

Scientific test: Protein Data Bank diagnostic

AUTHOR AND DATE

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FAILURES

The PDB diagnostic was run on **202,785** PDB files. **194,268** files passed the test and **8,517** 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/w/rosetta-2.hpc-c/rosetta/commits/main/source/test/timelimit.py 32 /home/benchmark/w/rosetta-2.hpc-c/rosetta/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 false -PDB_diagnostic::reading_only false

8,517 total PDBs failed with the following error codes:

6,090 [unrecognized_residue](#)
471 [zero_length_xyzVector](#)
354 [fill_missing_atoms](#)
258 [missing_disulfide_partner](#)
228 [rotlib_file](#)
194 [bad_patch](#)
142 [pseudobond_connection_change](#)
133 [duplicate_atom_name](#)
101 [no_orient_atoms](#)
100 [missing_bond](#)
93 [aa_difference](#)
83 [unknown](#)
78 [prepro_cyclic_pep](#)
60 [unknown_atom_name](#)
34 [zero_atom_restype](#)
30 [reroot_disconnected](#)
16 [alias_missing_atom](#)
14 [nu_conformer](#)
10 [unknown_hbond_acceptor](#)
10 [no_usable_coords](#)
6 [merge_with_next](#)
5 [base_of_chi](#)
4 [insufficient_mainchain](#)
2 [exceed_timeout](#)
1 [no_hbond_deriv](#)

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

PDB [114D](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [114D](#)
PDB [159D](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [159D](#)
PDB [199D](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [199D](#)
PDB [1A1V](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1A1V](#)
PDB [1A8R](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1A8R](#)
PDB [1A9C](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1A9C](#)
PDB [1BPY](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1BPY](#)
PDB [1BSU](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1BSU](#)
PDB [1BUA](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1BUA](#)
PDB [1C1Y](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1C1Y](#)
PDB [1C4K](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1C4K](#)
PDB [1C80](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1C80](#)
PDB [1CKM](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1CKM](#)
PDB [1CKN](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1CKN](#)
PDB [1C0Z](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1C0Z](#)
PDB [1D41](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1D41](#)
PDB [1D60](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1D60](#)

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PDB 286D	was passing test before but now failed with unrecognized_residue error!
PDB 297D	was passing test before but now failed with unrecognized_residue error!
PDB 2A5D	was passing test before but now failed with unrecognized_residue error!
PDB 2A5F	was passing test before but now failed with unrecognized_residue error!
PDB 2A5G	was passing test before but now failed with unrecognized_residue error!
PDB 2A5P	was passing test before but now failed with unrecognized_residue error!
PDB 2A5R	was passing test before but now failed with unrecognized_residue error!
PDB 2A8S	was passing test before but now failed with unrecognized_residue error!
PDB 2AD5	was passing test before but now failed with unrecognized_residue error!
PDB 2ADW	was passing test before but now failed with unknown error! Its run-log could be found in 2ADW
PDB 2AGP	was passing test before but now failed with unrecognized_residue error!
PDB 2AGQ	was passing test before but now failed with unrecognized_residue error!
PDB 2AJQ	was passing test before but now failed with unrecognized_residue error!
PDB 2ALZ	was passing test before but now failed with unrecognized_residue error!
PDB 2AQ4	was passing test before but now failed with unrecognized_residue error!
PDB 2AQY	was passing test before but now failed with unrecognized_residue error!
PDB 2ASD	was passing test before but now failed with unrecognized_residue error!
PDB 2ASJ	was passing test before but now failed with unrecognized_residue error!
PDB 2ASL	was passing test before but now failed with unrecognized_residue error!
PDB 2ATL	was passing test before but now failed with unrecognized_residue error!
PDB 2AU0	was passing test before but now failed with unrecognized_residue error!
PDB 2AU4	was passing test before but now failed with unrecognized_residue error!
PDB 2B0E	was passing test before but now failed with unrecognized_residue error!
PDB 2B0F	was passing test before but now failed with unrecognized_residue error!
PDB 2B51	was passing test before but now failed with unrecognized_residue error!
PDB 2B56	was passing test before but now failed with unrecognized_residue error!
PDB 2BE9	was passing test before but now failed with unrecognized_residue error!
PDB 2BKU	was passing test before but now failed with unrecognized_residue error!
PDB 2BNF	was passing test before but now failed with unrecognized_residue error!
PDB 2BT0	was passing test before but now failed with unrecognized_residue error!
PDB 2C2R	was passing test before but now failed with unrecognized_residue error!
PDB 2C5L	was passing test before but now failed with unrecognized_residue error!
PDB 2CL7	was passing test before but now failed with unrecognized_residue error!
PDB 2CLC	was passing test before but now failed with unrecognized_residue error!
PDB 2CLS	was passing test before but now failed with unrecognized_residue error!
PDB 2D3Y	was passing test before but now failed with unrecognized_residue error!

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PDB	3S9H	was passing test before but now failed with unrecognized_residue error!
PDB	3SKI	was passing test before but now failed with unrecognized_residue error!
PDB	3SKL	was passing test before but now failed with unrecognized_residue error!
PDB	3SKR	was passing test before but now failed with unrecognized_residue error!
PDB	3SKT	was passing test before but now failed with unrecognized_residue error!
PDB	3SKW	was passing test before but now failed with unrecognized_residue error!
PDB	3SKZ	was passing test before but now failed with unrecognized_residue error!
PDB	3SLQ	was passing test before but now failed with unrecognized_residue error!
PDB	3SNN	was passing test before but now failed with unrecognized_residue error!
PDB	3SQ0	was passing test before but now failed with unrecognized_residue error!
PDB	3SQ1	was passing test before but now failed with unrecognized_residue error!
PDB	3SQ2	was passing test before but now failed with unrecognized_residue error!
PDB	3SQ4	was passing test before but now failed with unrecognized_residue error!
PDB	3SUN	was passing test before but now failed with unrecognized_residue error!
PDB	3SU0	was passing test before but now failed with unrecognized_residue error!
PDB	3SUP	was passing test before but now failed with unrecognized_residue error!
PDB	3SUQ	was passing test before but now failed with unrecognized_residue error!
PDB	3SV3	was passing test before but now failed with unrecognized_residue error!
PDB	3SV4	was passing test before but now failed with unrecognized_residue error!
PDB	3SYZ	was passing test before but now failed with unrecognized_residue error!
PDB	3SZ2	was passing test before but now failed with unrecognized_residue error!
PDB	3T2K	was passing test before but now failed with bad_patch error! Its run-log could be found in 3T2K
PDB	3T2Z	was passing test before but now failed with bad_patch error! Its run-log could be found in 3T2Z
PDB	3T3F	was passing test before but now failed with unrecognized_residue error!
PDB	3THV	was passing test before but now failed with unrecognized_residue error!
PDB	3TI0	was passing test before but now failed with unrecognized_residue error!
PDB	3TKL	was passing test before but now failed with unrecognized_residue error!
PDB	3UCU	was passing test before but now failed with unrecognized_residue error!
PDB	3UCZ	was passing test before but now failed with unrecognized_residue error!
PDB	3UD3	was passing test before but now failed with unrecognized_residue error!
PDB	3UD4	was passing test before but now failed with unrecognized_residue error!
PDB	3UT5	was passing test before but now failed with unrecognized_residue error!
PDB	3V6H	was passing test before but now failed with unrecognized_residue error!
PDB	3V6J	was passing test before but now failed with unrecognized_residue error!
PDB	3V6K	was passing test before but now failed with unrecognized_residue error!
PDB	3VAF	was passing test before but now failed with unrecognized_residue error!

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Its run-log could be found in [7SJA](#)
 PDB [7T1B](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [7T1B](#)
 PDB [7TZR](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [7TZR](#)
 PDB [7TZS](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [7TZS](#)
 PDB [7UPI](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [7UPI](#)
 PDB [7V2B](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [7V2B](#)
 PDB [7VBW](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [7VBW](#)
 PDB [7VEX](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [7VEX](#)
 PDB [7VUI](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [7VUI](#)
 PDB [7Z01](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [7Z01](#)
 PDB [7Z02](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [7Z02](#)
 PDB [7Z0F](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [7Z0F](#)
 PDB [7Z0G](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [7Z0G](#)
 PDB [7Z6S](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [7Z6S](#)
 PDB [7Z7D](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [7Z7D](#)
 PDB [8MHT](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [8MHT](#)

NOTE: 11058 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.full.new.json](#) → [main repository](#) as [tests/benchmark/tests/scientific/protein_data_bank_diagnostic/reference-results.full.json](#)

[blocklist.full.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)