Brandeis

Zizhang Chen <zizhang2@brandeis.edu>

DB12731 is basically linear

100 messages

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 21, 2022 at 8:35 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

Hi Zizhang,

DB12731 is basically a linear glycan following all the usual patterns, + just one branch off the last residue. You can add that. I will email in this chain if I find more.

--
Dr. Ryan Badman
Postdoctoral Researcher
Pengyu Hong Lab
Computer Science Department
Brandeis University

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 21, 2022 at 9:00 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

added another linear glycan:

b-D-GlcpNAc-(1-4)-b-D-GlcpNAc

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 10:12 AM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB17331 is also a linear molecule you can add, it's full chemical name is too long for Windows OS to handle so files are named DB17331.csv/pdb:
`a-L-Rhap3Me-(1-[4)-a-D-Manp-(1-3)-a-L-Rhap-(1]n-4)-a-D-Manp-(1-3)-a-L-Rhap-(1-3)-a-L-Rhap-(1-3)-a-L-Rhap-(1-3)-b-D-Galp-(1-7)-Tyr`

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 10:28 AM
To: Zizhang Chen <zizhang2@brandeis.edu>

Added a-L-Rhap-(1-3)-b-D-GlcpNAc

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 10:41 AM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB22482 has one branch but the residue number in the PDB matches the csv order so you can include it in the linear molecules as a "simple branched".

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 10:45 AM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB22484 also has one branch residue, the order read is different than DB22482 but the residue number in the PDB matches the csv order so you can also include it in the current molecule set.

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 10:53 AM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB22485 the same as above, PDB order in number matches the csv shift order, so can include it in the current set.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 11:03 AM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB22505 and DB22506 are also easy to deal with. All the branches are phosphorous groups, "PO3" in the PDB which can be ignored, and there are no PO3 shifts in the shifts as these aren't carbohydrates, only the central chain glycan residues have shifts. So these molecules can be included by skipping the PO3 groups in the PDB, and otherwise the relative order of the residues in the PDB matches the shift order in the csv.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 11:07 AM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB22507 can also be included, the branch is an amino acid. The amino acid is omitted in the PDB (or maybe it's the blank residue 0 at the end), and the amino acid (Lys) is last in the shift and can be ignored. So the first 3 PDB residues match the first 3 shift residues in this molecule.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 2:04 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB22529 is another branched that can be included. The one branch residue is last in both PDB and the shifts.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 2:13 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB22544 also has the PDB residue number order match the shift order.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 2:18 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB22547 also has the PDB residue number order match the shift order, simple branched.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 2:31 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB22549 also has the PDB residue number order match the shift order,
simple branched.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 2:36 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB22550 also has the PDB residue number order match the shift order,
simple branched.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 2:57 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DBDB22551 also has the PDB residue number order match the shift order, simple branched.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 3:00 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB22552 also has the PDB residue number order match the shift order, simple branched.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 3:14 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB22553 also has the PDB residue number order match the shift order, simple branched.

I replaced the csv file for that one just now, had some ambiguity in the H6 I corrected H6? -> H62.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 3:20 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB22556 and DB22557 both have the PDB residue number order match the shift order,
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 3:26 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

a-D-Galp was missing the PDB, added it
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 4:09 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26302 both have the PDB residue number order match the shift order,
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 4:36 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26370 is another phosphorous one where the PO3 groups in the PDB can be skipped, and then the residue order (but not absolute number) matches between PDB and shift.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 5:34 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26378 is another phosphorous one where the PO3 groups in the PDB can be skipped, and then the residue order (but not absolute number) matches between PDB and shift.

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 5:41 PM

To: Zizhang Chen <zizhang2@brandeis.edu>

DB26379 is another phosphorous one where the PO3 groups in the PDB can be skipped, and then the residue order (but not absolute number) matches between PDB and shift.

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 5:45 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26380 is another phosphorous one where the PO3 groups in the PDB can be skipped, and then the residue order (but not absolute number) matches between PDB and shift.

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 5:48 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26383 the shift order matches the residue number in the PDB
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Oct 25, 2022 at 12:27 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26378 the shift order matches the residue number order in the PDB if PO3 is removed
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Oct 25, 2022 at 12:33 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26397 is the shift order matches the residue number in the PDB
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Oct 25, 2022 at 12:36 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26403 the shift order matches the residue number order in the PDB if PO3 is removed
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Oct 25, 2022 at 12:40 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26404 the shift order matches the residue number order in the PDB if PO3 is removed
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Oct 25, 2022 at 12:47 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26405 the shift order matches the residue number order in the PDB if PO3 is removed

---But one note the PO3 atoms needs to be in the graph
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Oct 25, 2022 at 3:37 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26428 the shift order matches the residue number order in the PDB
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Oct 25, 2022 at 4:20 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26431 the shift order matches the residue number order in the PDB if PO3 is removed, but Hepp is another name for MAN in bacteria (Man-hepp).
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Oct 25, 2022 at 4:54 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26467 the shift order matches the residue number order in the PDB if PO3 is removed,
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Oct 25, 2022 at 5:09 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26475 the shift order matches the residue number order in the PDB
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Oct 25, 2022 at 5:24 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26476 the shift order matches the residue number order in the PDB, but the second last residue is missing all but 1 and 5 carbons / hydrogens.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Oct 25, 2022 at 5:37 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26479 the shift order matches the residue number order in the PDB, but ME has to be removed from the shifts as it is a functional group not carbohydrate residue.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Oct 25, 2022 at 5:53 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

NeuAca2-3Galb1-3(NeuAca2-3Galb1-4GlcNAc b1-6)GalNAc can be corrected by SWECOM but it's more complicated than others.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 1:51 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26510 the shift order matches the residue number order in the PDB,
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 1:57 PM

To: Zizhang Chen <zizhang2@brandeis.edu>

DB26511 the shift order should match the residue number order in the PDB if it follows the template of the molecules uploaded around the same time, some ambiguity but consistent overall

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 2:31 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26517 the shift order matches the residue number order in the PDB,

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 2:45 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26521 is another phosphorous one where the PO3 group in the PDB can be skipped (last residue), and then the residue order (but not absolute number) matches between PDB and shift. The quip4n is equivalent to deoxy-Glcp4n in nomenclature

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 2:45 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

actually sorry absolute residue order number in PDB does match in 26521 still after the last PO3 omitted

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 2:51 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB4762 can be used, but PDB residue 5 -> csv shift residue 6, and 6 -> 5 respectively.

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 3:08 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB4858 can be used, residue 5 in the PDB is residue 3 in the shift file. Residue 3 and 4 in the PDB are residues 4 and 5 in the shift file. 1 and 2 match.

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 3:53 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB7424 the shift order matches the residue number order in the PDB,

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 4:01 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB8939 can be used, residue 5 in the PDB is residue 3 in the shift file. Residue 3 and 4 in the PDB are residues 4 and 5 in the shift file. 1 and 2 match.

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 4:07 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB9023 can be used, but residue 3 ->4 and 4-> 3 between the PDB and shift csv..
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 4:14 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB9078 can be used but residue 5 ->6 and 6-> 5 between the PDB and shift csv. Other residues have the csv order match the PDB order
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 4:17 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB9188 can be used but residue 3->4and 4-> 3between the PDB and shift csv. Other residues have the csv order match the PDB order

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 4:22 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB9213 is basically a linear glycan following all the usual patterns, + just one branch off the last residue.

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 4:26 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB9490 can be used but residue 3 ->4 and 4-> 3 between the PDB and > shift csv. Other residues have the csv order match the PDB order

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 4:30 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB9507 can be used, residue 5 in the PDB is residue 3 in the shift file. Residue 3 and 4 in the PDB are residues 4 and 5 in the shift file. 1 and 2 match.

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 4:35 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB9539 is basically a linear glycan following all the usual patterns, + just one branch off the last residue

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 4:37 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB9697can be used but residue 3 ->4 and 4-> 3 between the PDB and

shift csv. Other residues have the csv order match the PDB order

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 4:39 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB9708 can be used but residue 4 ->5 and 5-> 4 between the PDB and shift csv. Other residues have the csv order match the PDB order

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 4:45 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB9917 can be used but 5, 4, 3 in the PDB map to 3, 4, 5 in the csv (so 1,2,4 match but 3 and 5 flipped).
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 4:49 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB9919 can be used but residue 5 ->6 and 6-> 5 between the PDB and shift csv. Other residues have the csv order match the PDB order

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 4:54 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB9948 can be used, residue 5 in the shift is residue 3 in the pdb file. Residue 3 and 4 in the shift are residues 4 and 5 in the pdb. 1 and 2 match.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 5:11 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB9949 can be used, residue 5 in the shift is residue 3 in the pdb file. Residue 3 and 4 in the shift are residues 4 and 5 in the pdb. 1 and 2 match.

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Thu, Oct 27, 2022 at 4:30 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26550 can be used as is, the residue numbers in the PDB match the order in the csv shift.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Thu, Oct 27, 2022 at 4:37 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26552 can be used as is, the residue numbers in the PDB match the order in the csv shift.

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 12:06 AM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26691 can be used as is, the residue numbers in the PDB match the order in the csv shift.

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 12:13 AM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26692 can be used as is, the residue numbers in the PDB match the order in the csv shift.

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 12:18 AM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26693 can be used as is, the residue numbers in the PDB match the order in the csv shift.

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 12:20 AM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26694 can be used as is, the residue numbers in the PDB match the order in the csv shift.

[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 12:39 AM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26699 pdb order matches shift order.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 12:49 AM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26700 pdb order matches shift order.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 2:35 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26705 pdb order matches shift order.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 2:46 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26707 pdb order matches shift order.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 2:52 PM

To: Zizhang Chen <zizhang2@brandeis.edu>

DB26708 pdb order matches shift order.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 2:58 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

26709 pdb order matches shift order.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 4:50 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26712 pdb order matches shift order.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 5:23 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26715 pdb order matches shift order, but last PDB residue is PO3 (shouldn't affect shifts).
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 5:25 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26716 pdb order matches shift order, but last PDB residue
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 5:25 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

(ignore "but last PDB residue" in last email, copy/paste error)
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 5:41 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26718 pdb order matches shift order, but last PDB residue. Also I fixed the H6? in the csv file for this one
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 6:06 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

26719 pdb order matches shift order
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 7:41 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26720 pdb order matches shift order
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 7:44 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26722 pdb order matches shift order, there are two PO3 groups but they are the last PDB residues.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 7:47 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26723 pdb order matches shift order
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 7:50 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26724 pdb order matches shift order
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 31, 2022 at 3:08 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26812 pdb order matches shift order
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 31, 2022 at 5:39 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26813 pdb order matches shift order
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 31, 2022 at 5:56 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26879 pdb order matches shift order
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 31, 2022 at 6:04 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26881 pdb order matches shift order, but one PO3 group needs to be ignored in the residue order counting in the PDB (not in shift)
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 31, 2022 at 10:47 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26907 the relative PDB and shift order matches. But residue 2 and 7 in the PDB should be skipped in matching (CSC and PO3), and the first choline residue in the shifts should be skipped since these aren't carbohydrates.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 31, 2022 at 10:58 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

In DB26908, res 5 is actually res 1 in the PDB, and all other res need +1 added to them (e.g. 1 -> 2). Then Choline needs to be ignored in the shift, the one at the top of the shift, it's not a residue. The

high C numbers in the PDB correspond to Choline like C8, C9, C10, C11 etc. Just fit the C's in the shift list.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 31, 2022 at 11:02 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26909 relative residue order matches PDB and csv, but residue 2 and 7 need to be ignored in the PDB for shift matching since they are PO3 and CSC.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 31, 2022 at 11:06 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26910 relative residue order matches PDB and csv, but residue 3 and 6, and 7 need to be ignored in the PDB for shift matching since they are PO3
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Nov 1, 2022 at 2:25 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26918 residue order matches between PDB and csv
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Nov 1, 2022 at 2:30 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26919 residue order matches between PDB and csv
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Nov 1, 2022 at 2:34 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26920 residue order matches between PDB and csv
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Nov 1, 2022 at 2:39 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26921 residue order matches between PDB and csv
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Nov 1, 2022 at 3:39 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26922 residue order matches between PDB and csv
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Nov 1, 2022 at 4:37 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26938 residue order matches between PDB and csv
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Nov 1, 2022 at 4:48 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26945 residue order matches between PDB and csv
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Nov 1, 2022 at 6:10 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26957 residue order matches between PDB and csv
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Nov 1, 2022 at 6:16 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26959 residue order matches between PDB and csv
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Nov 2, 2022 at 4:21 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26960 there are two residues, and the PDB order is flipped. 1->2,
2->1 needs to be done in the PDB.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Nov 2, 2022 at 4:26 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26961 residue order matches between PDB and csv
[Quoted text hidden]