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【手続補正書】
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【手続補正１】
【補正対象書類名】特許請求の範囲
【補正対象項目名】全文
【補正方法】変更
【補正の内容】
【特許請求の範囲】
【請求項１】
インスリンＡ鎖ペプチドおよびインスリンＢ鎖ペプチドを含むペプチドであって、前記Ｂ鎖ペプチドは１０位のアミノ酸および２０位のアミノ酸で置換を含む、ペプチド。
【請求項２】
前記２０位のアミノ酸での置換がＧ２０Ｙ、Ｇ２０ＦもしくはＧ２０Ｐであるか、または前記１０位のアミノ酸での置換がＨ１０Ｅ、Ｈ１０ＤもしくはＨ１０Ｑである、請求項１に記載のペプチド。
【請求項３】
前記２０位のアミノ酸での置換がＧ２０Ｐであり、前記ペプチドが２１位のアミノ酸での置換をさらに含み、前記２１位のアミノ酸での置換がＧ２１Ｈである、請求項２に記載のペプチド。
【請求項４】
前記Ａ鎖ペプチド中に少なくとも１個の置換をさらに含む請求項１～３のいずれかに記載のペプチド。
【請求項５】
前記Ａ鎖ペプチド中の前記少なくとも１個の置換がＴ８Ｈ、Ｔ８Ｙ、Ｔ８ＫまたはＳ９Ｒである、請求項４に記載のペプチド。
【請求項６】
前記Ａ鎖ペプチド中に、Ｔ８Ｈ、Ｔ８Ｙ、Ｔ８ＫおよびＳ９Ｒから選択される少なくとも２個の置換をさらに含む請求項５に記載のペプチド。
【請求項７】

前記ペプチドがデス－オクタペプチドインスリンである、請求項１～６のいずれかに記載のペプチド。
【請求項８】
前記Ｂ鎖ペプチドがＦＶＮＱＨＬＣＧＳＥＬＶＥＡＬＹＬＶＣＹＥＲ（配列番号３０）の配列を含む、請求項１に記載のペプチド。
【請求項９】
前記Ａ鎖がＧＩＶＥＱＣＣＨＲＩＣＳＬＹＱＬＥＮＹＣＮ（配列番号３９）の配列を含む、請求項１に記載のペプチド。
【請求項１０】
前記Ａ鎖ペプチドおよびＢ鎖ペプチドが少なくとも１個のジスルフィド結合を介して結合している、請求項１～９のいずれかに記載のペプチド。
【請求項１１】
前記ペプチドが単量体である、請求項１～１０のいずれかに記載のペプチド。
【請求項１２】
前記インスリンＡ鎖ペプチドが野生型ヒトインスリンＡ鎖ペプチドと少なくとも７０％同一である、請求項１～１１のいずれかに記載のペプチド。
【請求項１３】
請求項１～１２のいずれかに記載のペプチドと、薬学的に許容される担体とを含む医薬組成物。
【請求項１４】
薬剤としての使用のための、請求項１～１２のいずれかに記載のペプチドを含む医薬組成物。
【請求項１５】
必要とする対象中のインスリンレセプター活性化の増加における使用のための、請求項１～１２のいずれかに記載のペプチドを含む医薬組成物。
【請求項１６】
必要とする対象の血糖の低下における使用のための、請求項１～１２のいずれかに記載のペプチドを含む医薬組成物。
【請求項１７】
１型糖尿病の処置における使用のための、請求項１～１２のいずれかに記載のペプチドを含む医薬組成物。
【請求項１８】
Ａ鎖ペプチドおよびＢ鎖ペプチドを含むインスリンアナログであって、前記Ｂ鎖は、ヒトインスリンのＢ鎖のアミノ酸番号２０に対応する位置で芳香族残基もしくは大きい脂肪族残基を含み、および／またはヒトインスリンのＢ鎖のアミノ酸番号１５に対応する位置で芳香族残基もしくは大きい脂肪族残基を含み、前記アナログは、ヒトインスリン中に見出される少なくとも１個のアミノ酸を含むがコヌス・ジオグラフス（Ｃｏｎｕｓ　ｇｅｏｇｒａｐｈｕｓ）毒液インスリンの対応する位置では欠いており、前記Ａ鎖ペプチドおよび前記Ｂ鎖ペプチドは少なくとも１対のシステイン残基を介して互いに結合している、インスリンアナログ。
【請求項１９】
インスリンレセプター（ＩＲ）に結合することが知られているポリペプチドを再設計するまたは改変する方法であって、下表の原子座標またはそのサブセットにより定義される構造の、構造に基づく評価を実施すること、および前記評価の結果として前記ポリペプチドを再設計するまたは化学的に改変することを含む方法：

【表１－１】

付録I: CON-INS G1インスリン(鎖Aおよび鎖B)に関する原子座標

フォーマットは、下記のコロンで区切られたフィールドを含む: (1) 原子の名称, (2) 残基タイプ, (3) 鎖の名称,(4) 残基番号,(5-7) xyz 座標,(8) 温度B因子(thermal B-factor)。

N:GLY:A:1:15.439:38.785:34.309:26.76
CA:GLY:A:1:14.11:39.14:33.733:22.21
C:GLY:A:1:14.251:39.976:32.492:21.3
O:GLY:A:1:15.353:40.312:32.093:22.73
H1:GLY:A:1:15.395:38.813:35.197:32.11
H2:GLY:A:1:15.666:37.965:34.049:32.11
H3:GLY:A:1:16.051:39.366:34.024:32.11
HA2:GLY:A:1:13.625:38.331:33.508:26.65
HA3:GLY:A:1:13.595:39.639:34.386:26.65
N:VAL:A:2:13.113:40.325:31.895:21.05
CA:VAL:A:2:13.122:41.169:30.72:22.11
C:VAL:A:2:13.696:42.561:31.01:20.41
O:VAL:A:2:14.274:43.187:30.116:20.06
CB:VAL:A:2:11.698:41.225:30.132:25.46
CG1:VAL:A:2:10.72:41.927:31.074:21.3
CG2:VAL:A:2:11.725:41.902:28.839:27.88
H:VAL:A:2:12.33:40.084:32.154:25.26
HA:VAL:A:2:13.693:40.756:30.053:26.54
HB:VAL:A:2:11.38:40.32:29.989:30.55
HG11:VAL:A:2:9.841:41.939:30.665:25.56
HG12:VAL:A:2:10.688:41.442:31.914:25.56
HG13:VAL:A:2:11.026:42.835:31.227:25.56
HG21:VAL:A:2:10.824:41.931:28.48:33.45
HG22:VAL:A:2:12.061:42.804:28.963:33.45
HG23:VAL:A:2:12.306:41.412:28.238:33.45
N:VAL:A:3:13.604:43.056:32.249:26.31
CA:VAL:A:3:14.092:44.414:32.525:22.38
C:VAL:A:3:15.618:44.365:32.529:26.64
O:VAL:A:3:16.283:45.246:31.982:21.94
CB:VAL:A:3:13.517:44.989:33.842:28.85
CG1:VAL:A:3:14.192:46.325:34.21:23.35
CG2:VAL:A:3:11.967:45.154:33.731:22.25
H:VAL:A:3:13.276:42.642:32.928:31.58
HA:VAL:A:3:13.816:44.998:31.802:26.85
HB:VAL:A:3:13.695:44.361:34.559:34.62
HG11:VAL:A:3:13.808:46.654:35.037:28.02
HG12:VAL:A:3:15.144:46.176:34.323:28.02
HG13:VAL:A:3:14.039:46.963:33.496:28.02
HG21:VAL:A:3:11.628:45.515:34.565:26.7
HG22:VAL:A:3:11.767:45.762:33.001:26.7
HG23:VAL:A:3:11.569:44.287:33.558:26.7
N:CGU:A:4:16.193:43.318:33.099:21.34
CA:CGU:A:4:17.68:43.233:33.107:21.52
CB:CGU:A:4:18.136:42.041:33.939:22.15
CG:CGU:A:4:17.867:42.164:35.47:27.83
CD1:CGU:A:4:16.419:42.187:35.88:25.08
OE12:CGU:A:4:16.135:42.812:36.937:28.6
OE11:CGU:A:4:15.531:41.542:35.211:22.71
CD2:CGU:A:4:18.45:40.98:36.25:48.38
OE21:CGU:A:4:18.448:39.819:35.754:54.62
OE22:CGU:A:4:18.871:41.181:37.42:85.42
C:CGU:A:4:18.255:43.089:31.618:20.98
O:CGU:A:4:19.303:43.691:31.269:21.08
HG:CGU:A:4:18.338:43.105:35.863:33.4
HB3:CGU:A:4:17.661:41.115:33.568:26.58
HB2:CGU:A:4:19.22:41.867:33.754:26.58
HA:CGU:A:4:18.079:44.185:33.551:25.82
N:HIS:A:5:17.548:42.333:30.786:21.02
CA:HIS:A:5:18.007:41.966:29.443:20.65
C:HIS:A:5:17.659:43.013:28.373:19.86
O:HIS:A:5:18.285:43.07:27.334:23.44
CB:HIS:A:5:17.391:40.584:29.071:20.16
CG:HIS:A:5:18.115:39.864:27.981:47.58
ND1:HIS:A:5:19.277:39.15:28.201:43.05
CD2:HIS:A:5:17.832:39.734:26.661:45.41
CE1:HIS:A:5:19.678:38.617:27.058:50.46
NE2:HIS:A:5:18.82:38.957:26.111:52.67
HA:HIS:A:5:18.972:41.867:29.458:24.79
HB2:HIS:A:5:17.402:40.017:29.858:24.19
HB3:HIS:A:5:16.476:40.72:28.778:24.19
HD2:HIS:A:5:17.106:40.104:26.213:54.49
HE1:HIS:A:5:20.437:38.093:26.94:60.55
HE2:HIS:A:5:18.873:38.729:25.284:63.2
H:HIS:A:5:16.775:42.01:30.98:25.23
N:CYS:A:6:16.641:43.84:28.616:19.88
CA:CYS:A:6:16.113:44.731:27.591:19.76
C:CYS:A:6:16.063:46.184:28.028:21.58
O:CYS:A:6:15.909:47.06:27.165:20.58
CB:CYS:A:6:14.695:44.308:27.194:21.07
SG:CYS:A:6:14.678:42.722:26.317:26
H:CYS:A:6:16.238:43.902:29.373:23.85
HA:CYS:A:6:16.676:44.674:26.803:23.71
HB2:CYS:A:6:14.154:44.217:27.994:25.29
HB3:CYS:A:6:14.315:44.981:26.608:25.29
N:CYS:A:7:16.128:46.463:29.323:21.05
CA:CYS:A:7:16.186:47.837:29.839:21.74
C:CYS:A:7:17.553:48.188:30.41:23.78
O:CYS:A:7:18.103:49.215:30.042:30.88
CB:CYS:A:7:15.098:48.081:30.895:21.43
SG:CYS:A:7:15.221:49.718:31.732:27.59
H:CYS:A:7:16.14:45.864:29.941:25.26
HA:CYS:A:7:16.016:48.446:29.103:26.09
HB2:CYS:A:7:14.229:48.033:30.465:25.71
HB3:CYS:A:7:15.165:47.394:31.576:25.71
N:HIS:A:8:18.157:47.348:31.264:28.49
CA:HIS:A:8:19.509:47.657:31.747:25.02
C:HIS:A:8:20.564:47.453:30.657:30.05
O:HIS:A:8:21.558:48.179:30.604:34.16

【表１－２】

CB:HIS:A:8:19.847:46.811:32.972:27.96
CG:HIS:A:8:18.916:47.03:34.125:33.4
ND1:HIS:A:8:18.619:46.043:35.044:34.99
CD2:HIS:A:8:18.234:48.129:34.521:27.24
CE1:HIS:A:8:17.767:46.516:35.936:33.7
NE2:HIS:A:8:17.527:47.782:35.648:38.53
H:HIS:A:8:17.818:46.619:31.57:34.19
HA:HIS:A:8:19.538:48.589:32.014:30.03
HB2:HIS:A:8:19.802:45.874:32.728:33.55
HB3:HIS:A:8:20.744:47.033:33.268:33.55
HD2:HIS:A:8:18.233:48.959:34.103:32.68
HE1:HIS:A:8:17.417:46.045:36.658:40.44
HE2:HIS:A:8:17.009:48.305:36.092:46.23
N:ARG:A:9:20.377:46.477:29.813:32.17
CA:ARG:A:9:21.026:46.221:28.542:24.61
C:ARG:A:9:19.985:46.413:27.464:24.55
O:ARG:A:9:18.838:46.063:27.712:22.58
CB:ARG:A:9:21.524:44.776:28.434:42.6
CG:ARG:A:9:22.966:44.545:28.786:89.14
CD:ARG:A:9:23.608:43.537:27.831:118.62
NE:ARG:A:9:25.059:43.702:27.796:137.92
CZ:ARG:A:9:25.928:42.745:27.485:154.54
NH1:ARG:A:9:25.517:41.519:27.184:170.53
NH2:ARG:A:9:27.224:43.02:27.49:152.73
H:ARG:A:9:19.797:45.864:29.977:38.61
HA:ARG:A:9:21.763:46.836:28.4:29.53
HB2:ARG:A:9:20.99:44.224:29.027:51.12
HB3:ARG:A:9:21.399:44.478:27.519:51.12
HG2:ARG:A:9:23.451:45.382:28.719:106.97
HG3:ARG:A:9:23.024:44.192:29.688:106.97
HD2:ARG:A:9:23.41:42.637:28.132:142.34
HD3:ARG:A:9:23.263:43.677:26.935:142.34
HE:ARG:A:9:25.375:44.477:27.991:165.51
HH11:ARG:A:9:24.676:41.336:27.181:204.63
HH12:ARG:A:9:26.09:40.909:26.987:204.63
HH21:ARG:A:9:27.495:43.812:27.686:183.27
HH22:ARG:A:9:27.794:42.407:27.293:183.27
N:PRO:A:10:20.315:46.922:26.273:21.04
CA:PRO:A:10:19.325:46.947:25.186:22.55
C:PRO:A:10:19.153:45.573:24.54:20.8
O:PRO:A:10:20.049:44.721:24.565:22.83
CB:PRO:A:10:19.914:47.951:24.205:21.44
CG:PRO:A:10:21.394:47.783:24.393:23.92
CD:PRO:A:10:21.581:47.551:25.858:26.07
HA:PRO:A:10:18.468:47.268:25.508:27.06
HB2:PRO:A:10:19.65:47.726:23.299:25.72
HB3:PRO:A:10:19.633:48.849:24.439:25.72
HG2:PRO:A:10:21.703:47.018:23.883:28.7
HG3:PRO:A:10:21.853:48.59:24.112:28.7
HD2:PRO:A:10:22.324:46.948:26.013:31.28
HD3:PRO:A:10:21.706:48.395:26.32:31.28
N:CYS:A:11:17.965:45.34:23.974:20.27
CA:CYS:A:11:17.735:44.077:23.278:20.11
C:CYS:A:11:17.021:44.299:21.95:20.29
O:CYS:A:11:16.249:45.24:21.766:20.43
CB:CYS:A:11:16.959:43.053:24.166:20.58
SG:CYS:A:11:15.186:43.358:24.401:23.25
H:CYS:A:11:17.296:45.881:23.98:24.33
HA:CYS:A:11:18.598:43.683:23.076:24.13
HB2:CYS:A:11:17.048:42.175:23.763:24.7
HB3:CYS:A:11:17.368:43.045:25.045:24.7
N:SER:A:12:17.349:43.443:21.002:19.95
CA:SER:A:12:16.64:43.374:19.734:20.24
C:SER:A:12:15.198:42.876:19.921:19.9
O:SER:A:12:14.82:42.314:20.95:19.48
CB:SER:A:12:17.365:42.442:18.794:20.66
OG:SER:A:12:17.226:41.115:19.254:20.36
H:SER:A:12:17.993:42.877:21.068:23.94
HA:SER:A:12:16.611:44.256:19.332:24.29
HB2:SER:A:12:16.978:42.517:17.908:24.79
HB3:SER:A:12:18.306:42.677:18.772:24.79
HG:SER:A:12:17.626:40.589:18.736:24.43
N:ASN:A:13:14.386:43.089:18.896:20.29
CA:ASN:A:13:13.05:42.486:18.857:20.21
C:ASN:A:13:13.113:40.969:18.999:19.99
O:ASN:A:13:12.303:40.375:19.72:19.76
CB:ASN:A:13:12.338:42.827:17.571:20.89
CG:ASN:A:13:11.993:44.254:17.455:21.34
OD1:ASN:A:13:12.063:45.022:18.425:21.1
ND2:ASN:A:13:11.561:44.637:16.254:22.2
H:ASN:A:13:14.577:43.575:18.213:24.35
HA:ASN:A:13:12.523:42.835:19.593:24.25
HB2:ASN:A:13:12.913:42.598:16.823:25.07
HB3:ASN:A:13:11.515:42.316:17.522:25.07
HD21:ASN:A:13:11.343:45.457:16.116:26.64
HD22:ASN:A:13:11.502:44.063:15.616:26.64
N:ALA:A:14:14.073:40.323:18.327:20.53
CA:ALA:A:14:14.136:38.865:18.34:20.59
C:ALA:A:14:14.514:38.344:19.713:20.2
O:ALA:A:14:13.966:37.34:20.17:20.42
CB:ALA:A:14:15.122:38.388:17.293:21.21
H:ALA:A:14:14.689:40.704:17.863:24.64
HA:ALA:A:14:13.262:38.509:18.115:24.71
HB1:ALA:A:14:15.156:37.419:17.311:25.45
HB2:ALA:A:14:14.827:38.694:16.421:25.45
HB3:ALA:A:14:15.997:38.755:17.494:25.45
N:GLU:A:15:15.393:39.048:20.418:19.99
CA:GLU:A:15:15.674:38.714:21.807:20.64
C:GLU:A:15:14.459:38.979:22.702:20.25
O:GLU:A:15:14.126:38.165:23.56:19.51
CB:GLU:A:15:16.886:39.507:22.306:24.27
CG:GLU:A:15:18.221:38.954:21.864:52.08
CD:GLU:A:15:18.481:37.555:22.399:68.3
OE1:GLU:A:15:18.414:37.354:23.638:37.34
OE2:GLU:A:15:18.75:36.655:21.573:92.14
H:GLU:A:15:15.838:39.719:20.116:23.99
HA:GLU:A:15:15.889:37.77:21.867:24.77
HB2:GLU:A:15:16.82:40.416:21.974:29.12
HB3:GLU:A:15:16.876:39.513:23.276:29.12
HG2:GLU:A:15:18.242:38.914:20.895:62.5
HG3:GLU:A:15:18.927:39.535:22.188:62.5
N:PHE:A:16:13.813:40.136:22.56:19.08

【表１－３】

CA:PHE:A:16:12.627:40.394:23.379:19.01
C:PHE:A:16:11.58:39.275:23.258:19.21
O:PHE:A:16:10.937:38.891:24.259:19.32
CB:PHE:A:16:12:41.738:23.008:19.12
CG:PHE:A:16:10.869:42.118:23.896:19.26
CD2:PHE:A:16:11.086:42.876:25.025:19.26
CD1:PHE:A:16:9.575:41.712:23.603:19.56
CE2:PHE:A:16:10.018:43.216:25.879:19.59
CE1:PHE:A:16:8.496:42.075:24.429:19.92
CZ:PHE:A:16:8.717:42.809:25.564:19.95
H:PHE:A:16:14.029:40.767:22.018:22.9
HA:PHE:A:16:12.898:40.443:24.309:22.81
HB2:PHE:A:16:12.677:42.43:23.073:22.95
HB3:PHE:A:16:11.663:41.689:22.1:22.95
HD2:PHE:A:16:11.95:43.143:25.241:23.11
HD1:PHE:A:16:9.416:41.209:22.837:23.48
HE2:PHE:A:16:10.173:43.731:26.637:23.51
HE1:PHE:A:16:7.635:41.79:24.221:23.9
HZ:PHE:A:16:8.006:43.046:26.114:23.93
N:LYS:A:17:11.394:38.736:22.051:19.63
CA:LYS:A:17:10.38:37.7:21.84:19.97
C:LYS:A:17:10.614:36.46:22.684:20.12
O:LYS:A:17:9.672:35.685:22.893:20.5
CB:LYS:A:17:10.329:37.289:20.362:20.31
CG:LYS:A:17:9.504:38.28:19.498:20.56
CD:LYS:A:17:9.689:38.041:18.044:21.03
CE:LYS:A:17:9.094:39.21:17.228:23.58
NZ:LYS:A:17:9.222:39.104:15.74:26.95
H:LYS:A:17:11.837:38.95:21.346:23.56
HA:LYS:A:17:9.512:38.061:22.078:23.96
HB2:LYS:A:17:11.232:37.262:20.009:24.37
HB3:LYS:A:17:9.917:36.413:20.291:24.37
HG2:LYS:A:17:8.562:38.173:19.703:24.67
HG3:LYS:A:17:9.788:39.186:19.694:24.67
HD2:LYS:A:17:10.636:37.977:17.845:25.23
HD3:LYS:A:17:9.232:37.224:17.789:25.23
HE2:LYS:A:17:8.148:39.275:17.433:28.3
HE3:LYS:A:17:9.539:40.028:17.499:28.3
HZ1:LYS:A:17:8.855:39.816:15.352:32.34
HZ2:LYS:A:17:10.081:39.061:15.511:32.34
HZ3:LYS:A:17:8.808:38.371:15.451:32.34
N:LYS:A:18:11.856:36.224:23.113:20.04
CA:LYS:A:18:12.144:35.116:24.033:21.82
C:LYS:A:18:11.301:35.19:25.294:20.55
O:LYS:A:18:11.071:34.163:25.936:21.12
CB:LYS:A:18:13.624:35.111:24.441:20.42
CG:LYS:A:18:14.518:34.782:23.279:20.61
CD:LYS:A:18:16.015:34.803:23.664:30.84
CE:LYS:A:18:16.866:34.3:22.484:38.22
NZ:LYS:A:18:18.269:33.984:22.906:62
H:LYS:A:18:12.546:36.685:22.889:24.05
HA:LYS:A:18:11.951:34.276:23.589:26.19
HB2:LYS:A:18:13.867:35.989:24.772:24.51
HB3:LYS:A:18:13.763:34.442:25.13:24.51
HG2:LYS:A:18:14.303:33.894:22.954:24.73
HG3:LYS:A:18:14.379:35.436:22.576:24.73
HD2:LYS:A:18:16.284:35.711:23.875:37
HD3:LYS:A:18:16.163:34.218:24.424:37
HE2:LYS:A:18:16.468:33.491:22.125:45.86
HE3:LYS:A:18:16.902:34.987:21.8:45.86
HZ1:LYS:A:18:18.739:33.696:22.207:74.4
HZ2:LYS:A:18:18.658:34.713:23.236:74.4
HZ3:LYS:A:18:18.263:33.351:23.531:74.4
N:TYR:A:19:10.88:36.384:25.687:25.2
CA:TYR:A:19:10.118:36.604:26.923:20.68
C:TYR:A:19:8.575:36.613:26.737:31.44
O:TYR:A:19:7.832:36.875:27.687:29.68
CB:TYR:A:19:10.538:37.943:27.555:20.37
CG:TYR:A:19:11.901:37.935:28.109:23.44
CD1:TYR:A:19:13:38.247:27.323:19.93
CD2:TYR:A:19:12.117:37.579:29.428:23.18
CE1:TYR:A:19:14.278:38.224:27.859:26.81
CE2:TYR:A:19:13.379:37.562:29.96:25.73
CZ:TYR:A:19:14.444:37.864:29.184:22.56
OH:TYR:A:19:15.682:37.826:29.75:22.36
H:TYR:A:19:11.025:37.107:25.245:30.24
HA:TYR:A:19:10.335:35.898:27.552:24.82
HB2:TYR:A:19:10.498:38.635:26.876:24.45
HB3:TYR:A:19:9.926:38.154:28.276:24.45
HD2:TYR:A:19:11.39:37.364:29.968:27.82
HD1:TYR:A:19:12.877:38.483:26.431:23.92
HE2:TYR:A:19:13.505:37.32:30.849:30.88
HE1:TYR:A:19:15.015:38.436:27.332:32.17
HH:TYR:A:19:16.265:38.03:29.18:26.83
O:CY3:A:20:6.334:34.016:25.918:46.46
C:CY3:A:20:5.968:35.121:26.067:39.6
N1:CY3:A:20:4.848:35.386:26.929:43.25
CA:CY3:A:20:6.666:36.307:25.294:21.87
N:CY3:A:20:8.084:36.362:25.53:22.5
CB:CY3:A:20:6.382:35.984:23.834:33.52
SG:CY3:A:20:6.832:37.458:22.767:39.89
H:CY3:A:20:8.534:36.217:24.812:27
HA:CY3:A:20:6.252:37.151:25.536:26.25
HB2:CY3:A:20:5.439:35.782:23.725:40.22
HB3:CY3:A:20:6.908:35.214:23.567:40.22
HN11:CY3:A:20:4.569:36.191:27.039:51.9
HN12:CY3:A:20:4.467:34.738:27.347:51.9
O:THR:B:-1:16.056:46.908:9.868:60.34
N:THR:B:-1:16.406:48.652:7.605:78.37
CA:THR:B:-1:17.132:48.822:8.897:76.87
C:THR:B:-1:17.109:47.519:9.689:64.38
CB:THR:B:-1:16.526:49.975:9.74:82.36
OG1:THR:B:-1:17.021:51.231:9.25:103.8
CG2:THR:B:-1:16.88:49.85:11.228:68.98
H1:THR:B:-1:16.283:49.449:7.227:94.05
H2:THR:B:-1:16.886:48.137:7.061:94.05
H3:THR:B:-1:15.617:48.27:7.756:94.05
HA:THR:B:-1:18.058:49.042:8.712:92.25
HB:THR:B:-1:15.56:49.958:9.656:98.83
HG1:THR:B:-1:16.698:51.862:9.7:124.55
HG21:THR:B:-1:16.486:50.584:11.725:82.78
HG22:THR:B:-1:16.538:49.013:11.58:82.78

【表１－４】

HG23:THR:B:-1:17.843:49.871:11.343:82.78
O:PHE:B:0:17.693:47.018:12.852:32.11
N:PHE:B:0:18.285:47.117:10.17:47.49
CA:PHE:B:0:18.434:45.859:10.88:33.82
C:PHE:B:0:17.777:45.945:12.258:30.41
CB:PHE:B:0:19.916:45.528:11.007:28.4
CG:PHE:B:0:20.185:44.138:11.419:27.64
CD2:PHE:B:0:20.443:43.17:10.471:29.44
CD1:PHE:B:0:20.187:43.786:12.753:26.31
CE2:PHE:B:0:20.706:41.883:10.832:27.99
CE1:PHE:B:0:20.454:42.477:13.135:27.97
CZ:PHE:B:0:20.702:41.517:12.166:27.51
H:PHE:B:0:19.016:47.564:10.094:56.99
HA:PHE:B:0:18.003:45.151:10.377:40.59
HB2:PHE:B:0:20.342:45.669:10.147:34.08
HB3:PHE:B:0:20.311:46.115:11.67:34.08
HD1:PHE:B:0:20.017:44.431:13.402:31.58
HD2:PHE:B:0:20.445:43.402:9.571:35.33
HE1:PHE:B:0:20.45:42.243:14.035:33.57
HE2:PHE:B:0:20.874:41.244:10.177:33.58
HZ:PHE:B:0:20.881:40.638:12.411:33.01
O:ASP:B:1:18.276:43.923:15.696:23.3
N:ASP:B:1:17.325:44.791:12.774:25.54
CA:ASP:B:1:16.642:44.721:14.072:24.29
C:ASP:B:1:17.702:44.882:15.159:25.42
CB:ASP:B:1:15.863:43.408:14.192:30.99
CG:ASP:B:1:15.425:43.112:15.613:33.34
OD1:ASP:B:1:15.172:44.1:16.35:26.15
OD2:ASP:B:1:15.36:41.913:16.004:22.1
H:ASP:B:1:17.404:44.028:12.384:30.65
HA:ASP:B:1:16.014:45.456:14.145:29.15
HB2:ASP:B:1:15.068:43.46:13.639:37.19
HB3:ASP:B:1:16.427:42.677:13.894:37.19
O:THR:B:2:17.54:46.872:18.038:27.96
N:THR:B:2:18.026:46.134:15.452:24.07
CA:THR:B:2:19.15:46.377:16.357:23.86
C:THR:B:2:18.686:46.539:17.782:24.18
CB:THR:B:2:19.911:47.632:15.99:31.47
OG1:THR:B:2:18.958:48.664:15.749:33.31
CG2:THR:B:2:20.815:47.367:14.758:33.17
H:THR:B:2:17.631:46.838:15.155:28.88
HA:THR:B:2:19.762:45.626:16.318:28.64
HB:THR:B:2:20.479:47.889:16.733:37.77
HG1:THR:B:2:19.352:49.376:15.542:39.98
HG21:THR:B:2:21.302:48.173:14.525:39.81
HG22:THR:B:2:21.45:46.662:14.959:39.81
HG23:THR:B:2:20.272:47.097:14.001:39.81
C:HYP:B:3:18.617:47.825:20.609:37.46
O:HYP:B:3:19.172:48.867:20.197:33.28
CA:HYP:B:3:19.208:46.443:20.27:30.06
CB:HYP:B:3:20.366:46.23:20.929:46.37
CG:HYP:B:3:21.21:45.388:19.961:34.65
OD1:HYP:B:3:20.787:44.116:19.901:37.02
CD:HYP:B:3:20.889:46.065:18.606:30.67
N:HYP:B:3:19.59:46.315:18.708:25.2
HD23:HYP:B:3:21.065:45.458:17.869:36.81
HD22:HYP:B:3:21.39:46.89:18.507:36.81
HG:HYP:B:3:22.156:45.447:20.171:41.58
HD1:HYP:B:3:21.078:43.754:19.188:44.43
HB3:HYP:B:3:20.807:47.074:21.115:55.65
HB2:HYP:B:3:20.201:45.739:21.749:55.65
HA:HYP:B:3:18.572:45.748:20.503:36.08
O:LYS:B:4:16.271:47.848:23.837:25.52
N:LYS:B:4:17.521:47.837:21.368:29.31
CA:LYS:B:4:16.899:49.058:21.865:26.28
C:LYS:B:4:16.634:48.93:23.365:21.83
CB:LYS:B:4:15.558:49.322:21.159:37.68
CG:LYS:B:4:15.666:49.595:19.675:65.23
CD:LYS:B:4:14.269:49.657:19.051:94.75
CE:LYS:B:4:14.289:50.089:17.586:109.16
NZ:LYS:B:4:12.904:50.217:17.038:105.24
H:LYS:B:4:17.109:47.124:21.616:35.17
HA:LYS:B:4:17.488:49.813:21.713:31.53
HB2:LYS:B:4:14.99:48.544:21.273:45.21
HB3:LYS:B:4:15.139:50.094:21.569:45.21
HG2:LYS:B:4:16.106:50.447:19.533:78.28
HG3:LYS:B:4:16.163:48.879:19.248:78.28
HD2:LYS:B:4:13.864:48.777:19.098:113.71
HD3:LYS:B:4:13.732:50.296:19.544:113.71
HE2:LYS:B:4:14.727:50.951:17.511:130.99
HE3:LYS:B:4:14.763:49.424:17.062:130.99
HZ1:LYS:B:4:12.937:50.469:16.185:126.28
HZ2:LYS:B:4:12.482:49.435:17.093:126.28
HZ3:LYS:B:4:12.449:50.825:17.502:126.28
O:HIS:B:5:14.227:50.871:24.963:32.55
N:HIS:B:5:16.734:50.025:24.109:21.79
CA:HIS:B:5:16.363:50.01:25.519:21.56
C:HIS:B:5:14.857:50.045:25.607:22.3
CB:HIS:B:5:16.937:51.202:26.275:22.18
CG:HIS:B:5:18.423:51.204:26.337:22.64
ND1:HIS:B:5:19.131:50.545:27.328:28.27
CD2:HIS:B:5:19.345:51.765:25.516:25.48
CE1:HIS:B:5:20.428:50.699:27.11:22.51
NE2:HIS:B:5:20.585:51.441:26.022:28.72
H:HIS:B:5:17.013:50.786:23.824:26.15
HA:HIS:B:5:16.682:49.193:25.934:25.87
HB2:HIS:B:5:16.657:52.018:25.832:26.62
HB3:HIS:B:5:16.601:51.188:27.185:26.62
HD1:HIS:B:5:18.784:50.097:27.975:33.93
HD2:HIS:B:5:19.173:52.273:24.756:30.58
HE1:HIS:B:5:21.112:50.36:27.64:27.01
N:ARG:B:6:14.278:49.126:26.37:20.97
CA:ARG:B:6:12.838:49.07:26.561:24.52
C:ARG:B:6:12.608:49.07:28.058:21.26
O:ARG:B:6:12.884:48.066:28.727:23.78
CB:ARG:B:6:12.238:47.832:25.893:20.69
CG:ARG:B:6:12.796:47.582:24.53:26.83
CD:ARG:B:6:12.576:46.115:24.096:33.07
NE:ARG:B:6:13.308:45.832:22.86:31.36
CZ:ARG:B:6:12.807:45.919:21.638:20.49
NH1:ARG:B:6:11.527:46.276:21.431:28.98
NH2:ARG:B:6:13.594:45.629:20.612:25.07

【表１－５】

H:ARG:B:6:14.707:48.515:26.795:25.17
HA:ARG:B:6:12.425:49.861:26.181:29.42
HB2:ARG:B:6:12.426:47.054:26.441:24.83
HB3:ARG:B:6:11.279:47.953:25.806:24.83
HG2:ARG:B:6:12.352:48.159:23.89:32.19
HG3:ARG:B:6:13.75:47.758:24.537:32.19
HD2:ARG:B:6:12.903:45.519:24.789:39.68
HD3:ARG:B:6:11.632:45.963:23.935:39.68
HE:ARG:B:6:14.13:45.591:22.934:37.64
HH11:ARG:B:6:11.019:46.461:22.1:34.78
HH12:ARG:B:6:11.218:46.324:20.63:34.78
HH21:ARG:B:6:14.411:45.398:20.748:30.08
HH22:ARG:B:6:13.289:45.676:19.809:30.08
N:CYS:B:7:12.125:50.193:28.588:22.09
CA:CYS:B:7:12.018:50.387:30.028:24.41
C:CYS:B:7:10.61:50.801:30.421:28.77
O:CYS:B:7:9.878:51.453:29.662:23.73
CB:CYS:B:7:12.995:51.452:30.534:25.61
SG:CYS:B:7:14.735:51.095:30.241:32.01
H:CYS:B:7:11.851:50.864:28.126:26.51
HA:CYS:B:7:12.223:49.551:30.477:29.3
HB2:CYS:B:7:12.791:52.292:30.093:30.73
HB3:CYS:B:7:12.874:51.551:31.492:30.73
N:GLY:B:8:10.246:50.438:31.636:23.3
CA:GLY:B:8:8.941:50.832:32.13:24.26
C:GLY:B:8:7.848:50.372:31.198:27.94
O:GLY:B:8:7.783:49.176:30.882:23.54
H:GLY:B:8:10.721:49.975:32.183:27.96
HA2:GLY:B:8:8.79:50.442:33.005:29.11
HA3:GLY:B:8:8.898:51.798:32.208:29.11
N:SER:B:9:7.045:51.325:30.7:25.43
CA:SER:B:9:5.825:51.05:29.947:28.83
C:SER:B:9:6.127:50.664:28.495:33.52
O:SER:B:9:5.335:49.988:27.841:31.13
CB:SER:B:9:4.914:52.281:29.986:36.62
OG:SER:B:9:5.573:53.396:29.4:36.38
H:SER:B:9:7.199:52.166:30.793:30.51
HA:SER:B:9:5.353:50.312:30.364:34.6
HB2:SER:B:9:4.104:52.092:29.487:43.94
HB3:SER:B:9:4.698:52.488:30.908:43.94
HG:SER:B:9:6.279:53.567:29.822:43.65
N:CGU:B:10:7.28:51.095:27.998:28.76
CA:CGU:B:10:7.81:50.596:26.686:28.05
CB:CGU:B:10:9.239:51.112:26.411:26.61
CG:CGU:B:10:9.333:52.622:26.497:48.2
CD1:CGU:B:10:10.796:53.099:26.309:43.27
OE12:CGU:B:10:10.997:54.252:25.818:32.43
OE11:CGU:B:10:11.775:52.332:26.659:28.59
CD2:CGU:B:10:8.34:53.322:25.507:61.07
OE21:CGU:B:10:8.191:52.877:24.334:60.62
OE22:CGU:B:10:7.665:54.311:25.914:71.45
C:CGU:B:10:7.888:49.082:26.653:29.41
O:CGU:B:10:7.883:48.518:25.527:30.26
HG:CGU:B:10:9.037:52.937:27.534:57.84
HB3:CGU:B:10:9.957:50.658:27.117:31.93
HB2:CGU:B:10:9.575:50.754:25.412:31.93
HA:CGU:B:10:7.113:50.935:25.873:33.66
N:ILE:B:11:8.048:48.421:27.803:25.25
CA:ILE:B:11:8.061:46.962:27.816:21.79
C:ILE:B:11:6.652:46.486:27.505:22.28
O:ILE:B:11:6.473:45.595:26.699:22.22
CB:ILE:B:11:8.584:46.402:29.14:29.42
CG1:ILE:B:11:10.089:46.697:29.267:30.34
CG2:ILE:B:11:8.328:44.893:29.247:23.17
CD1:ILE:B:11:10.655:46.443:30.653:34.61
H:ILE:B:11:8.15:48.789:28.574:30.3
HA:ILE:B:11:8.645:46.647:27.108:26.14
HB:ILE:B:11:8.12:46.846:29.867:35.31
HG12:ILE:B:11:10.571:46.133:28.643:36.41
HG13:ILE:B:11:10.243:47.63:29.052:36.41
HG21:ILE:B:11:8.671:44.574:30.097:27.8
HG22:ILE:B:11:7.373:44.731:29.195:27.8
HG23:ILE:B:11:8.781:44.443:28.517:27.8
HD11:ILE:B:11:11.603:46.651:30.649:41.53
HD12:ILE:B:11:10.194:47.009:31.291:41.53
HD13:ILE:B:11:10.522:45.509:30.881:41.53
N:THR:B:12:5.642:47.089:28.133:23.69
CA:THR:B:12:4.264:46.785:27.759:27.8
C:THR:B:12:4.051:46.987:26.269:32.55
O:THR:B:12:3.511:46.106:25.58:24.04
CB:THR:B:12:3.292:47.642:28.58:33.52
OG1:THR:B:12:3.502:47.358:29.965:32.74
CG2:THR:B:12:1.803:47.355:28.223:26.3
H:THR:B:12:5.726:47.666:28.765:28.42
HA:THR:B:12:4.082:45.854:27.961:33.36
HB:THR:B:12:3.471:48.581:28.413:40.23
HG1:THR:B:12:2.979:47.818:30.435:39.29
HG21:THR:B:12:1.22:47.914:28.761:31.56
HG22:THR:B:12:1.644:47.545:27.285:31.56
HG23:THR:B:12:1.594:46.424:28.396:31.56
N:ASN:B:13:4.453:48.15:25.751:24.48
CA:ASN:B:13:4.301:48.421:24.321:25.34
C:ASN:B:13:4.974:47.353:23.491:24.13
O:ASN:B:13:4.462:46.938:22.439:24.08
CB:ASN:B:13:4.909:49.776:23.943:28.08
CG:ASN:B:13:4.169:50.958:24.563:43.36
OD1:ASN:B:13:3.038:50.826:25.036:39.56
ND2:ASN:B:13:4.82:52.121:24.575:47.85
H:ASN:B:13:4.812:48.79:26.2:29.38
HA:ASN:B:13:3.358:48.435:24.096:30.41
HB2:ASN:B:13:5.829:49.805:24.249:33.69
HB3:ASN:B:13:4.877:49.876:22.978:33.69
HD21:ASN:B:13:4.449:52.819:24.913:57.42
HD22:ASN:B:13:5.612:52.174:24.244:57.42
N:SER:B:14:6.155:46.925:23.918:22.66
CA:SER:B:14:6.85:45.888:23.173:21.94
C:SER:B:14:6.098:44.563:23.22:21.87
O:SER:B:14:5.951:43.898:22.193:22.01
CB:SER:B:14:8.269:45.758:23.696:25.08
OG:SER:B:14:9.033:46.775:23.091:24.01
H:SER:B:14:6.565:47.209:24.618:27.19
HA:SER:B:14:6.904:46.16:22.243:26.33

【表１－６】

HB2:SER:B:14:8.274:45.874:24.659:30.1
HB3:SER:B:14:8.63:44.891:23.453:30.1
HG:SER:B:14:9.828:46.735:23.358:28.81
N:TYR:B:15:5.629:44.144:24.4:21.89
CA:TYR:B:15:4.768:42.964:24.454:22.13
C:TYR:B:15:3.609:43.089:23.478:22.94
O:TYR:B:15:3.283:42.128:22.771:23.01
CB:TYR:B:15:4.193:42.718:25.852:22.53
CG:TYR:B:15:5.115:42.148:26.893:22.01
CD1:TYR:B:15:5.679:40.889:26.759:37.65
CD2:TYR:B:15:5.351:42.85:28.079:48.14
CE1:TYR:B:15:6.507:40.375:27.747:62.89
CE2:TYR:B:15:6.165:42.337:29.078:52.81
CZ:TYR:B:15:6.748:41.113:28.908:60.82
OH:TYR:B:15:7.558:40.637:29.929:54.81
H:TYR:B:15:5.789:44.514:25.16:26.27
HA:TYR:B:15:5.287:42.185:24.203:26.56
HB2:TYR:B:15:3.868:43.565:26.195:27.03
HB3:TYR:B:15:3.448:42.104:25.765:27.03
HD1:TYR:B:15:5.53:40.399:25.982:45.19
HD2:TYR:B:15:4.966:43.688:28.195:57.77
HE1:TYR:B:15:6.897:39.537:27.638:75.46
HE2:TYR:B:15:6.328:42.83:29.85:63.37
HH:TYR:B:15:7.597:41.201:30.551:65.77
N:MET:B:16:2.967:44.255:23.427:23.8
CA:MET:B:16:1.803:44.423:22.544:28.09
C:MET:B:16:2.197:44.329:21.083:26.65
O:MET:B:16:1.471:43.748:20.275:36.43
CB:MET:B:16:1.118:45.775:22.768:30.99
CG:MET:B:16:0.499:45.977:24.148:42.33
SD:MET:B:16:-0.954:44.949:24.404:68.25
CE:MET:B:16:-0.206:43.67:25.426:42.42
H:MET:B:16:3.177:44.953:23.883:28.56
HA:MET:B:16:1.157:43.726:22.74:33.71
HB2:MET:B:16:1.775:46.477:22.639:37.19
HB3:MET:B:16:0.409:45.872:22.114:37.19
HG2:MET:B:16:1.153:45.748:24.826:50.79
HG3:MET:B:16:0.232:46.905:24.243:50.79
HE1:MET:B:16:-0.883:43.016:25.657:50.9
HE2:MET:B:16:0.508:43.245:24.926:50.9
HE3:MET:B:16:0.15:44.078:26.231:50.9
N:ASP:B:17:3.344:44.897:20.719:29.89
CA:ASP:B:17:3.758:44.849:19.322:34.2
C:ASP:B:17:4.362:43.503:18.931:30.46
O:ASP:B:17:4.224:43.095:17.781:28.87
CB:ASP:B:17:4.769:45.957:19.002:41.66
CG:ASP:B:17:4.239:47.347:19.307:78.78
OD1:ASP:B:17:3:47.511:19.374:89.35
OD2:ASP:B:17:5.064:48.277:19.478:72.64
H:ASP:B:17:3.887:45.306:21.246:35.87
HA:ASP:B:17:2.978:44.994:18.764:41.04
HB2:ASP:B:17:5.569:45.818:19.534:49.99
HB3:ASP:B:17:4.989:45.92:18.058:49.99
N:LEU:B:18:5.062:42.822:19.831:22.66
CA:LEU:B:18:5.868:41.669:19.444:22.1
C:LEU:B:18:5.314:40.329:19.885:22.41
O:LEU:B:18:5.69:39.304:19.308:24.4
CB:LEU:B:18:7.286:41.806:20.002:22.61
CG:LEU:B:18:7.948:43.093:19.512:21.46
CD1:LEU:B:18:9.302:43.234:20.155:24.5
CD2:LEU:B:18:8.07:43.128:17.966:28.1
H:LEU:B:18:5.088:43.006:20.671:27.19
HA:LEU:B:18:5.935:41.652:18.476:26.53
HB2:LEU:B:18:7.249:41.832:20.971:27.14
HB3:LEU:B:18:7.823:41.055:19.704:27.14
HG:LEU:B:18:7.407:43.85:19.787:25.75
HD11:LEU:B:18:9.717:44.053:19.841:29.4
HD12:LEU:B:18:9.192:43.267:21.118:29.4
HD13:LEU:B:18:9.848:42.471:19.91:29.4
HD21:LEU:B:18:8.494:43.959:17.702:33.72
HD22:LEU:B:18:8.607:42.375:17.675:33.72
HD23:LEU:B:18:7.183:43.071:17.578:33.72
N:CYS:B:19:4.481:40.285:20.912:26.31
CA:CYS:B:19:4.018:39.001:21.403:23.2
C:CYS:B:19:2.573:38.743:21.045:29.55
O:CYS:B:19:2.204:37.602:20.812:27.61
CB:CYS:B:19:4.199:38.915:22.923:25.28
SG:CYS:B:19:5.942:39.114:23.454:33.59
H:CYS:B:19:4.174:40.968:21.334:31.58
HA:CYS:B:19:4.553:38.3:21:27.84
HB2:CYS:B:19:3.677:39.617:23.342:30.34
HB3:CYS:B:19:3.891:38.047:23.227:30.34
O:TYR:B:20:0.453:40.693:18.643:58.94
N:TYR:B:20:1.763:39.78:20.969:30.88
CA:TYR:B:20:0.33:39.624:20.788:36.15
C:TYR:B:20:-0.046:39.793:19.324:48.21
CB:TYR:B:20:-0.44:40.615:21.651:29.56
CG:TYR:B:20:-0.651:40.122:23.065:55.92
CD1:TYR:B:20:-1.597:39.145:23.34:71.32
CD2:TYR:B:20:0.094:40.621:24.118:59.77
CE1:TYR:B:20:-1.8:38.679:24.621:72.77
CE2:TYR:B:20:-0.098:40.161:25.411:73.5
CZ:TYR:B:20:-1.058:39.185:25.659:74.33
OH:TYR:B:20:-1.29:38.681:26.931:61.61
H:TYR:B:20:2.02:40.599:21.019:37.06
HA:TYR:B:20:0.074:38.728:21.06:43.38
HB2:TYR:B:20:0.055:41.447:21.695:35.48
HB3:TYR:B:20:-1.312:40.768:21.254:35.48
HD1:TYR:B:20:-2.106:38.797:22.644:85.58
HD2:TYR:B:20:0.735:41.274:23.956:71.73
HE1:TYR:B:20:-2.44:38.024:24.782:87.33
HE2:TYR:B:20:0.409:40.506:26.11:88.2
HH:TYR:B:20:-0.786:39.058:27.486:73.93
O:ARG:B:21:-2.375:41.115:18.001:73.56
N:ARG:B:21:-0.904:38.888:18.851:48.09
CA:ARG:B:21:-1.505:38.926:17.518:54.86
C:ARG:B:21:-2.02:40.306:17.132:67.04
CB:ARG:B:21:-2.675:37.949:17.448:56.88
CG:ARG:B:21:-2.44:36.661:16.704:66.58
CD:ARG:B:21:-3.714:36.364:15.961:87.2
NE:ARG:B:21:-3.936:34.955:15.663:104.85
CZ:ARG:B:21:-5.147:34.397:15.619:123.5

【表１－７】

NH1:ARG:B:21:-6.239:35.129:15.88:136.71
NH2:ARG:B:21:-5.27:33.101:15.333:115.82
OXT:ARG:B:21:-2.121:40.62:15.939:68.47
H:ARG:B:21:-1.164:38.209:19.309:57.7
HA:ARG:B:21:-0.844:38.656:16.862:65.83
HB2:ARG:B:21:-2.926:37.714:18.355:68.25
HB3:ARG:B:21:-3.418:38.398:17.016:68.25
HG2:ARG:B:21:-1.716:36.768:16.067:79.9
HG3:ARG:B:21:-2.258:35.94:17.327:79.9
HD2:ARG:B:21:-4.462:36.672:16.495:104.64
HD3:ARG:B:21:-3.698:36.842:15.117:104.64
HE:ARG:B:21:-3.252:34.434:15.65:125.82
HH11:ARG:B:21:-6.162:35.965:16.065:164.05
HH12:ARG:B:21:-7.017:34.764:15.855:164.05
HH21:ARG:B:21:-4.571:32.628:15.17:138.98
HH22:ARG:B:21:-6.049:32.738:15.311:138.98

。

【請求項２０】

ＩＲアゴニストである単離分子であって、下表の原子座標またはそのサブセットにより定義されるＣｏｎ－Ｉｎｓ　Ｇ１の３Ｄ構造に基づいて同定されているおよび／または設計されている分子：

【表２－１】

付録I: CON-INS G1インスリン(鎖Aおよび鎖B)に関する原子座標

フォーマットは、下記のコロンで区切られたフィールドを含む: (1) 原子の名称, (2) 残基タイプ, (3) 鎖の名称,(4) 残基番号,(5-7) xyz 座標,(8) 温度B因子(thermal B-factor)。

N:GLY:A:1:15.439:38.785:34.309:26.76
CA:GLY:A:1:14.11:39.14:33.733:22.21
C:GLY:A:1:14.251:39.976:32.492:21.3
O:GLY:A:1:15.353:40.312:32.093:22.73
H1:GLY:A:1:15.395:38.813:35.197:32.11
H2:GLY:A:1:15.666:37.965:34.049:32.11
H3:GLY:A:1:16.051:39.366:34.024:32.11
HA2:GLY:A:1:13.625:38.331:33.508:26.65
HA3:GLY:A:1:13.595:39.639:34.386:26.65
N:VAL:A:2:13.113:40.325:31.895:21.05
CA:VAL:A:2:13.122:41.169:30.72:22.11
C:VAL:A:2:13.696:42.561:31.01:20.41
O:VAL:A:2:14.274:43.187:30.116:20.06
CB:VAL:A:2:11.698:41.225:30.132:25.46
CG1:VAL:A:2:10.72:41.927:31.074:21.3
CG2:VAL:A:2:11.725:41.902:28.839:27.88
H:VAL:A:2:12.33:40.084:32.154:25.26
HA:VAL:A:2:13.693:40.756:30.053:26.54
HB:VAL:A:2:11.38:40.32:29.989:30.55
HG11:VAL:A:2:9.841:41.939:30.665:25.56
HG12:VAL:A:2:10.688:41.442:31.914:25.56
HG13:VAL:A:2:11.026:42.835:31.227:25.56
HG21:VAL:A:2:10.824:41.931:28.48:33.45
HG22:VAL:A:2:12.061:42.804:28.963:33.45
HG23:VAL:A:2:12.306:41.412:28.238:33.45
N:VAL:A:3:13.604:43.056:32.249:26.31
CA:VAL:A:3:14.092:44.414:32.525:22.38
C:VAL:A:3:15.618:44.365:32.529:26.64
O:VAL:A:3:16.283:45.246:31.982:21.94
CB:VAL:A:3:13.517:44.989:33.842:28.85
CG1:VAL:A:3:14.192:46.325:34.21:23.35
CG2:VAL:A:3:11.967:45.154:33.731:22.25
H:VAL:A:3:13.276:42.642:32.928:31.58
HA:VAL:A:3:13.816:44.998:31.802:26.85
HB:VAL:A:3:13.695:44.361:34.559:34.62
HG11:VAL:A:3:13.808:46.654:35.037:28.02
HG12:VAL:A:3:15.144:46.176:34.323:28.02
HG13:VAL:A:3:14.039:46.963:33.496:28.02
HG21:VAL:A:3:11.628:45.515:34.565:26.7
HG22:VAL:A:3:11.767:45.762:33.001:26.7
HG23:VAL:A:3:11.569:44.287:33.558:26.7
N:CGU:A:4:16.193:43.318:33.099:21.34
CA:CGU:A:4:17.68:43.233:33.107:21.52
CB:CGU:A:4:18.136:42.041:33.939:22.15
CG:CGU:A:4:17.867:42.164:35.47:27.83
CD1:CGU:A:4:16.419:42.187:35.88:25.08
OE12:CGU:A:4:16.135:42.812:36.937:28.6
OE11:CGU:A:4:15.531:41.542:35.211:22.71
CD2:CGU:A:4:18.45:40.98:36.25:48.38
OE21:CGU:A:4:18.448:39.819:35.754:54.62
OE22:CGU:A:4:18.871:41.181:37.42:85.42
C:CGU:A:4:18.255:43.089:31.618:20.98
O:CGU:A:4:19.303:43.691:31.269:21.08
HG:CGU:A:4:18.338:43.105:35.863:33.4
HB3:CGU:A:4:17.661:41.115:33.568:26.58
HB2:CGU:A:4:19.22:41.867:33.754:26.58
HA:CGU:A:4:18.079:44.185:33.551:25.82
N:HIS:A:5:17.548:42.333:30.786:21.02
CA:HIS:A:5:18.007:41.966:29.443:20.65
C:HIS:A:5:17.659:43.013:28.373:19.86
O:HIS:A:5:18.285:43.07:27.334:23.44
CB:HIS:A:5:17.391:40.584:29.071:20.16
CG:HIS:A:5:18.115:39.864:27.981:47.58
ND1:HIS:A:5:19.277:39.15:28.201:43.05
CD2:HIS:A:5:17.832:39.734:26.661:45.41
CE1:HIS:A:5:19.678:38.617:27.058:50.46
NE2:HIS:A:5:18.82:38.957:26.111:52.67
HA:HIS:A:5:18.972:41.867:29.458:24.79
HB2:HIS:A:5:17.402:40.017:29.858:24.19
HB3:HIS:A:5:16.476:40.72:28.778:24.19
HD2:HIS:A:5:17.106:40.104:26.213:54.49
HE1:HIS:A:5:20.437:38.093:26.94:60.55
HE2:HIS:A:5:18.873:38.729:25.284:63.2
H:HIS:A:5:16.775:42.01:30.98:25.23
N:CYS:A:6:16.641:43.84:28.616:19.88
CA:CYS:A:6:16.113:44.731:27.591:19.76
C:CYS:A:6:16.063:46.184:28.028:21.58
O:CYS:A:6:15.909:47.06:27.165:20.58
CB:CYS:A:6:14.695:44.308:27.194:21.07
SG:CYS:A:6:14.678:42.722:26.317:26
H:CYS:A:6:16.238:43.902:29.373:23.85
HA:CYS:A:6:16.676:44.674:26.803:23.71
HB2:CYS:A:6:14.154:44.217:27.994:25.29
HB3:CYS:A:6:14.315:44.981:26.608:25.29
N:CYS:A:7:16.128:46.463:29.323:21.05
CA:CYS:A:7:16.186:47.837:29.839:21.74
C:CYS:A:7:17.553:48.188:30.41:23.78
O:CYS:A:7:18.103:49.215:30.042:30.88
CB:CYS:A:7:15.098:48.081:30.895:21.43
SG:CYS:A:7:15.221:49.718:31.732:27.59
H:CYS:A:7:16.14:45.864:29.941:25.26
HA:CYS:A:7:16.016:48.446:29.103:26.09
HB2:CYS:A:7:14.229:48.033:30.465:25.71
HB3:CYS:A:7:15.165:47.394:31.576:25.71
N:HIS:A:8:18.157:47.348:31.264:28.49
CA:HIS:A:8:19.509:47.657:31.747:25.02
C:HIS:A:8:20.564:47.453:30.657:30.05
O:HIS:A:8:21.558:48.179:30.604:34.16

【表２－２】

CB:HIS:A:8:19.847:46.811:32.972:27.96
CG:HIS:A:8:18.916:47.03:34.125:33.4
ND1:HIS:A:8:18.619:46.043:35.044:34.99
CD2:HIS:A:8:18.234:48.129:34.521:27.24
CE1:HIS:A:8:17.767:46.516:35.936:33.7
NE2:HIS:A:8:17.527:47.782:35.648:38.53
H:HIS:A:8:17.818:46.619:31.57:34.19
HA:HIS:A:8:19.538:48.589:32.014:30.03
HB2:HIS:A:8:19.802:45.874:32.728:33.55
HB3:HIS:A:8:20.744:47.033:33.268:33.55
HD2:HIS:A:8:18.233:48.959:34.103:32.68
HE1:HIS:A:8:17.417:46.045:36.658:40.44
HE2:HIS:A:8:17.009:48.305:36.092:46.23
N:ARG:A:9:20.377:46.477:29.813:32.17
CA:ARG:A:9:21.026:46.221:28.542:24.61
C:ARG:A:9:19.985:46.413:27.464:24.55
O:ARG:A:9:18.838:46.063:27.712:22.58
CB:ARG:A:9:21.524:44.776:28.434:42.6
CG:ARG:A:9:22.966:44.545:28.786:89.14
CD:ARG:A:9:23.608:43.537:27.831:118.62
NE:ARG:A:9:25.059:43.702:27.796:137.92
CZ:ARG:A:9:25.928:42.745:27.485:154.54
NH1:ARG:A:9:25.517:41.519:27.184:170.53
NH2:ARG:A:9:27.224:43.02:27.49:152.73
H:ARG:A:9:19.797:45.864:29.977:38.61
HA:ARG:A:9:21.763:46.836:28.4:29.53
HB2:ARG:A:9:20.99:44.224:29.027:51.12
HB3:ARG:A:9:21.399:44.478:27.519:51.12
HG2:ARG:A:9:23.451:45.382:28.719:106.97
HG3:ARG:A:9:23.024:44.192:29.688:106.97
HD2:ARG:A:9:23.41:42.637:28.132:142.34
HD3:ARG:A:9:23.263:43.677:26.935:142.34
HE:ARG:A:9:25.375:44.477:27.991:165.51
HH11:ARG:A:9:24.676:41.336:27.181:204.63
HH12:ARG:A:9:26.09:40.909:26.987:204.63
HH21:ARG:A:9:27.495:43.812:27.686:183.27
HH22:ARG:A:9:27.794:42.407:27.293:183.27
N:PRO:A:10:20.315:46.922:26.273:21.04
CA:PRO:A:10:19.325:46.947:25.186:22.55
C:PRO:A:10:19.153:45.573:24.54:20.8
O:PRO:A:10:20.049:44.721:24.565:22.83
CB:PRO:A:10:19.914:47.951:24.205:21.44
CG:PRO:A:10:21.394:47.783:24.393:23.92
CD:PRO:A:10:21.581:47.551:25.858:26.07
HA:PRO:A:10:18.468:47.268:25.508:27.06
HB2:PRO:A:10:19.65:47.726:23.299:25.72
HB3:PRO:A:10:19.633:48.849:24.439:25.72
HG2:PRO:A:10:21.703:47.018:23.883:28.7
HG3:PRO:A:10:21.853:48.59:24.112:28.7
HD2:PRO:A:10:22.324:46.948:26.013:31.28
HD3:PRO:A:10:21.706:48.395:26.32:31.28
N:CYS:A:11:17.965:45.34:23.974:20.27
CA:CYS:A:11:17.735:44.077:23.278:20.11
C:CYS:A:11:17.021:44.299:21.95:20.29
O:CYS:A:11:16.249:45.24:21.766:20.43
CB:CYS:A:11:16.959:43.053:24.166:20.58
SG:CYS:A:11:15.186:43.358:24.401:23.25
H:CYS:A:11:17.296:45.881:23.98:24.33
HA:CYS:A:11:18.598:43.683:23.076:24.13
HB2:CYS:A:11:17.048:42.175:23.763:24.7
HB3:CYS:A:11:17.368:43.045:25.045:24.7
N:SER:A:12:17.349:43.443:21.002:19.95
CA:SER:A:12:16.64:43.374:19.734:20.24
C:SER:A:12:15.198:42.876:19.921:19.9
O:SER:A:12:14.82:42.314:20.95:19.48
CB:SER:A:12:17.365:42.442:18.794:20.66
OG:SER:A:12:17.226:41.115:19.254:20.36
H:SER:A:12:17.993:42.877:21.068:23.94
HA:SER:A:12:16.611:44.256:19.332:24.29
HB2:SER:A:12:16.978:42.517:17.908:24.79
HB3:SER:A:12:18.306:42.677:18.772:24.79
HG:SER:A:12:17.626:40.589:18.736:24.43
N:ASN:A:13:14.386:43.089:18.896:20.29
CA:ASN:A:13:13.05:42.486:18.857:20.21
C:ASN:A:13:13.113:40.969:18.999:19.99
O:ASN:A:13:12.303:40.375:19.72:19.76
CB:ASN:A:13:12.338:42.827:17.571:20.89
CG:ASN:A:13:11.993:44.254:17.455:21.34
OD1:ASN:A:13:12.063:45.022:18.425:21.1
ND2:ASN:A:13:11.561:44.637:16.254:22.2
H:ASN:A:13:14.577:43.575:18.213:24.35
HA:ASN:A:13:12.523:42.835:19.593:24.25
HB2:ASN:A:13:12.913:42.598:16.823:25.07
HB3:ASN:A:13:11.515:42.316:17.522:25.07
HD21:ASN:A:13:11.343:45.457:16.116:26.64
HD22:ASN:A:13:11.502:44.063:15.616:26.64
N:ALA:A:14:14.073:40.323:18.327:20.53
CA:ALA:A:14:14.136:38.865:18.34:20.59
C:ALA:A:14:14.514:38.344:19.713:20.2
O:ALA:A:14:13.966:37.34:20.17:20.42
CB:ALA:A:14:15.122:38.388:17.293:21.21
H:ALA:A:14:14.689:40.704:17.863:24.64
HA:ALA:A:14:13.262:38.509:18.115:24.71
HB1:ALA:A:14:15.156:37.419:17.311:25.45
HB2:ALA:A:14:14.827:38.694:16.421:25.45
HB3:ALA:A:14:15.997:38.755:17.494:25.45
N:GLU:A:15:15.393:39.048:20.418:19.99
CA:GLU:A:15:15.674:38.714:21.807:20.64
C:GLU:A:15:14.459:38.979:22.702:20.25
O:GLU:A:15:14.126:38.165:23.56:19.51
CB:GLU:A:15:16.886:39.507:22.306:24.27
CG:GLU:A:15:18.221:38.954:21.864:52.08
CD:GLU:A:15:18.481:37.555:22.399:68.3
OE1:GLU:A:15:18.414:37.354:23.638:37.34
OE2:GLU:A:15:18.75:36.655:21.573:92.14
H:GLU:A:15:15.838:39.719:20.116:23.99
HA:GLU:A:15:15.889:37.77:21.867:24.77
HB2:GLU:A:15:16.82:40.416:21.974:29.12
HB3:GLU:A:15:16.876:39.513:23.276:29.12
HG2:GLU:A:15:18.242:38.914:20.895:62.5
HG3:GLU:A:15:18.927:39.535:22.188:62.5
N:PHE:A:16:13.813:40.136:22.56:19.08

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CA:PHE:A:16:12.627:40.394:23.379:19.01
C:PHE:A:16:11.58:39.275:23.258:19.21
O:PHE:A:16:10.937:38.891:24.259:19.32
CB:PHE:A:16:12:41.738:23.008:19.12
CG:PHE:A:16:10.869:42.118:23.896:19.26
CD2:PHE:A:16:11.086:42.876:25.025:19.26
CD1:PHE:A:16:9.575:41.712:23.603:19.56
CE2:PHE:A:16:10.018:43.216:25.879:19.59
CE1:PHE:A:16:8.496:42.075:24.429:19.92
CZ:PHE:A:16:8.717:42.809:25.564:19.95
H:PHE:A:16:14.029:40.767:22.018:22.9
HA:PHE:A:16:12.898:40.443:24.309:22.81
HB2:PHE:A:16:12.677:42.43:23.073:22.95
HB3:PHE:A:16:11.663:41.689:22.1:22.95
HD2:PHE:A:16:11.95:43.143:25.241:23.11
HD1:PHE:A:16:9.416:41.209:22.837:23.48
HE2:PHE:A:16:10.173:43.731:26.637:23.51
HE1:PHE:A:16:7.635:41.79:24.221:23.9
HZ:PHE:A:16:8.006:43.046:26.114:23.93
N:LYS:A:17:11.394:38.736:22.051:19.63
CA:LYS:A:17:10.38:37.7:21.84:19.97
C:LYS:A:17:10.614:36.46:22.684:20.12
O:LYS:A:17:9.672:35.685:22.893:20.5
CB:LYS:A:17:10.329:37.289:20.362:20.31
CG:LYS:A:17:9.504:38.28:19.498:20.56
CD:LYS:A:17:9.689:38.041:18.044:21.03
CE:LYS:A:17:9.094:39.21:17.228:23.58
NZ:LYS:A:17:9.222:39.104:15.74:26.95
H:LYS:A:17:11.837:38.95:21.346:23.56
HA:LYS:A:17:9.512:38.061:22.078:23.96
HB2:LYS:A:17:11.232:37.262:20.009:24.37
HB3:LYS:A:17:9.917:36.413:20.291:24.37
HG2:LYS:A:17:8.562:38.173:19.703:24.67
HG3:LYS:A:17:9.788:39.186:19.694:24.67
HD2:LYS:A:17:10.636:37.977:17.845:25.23
HD3:LYS:A:17:9.232:37.224:17.789:25.23
HE2:LYS:A:17:8.148:39.275:17.433:28.3
HE3:LYS:A:17:9.539:40.028:17.499:28.3
HZ1:LYS:A:17:8.855:39.816:15.352:32.34
HZ2:LYS:A:17:10.081:39.061:15.511:32.34
HZ3:LYS:A:17:8.808:38.371:15.451:32.34
N:LYS:A:18:11.856:36.224:23.113:20.04
CA:LYS:A:18:12.144:35.116:24.033:21.82
C:LYS:A:18:11.301:35.19:25.294:20.55
O:LYS:A:18:11.071:34.163:25.936:21.12
CB:LYS:A:18:13.624:35.111:24.441:20.42
CG:LYS:A:18:14.518:34.782:23.279:20.61
CD:LYS:A:18:16.015:34.803:23.664:30.84
CE:LYS:A:18:16.866:34.3:22.484:38.22
NZ:LYS:A:18:18.269:33.984:22.906:62
H:LYS:A:18:12.546:36.685:22.889:24.05
HA:LYS:A:18:11.951:34.276:23.589:26.19
HB2:LYS:A:18:13.867:35.989:24.772:24.51
HB3:LYS:A:18:13.763:34.442:25.13:24.51
HG2:LYS:A:18:14.303:33.894:22.954:24.73
HG3:LYS:A:18:14.379:35.436:22.576:24.73
HD2:LYS:A:18:16.284:35.711:23.875:37
HD3:LYS:A:18:16.163:34.218:24.424:37
HE2:LYS:A:18:16.468:33.491:22.125:45.86
HE3:LYS:A:18:16.902:34.987:21.8:45.86
HZ1:LYS:A:18:18.739:33.696:22.207:74.4
HZ2:LYS:A:18:18.658:34.713:23.236:74.4
HZ3:LYS:A:18:18.263:33.351:23.531:74.4
N:TYR:A:19:10.88:36.384:25.687:25.2
CA:TYR:A:19:10.118:36.604:26.923:20.68
C:TYR:A:19:8.575:36.613:26.737:31.44
O:TYR:A:19:7.832:36.875:27.687:29.68
CB:TYR:A:19:10.538:37.943:27.555:20.37
CG:TYR:A:19:11.901:37.935:28.109:23.44
CD1:TYR:A:19:13:38.247:27.323:19.93
CD2:TYR:A:19:12.117:37.579:29.428:23.18
CE1:TYR:A:19:14.278:38.224:27.859:26.81
CE2:TYR:A:19:13.379:37.562:29.96:25.73
CZ:TYR:A:19:14.444:37.864:29.184:22.56
OH:TYR:A:19:15.682:37.826:29.75:22.36
H:TYR:A:19:11.025:37.107:25.245:30.24
HA:TYR:A:19:10.335:35.898:27.552:24.82
HB2:TYR:A:19:10.498:38.635:26.876:24.45
HB3:TYR:A:19:9.926:38.154:28.276:24.45
HD2:TYR:A:19:11.39:37.364:29.968:27.82
HD1:TYR:A:19:12.877:38.483:26.431:23.92
HE2:TYR:A:19:13.505:37.32:30.849:30.88
HE1:TYR:A:19:15.015:38.436:27.332:32.17
HH:TYR:A:19:16.265:38.03:29.18:26.83
O:CY3:A:20:6.334:34.016:25.918:46.46
C:CY3:A:20:5.968:35.121:26.067:39.6
N1:CY3:A:20:4.848:35.386:26.929:43.25
CA:CY3:A:20:6.666:36.307:25.294:21.87
N:CY3:A:20:8.084:36.362:25.53:22.5
CB:CY3:A:20:6.382:35.984:23.834:33.52
SG:CY3:A:20:6.832:37.458:22.767:39.89
H:CY3:A:20:8.534:36.217:24.812:27
HA:CY3:A:20:6.252:37.151:25.536:26.25
HB2:CY3:A:20:5.439:35.782:23.725:40.22
HB3:CY3:A:20:6.908:35.214:23.567:40.22
HN11:CY3:A:20:4.569:36.191:27.039:51.9
HN12:CY3:A:20:4.467:34.738:27.347:51.9
O:THR:B:-1:16.056:46.908:9.868:60.34
N:THR:B:-1:16.406:48.652:7.605:78.37
CA:THR:B:-1:17.132:48.822:8.897:76.87
C:THR:B:-1:17.109:47.519:9.689:64.38
CB:THR:B:-1:16.526:49.975:9.74:82.36
OG1:THR:B:-1:17.021:51.231:9.25:103.8
CG2:THR:B:-1:16.88:49.85:11.228:68.98
H1:THR:B:-1:16.283:49.449:7.227:94.05
H2:THR:B:-1:16.886:48.137:7.061:94.05
H3:THR:B:-1:15.617:48.27:7.756:94.05
HA:THR:B:-1:18.058:49.042:8.712:92.25
HB:THR:B:-1:15.56:49.958:9.656:98.83
HG1:THR:B:-1:16.698:51.862:9.7:124.55
HG21:THR:B:-1:16.486:50.584:11.725:82.78
HG22:THR:B:-1:16.538:49.013:11.58:82.78

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HG23:THR:B:-1:17.843:49.871:11.343:82.78
O:PHE:B:0:17.693:47.018:12.852:32.11
N:PHE:B:0:18.285:47.117:10.17:47.49
CA:PHE:B:0:18.434:45.859:10.88:33.82
C:PHE:B:0:17.777:45.945:12.258:30.41
CB:PHE:B:0:19.916:45.528:11.007:28.4
CG:PHE:B:0:20.185:44.138:11.419:27.64
CD2:PHE:B:0:20.443:43.17:10.471:29.44
CD1:PHE:B:0:20.187:43.786:12.753:26.31
CE2:PHE:B:0:20.706:41.883:10.832:27.99
CE1:PHE:B:0:20.454:42.477:13.135:27.97
CZ:PHE:B:0:20.702:41.517:12.166:27.51
H:PHE:B:0:19.016:47.564:10.094:56.99
HA:PHE:B:0:18.003:45.151:10.377:40.59
HB2:PHE:B:0:20.342:45.669:10.147:34.08
HB3:PHE:B:0:20.311:46.115:11.67:34.08
HD1:PHE:B:0:20.017:44.431:13.402:31.58
HD2:PHE:B:0:20.445:43.402:9.571:35.33
HE1:PHE:B:0:20.45:42.243:14.035:33.57
HE2:PHE:B:0:20.874:41.244:10.177:33.58
HZ:PHE:B:0:20.881:40.638:12.411:33.01
O:ASP:B:1:18.276:43.923:15.696:23.3
N:ASP:B:1:17.325:44.791:12.774:25.54
CA:ASP:B:1:16.642:44.721:14.072:24.29
C:ASP:B:1:17.702:44.882:15.159:25.42
CB:ASP:B:1:15.863:43.408:14.192:30.99
CG:ASP:B:1:15.425:43.112:15.613:33.34
OD1:ASP:B:1:15.172:44.1:16.35:26.15
OD2:ASP:B:1:15.36:41.913:16.004:22.1
H:ASP:B:1:17.404:44.028:12.384:30.65
HA:ASP:B:1:16.014:45.456:14.145:29.15
HB2:ASP:B:1:15.068:43.46:13.639:37.19
HB3:ASP:B:1:16.427:42.677:13.894:37.19
O:THR:B:2:17.54:46.872:18.038:27.96
N:THR:B:2:18.026:46.134:15.452:24.07
CA:THR:B:2:19.15:46.377:16.357:23.86
C:THR:B:2:18.686:46.539:17.782:24.18
CB:THR:B:2:19.911:47.632:15.99:31.47
OG1:THR:B:2:18.958:48.664:15.749:33.31
CG2:THR:B:2:20.815:47.367:14.758:33.17
H:THR:B:2:17.631:46.838:15.155:28.88
HA:THR:B:2:19.762:45.626:16.318:28.64
HB:THR:B:2:20.479:47.889:16.733:37.77
HG1:THR:B:2:19.352:49.376:15.542:39.98
HG21:THR:B:2:21.302:48.173:14.525:39.81
HG22:THR:B:2:21.45:46.662:14.959:39.81
HG23:THR:B:2:20.272:47.097:14.001:39.81
C:HYP:B:3:18.617:47.825:20.609:37.46
O:HYP:B:3:19.172:48.867:20.197:33.28
CA:HYP:B:3:19.208:46.443:20.27:30.06
CB:HYP:B:3:20.366:46.23:20.929:46.37
CG:HYP:B:3:21.21:45.388:19.961:34.65
OD1:HYP:B:3:20.787:44.116:19.901:37.02
CD:HYP:B:3:20.889:46.065:18.606:30.67
N:HYP:B:3:19.59:46.315:18.708:25.2
HD23:HYP:B:3:21.065:45.458:17.869:36.81
HD22:HYP:B:3:21.39:46.89:18.507:36.81
HG:HYP:B:3:22.156:45.447:20.171:41.58
HD1:HYP:B:3:21.078:43.754:19.188:44.43
HB3:HYP:B:3:20.807:47.074:21.115:55.65
HB2:HYP:B:3:20.201:45.739:21.749:55.65
HA:HYP:B:3:18.572:45.748:20.503:36.08
O:LYS:B:4:16.271:47.848:23.837:25.52
N:LYS:B:4:17.521:47.837:21.368:29.31
CA:LYS:B:4:16.899:49.058:21.865:26.28
C:LYS:B:4:16.634:48.93:23.365:21.83
CB:LYS:B:4:15.558:49.322:21.159:37.68
CG:LYS:B:4:15.666:49.595:19.675:65.23
CD:LYS:B:4:14.269:49.657:19.051:94.75
CE:LYS:B:4:14.289:50.089:17.586:109.16
NZ:LYS:B:4:12.904:50.217:17.038:105.24
H:LYS:B:4:17.109:47.124:21.616:35.17
HA:LYS:B:4:17.488:49.813:21.713:31.53
HB2:LYS:B:4:14.99:48.544:21.273:45.21
HB3:LYS:B:4:15.139:50.094:21.569:45.21
HG2:LYS:B:4:16.106:50.447:19.533:78.28
HG3:LYS:B:4:16.163:48.879:19.248:78.28
HD2:LYS:B:4:13.864:48.777:19.098:113.71
HD3:LYS:B:4:13.732:50.296:19.544:113.71
HE2:LYS:B:4:14.727:50.951:17.511:130.99
HE3:LYS:B:4:14.763:49.424:17.062:130.99
HZ1:LYS:B:4:12.937:50.469:16.185:126.28
HZ2:LYS:B:4:12.482:49.435:17.093:126.28
HZ3:LYS:B:4:12.449:50.825:17.502:126.28
O:HIS:B:5:14.227:50.871:24.963:32.55
N:HIS:B:5:16.734:50.025:24.109:21.79
CA:HIS:B:5:16.363:50.01:25.519:21.56
C:HIS:B:5:14.857:50.045:25.607:22.3
CB:HIS:B:5:16.937:51.202:26.275:22.18
CG:HIS:B:5:18.423:51.204:26.337:22.64
ND1:HIS:B:5:19.131:50.545:27.328:28.27
CD2:HIS:B:5:19.345:51.765:25.516:25.48
CE1:HIS:B:5:20.428:50.699:27.11:22.51
NE2:HIS:B:5:20.585:51.441:26.022:28.72
H:HIS:B:5:17.013:50.786:23.824:26.15
HA:HIS:B:5:16.682:49.193:25.934:25.87
HB2:HIS:B:5:16.657:52.018:25.832:26.62
HB3:HIS:B:5:16.601:51.188:27.185:26.62
HD1:HIS:B:5:18.784:50.097:27.975:33.93
HD2:HIS:B:5:19.173:52.273:24.756:30.58
HE1:HIS:B:5:21.112:50.36:27.64:27.01
N:ARG:B:6:14.278:49.126:26.37:20.97
CA:ARG:B:6:12.838:49.07:26.561:24.52
C:ARG:B:6:12.608:49.07:28.058:21.26
O:ARG:B:6:12.884:48.066:28.727:23.78
CB:ARG:B:6:12.238:47.832:25.893:20.69
CG:ARG:B:6:12.796:47.582:24.53:26.83
CD:ARG:B:6:12.576:46.115:24.096:33.07
NE:ARG:B:6:13.308:45.832:22.86:31.36
CZ:ARG:B:6:12.807:45.919:21.638:20.49
NH1:ARG:B:6:11.527:46.276:21.431:28.98
NH2:ARG:B:6:13.594:45.629:20.612:25.07

【表２－５】

H:ARG:B:6:14.707:48.515:26.795:25.17
HA:ARG:B:6:12.425:49.861:26.181:29.42
HB2:ARG:B:6:12.426:47.054:26.441:24.83
HB3:ARG:B:6:11.279:47.953:25.806:24.83
HG2:ARG:B:6:12.352:48.159:23.89:32.19
HG3:ARG:B:6:13.75:47.758:24.537:32.19
HD2:ARG:B:6:12.903:45.519:24.789:39.68
HD3:ARG:B:6:11.632:45.963:23.935:39.68
HE:ARG:B:6:14.13:45.591:22.934:37.64
HH11:ARG:B:6:11.019:46.461:22.1:34.78
HH12:ARG:B:6:11.218:46.324:20.63:34.78
HH21:ARG:B:6:14.411:45.398:20.748:30.08
HH22:ARG:B:6:13.289:45.676:19.809:30.08
N:CYS:B:7:12.125:50.193:28.588:22.09
CA:CYS:B:7:12.018:50.387:30.028:24.41
C:CYS:B:7:10.61:50.801:30.421:28.77
O:CYS:B:7:9.878:51.453:29.662:23.73
CB:CYS:B:7:12.995:51.452:30.534:25.61
SG:CYS:B:7:14.735:51.095:30.241:32.01
H:CYS:B:7:11.851:50.864:28.126:26.51
HA:CYS:B:7:12.223:49.551:30.477:29.3
HB2:CYS:B:7:12.791:52.292:30.093:30.73
HB3:CYS:B:7:12.874:51.551:31.492:30.73
N:GLY:B:8:10.246:50.438:31.636:23.3
CA:GLY:B:8:8.941:50.832:32.13:24.26
C:GLY:B:8:7.848:50.372:31.198:27.94
O:GLY:B:8:7.783:49.176:30.882:23.54
H:GLY:B:8:10.721:49.975:32.183:27.96
HA2:GLY:B:8:8.79:50.442:33.005:29.11
HA3:GLY:B:8:8.898:51.798:32.208:29.11
N:SER:B:9:7.045:51.325:30.7:25.43
CA:SER:B:9:5.825:51.05:29.947:28.83
C:SER:B:9:6.127:50.664:28.495:33.52
O:SER:B:9:5.335:49.988:27.841:31.13
CB:SER:B:9:4.914:52.281:29.986:36.62
OG:SER:B:9:5.573:53.396:29.4:36.38
H:SER:B:9:7.199:52.166:30.793:30.51
HA:SER:B:9:5.353:50.312:30.364:34.6
HB2:SER:B:9:4.104:52.092:29.487:43.94
HB3:SER:B:9:4.698:52.488:30.908:43.94
HG:SER:B:9:6.279:53.567:29.822:43.65
N:CGU:B:10:7.28:51.095:27.998:28.76
CA:CGU:B:10:7.81:50.596:26.686:28.05
CB:CGU:B:10:9.239:51.112:26.411:26.61
CG:CGU:B:10:9.333:52.622:26.497:48.2
CD1:CGU:B:10:10.796:53.099:26.309:43.27
OE12:CGU:B:10:10.997:54.252:25.818:32.43
OE11:CGU:B:10:11.775:52.332:26.659:28.59
CD2:CGU:B:10:8.34:53.322:25.507:61.07
OE21:CGU:B:10:8.191:52.877:24.334:60.62
OE22:CGU:B:10:7.665:54.311:25.914:71.45
C:CGU:B:10:7.888:49.082:26.653:29.41
O:CGU:B:10:7.883:48.518:25.527:30.26
HG:CGU:B:10:9.037:52.937:27.534:57.84
HB3:CGU:B:10:9.957:50.658:27.117:31.93
HB2:CGU:B:10:9.575:50.754:25.412:31.93
HA:CGU:B:10:7.113:50.935:25.873:33.66
N:ILE:B:11:8.048:48.421:27.803:25.25
CA:ILE:B:11:8.061:46.962:27.816:21.79
C:ILE:B:11:6.652:46.486:27.505:22.28
O:ILE:B:11:6.473:45.595:26.699:22.22
CB:ILE:B:11:8.584:46.402:29.14:29.42
CG1:ILE:B:11:10.089:46.697:29.267:30.34
CG2:ILE:B:11:8.328:44.893:29.247:23.17
CD1:ILE:B:11:10.655:46.443:30.653:34.61
H:ILE:B:11:8.15:48.789:28.574:30.3
HA:ILE:B:11:8.645:46.647:27.108:26.14
HB:ILE:B:11:8.12:46.846:29.867:35.31
HG12:ILE:B:11:10.571:46.133:28.643:36.41
HG13:ILE:B:11:10.243:47.63:29.052:36.41
HG21:ILE:B:11:8.671:44.574:30.097:27.8
HG22:ILE:B:11:7.373:44.731:29.195:27.8
HG23:ILE:B:11:8.781:44.443:28.517:27.8
HD11:ILE:B:11:11.603:46.651:30.649:41.53
HD12:ILE:B:11:10.194:47.009:31.291:41.53
HD13:ILE:B:11:10.522:45.509:30.881:41.53
N:THR:B:12:5.642:47.089:28.133:23.69
CA:THR:B:12:4.264:46.785:27.759:27.8
C:THR:B:12:4.051:46.987:26.269:32.55
O:THR:B:12:3.511:46.106:25.58:24.04
CB:THR:B:12:3.292:47.642:28.58:33.52
OG1:THR:B:12:3.502:47.358:29.965:32.74
CG2:THR:B:12:1.803:47.355:28.223:26.3
H:THR:B:12:5.726:47.666:28.765:28.42
HA:THR:B:12:4.082:45.854:27.961:33.36
HB:THR:B:12:3.471:48.581:28.413:40.23
HG1:THR:B:12:2.979:47.818:30.435:39.29
HG21:THR:B:12:1.22:47.914:28.761:31.56
HG22:THR:B:12:1.644:47.545:27.285:31.56
HG23:THR:B:12:1.594:46.424:28.396:31.56
N:ASN:B:13:4.453:48.15:25.751:24.48
CA:ASN:B:13:4.301:48.421:24.321:25.34
C:ASN:B:13:4.974:47.353:23.491:24.13
O:ASN:B:13:4.462:46.938:22.439:24.08
CB:ASN:B:13:4.909:49.776:23.943:28.08
CG:ASN:B:13:4.169:50.958:24.563:43.36
OD1:ASN:B:13:3.038:50.826:25.036:39.56
ND2:ASN:B:13:4.82:52.121:24.575:47.85
H:ASN:B:13:4.812:48.79:26.2:29.38
HA:ASN:B:13:3.358:48.435:24.096:30.41
HB2:ASN:B:13:5.829:49.805:24.249:33.69
HB3:ASN:B:13:4.877:49.876:22.978:33.69
HD21:ASN:B:13:4.449:52.819:24.913:57.42
HD22:ASN:B:13:5.612:52.174:24.244:57.42
N:SER:B:14:6.155:46.925:23.918:22.66
CA:SER:B:14:6.85:45.888:23.173:21.94
C:SER:B:14:6.098:44.563:23.22:21.87
O:SER:B:14:5.951:43.898:22.193:22.01
CB:SER:B:14:8.269:45.758:23.696:25.08
OG:SER:B:14:9.033:46.775:23.091:24.01
H:SER:B:14:6.565:47.209:24.618:27.19
HA:SER:B:14:6.904:46.16:22.243:26.33

【表２－６】

HB2:SER:B:14:8.274:45.874:24.659:30.1
HB3:SER:B:14:8.63:44.891:23.453:30.1
HG:SER:B:14:9.828:46.735:23.358:28.81
N:TYR:B:15:5.629:44.144:24.4:21.89
CA:TYR:B:15:4.768:42.964:24.454:22.13
C:TYR:B:15:3.609:43.089:23.478:22.94
O:TYR:B:15:3.283:42.128:22.771:23.01
CB:TYR:B:15:4.193:42.718:25.852:22.53
CG:TYR:B:15:5.115:42.148:26.893:22.01
CD1:TYR:B:15:5.679:40.889:26.759:37.65
CD2:TYR:B:15:5.351:42.85:28.079:48.14
CE1:TYR:B:15:6.507:40.375:27.747:62.89
CE2:TYR:B:15:6.165:42.337:29.078:52.81
CZ:TYR:B:15:6.748:41.113:28.908:60.82
OH:TYR:B:15:7.558:40.637:29.929:54.81
H:TYR:B:15:5.789:44.514:25.16:26.27
HA:TYR:B:15:5.287:42.185:24.203:26.56
HB2:TYR:B:15:3.868:43.565:26.195:27.03
HB3:TYR:B:15:3.448:42.104:25.765:27.03
HD1:TYR:B:15:5.53:40.399:25.982:45.19
HD2:TYR:B:15:4.966:43.688:28.195:57.77
HE1:TYR:B:15:6.897:39.537:27.638:75.46
HE2:TYR:B:15:6.328:42.83:29.85:63.37
HH:TYR:B:15:7.597:41.201:30.551:65.77
N:MET:B:16:2.967:44.255:23.427:23.8
CA:MET:B:16:1.803:44.423:22.544:28.09
C:MET:B:16:2.197:44.329:21.083:26.65
O:MET:B:16:1.471:43.748:20.275:36.43
CB:MET:B:16:1.118:45.775:22.768:30.99
CG:MET:B:16:0.499:45.977:24.148:42.33
SD:MET:B:16:-0.954:44.949:24.404:68.25
CE:MET:B:16:-0.206:43.67:25.426:42.42
H:MET:B:16:3.177:44.953:23.883:28.56
HA:MET:B:16:1.157:43.726:22.74:33.71
HB2:MET:B:16:1.775:46.477:22.639:37.19
HB3:MET:B:16:0.409:45.872:22.114:37.19
HG2:MET:B:16:1.153:45.748:24.826:50.79
HG3:MET:B:16:0.232:46.905:24.243:50.79
HE1:MET:B:16:-0.883:43.016:25.657:50.9
HE2:MET:B:16:0.508:43.245:24.926:50.9
HE3:MET:B:16:0.15:44.078:26.231:50.9
N:ASP:B:17:3.344:44.897:20.719:29.89
CA:ASP:B:17:3.758:44.849:19.322:34.2
C:ASP:B:17:4.362:43.503:18.931:30.46
O:ASP:B:17:4.224:43.095:17.781:28.87
CB:ASP:B:17:4.769:45.957:19.002:41.66
CG:ASP:B:17:4.239:47.347:19.307:78.78
OD1:ASP:B:17:3:47.511:19.374:89.35
OD2:ASP:B:17:5.064:48.277:19.478:72.64
H:ASP:B:17:3.887:45.306:21.246:35.87
HA:ASP:B:17:2.978:44.994:18.764:41.04
HB2:ASP:B:17:5.569:45.818:19.534:49.99
HB3:ASP:B:17:4.989:45.92:18.058:49.99
N:LEU:B:18:5.062:42.822:19.831:22.66
CA:LEU:B:18:5.868:41.669:19.444:22.1
C:LEU:B:18:5.314:40.329:19.885:22.41
O:LEU:B:18:5.69:39.304:19.308:24.4
CB:LEU:B:18:7.286:41.806:20.002:22.61
CG:LEU:B:18:7.948:43.093:19.512:21.46
CD1:LEU:B:18:9.302:43.234:20.155:24.5
CD2:LEU:B:18:8.07:43.128:17.966:28.1
H:LEU:B:18:5.088:43.006:20.671:27.19
HA:LEU:B:18:5.935:41.652:18.476:26.53
HB2:LEU:B:18:7.249:41.832:20.971:27.14
HB3:LEU:B:18:7.823:41.055:19.704:27.14
HG:LEU:B:18:7.407:43.85:19.787:25.75
HD11:LEU:B:18:9.717:44.053:19.841:29.4
HD12:LEU:B:18:9.192:43.267:21.118:29.4
HD13:LEU:B:18:9.848:42.471:19.91:29.4
HD21:LEU:B:18:8.494:43.959:17.702:33.72
HD22:LEU:B:18:8.607:42.375:17.675:33.72
HD23:LEU:B:18:7.183:43.071:17.578:33.72
N:CYS:B:19:4.481:40.285:20.912:26.31
CA:CYS:B:19:4.018:39.001:21.403:23.2
C:CYS:B:19:2.573:38.743:21.045:29.55
O:CYS:B:19:2.204:37.602:20.812:27.61
CB:CYS:B:19:4.199:38.915:22.923:25.28
SG:CYS:B:19:5.942:39.114:23.454:33.59
H:CYS:B:19:4.174:40.968:21.334:31.58
HA:CYS:B:19:4.553:38.3:21:27.84
HB2:CYS:B:19:3.677:39.617:23.342:30.34
HB3:CYS:B:19:3.891:38.047:23.227:30.34
O:TYR:B:20:0.453:40.693:18.643:58.94
N:TYR:B:20:1.763:39.78:20.969:30.88
CA:TYR:B:20:0.33:39.624:20.788:36.15
C:TYR:B:20:-0.046:39.793:19.324:48.21
CB:TYR:B:20:-0.44:40.615:21.651:29.56
CG:TYR:B:20:-0.651:40.122:23.065:55.92
CD1:TYR:B:20:-1.597:39.145:23.34:71.32
CD2:TYR:B:20:0.094:40.621:24.118:59.77
CE1:TYR:B:20:-1.8:38.679:24.621:72.77
CE2:TYR:B:20:-0.098:40.161:25.411:73.5
CZ:TYR:B:20:-1.058:39.185:25.659:74.33
OH:TYR:B:20:-1.29:38.681:26.931:61.61
H:TYR:B:20:2.02:40.599:21.019:37.06
HA:TYR:B:20:0.074:38.728:21.06:43.38
HB2:TYR:B:20:0.055:41.447:21.695:35.48
HB3:TYR:B:20:-1.312:40.768:21.254:35.48
HD1:TYR:B:20:-2.106:38.797:22.644:85.58
HD2:TYR:B:20:0.735:41.274:23.956:71.73
HE1:TYR:B:20:-2.44:38.024:24.782:87.33
HE2:TYR:B:20:0.409:40.506:26.11:88.2
HH:TYR:B:20:-0.786:39.058:27.486:73.93
O:ARG:B:21:-2.375:41.115:18.001:73.56
N:ARG:B:21:-0.904:38.888:18.851:48.09
CA:ARG:B:21:-1.505:38.926:17.518:54.86
C:ARG:B:21:-2.02:40.306:17.132:67.04
CB:ARG:B:21:-2.675:37.949:17.448:56.88
CG:ARG:B:21:-2.44:36.661:16.704:66.58
CD:ARG:B:21:-3.714:36.364:15.961:87.2
NE:ARG:B:21:-3.936:34.955:15.663:104.85
CZ:ARG:B:21:-5.147:34.397:15.619:123.5

【表２－７】

NH1:ARG:B:21:-6.239:35.129:15.88:136.71
NH2:ARG:B:21:-5.27:33.101:15.333:115.82
OXT:ARG:B:21:-2.121:40.62:15.939:68.47
H:ARG:B:21:-1.164:38.209:19.309:57.7
HA:ARG:B:21:-0.844:38.656:16.862:65.83
HB2:ARG:B:21:-2.926:37.714:18.355:68.25
HB3:ARG:B:21:-3.418:38.398:17.016:68.25
HG2:ARG:B:21:-1.716:36.768:16.067:79.9
HG3:ARG:B:21:-2.258:35.94:17.327:79.9
HD2:ARG:B:21:-4.462:36.672:16.495:104.64
HD3:ARG:B:21:-3.698:36.842:15.117:104.64
HE:ARG:B:21:-3.252:34.434:15.65:125.82
HH11:ARG:B:21:-6.162:35.965:16.065:164.05
HH12:ARG:B:21:-7.017:34.764:15.855:164.05
HH21:ARG:B:21:-4.571:32.628:15.17:138.98
HH22:ARG:B:21:-6.049:32.738:15.311:138.98

。

【請求項２１】

ＩＲに結合する化合物を同定する方法であって、

ｉ）下記：

ａ）下表の原子座標もしくはそのサブセットにより定義される構造、または

ｂ）ａ）の対応する主鎖原子上で重ねた場合に約２．０Å未満の平均二乗偏差を有する構造

を有するポリペプチドの三次元構造モデルを作成すること、および

ｉｉ）前記ＩＲに潜在的に結合する化合物を設計するまたはスクリーニングすること

を含む方法：

【表３－１】

付録I: CON-INS G1インスリン(鎖Aおよび鎖B)に関する原子座標

フォーマットは、下記のコロンで区切られたフィールドを含む: (1) 原子の名称, (2) 残基タイプ, (3) 鎖の名称,(4) 残基番号,(5-7) xyz 座標,(8) 温度B因子(thermal B-factor)。

N:GLY:A:1:15.439:38.785:34.309:26.76
CA:GLY:A:1:14.11:39.14:33.733:22.21
C:GLY:A:1:14.251:39.976:32.492:21.3
O:GLY:A:1:15.353:40.312:32.093:22.73
H1:GLY:A:1:15.395:38.813:35.197:32.11
H2:GLY:A:1:15.666:37.965:34.049:32.11
H3:GLY:A:1:16.051:39.366:34.024:32.11
HA2:GLY:A:1:13.625:38.331:33.508:26.65
HA3:GLY:A:1:13.595:39.639:34.386:26.65
N:VAL:A:2:13.113:40.325:31.895:21.05
CA:VAL:A:2:13.122:41.169:30.72:22.11
C:VAL:A:2:13.696:42.561:31.01:20.41
O:VAL:A:2:14.274:43.187:30.116:20.06
CB:VAL:A:2:11.698:41.225:30.132:25.46
CG1:VAL:A:2:10.72:41.927:31.074:21.3
CG2:VAL:A:2:11.725:41.902:28.839:27.88
H:VAL:A:2:12.33:40.084:32.154:25.26
HA:VAL:A:2:13.693:40.756:30.053:26.54
HB:VAL:A:2:11.38:40.32:29.989:30.55
HG11:VAL:A:2:9.841:41.939:30.665:25.56
HG12:VAL:A:2:10.688:41.442:31.914:25.56
HG13:VAL:A:2:11.026:42.835:31.227:25.56
HG21:VAL:A:2:10.824:41.931:28.48:33.45
HG22:VAL:A:2:12.061:42.804:28.963:33.45
HG23:VAL:A:2:12.306:41.412:28.238:33.45
N:VAL:A:3:13.604:43.056:32.249:26.31
CA:VAL:A:3:14.092:44.414:32.525:22.38
C:VAL:A:3:15.618:44.365:32.529:26.64
O:VAL:A:3:16.283:45.246:31.982:21.94
CB:VAL:A:3:13.517:44.989:33.842:28.85
CG1:VAL:A:3:14.192:46.325:34.21:23.35
CG2:VAL:A:3:11.967:45.154:33.731:22.25
H:VAL:A:3:13.276:42.642:32.928:31.58
HA:VAL:A:3:13.816:44.998:31.802:26.85
HB:VAL:A:3:13.695:44.361:34.559:34.62
HG11:VAL:A:3:13.808:46.654:35.037:28.02
HG12:VAL:A:3:15.144:46.176:34.323:28.02
HG13:VAL:A:3:14.039:46.963:33.496:28.02
HG21:VAL:A:3:11.628:45.515:34.565:26.7
HG22:VAL:A:3:11.767:45.762:33.001:26.7
HG23:VAL:A:3:11.569:44.287:33.558:26.7
N:CGU:A:4:16.193:43.318:33.099:21.34
CA:CGU:A:4:17.68:43.233:33.107:21.52
CB:CGU:A:4:18.136:42.041:33.939:22.15
CG:CGU:A:4:17.867:42.164:35.47:27.83
CD1:CGU:A:4:16.419:42.187:35.88:25.08
OE12:CGU:A:4:16.135:42.812:36.937:28.6
OE11:CGU:A:4:15.531:41.542:35.211:22.71
CD2:CGU:A:4:18.45:40.98:36.25:48.38
OE21:CGU:A:4:18.448:39.819:35.754:54.62
OE22:CGU:A:4:18.871:41.181:37.42:85.42
C:CGU:A:4:18.255:43.089:31.618:20.98
O:CGU:A:4:19.303:43.691:31.269:21.08
HG:CGU:A:4:18.338:43.105:35.863:33.4
HB3:CGU:A:4:17.661:41.115:33.568:26.58
HB2:CGU:A:4:19.22:41.867:33.754:26.58
HA:CGU:A:4:18.079:44.185:33.551:25.82
N:HIS:A:5:17.548:42.333:30.786:21.02
CA:HIS:A:5:18.007:41.966:29.443:20.65
C:HIS:A:5:17.659:43.013:28.373:19.86
O:HIS:A:5:18.285:43.07:27.334:23.44
CB:HIS:A:5:17.391:40.584:29.071:20.16
CG:HIS:A:5:18.115:39.864:27.981:47.58
ND1:HIS:A:5:19.277:39.15:28.201:43.05
CD2:HIS:A:5:17.832:39.734:26.661:45.41
CE1:HIS:A:5:19.678:38.617:27.058:50.46
NE2:HIS:A:5:18.82:38.957:26.111:52.67
HA:HIS:A:5:18.972:41.867:29.458:24.79
HB2:HIS:A:5:17.402:40.017:29.858:24.19
HB3:HIS:A:5:16.476:40.72:28.778:24.19
HD2:HIS:A:5:17.106:40.104:26.213:54.49
HE1:HIS:A:5:20.437:38.093:26.94:60.55
HE2:HIS:A:5:18.873:38.729:25.284:63.2
H:HIS:A:5:16.775:42.01:30.98:25.23
N:CYS:A:6:16.641:43.84:28.616:19.88
CA:CYS:A:6:16.113:44.731:27.591:19.76
C:CYS:A:6:16.063:46.184:28.028:21.58
O:CYS:A:6:15.909:47.06:27.165:20.58
CB:CYS:A:6:14.695:44.308:27.194:21.07
SG:CYS:A:6:14.678:42.722:26.317:26
H:CYS:A:6:16.238:43.902:29.373:23.85
HA:CYS:A:6:16.676:44.674:26.803:23.71
HB2:CYS:A:6:14.154:44.217:27.994:25.29
HB3:CYS:A:6:14.315:44.981:26.608:25.29
N:CYS:A:7:16.128:46.463:29.323:21.05
CA:CYS:A:7:16.186:47.837:29.839:21.74
C:CYS:A:7:17.553:48.188:30.41:23.78
O:CYS:A:7:18.103:49.215:30.042:30.88
CB:CYS:A:7:15.098:48.081:30.895:21.43
SG:CYS:A:7:15.221:49.718:31.732:27.59
H:CYS:A:7:16.14:45.864:29.941:25.26
HA:CYS:A:7:16.016:48.446:29.103:26.09
HB2:CYS:A:7:14.229:48.033:30.465:25.71
HB3:CYS:A:7:15.165:47.394:31.576:25.71
N:HIS:A:8:18.157:47.348:31.264:28.49
CA:HIS:A:8:19.509:47.657:31.747:25.02
C:HIS:A:8:20.564:47.453:30.657:30.05
O:HIS:A:8:21.558:48.179:30.604:34.16

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CB:HIS:A:8:19.847:46.811:32.972:27.96
CG:HIS:A:8:18.916:47.03:34.125:33.4
ND1:HIS:A:8:18.619:46.043:35.044:34.99
CD2:HIS:A:8:18.234:48.129:34.521:27.24
CE1:HIS:A:8:17.767:46.516:35.936:33.7
NE2:HIS:A:8:17.527:47.782:35.648:38.53
H:HIS:A:8:17.818:46.619:31.57:34.19
HA:HIS:A:8:19.538:48.589:32.014:30.03
HB2:HIS:A:8:19.802:45.874:32.728:33.55
HB3:HIS:A:8:20.744:47.033:33.268:33.55
HD2:HIS:A:8:18.233:48.959:34.103:32.68
HE1:HIS:A:8:17.417:46.045:36.658:40.44
HE2:HIS:A:8:17.009:48.305:36.092:46.23
N:ARG:A:9:20.377:46.477:29.813:32.17
CA:ARG:A:9:21.026:46.221:28.542:24.61
C:ARG:A:9:19.985:46.413:27.464:24.55
O:ARG:A:9:18.838:46.063:27.712:22.58
CB:ARG:A:9:21.524:44.776:28.434:42.6
CG:ARG:A:9:22.966:44.545:28.786:89.14
CD:ARG:A:9:23.608:43.537:27.831:118.62
NE:ARG:A:9:25.059:43.702:27.796:137.92
CZ:ARG:A:9:25.928:42.745:27.485:154.54
NH1:ARG:A:9:25.517:41.519:27.184:170.53
NH2:ARG:A:9:27.224:43.02:27.49:152.73
H:ARG:A:9:19.797:45.864:29.977:38.61
HA:ARG:A:9:21.763:46.836:28.4:29.53
HB2:ARG:A:9:20.99:44.224:29.027:51.12
HB3:ARG:A:9:21.399:44.478:27.519:51.12
HG2:ARG:A:9:23.451:45.382:28.719:106.97
HG3:ARG:A:9:23.024:44.192:29.688:106.97
HD2:ARG:A:9:23.41:42.637:28.132:142.34
HD3:ARG:A:9:23.263:43.677:26.935:142.34
HE:ARG:A:9:25.375:44.477:27.991:165.51
HH11:ARG:A:9:24.676:41.336:27.181:204.63
HH12:ARG:A:9:26.09:40.909:26.987:204.63
HH21:ARG:A:9:27.495:43.812:27.686:183.27
HH22:ARG:A:9:27.794:42.407:27.293:183.27
N:PRO:A:10:20.315:46.922:26.273:21.04
CA:PRO:A:10:19.325:46.947:25.186:22.55
C:PRO:A:10:19.153:45.573:24.54:20.8
O:PRO:A:10:20.049:44.721:24.565:22.83
CB:PRO:A:10:19.914:47.951:24.205:21.44
CG:PRO:A:10:21.394:47.783:24.393:23.92
CD:PRO:A:10:21.581:47.551:25.858:26.07
HA:PRO:A:10:18.468:47.268:25.508:27.06
HB2:PRO:A:10:19.65:47.726:23.299:25.72
HB3:PRO:A:10:19.633:48.849:24.439:25.72
HG2:PRO:A:10:21.703:47.018:23.883:28.7
HG3:PRO:A:10:21.853:48.59:24.112:28.7
HD2:PRO:A:10:22.324:46.948:26.013:31.28
HD3:PRO:A:10:21.706:48.395:26.32:31.28
N:CYS:A:11:17.965:45.34:23.974:20.27
CA:CYS:A:11:17.735:44.077:23.278:20.11
C:CYS:A:11:17.021:44.299:21.95:20.29
O:CYS:A:11:16.249:45.24:21.766:20.43
CB:CYS:A:11:16.959:43.053:24.166:20.58
SG:CYS:A:11:15.186:43.358:24.401:23.25
H:CYS:A:11:17.296:45.881:23.98:24.33
HA:CYS:A:11:18.598:43.683:23.076:24.13
HB2:CYS:A:11:17.048:42.175:23.763:24.7
HB3:CYS:A:11:17.368:43.045:25.045:24.7
N:SER:A:12:17.349:43.443:21.002:19.95
CA:SER:A:12:16.64:43.374:19.734:20.24
C:SER:A:12:15.198:42.876:19.921:19.9
O:SER:A:12:14.82:42.314:20.95:19.48
CB:SER:A:12:17.365:42.442:18.794:20.66
OG:SER:A:12:17.226:41.115:19.254:20.36
H:SER:A:12:17.993:42.877:21.068:23.94
HA:SER:A:12:16.611:44.256:19.332:24.29
HB2:SER:A:12:16.978:42.517:17.908:24.79
HB3:SER:A:12:18.306:42.677:18.772:24.79
HG:SER:A:12:17.626:40.589:18.736:24.43
N:ASN:A:13:14.386:43.089:18.896:20.29
CA:ASN:A:13:13.05:42.486:18.857:20.21
C:ASN:A:13:13.113:40.969:18.999:19.99
O:ASN:A:13:12.303:40.375:19.72:19.76
CB:ASN:A:13:12.338:42.827:17.571:20.89
CG:ASN:A:13:11.993:44.254:17.455:21.34
OD1:ASN:A:13:12.063:45.022:18.425:21.1
ND2:ASN:A:13:11.561:44.637:16.254:22.2
H:ASN:A:13:14.577:43.575:18.213:24.35
HA:ASN:A:13:12.523:42.835:19.593:24.25
HB2:ASN:A:13:12.913:42.598:16.823:25.07
HB3:ASN:A:13:11.515:42.316:17.522:25.07
HD21:ASN:A:13:11.343:45.457:16.116:26.64
HD22:ASN:A:13:11.502:44.063:15.616:26.64
N:ALA:A:14:14.073:40.323:18.327:20.53
CA:ALA:A:14:14.136:38.865:18.34:20.59
C:ALA:A:14:14.514:38.344:19.713:20.2
O:ALA:A:14:13.966:37.34:20.17:20.42
CB:ALA:A:14:15.122:38.388:17.293:21.21
H:ALA:A:14:14.689:40.704:17.863:24.64
HA:ALA:A:14:13.262:38.509:18.115:24.71
HB1:ALA:A:14:15.156:37.419:17.311:25.45
HB2:ALA:A:14:14.827:38.694:16.421:25.45
HB3:ALA:A:14:15.997:38.755:17.494:25.45
N:GLU:A:15:15.393:39.048:20.418:19.99
CA:GLU:A:15:15.674:38.714:21.807:20.64
C:GLU:A:15:14.459:38.979:22.702:20.25
O:GLU:A:15:14.126:38.165:23.56:19.51
CB:GLU:A:15:16.886:39.507:22.306:24.27
CG:GLU:A:15:18.221:38.954:21.864:52.08
CD:GLU:A:15:18.481:37.555:22.399:68.3
OE1:GLU:A:15:18.414:37.354:23.638:37.34
OE2:GLU:A:15:18.75:36.655:21.573:92.14
H:GLU:A:15:15.838:39.719:20.116:23.99
HA:GLU:A:15:15.889:37.77:21.867:24.77
HB2:GLU:A:15:16.82:40.416:21.974:29.12
HB3:GLU:A:15:16.876:39.513:23.276:29.12
HG2:GLU:A:15:18.242:38.914:20.895:62.5
HG3:GLU:A:15:18.927:39.535:22.188:62.5
N:PHE:A:16:13.813:40.136:22.56:19.08

【表３－３】

CA:PHE:A:16:12.627:40.394:23.379:19.01
C:PHE:A:16:11.58:39.275:23.258:19.21
O:PHE:A:16:10.937:38.891:24.259:19.32
CB:PHE:A:16:12:41.738:23.008:19.12
CG:PHE:A:16:10.869:42.118:23.896:19.26
CD2:PHE:A:16:11.086:42.876:25.025:19.26
CD1:PHE:A:16:9.575:41.712:23.603:19.56
CE2:PHE:A:16:10.018:43.216:25.879:19.59
CE1:PHE:A:16:8.496:42.075:24.429:19.92
CZ:PHE:A:16:8.717:42.809:25.564:19.95
H:PHE:A:16:14.029:40.767:22.018:22.9
HA:PHE:A:16:12.898:40.443:24.309:22.81
HB2:PHE:A:16:12.677:42.43:23.073:22.95
HB3:PHE:A:16:11.663:41.689:22.1:22.95
HD2:PHE:A:16:11.95:43.143:25.241:23.11
HD1:PHE:A:16:9.416:41.209:22.837:23.48
HE2:PHE:A:16:10.173:43.731:26.637:23.51
HE1:PHE:A:16:7.635:41.79:24.221:23.9
HZ:PHE:A:16:8.006:43.046:26.114:23.93
N:LYS:A:17:11.394:38.736:22.051:19.63
CA:LYS:A:17:10.38:37.7:21.84:19.97
C:LYS:A:17:10.614:36.46:22.684:20.12
O:LYS:A:17:9.672:35.685:22.893:20.5
CB:LYS:A:17:10.329:37.289:20.362:20.31
CG:LYS:A:17:9.504:38.28:19.498:20.56
CD:LYS:A:17:9.689:38.041:18.044:21.03
CE:LYS:A:17:9.094:39.21:17.228:23.58
NZ:LYS:A:17:9.222:39.104:15.74:26.95
H:LYS:A:17:11.837:38.95:21.346:23.56
HA:LYS:A:17:9.512:38.061:22.078:23.96
HB2:LYS:A:17:11.232:37.262:20.009:24.37
HB3:LYS:A:17:9.917:36.413:20.291:24.37
HG2:LYS:A:17:8.562:38.173:19.703:24.67
HG3:LYS:A:17:9.788:39.186:19.694:24.67
HD2:LYS:A:17:10.636:37.977:17.845:25.23
HD3:LYS:A:17:9.232:37.224:17.789:25.23
HE2:LYS:A:17:8.148:39.275:17.433:28.3
HE3:LYS:A:17:9.539:40.028:17.499:28.3
HZ1:LYS:A:17:8.855:39.816:15.352:32.34
HZ2:LYS:A:17:10.081:39.061:15.511:32.34
HZ3:LYS:A:17:8.808:38.371:15.451:32.34
N:LYS:A:18:11.856:36.224:23.113:20.04
CA:LYS:A:18:12.144:35.116:24.033:21.82
C:LYS:A:18:11.301:35.19:25.294:20.55
O:LYS:A:18:11.071:34.163:25.936:21.12
CB:LYS:A:18:13.624:35.111:24.441:20.42
CG:LYS:A:18:14.518:34.782:23.279:20.61
CD:LYS:A:18:16.015:34.803:23.664:30.84
CE:LYS:A:18:16.866:34.3:22.484:38.22
NZ:LYS:A:18:18.269:33.984:22.906:62
H:LYS:A:18:12.546:36.685:22.889:24.05
HA:LYS:A:18:11.951:34.276:23.589:26.19
HB2:LYS:A:18:13.867:35.989:24.772:24.51
HB3:LYS:A:18:13.763:34.442:25.13:24.51
HG2:LYS:A:18:14.303:33.894:22.954:24.73
HG3:LYS:A:18:14.379:35.436:22.576:24.73
HD2:LYS:A:18:16.284:35.711:23.875:37
HD3:LYS:A:18:16.163:34.218:24.424:37
HE2:LYS:A:18:16.468:33.491:22.125:45.86
HE3:LYS:A:18:16.902:34.987:21.8:45.86
HZ1:LYS:A:18:18.739:33.696:22.207:74.4
HZ2:LYS:A:18:18.658:34.713:23.236:74.4
HZ3:LYS:A:18:18.263:33.351:23.531:74.4
N:TYR:A:19:10.88:36.384:25.687:25.2
CA:TYR:A:19:10.118:36.604:26.923:20.68
C:TYR:A:19:8.575:36.613:26.737:31.44
O:TYR:A:19:7.832:36.875:27.687:29.68
CB:TYR:A:19:10.538:37.943:27.555:20.37
CG:TYR:A:19:11.901:37.935:28.109:23.44
CD1:TYR:A:19:13:38.247:27.323:19.93
CD2:TYR:A:19:12.117:37.579:29.428:23.18
CE1:TYR:A:19:14.278:38.224:27.859:26.81
CE2:TYR:A:19:13.379:37.562:29.96:25.73
CZ:TYR:A:19:14.444:37.864:29.184:22.56
OH:TYR:A:19:15.682:37.826:29.75:22.36
H:TYR:A:19:11.025:37.107:25.245:30.24
HA:TYR:A:19:10.335:35.898:27.552:24.82
HB2:TYR:A:19:10.498:38.635:26.876:24.45
HB3:TYR:A:19:9.926:38.154:28.276:24.45
HD2:TYR:A:19:11.39:37.364:29.968:27.82
HD1:TYR:A:19:12.877:38.483:26.431:23.92
HE2:TYR:A:19:13.505:37.32:30.849:30.88
HE1:TYR:A:19:15.015:38.436:27.332:32.17
HH:TYR:A:19:16.265:38.03:29.18:26.83
O:CY3:A:20:6.334:34.016:25.918:46.46
C:CY3:A:20:5.968:35.121:26.067:39.6
N1:CY3:A:20:4.848:35.386:26.929:43.25
CA:CY3:A:20:6.666:36.307:25.294:21.87
N:CY3:A:20:8.084:36.362:25.53:22.5
CB:CY3:A:20:6.382:35.984:23.834:33.52
SG:CY3:A:20:6.832:37.458:22.767:39.89
H:CY3:A:20:8.534:36.217:24.812:27
HA:CY3:A:20:6.252:37.151:25.536:26.25
HB2:CY3:A:20:5.439:35.782:23.725:40.22
HB3:CY3:A:20:6.908:35.214:23.567:40.22
HN11:CY3:A:20:4.569:36.191:27.039:51.9
HN12:CY3:A:20:4.467:34.738:27.347:51.9
O:THR:B:-1:16.056:46.908:9.868:60.34
N:THR:B:-1:16.406:48.652:7.605:78.37
CA:THR:B:-1:17.132:48.822:8.897:76.87
C:THR:B:-1:17.109:47.519:9.689:64.38
CB:THR:B:-1:16.526:49.975:9.74:82.36
OG1:THR:B:-1:17.021:51.231:9.25:103.8
CG2:THR:B:-1:16.88:49.85:11.228:68.98
H1:THR:B:-1:16.283:49.449:7.227:94.05
H2:THR:B:-1:16.886:48.137:7.061:94.05
H3:THR:B:-1:15.617:48.27:7.756:94.05
HA:THR:B:-1:18.058:49.042:8.712:92.25
HB:THR:B:-1:15.56:49.958:9.656:98.83
HG1:THR:B:-1:16.698:51.862:9.7:124.55
HG21:THR:B:-1:16.486:50.584:11.725:82.78
HG22:THR:B:-1:16.538:49.013:11.58:82.78

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HG23:THR:B:-1:17.843:49.871:11.343:82.78
O:PHE:B:0:17.693:47.018:12.852:32.11
N:PHE:B:0:18.285:47.117:10.17:47.49
CA:PHE:B:0:18.434:45.859:10.88:33.82
C:PHE:B:0:17.777:45.945:12.258:30.41
CB:PHE:B:0:19.916:45.528:11.007:28.4
CG:PHE:B:0:20.185:44.138:11.419:27.64
CD2:PHE:B:0:20.443:43.17:10.471:29.44
CD1:PHE:B:0:20.187:43.786:12.753:26.31
CE2:PHE:B:0:20.706:41.883:10.832:27.99
CE1:PHE:B:0:20.454:42.477:13.135:27.97
CZ:PHE:B:0:20.702:41.517:12.166:27.51
H:PHE:B:0:19.016:47.564:10.094:56.99
HA:PHE:B:0:18.003:45.151:10.377:40.59
HB2:PHE:B:0:20.342:45.669:10.147:34.08
HB3:PHE:B:0:20.311:46.115:11.67:34.08
HD1:PHE:B:0:20.017:44.431:13.402:31.58
HD2:PHE:B:0:20.445:43.402:9.571:35.33
HE1:PHE:B:0:20.45:42.243:14.035:33.57
HE2:PHE:B:0:20.874:41.244:10.177:33.58
HZ:PHE:B:0:20.881:40.638:12.411:33.01
O:ASP:B:1:18.276:43.923:15.696:23.3
N:ASP:B:1:17.325:44.791:12.774:25.54
CA:ASP:B:1:16.642:44.721:14.072:24.29
C:ASP:B:1:17.702:44.882:15.159:25.42
CB:ASP:B:1:15.863:43.408:14.192:30.99
CG:ASP:B:1:15.425:43.112:15.613:33.34
OD1:ASP:B:1:15.172:44.1:16.35:26.15
OD2:ASP:B:1:15.36:41.913:16.004:22.1
H:ASP:B:1:17.404:44.028:12.384:30.65
HA:ASP:B:1:16.014:45.456:14.145:29.15
HB2:ASP:B:1:15.068:43.46:13.639:37.19
HB3:ASP:B:1:16.427:42.677:13.894:37.19
O:THR:B:2:17.54:46.872:18.038:27.96
N:THR:B:2:18.026:46.134:15.452:24.07
CA:THR:B:2:19.15:46.377:16.357:23.86
C:THR:B:2:18.686:46.539:17.782:24.18
CB:THR:B:2:19.911:47.632:15.99:31.47
OG1:THR:B:2:18.958:48.664:15.749:33.31
CG2:THR:B:2:20.815:47.367:14.758:33.17
H:THR:B:2:17.631:46.838:15.155:28.88
HA:THR:B:2:19.762:45.626:16.318:28.64
HB:THR:B:2:20.479:47.889:16.733:37.77
HG1:THR:B:2:19.352:49.376:15.542:39.98
HG21:THR:B:2:21.302:48.173:14.525:39.81
HG22:THR:B:2:21.45:46.662:14.959:39.81
HG23:THR:B:2:20.272:47.097:14.001:39.81
C:HYP:B:3:18.617:47.825:20.609:37.46
O:HYP:B:3:19.172:48.867:20.197:33.28
CA:HYP:B:3:19.208:46.443:20.27:30.06
CB:HYP:B:3:20.366:46.23:20.929:46.37
CG:HYP:B:3:21.21:45.388:19.961:34.65
OD1:HYP:B:3:20.787:44.116:19.901:37.02
CD:HYP:B:3:20.889:46.065:18.606:30.67
N:HYP:B:3:19.59:46.315:18.708:25.2
HD23:HYP:B:3:21.065:45.458:17.869:36.81
HD22:HYP:B:3:21.39:46.89:18.507:36.81
HG:HYP:B:3:22.156:45.447:20.171:41.58
HD1:HYP:B:3:21.078:43.754:19.188:44.43
HB3:HYP:B:3:20.807:47.074:21.115:55.65
HB2:HYP:B:3:20.201:45.739:21.749:55.65
HA:HYP:B:3:18.572:45.748:20.503:36.08
O:LYS:B:4:16.271:47.848:23.837:25.52
N:LYS:B:4:17.521:47.837:21.368:29.31
CA:LYS:B:4:16.899:49.058:21.865:26.28
C:LYS:B:4:16.634:48.93:23.365:21.83
CB:LYS:B:4:15.558:49.322:21.159:37.68
CG:LYS:B:4:15.666:49.595:19.675:65.23
CD:LYS:B:4:14.269:49.657:19.051:94.75
CE:LYS:B:4:14.289:50.089:17.586:109.16
NZ:LYS:B:4:12.904:50.217:17.038:105.24
H:LYS:B:4:17.109:47.124:21.616:35.17
HA:LYS:B:4:17.488:49.813:21.713:31.53
HB2:LYS:B:4:14.99:48.544:21.273:45.21
HB3:LYS:B:4:15.139:50.094:21.569:45.21
HG2:LYS:B:4:16.106:50.447:19.533:78.28
HG3:LYS:B:4:16.163:48.879:19.248:78.28
HD2:LYS:B:4:13.864:48.777:19.098:113.71
HD3:LYS:B:4:13.732:50.296:19.544:113.71
HE2:LYS:B:4:14.727:50.951:17.511:130.99
HE3:LYS:B:4:14.763:49.424:17.062:130.99
HZ1:LYS:B:4:12.937:50.469:16.185:126.28
HZ2:LYS:B:4:12.482:49.435:17.093:126.28
HZ3:LYS:B:4:12.449:50.825:17.502:126.28
O:HIS:B:5:14.227:50.871:24.963:32.55
N:HIS:B:5:16.734:50.025:24.109:21.79
CA:HIS:B:5:16.363:50.01:25.519:21.56
C:HIS:B:5:14.857:50.045:25.607:22.3
CB:HIS:B:5:16.937:51.202:26.275:22.18
CG:HIS:B:5:18.423:51.204:26.337:22.64
ND1:HIS:B:5:19.131:50.545:27.328:28.27
CD2:HIS:B:5:19.345:51.765:25.516:25.48
CE1:HIS:B:5:20.428:50.699:27.11:22.51
NE2:HIS:B:5:20.585:51.441:26.022:28.72
H:HIS:B:5:17.013:50.786:23.824:26.15
HA:HIS:B:5:16.682:49.193:25.934:25.87
HB2:HIS:B:5:16.657:52.018:25.832:26.62
HB3:HIS:B:5:16.601:51.188:27.185:26.62
HD1:HIS:B:5:18.784:50.097:27.975:33.93
HD2:HIS:B:5:19.173:52.273:24.756:30.58
HE1:HIS:B:5:21.112:50.36:27.64:27.01
N:ARG:B:6:14.278:49.126:26.37:20.97
CA:ARG:B:6:12.838:49.07:26.561:24.52
C:ARG:B:6:12.608:49.07:28.058:21.26
O:ARG:B:6:12.884:48.066:28.727:23.78
CB:ARG:B:6:12.238:47.832:25.893:20.69
CG:ARG:B:6:12.796:47.582:24.53:26.83
CD:ARG:B:6:12.576:46.115:24.096:33.07
NE:ARG:B:6:13.308:45.832:22.86:31.36
CZ:ARG:B:6:12.807:45.919:21.638:20.49
NH1:ARG:B:6:11.527:46.276:21.431:28.98
NH2:ARG:B:6:13.594:45.629:20.612:25.07

【表３－５】

H:ARG:B:6:14.707:48.515:26.795:25.17
HA:ARG:B:6:12.425:49.861:26.181:29.42
HB2:ARG:B:6:12.426:47.054:26.441:24.83
HB3:ARG:B:6:11.279:47.953:25.806:24.83
HG2:ARG:B:6:12.352:48.159:23.89:32.19
HG3:ARG:B:6:13.75:47.758:24.537:32.19
HD2:ARG:B:6:12.903:45.519:24.789:39.68
HD3:ARG:B:6:11.632:45.963:23.935:39.68
HE:ARG:B:6:14.13:45.591:22.934:37.64
HH11:ARG:B:6:11.019:46.461:22.1:34.78
HH12:ARG:B:6:11.218:46.324:20.63:34.78
HH21:ARG:B:6:14.411:45.398:20.748:30.08
HH22:ARG:B:6:13.289:45.676:19.809:30.08
N:CYS:B:7:12.125:50.193:28.588:22.09
CA:CYS:B:7:12.018:50.387:30.028:24.41
C:CYS:B:7:10.61:50.801:30.421:28.77
O:CYS:B:7:9.878:51.453:29.662:23.73
CB:CYS:B:7:12.995:51.452:30.534:25.61
SG:CYS:B:7:14.735:51.095:30.241:32.01
H:CYS:B:7:11.851:50.864:28.126:26.51
HA:CYS:B:7:12.223:49.551:30.477:29.3
HB2:CYS:B:7:12.791:52.292:30.093:30.73
HB3:CYS:B:7:12.874:51.551:31.492:30.73
N:GLY:B:8:10.246:50.438:31.636:23.3
CA:GLY:B:8:8.941:50.832:32.13:24.26
C:GLY:B:8:7.848:50.372:31.198:27.94
O:GLY:B:8:7.783:49.176:30.882:23.54
H:GLY:B:8:10.721:49.975:32.183:27.96
HA2:GLY:B:8:8.79:50.442:33.005:29.11
HA3:GLY:B:8:8.898:51.798:32.208:29.11
N:SER:B:9:7.045:51.325:30.7:25.43
CA:SER:B:9:5.825:51.05:29.947:28.83
C:SER:B:9:6.127:50.664:28.495:33.52
O:SER:B:9:5.335:49.988:27.841:31.13
CB:SER:B:9:4.914:52.281:29.986:36.62
OG:SER:B:9:5.573:53.396:29.4:36.38
H:SER:B:9:7.199:52.166:30.793:30.51
HA:SER:B:9:5.353:50.312:30.364:34.6
HB2:SER:B:9:4.104:52.092:29.487:43.94
HB3:SER:B:9:4.698:52.488:30.908:43.94
HG:SER:B:9:6.279:53.567:29.822:43.65
N:CGU:B:10:7.28:51.095:27.998:28.76
CA:CGU:B:10:7.81:50.596:26.686:28.05
CB:CGU:B:10:9.239:51.112:26.411:26.61
CG:CGU:B:10:9.333:52.622:26.497:48.2
CD1:CGU:B:10:10.796:53.099:26.309:43.27
OE12:CGU:B:10:10.997:54.252:25.818:32.43
OE11:CGU:B:10:11.775:52.332:26.659:28.59
CD2:CGU:B:10:8.34:53.322:25.507:61.07
OE21:CGU:B:10:8.191:52.877:24.334:60.62
OE22:CGU:B:10:7.665:54.311:25.914:71.45
C:CGU:B:10:7.888:49.082:26.653:29.41
O:CGU:B:10:7.883:48.518:25.527:30.26
HG:CGU:B:10:9.037:52.937:27.534:57.84
HB3:CGU:B:10:9.957:50.658:27.117:31.93
HB2:CGU:B:10:9.575:50.754:25.412:31.93
HA:CGU:B:10:7.113:50.935:25.873:33.66
N:ILE:B:11:8.048:48.421:27.803:25.25
CA:ILE:B:11:8.061:46.962:27.816:21.79
C:ILE:B:11:6.652:46.486:27.505:22.28
O:ILE:B:11:6.473:45.595:26.699:22.22
CB:ILE:B:11:8.584:46.402:29.14:29.42
CG1:ILE:B:11:10.089:46.697:29.267:30.34
CG2:ILE:B:11:8.328:44.893:29.247:23.17
CD1:ILE:B:11:10.655:46.443:30.653:34.61
H:ILE:B:11:8.15:48.789:28.574:30.3
HA:ILE:B:11:8.645:46.647:27.108:26.14
HB:ILE:B:11:8.12:46.846:29.867:35.31
HG12:ILE:B:11:10.571:46.133:28.643:36.41
HG13:ILE:B:11:10.243:47.63:29.052:36.41
HG21:ILE:B:11:8.671:44.574:30.097:27.8
HG22:ILE:B:11:7.373:44.731:29.195:27.8
HG23:ILE:B:11:8.781:44.443:28.517:27.8
HD11:ILE:B:11:11.603:46.651:30.649:41.53
HD12:ILE:B:11:10.194:47.009:31.291:41.53
HD13:ILE:B:11:10.522:45.509:30.881:41.53
N:THR:B:12:5.642:47.089:28.133:23.69
CA:THR:B:12:4.264:46.785:27.759:27.8
C:THR:B:12:4.051:46.987:26.269:32.55
O:THR:B:12:3.511:46.106:25.58:24.04
CB:THR:B:12:3.292:47.642:28.58:33.52
OG1:THR:B:12:3.502:47.358:29.965:32.74
CG2:THR:B:12:1.803:47.355:28.223:26.3
H:THR:B:12:5.726:47.666:28.765:28.42
HA:THR:B:12:4.082:45.854:27.961:33.36
HB:THR:B:12:3.471:48.581:28.413:40.23
HG1:THR:B:12:2.979:47.818:30.435:39.29
HG21:THR:B:12:1.22:47.914:28.761:31.56
HG22:THR:B:12:1.644:47.545:27.285:31.56
HG23:THR:B:12:1.594:46.424:28.396:31.56
N:ASN:B:13:4.453:48.15:25.751:24.48
CA:ASN:B:13:4.301:48.421:24.321:25.34
C:ASN:B:13:4.974:47.353:23.491:24.13
O:ASN:B:13:4.462:46.938:22.439:24.08
CB:ASN:B:13:4.909:49.776:23.943:28.08
CG:ASN:B:13:4.169:50.958:24.563:43.36
OD1:ASN:B:13:3.038:50.826:25.036:39.56
ND2:ASN:B:13:4.82:52.121:24.575:47.85
H:ASN:B:13:4.812:48.79:26.2:29.38
HA:ASN:B:13:3.358:48.435:24.096:30.41
HB2:ASN:B:13:5.829:49.805:24.249:33.69
HB3:ASN:B:13:4.877:49.876:22.978:33.69
HD21:ASN:B:13:4.449:52.819:24.913:57.42
HD22:ASN:B:13:5.612:52.174:24.244:57.42
N:SER:B:14:6.155:46.925:23.918:22.66
CA:SER:B:14:6.85:45.888:23.173:21.94
C:SER:B:14:6.098:44.563:23.22:21.87
O:SER:B:14:5.951:43.898:22.193:22.01
CB:SER:B:14:8.269:45.758:23.696:25.08
OG:SER:B:14:9.033:46.775:23.091:24.01
H:SER:B:14:6.565:47.209:24.618:27.19
HA:SER:B:14:6.904:46.16:22.243:26.33

【表３－６】

HB2:SER:B:14:8.274:45.874:24.659:30.1
HB3:SER:B:14:8.63:44.891:23.453:30.1
HG:SER:B:14:9.828:46.735:23.358:28.81
N:TYR:B:15:5.629:44.144:24.4:21.89
CA:TYR:B:15:4.768:42.964:24.454:22.13
C:TYR:B:15:3.609:43.089:23.478:22.94
O:TYR:B:15:3.283:42.128:22.771:23.01
CB:TYR:B:15:4.193:42.718:25.852:22.53
CG:TYR:B:15:5.115:42.148:26.893:22.01
CD1:TYR:B:15:5.679:40.889:26.759:37.65
CD2:TYR:B:15:5.351:42.85:28.079:48.14
CE1:TYR:B:15:6.507:40.375:27.747:62.89
CE2:TYR:B:15:6.165:42.337:29.078:52.81
CZ:TYR:B:15:6.748:41.113:28.908:60.82
OH:TYR:B:15:7.558:40.637:29.929:54.81
H:TYR:B:15:5.789:44.514:25.16:26.27
HA:TYR:B:15:5.287:42.185:24.203:26.56
HB2:TYR:B:15:3.868:43.565:26.195:27.03
HB3:TYR:B:15:3.448:42.104:25.765:27.03
HD1:TYR:B:15:5.53:40.399:25.982:45.19
HD2:TYR:B:15:4.966:43.688:28.195:57.77
HE1:TYR:B:15:6.897:39.537:27.638:75.46
HE2:TYR:B:15:6.328:42.83:29.85:63.37
HH:TYR:B:15:7.597:41.201:30.551:65.77
N:MET:B:16:2.967:44.255:23.427:23.8
CA:MET:B:16:1.803:44.423:22.544:28.09
C:MET:B:16:2.197:44.329:21.083:26.65
O:MET:B:16:1.471:43.748:20.275:36.43
CB:MET:B:16:1.118:45.775:22.768:30.99
CG:MET:B:16:0.499:45.977:24.148:42.33
SD:MET:B:16:-0.954:44.949:24.404:68.25
CE:MET:B:16:-0.206:43.67:25.426:42.42
H:MET:B:16:3.177:44.953:23.883:28.56
HA:MET:B:16:1.157:43.726:22.74:33.71
HB2:MET:B:16:1.775:46.477:22.639:37.19
HB3:MET:B:16:0.409:45.872:22.114:37.19
HG2:MET:B:16:1.153:45.748:24.826:50.79
HG3:MET:B:16:0.232:46.905:24.243:50.79
HE1:MET:B:16:-0.883:43.016:25.657:50.9
HE2:MET:B:16:0.508:43.245:24.926:50.9
HE3:MET:B:16:0.15:44.078:26.231:50.9
N:ASP:B:17:3.344:44.897:20.719:29.89
CA:ASP:B:17:3.758:44.849:19.322:34.2
C:ASP:B:17:4.362:43.503:18.931:30.46
O:ASP:B:17:4.224:43.095:17.781:28.87
CB:ASP:B:17:4.769:45.957:19.002:41.66
CG:ASP:B:17:4.239:47.347:19.307:78.78
OD1:ASP:B:17:3:47.511:19.374:89.35
OD2:ASP:B:17:5.064:48.277:19.478:72.64
H:ASP:B:17:3.887:45.306:21.246:35.87
HA:ASP:B:17:2.978:44.994:18.764:41.04
HB2:ASP:B:17:5.569:45.818:19.534:49.99
HB3:ASP:B:17:4.989:45.92:18.058:49.99
N:LEU:B:18:5.062:42.822:19.831:22.66
CA:LEU:B:18:5.868:41.669:19.444:22.1
C:LEU:B:18:5.314:40.329:19.885:22.41
O:LEU:B:18:5.69:39.304:19.308:24.4
CB:LEU:B:18:7.286:41.806:20.002:22.61
CG:LEU:B:18:7.948:43.093:19.512:21.46
CD1:LEU:B:18:9.302:43.234:20.155:24.5
CD2:LEU:B:18:8.07:43.128:17.966:28.1
H:LEU:B:18:5.088:43.006:20.671:27.19
HA:LEU:B:18:5.935:41.652:18.476:26.53
HB2:LEU:B:18:7.249:41.832:20.971:27.14
HB3:LEU:B:18:7.823:41.055:19.704:27.14
HG:LEU:B:18:7.407:43.85:19.787:25.75
HD11:LEU:B:18:9.717:44.053:19.841:29.4
HD12:LEU:B:18:9.192:43.267:21.118:29.4
HD13:LEU:B:18:9.848:42.471:19.91:29.4
HD21:LEU:B:18:8.494:43.959:17.702:33.72
HD22:LEU:B:18:8.607:42.375:17.675:33.72
HD23:LEU:B:18:7.183:43.071:17.578:33.72
N:CYS:B:19:4.481:40.285:20.912:26.31
CA:CYS:B:19:4.018:39.001:21.403:23.2
C:CYS:B:19:2.573:38.743:21.045:29.55
O:CYS:B:19:2.204:37.602:20.812:27.61
CB:CYS:B:19:4.199:38.915:22.923:25.28
SG:CYS:B:19:5.942:39.114:23.454:33.59
H:CYS:B:19:4.174:40.968:21.334:31.58
HA:CYS:B:19:4.553:38.3:21:27.84
HB2:CYS:B:19:3.677:39.617:23.342:30.34
HB3:CYS:B:19:3.891:38.047:23.227:30.34
O:TYR:B:20:0.453:40.693:18.643:58.94
N:TYR:B:20:1.763:39.78:20.969:30.88
CA:TYR:B:20:0.33:39.624:20.788:36.15
C:TYR:B:20:-0.046:39.793:19.324:48.21
CB:TYR:B:20:-0.44:40.615:21.651:29.56
CG:TYR:B:20:-0.651:40.122:23.065:55.92
CD1:TYR:B:20:-1.597:39.145:23.34:71.32
CD2:TYR:B:20:0.094:40.621:24.118:59.77
CE1:TYR:B:20:-1.8:38.679:24.621:72.77
CE2:TYR:B:20:-0.098:40.161:25.411:73.5
CZ:TYR:B:20:-1.058:39.185:25.659:74.33
OH:TYR:B:20:-1.29:38.681:26.931:61.61
H:TYR:B:20:2.02:40.599:21.019:37.06
HA:TYR:B:20:0.074:38.728:21.06:43.38
HB2:TYR:B:20:0.055:41.447:21.695:35.48
HB3:TYR:B:20:-1.312:40.768:21.254:35.48
HD1:TYR:B:20:-2.106:38.797:22.644:85.58
HD2:TYR:B:20:0.735:41.274:23.956:71.73
HE1:TYR:B:20:-2.44:38.024:24.782:87.33
HE2:TYR:B:20:0.409:40.506:26.11:88.2
HH:TYR:B:20:-0.786:39.058:27.486:73.93
O:ARG:B:21:-2.375:41.115:18.001:73.56
N:ARG:B:21:-0.904:38.888:18.851:48.09
CA:ARG:B:21:-1.505:38.926:17.518:54.86
C:ARG:B:21:-2.02:40.306:17.132:67.04
CB:ARG:B:21:-2.675:37.949:17.448:56.88
CG:ARG:B:21:-2.44:36.661:16.704:66.58
CD:ARG:B:21:-3.714:36.364:15.961:87.2
NE:ARG:B:21:-3.936:34.955:15.663:104.85
CZ:ARG:B:21:-5.147:34.397:15.619:123.5

【表３－７】

NH1:ARG:B:21:-6.239:35.129:15.88:136.71
NH2:ARG:B:21:-5.27:33.101:15.333:115.82
OXT:ARG:B:21:-2.121:40.62:15.939:68.47
H:ARG:B:21:-1.164:38.209:19.309:57.7
HA:ARG:B:21:-0.844:38.656:16.862:65.83
HB2:ARG:B:21:-2.926:37.714:18.355:68.25
HB3:ARG:B:21:-3.418:38.398:17.016:68.25
HG2:ARG:B:21:-1.716:36.768:16.067:79.9
HG3:ARG:B:21:-2.258:35.94:17.327:79.9
HD2:ARG:B:21:-4.462:36.672:16.495:104.64
HD3:ARG:B:21:-3.698:36.842:15.117:104.64
HE:ARG:B:21:-3.252:34.434:15.65:125.82
HH11:ARG:B:21:-6.162:35.965:16.065:164.05
HH12:ARG:B:21:-7.017:34.764:15.855:164.05
HH21:ARG:B:21:-4.571:32.628:15.17:138.98
HH22:ARG:B:21:-6.049:32.738:15.311:138.98

。

【請求項２２】

インスリン活性を模倣する化合物を同定するコンピュータベースの方法であって、

ｉ）下記：

ａ）下表の原子座標もしくはそのサブセットにより定義される構造、または

ｂ）ａ）の対応する主鎖原子上で重ねた場合に約２．０Å未満の平均二乗偏差を有する構造

を有するポリペプチドの三次元構造モデルを作成すること、および

ｉｉ）インスリン活性を模倣する化合物を設計するまたはスクリーニングすること

を含む方法：

【表４－１】

付録I: CON-INS G1インスリン(鎖Aおよび鎖B)に関する原子座標

フォーマットは、下記のコロンで区切られたフィールドを含む: (1) 原子の名称, (2) 残基タイプ, (3) 鎖の名称,(4) 残基番号,(5-7) xyz 座標,(8) 温度B因子(thermal B-factor)。

N:GLY:A:1:15.439:38.785:34.309:26.76
CA:GLY:A:1:14.11:39.14:33.733:22.21
C:GLY:A:1:14.251:39.976:32.492:21.3
O:GLY:A:1:15.353:40.312:32.093:22.73
H1:GLY:A:1:15.395:38.813:35.197:32.11
H2:GLY:A:1:15.666:37.965:34.049:32.11
H3:GLY:A:1:16.051:39.366:34.024:32.11
HA2:GLY:A:1:13.625:38.331:33.508:26.65
HA3:GLY:A:1:13.595:39.639:34.386:26.65
N:VAL:A:2:13.113:40.325:31.895:21.05
CA:VAL:A:2:13.122:41.169:30.72:22.11
C:VAL:A:2:13.696:42.561:31.01:20.41
O:VAL:A:2:14.274:43.187:30.116:20.06
CB:VAL:A:2:11.698:41.225:30.132:25.46
CG1:VAL:A:2:10.72:41.927:31.074:21.3
CG2:VAL:A:2:11.725:41.902:28.839:27.88
H:VAL:A:2:12.33:40.084:32.154:25.26
HA:VAL:A:2:13.693:40.756:30.053:26.54
HB:VAL:A:2:11.38:40.32:29.989:30.55
HG11:VAL:A:2:9.841:41.939:30.665:25.56
HG12:VAL:A:2:10.688:41.442:31.914:25.56
HG13:VAL:A:2:11.026:42.835:31.227:25.56
HG21:VAL:A:2:10.824:41.931:28.48:33.45
HG22:VAL:A:2:12.061:42.804:28.963:33.45
HG23:VAL:A:2:12.306:41.412:28.238:33.45
N:VAL:A:3:13.604:43.056:32.249:26.31
CA:VAL:A:3:14.092:44.414:32.525:22.38
C:VAL:A:3:15.618:44.365:32.529:26.64
O:VAL:A:3:16.283:45.246:31.982:21.94
CB:VAL:A:3:13.517:44.989:33.842:28.85
CG1:VAL:A:3:14.192:46.325:34.21:23.35
CG2:VAL:A:3:11.967:45.154:33.731:22.25
H:VAL:A:3:13.276:42.642:32.928:31.58
HA:VAL:A:3:13.816:44.998:31.802:26.85
HB:VAL:A:3:13.695:44.361:34.559:34.62
HG11:VAL:A:3:13.808:46.654:35.037:28.02
HG12:VAL:A:3:15.144:46.176:34.323:28.02
HG13:VAL:A:3:14.039:46.963:33.496:28.02
HG21:VAL:A:3:11.628:45.515:34.565:26.7
HG22:VAL:A:3:11.767:45.762:33.001:26.7
HG23:VAL:A:3:11.569:44.287:33.558:26.7
N:CGU:A:4:16.193:43.318:33.099:21.34
CA:CGU:A:4:17.68:43.233:33.107:21.52
CB:CGU:A:4:18.136:42.041:33.939:22.15
CG:CGU:A:4:17.867:42.164:35.47:27.83
CD1:CGU:A:4:16.419:42.187:35.88:25.08
OE12:CGU:A:4:16.135:42.812:36.937:28.6
OE11:CGU:A:4:15.531:41.542:35.211:22.71
CD2:CGU:A:4:18.45:40.98:36.25:48.38
OE21:CGU:A:4:18.448:39.819:35.754:54.62
OE22:CGU:A:4:18.871:41.181:37.42:85.42
C:CGU:A:4:18.255:43.089:31.618:20.98
O:CGU:A:4:19.303:43.691:31.269:21.08
HG:CGU:A:4:18.338:43.105:35.863:33.4
HB3:CGU:A:4:17.661:41.115:33.568:26.58
HB2:CGU:A:4:19.22:41.867:33.754:26.58
HA:CGU:A:4:18.079:44.185:33.551:25.82
N:HIS:A:5:17.548:42.333:30.786:21.02
CA:HIS:A:5:18.007:41.966:29.443:20.65
C:HIS:A:5:17.659:43.013:28.373:19.86
O:HIS:A:5:18.285:43.07:27.334:23.44
CB:HIS:A:5:17.391:40.584:29.071:20.16
CG:HIS:A:5:18.115:39.864:27.981:47.58
ND1:HIS:A:5:19.277:39.15:28.201:43.05
CD2:HIS:A:5:17.832:39.734:26.661:45.41
CE1:HIS:A:5:19.678:38.617:27.058:50.46
NE2:HIS:A:5:18.82:38.957:26.111:52.67
HA:HIS:A:5:18.972:41.867:29.458:24.79
HB2:HIS:A:5:17.402:40.017:29.858:24.19
HB3:HIS:A:5:16.476:40.72:28.778:24.19
HD2:HIS:A:5:17.106:40.104:26.213:54.49
HE1:HIS:A:5:20.437:38.093:26.94:60.55
HE2:HIS:A:5:18.873:38.729:25.284:63.2
H:HIS:A:5:16.775:42.01:30.98:25.23
N:CYS:A:6:16.641:43.84:28.616:19.88
CA:CYS:A:6:16.113:44.731:27.591:19.76
C:CYS:A:6:16.063:46.184:28.028:21.58
O:CYS:A:6:15.909:47.06:27.165:20.58
CB:CYS:A:6:14.695:44.308:27.194:21.07
SG:CYS:A:6:14.678:42.722:26.317:26
H:CYS:A:6:16.238:43.902:29.373:23.85
HA:CYS:A:6:16.676:44.674:26.803:23.71
HB2:CYS:A:6:14.154:44.217:27.994:25.29
HB3:CYS:A:6:14.315:44.981:26.608:25.29
N:CYS:A:7:16.128:46.463:29.323:21.05
CA:CYS:A:7:16.186:47.837:29.839:21.74
C:CYS:A:7:17.553:48.188:30.41:23.78
O:CYS:A:7:18.103:49.215:30.042:30.88
CB:CYS:A:7:15.098:48.081:30.895:21.43
SG:CYS:A:7:15.221:49.718:31.732:27.59
H:CYS:A:7:16.14:45.864:29.941:25.26
HA:CYS:A:7:16.016:48.446:29.103:26.09
HB2:CYS:A:7:14.229:48.033:30.465:25.71
HB3:CYS:A:7:15.165:47.394:31.576:25.71
N:HIS:A:8:18.157:47.348:31.264:28.49
CA:HIS:A:8:19.509:47.657:31.747:25.02
C:HIS:A:8:20.564:47.453:30.657:30.05
O:HIS:A:8:21.558:48.179:30.604:34.16

【表４－２】

CB:HIS:A:8:19.847:46.811:32.972:27.96
CG:HIS:A:8:18.916:47.03:34.125:33.4
ND1:HIS:A:8:18.619:46.043:35.044:34.99
CD2:HIS:A:8:18.234:48.129:34.521:27.24
CE1:HIS:A:8:17.767:46.516:35.936:33.7
NE2:HIS:A:8:17.527:47.782:35.648:38.53
H:HIS:A:8:17.818:46.619:31.57:34.19
HA:HIS:A:8:19.538:48.589:32.014:30.03
HB2:HIS:A:8:19.802:45.874:32.728:33.55
HB3:HIS:A:8:20.744:47.033:33.268:33.55
HD2:HIS:A:8:18.233:48.959:34.103:32.68
HE1:HIS:A:8:17.417:46.045:36.658:40.44
HE2:HIS:A:8:17.009:48.305:36.092:46.23
N:ARG:A:9:20.377:46.477:29.813:32.17
CA:ARG:A:9:21.026:46.221:28.542:24.61
C:ARG:A:9:19.985:46.413:27.464:24.55
O:ARG:A:9:18.838:46.063:27.712:22.58
CB:ARG:A:9:21.524:44.776:28.434:42.6
CG:ARG:A:9:22.966:44.545:28.786:89.14
CD:ARG:A:9:23.608:43.537:27.831:118.62
NE:ARG:A:9:25.059:43.702:27.796:137.92
CZ:ARG:A:9:25.928:42.745:27.485:154.54
NH1:ARG:A:9:25.517:41.519:27.184:170.53
NH2:ARG:A:9:27.224:43.02:27.49:152.73
H:ARG:A:9:19.797:45.864:29.977:38.61
HA:ARG:A:9:21.763:46.836:28.4:29.53
HB2:ARG:A:9:20.99:44.224:29.027:51.12
HB3:ARG:A:9:21.399:44.478:27.519:51.12
HG2:ARG:A:9:23.451:45.382:28.719:106.97
HG3:ARG:A:9:23.024:44.192:29.688:106.97
HD2:ARG:A:9:23.41:42.637:28.132:142.34
HD3:ARG:A:9:23.263:43.677:26.935:142.34
HE:ARG:A:9:25.375:44.477:27.991:165.51
HH11:ARG:A:9:24.676:41.336:27.181:204.63
HH12:ARG:A:9:26.09:40.909:26.987:204.63
HH21:ARG:A:9:27.495:43.812:27.686:183.27
HH22:ARG:A:9:27.794:42.407:27.293:183.27
N:PRO:A:10:20.315:46.922:26.273:21.04
CA:PRO:A:10:19.325:46.947:25.186:22.55
C:PRO:A:10:19.153:45.573:24.54:20.8
O:PRO:A:10:20.049:44.721:24.565:22.83
CB:PRO:A:10:19.914:47.951:24.205:21.44
CG:PRO:A:10:21.394:47.783:24.393:23.92
CD:PRO:A:10:21.581:47.551:25.858:26.07
HA:PRO:A:10:18.468:47.268:25.508:27.06
HB2:PRO:A:10:19.65:47.726:23.299:25.72
HB3:PRO:A:10:19.633:48.849:24.439:25.72
HG2:PRO:A:10:21.703:47.018:23.883:28.7
HG3:PRO:A:10:21.853:48.59:24.112:28.7
HD2:PRO:A:10:22.324:46.948:26.013:31.28
HD3:PRO:A:10:21.706:48.395:26.32:31.28
N:CYS:A:11:17.965:45.34:23.974:20.27
CA:CYS:A:11:17.735:44.077:23.278:20.11
C:CYS:A:11:17.021:44.299:21.95:20.29
O:CYS:A:11:16.249:45.24:21.766:20.43
CB:CYS:A:11:16.959:43.053:24.166:20.58
SG:CYS:A:11:15.186:43.358:24.401:23.25
H:CYS:A:11:17.296:45.881:23.98:24.33
HA:CYS:A:11:18.598:43.683:23.076:24.13
HB2:CYS:A:11:17.048:42.175:23.763:24.7
HB3:CYS:A:11:17.368:43.045:25.045:24.7
N:SER:A:12:17.349:43.443:21.002:19.95
CA:SER:A:12:16.64:43.374:19.734:20.24
C:SER:A:12:15.198:42.876:19.921:19.9
O:SER:A:12:14.82:42.314:20.95:19.48
CB:SER:A:12:17.365:42.442:18.794:20.66
OG:SER:A:12:17.226:41.115:19.254:20.36
H:SER:A:12:17.993:42.877:21.068:23.94
HA:SER:A:12:16.611:44.256:19.332:24.29
HB2:SER:A:12:16.978:42.517:17.908:24.79
HB3:SER:A:12:18.306:42.677:18.772:24.79
HG:SER:A:12:17.626:40.589:18.736:24.43
N:ASN:A:13:14.386:43.089:18.896:20.29
CA:ASN:A:13:13.05:42.486:18.857:20.21
C:ASN:A:13:13.113:40.969:18.999:19.99
O:ASN:A:13:12.303:40.375:19.72:19.76
CB:ASN:A:13:12.338:42.827:17.571:20.89
CG:ASN:A:13:11.993:44.254:17.455:21.34
OD1:ASN:A:13:12.063:45.022:18.425:21.1
ND2:ASN:A:13:11.561:44.637:16.254:22.2
H:ASN:A:13:14.577:43.575:18.213:24.35
HA:ASN:A:13:12.523:42.835:19.593:24.25
HB2:ASN:A:13:12.913:42.598:16.823:25.07
HB3:ASN:A:13:11.515:42.316:17.522:25.07
HD21:ASN:A:13:11.343:45.457:16.116:26.64
HD22:ASN:A:13:11.502:44.063:15.616:26.64
N:ALA:A:14:14.073:40.323:18.327:20.53
CA:ALA:A:14:14.136:38.865:18.34:20.59
C:ALA:A:14:14.514:38.344:19.713:20.2
O:ALA:A:14:13.966:37.34:20.17:20.42
CB:ALA:A:14:15.122:38.388:17.293:21.21
H:ALA:A:14:14.689:40.704:17.863:24.64
HA:ALA:A:14:13.262:38.509:18.115:24.71
HB1:ALA:A:14:15.156:37.419:17.311:25.45
HB2:ALA:A:14:14.827:38.694:16.421:25.45
HB3:ALA:A:14:15.997:38.755:17.494:25.45
N:GLU:A:15:15.393:39.048:20.418:19.99
CA:GLU:A:15:15.674:38.714:21.807:20.64
C:GLU:A:15:14.459:38.979:22.702:20.25
O:GLU:A:15:14.126:38.165:23.56:19.51
CB:GLU:A:15:16.886:39.507:22.306:24.27
CG:GLU:A:15:18.221:38.954:21.864:52.08
CD:GLU:A:15:18.481:37.555:22.399:68.3
OE1:GLU:A:15:18.414:37.354:23.638:37.34
OE2:GLU:A:15:18.75:36.655:21.573:92.14
H:GLU:A:15:15.838:39.719:20.116:23.99
HA:GLU:A:15:15.889:37.77:21.867:24.77
HB2:GLU:A:15:16.82:40.416:21.974:29.12
HB3:GLU:A:15:16.876:39.513:23.276:29.12
HG2:GLU:A:15:18.242:38.914:20.895:62.5
HG3:GLU:A:15:18.927:39.535:22.188:62.5
N:PHE:A:16:13.813:40.136:22.56:19.08

【表４－３】

CA:PHE:A:16:12.627:40.394:23.379:19.01
C:PHE:A:16:11.58:39.275:23.258:19.21
O:PHE:A:16:10.937:38.891:24.259:19.32
CB:PHE:A:16:12:41.738:23.008:19.12
CG:PHE:A:16:10.869:42.118:23.896:19.26
CD2:PHE:A:16:11.086:42.876:25.025:19.26
CD1:PHE:A:16:9.575:41.712:23.603:19.56
CE2:PHE:A:16:10.018:43.216:25.879:19.59
CE1:PHE:A:16:8.496:42.075:24.429:19.92
CZ:PHE:A:16:8.717:42.809:25.564:19.95
H:PHE:A:16:14.029:40.767:22.018:22.9
HA:PHE:A:16:12.898:40.443:24.309:22.81
HB2:PHE:A:16:12.677:42.43:23.073:22.95
HB3:PHE:A:16:11.663:41.689:22.1:22.95
HD2:PHE:A:16:11.95:43.143:25.241:23.11
HD1:PHE:A:16:9.416:41.209:22.837:23.48
HE2:PHE:A:16:10.173:43.731:26.637:23.51
HE1:PHE:A:16:7.635:41.79:24.221:23.9
HZ:PHE:A:16:8.006:43.046:26.114:23.93
N:LYS:A:17:11.394:38.736:22.051:19.63
CA:LYS:A:17:10.38:37.7:21.84:19.97
C:LYS:A:17:10.614:36.46:22.684:20.12
O:LYS:A:17:9.672:35.685:22.893:20.5
CB:LYS:A:17:10.329:37.289:20.362:20.31
CG:LYS:A:17:9.504:38.28:19.498:20.56
CD:LYS:A:17:9.689:38.041:18.044:21.03
CE:LYS:A:17:9.094:39.21:17.228:23.58
NZ:LYS:A:17:9.222:39.104:15.74:26.95
H:LYS:A:17:11.837:38.95:21.346:23.56
HA:LYS:A:17:9.512:38.061:22.078:23.96
HB2:LYS:A:17:11.232:37.262:20.009:24.37
HB3:LYS:A:17:9.917:36.413:20.291:24.37
HG2:LYS:A:17:8.562:38.173:19.703:24.67
HG3:LYS:A:17:9.788:39.186:19.694:24.67
HD2:LYS:A:17:10.636:37.977:17.845:25.23
HD3:LYS:A:17:9.232:37.224:17.789:25.23
HE2:LYS:A:17:8.148:39.275:17.433:28.3
HE3:LYS:A:17:9.539:40.028:17.499:28.3
HZ1:LYS:A:17:8.855:39.816:15.352:32.34
HZ2:LYS:A:17:10.081:39.061:15.511:32.34
HZ3:LYS:A:17:8.808:38.371:15.451:32.34
N:LYS:A:18:11.856:36.224:23.113:20.04
CA:LYS:A:18:12.144:35.116:24.033:21.82
C:LYS:A:18:11.301:35.19:25.294:20.55
O:LYS:A:18:11.071:34.163:25.936:21.12
CB:LYS:A:18:13.624:35.111:24.441:20.42
CG:LYS:A:18:14.518:34.782:23.279:20.61
CD:LYS:A:18:16.015:34.803:23.664:30.84
CE:LYS:A:18:16.866:34.3:22.484:38.22
NZ:LYS:A:18:18.269:33.984:22.906:62
H:LYS:A:18:12.546:36.685:22.889:24.05
HA:LYS:A:18:11.951:34.276:23.589:26.19
HB2:LYS:A:18:13.867:35.989:24.772:24.51
HB3:LYS:A:18:13.763:34.442:25.13:24.51
HG2:LYS:A:18:14.303:33.894:22.954:24.73
HG3:LYS:A:18:14.379:35.436:22.576:24.73
HD2:LYS:A:18:16.284:35.711:23.875:37
HD3:LYS:A:18:16.163:34.218:24.424:37
HE2:LYS:A:18:16.468:33.491:22.125:45.86
HE3:LYS:A:18:16.902:34.987:21.8:45.86
HZ1:LYS:A:18:18.739:33.696:22.207:74.4
HZ2:LYS:A:18:18.658:34.713:23.236:74.4
HZ3:LYS:A:18:18.263:33.351:23.531:74.4
N:TYR:A:19:10.88:36.384:25.687:25.2
CA:TYR:A:19:10.118:36.604:26.923:20.68
C:TYR:A:19:8.575:36.613:26.737:31.44
O:TYR:A:19:7.832:36.875:27.687:29.68
CB:TYR:A:19:10.538:37.943:27.555:20.37
CG:TYR:A:19:11.901:37.935:28.109:23.44
CD1:TYR:A:19:13:38.247:27.323:19.93
CD2:TYR:A:19:12.117:37.579:29.428:23.18
CE1:TYR:A:19:14.278:38.224:27.859:26.81
CE2:TYR:A:19:13.379:37.562:29.96:25.73
CZ:TYR:A:19:14.444:37.864:29.184:22.56
OH:TYR:A:19:15.682:37.826:29.75:22.36
H:TYR:A:19:11.025:37.107:25.245:30.24
HA:TYR:A:19:10.335:35.898:27.552:24.82
HB2:TYR:A:19:10.498:38.635:26.876:24.45
HB3:TYR:A:19:9.926:38.154:28.276:24.45
HD2:TYR:A:19:11.39:37.364:29.968:27.82
HD1:TYR:A:19:12.877:38.483:26.431:23.92
HE2:TYR:A:19:13.505:37.32:30.849:30.88
HE1:TYR:A:19:15.015:38.436:27.332:32.17
HH:TYR:A:19:16.265:38.03:29.18:26.83
O:CY3:A:20:6.334:34.016:25.918:46.46
C:CY3:A:20:5.968:35.121:26.067:39.6
N1:CY3:A:20:4.848:35.386:26.929:43.25
CA:CY3:A:20:6.666:36.307:25.294:21.87
N:CY3:A:20:8.084:36.362:25.53:22.5
CB:CY3:A:20:6.382:35.984:23.834:33.52
SG:CY3:A:20:6.832:37.458:22.767:39.89
H:CY3:A:20:8.534:36.217:24.812:27
HA:CY3:A:20:6.252:37.151:25.536:26.25
HB2:CY3:A:20:5.439:35.782:23.725:40.22
HB3:CY3:A:20:6.908:35.214:23.567:40.22
HN11:CY3:A:20:4.569:36.191:27.039:51.9
HN12:CY3:A:20:4.467:34.738:27.347:51.9
O:THR:B:-1:16.056:46.908:9.868:60.34
N:THR:B:-1:16.406:48.652:7.605:78.37
CA:THR:B:-1:17.132:48.822:8.897:76.87
C:THR:B:-1:17.109:47.519:9.689:64.38
CB:THR:B:-1:16.526:49.975:9.74:82.36
OG1:THR:B:-1:17.021:51.231:9.25:103.8
CG2:THR:B:-1:16.88:49.85:11.228:68.98
H1:THR:B:-1:16.283:49.449:7.227:94.05
H2:THR:B:-1:16.886:48.137:7.061:94.05
H3:THR:B:-1:15.617:48.27:7.756:94.05
HA:THR:B:-1:18.058:49.042:8.712:92.25
HB:THR:B:-1:15.56:49.958:9.656:98.83
HG1:THR:B:-1:16.698:51.862:9.7:124.55
HG21:THR:B:-1:16.486:50.584:11.725:82.78
HG22:THR:B:-1:16.538:49.013:11.58:82.78

【表４－４】

HG23:THR:B:-1:17.843:49.871:11.343:82.78
O:PHE:B:0:17.693:47.018:12.852:32.11
N:PHE:B:0:18.285:47.117:10.17:47.49
CA:PHE:B:0:18.434:45.859:10.88:33.82
C:PHE:B:0:17.777:45.945:12.258:30.41
CB:PHE:B:0:19.916:45.528:11.007:28.4
CG:PHE:B:0:20.185:44.138:11.419:27.64
CD2:PHE:B:0:20.443:43.17:10.471:29.44
CD1:PHE:B:0:20.187:43.786:12.753:26.31
CE2:PHE:B:0:20.706:41.883:10.832:27.99
CE1:PHE:B:0:20.454:42.477:13.135:27.97
CZ:PHE:B:0:20.702:41.517:12.166:27.51
H:PHE:B:0:19.016:47.564:10.094:56.99
HA:PHE:B:0:18.003:45.151:10.377:40.59
HB2:PHE:B:0:20.342:45.669:10.147:34.08
HB3:PHE:B:0:20.311:46.115:11.67:34.08
HD1:PHE:B:0:20.017:44.431:13.402:31.58
HD2:PHE:B:0:20.445:43.402:9.571:35.33
HE1:PHE:B:0:20.45:42.243:14.035:33.57
HE2:PHE:B:0:20.874:41.244:10.177:33.58
HZ:PHE:B:0:20.881:40.638:12.411:33.01
O:ASP:B:1:18.276:43.923:15.696:23.3
N:ASP:B:1:17.325:44.791:12.774:25.54
CA:ASP:B:1:16.642:44.721:14.072:24.29
C:ASP:B:1:17.702:44.882:15.159:25.42
CB:ASP:B:1:15.863:43.408:14.192:30.99
CG:ASP:B:1:15.425:43.112:15.613:33.34
OD1:ASP:B:1:15.172:44.1:16.35:26.15
OD2:ASP:B:1:15.36:41.913:16.004:22.1
H:ASP:B:1:17.404:44.028:12.384:30.65
HA:ASP:B:1:16.014:45.456:14.145:29.15
HB2:ASP:B:1:15.068:43.46:13.639:37.19
HB3:ASP:B:1:16.427:42.677:13.894:37.19
O:THR:B:2:17.54:46.872:18.038:27.96
N:THR:B:2:18.026:46.134:15.452:24.07
CA:THR:B:2:19.15:46.377:16.357:23.86
C:THR:B:2:18.686:46.539:17.782:24.18
CB:THR:B:2:19.911:47.632:15.99:31.47
OG1:THR:B:2:18.958:48.664:15.749:33.31
CG2:THR:B:2:20.815:47.367:14.758:33.17
H:THR:B:2:17.631:46.838:15.155:28.88
HA:THR:B:2:19.762:45.626:16.318:28.64
HB:THR:B:2:20.479:47.889:16.733:37.77
HG1:THR:B:2:19.352:49.376:15.542:39.98
HG21:THR:B:2:21.302:48.173:14.525:39.81
HG22:THR:B:2:21.45:46.662:14.959:39.81
HG23:THR:B:2:20.272:47.097:14.001:39.81
C:HYP:B:3:18.617:47.825:20.609:37.46
O:HYP:B:3:19.172:48.867:20.197:33.28
CA:HYP:B:3:19.208:46.443:20.27:30.06
CB:HYP:B:3:20.366:46.23:20.929:46.37
CG:HYP:B:3:21.21:45.388:19.961:34.65
OD1:HYP:B:3:20.787:44.116:19.901:37.02
CD:HYP:B:3:20.889:46.065:18.606:30.67
N:HYP:B:3:19.59:46.315:18.708:25.2
HD23:HYP:B:3:21.065:45.458:17.869:36.81
HD22:HYP:B:3:21.39:46.89:18.507:36.81
HG:HYP:B:3:22.156:45.447:20.171:41.58
HD1:HYP:B:3:21.078:43.754:19.188:44.43
HB3:HYP:B:3:20.807:47.074:21.115:55.65
HB2:HYP:B:3:20.201:45.739:21.749:55.65
HA:HYP:B:3:18.572:45.748:20.503:36.08
O:LYS:B:4:16.271:47.848:23.837:25.52
N:LYS:B:4:17.521:47.837:21.368:29.31
CA:LYS:B:4:16.899:49.058:21.865:26.28
C:LYS:B:4:16.634:48.93:23.365:21.83
CB:LYS:B:4:15.558:49.322:21.159:37.68
CG:LYS:B:4:15.666:49.595:19.675:65.23
CD:LYS:B:4:14.269:49.657:19.051:94.75
CE:LYS:B:4:14.289:50.089:17.586:109.16
NZ:LYS:B:4:12.904:50.217:17.038:105.24
H:LYS:B:4:17.109:47.124:21.616:35.17
HA:LYS:B:4:17.488:49.813:21.713:31.53
HB2:LYS:B:4:14.99:48.544:21.273:45.21
HB3:LYS:B:4:15.139:50.094:21.569:45.21
HG2:LYS:B:4:16.106:50.447:19.533:78.28
HG3:LYS:B:4:16.163:48.879:19.248:78.28
HD2:LYS:B:4:13.864:48.777:19.098:113.71
HD3:LYS:B:4:13.732:50.296:19.544:113.71
HE2:LYS:B:4:14.727:50.951:17.511:130.99
HE3:LYS:B:4:14.763:49.424:17.062:130.99
HZ1:LYS:B:4:12.937:50.469:16.185:126.28
HZ2:LYS:B:4:12.482:49.435:17.093:126.28
HZ3:LYS:B:4:12.449:50.825:17.502:126.28
O:HIS:B:5:14.227:50.871:24.963:32.55
N:HIS:B:5:16.734:50.025:24.109:21.79
CA:HIS:B:5:16.363:50.01:25.519:21.56
C:HIS:B:5:14.857:50.045:25.607:22.3
CB:HIS:B:5:16.937:51.202:26.275:22.18
CG:HIS:B:5:18.423:51.204:26.337:22.64
ND1:HIS:B:5:19.131:50.545:27.328:28.27
CD2:HIS:B:5:19.345:51.765:25.516:25.48
CE1:HIS:B:5:20.428:50.699:27.11:22.51
NE2:HIS:B:5:20.585:51.441:26.022:28.72
H:HIS:B:5:17.013:50.786:23.824:26.15
HA:HIS:B:5:16.682:49.193:25.934:25.87
HB2:HIS:B:5:16.657:52.018:25.832:26.62
HB3:HIS:B:5:16.601:51.188:27.185:26.62
HD1:HIS:B:5:18.784:50.097:27.975:33.93
HD2:HIS:B:5:19.173:52.273:24.756:30.58
HE1:HIS:B:5:21.112:50.36:27.64:27.01
N:ARG:B:6:14.278:49.126:26.37:20.97
CA:ARG:B:6:12.838:49.07:26.561:24.52
C:ARG:B:6:12.608:49.07:28.058:21.26
O:ARG:B:6:12.884:48.066:28.727:23.78
CB:ARG:B:6:12.238:47.832:25.893:20.69
CG:ARG:B:6:12.796:47.582:24.53:26.83
CD:ARG:B:6:12.576:46.115:24.096:33.07
NE:ARG:B:6:13.308:45.832:22.86:31.36
CZ:ARG:B:6:12.807:45.919:21.638:20.49
NH1:ARG:B:6:11.527:46.276:21.431:28.98
NH2:ARG:B:6:13.594:45.629:20.612:25.07

【表４－５】

H:ARG:B:6:14.707:48.515:26.795:25.17
HA:ARG:B:6:12.425:49.861:26.181:29.42
HB2:ARG:B:6:12.426:47.054:26.441:24.83
HB3:ARG:B:6:11.279:47.953:25.806:24.83
HG2:ARG:B:6:12.352:48.159:23.89:32.19
HG3:ARG:B:6:13.75:47.758:24.537:32.19
HD2:ARG:B:6:12.903:45.519:24.789:39.68
HD3:ARG:B:6:11.632:45.963:23.935:39.68
HE:ARG:B:6:14.13:45.591:22.934:37.64
HH11:ARG:B:6:11.019:46.461:22.1:34.78
HH12:ARG:B:6:11.218:46.324:20.63:34.78
HH21:ARG:B:6:14.411:45.398:20.748:30.08
HH22:ARG:B:6:13.289:45.676:19.809:30.08
N:CYS:B:7:12.125:50.193:28.588:22.09
CA:CYS:B:7:12.018:50.387:30.028:24.41
C:CYS:B:7:10.61:50.801:30.421:28.77
O:CYS:B:7:9.878:51.453:29.662:23.73
CB:CYS:B:7:12.995:51.452:30.534:25.61
SG:CYS:B:7:14.735:51.095:30.241:32.01
H:CYS:B:7:11.851:50.864:28.126:26.51
HA:CYS:B:7:12.223:49.551:30.477:29.3
HB2:CYS:B:7:12.791:52.292:30.093:30.73
HB3:CYS:B:7:12.874:51.551:31.492:30.73
N:GLY:B:8:10.246:50.438:31.636:23.3
CA:GLY:B:8:8.941:50.832:32.13:24.26
C:GLY:B:8:7.848:50.372:31.198:27.94
O:GLY:B:8:7.783:49.176:30.882:23.54
H:GLY:B:8:10.721:49.975:32.183:27.96
HA2:GLY:B:8:8.79:50.442:33.005:29.11
HA3:GLY:B:8:8.898:51.798:32.208:29.11
N:SER:B:9:7.045:51.325:30.7:25.43
CA:SER:B:9:5.825:51.05:29.947:28.83
C:SER:B:9:6.127:50.664:28.495:33.52
O:SER:B:9:5.335:49.988:27.841:31.13
CB:SER:B:9:4.914:52.281:29.986:36.62
OG:SER:B:9:5.573:53.396:29.4:36.38
H:SER:B:9:7.199:52.166:30.793:30.51
HA:SER:B:9:5.353:50.312:30.364:34.6
HB2:SER:B:9:4.104:52.092:29.487:43.94
HB3:SER:B:9:4.698:52.488:30.908:43.94
HG:SER:B:9:6.279:53.567:29.822:43.65
N:CGU:B:10:7.28:51.095:27.998:28.76
CA:CGU:B:10:7.81:50.596:26.686:28.05
CB:CGU:B:10:9.239:51.112:26.411:26.61
CG:CGU:B:10:9.333:52.622:26.497:48.2
CD1:CGU:B:10:10.796:53.099:26.309:43.27
OE12:CGU:B:10:10.997:54.252:25.818:32.43
OE11:CGU:B:10:11.775:52.332:26.659:28.59
CD2:CGU:B:10:8.34:53.322:25.507:61.07
OE21:CGU:B:10:8.191:52.877:24.334:60.62
OE22:CGU:B:10:7.665:54.311:25.914:71.45
C:CGU:B:10:7.888:49.082:26.653:29.41
O:CGU:B:10:7.883:48.518:25.527:30.26
HG:CGU:B:10:9.037:52.937:27.534:57.84
HB3:CGU:B:10:9.957:50.658:27.117:31.93
HB2:CGU:B:10:9.575:50.754:25.412:31.93
HA:CGU:B:10:7.113:50.935:25.873:33.66
N:ILE:B:11:8.048:48.421:27.803:25.25
CA:ILE:B:11:8.061:46.962:27.816:21.79
C:ILE:B:11:6.652:46.486:27.505:22.28
O:ILE:B:11:6.473:45.595:26.699:22.22
CB:ILE:B:11:8.584:46.402:29.14:29.42
CG1:ILE:B:11:10.089:46.697:29.267:30.34
CG2:ILE:B:11:8.328:44.893:29.247:23.17
CD1:ILE:B:11:10.655:46.443:30.653:34.61
H:ILE:B:11:8.15:48.789:28.574:30.3
HA:ILE:B:11:8.645:46.647:27.108:26.14
HB:ILE:B:11:8.12:46.846:29.867:35.31
HG12:ILE:B:11:10.571:46.133:28.643:36.41
HG13:ILE:B:11:10.243:47.63:29.052:36.41
HG21:ILE:B:11:8.671:44.574:30.097:27.8
HG22:ILE:B:11:7.373:44.731:29.195:27.8
HG23:ILE:B:11:8.781:44.443:28.517:27.8
HD11:ILE:B:11:11.603:46.651:30.649:41.53
HD12:ILE:B:11:10.194:47.009:31.291:41.53
HD13:ILE:B:11:10.522:45.509:30.881:41.53
N:THR:B:12:5.642:47.089:28.133:23.69
CA:THR:B:12:4.264:46.785:27.759:27.8
C:THR:B:12:4.051:46.987:26.269:32.55
O:THR:B:12:3.511:46.106:25.58:24.04
CB:THR:B:12:3.292:47.642:28.58:33.52
OG1:THR:B:12:3.502:47.358:29.965:32.74
CG2:THR:B:12:1.803:47.355:28.223:26.3
H:THR:B:12:5.726:47.666:28.765:28.42
HA:THR:B:12:4.082:45.854:27.961:33.36
HB:THR:B:12:3.471:48.581:28.413:40.23
HG1:THR:B:12:2.979:47.818:30.435:39.29
HG21:THR:B:12:1.22:47.914:28.761:31.56
HG22:THR:B:12:1.644:47.545:27.285:31.56
HG23:THR:B:12:1.594:46.424:28.396:31.56
N:ASN:B:13:4.453:48.15:25.751:24.48
CA:ASN:B:13:4.301:48.421:24.321:25.34
C:ASN:B:13:4.974:47.353:23.491:24.13
O:ASN:B:13:4.462:46.938:22.439:24.08
CB:ASN:B:13:4.909:49.776:23.943:28.08
CG:ASN:B:13:4.169:50.958:24.563:43.36
OD1:ASN:B:13:3.038:50.826:25.036:39.56
ND2:ASN:B:13:4.82:52.121:24.575:47.85
H:ASN:B:13:4.812:48.79:26.2:29.38
HA:ASN:B:13:3.358:48.435:24.096:30.41
HB2:ASN:B:13:5.829:49.805:24.249:33.69
HB3:ASN:B:13:4.877:49.876:22.978:33.69
HD21:ASN:B:13:4.449:52.819:24.913:57.42
HD22:ASN:B:13:5.612:52.174:24.244:57.42
N:SER:B:14:6.155:46.925:23.918:22.66
CA:SER:B:14:6.85:45.888:23.173:21.94
C:SER:B:14:6.098:44.563:23.22:21.87
O:SER:B:14:5.951:43.898:22.193:22.01
CB:SER:B:14:8.269:45.758:23.696:25.08
OG:SER:B:14:9.033:46.775:23.091:24.01
H:SER:B:14:6.565:47.209:24.618:27.19
HA:SER:B:14:6.904:46.16:22.243:26.33

【表４－６】

HB2:SER:B:14:8.274:45.874:24.659:30.1
HB3:SER:B:14:8.63:44.891:23.453:30.1
HG:SER:B:14:9.828:46.735:23.358:28.81
N:TYR:B:15:5.629:44.144:24.4:21.89
CA:TYR:B:15:4.768:42.964:24.454:22.13
C:TYR:B:15:3.609:43.089:23.478:22.94
O:TYR:B:15:3.283:42.128:22.771:23.01
CB:TYR:B:15:4.193:42.718:25.852:22.53
CG:TYR:B:15:5.115:42.148:26.893:22.01
CD1:TYR:B:15:5.679:40.889:26.759:37.65
CD2:TYR:B:15:5.351:42.85:28.079:48.14
CE1:TYR:B:15:6.507:40.375:27.747:62.89
CE2:TYR:B:15:6.165:42.337:29.078:52.81
CZ:TYR:B:15:6.748:41.113:28.908:60.82
OH:TYR:B:15:7.558:40.637:29.929:54.81
H:TYR:B:15:5.789:44.514:25.16:26.27
HA:TYR:B:15:5.287:42.185:24.203:26.56
HB2:TYR:B:15:3.868:43.565:26.195:27.03
HB3:TYR:B:15:3.448:42.104:25.765:27.03
HD1:TYR:B:15:5.53:40.399:25.982:45.19
HD2:TYR:B:15:4.966:43.688:28.195:57.77
HE1:TYR:B:15:6.897:39.537:27.638:75.46
HE2:TYR:B:15:6.328:42.83:29.85:63.37
HH:TYR:B:15:7.597:41.201:30.551:65.77
N:MET:B:16:2.967:44.255:23.427:23.8
CA:MET:B:16:1.803:44.423:22.544:28.09
C:MET:B:16:2.197:44.329:21.083:26.65
O:MET:B:16:1.471:43.748:20.275:36.43
CB:MET:B:16:1.118:45.775:22.768:30.99
CG:MET:B:16:0.499:45.977:24.148:42.33
SD:MET:B:16:-0.954:44.949:24.404:68.25
CE:MET:B:16:-0.206:43.67:25.426:42.42
H:MET:B:16:3.177:44.953:23.883:28.56
HA:MET:B:16:1.157:43.726:22.74:33.71
HB2:MET:B:16:1.775:46.477:22.639:37.19
HB3:MET:B:16:0.409:45.872:22.114:37.19
HG2:MET:B:16:1.153:45.748:24.826:50.79
HG3:MET:B:16:0.232:46.905:24.243:50.79
HE1:MET:B:16:-0.883:43.016:25.657:50.9
HE2:MET:B:16:0.508:43.245:24.926:50.9
HE3:MET:B:16:0.15:44.078:26.231:50.9
N:ASP:B:17:3.344:44.897:20.719:29.89
CA:ASP:B:17:3.758:44.849:19.322:34.2
C:ASP:B:17:4.362:43.503:18.931:30.46
O:ASP:B:17:4.224:43.095:17.781:28.87
CB:ASP:B:17:4.769:45.957:19.002:41.66
CG:ASP:B:17:4.239:47.347:19.307:78.78
OD1:ASP:B:17:3:47.511:19.374:89.35
OD2:ASP:B:17:5.064:48.277:19.478:72.64
H:ASP:B:17:3.887:45.306:21.246:35.87
HA:ASP:B:17:2.978:44.994:18.764:41.04
HB2:ASP:B:17:5.569:45.818:19.534:49.99
HB3:ASP:B:17:4.989:45.92:18.058:49.99
N:LEU:B:18:5.062:42.822:19.831:22.66
CA:LEU:B:18:5.868:41.669:19.444:22.1
C:LEU:B:18:5.314:40.329:19.885:22.41
O:LEU:B:18:5.69:39.304:19.308:24.4
CB:LEU:B:18:7.286:41.806:20.002:22.61
CG:LEU:B:18:7.948:43.093:19.512:21.46
CD1:LEU:B:18:9.302:43.234:20.155:24.5
CD2:LEU:B:18:8.07:43.128:17.966:28.1
H:LEU:B:18:5.088:43.006:20.671:27.19
HA:LEU:B:18:5.935:41.652:18.476:26.53
HB2:LEU:B:18:7.249:41.832:20.971:27.14
HB3:LEU:B:18:7.823:41.055:19.704:27.14
HG:LEU:B:18:7.407:43.85:19.787:25.75
HD11:LEU:B:18:9.717:44.053:19.841:29.4
HD12:LEU:B:18:9.192:43.267:21.118:29.4
HD13:LEU:B:18:9.848:42.471:19.91:29.4
HD21:LEU:B:18:8.494:43.959:17.702:33.72
HD22:LEU:B:18:8.607:42.375:17.675:33.72
HD23:LEU:B:18:7.183:43.071:17.578:33.72
N:CYS:B:19:4.481:40.285:20.912:26.31
CA:CYS:B:19:4.018:39.001:21.403:23.2
C:CYS:B:19:2.573:38.743:21.045:29.55
O:CYS:B:19:2.204:37.602:20.812:27.61
CB:CYS:B:19:4.199:38.915:22.923:25.28
SG:CYS:B:19:5.942:39.114:23.454:33.59
H:CYS:B:19:4.174:40.968:21.334:31.58
HA:CYS:B:19:4.553:38.3:21:27.84
HB2:CYS:B:19:3.677:39.617:23.342:30.34
HB3:CYS:B:19:3.891:38.047:23.227:30.34
O:TYR:B:20:0.453:40.693:18.643:58.94
N:TYR:B:20:1.763:39.78:20.969:30.88
CA:TYR:B:20:0.33:39.624:20.788:36.15
C:TYR:B:20:-0.046:39.793:19.324:48.21
CB:TYR:B:20:-0.44:40.615:21.651:29.56
CG:TYR:B:20:-0.651:40.122:23.065:55.92
CD1:TYR:B:20:-1.597:39.145:23.34:71.32
CD2:TYR:B:20:0.094:40.621:24.118:59.77
CE1:TYR:B:20:-1.8:38.679:24.621:72.77
CE2:TYR:B:20:-0.098:40.161:25.411:73.5
CZ:TYR:B:20:-1.058:39.185:25.659:74.33
OH:TYR:B:20:-1.29:38.681:26.931:61.61
H:TYR:B:20:2.02:40.599:21.019:37.06
HA:TYR:B:20:0.074:38.728:21.06:43.38
HB2:TYR:B:20:0.055:41.447:21.695:35.48
HB3:TYR:B:20:-1.312:40.768:21.254:35.48
HD1:TYR:B:20:-2.106:38.797:22.644:85.58
HD2:TYR:B:20:0.735:41.274:23.956:71.73
HE1:TYR:B:20:-2.44:38.024:24.782:87.33
HE2:TYR:B:20:0.409:40.506:26.11:88.2
HH:TYR:B:20:-0.786:39.058:27.486:73.93
O:ARG:B:21:-2.375:41.115:18.001:73.56
N:ARG:B:21:-0.904:38.888:18.851:48.09
CA:ARG:B:21:-1.505:38.926:17.518:54.86
C:ARG:B:21:-2.02:40.306:17.132:67.04
CB:ARG:B:21:-2.675:37.949:17.448:56.88
CG:ARG:B:21:-2.44:36.661:16.704:66.58
CD:ARG:B:21:-3.714:36.364:15.961:87.2
NE:ARG:B:21:-3.936:34.955:15.663:104.85
CZ:ARG:B:21:-5.147:34.397:15.619:123.5

【表４－７】

NH1:ARG:B:21:-6.239:35.129:15.88:136.71
NH2:ARG:B:21:-5.27:33.101:15.333:115.82
OXT:ARG:B:21:-2.121:40.62:15.939:68.47
H:ARG:B:21:-1.164:38.209:19.309:57.7
HA:ARG:B:21:-0.844:38.656:16.862:65.83
HB2:ARG:B:21:-2.926:37.714:18.355:68.25
HB3:ARG:B:21:-3.418:38.398:17.016:68.25
HG2:ARG:B:21:-1.716:36.768:16.067:79.9
HG3:ARG:B:21:-2.258:35.94:17.327:79.9
HD2:ARG:B:21:-4.462:36.672:16.495:104.64
HD3:ARG:B:21:-3.698:36.842:15.117:104.64
HE:ARG:B:21:-3.252:34.434:15.65:125.82
HH11:ARG:B:21:-6.162:35.965:16.065:164.05
HH12:ARG:B:21:-7.017:34.764:15.855:164.05
HH21:ARG:B:21:-4.571:32.628:15.17:138.98
HH22:ARG:B:21:-6.049:32.738:15.311:138.98

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【請求項２３】

あらゆる格子寸法において変動が最大約２％であるａ＝ｂ＝ｃ＝７４．９１Åの単位格子寸法を有する空間群Ｐ４３２を有するＣｏｎ－Ｉｎｓ　Ｇ１ポリペプチドの結晶。

【請求項２４】

下表の原子座標により定義される構造を有するポリペプチド：

【表５－１】

付録I: CON-INS G1インスリン(鎖Aおよび鎖B)に関する原子座標

フォーマットは、下記のコロンで区切られたフィールドを含む: (1) 原子の名称, (2) 残基タイプ, (3) 鎖の名称,(4) 残基番号,(5-7) xyz 座標,(8) 温度B因子(thermal B-factor)。

N:GLY:A:1:15.439:38.785:34.309:26.76
CA:GLY:A:1:14.11:39.14:33.733:22.21
C:GLY:A:1:14.251:39.976:32.492:21.3
O:GLY:A:1:15.353:40.312:32.093:22.73
H1:GLY:A:1:15.395:38.813:35.197:32.11
H2:GLY:A:1:15.666:37.965:34.049:32.11
H3:GLY:A:1:16.051:39.366:34.024:32.11
HA2:GLY:A:1:13.625:38.331:33.508:26.65
HA3:GLY:A:1:13.595:39.639:34.386:26.65
N:VAL:A:2:13.113:40.325:31.895:21.05
CA:VAL:A:2:13.122:41.169:30.72:22.11
C:VAL:A:2:13.696:42.561:31.01:20.41
O:VAL:A:2:14.274:43.187:30.116:20.06
CB:VAL:A:2:11.698:41.225:30.132:25.46
CG1:VAL:A:2:10.72:41.927:31.074:21.3
CG2:VAL:A:2:11.725:41.902:28.839:27.88
H:VAL:A:2:12.33:40.084:32.154:25.26
HA:VAL:A:2:13.693:40.756:30.053:26.54
HB:VAL:A:2:11.38:40.32:29.989:30.55
HG11:VAL:A:2:9.841:41.939:30.665:25.56
HG12:VAL:A:2:10.688:41.442:31.914:25.56
HG13:VAL:A:2:11.026:42.835:31.227:25.56
HG21:VAL:A:2:10.824:41.931:28.48:33.45
HG22:VAL:A:2:12.061:42.804:28.963:33.45
HG23:VAL:A:2:12.306:41.412:28.238:33.45
N:VAL:A:3:13.604:43.056:32.249:26.31
CA:VAL:A:3:14.092:44.414:32.525:22.38
C:VAL:A:3:15.618:44.365:32.529:26.64
O:VAL:A:3:16.283:45.246:31.982:21.94
CB:VAL:A:3:13.517:44.989:33.842:28.85
CG1:VAL:A:3:14.192:46.325:34.21:23.35
CG2:VAL:A:3:11.967:45.154:33.731:22.25
H:VAL:A:3:13.276:42.642:32.928:31.58
HA:VAL:A:3:13.816:44.998:31.802:26.85
HB:VAL:A:3:13.695:44.361:34.559:34.62
HG11:VAL:A:3:13.808:46.654:35.037:28.02
HG12:VAL:A:3:15.144:46.176:34.323:28.02
HG13:VAL:A:3:14.039:46.963:33.496:28.02
HG21:VAL:A:3:11.628:45.515:34.565:26.7
HG22:VAL:A:3:11.767:45.762:33.001:26.7
HG23:VAL:A:3:11.569:44.287:33.558:26.7
N:CGU:A:4:16.193:43.318:33.099:21.34
CA:CGU:A:4:17.68:43.233:33.107:21.52
CB:CGU:A:4:18.136:42.041:33.939:22.15
CG:CGU:A:4:17.867:42.164:35.47:27.83
CD1:CGU:A:4:16.419:42.187:35.88:25.08
OE12:CGU:A:4:16.135:42.812:36.937:28.6
OE11:CGU:A:4:15.531:41.542:35.211:22.71
CD2:CGU:A:4:18.45:40.98:36.25:48.38
OE21:CGU:A:4:18.448:39.819:35.754:54.62
OE22:CGU:A:4:18.871:41.181:37.42:85.42
C:CGU:A:4:18.255:43.089:31.618:20.98
O:CGU:A:4:19.303:43.691:31.269:21.08
HG:CGU:A:4:18.338:43.105:35.863:33.4
HB3:CGU:A:4:17.661:41.115:33.568:26.58
HB2:CGU:A:4:19.22:41.867:33.754:26.58
HA:CGU:A:4:18.079:44.185:33.551:25.82
N:HIS:A:5:17.548:42.333:30.786:21.02
CA:HIS:A:5:18.007:41.966:29.443:20.65
C:HIS:A:5:17.659:43.013:28.373:19.86
O:HIS:A:5:18.285:43.07:27.334:23.44
CB:HIS:A:5:17.391:40.584:29.071:20.16
CG:HIS:A:5:18.115:39.864:27.981:47.58
ND1:HIS:A:5:19.277:39.15:28.201:43.05
CD2:HIS:A:5:17.832:39.734:26.661:45.41
CE1:HIS:A:5:19.678:38.617:27.058:50.46
NE2:HIS:A:5:18.82:38.957:26.111:52.67
HA:HIS:A:5:18.972:41.867:29.458:24.79
HB2:HIS:A:5:17.402:40.017:29.858:24.19
HB3:HIS:A:5:16.476:40.72:28.778:24.19
HD2:HIS:A:5:17.106:40.104:26.213:54.49
HE1:HIS:A:5:20.437:38.093:26.94:60.55
HE2:HIS:A:5:18.873:38.729:25.284:63.2
H:HIS:A:5:16.775:42.01:30.98:25.23
N:CYS:A:6:16.641:43.84:28.616:19.88
CA:CYS:A:6:16.113:44.731:27.591:19.76
C:CYS:A:6:16.063:46.184:28.028:21.58
O:CYS:A:6:15.909:47.06:27.165:20.58
CB:CYS:A:6:14.695:44.308:27.194:21.07
SG:CYS:A:6:14.678:42.722:26.317:26
H:CYS:A:6:16.238:43.902:29.373:23.85
HA:CYS:A:6:16.676:44.674:26.803:23.71
HB2:CYS:A:6:14.154:44.217:27.994:25.29
HB3:CYS:A:6:14.315:44.981:26.608:25.29
N:CYS:A:7:16.128:46.463:29.323:21.05
CA:CYS:A:7:16.186:47.837:29.839:21.74
C:CYS:A:7:17.553:48.188:30.41:23.78
O:CYS:A:7:18.103:49.215:30.042:30.88
CB:CYS:A:7:15.098:48.081:30.895:21.43
SG:CYS:A:7:15.221:49.718:31.732:27.59
H:CYS:A:7:16.14:45.864:29.941:25.26
HA:CYS:A:7:16.016:48.446:29.103:26.09
HB2:CYS:A:7:14.229:48.033:30.465:25.71
HB3:CYS:A:7:15.165:47.394:31.576:25.71
N:HIS:A:8:18.157:47.348:31.264:28.49
CA:HIS:A:8:19.509:47.657:31.747:25.02
C:HIS:A:8:20.564:47.453:30.657:30.05
O:HIS:A:8:21.558:48.179:30.604:34.16

【表５－２】

CB:HIS:A:8:19.847:46.811:32.972:27.96
CG:HIS:A:8:18.916:47.03:34.125:33.4
ND1:HIS:A:8:18.619:46.043:35.044:34.99
CD2:HIS:A:8:18.234:48.129:34.521:27.24
CE1:HIS:A:8:17.767:46.516:35.936:33.7
NE2:HIS:A:8:17.527:47.782:35.648:38.53
H:HIS:A:8:17.818:46.619:31.57:34.19
HA:HIS:A:8:19.538:48.589:32.014:30.03
HB2:HIS:A:8:19.802:45.874:32.728:33.55
HB3:HIS:A:8:20.744:47.033:33.268:33.55
HD2:HIS:A:8:18.233:48.959:34.103:32.68
HE1:HIS:A:8:17.417:46.045:36.658:40.44
HE2:HIS:A:8:17.009:48.305:36.092:46.23
N:ARG:A:9:20.377:46.477:29.813:32.17
CA:ARG:A:9:21.026:46.221:28.542:24.61
C:ARG:A:9:19.985:46.413:27.464:24.55
O:ARG:A:9:18.838:46.063:27.712:22.58
CB:ARG:A:9:21.524:44.776:28.434:42.6
CG:ARG:A:9:22.966:44.545:28.786:89.14
CD:ARG:A:9:23.608:43.537:27.831:118.62
NE:ARG:A:9:25.059:43.702:27.796:137.92
CZ:ARG:A:9:25.928:42.745:27.485:154.54
NH1:ARG:A:9:25.517:41.519:27.184:170.53
NH2:ARG:A:9:27.224:43.02:27.49:152.73
H:ARG:A:9:19.797:45.864:29.977:38.61
HA:ARG:A:9:21.763:46.836:28.4:29.53
HB2:ARG:A:9:20.99:44.224:29.027:51.12
HB3:ARG:A:9:21.399:44.478:27.519:51.12
HG2:ARG:A:9:23.451:45.382:28.719:106.97
HG3:ARG:A:9:23.024:44.192:29.688:106.97
HD2:ARG:A:9:23.41:42.637:28.132:142.34
HD3:ARG:A:9:23.263:43.677:26.935:142.34
HE:ARG:A:9:25.375:44.477:27.991:165.51
HH11:ARG:A:9:24.676:41.336:27.181:204.63
HH12:ARG:A:9:26.09:40.909:26.987:204.63
HH21:ARG:A:9:27.495:43.812:27.686:183.27
HH22:ARG:A:9:27.794:42.407:27.293:183.27
N:PRO:A:10:20.315:46.922:26.273:21.04
CA:PRO:A:10:19.325:46.947:25.186:22.55
C:PRO:A:10:19.153:45.573:24.54:20.8
O:PRO:A:10:20.049:44.721:24.565:22.83
CB:PRO:A:10:19.914:47.951:24.205:21.44
CG:PRO:A:10:21.394:47.783:24.393:23.92
CD:PRO:A:10:21.581:47.551:25.858:26.07
HA:PRO:A:10:18.468:47.268:25.508:27.06
HB2:PRO:A:10:19.65:47.726:23.299:25.72
HB3:PRO:A:10:19.633:48.849:24.439:25.72
HG2:PRO:A:10:21.703:47.018:23.883:28.7
HG3:PRO:A:10:21.853:48.59:24.112:28.7
HD2:PRO:A:10:22.324:46.948:26.013:31.28
HD3:PRO:A:10:21.706:48.395:26.32:31.28
N:CYS:A:11:17.965:45.34:23.974:20.27
CA:CYS:A:11:17.735:44.077:23.278:20.11
C:CYS:A:11:17.021:44.299:21.95:20.29
O:CYS:A:11:16.249:45.24:21.766:20.43
CB:CYS:A:11:16.959:43.053:24.166:20.58
SG:CYS:A:11:15.186:43.358:24.401:23.25
H:CYS:A:11:17.296:45.881:23.98:24.33
HA:CYS:A:11:18.598:43.683:23.076:24.13
HB2:CYS:A:11:17.048:42.175:23.763:24.7
HB3:CYS:A:11:17.368:43.045:25.045:24.7
N:SER:A:12:17.349:43.443:21.002:19.95
CA:SER:A:12:16.64:43.374:19.734:20.24
C:SER:A:12:15.198:42.876:19.921:19.9
O:SER:A:12:14.82:42.314:20.95:19.48
CB:SER:A:12:17.365:42.442:18.794:20.66
OG:SER:A:12:17.226:41.115:19.254:20.36
H:SER:A:12:17.993:42.877:21.068:23.94
HA:SER:A:12:16.611:44.256:19.332:24.29
HB2:SER:A:12:16.978:42.517:17.908:24.79
HB3:SER:A:12:18.306:42.677:18.772:24.79
HG:SER:A:12:17.626:40.589:18.736:24.43
N:ASN:A:13:14.386:43.089:18.896:20.29
CA:ASN:A:13:13.05:42.486:18.857:20.21
C:ASN:A:13:13.113:40.969:18.999:19.99
O:ASN:A:13:12.303:40.375:19.72:19.76
CB:ASN:A:13:12.338:42.827:17.571:20.89
CG:ASN:A:13:11.993:44.254:17.455:21.34
OD1:ASN:A:13:12.063:45.022:18.425:21.1
ND2:ASN:A:13:11.561:44.637:16.254:22.2
H:ASN:A:13:14.577:43.575:18.213:24.35
HA:ASN:A:13:12.523:42.835:19.593:24.25
HB2:ASN:A:13:12.913:42.598:16.823:25.07
HB3:ASN:A:13:11.515:42.316:17.522:25.07
HD21:ASN:A:13:11.343:45.457:16.116:26.64
HD22:ASN:A:13:11.502:44.063:15.616:26.64
N:ALA:A:14:14.073:40.323:18.327:20.53
CA:ALA:A:14:14.136:38.865:18.34:20.59
C:ALA:A:14:14.514:38.344:19.713:20.2
O:ALA:A:14:13.966:37.34:20.17:20.42
CB:ALA:A:14:15.122:38.388:17.293:21.21
H:ALA:A:14:14.689:40.704:17.863:24.64
HA:ALA:A:14:13.262:38.509:18.115:24.71
HB1:ALA:A:14:15.156:37.419:17.311:25.45
HB2:ALA:A:14:14.827:38.694:16.421:25.45
HB3:ALA:A:14:15.997:38.755:17.494:25.45
N:GLU:A:15:15.393:39.048:20.418:19.99
CA:GLU:A:15:15.674:38.714:21.807:20.64
C:GLU:A:15:14.459:38.979:22.702:20.25
O:GLU:A:15:14.126:38.165:23.56:19.51
CB:GLU:A:15:16.886:39.507:22.306:24.27
CG:GLU:A:15:18.221:38.954:21.864:52.08
CD:GLU:A:15:18.481:37.555:22.399:68.3
OE1:GLU:A:15:18.414:37.354:23.638:37.34
OE2:GLU:A:15:18.75:36.655:21.573:92.14
H:GLU:A:15:15.838:39.719:20.116:23.99
HA:GLU:A:15:15.889:37.77:21.867:24.77
HB2:GLU:A:15:16.82:40.416:21.974:29.12
HB3:GLU:A:15:16.876:39.513:23.276:29.12
HG2:GLU:A:15:18.242:38.914:20.895:62.5
HG3:GLU:A:15:18.927:39.535:22.188:62.5
N:PHE:A:16:13.813:40.136:22.56:19.08

【表５－３】

CA:PHE:A:16:12.627:40.394:23.379:19.01
C:PHE:A:16:11.58:39.275:23.258:19.21
O:PHE:A:16:10.937:38.891:24.259:19.32
CB:PHE:A:16:12:41.738:23.008:19.12
CG:PHE:A:16:10.869:42.118:23.896:19.26
CD2:PHE:A:16:11.086:42.876:25.025:19.26
CD1:PHE:A:16:9.575:41.712:23.603:19.56
CE2:PHE:A:16:10.018:43.216:25.879:19.59
CE1:PHE:A:16:8.496:42.075:24.429:19.92
CZ:PHE:A:16:8.717:42.809:25.564:19.95
H:PHE:A:16:14.029:40.767:22.018:22.9
HA:PHE:A:16:12.898:40.443:24.309:22.81
HB2:PHE:A:16:12.677:42.43:23.073:22.95
HB3:PHE:A:16:11.663:41.689:22.1:22.95
HD2:PHE:A:16:11.95:43.143:25.241:23.11
HD1:PHE:A:16:9.416:41.209:22.837:23.48
HE2:PHE:A:16:10.173:43.731:26.637:23.51
HE1:PHE:A:16:7.635:41.79:24.221:23.9
HZ:PHE:A:16:8.006:43.046:26.114:23.93
N:LYS:A:17:11.394:38.736:22.051:19.63
CA:LYS:A:17:10.38:37.7:21.84:19.97
C:LYS:A:17:10.614:36.46:22.684:20.12
O:LYS:A:17:9.672:35.685:22.893:20.5
CB:LYS:A:17:10.329:37.289:20.362:20.31
CG:LYS:A:17:9.504:38.28:19.498:20.56
CD:LYS:A:17:9.689:38.041:18.044:21.03
CE:LYS:A:17:9.094:39.21:17.228:23.58
NZ:LYS:A:17:9.222:39.104:15.74:26.95
H:LYS:A:17:11.837:38.95:21.346:23.56
HA:LYS:A:17:9.512:38.061:22.078:23.96
HB2:LYS:A:17:11.232:37.262:20.009:24.37
HB3:LYS:A:17:9.917:36.413:20.291:24.37
HG2:LYS:A:17:8.562:38.173:19.703:24.67
HG3:LYS:A:17:9.788:39.186:19.694:24.67
HD2:LYS:A:17:10.636:37.977:17.845:25.23
HD3:LYS:A:17:9.232:37.224:17.789:25.23
HE2:LYS:A:17:8.148:39.275:17.433:28.3
HE3:LYS:A:17:9.539:40.028:17.499:28.3
HZ1:LYS:A:17:8.855:39.816:15.352:32.34
HZ2:LYS:A:17:10.081:39.061:15.511:32.34
HZ3:LYS:A:17:8.808:38.371:15.451:32.34
N:LYS:A:18:11.856:36.224:23.113:20.04
CA:LYS:A:18:12.144:35.116:24.033:21.82
C:LYS:A:18:11.301:35.19:25.294:20.55
O:LYS:A:18:11.071:34.163:25.936:21.12
CB:LYS:A:18:13.624:35.111:24.441:20.42
CG:LYS:A:18:14.518:34.782:23.279:20.61
CD:LYS:A:18:16.015:34.803:23.664:30.84
CE:LYS:A:18:16.866:34.3:22.484:38.22
NZ:LYS:A:18:18.269:33.984:22.906:62
H:LYS:A:18:12.546:36.685:22.889:24.05
HA:LYS:A:18:11.951:34.276:23.589:26.19
HB2:LYS:A:18:13.867:35.989:24.772:24.51
HB3:LYS:A:18:13.763:34.442:25.13:24.51
HG2:LYS:A:18:14.303:33.894:22.954:24.73
HG3:LYS:A:18:14.379:35.436:22.576:24.73
HD2:LYS:A:18:16.284:35.711:23.875:37
HD3:LYS:A:18:16.163:34.218:24.424:37
HE2:LYS:A:18:16.468:33.491:22.125:45.86
HE3:LYS:A:18:16.902:34.987:21.8:45.86
HZ1:LYS:A:18:18.739:33.696:22.207:74.4
HZ2:LYS:A:18:18.658:34.713:23.236:74.4
HZ3:LYS:A:18:18.263:33.351:23.531:74.4
N:TYR:A:19:10.88:36.384:25.687:25.2
CA:TYR:A:19:10.118:36.604:26.923:20.68
C:TYR:A:19:8.575:36.613:26.737:31.44
O:TYR:A:19:7.832:36.875:27.687:29.68
CB:TYR:A:19:10.538:37.943:27.555:20.37
CG:TYR:A:19:11.901:37.935:28.109:23.44
CD1:TYR:A:19:13:38.247:27.323:19.93
CD2:TYR:A:19:12.117:37.579:29.428:23.18
CE1:TYR:A:19:14.278:38.224:27.859:26.81
CE2:TYR:A:19:13.379:37.562:29.96:25.73
CZ:TYR:A:19:14.444:37.864:29.184:22.56
OH:TYR:A:19:15.682:37.826:29.75:22.36
H:TYR:A:19:11.025:37.107:25.245:30.24
HA:TYR:A:19:10.335:35.898:27.552:24.82
HB2:TYR:A:19:10.498:38.635:26.876:24.45
HB3:TYR:A:19:9.926:38.154:28.276:24.45
HD2:TYR:A:19:11.39:37.364:29.968:27.82
HD1:TYR:A:19:12.877:38.483:26.431:23.92
HE2:TYR:A:19:13.505:37.32:30.849:30.88
HE1:TYR:A:19:15.015:38.436:27.332:32.17
HH:TYR:A:19:16.265:38.03:29.18:26.83
O:CY3:A:20:6.334:34.016:25.918:46.46
C:CY3:A:20:5.968:35.121:26.067:39.6
N1:CY3:A:20:4.848:35.386:26.929:43.25
CA:CY3:A:20:6.666:36.307:25.294:21.87
N:CY3:A:20:8.084:36.362:25.53:22.5
CB:CY3:A:20:6.382:35.984:23.834:33.52
SG:CY3:A:20:6.832:37.458:22.767:39.89
H:CY3:A:20:8.534:36.217:24.812:27
HA:CY3:A:20:6.252:37.151:25.536:26.25
HB2:CY3:A:20:5.439:35.782:23.725:40.22
HB3:CY3:A:20:6.908:35.214:23.567:40.22
HN11:CY3:A:20:4.569:36.191:27.039:51.9
HN12:CY3:A:20:4.467:34.738:27.347:51.9
O:THR:B:-1:16.056:46.908:9.868:60.34
N:THR:B:-1:16.406:48.652:7.605:78.37
CA:THR:B:-1:17.132:48.822:8.897:76.87
C:THR:B:-1:17.109:47.519:9.689:64.38
CB:THR:B:-1:16.526:49.975:9.74:82.36
OG1:THR:B:-1:17.021:51.231:9.25:103.8
CG2:THR:B:-1:16.88:49.85:11.228:68.98
H1:THR:B:-1:16.283:49.449:7.227:94.05
H2:THR:B:-1:16.886:48.137:7.061:94.05
H3:THR:B:-1:15.617:48.27:7.756:94.05
HA:THR:B:-1:18.058:49.042:8.712:92.25
HB:THR:B:-1:15.56:49.958:9.656:98.83
HG1:THR:B:-1:16.698:51.862:9.7:124.55
HG21:THR:B:-1:16.486:50.584:11.725:82.78
HG22:THR:B:-1:16.538:49.013:11.58:82.78

【表５－４】

HG23:THR:B:-1:17.843:49.871:11.343:82.78
O:PHE:B:0:17.693:47.018:12.852:32.11
N:PHE:B:0:18.285:47.117:10.17:47.49
CA:PHE:B:0:18.434:45.859:10.88:33.82
C:PHE:B:0:17.777:45.945:12.258:30.41
CB:PHE:B:0:19.916:45.528:11.007:28.4
CG:PHE:B:0:20.185:44.138:11.419:27.64
CD2:PHE:B:0:20.443:43.17:10.471:29.44
CD1:PHE:B:0:20.187:43.786:12.753:26.31
CE2:PHE:B:0:20.706:41.883:10.832:27.99
CE1:PHE:B:0:20.454:42.477:13.135:27.97
CZ:PHE:B:0:20.702:41.517:12.166:27.51
H:PHE:B:0:19.016:47.564:10.094:56.99
HA:PHE:B:0:18.003:45.151:10.377:40.59
HB2:PHE:B:0:20.342:45.669:10.147:34.08
HB3:PHE:B:0:20.311:46.115:11.67:34.08
HD1:PHE:B:0:20.017:44.431:13.402:31.58
HD2:PHE:B:0:20.445:43.402:9.571:35.33
HE1:PHE:B:0:20.45:42.243:14.035:33.57
HE2:PHE:B:0:20.874:41.244:10.177:33.58
HZ:PHE:B:0:20.881:40.638:12.411:33.01
O:ASP:B:1:18.276:43.923:15.696:23.3
N:ASP:B:1:17.325:44.791:12.774:25.54
CA:ASP:B:1:16.642:44.721:14.072:24.29
C:ASP:B:1:17.702:44.882:15.159:25.42
CB:ASP:B:1:15.863:43.408:14.192:30.99
CG:ASP:B:1:15.425:43.112:15.613:33.34
OD1:ASP:B:1:15.172:44.1:16.35:26.15
OD2:ASP:B:1:15.36:41.913:16.004:22.1
H:ASP:B:1:17.404:44.028:12.384:30.65
HA:ASP:B:1:16.014:45.456:14.145:29.15
HB2:ASP:B:1:15.068:43.46:13.639:37.19
HB3:ASP:B:1:16.427:42.677:13.894:37.19
O:THR:B:2:17.54:46.872:18.038:27.96
N:THR:B:2:18.026:46.134:15.452:24.07
CA:THR:B:2:19.15:46.377:16.357:23.86
C:THR:B:2:18.686:46.539:17.782:24.18
CB:THR:B:2:19.911:47.632:15.99:31.47
OG1:THR:B:2:18.958:48.664:15.749:33.31
CG2:THR:B:2:20.815:47.367:14.758:33.17
H:THR:B:2:17.631:46.838:15.155:28.88
HA:THR:B:2:19.762:45.626:16.318:28.64
HB:THR:B:2:20.479:47.889:16.733:37.77
HG1:THR:B:2:19.352:49.376:15.542:39.98
HG21:THR:B:2:21.302:48.173:14.525:39.81
HG22:THR:B:2:21.45:46.662:14.959:39.81
HG23:THR:B:2:20.272:47.097:14.001:39.81
C:HYP:B:3:18.617:47.825:20.609:37.46
O:HYP:B:3:19.172:48.867:20.197:33.28
CA:HYP:B:3:19.208:46.443:20.27:30.06
CB:HYP:B:3:20.366:46.23:20.929:46.37
CG:HYP:B:3:21.21:45.388:19.961:34.65
OD1:HYP:B:3:20.787:44.116:19.901:37.02
CD:HYP:B:3:20.889:46.065:18.606:30.67
N:HYP:B:3:19.59:46.315:18.708:25.2
HD23:HYP:B:3:21.065:45.458:17.869:36.81
HD22:HYP:B:3:21.39:46.89:18.507:36.81
HG:HYP:B:3:22.156:45.447:20.171:41.58
HD1:HYP:B:3:21.078:43.754:19.188:44.43
HB3:HYP:B:3:20.807:47.074:21.115:55.65
HB2:HYP:B:3:20.201:45.739:21.749:55.65
HA:HYP:B:3:18.572:45.748:20.503:36.08
O:LYS:B:4:16.271:47.848:23.837:25.52
N:LYS:B:4:17.521:47.837:21.368:29.31
CA:LYS:B:4:16.899:49.058:21.865:26.28
C:LYS:B:4:16.634:48.93:23.365:21.83
CB:LYS:B:4:15.558:49.322:21.159:37.68
CG:LYS:B:4:15.666:49.595:19.675:65.23
CD:LYS:B:4:14.269:49.657:19.051:94.75
CE:LYS:B:4:14.289:50.089:17.586:109.16
NZ:LYS:B:4:12.904:50.217:17.038:105.24
H:LYS:B:4:17.109:47.124:21.616:35.17
HA:LYS:B:4:17.488:49.813:21.713:31.53
HB2:LYS:B:4:14.99:48.544:21.273:45.21
HB3:LYS:B:4:15.139:50.094:21.569:45.21
HG2:LYS:B:4:16.106:50.447:19.533:78.28
HG3:LYS:B:4:16.163:48.879:19.248:78.28
HD2:LYS:B:4:13.864:48.777:19.098:113.71
HD3:LYS:B:4:13.732:50.296:19.544:113.71
HE2:LYS:B:4:14.727:50.951:17.511:130.99
HE3:LYS:B:4:14.763:49.424:17.062:130.99
HZ1:LYS:B:4:12.937:50.469:16.185:126.28
HZ2:LYS:B:4:12.482:49.435:17.093:126.28
HZ3:LYS:B:4:12.449:50.825:17.502:126.28
O:HIS:B:5:14.227:50.871:24.963:32.55
N:HIS:B:5:16.734:50.025:24.109:21.79
CA:HIS:B:5:16.363:50.01:25.519:21.56
C:HIS:B:5:14.857:50.045:25.607:22.3
CB:HIS:B:5:16.937:51.202:26.275:22.18
CG:HIS:B:5:18.423:51.204:26.337:22.64
ND1:HIS:B:5:19.131:50.545:27.328:28.27
CD2:HIS:B:5:19.345:51.765:25.516:25.48
CE1:HIS:B:5:20.428:50.699:27.11:22.51
NE2:HIS:B:5:20.585:51.441:26.022:28.72
H:HIS:B:5:17.013:50.786:23.824:26.15
HA:HIS:B:5:16.682:49.193:25.934:25.87
HB2:HIS:B:5:16.657:52.018:25.832:26.62
HB3:HIS:B:5:16.601:51.188:27.185:26.62
HD1:HIS:B:5:18.784:50.097:27.975:33.93
HD2:HIS:B:5:19.173:52.273:24.756:30.58
HE1:HIS:B:5:21.112:50.36:27.64:27.01
N:ARG:B:6:14.278:49.126:26.37:20.97
CA:ARG:B:6:12.838:49.07:26.561:24.52
C:ARG:B:6:12.608:49.07:28.058:21.26
O:ARG:B:6:12.884:48.066:28.727:23.78
CB:ARG:B:6:12.238:47.832:25.893:20.69
CG:ARG:B:6:12.796:47.582:24.53:26.83
CD:ARG:B:6:12.576:46.115:24.096:33.07
NE:ARG:B:6:13.308:45.832:22.86:31.36
CZ:ARG:B:6:12.807:45.919:21.638:20.49
NH1:ARG:B:6:11.527:46.276:21.431:28.98
NH2:ARG:B:6:13.594:45.629:20.612:25.07

【表５－５】

H:ARG:B:6:14.707:48.515:26.795:25.17
HA:ARG:B:6:12.425:49.861:26.181:29.42
HB2:ARG:B:6:12.426:47.054:26.441:24.83
HB3:ARG:B:6:11.279:47.953:25.806:24.83
HG2:ARG:B:6:12.352:48.159:23.89:32.19
HG3:ARG:B:6:13.75:47.758:24.537:32.19
HD2:ARG:B:6:12.903:45.519:24.789:39.68
HD3:ARG:B:6:11.632:45.963:23.935:39.68
HE:ARG:B:6:14.13:45.591:22.934:37.64
HH11:ARG:B:6:11.019:46.461:22.1:34.78
HH12:ARG:B:6:11.218:46.324:20.63:34.78
HH21:ARG:B:6:14.411:45.398:20.748:30.08
HH22:ARG:B:6:13.289:45.676:19.809:30.08
N:CYS:B:7:12.125:50.193:28.588:22.09
CA:CYS:B:7:12.018:50.387:30.028:24.41
C:CYS:B:7:10.61:50.801:30.421:28.77
O:CYS:B:7:9.878:51.453:29.662:23.73
CB:CYS:B:7:12.995:51.452:30.534:25.61
SG:CYS:B:7:14.735:51.095:30.241:32.01
H:CYS:B:7:11.851:50.864:28.126:26.51
HA:CYS:B:7:12.223:49.551:30.477:29.3
HB2:CYS:B:7:12.791:52.292:30.093:30.73
HB3:CYS:B:7:12.874:51.551:31.492:30.73
N:GLY:B:8:10.246:50.438:31.636:23.3
CA:GLY:B:8:8.941:50.832:32.13:24.26
C:GLY:B:8:7.848:50.372:31.198:27.94
O:GLY:B:8:7.783:49.176:30.882:23.54
H:GLY:B:8:10.721:49.975:32.183:27.96
HA2:GLY:B:8:8.79:50.442:33.005:29.11
HA3:GLY:B:8:8.898:51.798:32.208:29.11
N:SER:B:9:7.045:51.325:30.7:25.43
CA:SER:B:9:5.825:51.05:29.947:28.83
C:SER:B:9:6.127:50.664:28.495:33.52
O:SER:B:9:5.335:49.988:27.841:31.13
CB:SER:B:9:4.914:52.281:29.986:36.62
OG:SER:B:9:5.573:53.396:29.4:36.38
H:SER:B:9:7.199:52.166:30.793:30.51
HA:SER:B:9:5.353:50.312:30.364:34.6
HB2:SER:B:9:4.104:52.092:29.487:43.94
HB3:SER:B:9:4.698:52.488:30.908:43.94
HG:SER:B:9:6.279:53.567:29.822:43.65
N:CGU:B:10:7.28:51.095:27.998:28.76
CA:CGU:B:10:7.81:50.596:26.686:28.05
CB:CGU:B:10:9.239:51.112:26.411:26.61
CG:CGU:B:10:9.333:52.622:26.497:48.2
CD1:CGU:B:10:10.796:53.099:26.309:43.27
OE12:CGU:B:10:10.997:54.252:25.818:32.43
OE11:CGU:B:10:11.775:52.332:26.659:28.59
CD2:CGU:B:10:8.34:53.322:25.507:61.07
OE21:CGU:B:10:8.191:52.877:24.334:60.62
OE22:CGU:B:10:7.665:54.311:25.914:71.45
C:CGU:B:10:7.888:49.082:26.653:29.41
O:CGU:B:10:7.883:48.518:25.527:30.26
HG:CGU:B:10:9.037:52.937:27.534:57.84
HB3:CGU:B:10:9.957:50.658:27.117:31.93
HB2:CGU:B:10:9.575:50.754:25.412:31.93
HA:CGU:B:10:7.113:50.935:25.873:33.66
N:ILE:B:11:8.048:48.421:27.803:25.25
CA:ILE:B:11:8.061:46.962:27.816:21.79
C:ILE:B:11:6.652:46.486:27.505:22.28
O:ILE:B:11:6.473:45.595:26.699:22.22
CB:ILE:B:11:8.584:46.402:29.14:29.42
CG1:ILE:B:11:10.089:46.697:29.267:30.34
CG2:ILE:B:11:8.328:44.893:29.247:23.17
CD1:ILE:B:11:10.655:46.443:30.653:34.61
H:ILE:B:11:8.15:48.789:28.574:30.3
HA:ILE:B:11:8.645:46.647:27.108:26.14
HB:ILE:B:11:8.12:46.846:29.867:35.31
HG12:ILE:B:11:10.571:46.133:28.643:36.41
HG13:ILE:B:11:10.243:47.63:29.052:36.41
HG21:ILE:B:11:8.671:44.574:30.097:27.8
HG22:ILE:B:11:7.373:44.731:29.195:27.8
HG23:ILE:B:11:8.781:44.443:28.517:27.8
HD11:ILE:B:11:11.603:46.651:30.649:41.53
HD12:ILE:B:11:10.194:47.009:31.291:41.53
HD13:ILE:B:11:10.522:45.509:30.881:41.53
N:THR:B:12:5.642:47.089:28.133:23.69
CA:THR:B:12:4.264:46.785:27.759:27.8
C:THR:B:12:4.051:46.987:26.269:32.55
O:THR:B:12:3.511:46.106:25.58:24.04
CB:THR:B:12:3.292:47.642:28.58:33.52
OG1:THR:B:12:3.502:47.358:29.965:32.74
CG2:THR:B:12:1.803:47.355:28.223:26.3
H:THR:B:12:5.726:47.666:28.765:28.42
HA:THR:B:12:4.082:45.854:27.961:33.36
HB:THR:B:12:3.471:48.581:28.413:40.23
HG1:THR:B:12:2.979:47.818:30.435:39.29
HG21:THR:B:12:1.22:47.914:28.761:31.56
HG22:THR:B:12:1.644:47.545:27.285:31.56
HG23:THR:B:12:1.594:46.424:28.396:31.56
N:ASN:B:13:4.453:48.15:25.751:24.48
CA:ASN:B:13:4.301:48.421:24.321:25.34
C:ASN:B:13:4.974:47.353:23.491:24.13
O:ASN:B:13:4.462:46.938:22.439:24.08
CB:ASN:B:13:4.909:49.776:23.943:28.08
CG:ASN:B:13:4.169:50.958:24.563:43.36
OD1:ASN:B:13:3.038:50.826:25.036:39.56
ND2:ASN:B:13:4.82:52.121:24.575:47.85
H:ASN:B:13:4.812:48.79:26.2:29.38
HA:ASN:B:13:3.358:48.435:24.096:30.41
HB2:ASN:B:13:5.829:49.805:24.249:33.69
HB3:ASN:B:13:4.877:49.876:22.978:33.69
HD21:ASN:B:13:4.449:52.819:24.913:57.42
HD22:ASN:B:13:5.612:52.174:24.244:57.42
N:SER:B:14:6.155:46.925:23.918:22.66
CA:SER:B:14:6.85:45.888:23.173:21.94
C:SER:B:14:6.098:44.563:23.22:21.87
O:SER:B:14:5.951:43.898:22.193:22.01
CB:SER:B:14:8.269:45.758:23.696:25.08
OG:SER:B:14:9.033:46.775:23.091:24.01
H:SER:B:14:6.565:47.209:24.618:27.19
HA:SER:B:14:6.904:46.16:22.243:26.33

【表５－６】

HB2:SER:B:14:8.274:45.874:24.659:30.1
HB3:SER:B:14:8.63:44.891:23.453:30.1
HG:SER:B:14:9.828:46.735:23.358:28.81
N:TYR:B:15:5.629:44.144:24.4:21.89
CA:TYR:B:15:4.768:42.964:24.454:22.13
C:TYR:B:15:3.609:43.089:23.478:22.94
O:TYR:B:15:3.283:42.128:22.771:23.01
CB:TYR:B:15:4.193:42.718:25.852:22.53
CG:TYR:B:15:5.115:42.148:26.893:22.01
CD1:TYR:B:15:5.679:40.889:26.759:37.65
CD2:TYR:B:15:5.351:42.85:28.079:48.14
CE1:TYR:B:15:6.507:40.375:27.747:62.89
CE2:TYR:B:15:6.165:42.337:29.078:52.81
CZ:TYR:B:15:6.748:41.113:28.908:60.82
OH:TYR:B:15:7.558:40.637:29.929:54.81
H:TYR:B:15:5.789:44.514:25.16:26.27
HA:TYR:B:15:5.287:42.185:24.203:26.56
HB2:TYR:B:15:3.868:43.565:26.195:27.03
HB3:TYR:B:15:3.448:42.104:25.765:27.03
HD1:TYR:B:15:5.53:40.399:25.982:45.19
HD2:TYR:B:15:4.966:43.688:28.195:57.77
HE1:TYR:B:15:6.897:39.537:27.638:75.46
HE2:TYR:B:15:6.328:42.83:29.85:63.37
HH:TYR:B:15:7.597:41.201:30.551:65.77
N:MET:B:16:2.967:44.255:23.427:23.8
CA:MET:B:16:1.803:44.423:22.544:28.09
C:MET:B:16:2.197:44.329:21.083:26.65
O:MET:B:16:1.471:43.748:20.275:36.43
CB:MET:B:16:1.118:45.775:22.768:30.99
CG:MET:B:16:0.499:45.977:24.148:42.33
SD:MET:B:16:-0.954:44.949:24.404:68.25
CE:MET:B:16:-0.206:43.67:25.426:42.42
H:MET:B:16:3.177:44.953:23.883:28.56
HA:MET:B:16:1.157:43.726:22.74:33.71
HB2:MET:B:16:1.775:46.477:22.639:37.19
HB3:MET:B:16:0.409:45.872:22.114:37.19
HG2:MET:B:16:1.153:45.748:24.826:50.79
HG3:MET:B:16:0.232:46.905:24.243:50.79
HE1:MET:B:16:-0.883:43.016:25.657:50.9
HE2:MET:B:16:0.508:43.245:24.926:50.9
HE3:MET:B:16:0.15:44.078:26.231:50.9
N:ASP:B:17:3.344:44.897:20.719:29.89
CA:ASP:B:17:3.758:44.849:19.322:34.2
C:ASP:B:17:4.362:43.503:18.931:30.46
O:ASP:B:17:4.224:43.095:17.781:28.87
CB:ASP:B:17:4.769:45.957:19.002:41.66
CG:ASP:B:17:4.239:47.347:19.307:78.78
OD1:ASP:B:17:3:47.511:19.374:89.35
OD2:ASP:B:17:5.064:48.277:19.478:72.64
H:ASP:B:17:3.887:45.306:21.246:35.87
HA:ASP:B:17:2.978:44.994:18.764:41.04
HB2:ASP:B:17:5.569:45.818:19.534:49.99
HB3:ASP:B:17:4.989:45.92:18.058:49.99
N:LEU:B:18:5.062:42.822:19.831:22.66
CA:LEU:B:18:5.868:41.669:19.444:22.1
C:LEU:B:18:5.314:40.329:19.885:22.41
O:LEU:B:18:5.69:39.304:19.308:24.4
CB:LEU:B:18:7.286:41.806:20.002:22.61
CG:LEU:B:18:7.948:43.093:19.512:21.46
CD1:LEU:B:18:9.302:43.234:20.155:24.5
CD2:LEU:B:18:8.07:43.128:17.966:28.1
H:LEU:B:18:5.088:43.006:20.671:27.19
HA:LEU:B:18:5.935:41.652:18.476:26.53
HB2:LEU:B:18:7.249:41.832:20.971:27.14
HB3:LEU:B:18:7.823:41.055:19.704:27.14
HG:LEU:B:18:7.407:43.85:19.787:25.75
HD11:LEU:B:18:9.717:44.053:19.841:29.4
HD12:LEU:B:18:9.192:43.267:21.118:29.4
HD13:LEU:B:18:9.848:42.471:19.91:29.4
HD21:LEU:B:18:8.494:43.959:17.702:33.72
HD22:LEU:B:18:8.607:42.375:17.675:33.72
HD23:LEU:B:18:7.183:43.071:17.578:33.72
N:CYS:B:19:4.481:40.285:20.912:26.31
CA:CYS:B:19:4.018:39.001:21.403:23.2
C:CYS:B:19:2.573:38.743:21.045:29.55
O:CYS:B:19:2.204:37.602:20.812:27.61
CB:CYS:B:19:4.199:38.915:22.923:25.28
SG:CYS:B:19:5.942:39.114:23.454:33.59
H:CYS:B:19:4.174:40.968:21.334:31.58
HA:CYS:B:19:4.553:38.3:21:27.84
HB2:CYS:B:19:3.677:39.617:23.342:30.34
HB3:CYS:B:19:3.891:38.047:23.227:30.34
O:TYR:B:20:0.453:40.693:18.643:58.94
N:TYR:B:20:1.763:39.78:20.969:30.88
CA:TYR:B:20:0.33:39.624:20.788:36.15
C:TYR:B:20:-0.046:39.793:19.324:48.21
CB:TYR:B:20:-0.44:40.615:21.651:29.56
CG:TYR:B:20:-0.651:40.122:23.065:55.92
CD1:TYR:B:20:-1.597:39.145:23.34:71.32
CD2:TYR:B:20:0.094:40.621:24.118:59.77
CE1:TYR:B:20:-1.8:38.679:24.621:72.77
CE2:TYR:B:20:-0.098:40.161:25.411:73.5
CZ:TYR:B:20:-1.058:39.185:25.659:74.33
OH:TYR:B:20:-1.29:38.681:26.931:61.61
H:TYR:B:20:2.02:40.599:21.019:37.06
HA:TYR:B:20:0.074:38.728:21.06:43.38
HB2:TYR:B:20:0.055:41.447:21.695:35.48
HB3:TYR:B:20:-1.312:40.768:21.254:35.48
HD1:TYR:B:20:-2.106:38.797:22.644:85.58
HD2:TYR:B:20:0.735:41.274:23.956:71.73
HE1:TYR:B:20:-2.44:38.024:24.782:87.33
HE2:TYR:B:20:0.409:40.506:26.11:88.2
HH:TYR:B:20:-0.786:39.058:27.486:73.93
O:ARG:B:21:-2.375:41.115:18.001:73.56
N:ARG:B:21:-0.904:38.888:18.851:48.09
CA:ARG:B:21:-1.505:38.926:17.518:54.86
C:ARG:B:21:-2.02:40.306:17.132:67.04
CB:ARG:B:21:-2.675:37.949:17.448:56.88
CG:ARG:B:21:-2.44:36.661:16.704:66.58
CD:ARG:B:21:-3.714:36.364:15.961:87.2
NE:ARG:B:21:-3.936:34.955:15.663:104.85
CZ:ARG:B:21:-5.147:34.397:15.619:123.5

【表５－７】

NH1:ARG:B:21:-6.239:35.129:15.88:136.71	HE:ARG:B:21:-3.252:34.434:15.65:125.82
NH2:ARG:B:21:-5.27:33.101:15.333:115.82	HH11:ARG:B:21:-6.162:35.965:16.065:164.05
OXT:ARG:B:21:-2.121:40.62:15.939:68.47	HH12:ARG:B:21:-7.017:34.764:15.855:164.05
H:ARG:B:21:-1.164:38.209:19.309:57.7	HH21:ARG:B:21:-4.571:32.628:15.17:138.98
HA:ARG:B:21:-0.844:38.656:16.862:65.83	HH22:ARG:B:21:-6.049:32.738:15.311:138.98
HB2:ARG:B:21:-2.926:37.714:18.355:68.25	
HB3:ARG:B:21:-3.418:38.398:17.016:68.25	
HG2:ARG:B:21:-1.716:36.768:16.067:79.9	
HG3:ARG:B:21:-2.258:35.94:17.327:79.9	
HD2:ARG:B:21:-4.462:36.672:16.495:104.64	
HD3:ARG:B:21:-3.698:36.842:15.117:104.64	

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【請求項２５】

少なくとも１個のジスルフィド結合を介してＢ鎖ペプチドに結合しているＡ鎖ペプチドを有する治療用タンパク質であって、前記Ａ鎖はＧＩＶＥＱＣＣＨＲＩＣＳＬＹＱＬＥＮＹＣＮ（配列番号３９）の配列を含み、前記Ｂ鎖ペプチドはＦＶＮＱＨＬＣＧＳＥＬＶＥＡＬＹＬＶＣＹＥＲ（配列番号３０）の配列を含む、治療用タンパク質。