23 | 10:I:82:VAL:HG12 | 1.92 | 0.51 |
| 10:I:47:ALA:CB | 10:I:80:ALA:HB1 | 2.40 | 0.51 |
| 31:A:300:G:H22 | 31:A:303:G:H5' | 1.76 | 0.51 |
| 31:A:1206:A:O2' | 31:A:1207:G:OP1 | 2.22 | 0.51 |
| 8:G:158:TYR:O | 8:G:160:GLY:N | 2.43 | 0.51 |
| 9:H:88:THR:O | 9:H:88:THR:HG22 | 2.11 | 0.51 |
| 10:I:46:SER:HB2 | 10:I:82:VAL:HG23 | 1.92 | 0.51 |
| 31:A:301:U:O2' | 31:A:302:U:OP1 | 2.23 | 0.51 |
| 31:A:2230:C:O2' | 31:A:3044:A:N3 | 2.43 | 0.51 |
| 10:I:90:ALA:O | 10:I:94:LYS:HG2 | 2.11 | 0.51 |
| 31:A:2544:U:O2 | 31:A:2545:G:N1 | 2.42 | 0.51 |
| 3:4:390:VAL:HG22 | 3:4:391:PHE:N | 2.26 | 0.51 |
| 9:H:90:LYS:C | 9:H:91:LEU:HD12 | 2.31 | 0.51 |
| 5:C:160:GLY:H | 5:C:196:VAL:HG13 | 1.76 | 0.51 |
| 3:4:105:GLU:O | 3:4:109:VAL:HG23 | 2.10 | 0.51 |
| 3:4:251:VAL:O | 3:4:330:HIS:HA | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:A:2510:A:H4' | 31:A:2511:A:O4' | 2.11 | 0.51 |
| 3:4:251:VAL:HG23 | 3:4:330:HIS:CB | 2.40 | 0.51 |
| 31:A:227:A:N1 | 31:A:505:C:O2' | 2.42 | 0.51 |
| 31:A:920:G:N2 | 31:A:944:A:OP1 | 2.44 | 0.51 |
| 31:A:2963:U:H2' | 31:A:2964:A:H5' | 1.92 | 0.51 |
| 31:A:718:C:O2' | 31:A:772:U:OP1 | 2.28 | 0.50 |
| 31:A:2006:A:H2' | 31:A:2007:C:O4' | 2.11 | 0.50 |
| 13:M:15:GLU:O | 31:A:690:G:N2 | 2.43 | 0.50 |
| 23:X:56:ASP:O | 23:X:57:ASP:HB2 | 2.11 | 0.50 |
| 31:A:327:U:O2 | 31:A:328:C:N4 | 2.43 | 0.50 |
| 22:W:71:ILE:HG22 | 22:W:72:GLU:H | 1.76 | 0.50 |
| 31:A:1532:G:N2 | 31:A:1804:G:C4 | 2.79 | 0.50 |
| 31:A:2161:A:H61 | 31:A:2193:A:H61 | 1.59 | 0.50 |
| 3:4:433:VAL:HG22 | 3:4:459:LEU:HD21 | 1.94 | 0.50 |
| 8:G:51:ILE:O | 8:G:53:VAL:HG13 | 2.11 | 0.50 |
| 22:W:71:ILE:HG22 | 22:W:72:GLU:N | 2.27 | 0.50 |
| 31:A:389:G:N1 | 31:A:392:A:OP2 | 2.36 | 0.50 |
| 31:A:637:G:O2' | 31:A:638:U:OP2 | 2.20 | 0.50 |
| 3:4:124:LEU:HD12 | 3:4:142:ASP:OD1 | 2.12 | 0.50 |
| 3:4:300:THR:HG22 | 3:4:318:THR:HG23 | 1.93 | 0.50 |
| 5:C:158:SER:OG | 5:C:159:ALA:N | 2.45 | 0.50 |
| 10:I:47:ALA:HA | 10:I:80:ALA:HB1 | 1.93 | 0.50 |
| 31:A:935:A:H4' | 31:A:951:G:H22 | 1.77 | 0.50 |
| 31:A:996:G:H2' | 31:A:997:G:C8 | 2.47 | 0.50 |
| 3:4:319:LEU:HD22 | 3:4:353:VAL:HG21 | 1.94 | 0.49 |
| 11:K:92:LEU:HD11 | 11:K:99:ARG:HD2 | 1.94 | 0.49 |
| 31:A:1221:A:OP2 | 31:A:1222:C:N4 | 2.45 | 0.49 |
| 16:Q:73:PHE:HB3 | 16:Q:80:ILE:HD11 | 1.93 | 0.49 |
| 31:A:2054:C:O2 | 31:A:2153:G:O2' | 2.21 | 0.49 |
| 3:4:331:VAL:HG22 | 3:4:367:VAL:CB | 2.40 | 0.49 |
| 3:4:442:THR:OG1 | 3:4:443:GLU:N | 2.44 | 0.49 |
| 31:A:380:A:N6 | 31:A:404:A:O2' | 2.40 | 0.49 |
| 31:A:1025:A:N3 | 31:A:2488:C:O2' | 2.39 | 0.49 |
| 31:A:2050:C:H4' | 31:A:2051:U:OP1 | 2.11 | 0.49 |
| 8:G:46:ALA:HA | 8:G:52:VAL:HG21 | 1.93 | 0.49 |
| 9:H:66:ASN:O | 9:H:136:LEU:HD23 | 2.12 | 0.49 |
| 23:X:38:VAL:HG12 | 23:X:40:GLN:OE1 | 2.13 | 0.49 |
| 4:B:26:A:H2 | 4:B:115:A:HO2' | 1.61 | 0.49 |
| 31:A:940:A:H3' | 31:A:940:A:C8 | 2.48 | 0.49 |
| 31:A:1630:U:O4 | 31:A:1631:A:N6 | 2.46 | 0.49 |
| 31:A:3107:G:O2' | 31:A:3108:G:OP2 | 2.26 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:L:25:LEU:HD13 | 12:L:40:VAL:HG23 | 1.94 | 0.49 |
| 12:L:80:ASP:OD1 | 12:L:80:ASP:O | 2.29 | 0.49 |
| 18:S:25:GLU:OE2 | 31:A:1111:G:N2 | 2.39 | 0.49 |
| 31:A:1402:A:C2' | 31:A:1403:C:O5' | 2.61 | 0.49 |
| 4:B:30:G:O2' | 4:B:59:A:N1 | 2.44 | 0.49 |
| 31:A:2018:G:H8 | 31:A:2426:C:HO2' | 1.59 | 0.49 |
| 3:4:34:ALA:HB3 | 3:4:48:ARG:NH1 | 2.28 | 0.49 |
| 3:4:332:VAL:HG21 | 3:4:343:ILE:CD1 | 2.42 | 0.49 |
| 9:H:26:GLY:O | 9:H:31:LEU:HD13 | 2.13 | 0.49 |
| 31:A:1294:U:HO2' | 31:A:1295:U:H6 | 1.55 | 0.49 |
| 31:A:1403:C:H2' | 31:A:1403:C:O2 | 2.13 | 0.49 |
| 31:A:1530:G:H22 | 31:A:1805:G:H1 | 1.59 | 0.49 |
| 31:A:2727:A:C8 | 33:A:3201:CLM:CL1 | 3.03 | 0.49 |
| 3:4:49:VAL:HG12 | 3:4:117:THR:CG2 | 2.43 | 0.49 |
| 4:B:33:C:O2' | 4:B:34:G:OP1 | 2.29 | 0.49 |
| 6:D:185:VAL:HG13 | 6:D:185:VAL:O | 2.13 | 0.49 |
| 23:X:56:ASP:OD2 | 31:A:2588:C:H5' | 2.13 | 0.49 |
| 31:A:2351:A:H2' | 31:A:2352:C:H6 | 1.78 | 0.49 |
| 10:I:48:THR:HG23 | 10:I:49:TYR:N | 2.24 | 0.49 |
| 31:A:388:U:H2' | 31:A:389:G:O4' | 2.13 | 0.49 |
| 13:M:20:THR:O | 13:M:20:THR:HG23 | 2.11 | 0.48 |
| 4:B:116:C:H2' | 4:B:117:A:O4' | 2.12 | 0.48 |
| 5:C:99:ASP:O | 31:A:1720:G:N2 | 2.45 | 0.48 |
| 31:A:1189:G:O2' | 31:A:1190:C:O4' | 2.24 | 0.48 |
| 31:A:2010:G:H2' | 31:A:2011:U:C6 | 2.48 | 0.48 |
| 31:A:2387:U:O4 | 31:A:2394:A:N6 | 2.46 | 0.48 |
| 3:4:12:THR:O | 3:4:12:THR:HG23 | 2.13 | 0.48 |
| 31:A:1179:U:O4' | 31:A:1188:A:O4' | 2.31 | 0.48 |
| 31:A:2630:A:OP2 | 31:A:2635:A:N6 | 2.39 | 0.48 |
| 9:H:124:ILE:O | 9:H:126:SER:N | 2.45 | 0.48 |
| 16:Q:18:THR:HG23 | 16:Q:18:THR:O | 2.13 | 0.48 |
| 31:A:2529:A:H2' | 31:A:2530:C:C6 | 2.49 | 0.48 |
| 5:C:244:ARG:O | 5:C:245:HIS:CG | 2.67 | 0.48 |
| 31:A:378:G:H2' | 31:A:379:G:C8 | 2.49 | 0.48 |
| 31:A:2351:A:O4' | 31:A:2396:A:O2' | 2.30 | 0.48 |
| 3:4:429:LEU:HD21 | 3:4:463:LEU:HD11 | 1.96 | 0.48 |
| 31:A:245:G:H2' | 31:A:246:U:C6 | 2.48 | 0.48 |
| 31:A:1938:G:HO2' | 31:A:1939:U:H6 | 1.59 | 0.48 |
| 31:A:3029:U:O2 | 31:A:3030:A:C8 | 2.67 | 0.47 |
| 3:4:251:VAL:HG11 | 3:4:322:VAL:HG22 | 1.96 | 0.47 |
| 5:C:235:GLY:HA2 | 5:C:240:THR:HB | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:G:48:ASP:OD1 | 8:G:49:GLY:N | 2.47 | 0.47 |
| 15:O:90:ARG:NH2 | 15:O:118:GLU:O | 2.46 | 0.47 |
| 21:V:81:THR:HG21 | 21:V:98:ALA:HB1 | 1.95 | 0.47 |
| 31:A:2043:C:H6 | 31:A:2043:C:O5' | 1.96 | 0.47 |
| 3:4:97:TYR:CD2 | 3:4:124:LEU:HD21 | 2.49 | 0.47 |
| 4:B:115:A:H2' | 4:B:116:C:O4' | 2.14 | 0.47 |
| 31:A:326:A:N6 | 31:A:450:G:C6 | 2.83 | 0.47 |
| 31:A:2025:C:O2 | 31:A:2025:C:O4' | 2.32 | 0.47 |
| 3:4:208:ILE:HD13 | 3:4:208:ILE:HA | 1.75 | 0.47 |
| 3:4:399:GLY:O | 3:4:402:LYS:HB2 | 2.14 | 0.47 |
| 9:H:95:VAL:HG12 | 9:H:96:THR:N | 2.29 | 0.47 |
| 3:4:433:VAL:HG11 | 3:4:451:ILE:CD1 | 2.44 | 0.47 |
| 31:A:1804:G:H2' | 31:A:1805:G:O4' | 2.14 | 0.47 |
| 7:E:151:ASN:ND2 | 7:E:193:ASP:OD1 | 2.43 | 0.47 |
| 10:I:25:VAL:O | 10:I:106:LYS:N | 2.48 | 0.47 |
| 10:I:45:ASP:N | 10:I:45:ASP:OD1 | 2.48 | 0.47 |
| 22:W:42:THR:HG22 | 22:W:42:THR:O | 2.15 | 0.47 |
| 31:A:162:A:O2' | 31:A:163:U:O5' | 2.33 | 0.47 |
| 31:A:844:G:O2' | 31:A:878:G:H4' | 2.15 | 0.47 |
| 31:A:1069:G:C6 | 31:A:1083:G:C6 | 3.03 | 0.47 |
| 31:A:1163:A:H4' | 31:A:1164:A:O5' | 2.13 | 0.47 |
| 3:4:330:HIS:O | 3:4:367:VAL:N | 2.38 | 0.47 |
| 3:4:330:HIS:CG | 3:4:346:VAL:HG11 | 2.49 | 0.47 |
| 10:I:99:ASP:OD1 | 10:I:99:ASP:N | 2.42 | 0.47 |
| 31:A:163:U:HO2' | 31:A:164:A:P | 2.30 | 0.47 |
| 31:A:273:A:H62 | 31:A:313:G:H21 | 1.63 | 0.47 |
| 31:A:318:U:O2' | 31:A:319:G:O5' | 2.19 | 0.47 |
| 31:A:1289:A:H2' | 31:A:1290:C:O4' | 2.15 | 0.47 |
| 31:A:979:G:H2' | 31:A:980:C:C6 | 2.50 | 0.47 |
| 9:H:5:LEU:O | 9:H:16:GLY:N | 2.44 | 0.47 |
| 17:R:89:GLU:HG3 | 17:R:89:GLU:O | 2.15 | 0.47 |
| 3:4:258:LYS:HB2 | 32:4:501:GCP:O2B | 2.15 | 0.46 |
| 9:H:38:VAL:O | 9:H:38:VAL:CG1 | 2.63 | 0.46 |
| 31:A:1350:G:O2' | 31:A:1351:G:C8 | 2.66 | 0.46 |
| 31:A:1473:G:N1 | 31:A:1487:U:OP2 | 2.35 | 0.46 |
| 3:4:293:ARG:NH2 | 3:4:412:GLU:O | 2.49 | 0.46 |
| 4:B:46:A:C4 | 4:B:47:A:C8 | 3.02 | 0.46 |
| 7:E:119:ALA:HB2 | 7:E:124:ILE:HD12 | 1.97 | 0.46 |
| 8:G:20:ASN:ND2 | 8:G:20:ASN:C | 2.64 | 0.46 |
| 13:M:96:ASP:N | 13:M:96:ASP:OD1 | 2.46 | 0.46 |
| 31:A:1203:A:O2' | 31:A:1204:A:P | 2.73 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2:5:LYS:HB3 | 1:2:57:GLU:O | 2.16 | 0.46 |
| 3:4:253:TYR:CD2 | 3:4:254:THR:HG22 | 2.50 | 0.46 |
| 31:A:243:U:O2 | 31:A:243:U:H2' | 2.15 | 0.46 |
| 31:A:899:G:H5' | 31:A:900:G:OP1 | 2.16 | 0.46 |
| 31:A:2573:G:C6 | 31:A:2593:A:C6 | 3.03 | 0.46 |
| 5:C:80:ALA:HB2 | 5:C:96:HIS:NE2 | 2.30 | 0.46 |
| 9:H:9:VAL:O | 9:H:9:VAL:HG13 | 2.14 | 0.46 |
| 10:I:24:VAL:HG12 | 10:I:80:ALA:HB3 | 1.97 | 0.46 |
| 22:W:39:GLY:HA3 | 22:W:98:LEU:HD12 | 1.98 | 0.46 |
| 31:A:546:G:O2' | 31:A:557:G:O6 | 2.29 | 0.46 |
| 31:A:1167:C:N3 | 31:A:1168:A:N6 | 2.63 | 0.46 |
| 31:A:1856:C:O2 | 31:A:2922:U:O2' | 2.33 | 0.46 |
| 31:A:2007:C:H2' | 31:A:2008:A:C8 | 2.51 | 0.46 |
| 3:4:261:LEU:CD1 | 3:4:367:VAL:HG11 | 2.46 | 0.46 |
| 31:A:244:A:C2 | 31:A:255:A:C2 | 3.04 | 0.46 |
| 31:A:617:U:O2 | 31:A:617:U:C2' | 2.64 | 0.46 |
| 3:4:420:VAL:HG13 | 3:4:422:ILE:HG23 | 1.97 | 0.46 |
| 8:G:45:ARG:O | 8:G:52:VAL:CB | 2.61 | 0.46 |
| 9:H:124:ILE:CG2 | 9:H:148:VAL:HG21 | 2.45 | 0.46 |
| 15:O:45:ARG:HB3 | 15:O:46:PRO:HD3 | 1.98 | 0.46 |
| 31:A:2328:G:C6 | 31:A:2408:G:O6 | 2.68 | 0.46 |
| 31:A:3019:C:N4 | 31:A:3024:A:C2 | 2.84 | 0.46 |
| 24:Y:36:VAL:HG11 | 24:Y:61:VAL:HG11 | 1.97 | 0.46 |
| 31:A:2196:G:HO2' | 31:A:2197:G:H8 | 1.64 | 0.46 |
| 31:A:2411:U:H2' | 31:A:2412:U:O4' | 2.16 | 0.46 |
| 31:A:2827:G:C2 | 31:A:2828:U:C5 | 3.04 | 0.46 |
| 6:D:161:PHE:O | 6:D:164:THR:OG1 | 2.32 | 0.46 |
| 10:I:50:THR:O | 10:I:50:THR:CG2 | 2.62 | 0.46 |
| 31:A:1159:C:H2' | 31:A:1160:G:H5' | 1.97 | 0.46 |
| 31:A:1178:U:H4' | 31:A:1179:U:H5' | 1.97 | 0.46 |
| 31:A:2334:U:O2' | 31:A:2342:A:OP1 | 2.34 | 0.46 |
| 5:C:257:THR:O | 5:C:257:THR:HG22 | 2.16 | 0.46 |
| 9:H:3:LEU:HD13 | 9:H:36:ALA:HB1 | 1.98 | 0.46 |
| 10:I:51:VAL:O | 10:I:51:VAL:HG13 | 2.16 | 0.46 |
| 19:T:8:PRO:HB2 | 19:T:71:LEU:HD21 | 1.98 | 0.46 |
| 31:A:1213:A:O2' | 31:A:1214:A:C5' | 2.64 | 0.46 |
| 4:B:81:U:H2' | 4:B:82:A:C8 | 2.51 | 0.45 |
| 8:G:156:ASP:OD2 | 8:G:158:TYR:O | 2.33 | 0.45 |
| 15:O:12:GLY:O | 15:O:13:SER:OG | 2.31 | 0.45 |
| 20:U:4:ILE:HD12 | 25:Z:22:LEU:HD22 | 1.98 | 0.45 |
| 10:I:43:LEU:HD13 | 10:I:46:SER:O | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:A:485:U:O2' | 31:A:2454:G:N2 | 2.49 | 0.45 |
| 6:D:60:ARG:O | 6:D:60:ARG:HG2 | 2.16 | 0.45 |
| 10:I:26:THR:HA | 10:I:104:VAL:O | 2.16 | 0.45 |
| 31:A:1202:A:N3 | 31:A:1223:U:H2' | 2.31 | 0.45 |
| 31:A:2008:A:C2 | 31:A:2046:A:H4' | 2.50 | 0.45 |
| 3:4:364:GLU:O | 3:4:365:LEU:C | 2.54 | 0.45 |
| 10:I:39:LEU:HD22 | 10:I:103:LEU:HB2 | 1.99 | 0.45 |
| 14:N:28:SER:O | 14:N:134:ARG:NH2 | 2.49 | 0.45 |
| 22:W:11:LEU:HD11 | 22:W:57:VAL:HG11 | 1.98 | 0.45 |
| 31:A:2164:U:O2' | 31:A:2165:C:OP2 | 2.27 | 0.45 |
| 2:3:22:PRO:HB3 | 31:A:1102:G:H2' | 1.98 | 0.45 |
| 8:G:50:ALA:HB3 | 8:G:52:VAL:CG2 | 2.46 | 0.45 |
| 13:M:54:GLN:OE1 | 31:A:940:A:H1' | 2.17 | 0.45 |
| 31:A:399:G:H2' | 31:A:400:C:O4' | 2.17 | 0.45 |
| 31:A:765:G:C6 | 31:A:766:G:N7 | 2.85 | 0.45 |
| 3:4:293:ARG:HG3 | 3:4:438:HIS:CG | 2.51 | 0.45 |
| 13:M:89:GLN:N | 13:M:89:GLN:OE1 | 2.49 | 0.45 |
| 31:A:602:A:H2 | 31:A:1376:C:HO2' | 1.65 | 0.45 |
| 3:4:365:LEU:HD22 | 3:4:410:LEU:HD12 | 1.99 | 0.45 |
| 7:E:141:ALA:HB1 | 7:E:169:VAL:HG12 | 1.98 | 0.45 |
| 31:A:2158:C:H1' | 31:A:2159:G:H2' | 1.98 | 0.45 |
| 31:A:2178:G:O2' | 31:A:2179:U:OP2 | 2.33 | 0.45 |
| 3:4:130:ASN:OD1 | 3:4:131:ALA:N | 2.49 | 0.45 |
| 10:I:47:ALA:CA | 10:I:80:ALA:HB1 | 2.46 | 0.45 |
| 31:A:107:G:C2 | 31:A:108:A:C8 | 3.05 | 0.45 |
| 3:4:329:ILE:HA | 3:4:365:LEU:O | 2.17 | 0.45 |
| 5:C:99:ASP:OD1 | 5:C:99:ASP:N | 2.50 | 0.45 |
| 8:G:48:ASP:OD1 | 8:G:50:ALA:HB2 | 2.17 | 0.45 |
| 8:G:122:ILE:HD11 | 8:G:134:VAL:HG11 | 1.99 | 0.45 |
| 31:A:2366:C:H3' | 31:A:2367:G:C5' | 2.46 | 0.45 |
| 9:H:136:LEU:HB2 | 9:H:140:VAL:HG13 | 1.98 | 0.45 |
| 31:A:1531:C:N4 | 31:A:1532:G:O6 | 2.50 | 0.45 |
| 31:A:1688:G:C6 | 31:A:1748:A:C2 | 3.05 | 0.45 |
| 7:E:144:PHE:O | 7:E:147:THR:HG22 | 2.18 | 0.44 |
| 9:H:136:LEU:HD22 | 9:H:140:VAL:CG2 | 2.47 | 0.44 |
| 17:R:73:ASP:O | 17:R:73:ASP:OD2 | 2.35 | 0.44 |
| 31:A:41:A:H2' | 31:A:42:G:O4' | 2.17 | 0.44 |
| 31:A:2031:G:OP2 | 31:A:2032:A:O2' | 2.20 | 0.44 |
| 31:A:2378:U:O2' | 31:A:2379:G:O4' | 2.35 | 0.44 |
| 31:A:2998:C:H2' | 31:A:2999:A:O4' | 2.17 | 0.44 |
| 3:4:284:THR:HG22 | 3:4:298:THR:HG22 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:4:332:VAL:HG21 | 3:4:343:ILE:HD11 | 1.99 | 0.44 |
| 31:A:317:G:O2' | 31:A:509:U:OP2 | 2.27 | 0.44 |
| 31:A:1640:A:H2' | 31:A:1642:G:N7 | 2.32 | 0.44 |
| 31:A:2675:A:C2 | 33:A:3201:CLM:H8 | 2.53 | 0.44 |
| 7:E:167:LYS:O | 31:A:403:U:H1' | 2.17 | 0.44 |
| 31:A:551:G:N2 | 31:A:554:A:OP2 | 2.46 | 0.44 |
| 31:A:2288:C:H2' | 31:A:2289:C:H6 | 1.82 | 0.44 |
| 5:C:75:VAL:HG23 | 5:C:75:VAL:O | 2.18 | 0.44 |
| 11:K:65:SER:OG | 11:K:66:GLY:N | 2.49 | 0.44 |
| 18:S:14:TYR:CE2 | 18:S:24:VAL:HG12 | 2.52 | 0.44 |
| 31:A:950:A:C4 | 31:A:951:G:C8 | 3.05 | 0.44 |
| 31:A:3014:A:N6 | 31:A:3113:A:OP2 | 2.51 | 0.44 |
| 9:H:124:ILE:O | 9:H:124:ILE:CG2 | 2.64 | 0.44 |
| 9:H:132:VAL:CG1 | 9:H:144:VAL:HG23 | 2.46 | 0.44 |
| 18:S:64:VAL:HG22 | 18:S:97:LEU:HD23 | 1.99 | 0.44 |
| 31:A:7:U:HO2' | 31:A:8:U:C1' | 2.30 | 0.44 |
| 31:A:2727:A:H8 | 33:A:3201:CLM:CL1 | 2.38 | 0.44 |
| 8:G:51:ILE:CD1 | 8:G:51:ILE:H | 2.21 | 0.44 |
| 31:A:940:A:C2' | 31:A:941:U:O5' | 2.66 | 0.44 |
| 31:A:2153:G:H2' | 31:A:2153:G:N3 | 2.32 | 0.44 |
| 31:A:2351:A:H2' | 31:A:2352:C:C6 | 2.52 | 0.44 |
| 3:4:48:ARG:HB3 | 3:4:82:LEU:HD23 | 1.99 | 0.44 |
| 5:C:145:VAL:HG12 | 5:C:191:ALA:CB | 2.48 | 0.44 |
| 16:Q:15:ASP:C | 16:Q:15:ASP:OD2 | 2.56 | 0.44 |
| 31:A:1334:C:H2' | 31:A:1335:G:O4' | 2.18 | 0.44 |
| 31:A:2244:A:C2 | 31:A:2246:U:O4' | 2.70 | 0.44 |
| 3:4:209:GLU:O | 3:4:215:ILE:HD11 | 2.18 | 0.44 |
| 12:L:25:LEU:CD1 | 12:L:40:VAL:HG23 | 2.48 | 0.44 |
| 14:N:42:ILE:CD1 | 14:N:97:VAL:HG11 | 2.48 | 0.44 |
| 31:A:9:U:H2' | 31:A:9:U:O2 | 2.18 | 0.44 |
| 4:B:1:G:C2 | 4:B:2:U:C4 | 3.06 | 0.43 |
| 9:H:11:HIS:HE2 | 31:A:2319:G:P | 2.41 | 0.43 |
| 31:A:137:G:H4' | 31:A:138:A:OP1 | 2.17 | 0.43 |
| 31:A:1196:C:H4' | 31:A:1197:C:OP1 | 2.18 | 0.43 |
| 31:A:1536:A:H2' | 31:A:1537:U:O4' | 2.18 | 0.43 |
| 3:4:291:ASP:OD1 | 3:4:291:ASP:N | 2.46 | 0.43 |
| 5:C:186:ASP:OD2 | 5:C:188:ARG:NH2 | 2.51 | 0.43 |
| 6:D:185:VAL:HG23 | 6:D:192:LEU:HD23 | 2.00 | 0.43 |
| 8:G:51:ILE:CA | 8:G:53:VAL:HG13 | 2.48 | 0.43 |
| 10:I:33:VAL:CG2 | 31:A:1173:G:O2' | 2.66 | 0.43 |
| 21:V:67:HIS:CE1 | 21:V:69:SER:HG | 2.35 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:A:1001:C:C5 | 31:A:1002:C:H1' | 2.53 | 0.43 |
| 31:A:1758:G:H2' | 31:A:1759:A:C8 | 2.53 | 0.43 |
| 16:Q:26:ASN:OD1 | 16:Q:41:VAL:CG1 | 2.66 | 0.43 |
| 21:V:15:LYS:NZ | 31:A:390:G:O2' | 2.30 | 0.43 |
| 31:A:681:C:H2' | 31:A:682:A:H8 | 1.82 | 0.43 |
| 31:A:2730:U:O2 | 31:A:2730:U:C2' | 2.66 | 0.43 |
| 3:4:14:GLU:O | 3:4:16:ALA:N | 2.51 | 0.43 |
| 5:C:20:ASP:OD1 | 5:C:20:ASP:N | 2.52 | 0.43 |
| 7:E:52:THR:HG22 | 7:E:53:LYS:N | 2.33 | 0.43 |
| 31:A:899:G:H4' | 31:A:900:G:O5' | 2.17 | 0.43 |
| 31:A:940:A:H2' | 31:A:941:U:O5' | 2.18 | 0.43 |
| 3:4:97:TYR:CG | 3:4:124:LEU:HD21 | 2.53 | 0.43 |
| 3:4:392:VAL:HG22 | 3:4:393:SER:N | 2.33 | 0.43 |
| 7:E:128:THR:HG22 | 7:E:129:GLU:N | 2.28 | 0.43 |
| 10:I:23:THR:O | 10:I:24:VAL:HG23 | 2.18 | 0.43 |
| 10:I:51:VAL:HG13 | 31:A:1202:A:C8 | 2.54 | 0.43 |
| 10:I:93:ILE:HD12 | 10:I:105:ILE:CG2 | 2.43 | 0.43 |
| 13:M:95:VAL:HG23 | 13:M:110:VAL:HG21 | 2.00 | 0.43 |
| 31:A:709:U:O2 | 31:A:709:U:O4' | 2.35 | 0.43 |
| 4:B:33:C:C2 | 4:B:52:G:N2 | 2.86 | 0.43 |
| 31:A:193:G:H2' | 31:A:194:A:O4' | 2.19 | 0.43 |
| 31:A:451:U:H2' | 31:A:452:G:C8 | 2.54 | 0.43 |
| 31:A:1010:U:H3' | 31:A:1012:C:H41 | 1.83 | 0.43 |
| 31:A:1083:G:O2' | 31:A:1084:U:H5' | 2.19 | 0.43 |
| 31:A:2288:C:H2' | 31:A:2289:C:C6 | 2.53 | 0.43 |
| 31:A:2731:C:O2 | 31:A:2731:C:H2' | 2.18 | 0.43 |
| 31:A:2787:U:C2 | 31:A:2789:A:OP2 | 2.71 | 0.43 |
| 3:4:36:VAL:O | 3:4:37:SER:HB2 | 2.19 | 0.43 |
| 3:4:49:VAL:HG12 | 3:4:117:THR:HG21 | 2.00 | 0.43 |
| 17:R:83:LEU:HD22 | 17:R:88:VAL:CG1 | 2.49 | 0.43 |
| 31:A:663:A:N3 | 31:A:663:A:H2' | 2.33 | 0.43 |
| 3:4:390:VAL:CG2 | 3:4:391:PHE:N | 2.81 | 0.43 |
| 10:I:24:VAL:CG1 | 10:I:105:ILE:HG22 | 2.48 | 0.43 |
| 10:I:47:ALA:H | 10:I:82:VAL:HA | 1.84 | 0.43 |
| 31:A:2294:A:H2' | 31:A:2295:C:C6 | 2.54 | 0.43 |
| 31:A:2963:U:C2' | 31:A:2964:A:H5' | 2.49 | 0.43 |
| 3:4:400:LEU:C | 3:4:402:LYS:N | 2.70 | 0.43 |
| 7:E:138:THR:OG1 | 31:A:403:U:O4' | 2.36 | 0.43 |
| 9:H:121:LYS:NZ | 31:A:158:G:OP2 | 2.45 | 0.43 |
| 10:I:31:LEU:O | 10:I:36:LEU:HD23 | 2.19 | 0.43 |
| 10:I:56:LEU:HB2 | 31:A:1165:G:OP2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:A:1173:G:H2' | 31:A:1174:G:C8 | 2.54 | 0.43 |
| 31:A:2349:A:N6 | 31:A:2386:U:O4' | 2.52 | 0.43 |
| 3:4:422:ILE:O | 3:4:448:GLY:HA2 | 2.19 | 0.43 |
| 7:E:101:ARG:O | 7:E:101:ARG:HG3 | 2.18 | 0.43 |
| 17:R:49:ASP:OD1 | 31:A:651:G:N2 | 2.52 | 0.43 |
| 18:S:64:VAL:HG22 | 18:S:97:LEU:CD2 | 2.49 | 0.43 |
| 31:A:241:A:H5' | 31:A:243:U:H1' | 2.00 | 0.43 |
| 31:A:243:U:C5 | 31:A:254:G:N2 | 2.87 | 0.43 |
| 31:A:714:U:O2 | 31:A:714:U:C2' | 2.67 | 0.43 |
| 31:A:1529:U:H2' | 31:A:1530:G:O4' | 2.19 | 0.42 |
| 31:A:2378:U:HO2' | 31:A:2379:G:C1' | 2.32 | 0.42 |
| 31:A:2706:A:C5 | 31:A:2707:C:C5 | 3.07 | 0.42 |
| 3:4:168:GLN:HB3 | 3:4:208:ILE:CG1 | 2.49 | 0.42 |
| 31:A:2351:A:O2' | 31:A:2352:C:O4' | 2.37 | 0.42 |
| 3:4:254:THR:OG1 | 3:4:255:ASN:N | 2.52 | 0.42 |
| 3:4:395:ARG:O | 3:4:396:THR:CB | 2.67 | 0.42 |
| 8:G:22:GLN:OE1 | 8:G:43:VAL:HG22 | 2.19 | 0.42 |
| 31:A:1937:U:H2' | 31:A:1938:G:O4' | 2.20 | 0.42 |
| 31:A:2035:U:HO2' | 31:A:2036:A:P | 2.42 | 0.42 |
| 31:A:2351:A:HO2' | 31:A:2352:C:C5' | 2.25 | 0.42 |
| 3:4:393:SER:O | 3:4:395:ARG:N | 2.52 | 0.42 |
| 4:B:113:G:H2' | 4:B:114:A:C8 | 2.54 | 0.42 |
| 9:H:32:PRO:HB3 | 24:Y:64:ALA:HB3 | 2.00 | 0.42 |
| 20:U:14:PRO:HB3 | 20:U:96:PHE:HD1 | 1.84 | 0.42 |
| 31:A:7:U:H2' | 31:A:8:U:C6 | 2.54 | 0.42 |
| 31:A:2186:C:H2' | 31:A:2187:U:O4' | 2.19 | 0.42 |
| 3:4:329:ILE:CG2 | 3:4:367:VAL:HG23 | 2.48 | 0.42 |
| 3:4:422:ILE:CD1 | 3:4:430:VAL:HG23 | 2.49 | 0.42 |
| 10:I:53:LYS:HE3 | 31:A:1224:G:OP2 | 2.18 | 0.42 |
| 10:I:58:LYS:HG3 | 10:I:70:ASP:HA | 2.01 | 0.42 |
| 13:M:84:ASN:OD1 | 13:M:84:ASN:C | 2.57 | 0.42 |
| 31:A:270:U:O2 | 31:A:270:U:H2' | 2.19 | 0.42 |
| 31:A:2552:A:H2' | 31:A:2553:G:C8 | 2.55 | 0.42 |
| 8:G:23:ASN:CG | 8:G:23:ASN:O | 2.57 | 0.42 |
| 10:I:75:GLY:O | 31:A:1225:G:O3' | 2.37 | 0.42 |
| 17:R:47:TYR:OH | 31:A:1110:C:OP1 | 2.36 | 0.42 |
| 18:S:71:PRO:O | 18:S:73:ILE:HD12 | 2.20 | 0.42 |
| 31:A:783:G:H2' | 31:A:785:A:H62 | 1.85 | 0.42 |
| 31:A:986:G:H2' | 31:A:987:A:O4' | 2.19 | 0.42 |
| 31:A:2299:C:OP2 | 31:A:2462:G:N2 | 2.47 | 0.42 |
| 5:C:256:ARG:HE | 5:C:271:ARG:NH1 | 2.17 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:I:21:THR:CG2 | 10:I:22:ALA:H | 2.23 | 0.42 |
| 17:R:26:GLY:O | 17:R:30:ARG:NH1 | 2.52 | 0.42 |
| 25:Z:18:LEU:O | 25:Z:22:LEU:HD13 | 2.20 | 0.42 |
| 31:A:273:A:C2 | 31:A:322:A:O4' | 2.72 | 0.42 |
| 31:A:3059:G:C4 | 31:A:3060:A:C8 | 3.08 | 0.42 |
| 3:4:332:VAL:HG22 | 3:4:368:VAL:HG12 | 2.01 | 0.42 |
| 3:4:364:GLU:O | 3:4:364:GLU:CD | 2.58 | 0.42 |
| 4:B:2:U:H2' | 4:B:3:U:O5' | 2.20 | 0.42 |
| 9:H:112:LEU:HD12 | 9:H:113:ASP:O | 2.20 | 0.42 |
| 13:M:81:GLY:O | 13:M:84:ASN:OD1 | 2.38 | 0.42 |
| 19:T:26:ARG:O | 19:T:29:ASP:OD1 | 2.38 | 0.42 |
| 19:T:56:LYS:NZ | 31:A:576:G:O2' | 2.45 | 0.42 |
| 31:A:1158:U:H2' | 31:A:1159:C:O4' | 2.19 | 0.42 |
| 31:A:1172:A:C6 | 31:A:1224:G:C6 | 3.08 | 0.42 |
| 31:A:1382:U:O2 | 31:A:1382:U:H2' | 2.20 | 0.42 |
| 31:A:1535:C:O2 | 31:A:1535:C:O4' | 2.35 | 0.42 |
| 31:A:1932:U:HO2' | 31:A:1933:G:P | 2.40 | 0.42 |
| 11:K:135:GLN:NE2 | 31:A:3:A:N3 | 2.67 | 0.42 |
| 31:A:781:C:C4 | 31:A:782:U:O4 | 2.73 | 0.42 |
| 31:A:1002:C:C2' | 31:A:1003:A:OP1 | 2.67 | 0.42 |
| 31:A:1762:C:H2' | 31:A:1763:G:O4' | 2.19 | 0.42 |
| 31:A:3046:C:O2 | 31:A:3046:C:O5' | 2.38 | 0.42 |
| 5:C:130:ASN:OD1 | 5:C:131:LEU:N | 2.53 | 0.42 |
| 10:I:28:TYR:OH | 31:A:1225:G:C1' | 2.67 | 0.42 |
| 14:N:42:ILE:HD12 | 14:N:97:VAL:HG11 | 2.01 | 0.42 |
| 31:A:447:A:H2' | 31:A:448:U:C6 | 2.54 | 0.42 |
| 31:A:735:U:H2' | 31:A:736:G:O4' | 2.20 | 0.42 |
| 31:A:1122:C:H2' | 31:A:1129:G:H2' | 2.01 | 0.42 |
| 31:A:1196:C:HO2' | 31:A:1197:C:P | 2.36 | 0.42 |
| 31:A:1758:G:O2' | 31:A:1759:A:O5' | 2.36 | 0.42 |
| 31:A:2490:A:H4' | 31:A:2491:A:O5' | 2.20 | 0.42 |
| 31:A:2521:C:O2 | 31:A:2521:C:H2' | 2.19 | 0.42 |
| 3:4:251:VAL:HG23 | 3:4:330:HIS:HB2 | 2.02 | 0.41 |
| 6:D:150:SER:OG | 31:A:2736:C:O2 | 2.38 | 0.41 |
| 9:H:75:LEU:HD21 | 9:H:104:ILE:HD12 | 2.02 | 0.41 |
| 10:I:28:TYR:OH | 31:A:1224:G:N3 | 2.53 | 0.41 |
| 13:M:49:MET:O | 13:M:49:MET:HG2 | 2.20 | 0.41 |
| 31:A:472:C:O2 | 31:A:472:C:H2' | 2.20 | 0.41 |
| 31:A:1216:A:C5 | 31:A:1217:G:C8 | 3.08 | 0.41 |
| 31:A:2194:A:H4' | 31:A:2195:U:O4' | 2.20 | 0.41 |
| 31:A:2327:C:N4 | 31:A:2328:G:O6 | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:D:212:ILE:HG23 | 6:D:213:LYS:N | 2.35 | 0.41 |
| 31:A:1087:G:H2' | 31:A:1088:U:C6 | 2.55 | 0.41 |
| 31:A:1183:U:H3 | 31:A:1187:A:HO2' | 1.68 | 0.41 |
| 31:A:1675:U:O2' | 31:A:1676:G:N7 | 2.53 | 0.41 |
| 31:A:2346:G:O6 | 31:A:2397:C:N4 | 2.53 | 0.41 |
| 31:A:2801:A:H5' | 31:A:2802:G:H5" | 2.02 | 0.41 |
| 3:4:464:ARG:HD3 | 3:4:464:ARG:C | 2.40 | 0.41 |
| 6:D:185:VAL:HG23 | 6:D:192:LEU:CD2 | 2.50 | 0.41 |
| 10:I:28:TYR:O | 10:I:29:ARG:HB2 | 2.20 | 0.41 |
| 31:A:2:A:C2 | 31:A:3119:A:C2 | 3.08 | 0.41 |
| 31:A:1444:U:OP2 | 31:A:1445:C:N4 | 2.53 | 0.41 |
| 31:A:2177:A:H3' | 31:A:2178:G:C5' | 2.51 | 0.41 |
| 4:B:112:C:O5' | 4:B:113:G:OP2 | 2.37 | 0.41 |
| 7:E:9:THR:HG23 | 7:E:10:PRO:HD2 | 2.01 | 0.41 |
| 10:I:3:LYS:O | 10:I:6:LYS:HG3 | 2.20 | 0.41 |
| 21:V:43:LYS:NZ | 31:A:568:A:OP2 | 2.49 | 0.41 |
| 25:Z:16:ASP:OD1 | 25:Z:17:GLU:N | 2.53 | 0.41 |
| 31:A:621:U:H2' | 31:A:622:C:C6 | 2.55 | 0.41 |
| 31:A:729:C:O2' | 31:A:733:U:OP1 | 2.36 | 0.41 |
| 31:A:940:A:C8 | 31:A:940:A:C3' | 3.03 | 0.41 |
| 31:A:1009:U:O3' | 31:A:1010:U:O4' | 2.38 | 0.41 |
| 31:A:1083:G:O4' | 31:A:2491:A:N6 | 2.53 | 0.41 |
| 3:4:150:ILE:HG21 | 3:4:277:PHE:HD2 | 1.84 | 0.41 |
| 3:4:254:THR:O | 3:4:255:ASN:C | 2.58 | 0.41 |
| 3:4:369:ASN:O | 3:4:370:LYS:CG | 2.69 | 0.41 |
| 3:4:393:SER:C | 3:4:395:ARG:N | 2.72 | 0.41 |
| 19:T:85:GLU:O | 31:A:21:G:O2' | 2.39 | 0.41 |
| 31:A:2729:G:O4' | 33:A:3201:CLM:CL2 | 2.75 | 0.41 |
| 3:4:93:ASP:C | 3:4:95:SER:N | 2.73 | 0.41 |
| 8:G:33:LEU:HD21 | 8:G:137:ILE:HD12 | 2.03 | 0.41 |
| 10:I:31:LEU:O | 10:I:32:THR:C | 2.59 | 0.41 |
| 10:I:59:ARG:HD3 | 31:A:1164:A:H5' | 2.03 | 0.41 |
| 17:R:109:LEU:O | 17:R:112:VAL:HG22 | 2.21 | 0.41 |
| 25:Z:66:LEU:O | 25:Z:66:LEU:HD23 | 2.21 | 0.41 |
| 31:A:361:A:H2' | 31:A:362:A:O5' | 2.20 | 0.41 |
| 31:A:997:G:O6 | 31:A:1010:U:H2' | 2.20 | 0.41 |
| 3:4:417:THR:HG22 | 3:4:454:ARG:HG2 | 2.02 | 0.41 |
| 10:I:54:ASN:OD1 | 31:A:1225:G:H5" | 2.21 | 0.41 |
| 19:T:65:ALA:O | 19:T:69:GLU:O | 2.39 | 0.41 |
| 31:A:93:A:H2' | 31:A:94:G:O4' | 2.21 | 0.41 |
| 31:A:244:A:C2 | 31:A:255:A:C4 | 3.09 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:A:2166:C:H4' | 31:A:2168:U:OP1 | 2.20 | 0.41 |
| 5:C:222:ARG:NH1 | 31:A:2006:A:OP2 | 2.54 | 0.41 |
| 10:I:69:LEU:HB2 | 10:I:72:LEU:HB2 | 2.03 | 0.41 |
| 31:A:239:U:C2' | 31:A:240:G:H5' | 2.50 | 0.41 |
| 31:A:619:C:O2 | 31:A:619:C:H2' | 2.20 | 0.41 |
| 31:A:905:U:O2 | 31:A:905:U:H2' | 2.21 | 0.41 |
| 31:A:2681:U:O2' | 31:A:2682:G:H5' | 2.21 | 0.41 |
| 1:2:22:SER:OG | 1:2:49:THR:HG21 | 2.20 | 0.41 |
| 3:4:346:VAL:O | 3:4:349:VAL:HG12 | 2.20 | 0.41 |
| 4:B:114:A:O5' | 4:B:114:A:H8 | 2.04 | 0.41 |
| 7:E:198:VAL:HG13 | 7:E:199:GLU:N | 2.36 | 0.41 |
| 9:H:75:LEU:HD12 | 9:H:76:GLY:N | 2.36 | 0.41 |
| 31:A:215:A:C4 | 31:A:216:A:C8 | 3.09 | 0.41 |
| 31:A:1807:C:C2 | 31:A:1808:A:C8 | 3.09 | 0.41 |
| 31:A:2603:G:H2' | 31:A:2604:U:C6 | 2.56 | 0.41 |
| 31:A:2980:U:H4' | 31:A:2981:A:OP1 | 2.21 | 0.41 |
| 8:G:4:ILE:O | 8:G:70:ARG:HD3 | 2.21 | 0.41 |
| 17:R:77:ASN:OD1 | 31:A:1270:G:C2' | 2.66 | 0.41 |
| 22:W:74:THR:HG22 | 22:W:75:GLU:N | 2.35 | 0.41 |
| 31:A:125:C:O2' | 31:A:126:C:OP2 | 2.27 | 0.41 |
| 31:A:401:C:H2' | 31:A:402:G:H5' | 2.03 | 0.41 |
| 31:A:658:U:C2' | 31:A:659:U:O5' | 2.70 | 0.41 |
| 31:A:1076:A:C2' | 31:A:1077:A:O5' | 2.69 | 0.41 |
| 31:A:1380:A:O4' | 31:A:1382:U:C6 | 2.74 | 0.41 |
| 31:A:2248:C:H2' | 31:A:2249:G:H8 | 1.85 | 0.41 |
| 31:A:2693:A:C6 | 31:A:2706:A:C8 | 3.09 | 0.41 |
| 31:A:3046:C:O2 | 31:A:3046:C:O4' | 2.39 | 0.41 |
| 3:4:48:ARG:HB2 | 3:4:115:ALA:CB | 2.51 | 0.40 |
| 7:E:171:ASN:ND2 | 31:A:406:A:OP1 | 2.55 | 0.40 |
| 31:A:294:G:N3 | 31:A:294:G:H2' | 2.36 | 0.40 |
| 31:A:752:C:C2 | 31:A:753:A:C8 | 3.09 | 0.40 |
| 31:A:1203:A:HO2' | 31:A:1204:A:P | 2.35 | 0.40 |
| 31:A:1292:U:HO2' | 31:A:1293:G:P | 2.42 | 0.40 |
| 3:4:21:ALA:HA | 3:4:24:ARG:HD2 | 2.03 | 0.40 |
| 3:4:176:LEU:HG | 3:4:176:LEU:O | 2.21 | 0.40 |
| 3:4:256:ALA:HB1 | 3:4:331:VAL:HG12 | 2.03 | 0.40 |
| 8:G:128:SER:OG | 8:G:129:PRO:HD2 | 2.21 | 0.40 |
| 10:I:43:LEU:HD12 | 10:I:44:GLY:O | 2.21 | 0.40 |
| 14:N:118:LEU:O | 14:N:122:ILE:HG13 | 2.22 | 0.40 |
| 31:A:1434:G:H2' | 31:A:1435:C:C6 | 2.55 | 0.40 |
| 3:4:73:LEU:O | 3:4:76:THR:HG22 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:4:93:ASP:OD2 | 3:4:99:GLY:HA2 | 2.21 | 0.40 |
| 3:4:201:ARG:O | 3:4:202:GLY:C | 2.58 | 0.40 |
| 3:4:232:ILE:HG23 | 31:A:2703:U:O2' | 2.22 | 0.40 |
| 3:4:393:SER:OG | 3:4:398:ASP:HB2 | 2.20 | 0.40 |
| 4:B:8:C:H2' | 4:B:9:G:O4' | 2.22 | 0.40 |
| 8:G:7:GLN:O | 8:G:51:ILE:HG23 | 2.22 | 0.40 |
| 13:M:93:VAL:HG13 | 13:M:93:VAL:O | 2.20 | 0.40 |
| 15:O:51:LEU:HD13 | 15:O:70:ILE:HD11 | 2.04 | 0.40 |
| 19:T:52:GLU:HB3 | 19:T:53:PRO:HD3 | 2.01 | 0.40 |
| 24:Y:18:VAL:HG22 | 24:Y:24:ARG:HG2 | 2.04 | 0.40 |
| 31:A:279:U:H2' | 31:A:280:G:H8 | 1.86 | 0.40 |
| 31:A:410:U:C2' | 31:A:411:G:OP1 | 2.69 | 0.40 |
| 31:A:1402:A:HO2' | 31:A:1403:C:P | 2.43 | 0.40 |
| 3:4:449:THR:O | 3:4:449:THR:HG22 | 2.21 | 0.40 |
| 10:I:87:VAL:HG11 | 10:I:124:ALA:O | 2.21 | 0.40 |
| 31:A:81:A:C2 | 31:A:100:A:C5 | 3.09 | 0.40 |
| 31:A:598:U:H2' | 31:A:599:G:C5' | 2.50 | 0.40 |
| 31:A:783:G:C5' | 31:A:784:G:OP2 | 2.70 | 0.40 |
| 31:A:1005:A:H2' | 31:A:1006:G:H5' | 2.04 | 0.40 |
| 31:A:1212:U:H2' | 31:A:1213:A:C8 | 2.56 | 0.40 |
| 31:A:2381:A:C4' | 31:A:2382:G:OP2 | 2.69 | 0.40 |
| 31:A:2764:C:O2' | 31:A:2964:A:N3 | 2.47 | 0.40 |
| 4:B:59:A:H2' | 4:B:59:A:N3 | 2.37 | 0.40 |
| 6:D:156:THR:HB | 6:D:157:PRO:CD | 2.52 | 0.40 |
| 13:M:22:VAL:HG12 | 13:M:29:LYS:HD2 | 2.03 | 0.40 |
| 31:A:248:G:O2' | 31:A:2656:A:OP1 | 2.30 | 0.40 |
| 31:A:502:C:N4 | 31:A:503:A:H62 | 2.19 | 0.40 |
| 31:A:1500:A:C4 | 31:A:1501:C:C5 | 3.10 | 0.40 |
| 31:A:1988:C:O2' | 31:A:2003:A:O4' | 2.39 | 0.40 |
| 31:A:2316:G:C2 | 31:A:2317:G:C8 | 3.09 | 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 | |
|---|---|---|---|---|---|---|---|
| 1 | 2 | 57/61 (93%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 2 | 3 | 21/24 (88%) | 20 (95%) | 1 (5%) | 0 | 100 | 100 |
| 3 | 4 | 454/470 (97%) | 389 (86%) | 65 (14%) | 0 | 100 | 100 |
| 5 | C | 273/278 (98%) | 254 (93%) | 19 (7%) | 0 | 100 | 100 |
| 6 | D | 212/217 (98%) | 202 (95%) | 10 (5%) | 0 | 100 | 100 |
| 7 | E | 207/215 (96%) | 194 (94%) | 13 (6%) | 0 | 100 | 100 |
| 8 | G | 174/179 (97%) | 156 (90%) | 18 (10%) | 0 | 100 | 100 |
| 9 | H | 149/151 (99%) | 136 (91%) | 13 (9%) | 0 | 100 | 100 |
| 10 | I | 124/175 (71%) | 85 (68%) | 39 (32%) | 0 | 100 | 100 |
| 11 | K | 144/147 (98%) | 142 (99%) | 2 (1%) | 0 | 100 | 100 |
| 12 | L | 120/122 (98%) | 114 (95%) | 6 (5%) | 0 | 100 | 100 |
| 13 | M | 143/147 (97%) | 130 (91%) | 13 (9%) | 0 | 100 | 100 |
| 14 | N | 134/138 (97%) | 129 (96%) | 5 (4%) | 0 | 100 | 100 |
| 15 | O | 116/199 (58%) | 109 (94%) | 7 (6%) | 0 | 100 | 100 |
| 16 | Q | 111/113 (98%) | 109 (98%) | 2 (2%) | 0 | 100 | 100 |
| 17 | R | 122/129 (95%) | 120 (98%) | 2 (2%) | 0 | 100 | 100 |
| 18 | S | 98/103 (95%) | 94 (96%) | 4 (4%) | 0 | 100 | 100 |
| 19 | T | 112/153 (73%) | 106 (95%) | 6 (5%) | 0 | 100 | 100 |
| 20 | U | 95/100 (95%) | 89 (94%) | 6 (6%) | 0 | 100 | 100 |
| 21 | V | 93/105 (89%) | 83 (89%) | 10 (11%) | 0 | 100 | 100 |
| 22 | W | 93/215 (43%) | 83 (89%) | 10 (11%) | 0 | 100 | 100 |
| 23 | X | 77/88 (88%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 24 | Y | 61/64 (95%) | 60 (98%) | 1 (2%) | 0 | 100 | 100 |
| 25 | Z | 62/77 (80%) | 62 (100%) | 0 | 0 | 100 | 100 |
| 26 | b | 52/57 (91%) | 52 (100%) | 0 | 0 | 100 | 100 |
| 27 | c | 47/55 (86%) | 47 (100%) | 0 | 0 | 100 | 100 |
| 28 | d | 44/47 (94%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 29 | e | 61/64 (95%) | 61 (100%) | 0 | 0 | 100 | 100 |
| 30 | f | 35/37 (95%) | 34 (97%) | 1 (3%) | 0 | 100 | 100 |
| All | All | 3491/3930 (89%) | 3232 (93%) | 259 (7%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains (i)

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 | |
|---|---|---|---|---|---|---|
| 1 | 2 | 52/54 (96%) | 52 (100%) | 0 | 100 | 100 |
| 2 | 3 | 18/19 (95%) | 18 (100%) | 0 | 100 | 100 |
| 3 | 4 | 359/372 (96%) | 355 (99%) | 4 (1%) | 70 | 81 |
| 5 | C | 215/218 (99%) | 215 (100%) | 0 | 100 | 100 |
| 6 | D | 160/163 (98%) | 160 (100%) | 0 | 100 | 100 |
| 7 | E | 169/173 (98%) | 169 (100%) | 0 | 100 | 100 |
| 8 | G | 148/150 (99%) | 145 (98%) | 3 (2%) | 50 | 70 |
| 9 | H | 90/116 (78%) | 90 (100%) | 0 | 100 | 100 |
| 10 | I | 89/120 (74%) | 88 (99%) | 1 (1%) | 70 | 81 |
| 11 | K | 119/120 (99%) | 119 (100%) | 0 | 100 | 100 |
| 12 | L | 100/100 (100%) | 100 (100%) | 0 | 100 | 100 |
| 13 | M | 112/114 (98%) | 111 (99%) | 1 (1%) | 75 | 84 |
| 14 | N | 114/116 (98%) | 114 (100%) | 0 | 100 | 100 |
| 15 | O | 97/158 (61%) | 97 (100%) | 0 | 100 | 100 |
| 16 | Q | 100/100 (100%) | 100 (100%) | 0 | 100 | 100 |
| 17 | R | 97/99 (98%) | 97 (100%) | 0 | 100 | 100 |
| 18 | S | 81/83 (98%) | 81 (100%) | 0 | 100 | 100 |
| 19 | T | 90/117 (77%) | 89 (99%) | 1 (1%) | 70 | 81 |
| 20 | U | 83/85 (98%) | 83 (100%) | 0 | 100 | 100 |
| 21 | V | 81/86 (94%) | 81 (100%) | 0 | 100 | 100 |
| 22 | W | 77/168 (46%) | 76 (99%) | 1 (1%) | 65 | 78 |
| 23 | X | 58/63 (92%) | 58 (100%) | 0 | 100 | 100 |
| 24 | Y | 50/51 (98%) | 50 (100%) | 0 | 100 | 100 |
| 25 | Z | 58/66 (88%) | 58 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 26 | b | 43/46 (94%) | 43 (100%) | 0 | 100 100 |
| 27 | c | 47/52 (90%) | 47 (100%) | 0 | 100 100 |
| 28 | d | 35/36 (97%) | 35 (100%) | 0 | 100 100 |
| 29 | e | 53/54 (98%) | 52 (98%) | 1 (2%) | 52 71 |
| 30 | f | 35/35 (100%) | 35 (100%) | 0 | 100 100 |
| All | All | 2830/3134 (90%) | 2818 (100%) | 12 (0%) | 88 92 |

All (12) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 4 | 93 | ASP |
| 3 | 4 | 208 | ILE |
| 3 | 4 | 209 | GLU |
| 3 | 4 | 464 | ARG |
| 8 | G | 20 | ASN |
| 8 | G | 51 | ILE |
| 8 | G | 52 | VAL |
| 10 | I | 6 | LYS |
| 13 | M | 49 | MET |
| 19 | T | 44 | ARG |
| 22 | W | 90 | ARG |
| 29 | e | 31 | HIS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | W | 9 | ASN |
| 22 | W | 94 | HIS |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 31 | A | 2947/3120 (94%) | 623 (21%) | 19 (0%) |
| 4 | B | 117/118 (99%) | 34 (29%) | 3 (2%) |
| All | All | 3064/3238 (94%) | 657 (21%) | 22 (0%) |

All (657) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | B | 2 | U |
| 4 | B | 3 | U |
| 4 | B | 4 | A |
| 4 | B | 5 | C |
| 4 | B | 8 | C |
| 4 | B | 9 | G |
| 4 | B | 12 | C |
| 4 | B | 13 | C |
| 4 | B | 14 | A |
| 4 | B | 26 | A |
| 4 | B | 27 | A |
| 4 | B | 28 | A |
| 4 | B | 29 | C |
| 4 | B | 33 | C |
| 4 | B | 34 | G |
| 4 | B | 42 | C |
| 4 | B | 43 | C |
| 4 | B | 44 | C |
| 4 | B | 46 | A |
| 4 | B | 53 | A |
| 4 | B | 57 | U |
| 4 | B | 58 | A |
| 4 | B | 59 | A |
| 4 | B | 67 | A |
| 4 | B | 75 | U |
| 4 | B | 76 | G |
| 4 | B | 88 | C |
| 4 | B | 89 | C |
| 4 | B | 90 | G |
| 4 | B | 107 | A |
| 4 | B | 112 | C |
| 4 | B | 113 | G |
| 4 | B | 115 | A |
| 4 | B | 117 | A |
| 31 | A | 7 | U |
| 31 | A | 9 | U |
| 31 | A | 31 | U |
| 31 | A | 41 | A |
| 31 | A | 42 | G |
| 31 | A | 52 | G |
| 31 | A | 57 | A |
| 31 | A | 60 | A |
| 31 | A | 68 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | A | 71 | A |
| 31 | A | 72 | G |
| 31 | A | 85 | G |
| 31 | A | 86 | U |
| 31 | A | 91 | C |
| 31 | A | 94 | G |
| 31 | A | 99 | G |
| 31 | A | 115 | A |
| 31 | A | 117 | U |
| 31 | A | 125 | C |
| 31 | A | 138 | A |
| 31 | A | 148 | A |
| 31 | A | 153 | G |
| 31 | A | 158 | G |
| 31 | A | 161 | U |
| 31 | A | 162 | A |
| 31 | A | 163 | U |
| 31 | A | 164 | A |
| 31 | A | 180 | A |
| 31 | A | 195 | A |
| 31 | A | 198 | A |
| 31 | A | 199 | U |
| 31 | A | 200 | C |
| 31 | A | 214 | G |
| 31 | A | 215 | A |
| 31 | A | 221 | A |
| 31 | A | 222 | A |
| 31 | A | 227 | A |
| 31 | A | 229 | U |
| 31 | A | 230 | G |
| 31 | A | 233 | A |
| 31 | A | 243 | U |
| 31 | A | 244 | A |
| 31 | A | 248 | G |
| 31 | A | 265 | A |
| 31 | A | 270 | U |
| 31 | A | 271 | A |
| 31 | A | 274 | C |
| 31 | A | 282 | A |
| 31 | A | 285 | U |
| 31 | A | 286 | G |
| 31 | A | 288 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | A | 289 | A |
| 31 | A | 290 | C |
| 31 | A | 291 | C |
| 31 | A | 292 | G |
| 31 | A | 295 | U |
| 31 | A | 296 | A |
| 31 | A | 300 | G |
| 31 | A | 301 | U |
| 31 | A | 302 | U |
| 31 | A | 303 | G |
| 31 | A | 313 | G |
| 31 | A | 314 | G |
| 31 | A | 315 | U |
| 31 | A | 319 | G |
| 31 | A | 326 | A |
| 31 | A | 327 | U |
| 31 | A | 329 | U |
| 31 | A | 330 | U |
| 31 | A | 331 | U |
| 31 | A | 336 | C |
| 31 | A | 337 | U |
| 31 | A | 338 | C |
| 31 | A | 340 | A |
| 31 | A | 342 | C |
| 31 | A | 343 | U |
| 31 | A | 350 | A |
| 31 | A | 352 | G |
| 31 | A | 353 | G |
| 31 | A | 355 | A |
| 31 | A | 356 | G |
| 31 | A | 357 | U |
| 31 | A | 359 | A |
| 31 | A | 361 | A |
| 31 | A | 367 | U |
| 31 | A | 368 | U |
| 31 | A | 369 | G |
| 31 | A | 370 | U |
| 31 | A | 371 | G |
| 31 | A | 372 | G |
| 31 | A | 376 | G |
| 31 | A | 378 | G |
| 31 | A | 379 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | A | 380 | A |
| 31 | A | 381 | A |
| 31 | A | 384 | G |
| 31 | A | 391 | G |
| 31 | A | 393 | U |
| 31 | A | 395 | G |
| 31 | A | 398 | U |
| 31 | A | 401 | C |
| 31 | A | 402 | G |
| 31 | A | 403 | U |
| 31 | A | 404 | A |
| 31 | A | 405 | G |
| 31 | A | 406 | A |
| 31 | A | 411 | G |
| 31 | A | 412 | A |
| 31 | A | 413 | G |
| 31 | A | 420 | G |
| 31 | A | 423 | C |
| 31 | A | 424 | G |
| 31 | A | 426 | G |
| 31 | A | 427 | A |
| 31 | A | 434 | G |
| 31 | A | 437 | G |
| 31 | A | 438 | U |
| 31 | A | 445 | U |
| 31 | A | 446 | G |
| 31 | A | 447 | A |
| 31 | A | 449 | G |
| 31 | A | 452 | G |
| 31 | A | 453 | U |
| 31 | A | 454 | U |
| 31 | A | 459 | A |
| 31 | A | 460 | G |
| 31 | A | 471 | C |
| 31 | A | 474 | G |
| 31 | A | 482 | U |
| 31 | A | 493 | U |
| 31 | A | 494 | G |
| 31 | A | 499 | G |
| 31 | A | 500 | A |
| 31 | A | 503 | A |
| 31 | A | 505 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | A | 509 | U |
| 31 | A | 512 | G |
| 31 | A | 543 | U |
| 31 | A | 544 | U |
| 31 | A | 553 | G |
| 31 | A | 561 | G |
| 31 | A | 569 | G |
| 31 | A | 572 | C |
| 31 | A | 578 | G |
| 31 | A | 591 | G |
| 31 | A | 592 | A |
| 31 | A | 594 | U |
| 31 | A | 595 | A |
| 31 | A | 596 | C |
| 31 | A | 597 | C |
| 31 | A | 599 | G |
| 31 | A | 614 | C |
| 31 | A | 617 | U |
| 31 | A | 618 | C |
| 31 | A | 619 | C |
| 31 | A | 620 | G |
| 31 | A | 636 | U |
| 31 | A | 637 | G |
| 31 | A | 638 | U |
| 31 | A | 639 | C |
| 31 | A | 640 | G |
| 31 | A | 642 | G |
| 31 | A | 655 | G |
| 31 | A | 659 | U |
| 31 | A | 660 | U |
| 31 | A | 662 | G |
| 31 | A | 665 | G |
| 31 | A | 667 | A |
| 31 | A | 678 | A |
| 31 | A | 679 | G |
| 31 | A | 684 | G |
| 31 | A | 696 | A |
| 31 | A | 706 | G |
| 31 | A | 707 | G |
| 31 | A | 708 | G |
| 31 | A | 715 | A |
| 31 | A | 721 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | A | 731 | A |
| 31 | A | 739 | U |
| 31 | A | 740 | A |
| 31 | A | 747 | A |
| 31 | A | 755 | A |
| 31 | A | 757 | G |
| 31 | A | 758 | A |
| 31 | A | 759 | G |
| 31 | A | 760 | U |
| 31 | A | 766 | G |
| 31 | A | 784 | G |
| 31 | A | 801 | U |
| 31 | A | 829 | U |
| 31 | A | 845 | C |
| 31 | A | 862 | U |
| 31 | A | 879 | A |
| 31 | A | 880 | G |
| 31 | A | 890 | G |
| 31 | A | 891 | G |
| 31 | A | 897 | A |
| 31 | A | 899 | G |
| 31 | A | 900 | G |
| 31 | A | 907 | A |
| 31 | A | 920 | G |
| 31 | A | 921 | C |
| 31 | A | 927 | C |
| 31 | A | 928 | U |
| 31 | A | 940 | A |
| 31 | A | 941 | U |
| 31 | A | 942 | U |
| 31 | A | 974 | G |
| 31 | A | 981 | U |
| 31 | A | 982 | A |
| 31 | A | 987 | A |
| 31 | A | 994 | A |
| 31 | A | 995 | U |
| 31 | A | 996 | G |
| 31 | A | 1002 | C |
| 31 | A | 1003 | A |
| 31 | A | 1005 | A |
| 31 | A | 1008 | G |
| 31 | A | 1010 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | A | 1011 | A |
| 31 | A | 1025 | A |
| 31 | A | 1030 | C |
| 31 | A | 1034 | U |
| 31 | A | 1042 | A |
| 31 | A | 1046 | C |
| 31 | A | 1047 | A |
| 31 | A | 1048 | A |
| 31 | A | 1049 | G |
| 31 | A | 1058 | A |
| 31 | A | 1063 | G |
| 31 | A | 1075 | U |
| 31 | A | 1076 | A |
| 31 | A | 1077 | A |
| 31 | A | 1078 | G |
| 31 | A | 1085 | G |
| 31 | A | 1090 | G |
| 31 | A | 1091 | A |
| 31 | A | 1092 | G |
| 31 | A | 1097 | A |
| 31 | A | 1101 | A |
| 31 | A | 1110 | C |
| 31 | A | 1114 | G |
| 31 | A | 1131 | G |
| 31 | A | 1144 | A |
| 31 | A | 1151 | U |
| 31 | A | 1159 | C |
| 31 | A | 1160 | G |
| 31 | A | 1161 | C |
| 31 | A | 1162 | G |
| 31 | A | 1164 | A |
| 31 | A | 1165 | G |
| 31 | A | 1170 | C |
| 31 | A | 1172 | A |
| 31 | A | 1173 | G |
| 31 | A | 1175 | A |
| 31 | A | 1176 | G |
| 31 | A | 1177 | G |
| 31 | A | 1178 | U |
| 31 | A | 1179 | U |
| 31 | A | 1180 | G |
| 31 | A | 1181 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | A | 1182 | C |
| 31 | A | 1184 | U |
| 31 | A | 1188 | A |
| 31 | A | 1189 | G |
| 31 | A | 1191 | A |
| 31 | A | 1192 | G |
| 31 | A | 1194 | C |
| 31 | A | 1197 | C |
| 31 | A | 1201 | G |
| 31 | A | 1202 | A |
| 31 | A | 1203 | A |
| 31 | A | 1204 | A |
| 31 | A | 1205 | G |
| 31 | A | 1206 | A |
| 31 | A | 1207 | G |
| 31 | A | 1208 | U |
| 31 | A | 1212 | U |
| 31 | A | 1213 | A |
| 31 | A | 1214 | A |
| 31 | A | 1215 | U |
| 31 | A | 1216 | A |
| 31 | A | 1217 | G |
| 31 | A | 1222 | C |
| 31 | A | 1223 | U |
| 31 | A | 1224 | G |
| 31 | A | 1240 | G |
| 31 | A | 1245 | U |
| 31 | A | 1247 | A |
| 31 | A | 1248 | U |
| 31 | A | 1250 | U |
| 31 | A | 1253 | C |
| 31 | A | 1254 | G |
| 31 | A | 1260 | C |
| 31 | A | 1262 | A |
| 31 | A | 1277 | C |
| 31 | A | 1292 | U |
| 31 | A | 1293 | G |
| 31 | A | 1294 | U |
| 31 | A | 1295 | U |
| 31 | A | 1307 | G |
| 31 | A | 1316 | U |
| 31 | A | 1335 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | A | 1343 | G |
| 31 | A | 1344 | A |
| 31 | A | 1351 | G |
| 31 | A | 1365 | G |
| 31 | A | 1368 | A |
| 31 | A | 1371 | G |
| 31 | A | 1377 | A |
| 31 | A | 1386 | G |
| 31 | A | 1387 | A |
| 31 | A | 1400 | G |
| 31 | A | 1403 | C |
| 31 | A | 1408 | C |
| 31 | A | 1415 | A |
| 31 | A | 1416 | A |
| 31 | A | 1436 | C |
| 31 | A | 1465 | C |
| 31 | A | 1466 | C |
| 31 | A | 1467 | U |
| 31 | A | 1480 | A |
| 31 | A | 1494 | U |
| 31 | A | 1499 | A |
| 31 | A | 1501 | C |
| 31 | A | 1502 | G |
| 31 | A | 1510 | A |
| 31 | A | 1511 | U |
| 31 | A | 1527 | U |
| 31 | A | 1532 | G |
| 31 | A | 1534 | C |
| 31 | A | 1536 | A |
| 31 | A | 1538 | G |
| 31 | A | 1541 | G |
| 31 | A | 1542 | A |
| 31 | A | 1543 | A |
| 31 | A | 1544 | U |
| 31 | A | 1624 | U |
| 31 | A | 1629 | G |
| 31 | A | 1631 | A |
| 31 | A | 1632 | G |
| 31 | A | 1640 | A |
| 31 | A | 1648 | A |
| 31 | A | 1649 | C |
| 31 | A | 1679 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | A | 1680 | A |
| 31 | A | 1681 | U |
| 31 | A | 1703 | G |
| 31 | A | 1710 | A |
| 31 | A | 1711 | G |
| 31 | A | 1712 | G |
| 31 | A | 1713 | U |
| 31 | A | 1714 | A |
| 31 | A | 1717 | U |
| 31 | A | 1729 | A |
| 31 | A | 1730 | U |
| 31 | A | 1737 | A |
| 31 | A | 1738 | G |
| 31 | A | 1753 | C |
| 31 | A | 1754 | G |
| 31 | A | 1755 | A |
| 31 | A | 1756 | G |
| 31 | A | 1769 | G |
| 31 | A | 1780 | G |
| 31 | A | 1786 | G |
| 31 | A | 1788 | G |
| 31 | A | 1789 | A |
| 31 | A | 1798 | U |
| 31 | A | 1803 | A |
| 31 | A | 1811 | C |
| 31 | A | 1825 | C |
| 31 | A | 1826 | A |
| 31 | A | 1828 | A |
| 31 | A | 1831 | A |
| 31 | A | 1852 | A |
| 31 | A | 1864 | U |
| 31 | A | 1866 | C |
| 31 | A | 1869 | G |
| 31 | A | 1870 | U |
| 31 | A | 1871 | G |
| 31 | A | 1872 | A |
| 31 | A | 1884 | G |
| 31 | A | 1887 | A |
| 31 | A | 1891 | G |
| 31 | A | 1892 | G |
| 31 | A | 1911 | U |
| 31 | A | 1933 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | A | 1945 | U |
| 31 | A | 1946 | U |
| 31 | A | 1947 | U |
| 31 | A | 1949 | C |
| 31 | A | 1950 | G |
| 31 | A | 1955 | A |
| 31 | A | 1967 | G |
| 31 | A | 1974 | A |
| 31 | A | 1975 | A |
| 31 | A | 1981 | U |
| 31 | A | 1990 | A |
| 31 | A | 2001 | A |
| 31 | A | 2017 | C |
| 31 | A | 2018 | G |
| 31 | A | 2025 | C |
| 31 | A | 2033 | U |
| 31 | A | 2046 | A |
| 31 | A | 2049 | C |
| 31 | A | 2051 | U |
| 31 | A | 2052 | G |
| 31 | A | 2053 | C |
| 31 | A | 2055 | C |
| 31 | A | 2152 | A |
| 31 | A | 2153 | G |
| 31 | A | 2154 | G |
| 31 | A | 2155 | U |
| 31 | A | 2156 | A |
| 31 | A | 2158 | C |
| 31 | A | 2159 | G |
| 31 | A | 2160 | A |
| 31 | A | 2162 | A |
| 31 | A | 2163 | U |
| 31 | A | 2164 | U |
| 31 | A | 2165 | C |
| 31 | A | 2166 | C |
| 31 | A | 2167 | U |
| 31 | A | 2168 | U |
| 31 | A | 2169 | G |
| 31 | A | 2170 | U |
| 31 | A | 2171 | C |
| 31 | A | 2176 | A |
| 31 | A | 2177 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | A | 2178 | G |
| 31 | A | 2182 | C |
| 31 | A | 2184 | A |
| 31 | A | 2186 | C |
| 31 | A | 2188 | G |
| 31 | A | 2189 | C |
| 31 | A | 2190 | A |
| 31 | A | 2191 | C |
| 31 | A | 2192 | G |
| 31 | A | 2193 | A |
| 31 | A | 2194 | A |
| 31 | A | 2195 | U |
| 31 | A | 2196 | G |
| 31 | A | 2197 | G |
| 31 | A | 2215 | U |
| 31 | A | 2217 | U |
| 31 | A | 2220 | C |
| 31 | A | 2221 | A |
| 31 | A | 2246 | U |
| 31 | A | 2247 | A |
| 31 | A | 2255 | A |
| 31 | A | 2256 | G |
| 31 | A | 2257 | A |
| 31 | A | 2258 | U |
| 31 | A | 2267 | C |
| 31 | A | 2275 | A |
| 31 | A | 2279 | C |
| 31 | A | 2280 | G |
| 31 | A | 2284 | A |
| 31 | A | 2285 | G |
| 31 | A | 2286 | A |
| 31 | A | 2315 | U |
| 31 | A | 2316 | G |
| 31 | A | 2320 | C |
| 31 | A | 2321 | U |
| 31 | A | 2323 | G |
| 31 | A | 2325 | U |
| 31 | A | 2326 | A |
| 31 | A | 2331 | U |
| 31 | A | 2332 | U |
| 31 | A | 2333 | G |
| 31 | A | 2335 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | A | 2336 | U |
| 31 | A | 2338 | G |
| 31 | A | 2339 | G |
| 31 | A | 2340 | A |
| 31 | A | 2341 | U |
| 31 | A | 2342 | A |
| 31 | A | 2343 | G |
| 31 | A | 2345 | U |
| 31 | A | 2348 | G |
| 31 | A | 2349 | A |
| 31 | A | 2350 | G |
| 31 | A | 2351 | A |
| 31 | A | 2353 | U |
| 31 | A | 2354 | G |
| 31 | A | 2355 | U |
| 31 | A | 2356 | G |
| 31 | A | 2357 | A |
| 31 | A | 2361 | U |
| 31 | A | 2362 | C |
| 31 | A | 2367 | G |
| 31 | A | 2368 | C |
| 31 | A | 2369 | C |
| 31 | A | 2370 | A |
| 31 | A | 2373 | G |
| 31 | A | 2375 | G |
| 31 | A | 2377 | G |
| 31 | A | 2380 | G |
| 31 | A | 2382 | G |
| 31 | A | 2384 | C |
| 31 | A | 2387 | U |
| 31 | A | 2388 | G |
| 31 | A | 2390 | U |
| 31 | A | 2391 | G |
| 31 | A | 2392 | A |
| 31 | A | 2393 | A |
| 31 | A | 2394 | A |
| 31 | A | 2395 | U |
| 31 | A | 2396 | A |
| 31 | A | 2398 | C |
| 31 | A | 2400 | C |
| 31 | A | 2402 | C |
| 31 | A | 2403 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | A | 2404 | G |
| 31 | A | 2405 | A |
| 31 | A | 2410 | A |
| 31 | A | 2415 | G |
| 31 | A | 2422 | A |
| 31 | A | 2427 | G |
| 31 | A | 2434 | A |
| 31 | A | 2436 | A |
| 31 | A | 2449 | A |
| 31 | A | 2462 | G |
| 31 | A | 2463 | G |
| 31 | A | 2470 | A |
| 31 | A | 2507 | C |
| 31 | A | 2510 | A |
| 31 | A | 2511 | A |
| 31 | A | 2512 | A |
| 31 | A | 2529 | A |
| 31 | A | 2530 | C |
| 31 | A | 2531 | G |
| 31 | A | 2532 | G |
| 31 | A | 2533 | C |
| 31 | A | 2534 | A |
| 31 | A | 2540 | G |
| 31 | A | 2546 | A |
| 31 | A | 2549 | G |
| 31 | A | 2558 | C |
| 31 | A | 2559 | A |
| 31 | A | 2571 | C |
| 31 | A | 2574 | C |
| 31 | A | 2585 | U |
| 31 | A | 2601 | A |
| 31 | A | 2607 | G |
| 31 | A | 2609 | A |
| 31 | A | 2620 | G |
| 31 | A | 2623 | A |
| 31 | A | 2647 | U |
| 31 | A | 2649 | A |
| 31 | A | 2652 | G |
| 31 | A | 2653 | G |
| 31 | A | 2654 | A |
| 31 | A | 2665 | C |
| 31 | A | 2672 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | A | 2693 | A |
| 31 | A | 2699 | C |
| 31 | A | 2700 | A |
| 31 | A | 2703 | U |
| 31 | A | 2704 | C |
| 31 | A | 2715 | U |
| 31 | A | 2726 | G |
| 31 | A | 2729 | G |
| 31 | A | 2730 | U |
| 31 | A | 2737 | G |
| 31 | A | 2742 | A |
| 31 | A | 2744 | C |
| 31 | A | 2753 | G |
| 31 | A | 2755 | A |
| 31 | A | 2758 | A |
| 31 | A | 2766 | A |
| 31 | A | 2775 | C |
| 31 | A | 2776 | U |
| 31 | A | 2777 | G |
| 31 | A | 2778 | U |
| 31 | A | 2779 | U |
| 31 | A | 2789 | A |
| 31 | A | 2790 | A |
| 31 | A | 2791 | G |
| 31 | A | 2796 | A |
| 31 | A | 2801 | A |
| 31 | A | 2826 | A |
| 31 | A | 2833 | U |
| 31 | A | 2834 | C |
| 31 | A | 2837 | U |
| 31 | A | 2839 | U |
| 31 | A | 2847 | G |
| 31 | A | 2854 | A |
| 31 | A | 2878 | A |
| 31 | A | 2884 | A |
| 31 | A | 2885 | G |
| 31 | A | 2893 | G |
| 31 | A | 2915 | C |
| 31 | A | 2926 | A |
| 31 | A | 2936 | C |
| 31 | A | 2938 | G |
| 31 | A | 2950 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | A | 2957 | A |
| 31 | A | 2964 | A |
| 31 | A | 2968 | G |
| 31 | A | 2972 | A |
| 31 | A | 2982 | A |
| 31 | A | 2989 | A |
| 31 | A | 3002 | A |
| 31 | A | 3013 | C |
| 31 | A | 3015 | C |
| 31 | A | 3021 | A |
| 31 | A | 3022 | G |
| 31 | A | 3023 | G |
| 31 | A | 3024 | A |
| 31 | A | 3029 | U |
| 31 | A | 3042 | A |
| 31 | A | 3082 | U |
| 31 | A | 3088 | C |
| 31 | A | 3093 | A |
| 31 | A | 3101 | C |
| 31 | A | 3104 | A |
| 31 | A | 3105 | C |
| 31 | A | 3108 | G |
| 31 | A | 3112 | A |
| 31 | A | 3115 | A |
| 31 | A | 3119 | A |
| 31 | A | 3120 | C |

All (22) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | B | 2 | U |
| 4 | B | 28 | A |
| 4 | B | 33 | C |
| 31 | A | 137 | G |
| 31 | A | 199 | U |
| 31 | A | 228 | A |
| 31 | A | 326 | A |
| 31 | A | 448 | U |
| 31 | A | 571 | A |
| 31 | A | 879 | A |
| 31 | A | 899 | G |
| 31 | A | 940 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | A | 942 | U |
| 31 | A | 980 | C |
| 31 | A | 981 | U |
| 31 | A | 1163 | A |
| 31 | A | 1196 | C |
| 31 | A | 1204 | A |
| 31 | A | 2050 | C |
| 31 | A | 2339 | G |
| 31 | A | 2356 | G |
| 31 | A | 2381 | 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 oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 33 | CLM | A | 3201 | - | 20,20,20 | 0.76 | 1 (5%) | 23,27,27 | 1.57 | 4 (17%) |
| 32 | GCP | 4 | 501 | - | 27,34,34 | 1.29 | 4 (14%) | 35,54,54 | 1.88 | 7 (20%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 33 | CLM | A | 3201 | - | - | 3/20/22/22 | 0/1/1/1 |
| 32 | GCP | 4 | 501 | - | - | 2/15/38/38 | 0/3/3/3 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 32 | 4 | 501 | GCP | C5-C6 | 3.49 | 1.47 | 1.41 |
| 32 | 4 | 501 | GCP | PG-O3G | 2.62 | 1.60 | 1.55 |
| 32 | 4 | 501 | GCP | PG-O2G | 2.36 | 1.60 | 1.55 |
| 33 | A | 3201 | CLM | O9A-N9 | -2.13 | 1.21 | 1.35 |
| 32 | 4 | 501 | GCP | PB-O1B | -2.01 | 1.46 | 1.51 |

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 32 | 4 | 501 | GCP | PB-O3A-PA | -4.93 | 116.28 | 132.37 |
| 32 | 4 | 501 | GCP | C2-N3-C4 | 4.91 | 120.78 | 115.48 |
| 32 | 4 | 501 | GCP | C2-N1-C6 | 4.36 | 122.02 | 115.96 |
| 33 | A | 3201 | CLM | C3-N2-C2 | -4.20 | 115.94 | 123.25 |
| 33 | A | 3201 | CLM | C5-C3-N2 | 3.66 | 116.64 | 110.03 |
| 32 | 4 | 501 | GCP | C5-C6-N1 | -3.55 | 118.67 | 123.42 |
| 32 | 4 | 501 | GCP | N3-C2-N1 | -3.45 | 122.83 | 127.21 |
| 33 | A | 3201 | CLM | C6-C5-C3 | 3.35 | 117.73 | 111.72 |
| 32 | 4 | 501 | GCP | C4-C5-C6 | -2.99 | 116.66 | 121.23 |
| 33 | A | 3201 | CLM | O5-C5-C3 | 2.53 | 114.62 | 107.90 |
| 32 | 4 | 501 | GCP | C4-C5-N7 | -2.28 | 106.93 | 109.34 |

There are no chirality outliers.

All (5) torsion outliers are listed below:

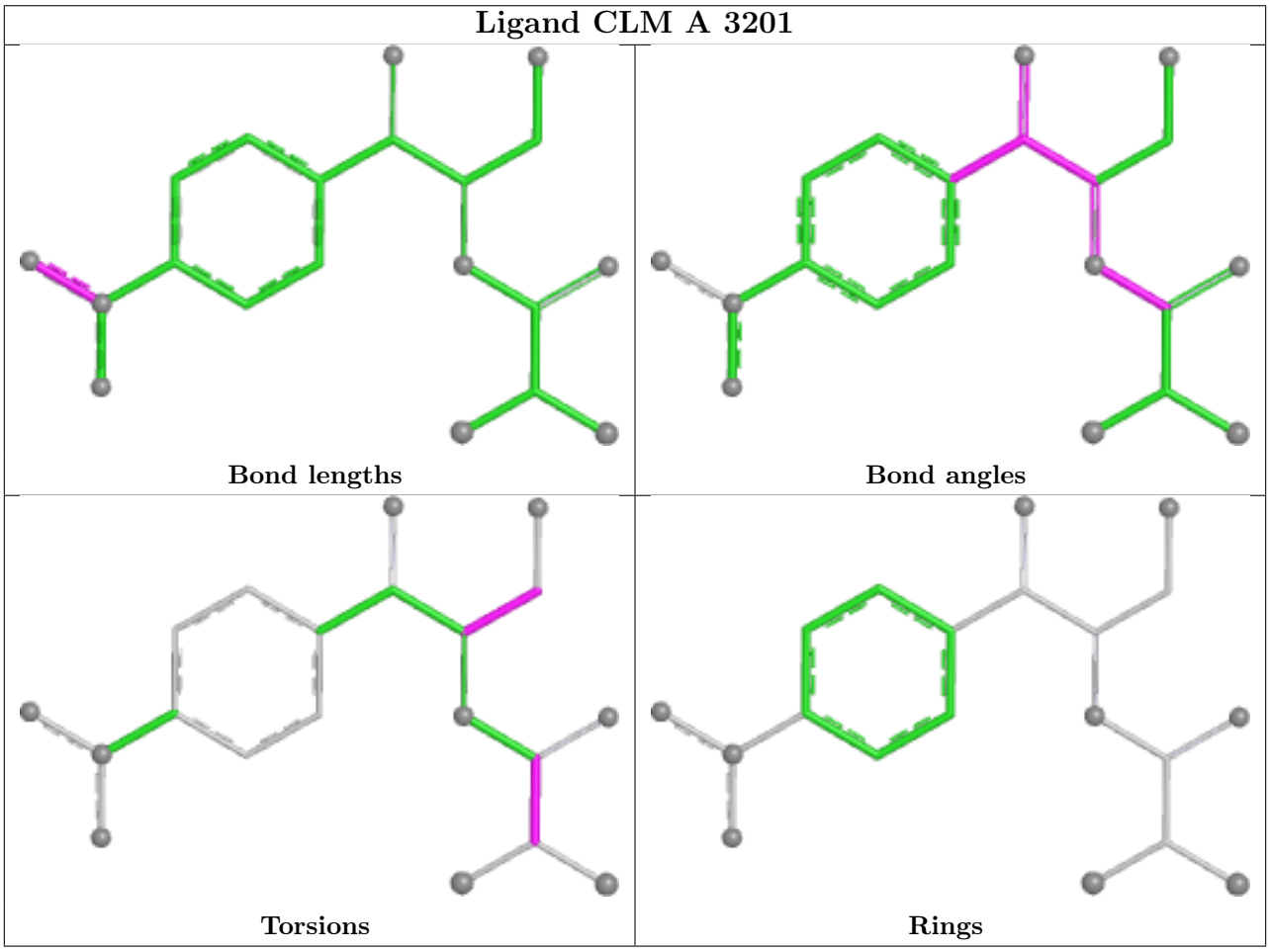
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 33 | A | 3201 | CLM | CL2-C1-C2-N2 |
| 32 | 4 | 501 | GCP | C4'-C5'-O5'-PA |
| 33 | A | 3201 | CLM | N2-C3-C4-O4 |
| 32 | 4 | 501 | GCP | O4'-C4'-C5'-O5' |
| 33 | A | 3201 | CLM | CL2-C1-C2-O2 |

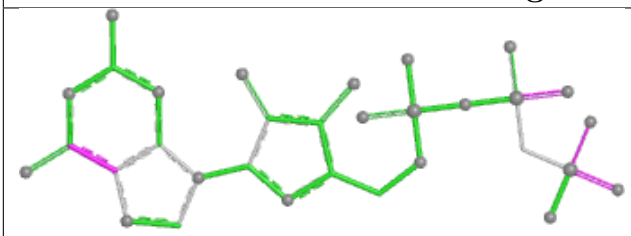
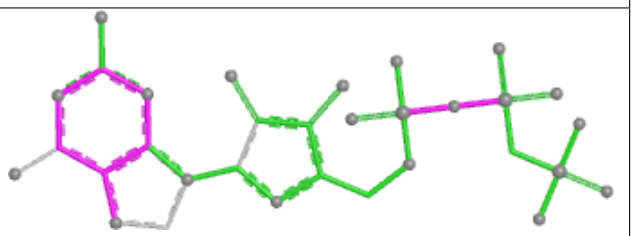
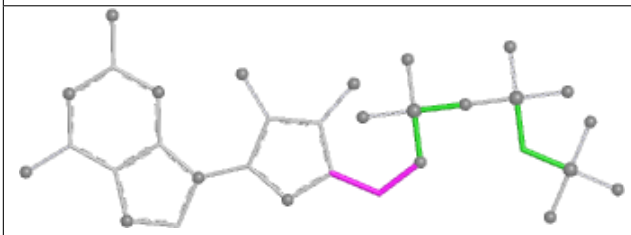
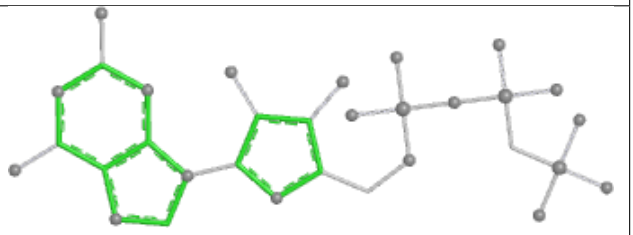
There are no ring outliers.

2 monomers are involved in 7 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 33 | A | 3201 | CLM | 4 | 0 |
| 32 | 4 | 501 | GCP | 3 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



| Ligand GCP 4 501 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

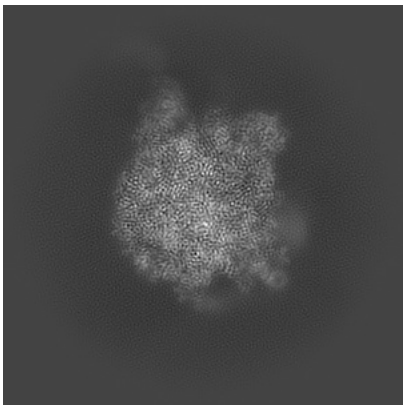
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43477. These allow visual inspection of the internal detail of the map and identification of artifacts.

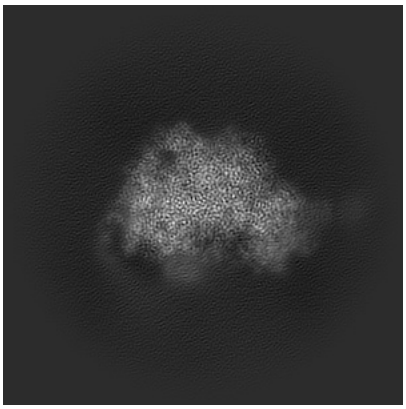
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

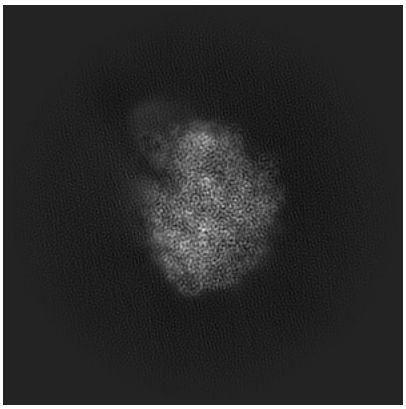
### 6.1.1 Primary map



X

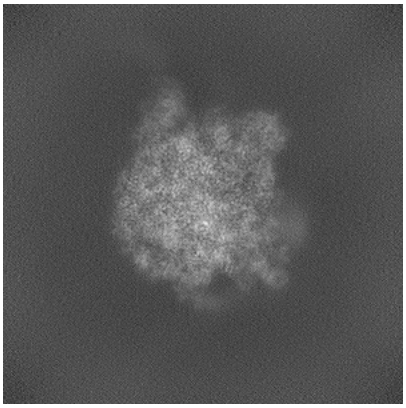


Y

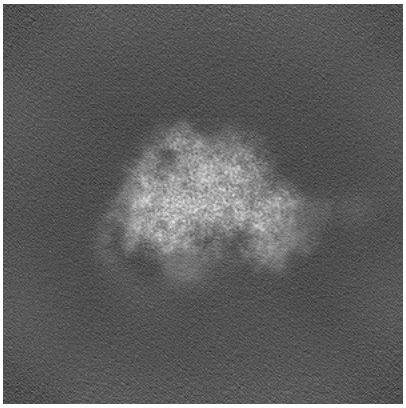


Z

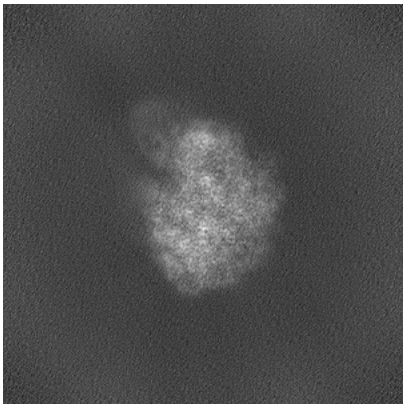
### 6.1.2 Raw map



X



Y

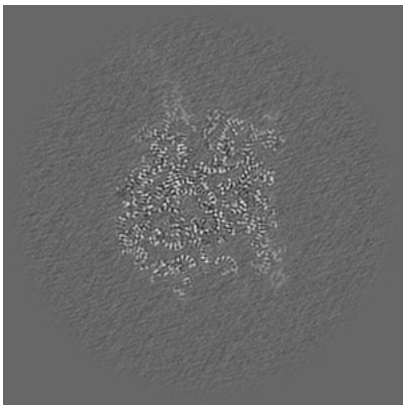


Z

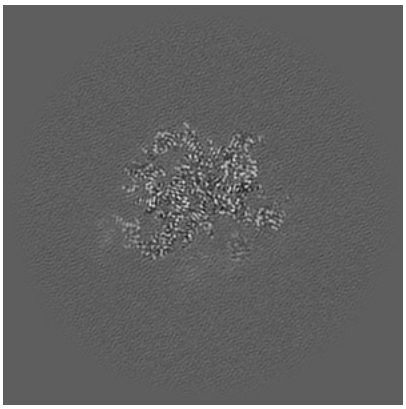
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

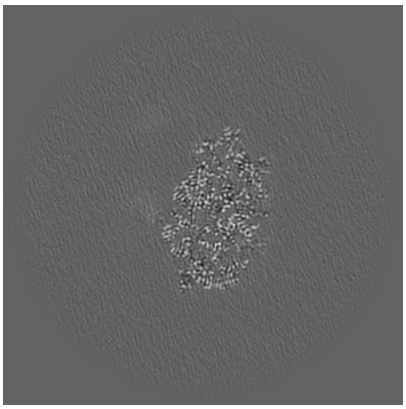
### 6.2.1 Primary map



X Index: 256

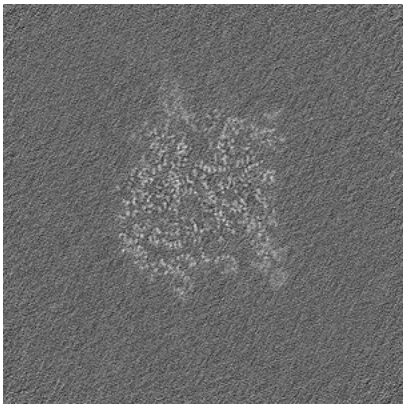


Y Index: 256

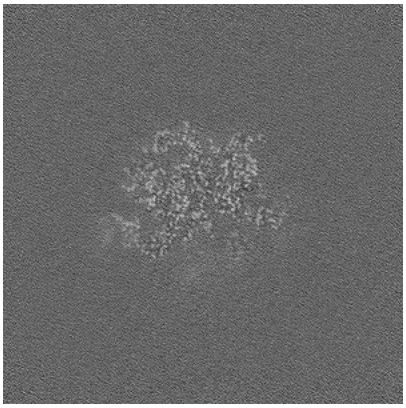


Z Index: 256

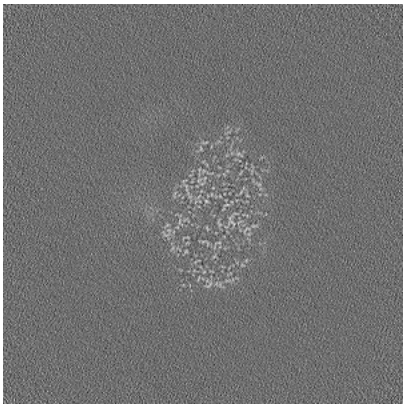
### 6.2.2 Raw map



X Index: 256



Y Index: 256

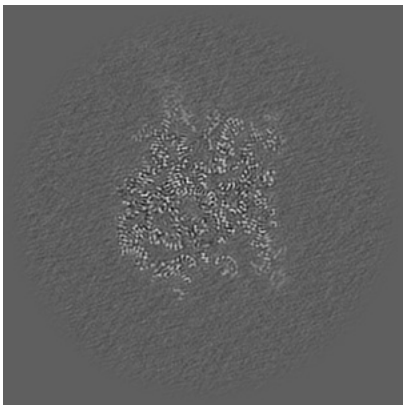


Z Index: 256

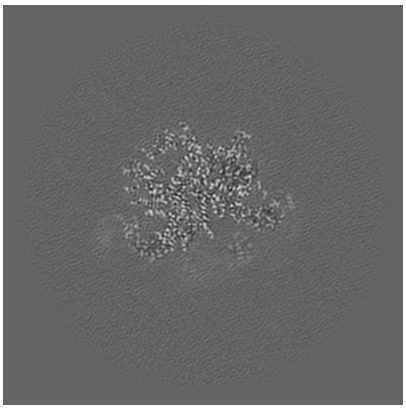
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

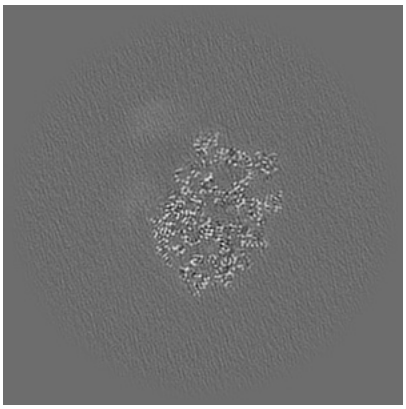
### 6.3.1 Primary map



X Index: 255

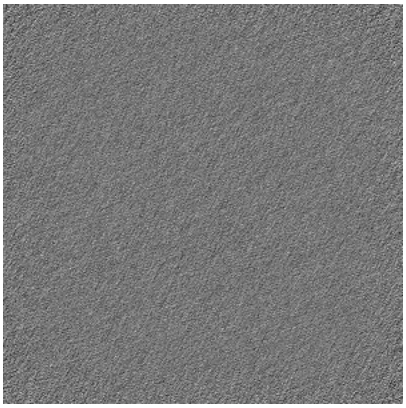


Y Index: 258

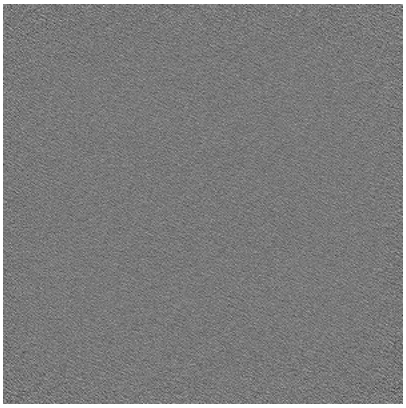


Z Index: 238

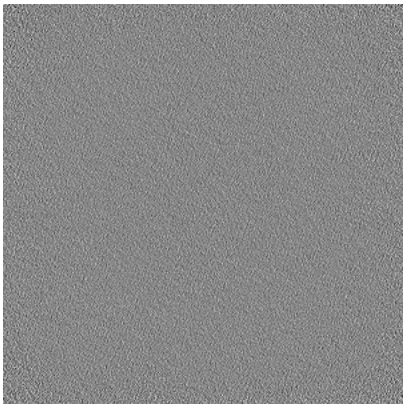
### 6.3.2 Raw map



X Index: 0



Y Index: 0

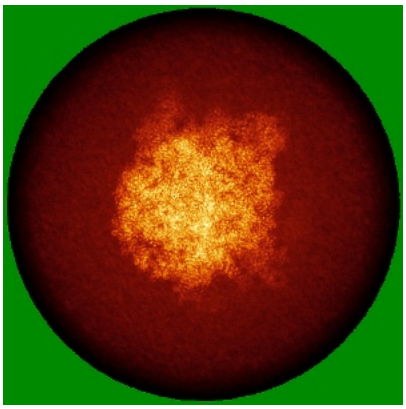


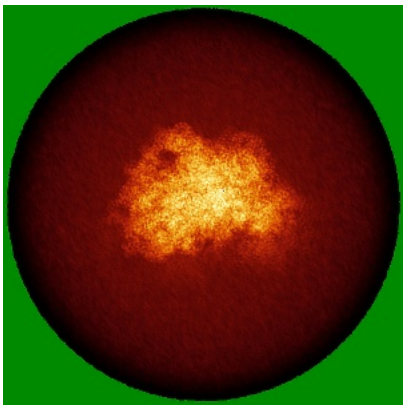
Z Index: 0

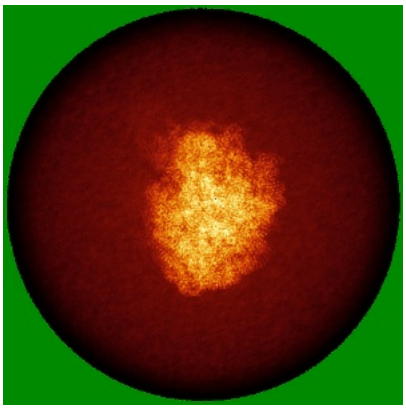
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) (i)

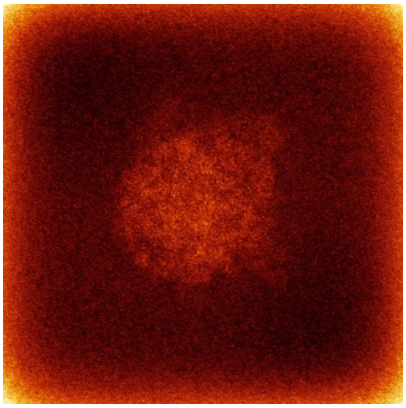
### 6.4.1 Primary map

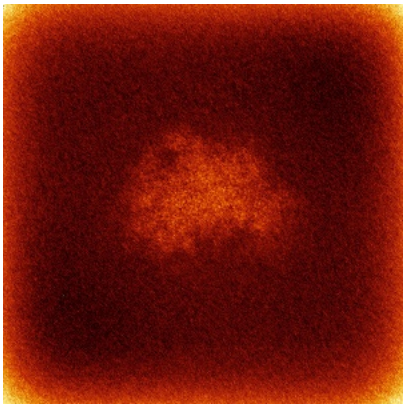

X

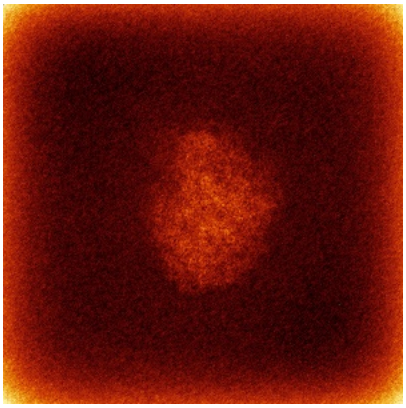

Y


Z

### 6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

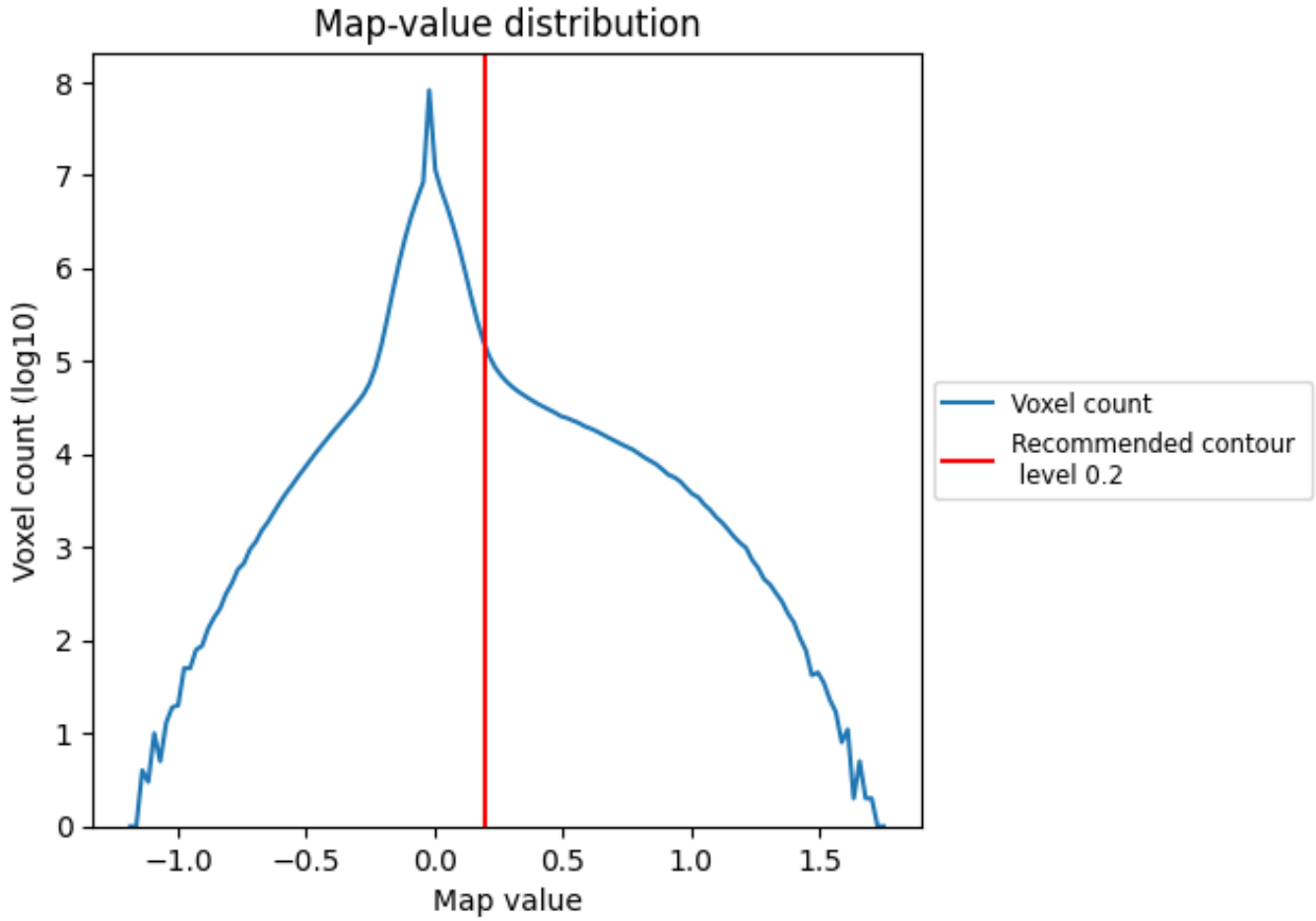
## 6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

# 7 Map analysis

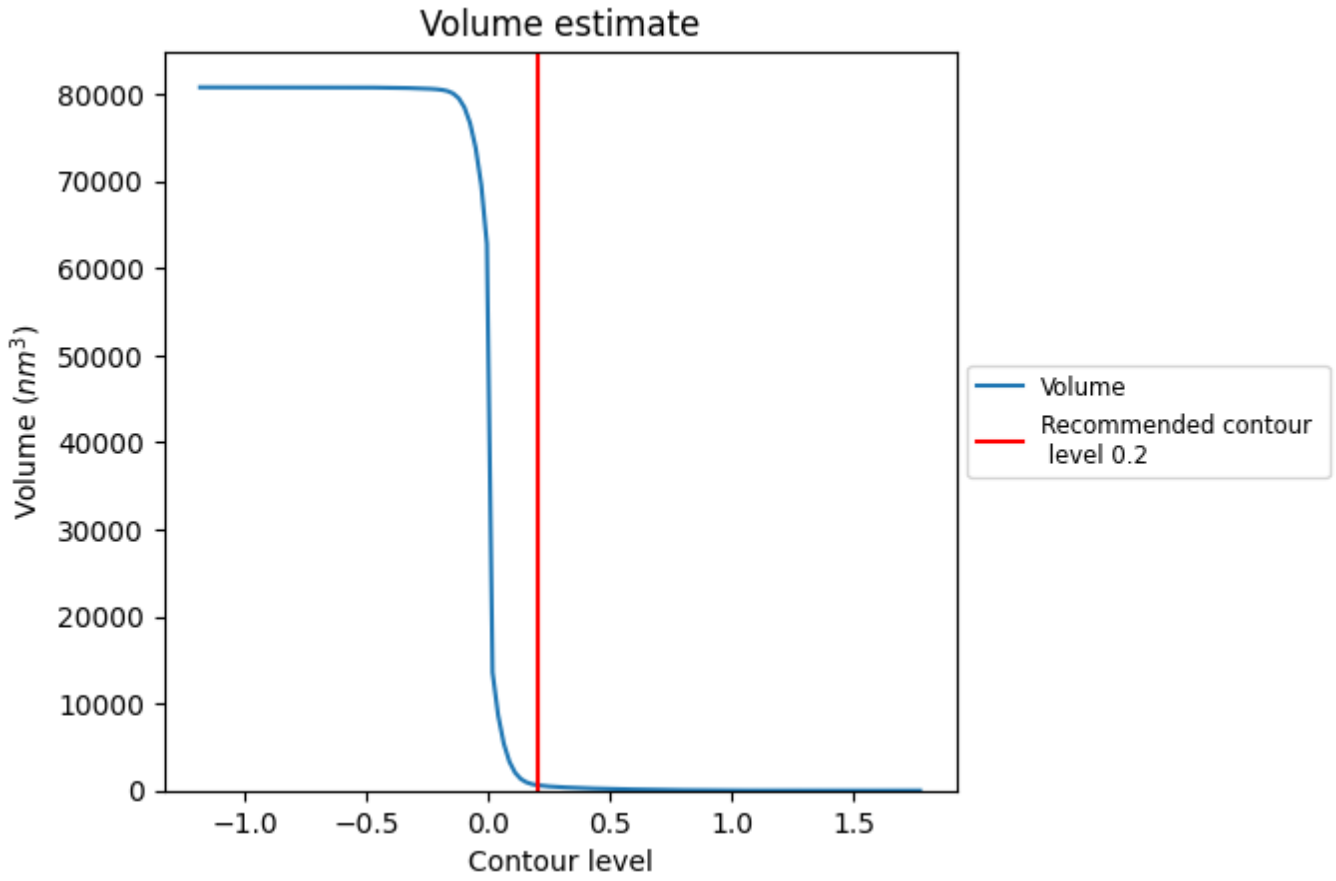
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

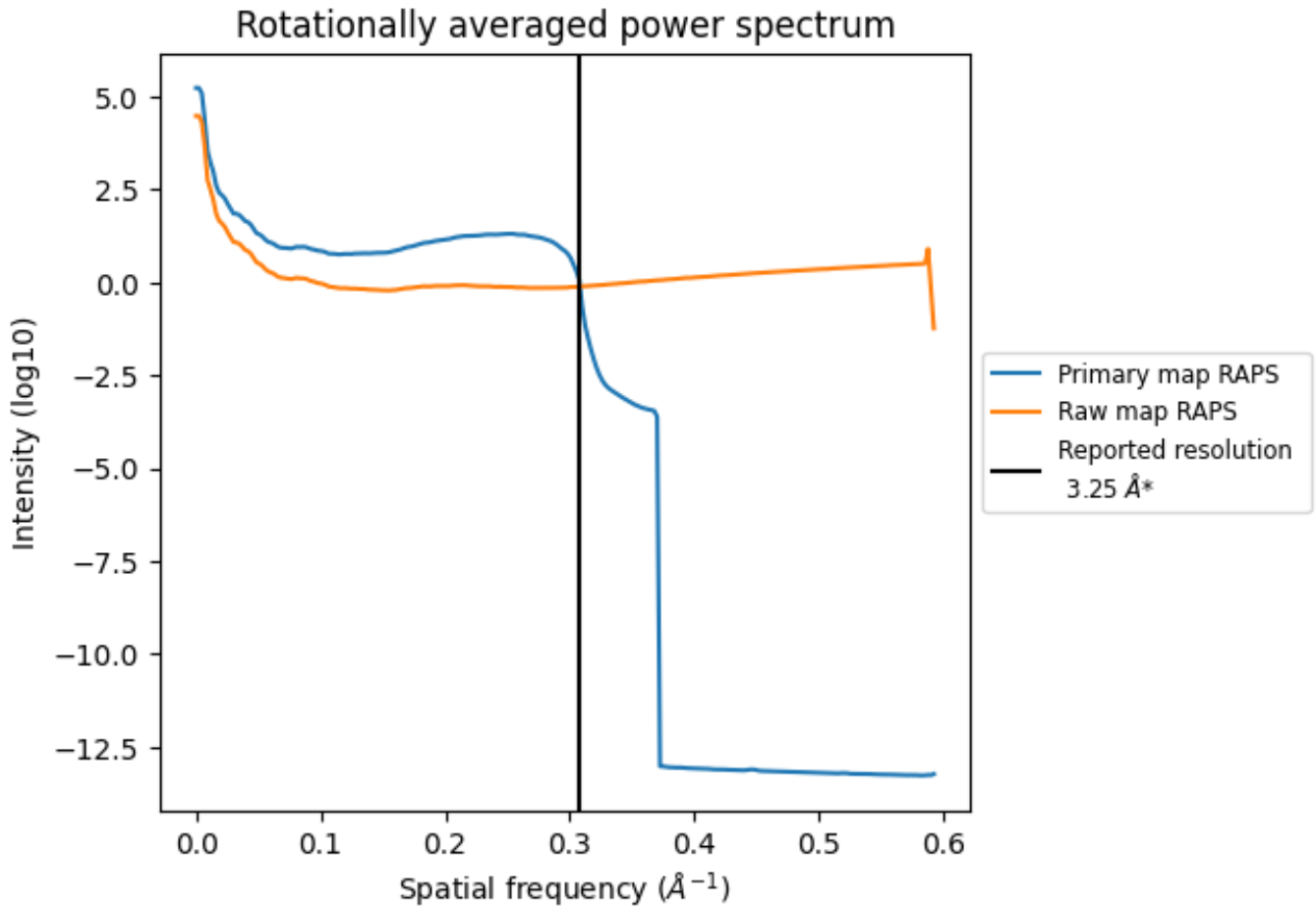
## 7.2 Volume estimate




The volume at the recommended contour level is 633 $nm^3$; this corresponds to an approximate mass of 571 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum (i)

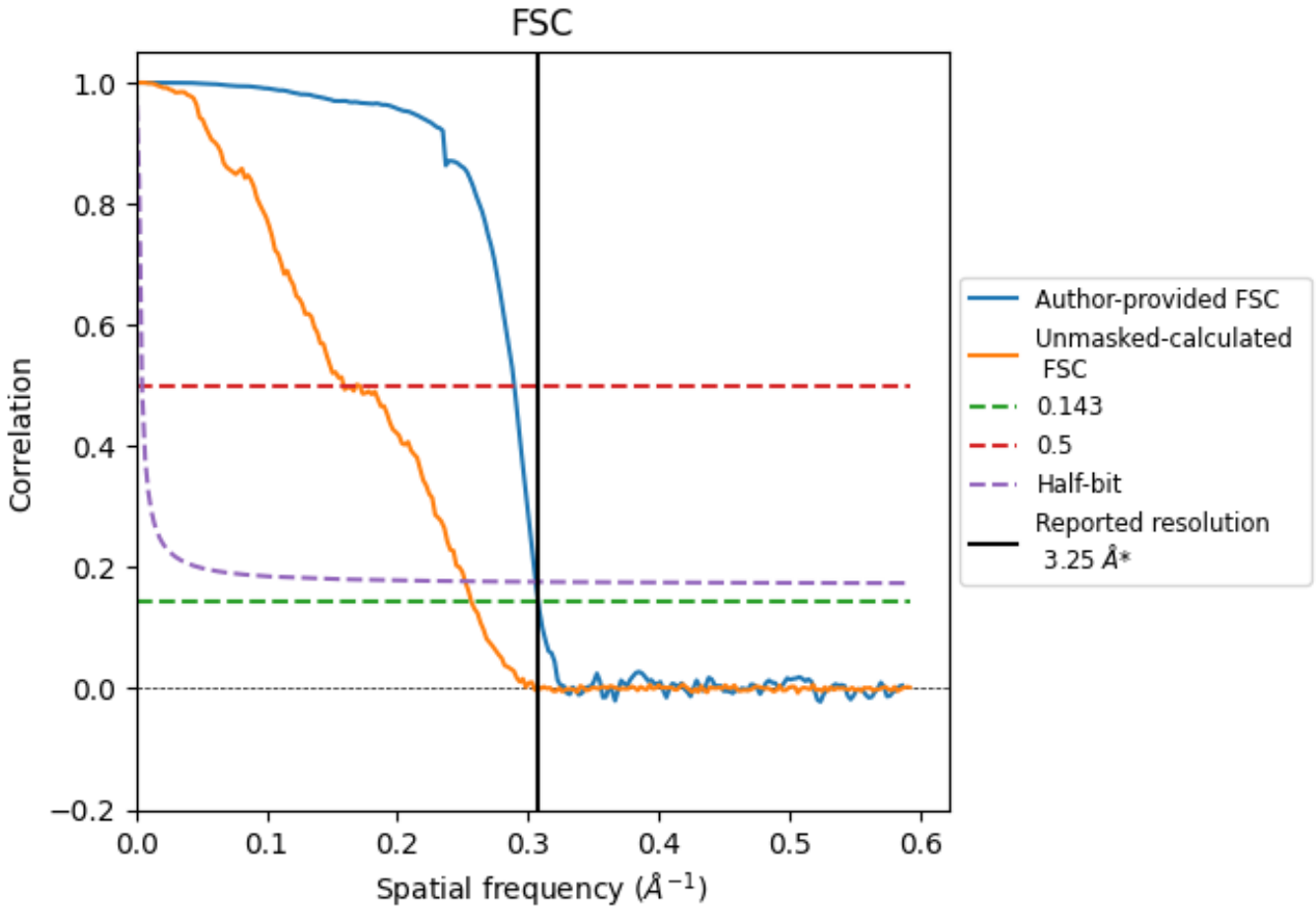



*Reported resolution corresponds to spatial frequency of 0.308 $Å^{-1}$

# 8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.308 Å$^{-1}$

## 8.2 Resolution estimates (i)

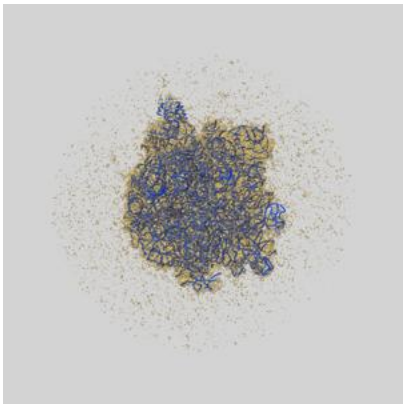
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.25 | - | - |
| Author-provided FSC curve | 3.25 | 3.45 | 3.27 |
| Unmasked-calculated* | 3.90 | 6.29 | 3.97 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.90 differs from the reported value 3.25 by more than 10 %

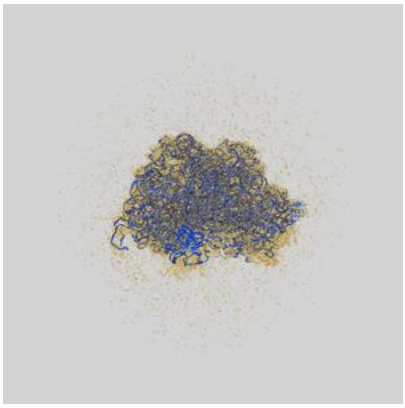
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43477 and PDB model 8VR8. Per-residue inclusion information can be found in section 3 on page 10.

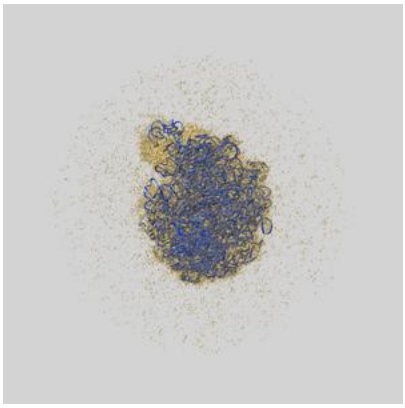
## 9.1 Map-model overlay



X



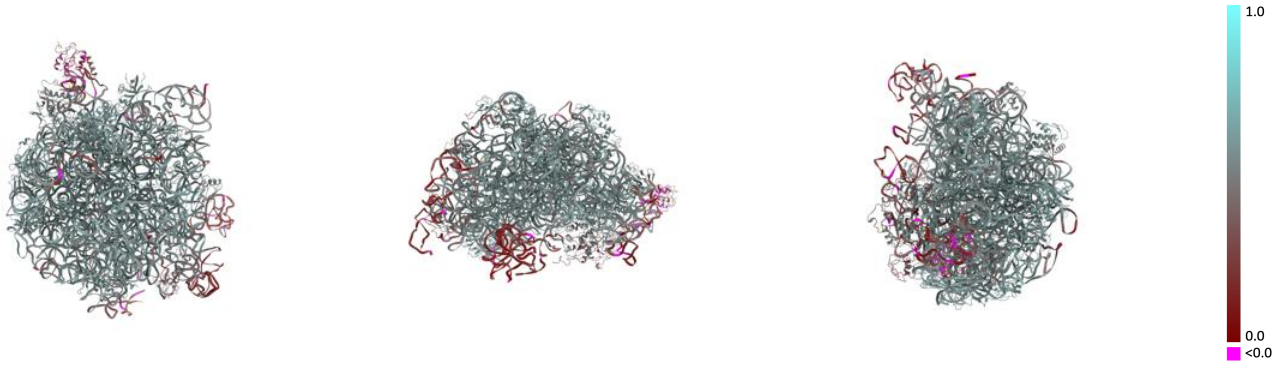
Y



Z

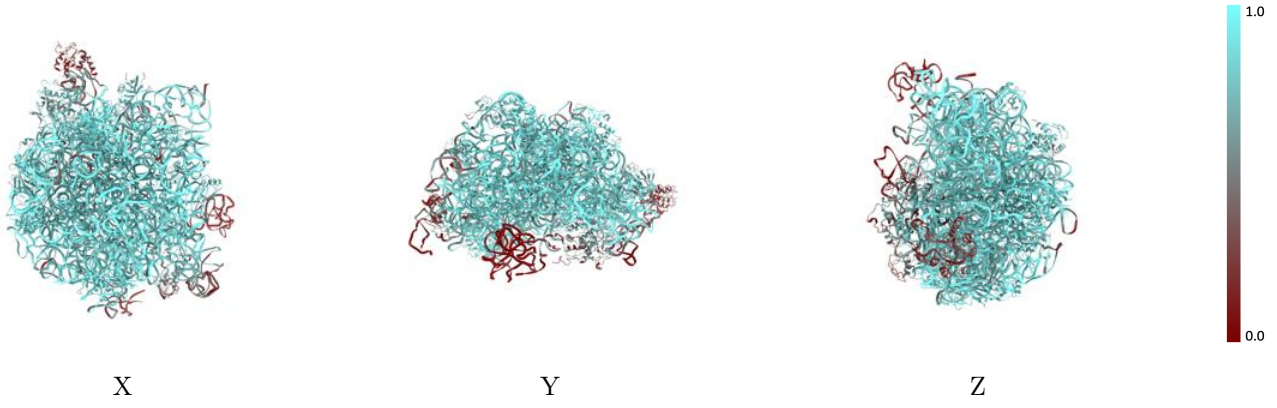
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model (i)



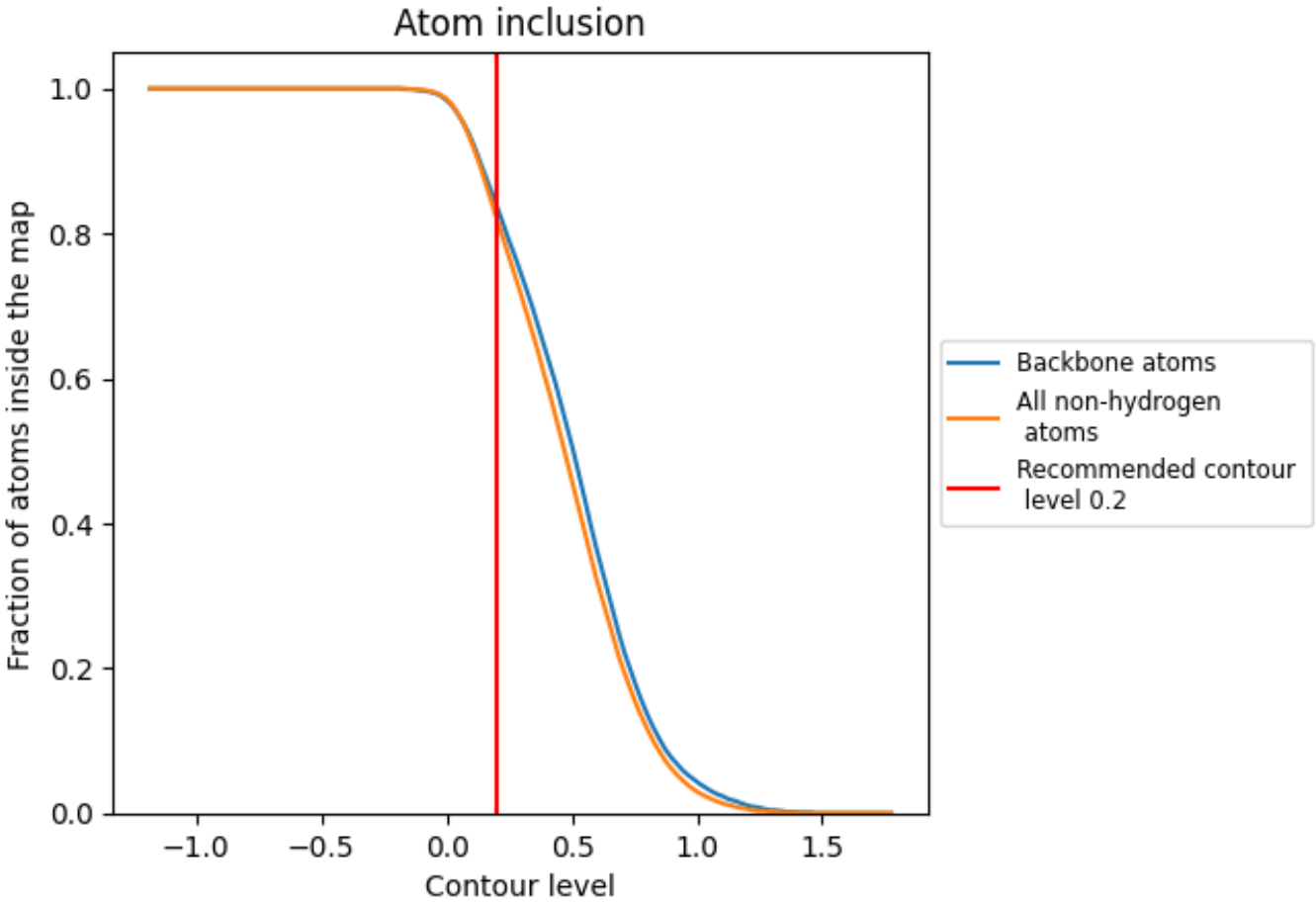

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model (i)




The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

## 9.4 Atom inclusion (i)




At the recommended contour level, 84% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8220 | 0.5120 |
| 2 | 0.8740 | 0.5680 |
| 3 | 0.8990 | 0.5840 |
| 4 | 0.5370 | 0.4270 |
| A | 0.8400 | 0.5070 |
| B | 0.8350 | 0.4910 |
| C | 0.8570 | 0.5670 |
| D | 0.8880 | 0.5820 |
| E | 0.8560 | 0.5630 |
| G | 0.7300 | 0.5010 |
| H | 0.4990 | 0.4260 |
| I | 0.1200 | 0.1720 |
| K | 0.8960 | 0.5790 |
| L | 0.8780 | 0.5730 |
| M | 0.8680 | 0.5670 |
| N | 0.8790 | 0.5710 |
| O | 0.8980 | 0.5730 |
| Q | 0.8100 | 0.5570 |
| R | 0.9010 | 0.5740 |
| S | 0.8870 | 0.5830 |
| T | 0.8730 | 0.5700 |
| U | 0.8310 | 0.5620 |
| V | 0.7680 | 0.5150 |
| W | 0.7550 | 0.5310 |
| X | 0.8590 | 0.5690 |
| Y | 0.8740 | 0.5630 |
| Z | 0.8220 | 0.5260 |
| b | 0.8710 | 0.5720 |
| c | 0.8730 | 0.5580 |
| d | 0.9170 | 0.5810 |
| e | 0.9080 | 0.5780 |
| f | 0.8950 | 0.5810 |