Testing InChI v1.7.0

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Test infrastructure

- InChI 1.7.0 compiled with GCC 14.1.0
- Debian bookworm
- 16 physical cores
- https://github.com/IUPAC-InChI/InChI/tree/main/INCHI-1-TEST

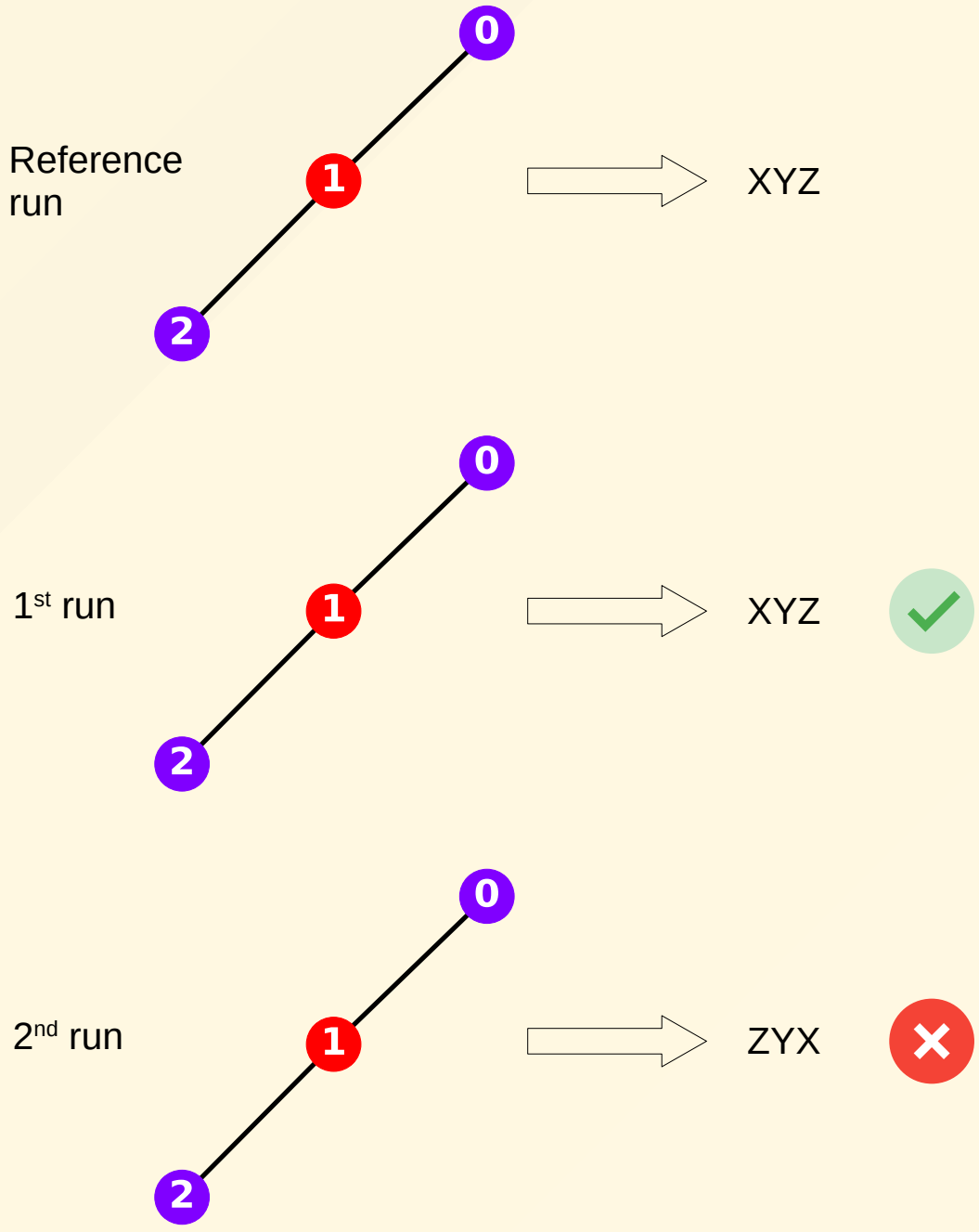
PubChem Datasets

https://ftp.ncbi.nlm.nih.gov/pubchem/

	Compound	Compound 3D	Substance
download[a]	Oct 13 2023	Oct 25 2023	Oct 23 2023
size in GB (gzip)[b]	99	37	81
N SDF[c]	338	1,103	895
N structures[d]	114,726,411	23,487,296	306,711,305

Regression

Are InChIs stable across version 1.06 and version 1.07?

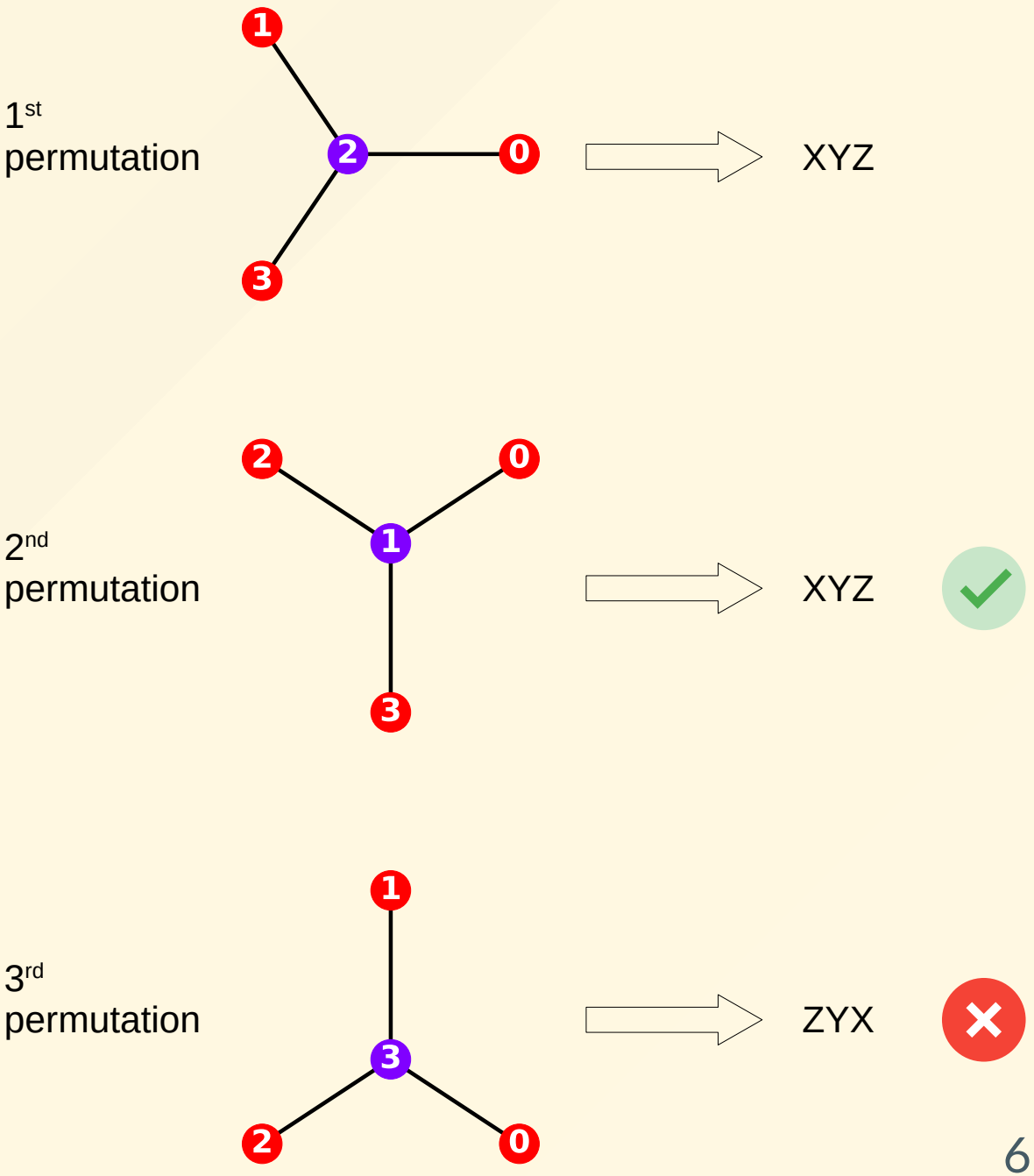


Regression Results

	Compound	Compound 3D	Substance
N structures passed[a]	114,726,411	23,487,296	306,711,303
N structures failed[b]	0	0	2
N structures error	0	0	0
percentage failed[c]	0	0	0.00000064
run-time total[d]	402 min (6 hrs, 42 min)	106 min (1 hr, 46 min)	585 min (9 hrs, 45 min)
avg run-time per structure[e]	0.21 ms	0.27 ms	0.114 ms

Invariance

Are InChIs canonical?



Invariance Results

	Compound	Compound 3D	Substance
N structures passed[a]	n/a	23,487,290	289,776,775
N structures failed[b]	n/a	6	2,131
N structures error	n/a	0	16,932,378[c,d] + 21[e,f] = 16,932,399
percentage failed[g]	n/a	0.000026	0.000735
run-time total[h]	n/a	389 min (6 hrs, 29 min)	4,063 min (2 days, 18 hrs, 43 min)
avg run-time per structure[i]	n/a	0.98 ms	0.84 ms

Details PubChem Datasets

a)

```
find . -type f -name "*.gz" -exec du -b {} + | awk '{ total += $1 } END { print total / 1024 / 1024 / 1024 " GB" }'
```

b) according to `.listing` file from PubChem FTP download

c) `ls *.sdf.gz | wc -l`

d)

```
totalCount=0; for file in ./*.sqlite; do count=$(sqlite3 "$file" "SELECT COUNT(*) FROM results;"); totalCount=$((totalCount + count)); done; echo $totalCount
```

Details Regression

a) N structures - (N structures error + N structures failed)

b) `grep -o "test failed" ./<log-name>.log | wc -l`

c) N structures failed / (N structures - N structures error) * 100

d) last timestamp - first timestamp from logs

e) run-time total / (N structures passed + N structures failed) * 60000

Details Invariance

a) N structures - (N structures error + N structures failed)

b) `grep -o "test failed" ./<log-name>.log | wc -l`

c) `grep -o "test didn't run" ./<log-name>.log | wc -l`

d) empty molfiles; see e.g., https://pubchem.ncbi.nlm.nih.gov/rest/pug/substance/sid/2167/record/SDF

Details Invariance (continued)

e) `grep -o "RuntimeError" ./<log-name>.log | wc -l`

f) InChI failed to process molfiles

g) N structures failed / (N structures - N structures error) * 100

h) last timestamp - first timestamp from logs

i) run-time total / (N structures passed + N structures failed) * 60000