

図 3-20 CgCBP-SO₄構造のグルコースおよび硫酸の $|F_{\text{obs}}| - |F_{\text{calc}}|$ 電子密度マップ(3σ)。
D490は一般酸触媒として働く触媒残基。

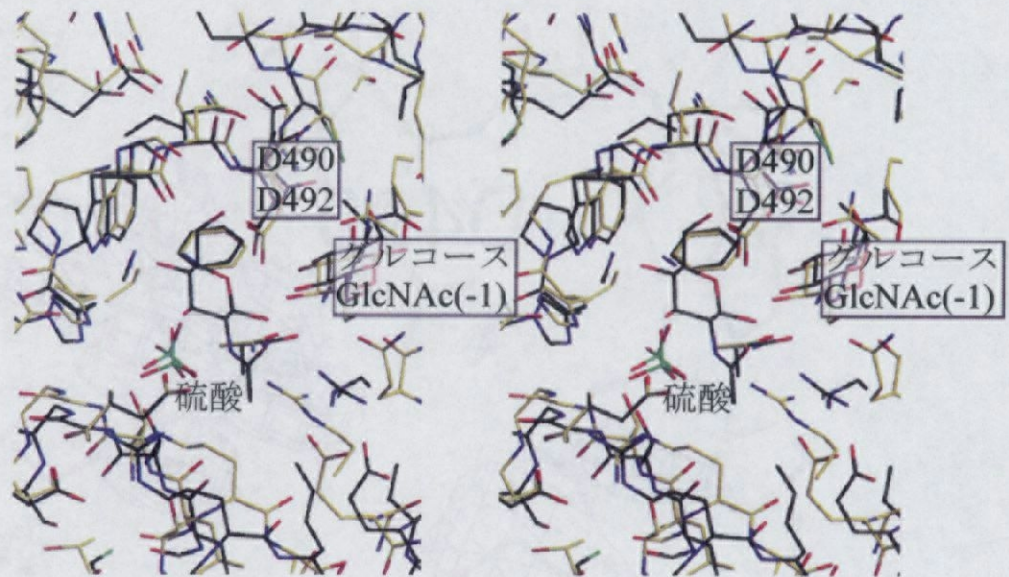


図 3-21 CgCBP-SO₄(黄)とChBP(黒)の活性中心部位の重ね合わせのステレオ図。触媒残基、糖受容体結合部位、硫酸結合部位が一致した。

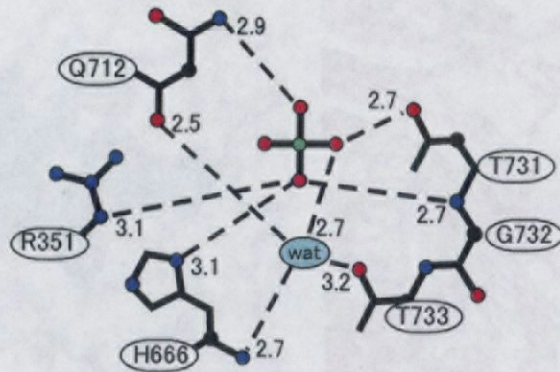


図 3-22a CgCBPと硫酸の相互作用

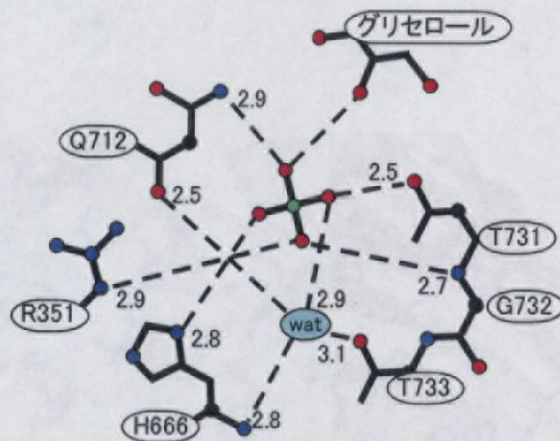


図 3-22b CgCBPとリン酸の相互作用

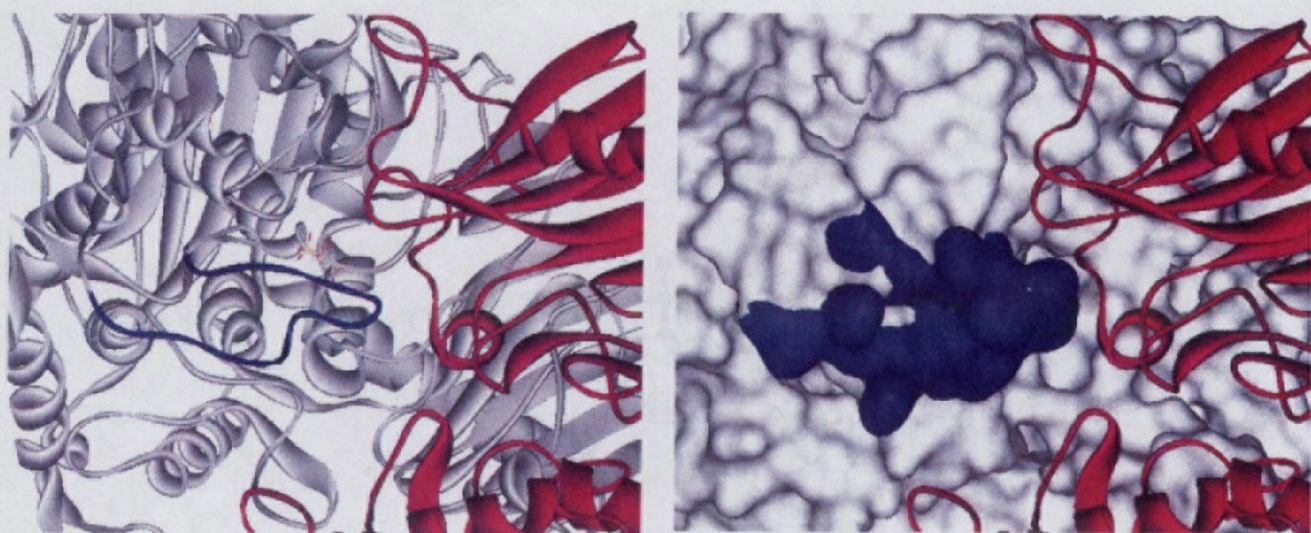


図 3-23a CgCBPの活性中心部位のリボン図(左)と分子表面(右)。隣のサブユニットを赤色で示した。青色で示した残基番号495-513のループで、活性中心部位は塞がれている。

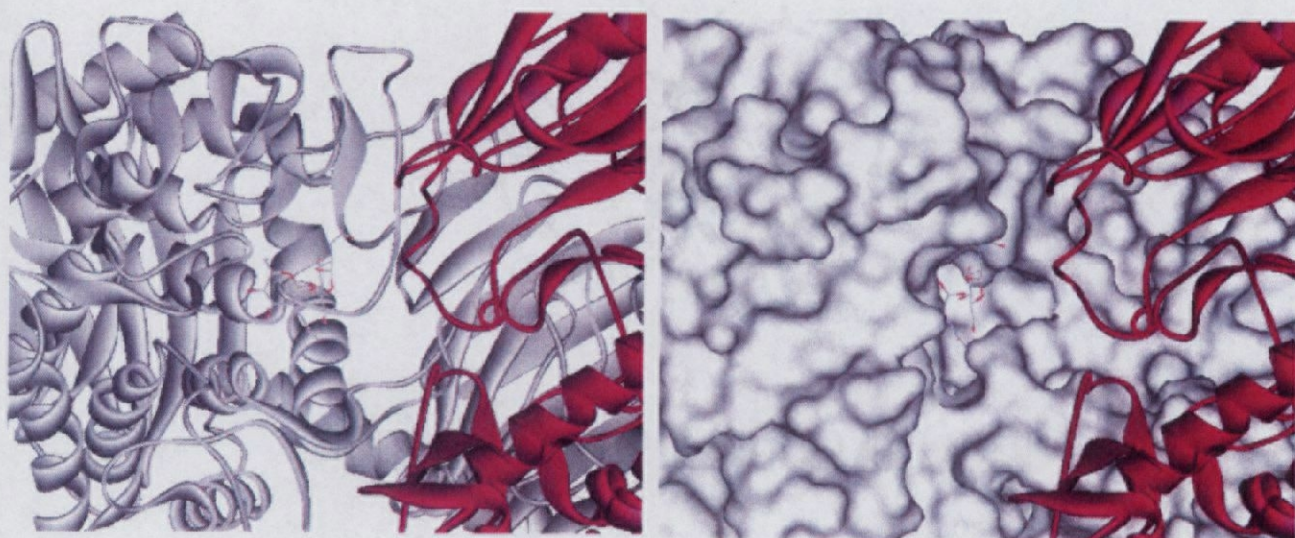


図 3-23b ChBPの活性中心部位のリボン図(左)と分子表面(右)。隣のサブユニットを赤色で示した。CgCBPと異なり、活性中心部位は分子表面に対し開いた構造である。

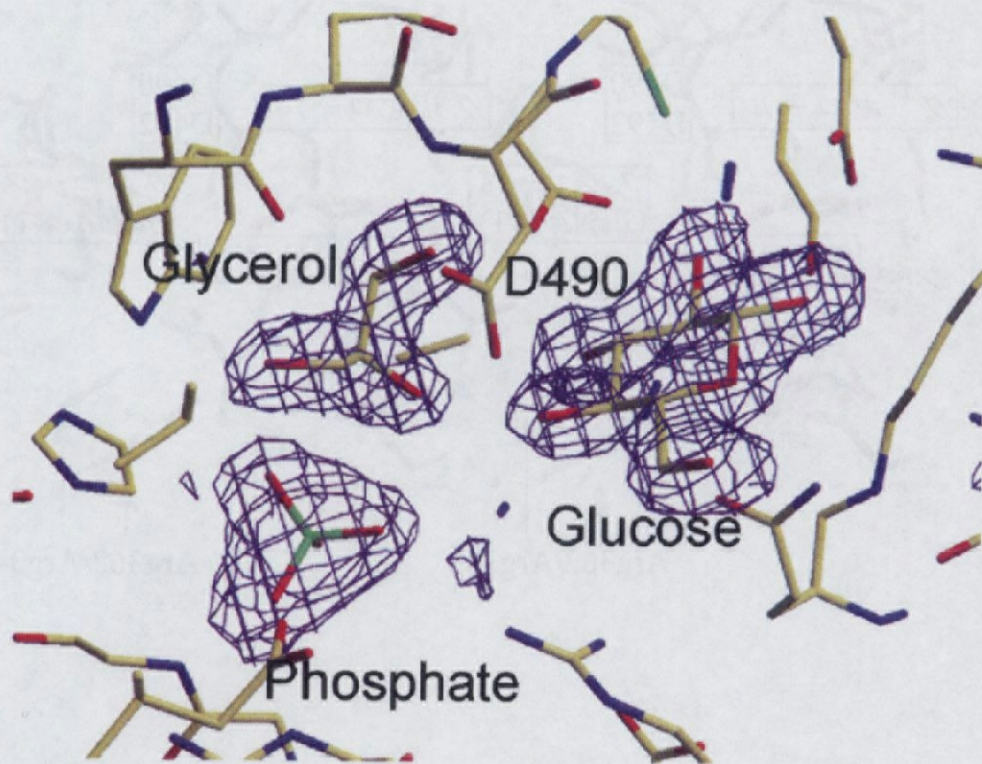


図 3-24 CgCBP-PO₄構造のグルコース、グリセロール、リン酸の $|F_{\text{obs}}| - |F_{\text{calc}}|$ 電子密度マップ(3 σ)。D490は一般酸触媒として働く触媒残基。

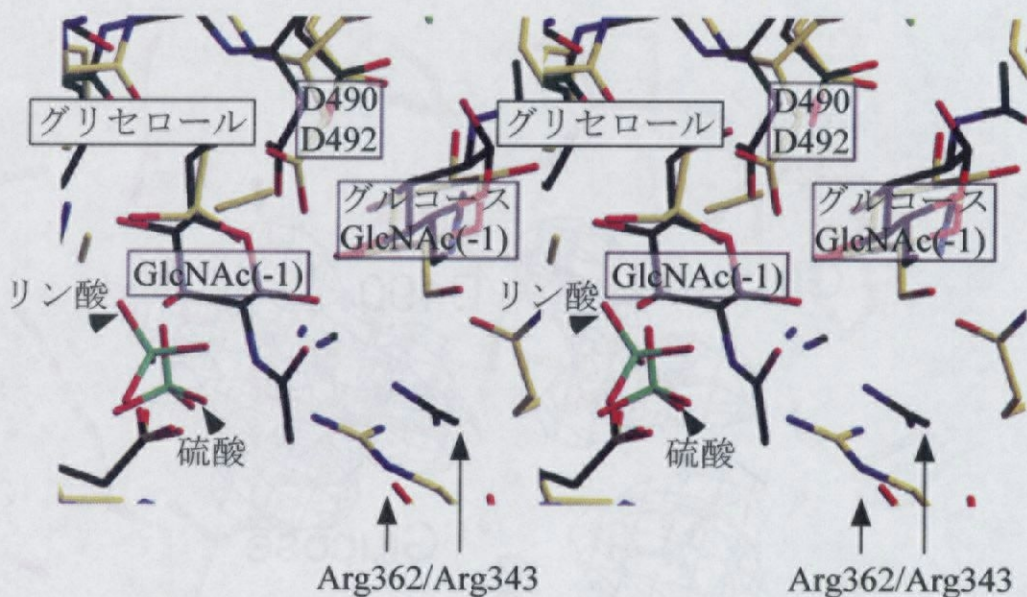


図 3-25 CgCBP-PO₄(黄)とChBP(黒)の活性中心部位の重ね合わせのステレオ図。触媒残基、糖受容体結合部位、リン酸結合部位が一致した。CgCBPのArg362は、ChBPのArg343に比べ活性中心部位に入り込んでおり、GlcNAc(-1)のN-アセチル基とは立体障害を起こす。

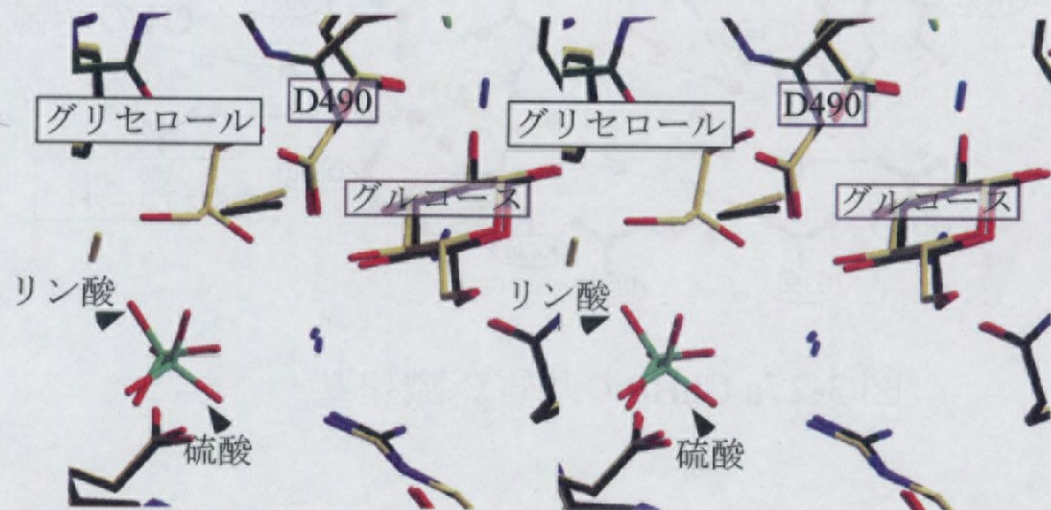


図 3-26 CgCBP-PO₄(黄)とCgCBP-SO₄(黒)の活性中心部位の重ね合わせのステレオ図。触媒残基、糖受容体結合部位が一致するが、リン酸、硫酸の結合方向が異なる。

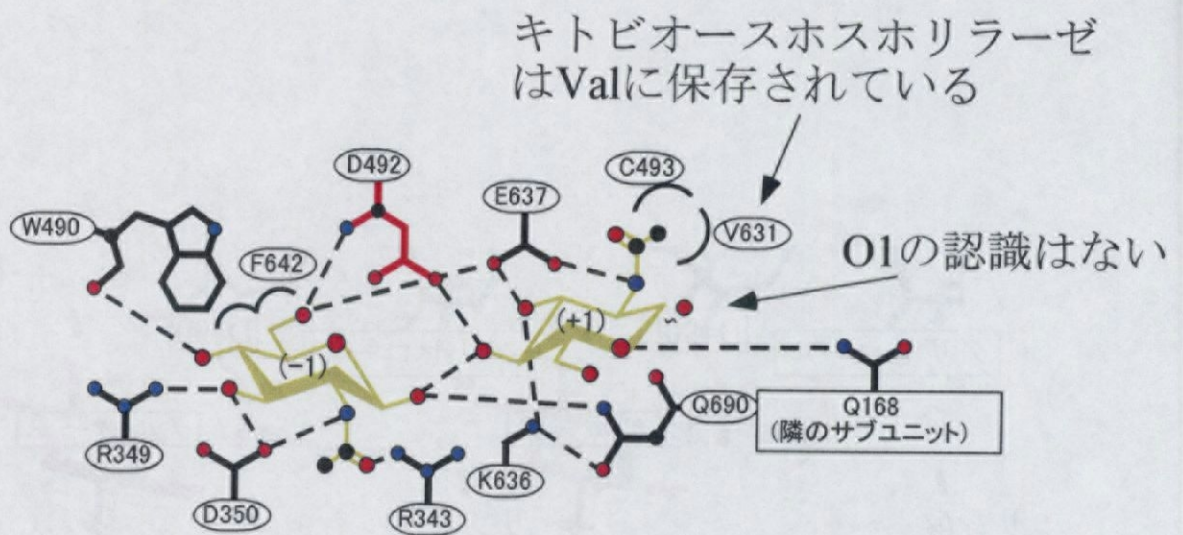
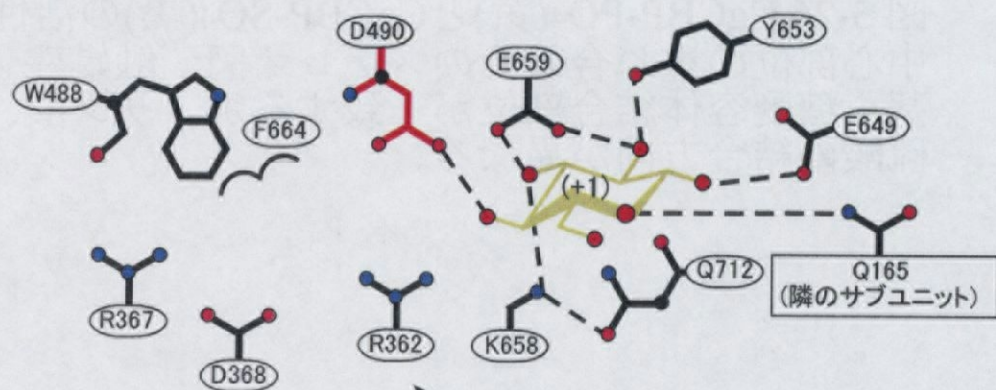


図 3-27a ChBPの基質認識残基。



ChBPに比べ、基質結合部位の内側に入り込んでいる

図 3-27b CgCBPの基質認識残基。

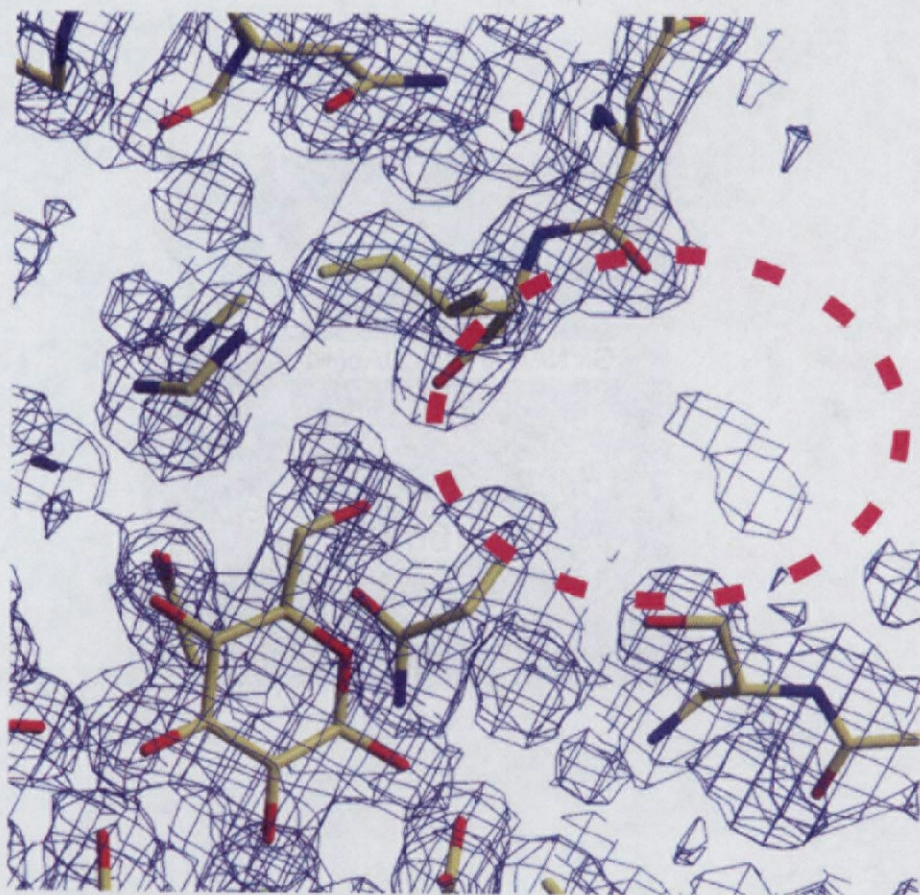


図 3-28 CgCBPの糖受容体結合部位まわりの $2|F_{\text{obs}}| - |F_{\text{calc}}|$ 電子密度マップ(1σ)。O6まわりは空間があり、O6に糖が結合したのもも糖受容体となり得る実験結果と一致する[6]。

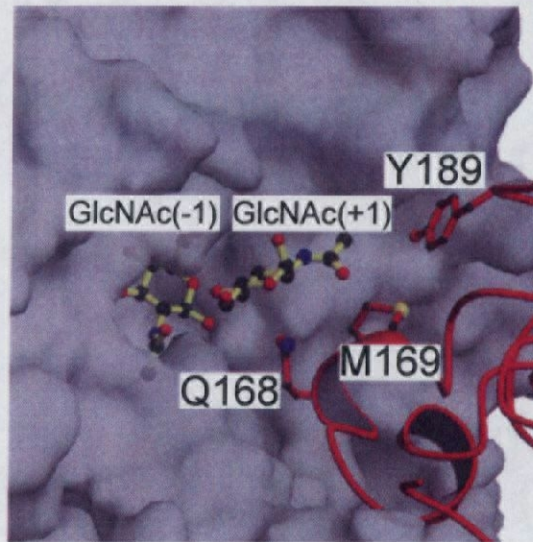


図 3-29 ChBPの二量体形成による基質結合部位のポケット化。隣のサブユニットのN末端ドメイン(赤)で基質結合部位の端が塞がれ、活性中心部位がポケット化している。

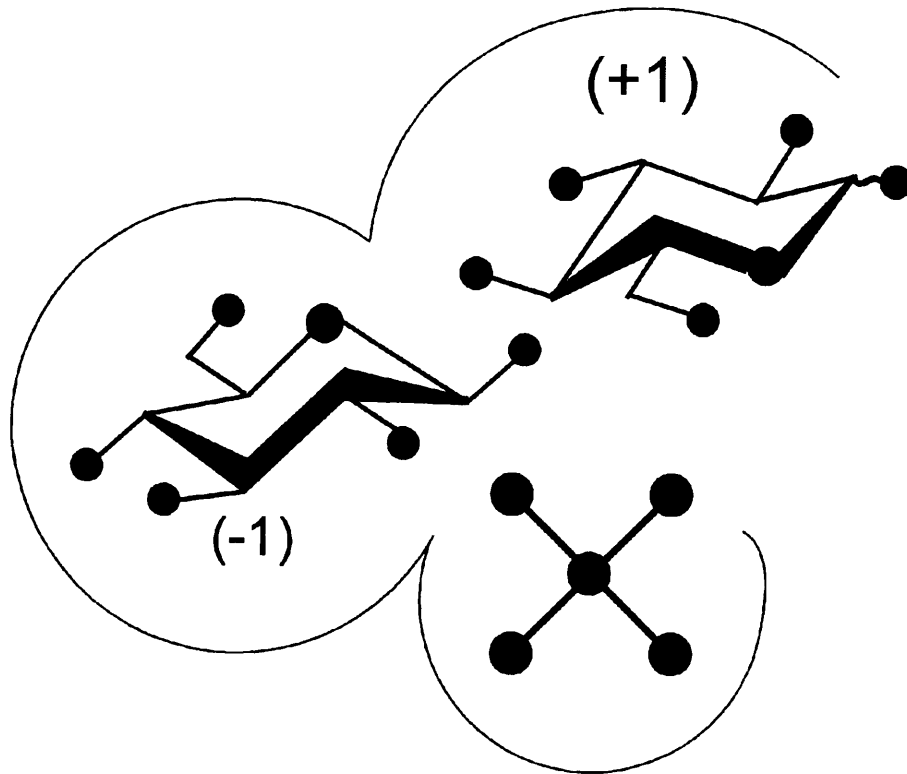


図 3-30 活性中心ポケットの模式図。サブサイト(-1)はポケットの奥側にあり、(+1)に糖が結合した状態では、(-1)に糖は結合できない。リン酸の結合、糖の結合は互いに影響を与えていない。

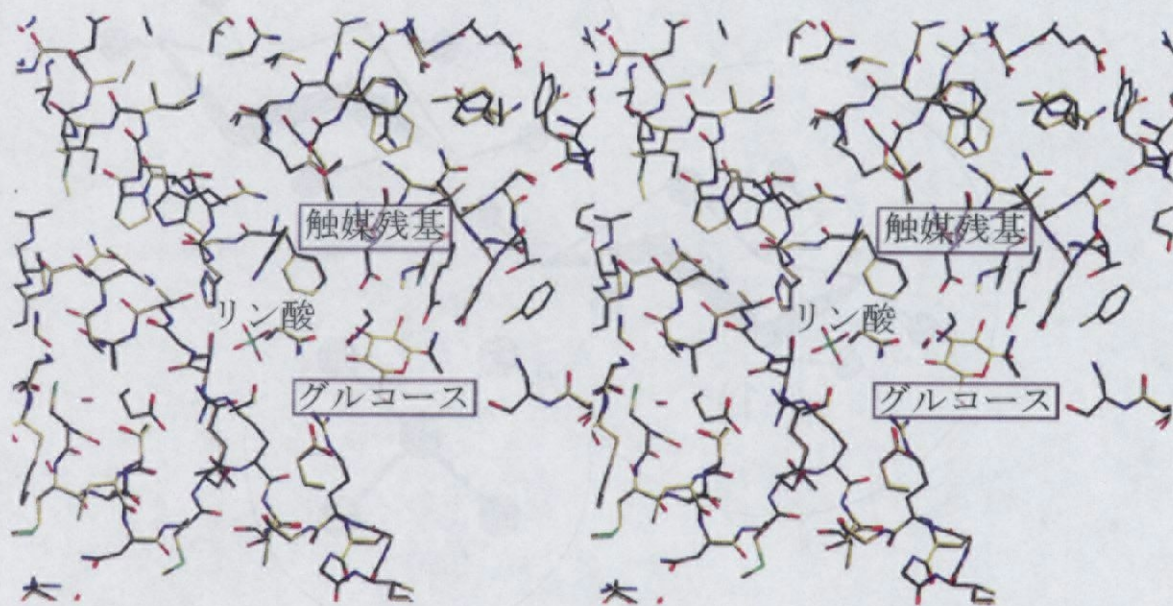


図 3-31 CgCBP(黄)とモデリングしたCtCBP(黒)の重ね合わせのステレオ図。活性中心部位はほぼ同じ構造を示している。

第3章の引用文献

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