

Scientific test: Protein Data Bank diagnostic

AUTHOR AND DATE

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FAILURES

The PDB diagnostic was run on **206,530** PDB files. **197,171** files passed the test and **9,359** 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-b/rosetta/commits/main/source/test/timelimit.py 32 /home/benchmark/w/rosetta-2.hpc-b/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

9,359 total PDBs failed with the following error codes:

6,900 unrecognized_residue
477 zero_length_xyzVector
359 fill_missing_atoms
258 missing_disulfide_partner
228 rotlib_file
200 bad_patch
142 pseudobond_connection_change
134 duplicate_atom_name
104 no_orient_atoms
103 missing_bond
96 aa_difference
83 unknown
78 prepro_cyclic_pep
63 unknown_atom_name
34 zero_atom_restype
30 reroot_disconnected
17 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
3 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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Its run-log could be found in 3EPI	now failed with unrecognized_residue error!
PDB 3ETD was passing test before but	Its run-log could be found in 3ETD
Its run-log could be found in 3ETE	PDB 3ETE was passing test before but
Its run-log could be found in 3ETG	PDB 3ETG was passing test before but
Its run-log could be found in 3ETG	PDB 3EVC was passing test before but
PDB 3EVC was passing test before but	Its run-log could be found in 3EVC
PDB 3EVD was passing test before but	Its run-log could be found in 3EVD
PDB 3F2Q was passing test before but	Its run-log could be found in 3F2Q
PDB 3F2T was passing test before but	Its run-log could be found in 3F2T
PDB 3F2W was passing test before but	Its run-log could be found in 3F2W
PDB 3F2X was passing test before but	Its run-log could be found in 3F2X
PDB 3F2Y was passing test before but	Its run-log could be found in 3F2Y
PDB 3F30 was passing test before but	Its run-log could be found in 3F30
PDB 3FC9 was passing test before but	Its run-log could be found in 3FC9
PDB 3FFU was passing test before but	Its run-log could be found in 3FFU
PDB 3FPI was passing test before but	Its run-log could be found in 3FPI
PDB 3G00 was passing test before but	Its run-log could be found in 3G00
PDB 3G0R was passing test before but	Its run-log could be found in 3G0R
PDB 3G2D was passing test before but	Its run-log could be found in 3G2D
PDB 3G38 was passing test before but	Its run-log could be found in 3G38
PDB 3G6V was passing test before but	Its run-log could be found in 3G6V
PDB 3G6W was passing test before but	Its run-log could be found in 3G6W
PDB 3G6X was passing test before but	Its run-log could be found in 3G6X
PDB 3G6Y was passing test before but	Its run-log could be found in 3G6Y
PDB 3G8S was passing test before but	Its run-log could be found in 3G8S
PDB 3G8T was passing test before but	Its run-log could be found in 3G8T
PDB 3G96 was passing test before but	Its run-log could be found in 3G96
PDB 3G9C was passing test before but	Its run-log could be found in 3G9C
PDB 3GA6 was passing test before but	Its run-log could be found in 3GA6
PDB 3GIJ was passing test before but	Its run-log could be found in 3GIJ
PDB 3GIK was passing test before but	Its run-log could be found in 3GIK
PDB 3GIL was passing test before but	Its run-log could be found in 3GIL
PDB 3GIM was passing test before but	Its run-log could be found in 3GIM
PDB 3GJX was passing test before but	Its run-log could be found in 3GJX
PDB 3G03 was passing test before but	could be found in 3G03
PDB 3GQC was passing test before but	Its run-log could be found in 3GQC
PDB 3H3A was passing test before but	Its run-log could be found in 3H3A

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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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PDB	4KXG	was passing test before but now failed with unrecognized_residue error!
PDB	4KGZ	was passing test before but now failed with unrecognized_residue error!
PDB	4KH1	was passing test before but now failed with unrecognized_residue error!
PDB	4KR2	was passing test before but now failed with unrecognized_residue error!
PDB	4KR3	was passing test before but now failed with unrecognized_residue error!
PDB	4KS6	was passing test before but now failed with bad_patch error! Its run-log could be found in 4KS6
PDB	4KTQ	was passing test before but now failed with unrecognized_residue error!
PDB	4KVA	was passing test before but now failed with unrecognized_residue error!
PDB	4KVG	was passing test before but now failed with unrecognized_residue error!
PDB	4KZE	was passing test before but now failed with unrecognized_residue error!
PDB	4LHZ	was passing test before but now failed with unrecognized_residue error!
PDB	4LIL	was passing test before but now failed with unrecognized_residue error!
PDB	4LNU	was passing test before but now failed with unrecognized_residue error!
PDB	4M80	was passing test before but now failed with unrecognized_residue error!
PDB	4MDF	was passing test before but now failed with unrecognized_residue error!
PDB	4MDX	was passing test before but now failed with unrecognized_residue error!
PDB	4MGN	was passing test before but now failed with unrecognized_residue error!
PDB	4MIT	was passing test before but now failed with unrecognized_residue error!
PDB	4MZL	was passing test before but now failed with unrecognized_residue error!
PDB	4N56	was passing test before but now failed with unrecognized_residue error!
PDB	4N5S	was passing test before but now failed with unrecognized_residue error!
PDB	4NCN	was passing test before but now failed with unrecognized_residue error!
PDB	4NYA	was passing test before but now failed with unrecognized_residue error!
PDB	4O25	was passing test before but now failed with unrecognized_residue error!
PDB	4O2A	was passing test before but now failed with unrecognized_residue error!
PDB	4O2B	was passing test before but now failed with unrecognized_residue error!
PDB	4O2L	was passing test before but now failed with unrecognized_residue error!
PDB	4O4H	was passing test before but now failed with unrecognized_residue error!
PDB	4O4I	was passing test before but now failed with unrecognized_residue error!
PDB	4O4J	was passing test before but now failed with unrecognized_residue error!
PDB	4O4L	was passing test before but now failed with unrecognized_residue error!
PDB	4O8E	was passing test before but now failed with unrecognized_residue error!
PDB	4OJI	was passing test before but now failed with unrecognized_residue error!
PDB	4OL0	was passing test before but now failed with unrecognized_residue error!
PDB	4OM8	was passing test before but now failed with bad_patch error! Its run-log could be foundin 4OM8
PDB	4OTS	was passing test before but now failed with unrecognized_residue error!

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Its run-log could be found in	5LEF	now failed with	unrecognized_residue	error!
PDB 5LJ5 was passing test before but	found in 5LJ5	now failed with	unrecognized_residue	error!
Its run-log could be found in	5LLX	now failed with	unrecognized_residue	error!
PDB 5LOV was passing test before but	found in 5LOV	now failed with	unrecognized_residue	error!
Its run-log could be found in	5LP6	now failed with	unrecognized_residue	error!
PDB 5LWJ was passing test before but	found in 5LWJ	now failed with	unrecognized_residue	error!
Its run-log could be found in	5LXS	now failed with	unrecognized_residue	error!
PDB 5LXT was passing test before but	found in 5LXT	now failed with	unrecognized_residue	error!
Its run-log could be found in	5LYJ	now failed with	unrecognized_residue	error!
PDB 5M3C was passing test before but	found in 5M3C	now failed with	unrecognized_residue	error!
Its run-log could be found in	5M4W	now failed with	unrecognized_residue	error!
PDB 5M50 was passing test before but	found in 5M50	now failed with	unrecognized_residue	error!
Its run-log could be found in	5M54	now failed with	unrecognized_residue	error!
PDB 5M5C was passing test before but	found in 5M5C	now failed with	unrecognized_residue	error!
Its run-log could be found in	5M5I	now failed with	unrecognized_residue	error!
PDB 5M5L was passing test before but	found in 5M5L	now failed with	unrecognized_residue	error!
Its run-log could be found in	5M5M	now failed with	unrecognized_residue	error!
PDB 5M5N was passing test before but	found in 5M5N	now failed with	unrecognized_residue	error!
Its run-log could be found in	5M5O	now failed with	unrecognized_residue	error!
PDB 5M73 was passing test before but	found in 5M73	now failed with	unrecognized_residue	error!
Its run-log could be found in	5M7E	now failed with	unrecognized_residue	error!
PDB 5M7G was passing test before but	found in 5M7G	now failed with	unrecognized_residue	error!
Its run-log could be found in	5M8D	now failed with	unrecognized_residue	error!
PDB 5M8G was passing test before but	found in 5M8G	now failed with	unrecognized_residue	error!
Its run-log could be found in	5MCV	now failed with	unrecognized_residue	error!
PDB 5MCW was passing test before but	found in 5MCW	now failed with	unrecognized_residue	error!
Its run-log could be found in	5MF4	now failed with	unrecognized_residue	error!
PDB 5MI0 was passing test before but	found in 5MI0	now failed with	unrecognized_residue	error!
Its run-log could be found in	5MJS	now failed with	unrecognized_residue	error!
PDB 5MM4 was passing test before but	found in 5MM4	now failed with	unrecognized_residue	error!
Its run-log could be found in	5MM7	now failed with	unrecognized_residue	error!
PDB 5MN5 was passing test before but	found in 5MN5	now failed with	unrecognized_residue	error!
Its run-log could be found in	5MN7	now failed with	unrecognized_residue	error!
PDB 5MN8 was passing test before but	found in 5MN8	now failed with	unrecognized_residue	error!
Its run-log could be found in	5MPS	now failed with	unrecognized_residue	error!
PDB 5MQ0 was passing test before but	found in 5MQ0	now failed with	unrecognized_residue	error!
Its run-log could be found in	5MQ0			

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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 6FM1	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 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!
PDB 6H DU	was passing test before but now failed with	unrecognized_residue	error!
PDB 6HX8	was passing test before but now failed with	unrecognized_residue	error!
PDB 6HXU	was passing test before but now failed with	unrecognized_residue	error!
PDB 6I00	was passing test before but now failed with	unrecognized_residue	error!
PDB 6I2I	was passing test before but now failed with	unrecognized_residue	error!
PDB 6I5C	was passing test before but now failed with	unrecognized_residue	error!
PDB 6I8A	was passing test before but now failed with	unrecognized_residue	error!
PDB 6IA7	was passing test before but now failed with	unrecognized_residue	error!
PDB 6IAE	was passing test before but now failed with	unrecognized_residue	error!
PDB 6IAN	was passing test before but now failed with	unrecognized_residue	error!
PDB 6IAO	was passing test before but now failed with	bad_patch	error! Its run-log could be found in 6IAO
PDB 6ICZ	was passing test before but now failed with	unrecognized_residue	error!
PDB 6ID0	was passing test before but now failed with	unrecognized_residue	error!
PDB 6ID1	was passing test before but now failed with	unrecognized_residue	error!
PDB 6IF2	was passing test before but now failed with	unrecognized_residue	error!

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Its run-log could be found in	6WVV	now failed with	unrecognized_residue	error!
PDB 6X1C was passing test before but	found in 6X1C	now failed with	unrecognized_residue	error!
Its run-log could be found in	6X1E	now failed with	unrecognized_residue	error!
PDB 6X1F was passing test before but	found in 6X1F	now failed with	unrecognized_residue	error!
Its run-log could be found in	6XER	now failed with	unrecognized_residue	error!
PDB 6XES was passing test before but	found in 6XES	now failed with	unrecognized_residue	error!
Its run-log could be found in	6XET	now failed with	unrecognized_residue	error!
PDB 6XH8 was passing test before but	found in 6XH8	now failed with	unrecognized_residue	error!
Its run-log could be found in	6XHS	now failed with	unrecognized_residue	error!
PDB 6XKN was passing test before but	found in 6XKN	now failed with	unrecognized_residue	error!
Its run-log could be found in	6XKO	now failed with	unrecognized_residue	error!
PDB 6XL9 was passing test before but	found in 6XL9	now failed with	unrecognized_residue	error!
Its run-log could be found in	6XLJ	now failed with	unrecognized_residue	error!
PDB 6XLL was passing test before but	found in 6XLL	now failed with	unrecognized_residue	error!
Its run-log could be found in	6XLV	now failed with	unrecognized_residue	error!
PDB 6XLW was passing test before but	found in 6XLW	now failed with	unrecognized_residue	error!
Its run-log could be found in	6XLX	now failed with	unrecognized_residue	error!
PDB 6XTZ was passing test before but	found in 6XTZ	now failed with	fill_missing_atoms	error! Its
run-log could be found in	6XU1	now failed with	unrecognized_residue	error!
PDB 6Y09 was passing test before but	found in 6Y09	now failed with	unrecognized_residue	error!
Its run-log could be found in	6Y4M	now failed with	unrecognized_residue	error!
PDB 6Y4N was passing test before but	found in 6Y4N	now failed with	unrecognized_residue	error!
Its run-log could be found in	6Y6D	now failed with	unrecognized_residue	error!
PDB 6YD4 was passing test before but	found in 6YD4	now failed with	unrecognized_residue	error!
Its run-log could be found in	6YD7	now failed with	unrecognized_residue	error!
PDB 6YMW was passing test before but	found in 6YMW	now failed with	unrecognized_residue	error!
Its run-log could be found in	6Z6Y	now failed with	unrecognized_residue	error!
PDB 6ZIZ was passing test before but	found in 6ZIZ	now failed with	unrecognized_residue	error!
Its run-log could be found in	6ZPI	now failed with	unrecognized_residue	error!
PDB 6ZWB was passing test before but	found in 6ZWB	now failed with	unrecognized_residue	error!
Its run-log could be found in	6ZWZ	now failed with	unrecognized_residue	error!
PDB 6ZYM was passing test before but	found in 6ZYM	now failed with	unrecognized_residue	error!
Its run-log could be found in	6ZYW	now failed with	unrecognized_residue	error!
PDB 6ZYX was passing test before but	found in 6ZYX	now failed with	unrecognized_residue	error!
Its run-log could be found in	7A5M	now failed with	unrecognized_residue	error!
PDB 7AAV was passing test before but	found in 7AAV	now failed with	unrecognized_residue	error!
Its run-log could be found in	7AAV			

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

Its run-log could be found in [7SJ8](#)
 PDB [7SJ9](#) was passing test before but now failed with [unrecognized_residue](#) error!
 Its run-log could be found in [7SJ9](#)
 PDB [7SJA](#) was passing test before but now failed with [unrecognized_residue](#) error!
 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: 14006 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)