# Scientific test: Protein Data Bank diagnostic

## ## AUTHOR AND DATE

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## FAILURES

The PDB diagnostic was run on **191,312** PDB files. **189,825** files passed the test and **1,487** failed!

## ## PURPOSE OF THE TEST

This test tries to load every PDB file in the PDB database and classifies the failures that occur. The command line below shows what was done; broadly all versions of this test examine load-time problems and more expensive versions (`-PDB_diagnostic::skip_pack_and_min false`) also check for errors during scoring, packing, and minimization.

*"Hunting down these bugs is the most fun thing you can do on a Thursday morning"* - Andy Watkins, probably.

An individual PDB passes or fails this test based on whether it errors out or completes the diagnostic. The test as a whole passes or fails based on a "reference results" system, like an expected result in a unit test. About 700 PDBs and 1200 CIFs fail at the time of this writing; the purpose of the test is to document the failures and watch for new ones, so PDBs failing in an expected manner does not constitute an overall test failure. The test will fail if PDBs pass or fail **UNEXPECTEDLY**, where the expectation is defined by the reference results (see below).

If you find that this page is telling you the test failed because there are **FEWER** errors: **GREAT**! You fixed some bugs! You can update the reference results following the instructions at the bottom of the page.

If you find that there are **MORE** failures than expected, especially non-timeout failures, consider it a warning that recent code changes may have introduced bugs into the PDB reading machinery. If you don't know what's going on: post to Slack or devel. **DO NOT** just update the reference results in this case.

If you want to know more about what this test does - pester Steven Lewis to write proper documentation.

Command line used: `/home/benchmark/benchmark/W.rosetta-2.hpc-c/rosetta.Rosetta-2.hpc-c/_commits_/main/source/test/timelimit.py 8 /home/benchmark/benchmark/W.rosetta-2.hpc-c/rosetta.Rosetta-2.hpc-c/_commits_/main/source/bin/PDB_diagnostic.default.linuxclangrelease -no_color -out:file:score_only /dev/null -jd2::delete_old_poses true -ignore_unrecognized_res false -load_PDB_components true -packing::pack_missing_sidechains false -packing::repack_only true -s {input_file} -`

```
ignore_zero_occupancy false -in:file:obey_ENDMDL true -
PDB_diagnostic::skip_pack_and_min true   -PDB_diagnostic::reading_only true
```

**1,487** total PDBs failed with the following error codes:

```
475 ▉unrecognized_residue▉
344 ▉fill_missing_atoms▉
227 ▉multiple_disulfides▉
140 ▉missing_disulfide_partner▉
 76 ▉bad_patch▉
 49 ▉unknown_atom_name▉
 35 ▉reroot_disconnected▉
 31 ▉exceed_timeout▉
 21 ▉duplicate_atom_name▉
 17 ▉zero_atom_restype▉
 17 ▉ld_chirality▉
 13 ▉unknown▉
 12 ▉nu_conformer▉
 10 ▉no_usable_coords▉
  5 ▉merge_with_next▉
  4 ▉insufficient_mainchain▉
  3 ▉base_of_chi▉
  3 ▉partly_recognized▉
  2 ▉cutpoint_neighbour▉
  2 ▉incompatible_w_polymer▉
  1 ▉zero_length_xyzVector▉
```

Test marked as **FAILED** due to following errors:

PDB 1A08 was passing test before but now failed with ▉duplicate_atom_name▉ error! Its run-log could be found in ▉1A08▉
PDB 1A09 was passing test before but now failed with ▉duplicate_atom_name▉ error! Its run-log could be found in ▉1A09▉
PDB 1A1A was passing test before but now failed with ▉duplicate_atom_name▉ error! Its run-log could be found in ▉1A1A▉
PDB 1A1V was passing test before but now failed with ▉unrecognized_residue▉ error! Its run-log could be found in ▉1A1V▉
PDB 1A9Y was passing test before but now failed with ▉unrecognized_residue▉ error! Its run-log could be found in ▉1A9Y▉
PDB 1A9Z was passing test before but now failed with ▉unrecognized_residue▉ error! Its run-log could be found in ▉1A9Z▉
PDB 1AC3 was passing test before but now failed with ▉bad_patch▉ error! Its run-log could be found in ▉1AC3▉
PDB 1AMJ was passing test before but now failed with ▉fill_missing_atoms▉ error! Its run-log could be found in ▉1AMJ▉
PDB 1APO was passing test before but now failed with ▉fill_missing_atoms▉ error! Its run-log could be found in ▉1APO▉
PDB 1ASO was passing test before but now failed with ▉fill_missing_atoms▉ error! Its run-log could be found in ▉1ASO▉
PDB 1ASP was passing test before but now failed with ▉fill_missing_atoms▉ error! Its run-log could be found in ▉1ASP▉
PDB 1ASQ was passing test before but now failed with ▉fill_missing_atoms▉ error! Its run-log could be found in ▉1ASQ▉
PDB 1BIQ was passing test before but now failed with ▉fill_missing_atoms▉ error! Its run-log could be found in ▉1BIQ▉
PDB 1BL9 was passing test before but now failed with ▉fill_missing_atoms▉ error! Its run-log could be found in ▉1BL9▉
PDB 1C23 was passing test before but now failed with ▉bad_patch▉ error! Its run-log could be found in ▉1C23▉
PDB 1CPX was passing test before but now failed with ▉fill_missing_atoms▉ error! Its run-log could be found in ▉1CPX▉
PDB 1D40 was passing test before but now failed with ▉unrecognized_residue▉ error! Its run-log could be found in ▉1D40▉
PDB 1D41 was passing test before but now failed with ▉unrecognized_residue▉ error! Its run-log could be found in ▉1D41▉
PDB 1D76 was passing test before but now failed with ▉unrecognized_residue▉ error!

Its run-log could be found in 🔗1D76🔗
PDB 1DGO was passing test before but now failed with 🔗unrecognized_residue🔗 error!
Its run-log could be found in 🔗1DGO🔗
PDB 1DOA was passing test before but now failed with 🔗reroot_disconnected🔗 error! Its run-log could be found in 🔗1DOA🔗
PDB 1E8X was passing test before but now failed with 🔗nu_conformer🔗 error! Its run-log could be found in 🔗1E8X🔗
PDB 1E98 was passing test before but now failed with 🔗duplicate_atom_name🔗 error! Its run-log could be found in 🔗1E98🔗
PDB 1E99 was passing test before but now failed with 🔗duplicate_atom_name🔗 error! Its run-log could be found in 🔗1E99🔗
PDB 1E9B was passing test before but now failed with 🔗duplicate_atom_name🔗 error! Its run-log could be found in 🔗1E9B🔗
PDB 1E9D was passing test before but now failed with 🔗duplicate_atom_name🔗 error! Its run-log could be found in 🔗1E9D🔗
PDB 1EG6 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1EG6🔗
PDB 1EK6 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1EK6🔗
PDB 1EL2 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1EL2🔗
PDB 1ELN was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1ELN🔗
PDB 1EQ8 was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1EQ8🔗
PDB 1F91 was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1F91🔗
PDB 1FGG was passing test before but now failed with 🔗bad_patch🔗 error! Its run-log could be found in 🔗1FGG🔗
PDB 1G22 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1G22🔗
PDB 1G93 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1G93🔗
PDB 1GBT was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1GBT🔗
PDB 1GJN was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1GJN🔗
PDB 1GUQ was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1GUQ🔗
PDB 1I24 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1I24🔗
PDB 1I2B was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1I2B🔗
PDB 1I2C was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1I2C🔗
PDB 1I3K was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1I3K🔗
PDB 1IDX was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1IDX🔗
PDB 1II1 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1II1🔗
PDB 1IIN was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1IIN🔗
PDB 1IT0 was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1IT0🔗
PDB 1J39 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1J39🔗
PDB 1J90 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1J90🔗
PDB 1JGU was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1JGU🔗
PDB 1JKU was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1JKU🔗
PDB 1JKV was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1JKV🔗
PDB 1JS5 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1JS5🔗
PDB 1JS7 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1JS7🔗
PDB 1K1H was passing test before but now failed with 🔗unknown_atom_name🔗 error! Its run-log could be found in 🔗1K1H🔗

PDB 1KO3 was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨1KO3▨▨

PDB 1KTG was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨1KTG▨▨

PDB 1KVQ was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨1KVQ▨▨

PDB 1KVS was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨1KVS▨▨

PDB 1KVT was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨1KVT▨▨

PDB 1KVU was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨1KVU▨▨

PDB 1LL2 was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨1LL2▨▨

PDB 1LLP was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨1LLP▨▨

PDB 1LRL was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨1LRL▨▨

PDB 1MBN was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨1MBN▨▨

PDB 1MMM was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨1MMM▨▨

PDB 1MMS was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨1MMS▨▨

PDB 1MP4 was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨1MP4▨▨

PDB 1MP5 was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨1MP5▨▨

PDB 1MUW was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨1MUW▨▨

PDB 1MWJ was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨1MWJ▨▨

PDB 1MXD was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨1MXD▨▨

PDB 1N9F was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨1N9F▨▨

PDB 1N9H was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨1N9H▨▨

PDB 1N9I was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨1N9I▨▨

PDB 1N9X was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨1N9X▨▨

PDB 1NAZ was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨1NAZ▨▨

PDB 1NH3 was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨1NH3▨▨

PDB 1NIR was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨1NIR▨▨

PDB 1NTQ was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨1NTQ▨▨

PDB 1NZ1 was passing test before but now failed with ▨▨unknown▨▨ error! Its run-log could be found in ▨▨1NZ1▨▨

PDB 1NZD was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨1NZD▨▨

PDB 1NZF was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨1NZF▨▨

PDB 1O23 was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨1O23▨▨

PDB 1OMW was passing test before but now failed with ▨▨reroot_disconnected▨▨ error! Its run-log could be found in ▨▨1OMW▨▨

PDB 1P60 was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨1P60▨▨

PDB 1P61 was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨1P61▨▨

PDB 1P7P was passing test before but now failed with ▨▨bad_patch▨▨ error! Its run-log could be found in ▨▨1P7P▨▨

PDB 1PAJ was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨1PAJ▨▨

PDB 1PAK was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨1PAK▨▨

PDB 1PCN was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its

run-log could be found in 🔗1PCN🔗
PDB 1PCO was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1PCO🔗
PDB 1QE7 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1QE7🔗
PDB 1QRR was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1QRR🔗
PDB 1QY9 was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1QY9🔗
PDB 1R0B was passing test before but now failed with 🔗multiple_disulfides🔗 error! Its run-log could be found in 🔗1R0B🔗
PDB 1R9S was passing test before but now failed with 🔗bad_patch🔗 error! Its run-log could be found in 🔗1R9S🔗
PDB 1RMY was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1RMY🔗
PDB 1S4G was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1S4G🔗
PDB 1S5N was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1S5N🔗
PDB 1SB9 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1SB9🔗
PDB 1STO was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1STO🔗
PDB 1T0Q was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1T0Q🔗
PDB 1T0R was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1T0R🔗
PDB 1T0S was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1T0S🔗
PDB 1TEQ was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1TEQ🔗
PDB 1UDC was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1UDC🔗
PDB 1UQU was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1UQU🔗
PDB 1VEW was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1VEW🔗
PDB 1VQ5 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1VQ5🔗
PDB 1VQP was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1VQP🔗
PDB 1W2H was passing test before but now failed with 🔗duplicate_atom_name🔗 error! Its run-log could be found in 🔗1W2H🔗
PDB 1XEL was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1XEL🔗
PDB 1XU5 was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1XU5🔗
PDB 1XYA was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1XYA🔗
PDB 1XYL was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1XYL🔗
PDB 1XYM was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗1XYM🔗
PDB 1Y6F was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1Y6F🔗
PDB 1Z45 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1Z45🔗
PDB 1ZDF was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1ZDF🔗
PDB 1ZDG was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗1ZDG🔗
PDB 271D was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗271D🔗
PDB 2A2Z was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗2A2Z🔗
PDB 2A30 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗2A30🔗
PDB 2ACW was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗2ACW🔗
PDB 2AH4 was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗2AH4🔗

PDB 2AM3 was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2AM3▨▨

PDB 2AT1 was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨2AT1▨▨

PDB 2B0E was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2B0E▨▨

PDB 2BUM was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨2BUM▨▨

PDB 2BUT was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨2BUT▨▨

PDB 2BUX was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨2BUX▨▨

PDB 2C01 was passing test before but now failed with ▨▨ld_chirality▨▨ error! Its run-log could be found in ▨▨2C01▨▨

PDB 2CCH was passing test before but now failed with ▨▨bad_patch▨▨ error! Its run-log could be found in ▨▨2CCH▨▨

PDB 2CG9 was passing test before but now failed with ▨▨bad_patch▨▨ error! Its run-log could be found in ▨▨2CG9▨▨

PDB 2D3Y was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2D3Y▨▨

PDB 2DP7 was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2DP7▨▨

PDB 2DPB was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2DPB▨▨

PDB 2F55 was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2F55▨▨

PDB 2GJW was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2GJW▨▨

PDB 2GN9 was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2GN9▨▨

PDB 2GSM was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨2GSM▨▨

PDB 2GXB was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2GXB▨▨

PDB 2H2Q was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2H2Q▨▨

PDB 2HUO was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨2HUO▨▨

PDB 2I5S was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2I5S▨▨

PDB 2ICY was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2ICY▨▨

PDB 2IMH was passing test before but now failed with ▨▨bad_patch▨▨ error! Its run-log could be found in ▨▨2IMH▨▨

PDB 2IX8 was passing test before but now failed with ▨▨bad_patch▨▨ error! Its run-log could be found in ▨▨2IX8▨▨

PDB 2JAU was passing test before but now failed with ▨▨duplicate_atom_name▨▨ error! Its run-log could be found in ▨▨2JAU▨▨

PDB 2JAX was passing test before but now failed with ▨▨bad_patch▨▨ error! Its run-log could be found in ▨▨2JAX▨▨

PDB 2LZV was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2LZV▨▨

PDB 2NO1 was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2NO1▨▨

PDB 2NX3 was passing test before but now failed with ▨▨unknown▨▨ error! Its run-log could be found in ▨▨2NX3▨▨

PDB 2NXG was passing test before but now failed with ▨▨unknown▨▨ error! Its run-log could be found in ▨▨2NXG▨▨

PDB 2O8D was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2O8D▨▨

PDB 2OEG was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2OEG▨▨

PDB 2ORH was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2ORH▨▨

PDB 2P10 was passing test before but now failed with ▨▨bad_patch▨▨ error! Its run-log could be found in ▨▨2P10▨▨

PDB 2P72 was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2P72▨▨

PDB 2PA4 was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨2PA4▨▨

PDB 2Q3E was passing test before but now failed with ▨▨unrecognized_residue▨▨ error!

Its run-log could be found in ⍰2Q3E⍰

PDB 2TMK was passing test before but now failed with ⍰duplicate_atom_name⍰ error! Its run-log could be found in ⍰2TMK⍰

PDB 2V1E was passing test before but now failed with ⍰fill_missing_atoms⍰ error! Its run-log could be found in ⍰2V1E⍰

PDB 2V1F was passing test before but now failed with ⍰fill_missing_atoms⍰ error! Its run-log could be found in ⍰2V1F⍰

PDB 2V1G was passing test before but now failed with ⍰fill_missing_atoms⍰ error! Its run-log could be found in ⍰2V1G⍰

PDB 2V92 was passing test before but now failed with ⍰nu_conformer⍰ error! Its run-log could be found in ⍰2V92⍰

PDB 2VAH was passing test before but now failed with ⍰unrecognized_residue⍰ error! Its run-log could be found in ⍰2VAH⍰

PDB 2VAI was passing test before but now failed with ⍰unrecognized_residue⍰ error! Its run-log could be found in ⍰2VAI⍰

PDB 2VKD was passing test before but now failed with ⍰unrecognized_residue⍰ error! Its run-log could be found in ⍰2VKD⍰

PDB 2VKH was passing test before but now failed with ⍰unrecognized_residue⍰ error! Its run-log could be found in ⍰2VKH⍰

PDB 2VM0 was passing test before but now failed with ⍰fill_missing_atoms⍰ error! Its run-log could be found in ⍰2VM0⍰

PDB 2VP5 was passing test before but now failed with ⍰unrecognized_residue⍰ error! Its run-log could be found in ⍰2VP5⍰

PDB 2VWJ was passing test before but now failed with ⍰unrecognized_residue⍰ error! Its run-log could be found in ⍰2VWJ⍰

PDB 2WWI was passing test before but now failed with ⍰duplicate_atom_name⍰ error! Its run-log could be found in ⍰2WWI⍰

PDB 2WZG was passing test before but now failed with ⍰unrecognized_residue⍰ error! Its run-log could be found in ⍰2WZG⍰

PDB 2X2I was passing test before but now failed with ⍰fill_missing_atoms⍰ error! Its run-log could be found in ⍰2X2I⍰

PDB 2X87 was passing test before but now failed with ⍰fill_missing_atoms⍰ error! Its run-log could be found in ⍰2X87⍰

PDB 2XA2 was passing test before but now failed with ⍰unrecognized_residue⍰ error! Its run-log could be found in ⍰2XA2⍰

PDB 2XA9 was passing test before but now failed with ⍰unrecognized_residue⍰ error! Its run-log could be found in ⍰2XA9⍰

PDB 2XU9 was passing test before but now failed with ⍰fill_missing_atoms⍰ error! Its run-log could be found in ⍰2XU9⍰

PDB 2YAF was passing test before but now failed with ⍰fill_missing_atoms⍰ error! Its run-log could be found in ⍰2YAF⍰

PDB 2YAH was passing test before but now failed with ⍰fill_missing_atoms⍰ error! Its run-log could be found in ⍰2YAH⍰

PDB 2YAM was passing test before but now failed with ⍰fill_missing_atoms⍰ error! Its run-log could be found in ⍰2YAM⍰

PDB 2YAO was passing test before but now failed with ⍰fill_missing_atoms⍰ error! Its run-log could be found in ⍰2YAO⍰

PDB 2YAQ was passing test before but now failed with ⍰fill_missing_atoms⍰ error! Its run-log could be found in ⍰2YAQ⍰

PDB 2YAR was passing test before but now failed with ⍰fill_missing_atoms⍰ error! Its run-log could be found in ⍰2YAR⍰

PDB 2Z2C was passing test before but now failed with ⍰bad_patch⍰ error! Its run-log could be found in ⍰2Z2C⍰

PDB 2Z6Q was passing test before but now failed with ⍰unrecognized_residue⍰ error! Its run-log could be found in ⍰2Z6Q⍰

PDB 357D was passing test before but now failed with ⍰unknown⍰ error! Its run-log could be found in ⍰357D⍰

PDB 367D was passing test before but now failed with ⍰unrecognized_residue⍰ error! Its run-log could be found in ⍰367D⍰

PDB 3BXD was passing test before but now failed with ⍰fill_missing_atoms⍰ error! Its run-log could be found in ⍰3BXD⍰

PDB 3CIK was passing test before but now failed with ⍰reroot_disconnected⍰ error! Its run-log could be found in ⍰3CIK⍰

PDB 3CKQ was passing test before but now failed with ⍰unrecognized_residue⍰ error! Its run-log could be found in ⍰3CKQ⍰

PDB 3CWH was passing test before but now failed with ⍰fill_missing_atoms⍰ error! Its run-log could be found in ⍰3CWH⍰

PDB 3DTU was passing test before but now failed with ⍰fill_missing_atoms⍰ error! Its run-log could be found in ⍰3DTU⍰

PDB 3ENK was passing test before but now failed with ⍰unrecognized_residue⍰ error! Its run-log could be found in ⍰3ENK⍰

PDB 3G00 was passing test before but now failed with ▨unrecognized_residue▨ error!
Its run-log could be found in ▨▨3G00▨▨
PDB 3G0R was passing test before but now failed with ▨unrecognized_residue▨ error!
Its run-log could be found in ▨▨3G0R▨▨
PDB 3G2D was passing test before but now failed with ▨unrecognized_residue▨ error!
Its run-log could be found in ▨▨3G2D▨▨
PDB 3G38 was passing test before but now failed with ▨unrecognized_residue▨ error!
Its run-log could be found in ▨▨3G38▨▨
PDB 3GA6 was passing test before but now failed with ▨unrecognized_residue▨ error!
Its run-log could be found in ▨▨3GA6▨▨
PDB 3GCH was passing test before but now failed with ▨unknown▨ error! Its run-log
could be found in ▨▨3GCH▨▨
PDB 3GF4 was passing test before but now failed with ▨unrecognized_residue▨ error!
Its run-log could be found in ▨▨3GF4▨▨
PDB 3GUE was passing test before but now failed with ▨unrecognized_residue▨ error!
Its run-log could be found in ▨▨3GUE▨▨
PDB 3IVA was passing test before but now failed with ▨nu_conformer▨ error! Its run-
log could be found in ▨▨3IVA▨▨
PDB 3JSZ was passing test before but now failed with ▨unrecognized_residue▨ error!
Its run-log could be found in ▨▨3JSZ▨▨
PDB 3JUK was passing test before but now failed with ▨unrecognized_residue▨ error!
Its run-log could be found in ▨▨3JUK▨▨
PDB 3KHU was passing test before but now failed with ▨unrecognized_residue▨ error!
Its run-log could be found in ▨▨3KHU▨▨
PDB 3KLH was passing test before but now failed with ▨duplicate_atom_name▨ error! Its
run-log could be found in ▨▨3KLH▨▨
PDB 3KRW was passing test before but now failed with ▨reroot_disconnected▨ error! Its
run-log could be found in ▨▨3KRW▨▨
PDB 3KRX was passing test before but now failed with ▨reroot_disconnected▨ error! Its
run-log could be found in ▨▨3KRX▨▨
PDB 3L4J was passing test before but now failed with ▨bad_patch▨ error! Its run-log
could be found in ▨▨3L4J▨▨
PDB 3L4K was passing test before but now failed with ▨bad_patch▨ error! Its run-log
could be found in ▨▨3L4K▨▨
PDB 3N1X was passing test before but now failed with ▨fill_missing_atoms▨ error! Its
run-log could be found in ▨▨3N1X▨▨
PDB 3NPE was passing test before but now failed with ▨fill_missing_atoms▨ error! Its
run-log could be found in ▨▨3NPE▨▨
PDB 3OH4 was passing test before but now failed with ▨unrecognized_residue▨ error!
Its run-log could be found in ▨▨3OH4▨▨
PDB 3OMA was passing test before but now failed with ▨fill_missing_atoms▨ error! Its
run-log could be found in ▨▨3OMA▨▨
PDB 3OMI was passing test before but now failed with ▨fill_missing_atoms▨ error! Its
run-log could be found in ▨▨3OMI▨▨
PDB 3OMN was passing test before but now failed with ▨fill_missing_atoms▨ error! Its
run-log could be found in ▨▨3OMN▨▨
PDB 3PER was passing test before but now failed with ▨fill_missing_atoms▨ error! Its
run-log could be found in ▨▨3PER▨▨
PDB 3PF7 was passing test before but now failed with ▨fill_missing_atoms▨ error! Its
run-log could be found in ▨▨3PF7▨▨
PDB 3PSC was passing test before but now failed with ▨reroot_disconnected▨ error! Its
run-log could be found in ▨▨3PSC▨▨
PDB 3PVU was passing test before but now failed with ▨reroot_disconnected▨ error! Its
run-log could be found in ▨▨3PVU▨▨
PDB 3PVW was passing test before but now failed with ▨reroot_disconnected▨ error! Its
run-log could be found in ▨▨3PVW▨▨
PDB 3Q1G was passing test before but now failed with ▨fill_missing_atoms▨ error! Its
run-log could be found in ▨▨3Q1G▨▨
PDB 3Q8K was passing test before but now failed with ▨fill_missing_atoms▨ error! Its
run-log could be found in ▨▨3Q8K▨▨
PDB 3QBA was passing test before but now failed with ▨unrecognized_residue▨ error!
Its run-log could be found in ▨▨3QBA▨▨
PDB 3QDX was passing test before but now failed with ▨fill_missing_atoms▨ error! Its
run-log could be found in ▨▨3QDX▨▨
PDB 3QDY was passing test before but now failed with ▨fill_missing_atoms▨ error! Its
run-log could be found in ▨▨3QDY▨▨
PDB 3RME was passing test before but now failed with ▨unknown▨ error! Its run-log
could be found in ▨▨3RME▨▨
PDB 3RMW was passing test before but now failed with ▨unrecognized_residue▨ error!
Its run-log could be found in ▨▨3RMW▨▨
PDB 3RN9 was passing test before but now failed with ▨fill_missing_atoms▨ error! Its

run-log could be found in ▢▢3RN9▢▢
PDB 3RNA was passing test before but now failed with ▢▢fill_missing_atoms▢▢ error! Its run-log could be found in ▢▢3RNA▢▢
PDB 3RNB was passing test before but now failed with ▢▢fill_missing_atoms▢▢ error! Its run-log could be found in ▢▢3RNB▢▢
PDB 3RNC was passing test before but now failed with ▢▢fill_missing_atoms▢▢ error! Its run-log could be found in ▢▢3RNC▢▢
PDB 3RNE was passing test before but now failed with ▢▢fill_missing_atoms▢▢ error! Its run-log could be found in ▢▢3RNE▢▢
PDB 3RNG was passing test before but now failed with ▢▢fill_missing_atoms▢▢ error! Its run-log could be found in ▢▢3RNG▢▢
PDB 3RXJ was passing test before but now failed with ▢▢fill_missing_atoms▢▢ error! Its run-log could be found in ▢▢3RXJ▢▢
PDB 3SAS was passing test before but now failed with ▢▢unknown_atom_name▢▢ error! Its run-log could be found in ▢▢3SAS▢▢
PDB 3SAT was passing test before but now failed with ▢▢unknown_atom_name▢▢ error! Its run-log could be found in ▢▢3SAT▢▢
PDB 3SAU was passing test before but now failed with ▢▢unknown_atom_name▢▢ error! Its run-log could be found in ▢▢3SAU▢▢
PDB 3SRZ was passing test before but now failed with ▢▢unrecognized_residue▢▢ error! Its run-log could be found in ▢▢3SRZ▢▢
PDB 3T5G was passing test before but now failed with ▢▢reroot_disconnected▢▢ error! Its run-log could be found in ▢▢3T5G▢▢
PDB 3T5I was passing test before but now failed with ▢▢reroot_disconnected▢▢ error! Its run-log could be found in ▢▢3T5I▢▢
PDB 3T7O was passing test before but now failed with ▢▢unrecognized_residue▢▢ error! Its run-log could be found in ▢▢3T7O▢▢
PDB 3TA2 was passing test before but now failed with ▢▢nu_conformer▢▢ error! Its run-log could be found in ▢▢3TA2▢▢
PDB 3TDK was passing test before but now failed with ▢▢unrecognized_residue▢▢ error! Its run-log could be found in ▢▢3TDK▢▢
PDB 3UGW was passing test before but now failed with ▢▢unrecognized_residue▢▢ error! Its run-log could be found in ▢▢3UGW▢▢
PDB 3UZS was passing test before but now failed with ▢▢reroot_disconnected▢▢ error! Its run-log could be found in ▢▢3UZS▢▢
PDB 3V91 was passing test before but now failed with ▢▢unrecognized_residue▢▢ error! Its run-log could be found in ▢▢3V91▢▢
PDB 3VAF was passing test before but now failed with ▢▢unrecognized_residue▢▢ error! Its run-log could be found in ▢▢3VAF▢▢
PDB 3VAG was passing test before but now failed with ▢▢unrecognized_residue▢▢ error! Its run-log could be found in ▢▢3VAG▢▢
PDB 3VAH was passing test before but now failed with ▢▢unrecognized_residue▢▢ error! Its run-log could be found in ▢▢3VAH▢▢
PDB 3VAI was passing test before but now failed with ▢▢unrecognized_residue▢▢ error! Its run-log could be found in ▢▢3VAI▢▢
PDB 3VAJ was passing test before but now failed with ▢▢unrecognized_residue▢▢ error! Its run-log could be found in ▢▢3VAJ▢▢
PDB 3VAK was passing test before but now failed with ▢▢unrecognized_residue▢▢ error! Its run-log could be found in ▢▢3VAK▢▢
PDB 3VAL was passing test before but now failed with ▢▢unrecognized_residue▢▢ error! Its run-log could be found in ▢▢3VAL▢▢
PDB 3VAM was passing test before but now failed with ▢▢unrecognized_residue▢▢ error! Its run-log could be found in ▢▢3VAM▢▢
PDB 3VSJ was passing test before but now failed with ▢▢fill_missing_atoms▢▢ error! Its run-log could be found in ▢▢3VSJ▢▢
PDB 3VTF was passing test before but now failed with ▢▢unrecognized_residue▢▢ error! Its run-log could be found in ▢▢3VTF▢▢
PDB 3VV9 was passing test before but now failed with ▢▢fill_missing_atoms▢▢ error! Its run-log could be found in ▢▢3VV9▢▢
PDB 3VVA was passing test before but now failed with ▢▢fill_missing_atoms▢▢ error! Its run-log could be found in ▢▢3VVA▢▢
PDB 3W54 was passing test before but now failed with ▢▢fill_missing_atoms▢▢ error! Its run-log could be found in ▢▢3W54▢▢
PDB 3ZFO was passing test before but now failed with ▢▢fill_missing_atoms▢▢ error! Its run-log could be found in ▢▢3ZFO▢▢
PDB 3ZFR was passing test before but now failed with ▢▢fill_missing_atoms▢▢ error! Its run-log could be found in ▢▢3ZFR▢▢
PDB 4A68 was passing test before but now failed with ▢▢fill_missing_atoms▢▢ error! Its run-log could be found in ▢▢4A68▢▢
PDB 4AC7 was passing test before but now failed with ▢▢fill_missing_atoms▢▢ error! Its run-log could be found in ▢▢4AC7▢▢

PDB 4BQF was passing test before but now failed with ⬜⬜fill_missing_atoms⬜⬜ error! Its run-log could be found in ⬜⬜4BQF⬜⬜

PDB 4C0N was passing test before but now failed with ⬜⬜fill_missing_atoms⬜⬜ error! Its run-log could be found in ⬜⬜4C0N⬜⬜

PDB 4CDR was passing test before but now failed with ⬜⬜bad_patch⬜⬜ error! Its run-log could be found in ⬜⬜4CDR⬜⬜

PDB 4CEU was passing test before but now failed with ⬜⬜fill_missing_atoms⬜⬜ error! Its run-log could be found in ⬜⬜4CEU⬜⬜

PDB 4D4Z was passing test before but now failed with ⬜⬜fill_missing_atoms⬜⬜ error! Its run-log could be found in ⬜⬜4D4Z⬜⬜

PDB 4E7B was passing test before but now failed with ⬜⬜unrecognized_residue⬜⬜ error! Its run-log could be found in ⬜⬜4E7B⬜⬜

PDB 4E7E was passing test before but now failed with ⬜⬜unrecognized_residue⬜⬜ error! Its run-log could be found in ⬜⬜4E7E⬜⬜

PDB 4E9V was passing test before but now failed with ⬜⬜fill_missing_atoms⬜⬜ error! Its run-log could be found in ⬜⬜4E9V⬜⬜

PDB 4EAQ was passing test before but now failed with ⬜⬜duplicate_atom_name⬜⬜ error! Its run-log could be found in ⬜⬜4EAQ⬜⬜

PDB 4EDF was passing test before but now failed with ⬜⬜unrecognized_residue⬜⬜ error! Its run-log could be found in ⬜⬜4EDF⬜⬜

PDB 4EF3 was passing test before but now failed with ⬜⬜fill_missing_atoms⬜⬜ error! Its run-log could be found in ⬜⬜4EF3⬜⬜

PDB 4FLY was passing test before but now failed with ⬜⬜unrecognized_residue⬜⬜ error! Its run-log could be found in ⬜⬜4FLY⬜⬜

PDB 4FM0 was passing test before but now failed with ⬜⬜unrecognized_residue⬜⬜ error! Its run-log could be found in ⬜⬜4FM0⬜⬜

PDB 4FM1 was passing test before but now failed with ⬜⬜unrecognized_residue⬜⬜ error! Its run-log could be found in ⬜⬜4FM1⬜⬜

PDB 4FM2 was passing test before but now failed with ⬜⬜unrecognized_residue⬜⬜ error! Its run-log could be found in ⬜⬜4FM2⬜⬜

PDB 4G4N was passing test before but now failed with ⬜⬜unknown_atom_name⬜⬜ error! Its run-log could be found in ⬜⬜4G4N⬜⬜

PDB 4G4O was passing test before but now failed with ⬜⬜unknown_atom_name⬜⬜ error! Its run-log could be found in ⬜⬜4G4O⬜⬜

PDB 4G4Q was passing test before but now failed with ⬜⬜unknown_atom_name⬜⬜ error! Its run-log could be found in ⬜⬜4G4Q⬜⬜

PDB 4G4R was passing test before but now failed with ⬜⬜unknown_atom_name⬜⬜ error! Its run-log could be found in ⬜⬜4G4R⬜⬜

PDB 4GFH was passing test before but now failed with ⬜⬜bad_patch⬜⬜ error! Its run-log could be found in ⬜⬜4GFH⬜⬜

PDB 4GMD was passing test before but now failed with ⬜⬜duplicate_atom_name⬜⬜ error! Its run-log could be found in ⬜⬜4GMD⬜⬜

PDB 4H9U was passing test before but now failed with ⬜⬜fill_missing_atoms⬜⬜ error! Its run-log could be found in ⬜⬜4H9U⬜⬜

PDB 4H9V was passing test before but now failed with ⬜⬜fill_missing_atoms⬜⬜ error! Its run-log could be found in ⬜⬜4H9V⬜⬜

PDB 4H9X was passing test before but now failed with ⬜⬜fill_missing_atoms⬜⬜ error! Its run-log could be found in ⬜⬜4H9X⬜⬜

PDB 4H9Y was passing test before but now failed with ⬜⬜fill_missing_atoms⬜⬜ error! Its run-log could be found in ⬜⬜4H9Y⬜⬜

PDB 4HA0 was passing test before but now failed with ⬜⬜fill_missing_atoms⬜⬜ error! Its run-log could be found in ⬜⬜4HA0⬜⬜

PDB 4HAK was passing test before but now failed with ⬜⬜fill_missing_atoms⬜⬜ error! Its run-log could be found in ⬜⬜4HAK⬜⬜

PDB 4HAL was passing test before but now failed with ⬜⬜fill_missing_atoms⬜⬜ error! Its run-log could be found in ⬜⬜4HAL⬜⬜

PDB 4HO6 was passing test before but now failed with ⬜⬜unrecognized_residue⬜⬜ error! Its run-log could be found in ⬜⬜4HO6⬜⬜

PDB 4HO8 was passing test before but now failed with ⬜⬜unrecognized_residue⬜⬜ error! Its run-log could be found in ⬜⬜4HO8⬜⬜

PDB 4JXG was passing test before but now failed with ⬜⬜fill_missing_atoms⬜⬜ error! Its run-log could be found in ⬜⬜4JXG⬜⬜

PDB 4KAS was passing test before but now failed with ⬜⬜unrecognized_residue⬜⬜ error! Its run-log could be found in ⬜⬜4KAS⬜⬜

PDB 4KAT was passing test before but now failed with ⬜⬜unrecognized_residue⬜⬜ error! Its run-log could be found in ⬜⬜4KAT⬜⬜

PDB 4LIS was passing test before but now failed with ⬜⬜unrecognized_residue⬜⬜ error! Its run-log could be found in ⬜⬜4LIS⬜⬜

PDB 4M2A was passing test before but now failed with ⬜⬜unrecognized_residue⬜⬜ error! Its run-log could be found in ⬜⬜4M2A⬜⬜

PDB 4M2B was passing test before but now failed with ⬜⬜unrecognized_residue⬜⬜ error!

Its run-log could be found in 🔗4M2B🔗

PDB 4MDX was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗4MDX🔗

PDB 4NER was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗4NER🔗

PDB 4OJI was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗4OJI🔗

PDB 4P9C was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗4P9C🔗

PDB 4R7P was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗4R7P🔗

PDB 4RGE was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗4RGE🔗

PDB 4RGF was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗4RGF🔗

PDB 4RYK was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗4RYK🔗

PDB 4TU7 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗4TU7🔗

PDB 4TU8 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗4TU8🔗

PDB 4TU9 was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗4TU9🔗

PDB 4UCW was passing test before but now failed with 🔗missing_disulfide_partner🔗 error! Its run-log could be found in 🔗4UCW🔗

PDB 4WMA was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗4WMA🔗

PDB 4XSR was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗4XSR🔗

PDB 4XWO was passing test before but now failed with 🔗bad_patch🔗 error! Its run-log could be found in 🔗4XWO🔗

PDB 4Y27 was passing test before but now failed with 🔗unknown🔗 error! Its run-log could be found in 🔗4Y27🔗

PDB 4Y6N was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗4Y6N🔗

PDB 4Y6U was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗4Y6U🔗

PDB 4Y7F was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗4Y7F🔗

PDB 4Y7G was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗4Y7G🔗

PDB 4Y9X was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗4Y9X🔗

PDB 4YGK was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗4YGK🔗

PDB 4YGL was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗4YGL🔗

PDB 4YZ5 was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗4YZ5🔗

PDB 4ZRN was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗4ZRN🔗

PDB 4ZTT was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗4ZTT🔗

PDB 5ACU was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗5ACU🔗

PDB 5ACV was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗5ACV🔗

PDB 5ACW was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗5ACW🔗

PDB 5ACX was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗5ACX🔗

PDB 5AFA was passing test before but now failed with 🔗fill_missing_atoms🔗 error! Its run-log could be found in 🔗5AFA🔗

PDB 5B2O was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗5B2O🔗

PDB 5B2Q was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗5B2Q🔗

PDB 5C4B was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗5C4B🔗

PDB 5C4C was passing test before but now failed with 🔗unrecognized_residue🔗 error! Its run-log could be found in 🔗5C4C🔗

PDB 5C4D was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5C4D▤▤

PDB 5C4F was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5C4F▤▤

PDB 5C8R was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5C8R▤▤

PDB 5CJH was passing test before but now failed with ▤fill_missing_atoms▤ error! Its run-log could be found in ▤▤5CJH▤▤

PDB 5CR2 was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5CR2▤▤

PDB 5D15 was passing test before but now failed with ▤bad_patch▤ error! Its run-log could be found in ▤▤5D15▤▤

PDB 5DLO was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5DLO▤▤

PDB 5E8F was passing test before but now failed with ▤reroot_disconnected▤ error! Its run-log could be found in ▤▤5E8F▤▤

PDB 5EV1 was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5EV1▤▤

PDB 5EV2 was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5EV2▤▤

PDB 5EV3 was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5EV3▤▤

PDB 5EV4 was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5EV4▤▤

PDB 5F2U was passing test before but now failed with ▤reroot_disconnected▤ error! Its run-log could be found in ▤▤5F2U▤▤

PDB 5FBD was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5FBD▤▤

PDB 5FBG was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5FBG▤▤

PDB 5FQA was passing test before but now failed with ▤fill_missing_atoms▤ error! Its run-log could be found in ▤▤5FQA▤▤

PDB 5FSD was passing test before but now failed with ▤fill_missing_atoms▤ error! Its run-log could be found in ▤▤5FSD▤▤

PDB 5FSE was passing test before but now failed with ▤fill_missing_atoms▤ error! Its run-log could be found in ▤▤5FSE▤▤

PDB 5G4H was passing test before but now failed with ▤fill_missing_atoms▤ error! Its run-log could be found in ▤▤5G4H▤▤

PDB 5GL5 was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5GL5▤▤

PDB 5GN7 was passing test before but now failed with ▤fill_missing_atoms▤ error! Its run-log could be found in ▤▤5GN7▤▤

PDB 5H18 was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5H18▤▤

PDB 5HK0 was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5HK0▤▤

PDB 5HK3 was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5HK3▤▤

PDB 5HKC was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5HKC▤▤

PDB 5HPO was passing test before but now failed with ▤fill_missing_atoms▤ error! Its run-log could be found in ▤▤5HPO▤▤

PDB 5HUT was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5HUT▤▤

PDB 5HUV was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5HUV▤▤

PDB 5I1F was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5I1F▤▤

PDB 5JSX was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5JSX▤▤

PDB 5K73 was passing test before but now failed with ▤fill_missing_atoms▤ error! Its run-log could be found in ▤▤5K73▤▤

PDB 5K77 was passing test before but now failed with ▤fill_missing_atoms▤ error! Its run-log could be found in ▤▤5K77▤▤

PDB 5K8Z was passing test before but now failed with ▤fill_missing_atoms▤ error! Its run-log could be found in ▤▤5K8Z▤▤

PDB 5KVY was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5KVY▤▤

PDB 5KW1 was passing test before but now failed with ▤unrecognized_residue▤ error! Its run-log could be found in ▤▤5KW1▤▤

PDB 5KW6 was passing test before but now failed with ▤unrecognized_residue▤ error!

Its run-log could be found in ▨▨5KW6▨▨
PDB 5LOR was passing test before but now failed with ▨▨unrecognized_residue▨▨ error!
Its run-log could be found in ▨▨5LOR▨▨
PDB 5M4G was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5M4G▨▨
PDB 5M4L was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5M4L▨▨
PDB 5M4Q was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5M4Q▨▨
PDB 5MBY was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5MBY▨▨
PDB 5MBZ was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5MBZ▨▨
PDB 5MC0 was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5MC0▨▨
PDB 5MC3 was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5MC3▨▨
PDB 5MC4 was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5MC4▨▨
PDB 5MC5 was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5MC5▨▨
PDB 5NFV was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨5NFV▨▨
PDB 5NJW was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5NJW▨▨
PDB 5NKU was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5NKU▨▨
PDB 5NN8 was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5NN8▨▨
PDB 5NZG was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨5NZG▨▨
PDB 5NZI was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨5NZI▨▨
PDB 5NZJ was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨5NZJ▨▨
PDB 5OCZ was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨5OCZ▨▨
PDB 5ODF was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨5ODF▨▨
PDB 5ODM was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨5ODM▨▨
PDB 5OE1 was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨5OE1▨▨
PDB 5TAR was passing test before but now failed with ▨▨reroot_disconnected▨▨ error! Its run-log could be found in ▨▨5TAR▨▨
PDB 5TB5 was passing test before but now failed with ▨▨reroot_disconnected▨▨ error! Its run-log could be found in ▨▨5TB5▨▨
PDB 5TJH was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨5TJH▨▨
PDB 5UBQ was passing test before but now failed with ▨▨bad_patch▨▨ error! Its run-log could be found in ▨▨5UBQ▨▨
PDB 5UCY was passing test before but now failed with ▨▨bad_patch▨▨ error! Its run-log could be found in ▨▨5UCY▨▨
PDB 5UKM was passing test before but now failed with ▨▨reroot_disconnected▨▨ error! Its run-log could be found in ▨▨5UKM▨▨
PDB 5UQ6 was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5UQ6▨▨
PDB 5VC7 was passing test before but now failed with ▨▨bad_patch▨▨ error! Its run-log could be found in ▨▨5VC7▨▨
PDB 5X7Q was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5X7Q▨▨
PDB 5X7R was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5X7R▨▨
PDB 5X8B was passing test before but now failed with ▨▨nu_conformer▨▨ error! Its run-log could be found in ▨▨5X8B▨▨
PDB 5XP6 was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5XP6▨▨
PDB 5Y5R was passing test before but now failed with ▨▨bad_patch▨▨ error! Its run-log could be found in ▨▨5Y5R▨▨
PDB 5ZDQ was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5ZDQ▨▨

PDB 5ZDR was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5ZDR▨▨
PDB 5ZGE was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5ZGE▨▨
PDB 5ZGF was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5ZGF▨▨
PDB 5ZGI was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5ZGI▨▨
PDB 5ZGQ was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5ZGQ▨▨
PDB 5ZGT was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5ZGT▨▨
PDB 5ZGU was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5ZGU▨▨
PDB 5ZGV was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5ZGV▨▨
PDB 5ZGW was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5ZGW▨▨
PDB 5ZGX was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5ZGX▨▨
PDB 5ZGY was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5ZGY▨▨
PDB 5ZGZ was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5ZGZ▨▨
PDB 5ZH1 was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨5ZH1▨▨
PDB 6ALS was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨6ALS▨▨
PDB 6ALT was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨6ALT▨▨
PDB 6ALU was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨6ALU▨▨
PDB 6BHJ was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨6BHJ▨▨
PDB 6C4J was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨6C4J▨▨
PDB 6C5A was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨6C5A▨▨
PDB 6C5Z was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨6C5Z▨▨
PDB 6D9B was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨6D9B▨▨
PDB 6D9C was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨6D9C▨▨
PDB 6F5K was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨6F5K▨▨
PDB 6FSN was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨6FSN▨▨
PDB 6G48 was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨6G48▨▨
PDB 6HA8 was passing test before but now failed with ▨▨bad_patch▨▨ error! Its run-log could be found in ▨▨6HA8▨▨
PDB 6I9Y was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨6I9Y▨▨
PDB 6IG0 was passing test before but now failed with ▨▨bad_patch▨▨ error! Its run-log could be found in ▨▨6IG0▨▨
PDB 6ILD was passing test before but now failed with ▨▨unknown▨▨ error! Its run-log could be found in ▨▨6ILD▨▨
PDB 6M9C was passing test before but now failed with ▨▨bad_patch▨▨ error! Its run-log could be found in ▨▨6M9C▨▨
PDB 6N30 was passing test before but now failed with ▨▨bad_patch▨▨ error! Its run-log could be found in ▨▨6N30▨▨
PDB 6NKN was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨6NKN▨▨
PDB 7AT1 was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨7AT1▨▨
PDB 8AT1 was passing test before but now failed with ▨▨fill_missing_atoms▨▨ error! Its run-log could be found in ▨▨8AT1▨▨
PDB 8MHT was passing test before but now failed with ▨▨unrecognized_residue▨▨ error! Its run-log could be found in ▨▨8MHT▨▨

NOTE: 42213 PDB's passed the tests but was not listed in reference results.



To update reference results please copy the files below into the main repository:

reference-results.cif.new.json → ⸤main repository⸣ as tests/benchmark/tests/scientific/ protein_data_bank_diagnostic/reference-results.cif.json

blocklist.cif.new.json → ⸤main repository⸣ as tests/benchmark/tests/scientific/ protein_data_bank_diagnostic/blocklist.json (note the cif/pdb/fast mode is ignored: the blocklist is segfaults and huge PDBs and is shared)