

Supporting Information: A Workflow to Create a High-Quality Protein-Ligand Binding Dataset for Training, Validation, and Prediction Tasks

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1 Data Usage

The HiQBind dataset can be found in the following Figshare repository:

- <https://doi.org/10.6084/m9.figshare.27430305>

which contains the following files:

- `hiqbind.tar.gz`: Protein-Ligand complexes structures in HiQBind
- `hiqbind_metadata.csv`: Metadata for HiQBind dataset
- `hiqbind_sm_metadata.csv`: Metadata for subset of HiQBind in which ligands all small molecules
- `hiqbind_poly_metadata.csv`: Metadata for subset of HiQBind in which ligands are polymers
- `README.md`: Description of the structural dataset and columns in the metadata csv file

The metadata files are also provided in the Github repository:

- <https://github.com/THGLab/HiQBind/blob/main/figshare>

Unzipping the data tarball with command `tar -xzf hiqbind.tar.gz` will yield two directories `raw_data_hiq_sm` and `raw_data_hiq_poly` corresponding to the "small molecule" and "polymer" subset of HiQBind, respectively. In each directory, you will see a file structure like this:

```
-- 1a69/
  |-- 1a69_FMB_A_240/
    |-- 1a69_FMB_A_240_ligand.pdb
    |-- 1a69_FMB_A_240_protein.pdb
    |-- 1a69_FMB_A_240_protein_hetatm.pdb
    |-- 1a69_FMB_A_240_hetatm.pdb
    |-- 1a69_FMB_A_240_ligand_refined.sdf
    |-- 1a69_FMB_A_240_protein_refined.pdb
  |-- 1a4m_FMB_B_240/
  |-- 1a4m_FMB_C_240/
-- 1a85/
```

An overview of the file contents is in Table S1 and here is a description of the naming conventions of the files:

- **1a69:** 4-letter PDB ID
- **FMB:** Name of the ligand. If the ligand is a polymer, it will be format like "ACE-DIP", where "ACE" is the name of the first residue and "DIP" is the name of the last residue.
- **A:** Ligand chain ID.
- **240:** Ligand residue number. If the ligand is a polymer, it will be format like "1-3", where "1" is the residue number of the first residue and "3" is the number of the last residue. Note the residue number may contain insertion code, or be a negative integer or zero.

Table S1: Overview of the files in HiQBind.

File	Description
*_ligand_refined.sdf	Refined ligand structures (hydrogen added, correct bond order, better tautomer states/protonation states) with HiQBind-WF workflow
*_protein_refined.pdb	Refined protein structures (hydrogen added, missing atoms/residues added) with HiQBind-WF workflow
*_ligand.pdb	Ligand structure extracted from the original PDB (not processed)
*_protein.pdb	Protein structure extracted from the original PDB (not processed). A protein is defined as chains within 10 angstrom of the ligand structure.
*_hetatm.pdb	Additives' structure extracted from the original PDB (not processed)
*_protein_hetatm.pdb	Protein structure with additives (solvents, ions) extracted from the original PDB (not processed). Additives are specified with "HETATM" atoms that are within 4 angstroms of the protein chains.

A description of all fields in the csv-formatted metadata file in Table S2.

Table S2: Overview of the HiQBind metadata fields.

Field	Type	Description
PDBID	string	Four-letter PDB code
Resolution	string / float	Resolution of the structure or "NMR"
Year	int	Initial release year in RCSB PDB database
Ligand Name	string	Name of the ligand. ^a
Ligand Chain	string	Chain ID of the ligand.
Ligand Residue Number	string	Residue number of the ligand. ^b
Binding Affinity Measurement	string	Type of binding affinity assay: "kd", "ki", "ic50" or "ec50". ^c
Binding Affinity Sign	string	Sign of the binding affinity measurement: "=", ">=", "<=" or "~".
Binding Affinity Value	float	Value of the binding affinity
Binding Affinity Unit	string	Unit of the binding affinity: "fM", "pM", "nM", "uM", "mM" and "M".
Log Binding Affinity	float	Binding affinity in log unit.
Binding Affinity Source	string	Source of the binding affinity annotations: "BindingMOAD", "BindingDB" or "BioLiP"
Binding Affinity Annotation	string	The annotation in the original source.
Protein UniProtID	string	UniProtID of the proteins, seperated by a comma if the ligand bound to more than one chain.
Protein UniProtName	string	Name of the proteins, separated by a comma if the ligand bound to more than one chain.
Ligand SMILES	string	SMILES of the ligand.
Ligand MW	float	Molecular weight of the ligand.
Ligand LogP	float	LogP value of the ligand computed by RDKit.
Ligand TPSA	float	TPSA value of the ligand computed by RDKit.
Ligand NumRotBond	int	Number of rotatable bonds in the ligand.
Ligand NumHeavyAtoms	int	Number of heavy atoms in the ligand.
Ligand NumHDon	int	Number of hydrogen bond donors in the ligand.
Ligand NumHAcc	int	Number of hydrogen bond acceptors in the ligand.
Ligand QED	float	QED value of the ligand computed by RDKit.

^a If the ligand is a polymer, its name will be format like "ACE-DIP", where "ACE" is the name of the first residue and "DIP" is the name of the last residue.

^b If the ligand is a polymer, its residue number will be format like "1-3", where "1" is the number of the first residue and "3" is the number of the last one. Note the residue number may contain insertion code, or be a negative integer or zero.

^c In some sources where binding data is labeled as K_a or K_b , they are converted to K_d using $K_a = 1/K_d$.

Since users may want to create their own data splits based on time or create subset that does not overlap with existing dataset, such as PDBbind v2020, here we provide some relevant analysis in Figure S1. All entries in PDBbind v2020 are before 1/1/2020, and HiQBind contains 1,463 PDB entries deposited after this date. Overall, 11,615 PDB entries out of HiQBind's total 18,160 entries are in PDBbind v2020. This overlapping is due to the

fact that many entries in also appear in Binding MOAD and BindingDB, which are datasets that HiQBind queries binding-affiniy annotation from.

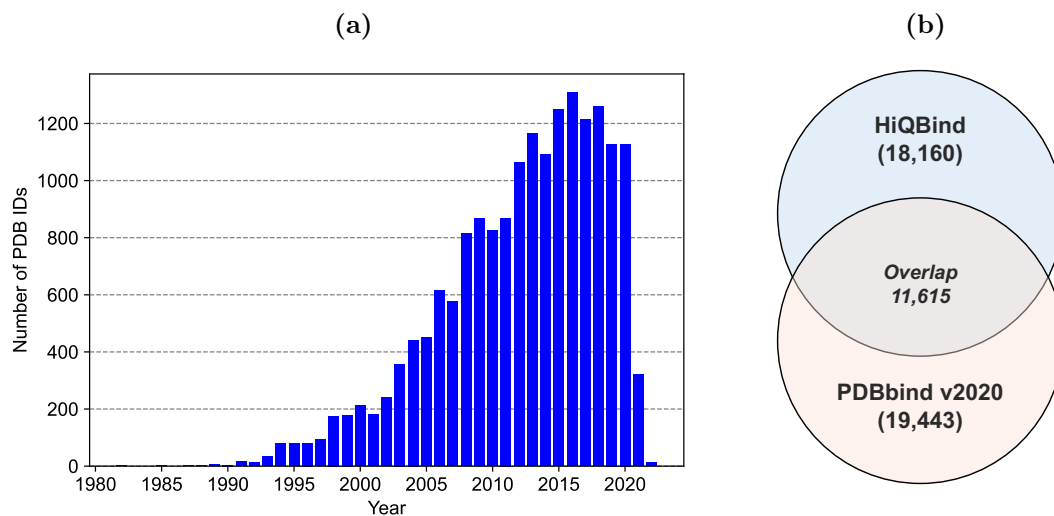


Figure S1: (a) The year distribution of PDB entries in HiQBind. HiQBind contains 1,463 PDB entries deposited after 1/1/2020. (b) HiQBind PDB entries overlapping with those in PDBbind v2020. Among 18,160 unique PDB IDs in HiQBind, 11,615 of them appear in PDBbind v2020.

2 Failed cases in processing HiQBind

Table S3: Overview of the number of entries during filter and structure fixing process of HiQBind.

	Number of unique PDB IDs		
	Small Molecule	Polymer	Total
Before processing	19105	1250	20349 ^a
Successfully processed ^d	17725 (31572)	438 (703)	18160 ^b (32275)
Failed	1380	812	2189 ^c
Covalent binders	262	16	278
Steric clashes	105	7	112
Contain uncommon elements	355	6	361
Small ligands	10	0	10
Fail to fix structures	638	783	1428 ^c

^a 6 PDB entries are included in both small molecule set and polymer set: 1ga8, 1gwv, 1gx4, 1o7o, 1o9f, 4d4u.

^b 3 PDB entries are successfully processed in both small molecule set and polymer set: 1gwv, 1o7o, 1o9f.

^c 1ga8 and 4d4u are failed in both small molecule set and polymer set; 1gx4 is successful in small molecule set but failed in polymer set.

^d In parenthesis is the number of protein-ligand structures.

278 entries are identified with covalent binders:

1au0, 1ayu, 1ayv, 1ayw, 1b0f, 1b4e, 1b6a, 1c3b, 1dru, 1drw, 1erm, 1eta, 1etb, 1fsw, 1fsy, 1ga9, 1gfw, 1h2y, 1hbj, 1i72, 1iau, 1kds, 1kdw, 1ke0, 1ke3, 1lhc, 1lhd, 1ms0, 1mt5, 1my8, 1nl6, 1nlj, 1o2t, 1o4l, 1o45, 1o4d, 1o4e, 1o4i, 1o5f, 1o5w, 1pi4, 1pi5, 1q6k, 1qfs, 1qhr, 1qm5, 1rel, 1rhm, 1rrh, 1rhu, 1rwm, 1rww, 1s2y, 1s3b, 1s3e, 1snk, 1sri, 1tu6, 1u9v, 1u9w, 1u9x, 1uks, 1w3l, 1wof, 1yt7, 2abe, 2alv, 2amd, 2aux, 2auz, 2bxx, 2bxs, 2c72, 2c73, 2c75, 2c76, 2clx, 2dc6, 2dc8, 2dc9, 2dca, 2dcc, 2dcd, 2fj0, 2fs9, 2fzi, 2g5p, 2g5t, 2g63, 2gsu, 2hpp, 2hpq, 2hwp, 2j5f, 2jai, 2jdh, 2jdk, 2op9, 2qky, 2ql5, 2ql7, 2ql9, 2qlb, 2qlq, 2qq7, 2v6n, 2wn2, 2y4a, 2y55, 2yld, 2zu4, 2zu5, 2zz3, 2zz4, 2zz6, 3afk, 3b0r, 3bls, 3dww, 3dz5, 3fkv, 3g3d, 3g3m, 3gzn, 3hj0, 3i06, 3i4a, 3ika, 3jwe, 3k7f, 3k83, 3k84, 3kjq, 3kw9, 3kwb, 3kwz, 3lok, 3m3c, 3m3e, 3o1g, 3ovx, 3qug, 3rdh, 3sgu, 3sw6, 3uli, 3w2t, 3zim, 3zs0, 3zs1, 3zvt, 3zvw, 4an0, 4b16, 4bxn, 4d0l, 4dmx, 4e3n, 4hbp, 4hjs, 4hpc, 4i24, 4ll0, 4lqm, 4lrm, 4lv0, 4oyq, 4rus, 4twy, 4wkt, 4x21, 4yqm, 4ywb, 4z16, 4zzm, 4zzo, 5cyi, 5f2e, 5fct, 5feq, 5gmp, 5i3k, 5j87, 5j9y, 5j9z, 5lf3, 5lf7, 5mxq, 5u4f, 5weu, 5xdk, 5xdl, 5xxd, 5xxg, 5y9t, 5yu9, 5za2, 6alj, 6avi, 6ax1, 6b1e, 6bl1, 6cli, 6cge, 6cha, 6di9, 6e6e, 6ezp, 6hhf, 6hhi, 6iuo, 6j99, 6jjp, 6jwl, 6jx0, 6jx4, 6jxt, 6k1s, 6lw2, 6lze, 6m0k, 6md1, 6mzw, 6o0e, 6o0f, 6oni, 6p69, 6p7i, 6pdz, 6pnm, 6pnn, 6pno, 6qw7, 6r4v, 6rnu, 6swm, 6t5y, 6tfp, 6tpm, 6v6k, 6v6o, 6v9c, 6vh4, 6vim, 6why, 6wi0, 6wtj, 6wtt, 6wxz, 6xd3, 6xhm, 6xmk, 6xr3, 6y2f, 6yi8, 6yzt, 6zpi, 7b3e, 7bwd, 7c6u, 7c8u, 7cb7, 7cbt, 7d1m, 7dpp, 7jkw, 7jxl, 7jxp, 7jxw, 7k0e, 7k1h, 7lel, 7ltm, 7mlf, 7orf, 7rbz, 7rc0, 7tob

112 entries are identified to exhibit steric clashes:

1bb0, 1ca8, 1e55, 1fbp, 1h00, 1qga, 1rly, 1vyr, 1w6p, 1ykl, 1ykp, 1z8a, 2c01, 2ime, 2j9m, 2jjk, 2r24, 2r9m, 2vj1, 2w68, 2w92, 2wnj, 2xuc, 2zyk, 3a23, 3cud, 3d04, 3fck, 3kfy, 3lb4, 3mdj, 3n8y, 3pch, 3qce, 3qcf, 3rho, 3rv7, 3uo9, 3w4k, 3wzu, 3zrc, 4bii, 4d0m, 4e26, 4ele, 4fh7, 4fm5, 4g5y, 4gs9, 4he9, 4ic0, 4jlm, 4otj, 4ucf, 4v04, 4xi3, 4yx9, 4zx6, 4zzw, 5afk, 5dx3, 5dxb, 5ewa, 5fb7, 5fry, 5glt, 5glz, 5gm0, 5h5o, 5hjc, 5hk9, 5hn7, 5hn9, 5hyr, 5i3b, 5is0, 5ivt, 5sye, 5syf, 5t6p, 5vn1, 5wbk, 5xg4, 5z75,

6a6k, 6ah4, 6ah5, 6c7g, 6ch5, 6co5, 6cup, 6eum, 6gno, 6jz0, 6kiu, 6kiv, 6kix, 6kiz, 6n92, 6n94, 6n96, 6ncf, 6ohu, 6oo8, 6ppl, 6pww, 6qdf, 6ula, 6whv, 6wv1, 7c7h, 7cr4

361 entries are identified contain ligand with uncommon elements:

1cp6, 1cws, 1d3v, 1dd7, 1dzj, 1el7, 1el8, 1esz, 1hq5, 1hyv, 1hyz, 1k2v, 1lvk, 1mu9, 1nop, 1rff, 1rfi, 1rg1, 1rg2, 1rgt, 1rgu, 1rh0, 1suo, 1svk, 1tqv, 1tqw, 1v97, 1w0g, 1wva, 1xuf, 1xuj, 1y3g, 1ztz, 2aeb, 2ato, 2bdm, 2bt3, 2c2s, 2c2t, 2cfd, 2ci0, 2cib, 2d0t, 2dy5, 2fb3, 2fdu, 2fdv, 2fdw, 2fou, 2fov, 2foy, 2gj8, 2h7r, 2ij7, 2jpp, 2jld, 2nz5, 2oi4, 2oro, 2orp, 2p8o, 2pll, 2rar, 2rav, 2rb5, 2rbk, 2v0m, 2v96, 2v97, 2w09, 2w0b, 2wfg, 2wh8, 2whf, 2wpu, 2wuz, 2wv2, 2wx2, 2xfh, 2yak, 2ydm, 3b6h, 3b99, 3ben, 3bwf, 3e6k, 3e6v, 3e9b, 3fxz, 3fy0, 3g5n, 3gph, 3i7z, 3i80, 3i8w, 3ixb, 3ixg, 3jt4, 3jt9, 3jus, 3khm, 3koh, 3ksw, 3lc4, 3mdt, 3mke, 3mmr, 3mnu, 3nxu, 3o0j, 3ozu, 3ozv, 3ozw, 3qoa, 3r9c, 3ruk, 3swz, 3t3q, 3t3r, 3t3s, 3t3z, 3tmz, 3vjs, 3vjt, 3wax, 3way, 3zg2, 3zg3, 4c0c, 4c4r, 4c4s, 4coh, 4d2y, 4d2z, 4d30, 4d31, 4d32, 4d33, 4d34, 4d35, 4d36, 4d37, 4d38, 4d39, 4d3a, 4d3b, 4d75, 4d78, 4d7d, 4dtw, 4dtz, 4du2, 4dub, 4due, 4duf, 4ehr, 4ejh, 4eji, 4enh, 4fdh, 4fil, 4g0c, 4g44, 4g45, 4h4d, 4h4e, 4hpd, 4hww, 4hxq, 4hze, 4i06, 4i4g, 4i60, 4ie2, 4ie3, 4iu0, 4iu4, 4ixu, 4ixv, 4j14, 4jfv, 4jfw, 4jjf, 4jjg, 4k9t, 4k9v, 4k9w, 4k9x, 4mdg, 4mdl, 4mdm, 4nkx, 4ob0, 4pf7, 4pk5, 4pk6, 4q3q, 4q3r, 4q3s, 4u72, 4u74, 4uch, 4uhi, 4uhl, 4uqh, 4uzi, 4v3u, 4v3v, 4v3w, 4v3x, 4v3y, 4v3z, 4wmz, 4xrz, 4xud, 4z0l, 4zdy, 4zdz, 4ze0, 4ze1, 4ze2, 4ze3, 4zee, 4zgx, 5agp, 5brv, 5c8i, 5cg5, 5cg6, 5cjh, 5e58, 5e7v, 5ek2, 5ek3, 5ek4, 5etw, 5fom, 5fqb, 5fqe, 5fsa, 5hs1, 5ibe, 5ibf, 5ibg, 5irq, 5irv, 5jqt, 5jws, 5jwu, 5jww, 5k1l, 5k7k, 5l2r, 5l92, 5l94, 5mon, 5moo, 5tz1, 5u48, 5u4a, 5u4c, 5u4e, 5vc0, 5vce, 5veu, 5wmu, 5wn8, 6a16, 6a17, 6abk, 6bbs, 6bc9, 6bcc, 6c6n, 6c8x, 6ceh, 6chi, 6cir, 6ciz, 6cr2, 6d1l, 6d1m, 6da3, 6da5, 6daa, 6dab, 6dac, 6dag, 6daj, 6e40, 6e41, 6f0a, 6ffk, 6frj, 6gcy, 6h1l, 6h1t, 6h3q, 6hwz, 6hx5, 6i96, 6j8r, 6jn6, 6kof, 6kps, 6kvq, 6kw7, 6m7x, 6ma6, 6ma7, 6msn, 6mso, 6o3i, 6pgx, 6pht, 6pu7, 6q2t, 6q37, 6q39, 6qfu, 6qfv, 6qfw, 6qfx, 6qou, 6rpn, 6rvf, 6rvk, 6rvl, 6rw1, 6sp7, 6t7u, 6t9z, 6u30, 6u7o, 6ung, 6unh, 6uni, 6unk, 6unl, 6v7c, 6v7d, 6v7e, 6v7f, 6vbn, 6wpl, 6wr0, 6wr1, 6xz8, 6xz9, 6yzq, 6yzs, 6yzt, 6yzu, 6yzv, 6yzw, 6yzx, 6zjc, 7e0p, 7e7f, 7m8v, 9nse

10 entries are identified to contain small ligands:

1lg6, 1ray, 1ugb, 1ugf, 1zdq, 2ca2, 2hds, 4e5q, 4qef, 6pdv

1428 entries failed the structure fixing:

1lgs, 1a07, 1a2c, 1a5v, 1ad8, 1agm, 1apv, 1apw, 1aqc, 1at5, 1at6, 1axw, 1b11, 1b40, 1b5q, 1b6j, 1bdq, 1bfn, 1bm2, 1bzh, 1c0p, 1c5o, 1c5p, 1c5z, 1cka, 1ckb, 1ckp, 1clu, 1d6s, 1deh, 1dmb, 1e4w, 1e5j, 1eb1, 1ec9, 1eef, 1epq, 1evh, 1eyn, 1ez9, 1f5k, 1f86, 1fh7, 1fh8, 1fh9, 1fhd, 1fls, 1fm1, 1fwu, 1fwv, 1g3c, 1g42, 1g9r, 1ga8, 1gah, 1gai, 1gbn, 1gni, 1gnm, 1gnn, 1gno, 1gny, 1gse, 1gu3, 1gui, 1gvu, 1gvx, 1gwl, 1gwq, 1gwr, 1gww, 1h24, 1h2t, 1h2u, 1h9g, 1hew, 1hkk, 1hpb, 1hps, 1htb, 1htg, 1hut, 1i30, 1i7c, 1i7m, 1igj, 1is0, 1it6, 1j1a, 1j84, 1j8v, 1jd5, 1jfh, 1jlx, 1jn2, 1ju9, 1jvp, 1k1y, 1k7t, 1k7u, 1kjl, 1kjr, 1kl3, 1kl5, 1l6m, 1l7z, 1lax, 1lek, 1lf9, 1lkk, 1lqe, 1lr8, 1lzb, 1lze, 1lzg, 1m7d, 1m7i, 1md2, 1mf4, 1mfa, 1mfd, 1mfl, 1mhw, 1n92, 1nm5, 1nzy, 1oau, 1obx, 1oby, 1ocq, 1of4, 1ogg, 1oh3, 1oh4, 1ols, 1olu, 1olx, 1oxn, 1oxq, 1p2g, 1ph0, 1phw, 1pig, 1pl0, 1pmh, 1ppi, 1pzi, 1pzk, 1q0y, 1q4k, 1qaw, 1qiw, 1qj6, 1qj7, 1qja, 1qjb, 1qlu, 1qsc, 1ra1, 1ra9, 1rbm, 1rbz, 1rc0, 1rev, 1rd9, 1rdj, 1rdl, 1rdm, 1rdp, 1rf2, 1rr8, 1rrj, 1rsu, 1rx9, 1s7y, 1sem, 1seu, 1shd, 1skx, 1sld, 1sle, 1slg, 1sln, 1ssq, 1str, 1sts, 1syn, 1t7d, 1t8i, 1tb4, 1tc1, 1tf8, 1tlc, 1tps, 1tsd, 1tw6, 1u5b, 1ua7, 1ugx, 1ugy, 1ukq, 1ukt, 1uld, 1ule, 1ulg, 1umw, 1ur8, 1ur9, 1utc, 1ux7, 1uxa, 1uxb, 1uz8, 1uzn, 1v0k, 1v0l, 1v11, 1v16, 1v1m, 1vwl, 1vwn, 1w1g, 1w2h, 1w3k, 1w3l, 1w3y, 1w8f, 1w8h, 1w9d, 1w9e, 1w9o, 1w9w, 1wdn, 1wdr, 1wgc, 1wu1, 1x08, 1x09, 1x7w, 1x7x, 1x7y, 1x7z, 1x80, 1xff, 1xkx, 1xl1, 1xnk, 1xt3, 1xt8, 1xxz, 1y3n, 1y3p, 1y3y, 1y79, 1y7l, 1yf4, 1yhm, 1yp9, 1yxd, 1zfp, 1zhs, 1zkk, 1zky, 2a3y, 2ak5, 2aoc, 2aod, 2aoh, 2aou, 2ar6, 2arb, 2ay7, 2az8, 2az9, 2azb, 2azc, 2bcd, 2bel, 2bgr, 2bmz, 2c05, 2c7u, 2cb8, 2cdp, 2chn, 2cju, 2cvq, 2dt3, 2e95, 2eax, 2er9, 2euk, 2eum, 2evl, 2ff4, 2fgu, 2fgv, 2foq, 2fos, 2gfa, 2gfj, 2ggg, 2gh9,

2h13, 2h6k, 2h6n, 2h6q, 2hah, 2hj4, 2hjb, 2hl3, 2ho2, 2i74, 2ifw, 2ii3, 2imf, 2iqd, 2itk, 2j1t, 2j6o,
 2jg8, 2jjb, 2mip, 2msb, 2ntb, 2nwl, 2nwx, 2nxd, 2nxl, 2nxm, 2o9v, 2oei, 2ok0, 2oor, 2ooz, 2orv, 2p4t,
 2peh, 2q5a, 2q7q, 2q8y, 2qmj, 2qt5, 2qta, 2qtz, 2r0h, 2r1w, 2r1x, 2r1y, 2r23, 2r3y, 2rca, 2ri9, 2rkm,
 2rkn, 2tpi, 2uue, 2uvh, 2uvi, 2uvj, 2uyq, 2v7d, 2v83, 2v86, 2v88, 2v8l, 2vco, 2vj0, 2v1l, 2vnf, 2vnk,
 2vpe, 2vqz, 2vsl, 2vt5, 2vuz, 2vzl, 2w1u, 2w3o, 2w5k, 2w5l, 2w7y, 2wa8, 2wcg, 2wd3, 2wdb, 2wev,
 2wgc, 2whp, 2wk2, 2wly, 2wm0, 2wn3, 2wra, 2wt0, 2wt1, 2wt2, 2wyf, 2wyn, 2x4t, 2xd3, 2xg3, 2xg9,
 2xog, 2xoi, 2xom, 2xon, 2xqq, 2xwe, 2y4s, 2y64, 2y6g, 2y6l, 2y7z, 2yg0, 2yjq, 2ylg, 2yln, 2ypp, 2z8d,
 2z8e, 2z8f, 2zcr, 2zcs, 2zex, 2zey, 2zga, 2zhf, 2zhk, 2zhl, 2zhp, 2zm3, 2zno, 2zq0, 2zy1, 3a06, 3ach,
 3aci, 3al3, 3avf, 3ayc, 3ayd, 3b4y, 3b9a, 3bbt, 3bho, 3bib, 3biv, 3boo, 3bpc, 3bwr, 3bzi, 3c0z, 3c3d,
 3c9e, 3cbs, 3d3x, 3d6o, 3d9t, 3db3, 3dcq, 3diw, 3drg, 3dz2, 3dz4, 3dz6, 3e7a, 3ebb, 3er3, 3eys, 3f3a,
 3f5j, 3f5k, 3f5o, 3f5p, 3f70, 3f81, 3f9w, 3f9y, 3fi2, 3fn0, 3g0e, 3g0f, 3g3r, 3g42, 3gjf, 3gl6, 3gss, 3gxz,
 3h9f, 3hkn, 3hlo, 3hzk, 3hzy, 3i6c, 3iet, 3if7, 3iiq, 3iit, 3iqg, 3iqh, 3iqi, 3iqj, 3iqv, 3isd, 3ivv, 3jvk,
 3jyr, 3jzj, 3k00, 3k45, 3k8d, 3ka2, 3kce, 3kmc, 3kyf, 3kyg, 3lbl, 3lex, 3lgs, 3ll2, 3lpl, 3lq2, 3lq4, 3lqi,
 3lqj, 3lsj, 3lug, 3luh, 3lw1, 3m3o, 3m3r, 3mbp, 3muk, 3mxc, 3mxy, 3n0i, 3n7y, 3n8m, 3n8w, 3nf3,
 3nkx, 3nq6, 3nw3, 3nrx, 3ny3, 3o0w, 3o0x, 3o6m, 3oea, 3oeb, 3oka, 3okp, 3old, 3ole, 3olg, 3oli, 3oy8,
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 3voz, 3vp1, 3vp2, 3vtr, 3vyk, 3waw, 3wch, 3wel, 3weo, 3wol, 3wom, 3won, 3wqd, 3wqv, 3zdvd, 3zkk,
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5vdk, 5vnf, 5vrw, 5vrz, 5vrx, 5vry, 5vrz, 5vs1, 5vs2, 5vs3, 5vv8, 5w3y, 5w7i, 5w7x, 5wei, 5wje, 5x2a, 5xo2, 5xof, 5y5u, 5yba, 5yd3, 5yd4, 5yd5, 5ygf, 5yqw, 5ysd, 5yse, 5ysf, 5yto, 5ytu, 5yx2, 5yy4, 5zbz, 5zrf, 6a56, 6a80, 6a8n, 6apr, 6apu, 6asz, 6at0, 6ayh, 6b2c, 6b3p, 6b67, 6bn0, 6brr, 6c19, 6c5h, 6c5j, 6c5k, 6c9n, 6c9p, 6c9r, 6cb5, 6cbz, 6ccu, 6cd8, 6cdg, 6cff, 6cy7, 6d6t, 6dfr, 6dmf, 6dqn, 6dqs, 6dqv, 6dqz, 6dr0, 6drc, 6e3d, 6ecz, 6eeh, 6ek3, 6eor, 6eq1, 6eqv, 6eqw, 6eqx, 6f4p, 6f4r, 6f4t, 6f57, 6f5u, 6f6i, 6f6n, 6f6s, 6f8n, 6fau, 6fav, 6faw, 6fbw, 6fby, 6ffl, 6fft, 6fhu, 6fi4, 6fi5, 6fiv, 6fjj, 6flg, 6fmn, 6fn9, 6fpu, 6fqr, 6ful, 6fuv, 6g15, 6g9b, 6g9i, 6gd0, 6gdo, 6gex, 6gtx, 6gty, 6gtz, 6gu0, 6gw1, 6gx6, 6h0h, 6h4o, 6h4p, 6h4r, 6h4s, 6h4u, 6h4v, 6h4w, 6h4x, 6h4y, 6h50, 6h51, 6h52, 6h5w, 6hcu, 6hhp, 6hi4, 6hi6, 6hi8, 6hm0, 6hmt, 6how, 6hpg, 6hqx, 6hro, 6hs4, 6i0l, 6i1u, 6i41, 6i5p, 6i5v, 6i5w, 6i68, 6i7a, 6ial, 6iam, 6idg, 6im4, 6inz, 6jad, 6jao, 6jba, 6jue, 6kgo, 6kgq, 6kxa, 6kxb, 6l1f, 6lcf, 6ld3, 6ld4, 6ld5, 6lf2, 6lfj, 6lj2, 6lk4, 6lra, 6lrd, 6m6p, 6m8p, 6mle, 6mlo, 6n19, 6n93, 6n97, 6nlk, 6nll, 6nlm, 6nxz, 6ny0, 6o5i, 6o6n, 6orv, 6p02, 6pa7, 6phx, 6pre, 6prg, 6pwv, 6q9w, 6qdx, 6qpl, 6qsw, 6qsx, 6qux, 6r18, 6r3m, 6r6v, 6r6w, 6rav, 6rd2, 6rfh, 6rk4, 6rt6, 6rt7, 6rti, 6ryo, 6sli, 6sey, 6sgf, 6slo, 6spw, 6spx, 6sq0, 6swm, 6swo, 6swq, 6swx, 6t1d, 6t7z, 6tg4, 6th7, 6tkm, 6tmp, 6tmq, 6tmz, 6tn0, 6tn2, 6tpk, 6tpx, 6tpy, 6tpz, 6tv4, 6twu, 6twx, 6u4q, 6u4t, 6u5m, 6u67, 6u8p, 6u8v, 6u8w, 6u8x, 6u90, 6u91, 6uc3, 6udc, 6v2e, 6vzh, 6vuf, 6vw7, 6wf5, 6wj7, 6wm1, 6wo2, 6wp5, 6wy7, 6x23, 6x3v, 6x9c, 6x9i, 6x9j, 6xwd, 6y2g, 6y58, 6yb4, 6yqn, 6yqo, 6yqr, 6yqs, 6yt1, 6yt2, 6z4q, 6z4s, 6z84, 6zb0, 6zb1, 6zb2, 6zb3, 6zfm, 6zin, 6zpd, 7a5m, 7at8, 7bvt, 7c67, 7c68, 7c69, 7c6g, 7c6i, 7c6k, 7c6m, 7c6t, 7c6w, 7c70, 7jjc, 7k0l, 7k0q, 7k5e, 7k5f, 7k5g, 7k5h, 7kkp, 7kme, 7lan, 7luf, 7n7x, 7otm, 7oty, 7pw4, 7pw5, 7pw6, 7pw7, 8icj, 8ico, 8icw, 8icx, 8icy, 8kme, 9icd, 9icu

Note: 1gx4 failed only in small molecule set.

3 Failed cases in processing PDBBind

Table S4: Overview of the number of entries during filter and structure fixing process of PDBBind.

	Number of unique PDB IDs		
	Small Molecule	Polymer	Total
Before processing	16738	2705	19443
Successfully processed ^a	14915 (26626)	746 (1131)	15661 (27757)
Failed	1823	1959	3782
Covalent binders	857	101	958
Steric clashes	128	37	165
Contain uncommon elements	197	9	206
Small ligands	1	0	1
Fail to fix structures	640	1812	2452 ^c

^a In parenthesis is the number of protein-ligand structures.

958 entries are identified with covalent binders:

1a09, 1a46, 1a5g, 1a61, 1ad8, 1aht, 1amn, 1au0, 1au2, 1auj, 1avp, 1awf, 1awh, 1ayu, 1ayv, 1b0f, 1b5g, 1bgo, 1bio, 1bjr, 1bmq, 1bwn, 1c3b, 1doj, 1e34, 1e37, 1eas, 1eat, 1ekb, 1ero, 1erq, 1exw, 1flj, 1f7b, 1f9e, 1fsw, 1fsy, 1ft4, 1g37, 1ga9, 1gbt, 1gfw, 1ggd, 1gzg, 1gzv, 1h0w, 1h1b, 1h8y, 1hbj, 1i72, 1i8j, 1iau, 1iem, 1iew, 1inc, 1jlx, 1k2i, 1kds, 1kdw, 1ke0, 1ke3, 1l6s, 1l6y, 1lhc, 1lhd, 1lhe, 1lhf, 1lhg, 1llb, 1me3, 1me4, 1mem, 1mns, 1mpl, 1ms0, 1ms6, 1mwt, 1mxo, 1my8, 1nc6, 1njt, 1nju, 1nkm, 1nl6, 1nlj, 1nms, 1no9, 1npz, 1nqc, 1ny0, 1nyy, 1o2t, 1o41, 1o43, 1o45, 1o4a, 1o4d, 1o4e, 1o4i, 1o4k, 1o5f,

long, lonh, 1p01, 1p02, 1p03, 1p04, 1p05, 1p06, 1p10, 1pau, 1pi4, 1pi5, 1q6k, 1qcp, 1qfs, 1qhr, 1qj1,
 1qj6, 1qj7, 1qtn, 1qw, 1qx1, 1re1, 1rhj, 1rhk, 1rhm, 1rhq, 1rhr, 1rhu, 1rtl, 1rww, 1rwx, 1rxp, 1snk,
 1sre, 1sri, 1tbz, 1tlo, 1tmb, 1tu6, 1tyn, 1u9v, 1u9w, 1u9x, 1ukt, 1uod, 1vgc, 1vs, 1w10, 1w12, 1w14,
 1w31, 1x6u, 1y19, 1yk7, 1ylv, 1yly, 1ym1, 1yms, 1yt7, 1z6f, 1zom, 1zpb, 1zpc, 2a4g, 2a4q, 2ajb,
 2ajd, 2ajl, 2alv, 2asu, 2aux, 2auz, 2bdl, 2bz5, 2clx, 2eep, 2f9u, 2f9v, 2fda, 2fj0, 2fm2, 2fs8, 2fs9,
 2ftd, 2fxr, 2g5p, 2g5t, 2g63, 2g83, 2gbf, 2gbg, 2gph, 2gsu, 2gvf, 2h5d, 2h5i, 2h5j, 2h65, 2ha0, 2hds,
 2hob, 2hwo, 2hwp, 2i03, 2i72, 2jal, 2jbv, 2jdh, 2k0x, 2lpr, 2mlm, 2nqg, 2nqi, 2o7e, 2o7v, 2o9a, 2obo,
 2oc0, 2oc1, 2oc7, 2op3, 2op9, 2oz2, 2q3z, 2q80, 2q9m, 2q9n, 2qaf, 2qcn, 2qky, 2ql5, 2ql7, 2ql9, 2qlb,
 2qlf, 2qlj, 2qlq, 2qnz, 2qq7, 2qve, 2r4b, 2r6n, 2rcx, 2rjr, 2rjs, 2uzj, 2v6n, 2vgc, 2wap, 2wgi, 2wig,
 2wij, 2wik, 2wj1, 2wj2, 2woq, 2wzx, 2wzz, 2xcn, 2xdm, 2xdw, 2xe4, 2xk1, 2xlc, 2xln, 2xni, 2xow,
 2xu1, 2xu3, 2xu4, 2xu5, 2xzc, 2y2h, 2y2i, 2y2j, 2y2k, 2y2n, 2y2p, 2y4a, 2y55, 2y59, 2yj2, 2yj8, 2yj9,
 2yjb, 2yjc, 2z3z, 2zu3, 2zu4, 2zu5, 2zz6, 3a73, 3b1t, 3b1u, 3b9s, 3bar, 3bh3, 3bjm, 3bls, 3blt, 3blu,
 3bm6, 3bm8, 3bwk, 3c9e, 3d4f, 3d62, 3dz5, 3e90, 3ewu, 3ex3, 3ex6, 3eyd, 3fkv, 3fmq, 3fmr, 3fnn,
 3g3d, 3g3m, 3gjs, 3gpj, 3gzn, 3h0e, 3hd3, 3hha, 3hj0, 3hwn, 3i06, 3i4a, 3ibc, 3ika, 3iut, 3k7f, 3k83,
 3k84, 3kjf, 3kjin, 3kjq, 3kqa, 3kw9, 3kwb, 3kwz, 3lj7, 3lle, 3lok, 3lox, 3lpr, 3lxs, 3m3c, 3m3e, 3mbz,
 3mkf, 3mxr, 3mxs, 3n4c, 3n5e, 3ns7, 3nzi, 3o1g, 3o6t, 3o86, 3o87, 3o88, 3of8, 3oj8, 3oli, 3opp, 3opr,
 3ovx, 3oyp, 3p8e, 3pa8, 3pcb, 3pcf, 3pch, 3pr0, 3qkv, 3qsd, 3rdh, 3rjm, 3s1y, 3s22, 3s3q, 3s3r, 3sji,
 3sjo, 3sn8, 3sna, 3snb, 3snc, 3snd, 3sv6, 3sv7, 3sv8, 3svv, 3sz9, 3szb, 3t9t, 3tdz, 3tjm, 3uli, 3ufa,
 3ur9, 3v4j, 3v4x, 3v6r, 3v6s, 3vb4, 3vb5, 3vb6, 3vb7, 3vgc, 3w2p, 3w2q, 3w2t, 3wnr, 3wns, 3wnt,
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 4axm, 4bcb, 4bcc, 4bs5, 4bsq, 4bxn, 4ccd, 4d8e, 4d8i, 4dcd, 4dkt, 4dmy, 4e3i, 4e3j, 4e3k, 4e3l, 4e3m,
 4e3n, 4e3o, 4ede, 4eej, 4efg, 4ehm, 4ejf, 4est, 4exz, 4f49, 4fgt, 4fzc, 4fzg, 4gd6, 4ght, 4gk7, 4gkc, 4gs6,
 4hbp, 4hcu, 4hcv, 4hnp, 4hrc, 4hrd, 4i7c, 4i7d, 4i9o, 4i9r, 4i9s, 4imq, 4imz, 4inh, 4inr, 4int, 4inu,
 4ivk, 4j5p, 4j70, 4jg6, 4jg7, 4jg8, 4jj7, 4jj8, 4jje, 4jmx, 4jr0, 4kqo, 4kw6, 4l0l, 4len, 4lv1, 4lv2, 4lv3,
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 6e5b, 6e5g, 6e5s, 6e7m, 6ert, 6euv, 6eyz, 6f34, 6f6r, 6fdq, 6fdu, 6ffn, 6ffs, 6fv1, 6fv2, 6g7f, 6g8m,
 6g8n, 6g9f, 6g9s, 6gch, 6gcr, 6gop, 6gxy, 6gzy, 6h0u, 6hgy, 6hhg, 6hhh, 6hhi, 6hhj, 6htc, 6htd, 6htp,

6htr, 6hub, 6huc, 6huq, 6huu, 6huv, 6hv4, 6hv5, 6hv7, 6hva, 6hvr, 6hvs, 6hvt, 6hvu, 6hvv, 6hvw, 6i0x, 6ib0, 6ib2, 6ic5, 6ic6, 6iuo, 6iyv, 6iyw, 6j6m, 6jpp, 6k1s, 6lpr, 6m8w, 6m8y, 6m9c, 6m9d, 6m9f, 6mhb, 6mhc, 6mhd, 6mhm, 6mkq, 6mny, 6mu1, 6mzw, 6n4t, 6n9p, 6n9t, 6nd3, 6nng, 6nnr, 6nvg, 6nvh, 6nvi, 6nvj, 6nvl, 6o8i, 6oim, 6ovz, 6p8x, 6p8y, 6p8z, 6pgo, 6pgp, 6pnm, 6pnn, 6pno, 6q35, 6q5b, 6qft, 6qg4, 6qg7, 6qho, 6qhr, 6qmu, 6qw7, 6qw8, 6qw9, 6qwa, 6qwb, 6r4v, 6rjp, 6rmm, 6rn6, 6rn7, 6rn9, 6rne, 6rni, 6rnu, 6rrm, 6rtu, 6s1s, 6s9w, 6s9x, 6skb, 6skd, 6un1, 6un3, 7gch, 7lpr, 8lpr, 9lpr

165 entries are identified to exhibit steric clashes:

1ba8, 1bb0, 1ca8, 1e55, 1gj5, 1gvk, 1h9l, 1ibc, 1jbd, 1jrs, 1nu8, 1oxg, 1pop, 1xxh, 1ykp, 1yyy, 1zzz, 2a4r, 2jjk, 2l75, 2p59, 2pre, 2psx, 2q6f, 2qpj, 2qq5, 2r9m, 2vcb, 2vj1, 2w68, 2w92, 2wnj, 2ww0, 2xuc, 3aav, 3atp, 3b3x, 3bcn, 3d04, 3dkj, 3e0p, 3e16, 3fck, 3fv7, 3fyz, 3fzc, 3gjq, 3gjt, 3gpe, 3gxy, 3kl8, 3lce, 3lpg, 3mo0, 3o0u, 3qce, 3qcf, 3qzq, 3rsb, 3rv7, 3sgv, 3t2c, 3tyq, 3uo9, 3wdc, 3wdd, 3wde, 3wzu, 3zmq, 3zrc, 4a2a, 4e26, 4ele, 4f3h, 4g5y, 4ga3, 4gs9, 4h38, 4h3a, 4he9, 4jlm, 4kiu, 4li5, 4lil, 4loj, 4p00, 4ps0, 4ps1, 4qlq, 4qls, 4qlt, 4qlu, 4qlv, 4v04, 4w5j, 4whs, 4ym4, 4yv2, 4yx9, 4z7f, 4z7q, 4zx6, 5afk, 5dpw, 5dx3, 5ewa, 5f5b, 5fb7, 5g1p, 5gsw, 5h5o, 5hk9, 5hn7, 5hn9, 5htb, 5hvp, 5ivt, 5izk, 5jer, 5n6s, 5ngb, 5npf, 5nqe, 5ouh, 5t6p, 5v5o, 5vfn, 5wbf, 5xg4, 5xw6, 5yjo, 5ykp, 5yr4, 5yr5, 5yr6, 5yun, 5z1d, 6a6k, 6a73, 6b22, 6byz, 6c7g, 6ccx, 6ddb, 6eqs, 6eum, 6fmp, 6hmy, 6ijl, 6ikm, 6jjj, 6jki, 6jz0, 6k4r, 6kjj, 6myn, 6n55, 6n92, 6n94, 6n96, 6nt2, 6nzz, 6ohu, 6pk7, 6pvs

206 entries are identified to contain ligand with uncommon elements:

1cp6, 1d3v, 1dzj, 1esz, 1hq5, 1hyv, 1hyz, 1k2v, 1lkx, 1lvk, 1nxy, 1nym, 1pq3, 1wva, 1y3g, 2aeb, 2cfd, 2cfg, 2fou, 2fov, 2foy, 2jld, 2p8o, 2pll, 2v0c, 2v96, 2wf5, 2wfg, 2wq4, 2yak, 2ydm, 2z97, 3bwf, 3c7n, 3csl, 3cst, 3e6k, 3e6v, 3e81, 3e9b, 3fxz, 3fy0, 3ixg, 3m1s, 3mg0, 3mke, 3mmr, 3mnu, 3o0j, 3p3h, 3p3j, 3p44, 3p55, 3pup, 3q4c, 3qlb, 3qo9, 3rj7, 3ro0, 3sjt, 3skk, 3sl0, 3sl1, 3vjs, 3vjt, 3w8o, 3wax, 3way, 3wc5, 3whw, 3zp9, 4aw8, 4daw, 4dcx, 4dcy, 4ehr, 4fea, 4fil, 4g0c, 4h4d, 4h4e, 4hmq, 4hww, 4hxq, 4hze, 4i06, 4i60, 4ido, 4ie2, 4ie3, 4iu0, 4iu4, 4ixu, 4ixv, 4jfv, 4jfw, 4jhq, 4jjf, 4jjg, 4k6t, 4kai, 4kb7, 4kbi, 4kii, 4l6q, 4ob0, 4ob1, 4q3q, 4q3r, 4q3s, 4rlp, 4u5t, 4xkc, 4z46, 5agi, 5agj, 5agr, 5ags, 5agt, 5dhf, 5fjw, 5fom, 5fqb, 5fqc, 5fsb, 5hj9, 5hja, 5hki, 5hlm, 5ll7, 5m29, 5m2q, 5m34, 5m3b, 5mgi, 5mnx, 5mny, 5mo2, 5mon, 5moo, 5mos, 5nxx, 5nxy, 5od5, 5tgy, 5u48, 5u4a, 5u4c, 5u4e, 5ujo, 5vrl, 5wys, 5zeq, 6abk, 6ajz, 6b30, 6bbs, 6bc9, 6c8x, 6ceh, 6d1l, 6d1m, 6e4v, 6frj, 6h3q, 6hwz, 6hx5, 6i0k, 6i0p, 6i96, 6i97, 6ibs, 6ibv, 6j8q, 6j8r, 6jn3, 6jn4, 6jn5, 6jn6, 6msn, 6mso, 6naf, 6nti, 6ntj, 6pgx, 6pht, 6q2y, 6q30, 6q37, 6q39, 6qaf, 6qfu, 6qfv, 6qfw, 6qfx, 6rmf, 6rsa, 6rvf, 6rvk, 6rvl, 6rw1, 6skc, 6u7o, 6u7p, 6uhu

1 entry are identified to contain small ligands:

6eu6

2452 entries failed the structure fixing:

1lgs, 1a07, 1a0t, 1a2c, 1a37, 1a3e, 1abf, 1abt, 1af2, 1agm, 1apb, 1apv, 1apw, 1aqc, 1at5, 1at6, 1atl, 1aze, 1azx, 1b11, 1b2m, 1b40, 1b6j, 1bap, 1bd1, 1bdq, 1bm2, 1bm6, 1bsk, 1bt6, 1bux, 1bzh, 1c5o, 1c5p, 1c5z, 1cka, 1ckb, 1clu, 1cpi, 1cyn, 1czq, 1d4w, 1d6s, 1d8e, 1dkd, 1dmb, 1dva, 1dyp, 1e03, 1e5j, 1eb1, 1ec9, 1eef, 1ej4, 1eoj, 1eol, 1epq, 1eub, 1evh, 1ez9, 1f47, 1f4y, 1f5k, 1ff1, 1fh7, 1fh8, 1fh9, 1fhd, 1fls, 1fwu, 1fwv, 1g42, 1g6g, 1g9r, 1ga8, 1gag, 1gah, 1gai, 1gmy, 1gni, 1gnj, 1gnm, 1gno, 1gny, 1gu3, 1gui, 1gvu, 1gvx, 1gwm, 1gwq, 1gwr, 1gww, 1gzc, 1h00, 1h07, 1h24, 1h25, 1h26, 1h27, 1h28, 1h2t, 1h2u, 1h5v, 1h6e, 1hc9, 1hgt, 1hkj, 1hkk, 1hkm, 1hps, 1htg, 1i3z, 1i6v, 1i7c, 1i7m, 1i8h, 1i8i, 1idg, 1igj, 1iht, 1ikt, 1ilq, 1iq1, 1is0, 1it6, 1iwq, 1j19, 1j1a, 1j4q, 1jd5, 1jd6, 1jfh, 1jh1, 1jm4, 1jmq, 1jn2, 1jp5, 1jpl, 1juq, 1jvp, 1k1y, 1k9q, 1kat, 1kc5, 1kcs, 1kjr, 1kl3, 1kl5, 1kna, 1kne, 1l6m, 1lek, 1lf8, 1lf9, 1lkk, 1ll4, 1lqe, 1lt5, 1lxh, 1m7d, 1m7i, 1mf4, 1mfa, 1mfd, 1mhw, 1mpa, 1mv0,

1n3w, 1n4m, 1n5z, 1n7m, 1nde, 1ngw, 1nlo, 1nlp, 1nlt, 1ny2, 1o9k, 1oau, 1obx, 1ocn, 1ocq, 1od8,
1oeb, 1ogg, 1oh4, 1oj5, 1ok7, 1oko, 1ols, 1olu, 1olx, 1om9, 1orw, 1osg, 1osv, 1ov3, 1ow6, 1ow7, 1ow8,
1oxn, 1oxq, 1oy7, 1ozv, 1p28, 1p2g, 1p4u, 1pcg, 1pdq, 1ph0, 1pig, 1pl0, 1pmx, 1ppi, 1pum, 1pxh,
1py1, 1pyw, 1pzi, 1q4k, 1qaw, 1qi0, 1qiw, 1qja, 1qjb, 1qm5, 1qsc, 1r17, 1r2b, 1r6z, 1rdj, 1rdl, 1rdn,
1rgj, 1s9v, 1shd, 1sje, 1sld, 1sle, 1slg, 1sln, 1sm3, 1sps, 1ssq, 1str, 1sts, 1szm, 1t29, 1t2v, 1t37, 1t79,
1t7d, 1t7f, 1t7r, 1tc1, 1tet, 1ths, 1tl9, 1tps, 1ttv, 1tyr, 1u8t, 1uef, 1ugx, 1ugy, 1uh1, 1uj0, 1ujj, 1ujk,
1ukh, 1ule, 1ulg, 1umw, 1upk, 1ur9, 1urc, 1urg, 1utc, 1uti, 1uvu, 1ux7, 1uxa, 1uxb, 1uz8, 1v0k, 1v0l,
1v0m, 1v0n, 1v11, 1v16, 1v1m, 1vj6, 1vr1, 1vwl, 1vwn, 1w1g, 1w2h, 1w3k, 1w3l, 1w70, 1w80, 1wdn,
1wdq, 1wdr, 1ws5, 1wu1, 1x11, 1x8s, 1x9d, 1xb7, 1xff, 1xhm, 1xn2, 1xn3, 1xt3, 1xt8, 1y3a, 1y3n,
1y3p, 1y3y, 1ybg, 1ybo, 1yhm, 1ymx, 1yp9, 1yvh, 1ywi, 1yxd, 1yy6, 1z3t, 1z3v, 1zfp, 1zkk, 1zky,
1zub, 2a25, 2aez, 2aof, 2aoh, 2aoi, 2aoj, 2aou, 2aq9, 2auc, 2ay7, 2az8, 2az9, 2azb, 2azc, 2azm, 2b1q,
2b1r, 2b2v, 2b7f, 2bba, 2bcd, 2bgn, 2bgr, 2bmz, 2br8, 2byp, 2c1n, 2c9t, 2ce9, 2cht, 2ci9, 2cia, 2co0,
2d1x, 2d2v, 2df6, 2dwx, 2e7l, 2e95, 2e98, 2e9a, 2e9c, 2eh8, 2emt, 2er0, 2er9, 2euk, 2eum, 2evl, 2ez5,
2f5t, 2f6j, 2fci, 2fgu, 2fgv, 2flu, 2fr8, 2frd, 2fsa, 2fts, 2fuu, 2fx9, 2fys, 2g6q, 2gfa, 2ggg, 2gh9, 2h13,
2h2d, 2h2e, 2h2g, 2h2h, 2h6k, 2h6q, 2h9m, 2h9n, 2h9p, 2hah, 2hdx, 2hj4, 2hjb, 2hkf, 2hnh, 2hrp,
2ig0, 2igv, 2igw, 2itk, 2iv9, 2ivz, 2j7w, 2j9n, 2jb5, 2jbu, 2jdk, 2jdl, 2jg8, 2jjb, 2jk9, 2jkr, 2jkt, 2jnj,
2jnw, 2jq9, 2jqk, 2k1q, 2k3w, 2kgi, 2knh, 2kup, 2l0i, 2l65, 2l7u, 2l8j, 2lcs, 2lct, 2liq, 2llq, 2lp8, 2m0o,
2m3o, 2mg5, 2mip, 2mkr, 2mov, 2mow, 2mpa, 2mwy, 2n3k, 2n7b, 2nn8, 2nwl, 2nwn, 2nxd, 2nxl,
2nxm, 2o9k, 2o9r, 2o9v, 2odd, 2oei, 2oi9, 2ooz, 2peh, 2pem, 2pl9, 2pmc, 2pnx, 2pv3, 2q7q, 2q7y,
2q8y, 2qbx, 2qic, 2qki, 2qmj, 2qt5, 2qta, 2qtr, 2qv7, 2qwe, 2r02, 2r03, 2r05, 2r0h, 2r0y, 2r1w, 2r1x,
2r1y, 2r23, 2r2b, 2r3c, 2r3y, 2r5b, 2r7g, 2rfy, 2ri9, 2rkm, 2rkn, 2rok, 2rol, 2rvn, 2srt, 2tpi, 2uw0,
2uyq, 2uz6, 2v7d, 2v83, 2v85, 2v86, 2v87, 2v88, 2vl1, 2vnf, 2vpe, 2vpg, 2vr3, 2vsl, 2vwf, 2vxj, 2w0p,
2w0z, 2w10, 2w16, 2w2u, 2w3o, 2w47, 2w6c, 2w6t, 2w6u, 2w73, 2w76, 2w77, 2w78, 2w7y, 2w9r,
2wa8, 2wgc, 2wd3, 2whp, 2wk2, 2wly, 2wlz, 2wm0, 2wp1, 2wyf, 2wyn, 2wzf, 2x2i, 2x3t, 2x4t, 2x4z,
2x52, 2x6w, 2x6x, 2x6y, 2x85, 2xaf, 2xag, 2xah, 2xaj, 2xaq, 2xas, 2xcs, 2xct, 2xg3, 2xg9, 2xhs, 2xl2,
2xl3, 2xn6, 2xn7, 2xog, 2xoi, 2xqq, 2xrw, 2xs0, 2xs8, 2xwd, 2xwe, 2xxn, 2xzq, 2y06, 2y07, 2y1n,
2y36, 2y4m, 2y4s, 2y6s, 2y8i, 2y8o, 2y9g, 2y9q, 2ydt, 2yhw, 2yjq, 2ylc, 2yln, 2ymt, 2ynr, 2yns, 2ypp,
2yq6, 2z5o, 2z5s, 2z5t, 2zcr, 2zcs, 2zg3, 2zga, 2zgm, 2zm3, 2zpk, 2zq0, 2zy1, 2zym, 2zyn, 2afk, 2al3,
2alt, 2ap4, 2ap7, 2ary, 2arz, 2as3, 2ask, 2asl, 2au6, 2avf, 2avg, 2avh, 2ax5, 2aya, 2ayc, 2ayd, 2b3s,
2b95, 2bbb, 2bbt, 2bg8, 2bho, 2bim, 2bpc, 2btr, 2bu6, 2bu8, 2bum, 2bun, 2buo, 2buw, 2bux, 2bzi,
2c0z, 2c1n, 2c6w, 2c94, 2cbs, 2cfs, 2cfv, 2ck7, 2ck8, 2ckb, 2coj, 2cs8, 2d1e, 2d1f, 2d3x, 2d45, 2d6o,
2d9k, 2d9l, 2d9m, 2d9n, 2d9o, 2d9p, 2dab, 2dcq, 2diw, 2dla, 2dnj, 2dow, 2dpo, 2drf, 2drg, 2dri,
2ds1, 2ds9, 2dvp, 2dz2, 2dz4, 2dz6, 2e7a, 2e8u, 2ebb, 2eg6, 2ehn, 2eht, 2emh, 2eqs, 2er3, 2ery, 2eu7,
2evc, 2evd, 2evf, 2eyf, 2eys, 2eyu, 2f3a, 2f5j, 2f5k, 2f5l, 2f5p, 2f69, 2f70, 2f81, 2f9w, 2f9y, 2fbr, 2fdm,
2fdt, 2fi2, 2fn0, 2fqa, 2fuc, 2fv8, 2g0e, 2g0f, 2g2s, 2g2t, 2g2u, 2g2v, 2g2w, 2g3r, 2g42, 2g5v, 2g5y,
2g7l, 2gds, 2ggw, 2ghe, 2gl6, 2gsm, 2gss, 2gv6, 2gxz, 2h52, 2h6z, 2h91, 2h9f, 2hkn, 2hkt, 2hlo, 2hqh,
2hs8, 2hs9, 2hzk, 2hzv, 2hzy, 2i02, 2i5r, 2i6c, 2i8t, 2i90, 2i91, 2iet, 2if7, 2ifl, 2ifo, 2ifp, 2iit, 2iiw, 2iiy,
2ij0, 2ij1, 2ijy, 2ikc, 2iqg, 2iqh, 2iqi, 2iqj, 2iqq, 2iss, 2isw, 2iux, 2ivq, 2ivv, 2iw7, 2jpx, 2juq, 2jvk,
2jyr, 2jzg, 2jzh, 2jzj, 2k00, 2k26, 2k27, 2k48, 2k8d, 2ka2, 2kmc, 2krd, 2ktr, 2kyf, 2kyg, 2kze, 2l3q,
2l3x, 2l3z, 2l6x, 2lbl, 2lgl, 2lgs, 2lk1, 2lnj, 2lnz, 2lpl, 2lq2, 2lq4, 2lqi, 2lqj, 2luo, 2m3o, 2m3r, 2m53,
2m54, 2m55, 2m56, 2m57, 2m58, 2m59, 2m5a, 2mbp, 2me9, 2mea, 2met, 2meu, 2ml4, 2mp1, 2mp6,
2muk, 2mxc, 2mxy, 2n5u, 2nf3, 2nfl, 2nfl, 2nii, 2nij, 2nil, 2nin, 2nkx, 2nsn, 2nti, 2nw3, 2ny3, 2o0e,
2o1d, 2o1e, 2o6l, 2o6m, 2ob0, 2ob1, 2ob2, 2odi, 2odl, 2ogx, 2oka, 2okp, 2old, 2ole, 2olg, 2omc, 2omg,
2oq5, 2oy8, 2oyw, 2p4f, 2pdh, 2pfp, 2pgu, 2pjl, 2pkn, 2plu, 2pma, 2poa, 2pp7, 2pqz, 2psl, 2puj,
2puk, 2pxe, 2q5u, 2q6s, 2q8d, 2qfy, 2qfz, 2qg6, 2ql9, 2qlc, 2qmk, 2qn7, 2qnj, 2qo2, 2qs4, 2qxd, 2qyv,

3qzt, 3qzv, 3r42, 3r93, 3rbq, 3rdv, 3rg2, 3rl7, 3rl8, 3rme, 3rqe, 3rqf, 3rqg, 3rtx, 3rul, 3rum, 3run,
 3rv6, 3rv8, 3rz9, 3rzi, 3s7f, 3shb, 3shv, 3sm1, 3so6, 3sou, 3sov, 3sow, 3stj, 3sw9, 3sxu, 3szm, 3t5i,
 3t6r, 3t7g, 3t83, 3t8v, 3tcg, 3tdu, 3tf6, 3tf7, 3tg5, 3th0, 3ti4, 3tib, 3tiw, 3tkz, 3tl0, 3tlh, 3tpx, 3tsz,
 3twr, 3tws, 3twu, 3twv, 3tww, 3twx, 3tzd, 3u3f, 3u78, 3ual, 3uat, 3ud7, 3ud8, 3ud9, 3uda, 3ued,
 3uef, 3ueo, 3ui2, 3uig, 3uih, 3uii, 3uij, 3uik, 3upk, 3ur0, 3uri, 3uvk, 3uyl, 3uvm, 3uvm, 3uvo, 3uvu,
 3uvw, 3uvx, 3uw9, 3uwl, 3ux0, 3uxg, 3uyr, 3uzd, 3v2o, 3v30, 3v3b, 3v43, 3v4t, 3v7d, 3va4, 3vf9,
 3vfj, 3voz, 3vp1, 3vp2, 3vp3, 3vp4, 3vtr, 3vzg, 3w37, 3waw, 3wcb, 3wch, 3wdz, 3wp0, 3wp1, 3wqv,
 3wqw, 3wsy, 3wut, 3wu, 3wuv, 3zdv, 3zev, 3zha, 3zhf, 3zi8, 3zjt, 3zju, 3zjv, 3zke, 3zkf, 3zlv, 3zmp,
 3zmt, 3zmu, 3zmv, 3zmz, 3zn0, 3zn1, 3zq9, 3zqi, 3zst, 3zvy, 3zyb, 3zyh, 3zyr, 4a0j, 4a1w, 4a23, 4a4c,
 4a50, 4a7j, 4a9t, 4a9u, 4aa1, 4aa2, 4abi, 4abj, 4ad2, 4ad3, 4agl, 4aif, 4aom, 4ap0, 4aph, 4apr, 4aui,
 4av0, 4av5, 4avi, 4avj, 4ay6, 4ayp, 4aze, 4b4n, 4b4q, 4b60, 4b83, 4b8o, 4b8p, 4b8y, 4b9h, 4b9w,
 4b9z, 4ba3, 4bea, 4bg6, 4bgx, 4blb, 4bpi, 4bpj, 4btl, 4bv2, 4bxu, 4c0r, 4c16, 4c1t, 4c1u, 4c1w, 4c4n,
 4c5w, 4c9w, 4cc2, 4cc7, 4cd4, 4cd5, 4cd6, 4cd8, 4cdr, 4ch2, 4ch8, 4ciz, 4cpq, 4cps, 4cpx, 4csy, 4cy1,
 4czs, 4d1d, 4d4d, 4de7, 4dhl, 4djs, 4dma, 4dow, 4dro, 4ds1, 4dx9, 4e35, 4e3b, 4e6c, 4e81, 4e9c, 4e9d,
 4edu, 4egi, 4elb, 4elg, 4elh, 4ep2, 4eqf, 4eqj, 4er4, 4erq, 4ery, 4erz, 4es0, 4esg, 4ewr, 4exh, 4ezo, 4ezq,
 4ezt, 4ezy, 4f14, 4f20, 4fbx, 4fcm, 4fe9, 4fem, 4fgx, 4fgy, 4fk7, 4fmn, 4fmo, 4fmq, 4fn5, 4ft2, 4fut,
 4g0a, 4g5f, 4g68, 4g69, 4gah, 4gao, 4gj8, 4glr, 4glx, 4gne, 4gnf, 4gng, 4gq6, 4gvc, 4gvd, 4gw1, 4gw5,
 4gwi, 4gxl, 4gy5, 4gye, 4gzf, 4gzw, 4gzx, 4h36, 4h39, 4h3b, 4h3q, 4hcz, 4hcz, 4hgc, 4hp0, 4hpi, 4hpy,
 4hs6, 4hs8, 4htp, 4hva, 4hy9, 4hyb, 4i2z, 4i31, 4i32, 4i33, 4i67, 4i7b, 4iaw, 4iax, 4ib5, 4ifi, 4igk, 4igq,
 4ii9, 4ikn, 4ipn, 4is6, 4iur, 4iut, 4iuu, 4iuv, 4iwd, 4j09, 4j24, 4j26, 4j2c, 4j3u, 4j48, 4j4v, 4j73, 4j77,
 4j7i, 4j84, 4j8g, 4j8r, 4j8s, 4jc1, 4jck, 4je8, 4jfx, 4jz, 4jg0, 4jg1, 4jiz, 4jjq, 4jmg, 4jmh, 4jof, 4jog,
 4joh, 4joj, 4jok, 4k0o, 4k0u, 4k3l, 4k3m, 4k63, 4k64, 4k66, 4k67, 4k6u, 4k6v, 4k6w, 4k6y, 4k72, 4k75,
 4k76, 4kc1, 4kc2, 4kc4, 4kmd, 4kn7, 4kom, 4kon, 4ktu, 4kup, 4kvm, 4kx8, 4l1u, 4l58, 4l6t, 4lbl, 4lbo,
 4lg6, 4ljh, 4lk6, 4lk7, 4lkd, 4lke, 4lkf, 4lkg, 4lkh, 4lkk, 4lkm, 4ln2, 4lnf, 4lno, 4lnp, 4lp6, 4lq3, 4lte,
 4m1d, 4m7j, 4mbp, 4mdn, 4mdr, 4mg5, 4mo4, 4mr3, 4mr5, 4mrd, 4mx5, 4mz5, 4mz6, 4mzf, 4mzh,
 4mzj, 4mzk, 4mzl, 4n3w, 4n6g, 4n7g, 4n7h, 4n7j, 4n7y, 4n84, 4nb3, 4ngn, 4ngp, 4ngq, 4ngs, 4ngt,
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