

Scientific test: Protein Data Bank diagnostic

AUTHOR AND DATE

Steven M Lewis, smlewi@gmail.com, Cyrus Biotechnology, Oct 2018

Sergey Lyskov, sergey.lyskov@gmail.com, Gray lab, Johns Hopkins University, Oct 2018

FAILURES

The PDB diagnostic was run on **209,593** PDB files. **201,644** files passed the test and **7,949** 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 8 /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 true -PDB_diagnostic::reading_only true

7,949 total PDBs failed with the following error codes:

7,176 [unrecognized_residue](#)
360 [fill_missing_atoms](#)
124 [bad_patch](#)
60 [unknown_atom_name](#)
50 [duplicate_atom_name](#)
42 [unknown](#)
34 [reroot_disconnected](#)
24 [zero_atom_restype](#)
21 [old_chirality](#)
15 [nu_conformer](#)
11 [no_usable_coords](#)
6 [merge_with_next](#)
6 [exceed_timeout](#)
5 [alias_missing_atom](#)
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 [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 [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 [1C6K](#) was passing test before but now failed with [unknown](#) error! Its run-log
could be found in [1C6K](#)
PDB [1C6M](#) was passing test before but now failed with [unknown](#) error! Its run-log
could be found in [1C6M](#)
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 [1COZ](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1COZ](#)
PDB [1DEK](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1DEK](#)
PDB [1DEL](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1DEL](#)
PDB [1E96](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1E96](#)
PDB [1ETL](#) was passing test before but now failed with [unknown](#) error! Its run-log
could be found in [1ETL](#)
PDB [1ETM](#) was passing test before but now failed with [unknown](#) error! Its run-log
could be found in [1ETM](#)
PDB [1ETN](#) was passing test before but now failed with [unknown](#) error! Its run-log
could be found in [1ETN](#)
PDB [1FFX](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1FFX](#)
PDB [1FRW](#) was passing test before but now failed with [unrecognized_residue](#) error!
Its run-log could be found in [1FRW](#)
PDB [1FVG](#) was passing test before but now failed with [bad_patch](#) error! Its run-log

could be found in [1FVG](#)

PDB [1GQ9](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1GQ9](#)

PDB [1GWN](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1GWN](#)

PDB [1GX5](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1GX5](#)

PDB [1GX6](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1GX6](#)

PDB [1H7G](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1H7G](#)

PDB [1HC8](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1HC8](#)

PDB [1HI0](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1HI0](#)

PDB [1I52](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1I52](#)

PDB [1IA0](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1IA0](#)

PDB [1IG9](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1IG9](#)

PDB [1III](#) was passing test before but now failed with [bad_patch](#) error! Its run-log
 could be found in [1III](#)

PDB [1IIK](#) was passing test before but now failed with [bad_patch](#) error! Its run-log
 could be found in [1IIK](#)

PDB [1IJN](#) was passing test before but now failed with [bad_patch](#) error! Its run-log
 could be found in [1IJN](#)

PDB [1J2J](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1J2J](#)

PDB [1JFF](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1JFF](#)

PDB [1JLR](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1JLR](#)

PDB [1K1R](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1K1R](#)

PDB [1KCG](#) was passing test before but now failed with [unknown](#) error! Its run-log
 could be found in [1KCG](#)

PDB [1KDT](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1KDT](#)

PDB [1KFD](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1KFD](#)

PDB [1KQE](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1KQE](#)

PDB [1KSG](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1KSG](#)

PDB [1KSJ](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1KSJ](#)

PDB [1L2X](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1L2X](#)

PDB [1L3D](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1L3D](#)

PDB [1L00](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1L00](#)

PDB [1M5K](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1M5K](#)

PDB [1M7B](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1M7B](#)

PDB [1MIY](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1MIY](#)

PDB [1MQ2](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1MQ2](#)

PDB [1MQ3](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1MQ3](#)

PDB [1N3R](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1N3R](#)

PDB [1N3S](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1N3S](#)

PDB [1N3T](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [1N3T](#)

PDB [1N5Y](#) was passing test before but now failed with [duplicate_atom_name](#) error! Its
 run-log could be found in [1N5Y](#)

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

PDB	5DCV	was passing test before but now failed with unrecognized_residue error!
PDB	5DIS	was passing test before but now failed with unrecognized_residue error!
PDB	5DLQ	was passing test before but now failed with unrecognized_residue error!
PDB	5DX9	was passing test before but now failed with unknown error! Its run-log could be found in 5DX9
PDB	5E41	was passing test before but now failed with unrecognized_residue error!
PDB	5E6M	was passing test before but now failed with unrecognized_residue error!
PDB	5EE5	was passing test before but now failed with unrecognized_residue error!
PDB	5EFC	was passing test before but now failed with unrecognized_residue error!
PDB	5EIB	was passing test before but now failed with unrecognized_residue error!
PDB	5EIN	was passing test before but now failed with unrecognized_residue error!
PDB	5EOM	was passing test before but now failed with unrecognized_residue error!
PDB	5EWE	was passing test before but now failed with unrecognized_residue error!
PDB	5EWF	was passing test before but now failed with unrecognized_residue error!
PDB	5EXY	was passing test before but now failed with unrecognized_residue error!
PDB	5EXZ	was passing test before but now failed with unrecognized_residue error!
PDB	5EY0	was passing test before but now failed with unrecognized_residue error!
PDB	5EY1	was passing test before but now failed with unrecognized_residue error!
PDB	5EYP	was passing test before but now failed with unrecognized_residue error!
PDB	5EZ5	was passing test before but now failed with unrecognized_residue error!
PDB	5EZY	was passing test before but now failed with unrecognized_residue error!
PDB	5F0Q	was passing test before but now failed with unrecognized_residue error!
PDB	5F0S	was passing test before but now failed with unrecognized_residue error!
PDB	5F8I	was passing test before but now failed with unrecognized_residue error!
PDB	5F9H	was passing test before but now failed with unrecognized_residue error!
PDB	5F9R	was passing test before but now failed with unrecognized_residue error!
PDB	5FH0	was passing test before but now failed with unrecognized_residue error!
PDB	5FH1	was passing test before but now failed with unrecognized_residue error!
PDB	5FH2	was passing test before but now failed with unrecognized_residue error!
PDB	5FH3	was passing test before but now failed with unrecognized_residue error!
PDB	5FH4	was passing test before but now failed with unrecognized_residue error!
PDB	5FJC	was passing test before but now failed with unrecognized_residue error!
PDB	5FNV	was passing test before but now failed with unrecognized_residue error!
PDB	5GAM	was passing test before but now failed with unrecognized_residue error!
PDB	5GAN	was passing test before but now failed with unrecognized_residue error!
PDB	5GIX	was passing test before but now failed with unknown error! Its run-log could be found in 5GIX
PDB	5GIY	was passing test before but now failed with unknown error! Its run-log could be found in 5GIY

[illegible]

[illegible]

[illegible]

Its run-log could be found in 5S4L	now failed with unrecognized_residue error!
PDB 5S4M was passing test before but	Its run-log could be found in 5S4M
Its run-log could be found in 5S4N	PDB 5S4N was passing test before but
Its run-log could be found in 5S4O	PDB 5S4O was passing test before but
Its run-log could be found in 5S4P	PDB 5S4P was passing test before but
Its run-log could be found in 5S4Q	PDB 5S4Q was passing test before but
Its run-log could be found in 5S4R	PDB 5S4R was passing test before but
Its run-log could be found in 5S4S	PDB 5S4S was passing test before but
Its run-log could be found in 5S4T	PDB 5S4T was passing test before but
Its run-log could be found in 5S4U	PDB 5S4U was passing test before but
Its run-log could be found in 5S4V	PDB 5S4V was passing test before but
Its run-log could be found in 5S4W	PDB 5S4W was passing test before but
Its run-log could be found in 5S4X	PDB 5S4X was passing test before but
Its run-log could be found in 5S4Y	PDB 5S4Y was passing test before but
Its run-log could be found in 5S4Z	PDB 5S4Z was passing test before but
Its run-log could be found in 5S50	PDB 5S50 was passing test before but
Its run-log could be found in 5S51	PDB 5S51 was passing test before but
Its run-log could be found in 5S52	PDB 5S52 was passing test before but
Its run-log could be found in 5S53	PDB 5S53 was passing test before but
Its run-log could be found in 5S54	PDB 5S54 was passing test before but
Its run-log could be found in 5S55	PDB 5S55 was passing test before but
Its run-log could be found in 5S56	PDB 5S56 was passing test before but
Its run-log could be found in 5S57	PDB 5S57 was passing test before but
Its run-log could be found in 5S58	PDB 5S58 was passing test before but
Its run-log could be found in 5S59	PDB 5S59 was passing test before but
Its run-log could be found in 5S5A	PDB 5S5A was passing test before but
Its run-log could be found in 5S5B	PDB 5S5B was passing test before but
Its run-log could be found in 5S5C	PDB 5S5C was passing test before but
Its run-log could be found in 5S5D	PDB 5S5D was passing test before but
Its run-log could be found in 5S5E	PDB 5S5E was passing test before but
Its run-log could be found in 5S5F	PDB 5S5F was passing test before but
Its run-log could be found in 5S5G	PDB 5S5G was passing test before but
Its run-log could be found in 5S5H	PDB 5S5H was passing test before but
Its run-log could be found in 5S5I	PDB 5S5I was passing test before but
Its run-log could be found in 5S5J	PDB 5S5J was passing test before but
Its run-log could be found in 5S5K	PDB 5S5K was passing test before but

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

PDB	6EG5	was passing test before but now failed with unrecognized_residue error!
PDB	6EVW	was passing test before but now failed with unrecognized_residue error!
PDB	6EVX	was passing test before but now failed with unrecognized_residue error!
PDB	6EVY	was passing test before but now failed with unrecognized_residue error!
PDB	6EVZ	was passing test before but now failed with unrecognized_residue error!
PDB	6EW0	was passing test before but now failed with unrecognized_residue error!
PDB	6EWZ	was passing test before but now failed with unrecognized_residue error!
PDB	6EXN	was passing test before but now failed with unrecognized_residue error!
PDB	6F7C	was passing test before but now failed with unrecognized_residue error!
PDB	6FF4	was passing test before but now failed with unrecognized_residue error!
PDB	6FF7	was passing test before but now failed with unrecognized_residue error!
PDB	6FF8	was passing test before but now failed with unrecognized_residue error!
PDB	6FII	was passing test before but now failed with unrecognized_residue error!
PDB	6FJF	was passing test before but now failed with unrecognized_residue error!
PDB	6FJM	was passing test before but now failed with unrecognized_residue error!
PDB	6FKJ	was passing test before but now failed with unrecognized_residue error!
PDB	6FKL	was passing test before but now failed with unrecognized_residue error!
PDB	6FKO	was passing test before but now failed with unrecognized_residue error!
PDB	6FM1	was passing test before but now failed with unrecognized_residue error!
PDB	6FRK	was passing test before but now failed with unrecognized_residue error!
PDB	6FWK	was passing test before but now failed with unrecognized_residue error!
PDB	6FXE	was passing test before but now failed with unknown error! Its run-log could be found in 6FXE
PDB	6G0A	was passing test before but now failed with unrecognized_residue error!
PDB	6G2Q	was passing test before but now failed with unrecognized_residue error!
PDB	6G9W	was passing test before but now failed with unrecognized_residue error!
PDB	6GF3	was passing test before but now failed with unrecognized_residue error!
PDB	6GJ4	was passing test before but now failed with unrecognized_residue error!
PDB	6GSM	was passing test before but now failed with unrecognized_residue error!
PDB	6GVM	was passing test before but now failed with unrecognized_residue error!
PDB	6GVN	was passing test before but now failed with unrecognized_residue error!
PDB	6GWC	was passing test before but now failed with unrecognized_residue error!
PDB	6GWD	was passing test before but now failed with unrecognized_residue error!
PDB	6GX7	was passing test before but now failed with unrecognized_residue error!
PDB	6GZE	was passing test before but now failed with unrecognized_residue error!
PDB	6H1V	was passing test before but now failed with unrecognized_residue error!
PDB	6H9B	was passing test before but now failed with unrecognized_residue error!

[illegible]

PDB	6KNZ	was passing test before but now failed with unrecognized_residue error!
PDB	6KPP	was passing test before but now failed with unrecognized_residue error!
PDB	6KQL	was passing test before but now failed with unrecognized_residue error!
PDB	6KQM	was passing test before but now failed with unrecognized_residue error!
PDB	6KQN	was passing test before but now failed with unrecognized_residue error!
PDB	6KSF	was passing test before but now failed with bad_patch error! Its run-log could be found in 6KSF
PDB	6KWR	was passing test before but now failed with unrecognized_residue error!
PDB	6L54	was passing test before but now failed with unrecognized_residue error!
PDB	6L74	was passing test before but now failed with unrecognized_residue error!
PDB	6L8K	was passing test before but now failed with unrecognized_residue error!
PDB	6LAU	was passing test before but now failed with unrecognized_residue error!
PDB	6LAZ	was passing test before but now failed with unrecognized_residue error!
PDB	6LK4	was passing test before but now failed with unrecognized_residue error!
PDB	6LQ9	was passing test before but now failed with unrecognized_residue error!
PDB	6LQP	was passing test before but now failed with unrecognized_residue error!
PDB	6LQQ	was passing test before but now failed with unrecognized_residue error!
PDB	6LQR	was passing test before but now failed with unrecognized_residue error!
PDB	6LQS	was passing test before but now failed with unrecognized_residue error!
PDB	6LQT	was passing test before but now failed with unrecognized_residue error!
PDB	6LQU	was passing test before but now failed with unrecognized_residue error!
PDB	6LQV	was passing test before but now failed with unrecognized_residue error!
PDB	6LS4	was passing test before but now failed with unrecognized_residue error!
PDB	6LSM	was passing test before but now failed with unrecognized_residue error!
PDB	6LSN	was passing test before but now failed with unrecognized_residue error!
PDB	6M60	was passing test before but now failed with unrecognized_residue error!
PDB	6M6R	was passing test before but now failed with unrecognized_residue error!
PDB	6M6S	was passing test before but now failed with unrecognized_residue error!
PDB	6M6X	was passing test before but now failed with unrecognized_residue error!
PDB	6MCB	was passing test before but now failed with unrecognized_residue error!
PDB	6MCC	was passing test before but now failed with unrecognized_residue error!
PDB	6MLQ	was passing test before but now failed with unrecognized_residue error!
PDB	6MLR	was passing test before but now failed with unrecognized_residue error!
PDB	6MNX	was passing test before but now failed with unrecognized_residue error!
PDB	6MWN	was passing test before but now failed with unrecognized_residue error!
PDB	6MZE	was passing test before but now failed with unrecognized_residue error!
PDB	6MZF	was passing test before but now failed with unrecognized_residue error!

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

Its run-log could be found in	7MIF	now failed with	unrecognized_residue	error!
PDB 7MIG was passing test before but	found in 7MIG			
Its run-log could be found in	7MIH	now failed with	unrecognized_residue	error!
PDB 7MII was passing test before but	found in 7MII	now failed with	unrecognized_residue	error!
Its run-log could be found in	7MIP	now failed with	unrecognized_residue	error!
PDB 7MIU was passing test before but	found in 7MIU	now failed with	unrecognized_residue	error!
Its run-log could be found in	7MIV	now failed with	unrecognized_residue	error!
PDB 7MIZ was passing test before but	found in 7MIZ	now failed with	unrecognized_residue	error!
Its run-log could be found in	7MOQ	now failed with	unrecognized_residue	error!
PDB 7MQ8 was passing test before but	found in 7MQ8	now failed with	alias_missing_atom	error! Its run-log could be found in
PDB 7MQ9 was passing test before but	found in 7MQ9	now failed with	unrecognized_residue	error!
Its run-log could be found in	7MSV	now failed with	unrecognized_residue	error!
PDB 7MWG was passing test before but	found in 7MWG	now failed with	unrecognized_residue	error!
Its run-log could be found in	7N2V	now failed with	unrecognized_residue	error!
PDB 7N32 was passing test before but	found in 7N32	now failed with	unrecognized_residue	error!
Its run-log could be found in	7N7H	now failed with	unrecognized_residue	error!
PDB 7N7I was passing test before but	found in 7N7I	now failed with	unrecognized_residue	error!
Its run-log could be found in	7NB8	now failed with	unrecognized_residue	error!
PDB 7NBA was passing test before but	found in 7NBA	now failed with	unrecognized_residue	error!
Its run-log could be found in	7NFX	now failed with	unrecognized_residue	error!
PDB 7NV0 was passing test before but	found in 7NV0	now failed with	unrecognized_residue	error!
Its run-log could be found in	7NV1	now failed with	unrecognized_residue	error!
PDB 7O35 was passing test before but	found in 7O35	now failed with	unrecognized_residue	error!
Its run-log could be found in	7O36	now failed with	unrecognized_residue	error!
PDB 7O7Y was passing test before but	found in 7O7Y	now failed with	unrecognized_residue	error!
Its run-log could be found in	7O7Z	now failed with	unrecognized_residue	error!
PDB 7O80 was passing test before but	found in 7O80	now failed with	unrecognized_residue	error!
Its run-log could be found in	7O81	now failed with	unrecognized_residue	error!
PDB 7OA3 was passing test before but	found in 7OA3	now failed with	unrecognized_residue	error!
Its run-log could be found in	7OAV	now failed with	unrecognized_residue	error!
PDB 7OAW was passing test before but	found in 7OAW	now failed with	unrecognized_residue	error!
Its run-log could be found in	7OAX	now failed with	unrecognized_residue	error!
PDB 7OBQ was passing test before but	found in 7OBQ	now failed with	unrecognized_residue	error!
Its run-log could be found in	7ODN	now failed with	unrecognized_residue	error!
PDB 7ODX was passing test before but	found in 7ODX	now failed with	unrecognized_residue	error!
Its run-log could be found in	7OF2	now failed with	unrecognized_residue	error!

[illegible]

[illegible]

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](#)

NOTE: 14494 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)