Example 1 pdb_chain_id = 372595 pdb_chain_dbref_id = 5584953

seqres (the raf do has 0 mm)

vnwaavvddfyqelfkahpeyqnkfgfkgvalgslkgnaayktqagkvvdyinaaiggsadaaglasrhkgrnvgsaefhnakaclakacsahgapdlghaiddilshl

uniprot

mvnwaavvddfyqelfkahpeyqnkfgfkgvalgslkgnaayktqagktvdyinaaiggsadaaglasrhkgrnvgsaefhnakaclakacsahgapdlghaiddilsh

Corresponding PDB submission

DBREF 1V07 A 0 0 PDB 1V07 1V07 0 0
DBREF 1V07 A 1 109 UNP O76242 GLBN_CERLA 1 109
SEQADV 1V07 VAL A 48 UNP O76242 THR 48 ENGINEERED MUTATION

1. V --> T is captured, but the sequence is still different
2. Don't know why the pdb_chain_dbref_id is not present in the pdb_chain_diff table
3. The pdb_align_start and pdb_align_end for above case should be 0 108

in the debug code, the SEQADV matches up its DBREF as the PDB one, as alignIDMap has key as struct_ref id="1" for the PDB reference

```
 <PDBx:struct_refCategory>
     <PDBx:struct_ref id="1">
         <PDBx:biol_id></PDBx:biol_id>
         <PDBx:db_code>1V07</PDBx:db_code>
         <PDBx:db_name>PDB</PDBx:db_name>
         <PDBx:entity_id>1</PDBx:entity_id>
         <PDBx:pdbx_align_begin xsi:nil="true" />
         <PDBx:pdbx_seq_one_letter_code xsi:nil="true" />
     </PDBx:struct_ref>
     <PDBx:struct_ref id="2">
         <PDBx:biol_id></PDBx:biol_id>
         <PDBx:db_code>GLBN_CERLA</PDBx:db_code>
         <PDBx:db_name>UNP</PDBx:db_name>
```

```
            <PDBx:entity_id>1</PDBx:entity_id>
            <PDBx:pdbx_align_begin xsi:nil="true" />
            <PDBx:pdbx_seq_one_letter_code xsi:nil="true" />
        </PDBx:struct_ref>
    </PDBx:struct_refCategory>

 <PDBx:struct_ref_seq_difCategory>
      <PDBx:struct_ref_seq_dif pdbx_ordinal="1">
          <PDBx:align_id>1</PDBx:align_id>
          <PDBx:db_mon_id>THR</PDBx:db_mon_id>
          <PDBx:details>ENGINEERED MUTATION</PDBx:details>
          <PDBx:mon_id>VAL</PDBx:mon_id>
          <PDBx:pdbx_auth_seq_num>48</PDBx:pdbx_auth_seq_num>
          <PDBx:pdbx_pdb_id_code>1V07</PDBx:pdbx_pdb_id_code>
          <PDBx:pdbx_pdb_ins_code xsi:nil="true" />
          <PDBx:pdbx_pdb_strand_id>A</PDBx:pdbx_pdb_strand_id>
          <PDBx:pdbx_seq_db_accession_code>O76242</PDBx:pdbx_seq_db_accession_code>
          <PDBx:pdbx_seq_db_name>UNP</PDBx:pdbx_seq_db_name>
          <PDBx:pdbx_seq_db_seq_num>48</PDBx:pdbx_seq_db_seq_num>
          <PDBx:seq_num>49</PDBx:seq_num>
      </PDBx:struct_ref_seq_dif>
    </PDBx:struct_ref_seq_difCategory>

 seqadvs: [SEQADV: ENGINEERED MUTATION 48 v 0 0 DBRef: PDB 1V07 1V07 1 1 A 0 0]
```

The code did perform as expected to match the ref_id = 1 of dbref and align_id = 1 in diff

Example 3 pdb_chain_id = 323001 pdb_chain_dbref_id = 5565018

seqres

glsaaqrqvvastwkdiagsdngagvgkecftkflsahhd**m**aavfgfsgasdpgvadlgakvlaqigvavshlgdegkmvaemkavgvrhkgygnkhikaeyfeplgasllsa
mehriggkmnaaakdawaaayadisgalisglqs

uniprot

mglsaaqrqvvastwkdiagsdngagvgkecftkflsahhd**i**aavfgfsgasdpgvadlgakvlaqigvavshlgdegkmvaemkavgvrhkgygykhikaeyfeplgaslls amehriggkmtaaakdawaaayadisgalisglq

Corresponding PDB submission

REMARK 800 SITE_DESCRIPTION: BINDING SITE FOR RESIDUE HEM A 148
DBREF 1JL6 A 1 147 UNP P15447 GLB4_GLYDI 1 147
SEQRES 1 A 147 GLY LEU SER ALA ALA GLN ARG GLN VAL VAL ALA SER THR

1. No SEQADV documenting the difference I --> M
2. pdb_align_start and pdb_align_end are indexed correctly

In [ ]: