



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:30 AM UTC

PDB ID : 8CAT / pdb\_00008cat  
Title : The NADPH binding site on beef liver catalase  
Authors : Murthy, M.R.N.; Reid III, T.J.; Sicignano, A.; Tanaka, N.; Fita, I.; Rossmann, M.G.  
Deposited on : 1984-11-15  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

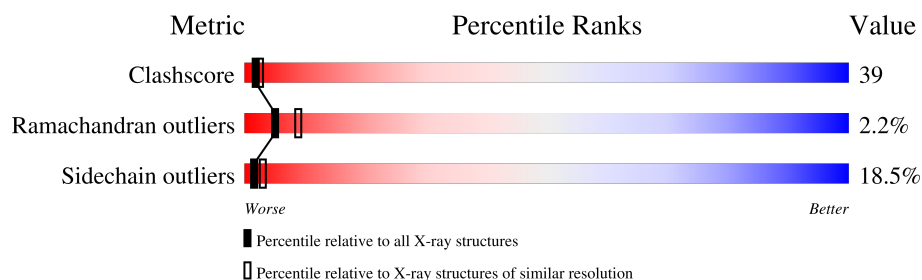
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 6492 (2.50-2.50)                                      |
| Ramachandran outliers | 187476                      | 6378 (2.50-2.50)                                      |
| Sidechain outliers    | 187428                      | 6380 (2.50-2.50)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 506    |                  |
| 1   | B     | 506    |                  |

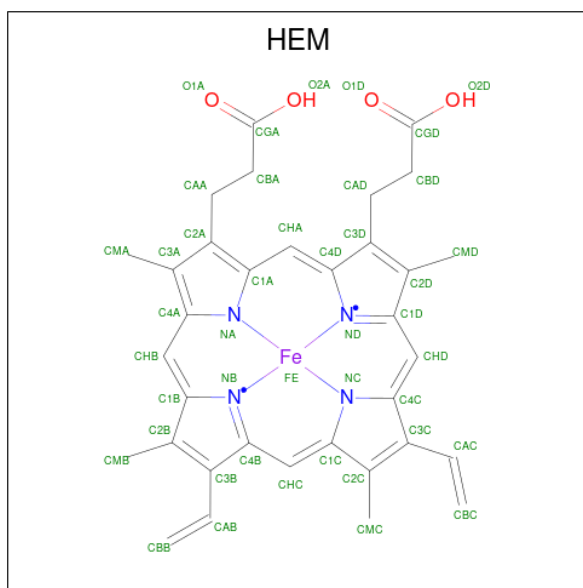
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | NDP  | A     | 508 | X         | -        | -       | -                |
| 3   | NDP  | B     | 508 | X         | -        | -       | -                |



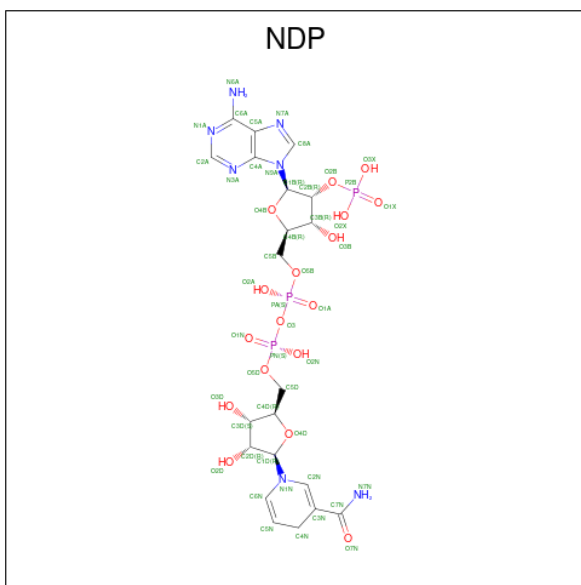
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$ ).



| Mol | Chain | Residues | Atoms       |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 3   | A     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 3   | B     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |

- Molecule 4 is water.

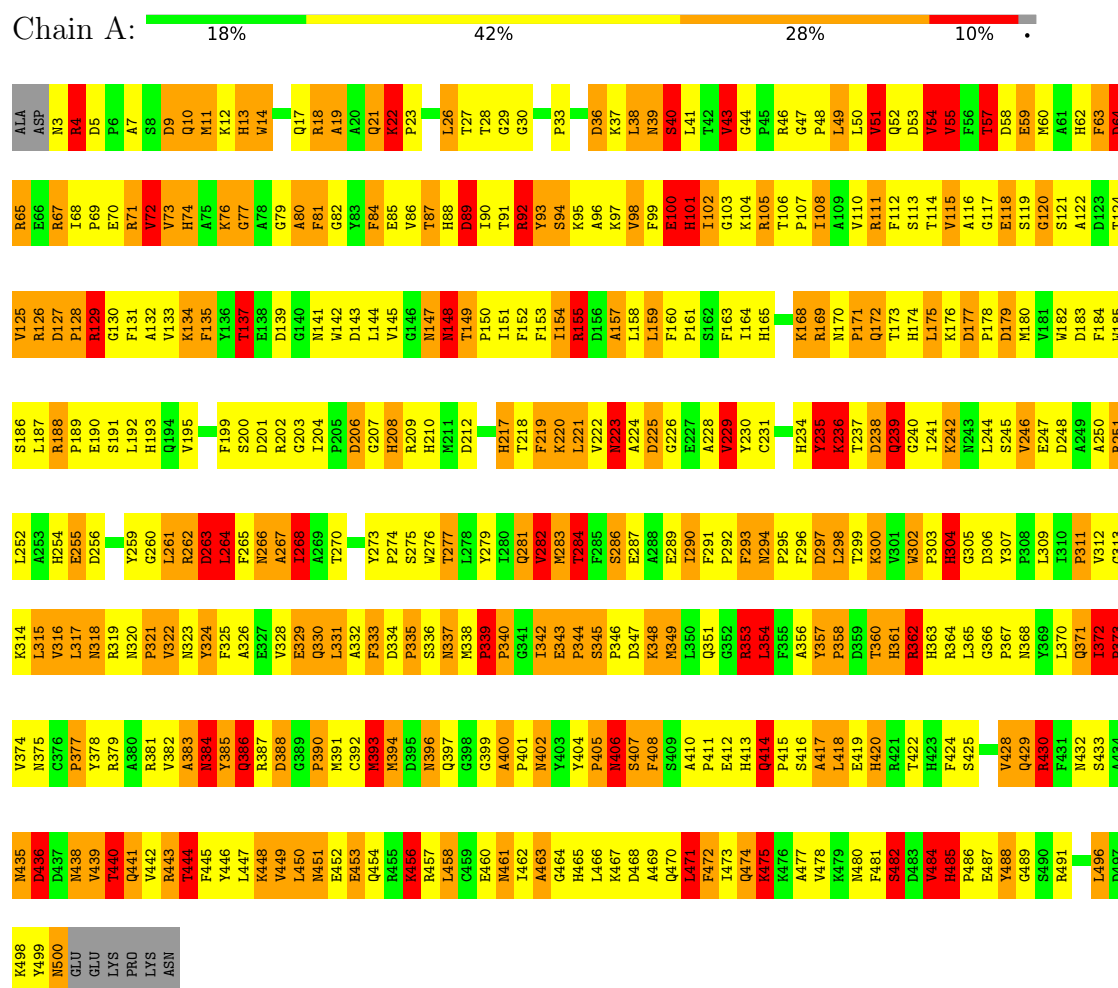
| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 4   | A     | 48       | Total O<br>48 48 | 0       | 0       |
| 4   | B     | 50       | Total O<br>50 50 | 0       | 0       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: CATALASE



|      |      |      |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     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| D497 | D498 | Y499 | GLU | GLU | LYS | PRO | LYS | ASN | D436 | D437 | N438 | V439 | T440 | Q441 | V442 | R443 | T444 | Y445 | Y446 | L447 | K448 | V449 | N450 | L451 | E452 | E453 | Q454 | R455 | K456 | R457 | L458 | C459 | E460 | N461 | I462 | A463 | G464 | H465 | L466 | K467 | D468 | A469 | Q470 | L471 | F472 | I473 | Q474 | K475 | K476 | A477 | V478 | K479 | N480 | F481 | S482 | D483 | V484 | H485 | P486 | E487 | Y488 | R491 | I492 | Q493 | A494 | L495 | L496 | N495 | M496 | N497 | N498 | N499 | N500 | V501 | T502 | T503 | T504 | T505 | T506 | T507 | T508 | T509 | T510 | T511 | T512 | T513 | T514 | T515 | T516 | T517 | T518 | T519 | T520 | T521 | T522 | T523 | T524 | T525 | T526 | T527 | T528 | T529 | T530 | T531 | T532 | T533 | T534 | T535 | T536 | T537 | T538 | T539 | T540 | T541 | T542 | T543 | T544 | T545 | T546 | T547 | T548 | T549 | T550 | T551 | T552 | T553 | T554 | T555 | T556 | T557 | T558 | T559 | T560 | T561 | T562 | T563 | T564 | T565 | T566 | T567 | T568 | T569 | T570 | T571 | T572 | T573 | T574 | T575 | T576 | T577 | T578 | T579 | T580 | T581 | T582 | T583 | T584 | T585 | T586 | T587 | T588 | T589 | T590 | T591 | T592 | T593 | T594 | T595 | T596 | T597 | T598 | T599 | T600 | T601 | T602 | T603 | T604 | T605 | T606 | T607 | T608 | T609 | T610 | T611 | T612 | T613 | T614 | T615 | T616 | T617 | T618 | T619 | T620 | T621 | T622 | T623 | T624 | T625 | T626 | T627 | T628 | T629 | T630 | T631 | T632 | T633 | T634 | T635 | T636 | T637 | T638 | T639 | T640 | T641 | T642 | T643 | T644 | T645 | T646 | T647 | T648 | T649 | T650 | T651 | T652 | T653 | T654 | T655 | T656 | T657 | T658 | T659 | T660 | T661 | T662 | T663 | T664 | T665 | T666 | T667 | T668 | T669 | T670 | T671 | T672 | T673 | T674 | T675 | T676 | T677 | T678 | T679 | T680 | T681 | T682 | T683 | T684 | T685 | T686 | T687 | T688 | T689 | T690 | T691 | T692 | T693 | T694 | T695 | T696 | T697 | T698 | T699 | T700 | T701 | T702 | T703 | T704 | T705 | T706 | T707 | T708 | T709 | T710 | T711 | T712 | T713 | T714 | T715 | T716 | T717 | T718 | T719 | T720 | T721 | T722 | T723 | T724 | T725 | T726 | T727 | T728 | T729 | T730 | T731 | T732 | T733 | T734 | T735 | T736 | T737 | T738 | T739 | T740 | T741 | T742 | T743 | T744 | T745 | T746 | T747 | T748 | T749 | T750 | T751 | T752 | T753 | T754 | T755 | T756 | T757 | T758 | T759 | T760 | T761 | T762 | T763 | T764 | T765 | T766 | T767 | T768 | T769 | T770 | T771 | T772 | T773 | T774 | T775 | T776 | T777 | T778 | T779 | T780 | T781 | T782 | T783 | T784 | T785 | T786 | T787 | T788 | T789 | T790 | T791 | T792 | T793 | T794 | T795 | T796 | T797 | T798 | T799 | T800 | T801 | T802 | T803 | T804 | T805 | T806 | T807 | T808 | T809 | T810 | T811 | T812 | T813 | T814 | T815 | T816 | T817 | T818 | T819 | T820 | T821 | T822 | T823 | T824 | T825 | T826 | T827 | T828 | T829 | T830 | T831 | T832 | T833 | T834 | T835 | T836 | T837 | T838 | T839 | T840 | T841 | T842 | T843 | T844 | T845 | T846 | T847 | T848 | T849 | T850 | T851 | T852 | T853 | T854 | T855 | T856 | T857 | T858 | T859 | T860 | T861 | T862 | T863 | T864 | T865 | T866 | T867 | T868 | T869 | T870 | T871 | T872 | T873 | T874 | T875 | T876 | T877 | T878 | T879 | T880 | T881 | T882 | T883 | T884 | T885 | T886 | T887 | T888 | T889 | T890 | T891 | T892 | T893 | T894 | T895 | T896 | T897 | T898 | T899 | T900 | T901 | T902 | T903 | T904 | T905 | T906 | T907 | T908 | T909 | T910 | T911 | T912 | T913 | T914 | T915 | T916 | T917 | T918 | T919 | T920 | T921 | T922 | T923 | T924 | T925 | T926 | T927 | T928 | T929 | T930 | T931 | T932 | T933 | T934 | T935 | T936 | T937 | T938 | T939 | T940 | T941 | T942 | T943 | T944 | T945 | T946 | T947 | T948 | T949 | T950 | T951 | T952 | T953 | T954 | T955 | T956 | T957 | T958 | T959 | T960 | T961 | T962 | T963 | T964 | T965 | T966 | T967 | T968 | T969 | T970 | T971 | T972 | T973 | T974 | T975 | T976 | T977 | T978 | T979 | T980 | T981 | T982 | T983 | T984 | T985 | T986 | T987 | T988 | T989 | T990 | T991 | T992 | T993 | T994 | T995 | T996 | T997 | T998 | T999 | 1000 | 1001 | 1002 | 1003 | 1004 | 1005 | 1006 | 1007 | 1008 | 1009 | 1010 | 1011 | 1012 | 1013 | 1014 | 1015 | 1016 | 1017 | 1018 | 1019 | 1020 | 1021 | 1022 | 1023 | 1024 | 1025 | 1026 | 1027 | 1028 | 1029 | 1030 | 1031 | 1032 | 1033 | 1034 | 1035 | 1036 | 1037 | 1038 | 1039 | 1040 | 1041 | 1042 | 1043 | 1044 | 1045 | 1046 | 1047 | 1048 | 1049 | 1050 | 1051 | 1052 | 1053 | 1054 | 1055 | 1056 | 1057 | 1058 | 1059 | 1060 | 1061 | 1062 | 1063 | 1064 | 1065 | 1066 | 1067 | 1068 | 1069 | 1070 | 1071 | 1072 | 1073 | 1074 | 1075 | 1076 | 1077 | 1078 | 1079 | 1080 | 1081 | 1082 | 1083 | 1084 | 1085 | 1086 | 1087 | 1088 | 1089 | 1090 | 1091 | 1092 | 1093 | 1094 | 1095 | 1096 | 1097 | 1098 | 1099 | 1100 | 1101 | 1102 | 1103 | 1104 | 1105 | 1106 | 1107 | 1108 | 1109 | 1110 | 1111 | 1112 | 1113 | 1114 | 1115 | 1116 | 1117 | 1118 | 1119 | 1120 | 1121 | 1122 | 1123 | 1124 | 1125 | 1126 | 1127 | 1128 | 1129 | 1130 | 1131 | 1132 | 1133 | 1134 | 1135 | 1136 | 1137 | 1138 | 1139 | 1140 | 1141 | 1142 | 1143 | 1144 | 1145 | 1146 | 1147 | 1148 | 1149 | 1150 | 1151 | 1152 | 1153 | 1154 | 1155 | 1156 | 1157 | 1158 | 1159 | 1160 | 1161 | 1162 | 1163 | 1164 | 1165 | 1166 | 1167 | 1168 | 1169 | 1170 | 1171 | 1172 | 1173 | 1174 | 1175 | 1176 | 1177 | 1178 | 1179 | 1180 | 1181 | 1182 | 1183 | 1184 | 1185 | 1186 | 1187 | 1188 | 1189 | 1190 | 1191 | 1192 | 1193 | 1194 | 1195 | 1196 | 1197 | 1198 | 1199 | 1200 | 1201 | 1202 | 1203 | 1204 | 1205 | 1206 | 1207 | 1208 | 1209 | 1210 | 1211 | 1212 | 1213 | 1214 | 1215 | 1216 | 1217 | 1218 | 1219 | 1220 | 1221 | 1222 | 1223 | 1224 | 1225 | 1226 | 1227 | 1228 | 1229 | 1230 | 1231 | 1232 | 1233 | 1234 | 1235 | 1236 | 1237 | 1238 | 1239 | 1240 | 1241 | 1242 | 1243 | 1244 | 1245 | 1246 | 1247 | 1248 | 1249 | 1250 | 1251 | 1252 | 1253 | 1254 | 1255 | 1256 | 1257 | 1258 | 1259 | 1260 | 1261 | 1262 | 1263 | 1264 | 1265 | 1266 | 1267 | 1268 | 1269 | 1270 | 1271 | 1272 | 1273 | 1274 | 1275 | 1276 | 1277 | 1278 | 1279 | 1280 | 1281 | 1282 | 1283 | 1284 | 1285 | 1286 | 1287 | 1288 | 1289 | 1290 | 1291 | 1292 | 1293 | 1294 | 1295 | 1296 | 1297 | 1298 | 1299 | 1300 | 1301 | 1302 | 1303 | 1304 | 1305 | 1306 | 1307 | 1308 | 1309 | 1310 | 1311 | 1312 | 1313 | 1314 | 1315 | 1316 | 1317 | 1318 | 1319 | 1320 | 1321 | 1322 | 1323 | 1324 | 1325 | 1326 | 1327 | 1328 | 1329 | 1330 | 1331 | 1332 | 1333 | 1334 | 1335 | 1336 | 1337 | 1338 | 1339 | 1340 | 1341 | 1342 | 1343 | 1344 | 1345 | 1346 | 1347 | 1348 | 1349 | 1350 | 1351 | 1352 | 1353 | 1354 | 1355 | 1356 | 1357 | 1358 | 1359 | 1360 | 1361 | 1362 | 1363 | 1364 | 1365 | 1366 | 1367 | 1368 | 1369 | 1370 | 1371 | 1372 | 1373 | 1374 | 1375 | 1376 | 1377 | 1378 | 1379 | 1380 | 1381 | 1382 | 1383 | 1384 | 1385 | 1386 | 1387 | 1388 | 1389 | 1390 | 1391 | 1392 | 1393 | 1394 | 1395 | 1396 | 1397 | 1398 | 1399 | 1400 | 1401 | 1402 | 1403 | 1404 | 1405 | 1406 | 1407 | 1408 | 1409 | 1410 | 1411 | 1412 | 1413 | 1414 | 1415 | 1416 | 1417 | 1418 | 1419 | 1420 | 1421 | 1422 | 1423 | 1424 | 1425 | 1426 | 1427 | 1428 | 1429 | 1430 | 1431 | 1432 | 1433 | 1434 | 1435 | 1436 | 1437 | 1438 | 1439 | 1440 | 1441 | 1442 | 1443 | 1444 | 1445 | 1446 | 1447 | 1448 | 1449 | 1450 | 1451 | 1452 | 1453 | 1454 | 1455 | 1456 | 1457 | 1458 | 1459 | 1460 | 1461 | 1462 | 1463 | 1464 | 1465 | 1466 | 1467 | 1468 | 1469 | 1470 | 1471 | 1472 | 1473 | 1474 | 1475 | 1476 | 1477 | 1478 | 1479 | 1480 | 1481 | 1482 | 1483 | 1484 | 1485 | 1486 | 1487 | 1488 | 1489 | 1490 | 1491 | 1492 | 1493 | 1494 | 1495 | 1496 | 1497 | 1498 | 1499 | 1500 | 1501 | 1502 | 1503 | 1504 | 1505 | 1506 | 1507 | 1508 | 1509 | 1510 | 1511 | 1512 | 1513 | 1514 | 1515 | 1516 | 1517 | 1518 | 1519 | 1520 | 1521 | 1522 | 1523 | 1524 | 1525 | 1526 | 1527 | 1528 | 1529 | 1530 | 1531 | 1532 | 1533 | 1534 | 1535 | 1536 | 1537 | 1538 | 1539 | 1540 | 1541 | 1542 | 1543 | 1544 | 1545 | 1546 | 1547 | 1548 | 1549 | 1550 | 1551 | 1552 | 1553 | 1554 | 1555 | 1556 | 1557 | 1558 | 1559 | 1560 | 1561 | 1562 | 1563 | 1564 | 1565 | 1566 | 1567 | 1568 | 1569 | 1570 | 1571 | 1572 | 1573 | 1574 | 1575 | 1576 | 1577 | 1578 | 1579 | 1580 | 1581 | 1582 | 1583 | 1584 | 1585 | 1586 | 1587 | 1588 | 1589 | 1590 | 1591 | 1592 | 1593 | 1594 | 1595 | 1596 | 1597 | 1598 | 1599 | 1600 | 1601 | 1602 | 1603 | 1604 | 1605 | 1606 | 1607 | 1608 | 1609 | 1610 | 1611 | 1612 | 1613 | 1614 | 1615 | 1616 | 1617 | 1618 | 1619 | 1620 | 1621 | 1622 | 1623 | 1624 | 1625 | 1626 | 1627 | 1628 | 1629 | 1630 | 1631 | 1632 | 1633 | 1634 | 1635 | 1636 | 1637 | 1638 | 1639 | 1640 | 1641 | 1642 | 1643 | 1644 | 1645 | 1646 | 1647 | 1648 | 1649 | 1650 | 1651 | 1652 | 1653 | 1654 | 1655 | 1656 | 1657 | 1658 | 1659 | 1660 | 1661 | 1662 | 1663 | 1664 | 1665 | 1666 | 1667 | 1668 | 1669 | 1670 | 1671 | 1672 | 1673 | 1674 | 1675 | 1676 | 1677 | 1678 | 1679 | 1680 | 1681 | 1682 | 1683 | 1684 | 1685 | 1686 | 1687 | 1688 | 1689 | 1690 | 1691 | 1692 | 1693 | 1694 | 1695 | 1696 | 1697 | 1698 | 1699 | 1700 | 1701 | 1702 | 1703 | 1704 | 1705 | 1706 | 1707 | 1708 | 1709 | 1710 | 1711 | 1712 | 1713 | 1714 | 1715 | 1716 | 1717 | 1718 | 1719 | 1720 | 1721 | 1722 | 1723 | 1724 | 1725 | 1726 | 1727 | 1728 | 1729 | 1730 | 1731 | 1732 | 1733 | 1734 | 1735 | 1736 | 1737 | 1738 | 1739 | 1740 | 1741 | 1742 | 1743 | 1744 | 1745 | 1746 | 1747 | 1748 | 1749 | 1750 | 1751 | 1752 | 1753 | 1754 | 1755 | 1756 | 1757 | 1758 | 1759 | 1760 | 1761 | 1762 | 1763 | 1764 | 1765 | 1766 | 1767 | 1768 | 1769 | 1770 | 1771 | 1772 | 1773 | 1774 | 1775 | 1776 | 1777 | 1778 | 1779 | 1780 | 1781 | 1782 | 1783 | 1784 | 1785 | 1786 | 1787 | 1788 | 1789 | 1790 | 1791 | 1792 | 1793 | 1794 | 1795 | 1796 | 1797 | 1798 | 1799 | 1800 | 1801 | 1802 | 1803 | 1804 | 1805 | 1806 | 1807 | 1808 | 1809 | 1810 | 1811 | 1812 | 1813 | 1814 | 1815 | 1816 | 1817 | 1818 | 1819 | 1820 | 1821 | 1822 | 1823 | 1824 | 1825 | 1826 | 1827 | 1828 | 1829 | 1830 | 1831 | 1832 | 1833 | 1834 | 1835 | 1836 | 1837 | 1838 | 1839 | 1840 | 1841 | 1842 | 1843 | 1844 | 1845 | 1846 | 1847 | 1848 | 1849 | 1850 | 1851 | 1852 | 1853 | 1854 | 1855 | 1856 | 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|------|------|------|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                            | Source    |
|----------------------------------------------------------|--------------------------------------------------|-----------|
| Space group                                              | P 32 2 1                                         | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 142.00Å 142.00Å 103.70Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å)                                           | 8.50 – 2.50                                      | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (8.50-2.50)                      | Depositor |
| $R_{merge}$                                              | (Not available)                                  | Depositor |
| $R_{sym}$                                                | (Not available)                                  | Depositor |
| Refinement program                                       | unknown                                          | Depositor |
| R, $R_{free}$                                            | 0.191 , (Not available)                          | Depositor |
| Estimated twinning fraction                              | No twinning to report.                           | Xtriage   |
| Total number of atoms                                    | 8296                                             | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 21.0                                             | wwPDB-VP  |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, NDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 1.98         | 98/4128 (2.4%)  | 2.84        | 444/5607 (7.9%)  |
| 1   | B     | 2.05         | 110/4128 (2.7%) | 2.95        | 505/5607 (9.0%)  |
| All | All   | 2.01         | 208/8256 (2.5%) | 2.90        | 949/11214 (8.5%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 4                   |
| 1   | B     | 0                   | 2                   |
| All | All   | 0                   | 6                   |

All (208) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 343 | GLU  | N-CA   | 9.37  | 1.59        | 1.46     |
| 1   | B     | 228 | ALA  | C-N    | -9.04 | 1.25        | 1.33     |
| 1   | B     | 426 | GLY  | N-CA   | 8.86  | 1.54        | 1.45     |
| 1   | B     | 151 | ILE  | N-CA   | 8.80  | 1.57        | 1.46     |
| 1   | A     | 122 | ALA  | N-CA   | 8.59  | 1.56        | 1.46     |
| 1   | B     | 291 | PHE  | N-CA   | 8.47  | 1.55        | 1.45     |
| 1   | B     | 261 | LEU  | CA-CB  | -8.43 | 1.40        | 1.53     |
| 1   | A     | 300 | LYS  | C-O    | 8.38  | 1.34        | 1.23     |
| 1   | A     | 67  | ARG  | CD-NE  | -8.16 | 1.34        | 1.46     |
| 1   | A     | 165 | HIS  | CG-CD2 | -8.06 | 1.26        | 1.35     |
| 1   | B     | 28  | THR  | C-O    | 8.03  | 1.33        | 1.23     |
| 1   | A     | 384 | ASN  | C-O    | 7.99  | 1.31        | 1.24     |
| 1   | A     | 360 | THR  | C-O    | 7.91  | 1.34        | 1.24     |
| 1   | B     | 241 | ILE  | N-CA   | 7.88  | 1.56        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 450 | LEU  | N-CA    | 7.86  | 1.55        | 1.45     |
| 1   | B     | 469 | ALA  | N-CA    | 7.76  | 1.55        | 1.45     |
| 1   | A     | 385 | TYR  | N-CA    | 7.71  | 1.55        | 1.46     |
| 1   | A     | 261 | LEU  | N-CA    | 7.59  | 1.55        | 1.46     |
| 1   | B     | 222 | VAL  | C-O     | 7.58  | 1.32        | 1.24     |
| 1   | B     | 361 | HIS  | ND1-CE1 | -7.53 | 1.25        | 1.32     |
| 1   | A     | 329 | GLU  | CA-CB   | -7.51 | 1.41        | 1.53     |
| 1   | B     | 370 | LEU  | C-N     | -7.43 | 1.23        | 1.33     |
| 1   | B     | 124 | THR  | CA-CB   | 7.30  | 1.62        | 1.52     |
| 1   | B     | 294 | ASN  | N-CA    | 7.26  | 1.58        | 1.46     |
| 1   | A     | 364 | ARG  | NE-CZ   | 7.19  | 1.41        | 1.33     |
| 1   | A     | 436 | ASP  | N-CA    | 7.16  | 1.55        | 1.46     |
| 1   | A     | 148 | ASN  | N-CA    | 7.15  | 1.54        | 1.46     |
| 1   | A     | 185 | TRP  | C-O     | 7.14  | 1.32        | 1.24     |
| 1   | B     | 275 | SER  | C-N     | -7.09 | 1.24        | 1.33     |
| 1   | B     | 355 | PHE  | C-N     | -7.07 | 1.23        | 1.33     |
| 1   | B     | 120 | GLY  | N-CA    | 7.06  | 1.53        | 1.45     |
| 1   | A     | 252 | LEU  | C-O     | 6.98  | 1.32        | 1.24     |
| 1   | A     | 417 | ALA  | N-CA    | 6.96  | 1.53        | 1.46     |
| 1   | B     | 76  | LYS  | C-N     | 6.96  | 1.41        | 1.33     |
| 1   | A     | 14  | TRP  | NE1-CE2 | 6.92  | 1.45        | 1.37     |
| 1   | A     | 124 | THR  | CA-CB   | 6.86  | 1.61        | 1.52     |
| 1   | A     | 165 | HIS  | C-N     | -6.78 | 1.24        | 1.33     |
| 1   | B     | 363 | HIS  | C-O     | 6.76  | 1.29        | 1.23     |
| 1   | B     | 157 | ALA  | N-CA    | 6.76  | 1.54        | 1.46     |
| 1   | B     | 234 | HIS  | N-CA    | 6.75  | 1.54        | 1.46     |
| 1   | A     | 120 | GLY  | N-CA    | 6.72  | 1.53        | 1.45     |
| 1   | B     | 83  | TYR  | N-CA    | 6.65  | 1.54        | 1.45     |
| 1   | B     | 311 | PRO  | C-N     | 6.62  | 1.42        | 1.33     |
| 1   | B     | 240 | GLY  | N-CA    | 6.61  | 1.51        | 1.45     |
| 1   | A     | 364 | ARG  | C-O     | 6.60  | 1.31        | 1.24     |
| 1   | B     | 373 | PRO  | C-O     | 6.56  | 1.32        | 1.24     |
| 1   | B     | 321 | PRO  | C-O     | -6.55 | 1.16        | 1.23     |
| 1   | A     | 26  | LEU  | C-O     | 6.52  | 1.31        | 1.24     |
| 1   | B     | 213 | GLY  | CA-C    | 6.50  | 1.57        | 1.52     |
| 1   | B     | 305 | GLY  | N-CA    | 6.44  | 1.54        | 1.45     |
| 1   | B     | 318 | ASN  | N-CA    | 6.44  | 1.52        | 1.46     |
| 1   | B     | 40  | SER  | N-CA    | 6.42  | 1.54        | 1.45     |
| 1   | B     | 89  | ASP  | N-CA    | 6.40  | 1.53        | 1.46     |
| 1   | A     | 382 | VAL  | CA-CB   | 6.39  | 1.61        | 1.54     |
| 1   | B     | 296 | PHE  | N-CA    | -6.35 | 1.38        | 1.46     |
| 1   | B     | 312 | VAL  | C-N     | -6.33 | 1.27        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 310 | ILE  | CA-CB   | 6.32  | 1.61        | 1.54     |
| 1   | B     | 108 | ILE  | CA-CB   | 6.31  | 1.66        | 1.55     |
| 1   | B     | 219 | PHE  | C-N     | -6.23 | 1.25        | 1.33     |
| 1   | A     | 188 | ARG  | CD-NE   | 6.19  | 1.54        | 1.46     |
| 1   | B     | 74  | HIS  | C-N     | -6.19 | 1.25        | 1.33     |
| 1   | B     | 425 | SER  | C-O     | 6.18  | 1.31        | 1.24     |
| 1   | A     | 336 | SER  | N-CA    | -6.17 | 1.38        | 1.46     |
| 1   | B     | 435 | ASN  | N-CA    | 6.17  | 1.53        | 1.46     |
| 1   | B     | 206 | ASP  | N-CA    | 6.16  | 1.54        | 1.46     |
| 1   | B     | 67  | ARG  | C-O     | 6.14  | 1.31        | 1.24     |
| 1   | A     | 171 | PRO  | N-CD    | 6.11  | 1.56        | 1.47     |
| 1   | A     | 11  | MET  | N-CA    | 6.10  | 1.54        | 1.46     |
| 1   | B     | 220 | LYS  | CA-CB   | -6.10 | 1.43        | 1.53     |
| 1   | B     | 325 | PHE  | C-N     | -6.10 | 1.25        | 1.33     |
| 1   | A     | 384 | ASN  | N-CA    | 6.06  | 1.56        | 1.46     |
| 1   | A     | 238 | ASP  | N-CA    | 6.04  | 1.54        | 1.46     |
| 1   | B     | 247 | GLU  | N-CA    | 6.04  | 1.53        | 1.46     |
| 1   | B     | 410 | ALA  | CA-CB   | -6.02 | 1.43        | 1.53     |
| 1   | B     | 261 | LEU  | CB-CG   | -6.01 | 1.41        | 1.53     |
| 1   | B     | 354 | LEU  | C-O     | 6.00  | 1.31        | 1.24     |
| 1   | B     | 127 | ASP  | N-CA    | 5.99  | 1.51        | 1.46     |
| 1   | A     | 164 | ILE  | CA-CB   | 5.98  | 1.61        | 1.54     |
| 1   | A     | 64  | ASP  | C-N     | -5.96 | 1.26        | 1.33     |
| 1   | B     | 329 | GLU  | C-O     | 5.95  | 1.31        | 1.24     |
| 1   | B     | 42  | THR  | N-CA    | 5.91  | 1.53        | 1.45     |
| 1   | A     | 164 | ILE  | C-N     | -5.91 | 1.26        | 1.33     |
| 1   | B     | 409 | SER  | N-CA    | -5.88 | 1.38        | 1.46     |
| 1   | A     | 428 | VAL  | C-O     | 5.87  | 1.31        | 1.23     |
| 1   | A     | 348 | LYS  | C-O     | 5.87  | 1.30        | 1.24     |
| 1   | B     | 126 | ARG  | C-N     | -5.86 | 1.26        | 1.33     |
| 1   | B     | 463 | ALA  | C-O     | 5.86  | 1.31        | 1.24     |
| 1   | A     | 155 | ARG  | CZ-NH2  | -5.85 | 1.25        | 1.33     |
| 1   | B     | 62  | HIS  | CE1-NE2 | 5.85  | 1.38        | 1.32     |
| 1   | A     | 344 | PRO  | N-CD    | 5.85  | 1.55        | 1.47     |
| 1   | B     | 143 | ASP  | C-N     | -5.85 | 1.26        | 1.33     |
| 1   | A     | 219 | PHE  | N-CA    | 5.82  | 1.52        | 1.45     |
| 1   | B     | 203 | GLY  | N-CA    | 5.80  | 1.52        | 1.45     |
| 1   | B     | 119 | SER  | C-O     | 5.78  | 1.31        | 1.24     |
| 1   | B     | 168 | LYS  | CA-CB   | -5.76 | 1.43        | 1.53     |
| 1   | A     | 353 | ARG  | N-CA    | 5.75  | 1.53        | 1.46     |
| 1   | A     | 284 | THR  | CA-CB   | 5.74  | 1.62        | 1.53     |
| 1   | A     | 80  | ALA  | N-CA    | 5.74  | 1.54        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 323 | ASN  | C-N     | -5.73 | 1.26        | 1.33     |
| 1   | A     | 343 | GLU  | CA-C    | -5.73 | 1.45        | 1.52     |
| 1   | B     | 241 | ILE  | C-N     | -5.71 | 1.25        | 1.33     |
| 1   | B     | 372 | ILE  | C-O     | 5.70  | 1.31        | 1.24     |
| 1   | A     | 29  | GLY  | N-CA    | 5.70  | 1.54        | 1.45     |
| 1   | A     | 69  | PRO  | CA-CB   | -5.70 | 1.46        | 1.53     |
| 1   | A     | 226 | GLY  | N-CA    | 5.69  | 1.52        | 1.45     |
| 1   | B     | 144 | LEU  | N-CA    | -5.69 | 1.38        | 1.46     |
| 1   | A     | 469 | ALA  | N-CA    | 5.69  | 1.53        | 1.45     |
| 1   | B     | 364 | ARG  | NE-CZ   | 5.68  | 1.39        | 1.33     |
| 1   | B     | 204 | ILE  | C-O     | 5.67  | 1.31        | 1.24     |
| 1   | A     | 264 | LEU  | C-N     | -5.64 | 1.26        | 1.33     |
| 1   | B     | 355 | PHE  | C-O     | 5.62  | 1.31        | 1.23     |
| 1   | B     | 310 | ILE  | C-O     | 5.60  | 1.30        | 1.24     |
| 1   | B     | 95  | LYS  | CA-CB   | 5.58  | 1.61        | 1.53     |
| 1   | A     | 73  | VAL  | C-O     | 5.58  | 1.29        | 1.23     |
| 1   | B     | 185 | TRP  | C-O     | 5.58  | 1.31        | 1.24     |
| 1   | A     | 84  | PHE  | N-CA    | 5.57  | 1.52        | 1.46     |
| 1   | A     | 413 | HIS  | CE1-NE2 | -5.55 | 1.26        | 1.32     |
| 1   | B     | 368 | ASN  | C-O     | -5.55 | 1.17        | 1.23     |
| 1   | A     | 65  | ARG  | C-N     | -5.54 | 1.26        | 1.34     |
| 1   | A     | 62  | HIS  | CE1-NE2 | 5.52  | 1.38        | 1.32     |
| 1   | A     | 261 | LEU  | CA-CB   | -5.51 | 1.44        | 1.53     |
| 1   | B     | 155 | ARG  | CD-NE   | -5.51 | 1.38        | 1.46     |
| 1   | B     | 116 | ALA  | N-CA    | 5.51  | 1.53        | 1.46     |
| 1   | A     | 475 | LYS  | C-O     | -5.48 | 1.17        | 1.24     |
| 1   | A     | 474 | GLN  | C-O     | 5.46  | 1.30        | 1.24     |
| 1   | A     | 363 | HIS  | C-N     | -5.46 | 1.27        | 1.33     |
| 1   | A     | 477 | ALA  | C-N     | -5.44 | 1.27        | 1.33     |
| 1   | B     | 161 | PRO  | CA-CB   | -5.42 | 1.46        | 1.53     |
| 1   | A     | 343 | GLU  | CA-CB   | -5.42 | 1.44        | 1.53     |
| 1   | A     | 393 | MET  | N-CA    | -5.42 | 1.39        | 1.46     |
| 1   | B     | 88  | HIS  | CG-CD2  | -5.41 | 1.29        | 1.35     |
| 1   | A     | 353 | ARG  | CZ-NH2  | 5.41  | 1.40        | 1.33     |
| 1   | B     | 60  | MET  | N-CA    | 5.40  | 1.52        | 1.46     |
| 1   | B     | 10  | GLN  | C-O     | 5.39  | 1.30        | 1.24     |
| 1   | A     | 472 | PHE  | N-CA    | 5.38  | 1.52        | 1.46     |
| 1   | B     | 438 | ASN  | C-O     | 5.37  | 1.31        | 1.24     |
| 1   | A     | 480 | ASN  | C-N     | -5.36 | 1.26        | 1.33     |
| 1   | B     | 171 | PRO  | N-CA    | -5.36 | 1.40        | 1.47     |
| 1   | B     | 134 | LYS  | CA-C    | 5.36  | 1.59        | 1.52     |
| 1   | A     | 33  | PRO  | C-O     | 5.34  | 1.29        | 1.23     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 393 | MET  | CA-CB   | 5.34  | 1.61        | 1.53     |
| 1   | B     | 373 | PRO  | C-N     | -5.33 | 1.28        | 1.34     |
| 1   | B     | 48  | PRO  | N-CD    | 5.33  | 1.55        | 1.47     |
| 1   | B     | 160 | PHE  | C-O     | 5.33  | 1.30        | 1.24     |
| 1   | A     | 432 | ASN  | N-CA    | 5.32  | 1.52        | 1.46     |
| 1   | B     | 65  | ARG  | C-N     | -5.31 | 1.26        | 1.34     |
| 1   | B     | 354 | LEU  | C-N     | -5.31 | 1.26        | 1.33     |
| 1   | A     | 44  | GLY  | N-CA    | 5.30  | 1.51        | 1.44     |
| 1   | B     | 404 | TYR  | CA-C    | 5.29  | 1.57        | 1.52     |
| 1   | B     | 54  | VAL  | C-N     | -5.29 | 1.26        | 1.33     |
| 1   | A     | 126 | ARG  | CA-CB   | -5.28 | 1.45        | 1.53     |
| 1   | B     | 377 | PRO  | CA-CB   | -5.28 | 1.48        | 1.53     |
| 1   | A     | 351 | GLN  | C-O     | 5.28  | 1.30        | 1.24     |
| 1   | B     | 171 | PRO  | C-N     | 5.27  | 1.40        | 1.33     |
| 1   | B     | 11  | MET  | CA-CB   | -5.27 | 1.44        | 1.53     |
| 1   | B     | 277 | THR  | CA-CB   | 5.26  | 1.60        | 1.53     |
| 1   | A     | 354 | LEU  | N-CA    | 5.25  | 1.52        | 1.46     |
| 1   | A     | 208 | HIS  | CA-CB   | 5.24  | 1.61        | 1.53     |
| 1   | A     | 418 | LEU  | C-N     | -5.24 | 1.26        | 1.33     |
| 1   | B     | 297 | ASP  | N-CA    | 5.24  | 1.52        | 1.46     |
| 1   | A     | 328 | VAL  | C-O     | 5.23  | 1.30        | 1.24     |
| 1   | A     | 400 | ALA  | CA-CB   | 5.22  | 1.63        | 1.53     |
| 1   | A     | 229 | VAL  | C-O     | 5.21  | 1.30        | 1.23     |
| 1   | B     | 465 | HIS  | CE1-NE2 | -5.21 | 1.27        | 1.32     |
| 1   | B     | 142 | TRP  | C-O     | -5.21 | 1.17        | 1.24     |
| 1   | B     | 298 | LEU  | N-CA    | 5.19  | 1.53        | 1.46     |
| 1   | A     | 179 | ASP  | CA-CB   | -5.18 | 1.45        | 1.53     |
| 1   | B     | 381 | ARG  | CZ-NH1  | 5.17  | 1.40        | 1.32     |
| 1   | A     | 329 | GLU  | N-CA    | 5.17  | 1.52        | 1.46     |
| 1   | B     | 52  | GLN  | N-CA    | -5.16 | 1.39        | 1.46     |
| 1   | B     | 477 | ALA  | N-CA    | 5.15  | 1.52        | 1.46     |
| 1   | A     | 185 | TRP  | CA-CB   | 5.15  | 1.61        | 1.53     |
| 1   | A     | 101 | HIS  | N-CA    | 5.14  | 1.52        | 1.46     |
| 1   | A     | 381 | ARG  | CD-NE   | 5.14  | 1.53        | 1.46     |
| 1   | A     | 117 | GLY  | CA-C    | 5.13  | 1.56        | 1.52     |
| 1   | B     | 363 | HIS  | ND1-CE1 | 5.12  | 1.37        | 1.32     |
| 1   | A     | 338 | MET  | CG-SD   | 5.12  | 1.93        | 1.80     |
| 1   | A     | 342 | ILE  | C-O     | 5.12  | 1.29        | 1.23     |
| 1   | A     | 65  | ARG  | CZ-NH2  | 5.12  | 1.40        | 1.33     |
| 1   | A     | 287 | GLU  | N-CA    | 5.12  | 1.52        | 1.46     |
| 1   | B     | 379 | ARG  | CD-NE   | 5.12  | 1.53        | 1.46     |
| 1   | B     | 164 | ILE  | CA-CB   | 5.11  | 1.61        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 361 | HIS  | C-N     | -5.10 | 1.26        | 1.33     |
| 1   | A     | 250 | ALA  | C-N     | -5.10 | 1.27        | 1.33     |
| 1   | A     | 424 | PHE  | C-N     | -5.10 | 1.26        | 1.33     |
| 1   | A     | 135 | PHE  | C-O     | 5.10  | 1.29        | 1.24     |
| 1   | A     | 137 | THR  | CA-CB   | 5.09  | 1.60        | 1.53     |
| 1   | B     | 79  | GLY  | CA-C    | -5.09 | 1.46        | 1.52     |
| 1   | A     | 218 | THR  | C-O     | 5.09  | 1.30        | 1.24     |
| 1   | B     | 174 | HIS  | CE1-NE2 | -5.09 | 1.27        | 1.32     |
| 1   | A     | 63  | PHE  | N-CA    | 5.08  | 1.52        | 1.46     |
| 1   | B     | 173 | THR  | CA-CB   | 5.07  | 1.61        | 1.53     |
| 1   | A     | 28  | THR  | C-O     | 5.07  | 1.30        | 1.23     |
| 1   | B     | 330 | GLN  | C-O     | 5.06  | 1.30        | 1.24     |
| 1   | A     | 283 | MET  | C-N     | -5.06 | 1.26        | 1.33     |
| 1   | B     | 36  | ASP  | N-CA    | 5.06  | 1.52        | 1.46     |
| 1   | B     | 355 | PHE  | N-CA    | 5.05  | 1.52        | 1.46     |
| 1   | B     | 166 | SER  | C-O     | 5.05  | 1.30        | 1.24     |
| 1   | A     | 379 | ARG  | NE-CZ   | 5.05  | 1.38        | 1.33     |
| 1   | B     | 13  | HIS  | CD2-NE2 | 5.04  | 1.43        | 1.37     |
| 1   | A     | 336 | SER  | C-N     | -5.04 | 1.26        | 1.33     |
| 1   | A     | 121 | SER  | C-O     | 5.04  | 1.30        | 1.24     |
| 1   | B     | 338 | MET  | C-N     | -5.03 | 1.27        | 1.33     |
| 1   | B     | 363 | HIS  | C-N     | -5.02 | 1.27        | 1.33     |
| 1   | A     | 254 | HIS  | N-CA    | 5.02  | 1.52        | 1.46     |
| 1   | A     | 103 | GLY  | N-CA    | 5.01  | 1.52        | 1.44     |
| 1   | B     | 408 | PHE  | C-N     | -5.00 | 1.26        | 1.33     |
| 1   | A     | 303 | PRO  | CA-CB   | -5.00 | 1.47        | 1.53     |

All (949) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | A     | 67  | ARG  | CD-NE-CZ | 25.30  | 159.81      | 124.40   |
| 1   | B     | 472 | PHE  | CA-CB-CG | 19.95  | 133.75      | 113.80   |
| 1   | A     | 179 | ASP  | CA-CB-CG | 18.22  | 130.82      | 112.60   |
| 1   | A     | 263 | ASP  | CA-CB-CG | 15.93  | 128.53      | 112.60   |
| 1   | B     | 71  | ARG  | CD-NE-CZ | 15.40  | 145.96      | 124.40   |
| 1   | B     | 254 | HIS  | CA-CB-CG | 14.51  | 128.31      | 113.80   |
| 1   | B     | 89  | ASP  | CA-CB-CG | -14.25 | 98.35       | 112.60   |
| 1   | B     | 74  | HIS  | CA-C-N   | 13.83  | 138.81      | 120.28   |
| 1   | B     | 74  | HIS  | C-N-CA   | 13.83  | 138.81      | 120.28   |
| 1   | B     | 99  | PHE  | CA-CB-CG | 13.51  | 127.31      | 113.80   |
| 1   | B     | 386 | GLN  | CB-CG-CD | 13.30  | 135.21      | 112.60   |
| 1   | B     | 261 | LEU  | CA-CB-CG | 13.13  | 162.25      | 116.30   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | B     | 293 | PHE  | CA-CB-CG  | 12.97  | 126.77      | 113.80   |
| 1   | B     | 126 | ARG  | NE-CZ-NH2 | 12.93  | 130.84      | 119.20   |
| 1   | A     | 461 | ASN  | CA-CB-CG  | 12.56  | 125.16      | 112.60   |
| 1   | B     | 240 | GLY  | CA-C-O    | -12.31 | 112.79      | 122.52   |
| 1   | B     | 408 | PHE  | CA-C-N    | 12.18  | 142.10      | 123.47   |
| 1   | B     | 408 | PHE  | C-N-CA    | 12.18  | 142.10      | 123.47   |
| 1   | B     | 338 | MET  | O-C-N     | 12.17  | 132.22      | 121.39   |
| 1   | A     | 393 | MET  | N-CA-C    | 11.76  | 123.84      | 111.14   |
| 1   | B     | 461 | ASN  | CA-CB-CG  | 11.72  | 124.32      | 112.60   |
| 1   | A     | 127 | ASP  | CA-CB-CG  | 11.34  | 123.94      | 112.60   |
| 1   | A     | 221 | LEU  | CA-C-O    | -11.31 | 108.05      | 120.38   |
| 1   | B     | 155 | ARG  | CD-NE-CZ  | 11.23  | 140.12      | 124.40   |
| 1   | B     | 28  | THR  | CA-C-O    | -11.21 | 107.48      | 121.50   |
| 1   | B     | 343 | GLU  | CB-CG-CD  | 11.21  | 131.65      | 112.60   |
| 1   | A     | 184 | PHE  | CA-C-N    | 11.14  | 135.64      | 120.38   |
| 1   | A     | 184 | PHE  | C-N-CA    | 11.14  | 135.64      | 120.38   |
| 1   | A     | 65  | ARG  | CD-NE-CZ  | 11.04  | 139.86      | 124.40   |
| 1   | B     | 291 | PHE  | CA-CB-CG  | 10.82  | 124.62      | 113.80   |
| 1   | B     | 261 | LEU  | O-C-N     | 10.82  | 133.77      | 122.09   |
| 1   | A     | 335 | PRO  | CA-C-N    | 10.74  | 143.42      | 121.94   |
| 1   | A     | 335 | PRO  | C-N-CA    | 10.74  | 143.42      | 121.94   |
| 1   | A     | 74  | HIS  | CA-C-N    | 10.69  | 135.67      | 120.28   |
| 1   | A     | 74  | HIS  | C-N-CA    | 10.69  | 135.67      | 120.28   |
| 1   | B     | 338 | MET  | CA-C-O    | -10.68 | 108.80      | 119.69   |
| 1   | A     | 343 | GLU  | CA-CB-CG  | 10.65  | 135.40      | 114.10   |
| 1   | B     | 51  | VAL  | CA-C-N    | 10.65  | 138.50      | 120.72   |
| 1   | B     | 51  | VAL  | C-N-CA    | 10.65  | 138.50      | 120.72   |
| 1   | A     | 418 | LEU  | CA-C-O    | -10.60 | 110.00      | 121.56   |
| 1   | A     | 430 | ARG  | NE-CZ-NH1 | -10.58 | 110.92      | 121.50   |
| 1   | B     | 92  | ARG  | CA-C-N    | 10.55  | 138.33      | 120.71   |
| 1   | B     | 92  | ARG  | C-N-CA    | 10.55  | 138.33      | 120.71   |
| 1   | A     | 472 | PHE  | CA-CB-CG  | 10.52  | 124.32      | 113.80   |
| 1   | B     | 92  | ARG  | NE-CZ-NH1 | 10.46  | 131.96      | 121.50   |
| 1   | A     | 303 | PRO  | CA-C-O    | -10.35 | 110.15      | 121.23   |
| 1   | B     | 126 | ARG  | CA-C-O    | -10.21 | 108.73      | 120.58   |
| 1   | B     | 420 | HIS  | CA-C-N    | 10.20  | 135.93      | 121.24   |
| 1   | B     | 420 | HIS  | C-N-CA    | 10.20  | 135.93      | 121.24   |
| 1   | A     | 10  | GLN  | CB-CG-CD  | 10.18  | 129.90      | 112.60   |
| 1   | B     | 334 | ASP  | CA-CB-CG  | 10.14  | 122.74      | 112.60   |
| 1   | A     | 362 | ARG  | NE-CZ-NH2 | -10.10 | 110.11      | 119.20   |
| 1   | B     | 275 | SER  | CA-C-N    | 10.10  | 139.71      | 121.94   |
| 1   | B     | 275 | SER  | C-N-CA    | 10.10  | 139.71      | 121.94   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 111 | ARG  | NE-CZ-NH2  | -10.02 | 110.19      | 119.20   |
| 1   | A     | 28  | THR  | CA-C-O     | -9.96  | 110.24      | 121.89   |
| 1   | A     | 147 | ASN  | CA-C-O     | -9.91  | 109.61      | 121.60   |
| 1   | A     | 155 | ARG  | CD-NE-CZ   | -9.91  | 110.52      | 124.40   |
| 1   | A     | 384 | ASN  | CA-CB-CG   | -9.90  | 102.70      | 112.60   |
| 1   | A     | 93  | TYR  | CA-C-O     | -9.90  | 110.42      | 120.82   |
| 1   | A     | 239 | GLN  | OE1-CD-NE2 | -9.89  | 112.71      | 122.60   |
| 1   | B     | 396 | ASN  | CA-C-N     | 9.84   | 136.67      | 122.40   |
| 1   | B     | 396 | ASN  | C-N-CA     | 9.84   | 136.67      | 122.40   |
| 1   | A     | 92  | ARG  | CA-C-N     | 9.79   | 133.16      | 120.44   |
| 1   | A     | 92  | ARG  | C-N-CA     | 9.79   | 133.16      | 120.44   |
| 1   | A     | 116 | ALA  | CA-C-N     | 9.76   | 129.37      | 120.10   |
| 1   | A     | 116 | ALA  | C-N-CA     | 9.76   | 129.37      | 120.10   |
| 1   | A     | 169 | ARG  | NE-CZ-NH2  | -9.72  | 110.45      | 119.20   |
| 1   | A     | 353 | ARG  | NE-CZ-NH2  | -9.67  | 110.50      | 119.20   |
| 1   | B     | 375 | ASN  | CB-CG-ND2  | 9.63   | 130.84      | 116.40   |
| 1   | A     | 306 | ASP  | CA-CB-CG   | 9.62   | 122.22      | 112.60   |
| 1   | B     | 432 | ASN  | OD1-CG-ND2 | -9.55  | 113.05      | 122.60   |
| 1   | B     | 118 | GLU  | CA-C-O     | -9.53  | 111.11      | 121.88   |
| 1   | A     | 404 | TYR  | CA-C-O     | 9.53   | 128.39      | 119.72   |
| 1   | B     | 135 | PHE  | CA-C-O     | -9.49  | 110.03      | 120.38   |
| 1   | A     | 364 | ARG  | CD-NE-CZ   | -9.48  | 111.12      | 124.40   |
| 1   | B     | 127 | ASP  | N-CA-C     | -9.46  | 99.62       | 108.13   |
| 1   | B     | 370 | LEU  | CA-C-N     | 9.44   | 137.13      | 122.49   |
| 1   | B     | 370 | LEU  | C-N-CA     | 9.44   | 137.13      | 122.49   |
| 1   | B     | 228 | ALA  | CA-C-N     | 9.40   | 134.56      | 121.96   |
| 1   | B     | 228 | ALA  | C-N-CA     | 9.40   | 134.56      | 121.96   |
| 1   | B     | 343 | GLU  | CA-CB-CG   | 9.36   | 132.82      | 114.10   |
| 1   | A     | 408 | PHE  | CA-CB-CG   | 9.36   | 123.16      | 113.80   |
| 1   | A     | 139 | ASP  | CA-CB-CG   | 9.26   | 121.86      | 112.60   |
| 1   | B     | 368 | ASN  | OD1-CG-ND2 | -9.26  | 113.34      | 122.60   |
| 1   | A     | 392 | CYS  | CA-C-N     | 9.24   | 133.01      | 120.44   |
| 1   | A     | 392 | CYS  | C-N-CA     | 9.24   | 133.01      | 120.44   |
| 1   | B     | 168 | LYS  | CA-CB-CG   | 9.24   | 132.59      | 114.10   |
| 1   | A     | 371 | GLN  | OE1-CD-NE2 | -9.22  | 113.38      | 122.60   |
| 1   | A     | 407 | SER  | CA-C-O     | -9.20  | 107.47      | 119.80   |
| 1   | B     | 364 | ARG  | CD-NE-CZ   | -9.19  | 111.53      | 124.40   |
| 1   | B     | 386 | GLN  | CA-CB-CG   | 9.16   | 132.42      | 114.10   |
| 1   | B     | 71  | ARG  | NE-CZ-NH2  | 9.15   | 127.43      | 119.20   |
| 1   | B     | 451 | ASN  | CA-CB-CG   | 9.10   | 121.70      | 112.60   |
| 1   | B     | 328 | VAL  | CB-CA-C    | 9.07   | 119.12      | 111.05   |
| 1   | A     | 155 | ARG  | NE-CZ-NH1  | -9.07  | 112.43      | 121.50   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 251 | ARG  | CA-CB-CG   | 9.05  | 132.20      | 114.10   |
| 1   | A     | 420 | HIS  | CA-CB-CG   | 9.03  | 122.83      | 113.80   |
| 1   | A     | 224 | ALA  | CA-C-O     | -8.99 | 108.61      | 119.49   |
| 1   | A     | 384 | ASN  | OD1-CG-ND2 | 8.98  | 131.59      | 122.60   |
| 1   | A     | 373 | PRO  | N-CA-CB    | -8.97 | 93.83       | 103.25   |
| 1   | B     | 174 | HIS  | CA-CB-CG   | -8.96 | 104.84      | 113.80   |
| 1   | B     | 255 | GLU  | CA-CB-CG   | 8.94  | 131.97      | 114.10   |
| 1   | A     | 383 | ALA  | CA-C-O     | -8.93 | 110.78      | 120.24   |
| 1   | B     | 429 | GLN  | CA-CB-CG   | 8.92  | 131.94      | 114.10   |
| 1   | A     | 221 | LEU  | O-C-N      | 8.92  | 133.81      | 123.29   |
| 1   | B     | 66  | GLU  | CA-C-N     | 8.90  | 134.74      | 122.19   |
| 1   | B     | 66  | GLU  | C-N-CA     | 8.90  | 134.74      | 122.19   |
| 1   | A     | 353 | ARG  | NE-CZ-NH1  | 8.88  | 130.38      | 121.50   |
| 1   | B     | 450 | LEU  | CB-CA-C    | 8.86  | 126.79      | 109.33   |
| 1   | A     | 137 | THR  | CA-C-O     | -8.85 | 111.11      | 121.82   |
| 1   | A     | 362 | ARG  | NE-CZ-NH1  | 8.82  | 130.32      | 121.50   |
| 1   | B     | 188 | ARG  | NE-CZ-NH1  | -8.75 | 112.75      | 121.50   |
| 1   | B     | 311 | PRO  | CA-C-N     | -8.74 | 113.59      | 122.77   |
| 1   | B     | 311 | PRO  | C-N-CA     | -8.74 | 113.59      | 122.77   |
| 1   | B     | 438 | ASN  | CA-C-O     | -8.74 | 109.18      | 119.15   |
| 1   | B     | 24  | ASP  | CA-CB-CG   | 8.71  | 121.31      | 112.60   |
| 1   | B     | 261 | LEU  | N-CA-CB    | 8.68  | 122.66      | 110.07   |
| 1   | A     | 430 | ARG  | CD-NE-CZ   | -8.68 | 112.25      | 124.40   |
| 1   | B     | 138 | GLU  | CB-CG-CD   | 8.63  | 127.27      | 112.60   |
| 1   | A     | 19  | ALA  | N-CA-C     | -8.63 | 102.89      | 113.41   |
| 1   | B     | 445 | PHE  | O-C-N      | 8.59  | 131.99      | 122.11   |
| 1   | A     | 261 | LEU  | N-CA-C     | -8.58 | 101.87      | 111.14   |
| 1   | B     | 54  | VAL  | CA-C-O     | -8.53 | 110.12      | 120.78   |
| 1   | A     | 9   | ASP  | CA-CB-CG   | 8.49  | 121.09      | 112.60   |
| 1   | A     | 59  | GLU  | CB-CG-CD   | 8.48  | 127.01      | 112.60   |
| 1   | B     | 140 | GLY  | O-C-N      | 8.47  | 130.96      | 122.91   |
| 1   | B     | 256 | ASP  | CA-CB-CG   | 8.46  | 121.06      | 112.60   |
| 1   | B     | 468 | ASP  | CA-CB-CG   | 8.45  | 121.05      | 112.60   |
| 1   | B     | 57  | THR  | CB-CA-C    | 8.44  | 127.59      | 110.38   |
| 1   | A     | 468 | ASP  | CA-CB-CG   | 8.43  | 121.03      | 112.60   |
| 1   | B     | 314 | LYS  | CA-CB-CG   | 8.42  | 130.94      | 114.10   |
| 1   | A     | 318 | ASN  | CA-CB-CG   | 8.41  | 121.01      | 112.60   |
| 1   | A     | 238 | ASP  | CA-CB-CG   | 8.40  | 121.00      | 112.60   |
| 1   | B     | 139 | ASP  | CA-CB-CG   | 8.37  | 120.97      | 112.60   |
| 1   | A     | 364 | ARG  | NE-CZ-NH1  | -8.36 | 113.14      | 121.50   |
| 1   | A     | 169 | ARG  | N-CA-C     | 8.36  | 123.04      | 109.59   |
| 1   | A     | 432 | ASN  | OD1-CG-ND2 | 8.36  | 130.96      | 122.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 191 | SER  | CA-C-N    | 8.34  | 134.84      | 120.58   |
| 1   | B     | 191 | SER  | C-N-CA    | 8.34  | 134.84      | 120.58   |
| 1   | B     | 365 | LEU  | N-CA-CB   | -8.33 | 97.82       | 110.07   |
| 1   | A     | 412 | GLU  | CA-CB-CG  | 8.29  | 130.69      | 114.10   |
| 1   | B     | 188 | ARG  | NE-CZ-NH2 | 8.27  | 126.65      | 119.20   |
| 1   | B     | 377 | PRO  | CA-C-O    | -8.27 | 110.84      | 123.16   |
| 1   | B     | 212 | ASP  | CA-C-N    | 8.23  | 128.34      | 122.33   |
| 1   | B     | 212 | ASP  | C-N-CA    | 8.23  | 128.34      | 122.33   |
| 1   | A     | 102 | ILE  | CA-C-O    | -8.20 | 110.53      | 120.78   |
| 1   | B     | 187 | LEU  | CB-CA-C   | 8.20  | 125.46      | 109.72   |
| 1   | B     | 465 | HIS  | CA-C-O    | 8.19  | 128.66      | 119.41   |
| 1   | A     | 67  | ARG  | CA-CB-CG  | 8.16  | 130.43      | 114.10   |
| 1   | A     | 143 | ASP  | O-C-N     | 8.14  | 132.61      | 123.16   |
| 1   | A     | 260 | GLY  | CA-C-N    | -8.13 | 109.38      | 120.44   |
| 1   | A     | 260 | GLY  | C-N-CA    | -8.13 | 109.38      | 120.44   |
| 1   | B     | 55  | VAL  | CA-C-N    | 8.12  | 131.48      | 120.44   |
| 1   | B     | 55  | VAL  | C-N-CA    | 8.12  | 131.48      | 120.44   |
| 1   | A     | 261 | LEU  | CA-CB-CG  | 8.12  | 144.70      | 116.30   |
| 1   | A     | 64  | ASP  | CA-C-N    | 8.11  | 135.25      | 122.60   |
| 1   | A     | 64  | ASP  | C-N-CA    | 8.11  | 135.25      | 122.60   |
| 1   | A     | 68  | ILE  | O-C-N     | 8.10  | 128.12      | 121.40   |
| 1   | A     | 135 | PHE  | CA-CB-CG  | 8.10  | 121.90      | 113.80   |
| 1   | B     | 450 | LEU  | CA-C-O    | -8.10 | 111.96      | 121.11   |
| 1   | B     | 127 | ASP  | CA-CB-CG  | 8.09  | 120.69      | 112.60   |
| 1   | A     | 57  | THR  | CB-CA-C   | 8.09  | 124.59      | 110.85   |
| 1   | A     | 468 | ASP  | CA-C-O    | -8.08 | 110.10      | 119.56   |
| 1   | A     | 62  | HIS  | CA-CB-CG  | -8.05 | 105.75      | 113.80   |
| 1   | B     | 143 | ASP  | CA-C-N    | 8.05  | 135.36      | 123.12   |
| 1   | B     | 143 | ASP  | C-N-CA    | 8.05  | 135.36      | 123.12   |
| 1   | B     | 25  | VAL  | CA-C-N    | 8.02  | 132.79      | 121.24   |
| 1   | B     | 25  | VAL  | C-N-CA    | 8.02  | 132.79      | 121.24   |
| 1   | B     | 157 | ALA  | CA-C-N    | 8.02  | 132.09      | 120.38   |
| 1   | B     | 157 | ALA  | C-N-CA    | 8.02  | 132.09      | 120.38   |
| 1   | B     | 117 | GLY  | CA-C-N    | 8.01  | 137.03      | 121.66   |
| 1   | B     | 117 | GLY  | C-N-CA    | 8.01  | 137.03      | 121.66   |
| 1   | A     | 217 | HIS  | CA-C-N    | 8.00  | 133.40      | 122.77   |
| 1   | A     | 217 | HIS  | C-N-CA    | 8.00  | 133.40      | 122.77   |
| 1   | A     | 266 | ASN  | CA-C-O    | -7.99 | 112.67      | 120.90   |
| 1   | A     | 234 | HIS  | CA-C-O    | -7.98 | 111.46      | 120.32   |
| 1   | A     | 386 | GLN  | CB-CG-CD  | 7.96  | 126.13      | 112.60   |
| 1   | B     | 119 | SER  | N-CA-C    | 7.95  | 122.07      | 112.38   |
| 1   | B     | 66  | GLU  | N-CA-C    | 7.94  | 121.03      | 111.82   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 368 | ASN  | CB-CG-ND2  | 7.93  | 128.30      | 116.40   |
| 1   | A     | 290 | ILE  | CA-CB-CG2  | 7.93  | 123.98      | 110.50   |
| 1   | A     | 190 | GLU  | CB-CG-CD   | 7.92  | 126.07      | 112.60   |
| 1   | B     | 19  | ALA  | N-CA-C     | -7.92 | 103.75      | 113.50   |
| 1   | B     | 281 | GLN  | CA-C-O     | -7.92 | 112.01      | 120.80   |
| 1   | A     | 435 | ASN  | CB-CA-C    | 7.89  | 124.22      | 110.01   |
| 1   | A     | 157 | ALA  | CA-C-N     | 7.89  | 131.90      | 120.38   |
| 1   | A     | 157 | ALA  | C-N-CA     | 7.89  | 131.90      | 120.38   |
| 1   | A     | 313 | GLY  | CA-C-O     | -7.89 | 113.79      | 121.83   |
| 1   | B     | 449 | VAL  | N-CA-C     | -7.85 | 105.11      | 112.96   |
| 1   | B     | 74  | HIS  | CB-CA-C    | -7.85 | 99.23       | 111.39   |
| 1   | A     | 281 | GLN  | OE1-CD-NE2 | -7.81 | 114.79      | 122.60   |
| 1   | B     | 115 | VAL  | CA-C-O     | -7.81 | 113.23      | 120.34   |
| 1   | A     | 264 | LEU  | CA-C-O     | -7.81 | 111.88      | 121.02   |
| 1   | A     | 429 | GLN  | CA-C-N     | 7.80  | 134.68      | 123.14   |
| 1   | A     | 429 | GLN  | C-N-CA     | 7.80  | 134.68      | 123.14   |
| 1   | B     | 219 | PHE  | CA-CB-CG   | -7.79 | 106.01      | 113.80   |
| 1   | A     | 449 | VAL  | O-C-N      | 7.78  | 130.73      | 122.17   |
| 1   | B     | 89  | ASP  | CB-CA-C    | 7.77  | 123.37      | 109.38   |
| 1   | B     | 481 | PHE  | CA-CB-CG   | -7.77 | 106.03      | 113.80   |
| 1   | B     | 265 | PHE  | CA-C-N     | 7.74  | 130.51      | 120.44   |
| 1   | B     | 265 | PHE  | C-N-CA     | 7.74  | 130.51      | 120.44   |
| 1   | B     | 111 | ARG  | O-C-N      | 7.74  | 133.29      | 123.23   |
| 1   | B     | 234 | HIS  | CA-C-O     | -7.73 | 111.73      | 120.32   |
| 1   | A     | 261 | LEU  | N-CA-CB    | 7.73  | 121.28      | 110.07   |
| 1   | B     | 10  | GLN  | OE1-CD-NE2 | -7.72 | 114.88      | 122.60   |
| 1   | B     | 318 | ASN  | OD1-CG-ND2 | 7.71  | 130.31      | 122.60   |
| 1   | A     | 488 | TYR  | CA-C-N     | 7.70  | 128.33      | 119.94   |
| 1   | A     | 488 | TYR  | C-N-CA     | 7.70  | 128.33      | 119.94   |
| 1   | A     | 284 | THR  | OG1-CB-CG2 | 7.68  | 124.65      | 109.30   |
| 1   | A     | 176 | LYS  | N-CA-C     | -7.67 | 98.08       | 110.20   |
| 1   | A     | 457 | ARG  | CD-NE-CZ   | 7.67  | 135.14      | 124.40   |
| 1   | B     | 284 | THR  | CA-C-O     | -7.66 | 113.37      | 122.03   |
| 1   | B     | 126 | ARG  | N-CA-C     | -7.65 | 98.34       | 109.59   |
| 1   | B     | 247 | GLU  | CA-CB-CG   | 7.65  | 129.39      | 114.10   |
| 1   | B     | 48  | PRO  | CA-C-N     | 7.63  | 132.78      | 121.72   |
| 1   | B     | 48  | PRO  | C-N-CA     | 7.63  | 132.78      | 121.72   |
| 1   | B     | 368 | ASN  | CA-C-O     | -7.62 | 112.06      | 121.89   |
| 1   | B     | 64  | ASP  | CA-CB-CG   | 7.61  | 120.21      | 112.60   |
| 1   | B     | 430 | ARG  | NE-CZ-NH2  | 7.61  | 126.05      | 119.20   |
| 1   | A     | 226 | GLY  | N-CA-C     | -7.60 | 104.30      | 115.63   |
| 1   | A     | 188 | ARG  | CD-NE-CZ   | -7.59 | 113.77      | 124.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 385 | TYR  | CB-CA-C    | 7.59  | 123.25      | 111.02   |
| 1   | B     | 159 | LEU  | CA-CB-CG   | 7.57  | 142.79      | 116.30   |
| 1   | B     | 374 | VAL  | CA-C-O     | -7.54 | 110.49      | 119.85   |
| 1   | A     | 328 | VAL  | CB-CA-C    | 7.54  | 118.30      | 110.91   |
| 1   | B     | 163 | PHE  | N-CA-CB    | 7.54  | 121.29      | 109.82   |
| 1   | A     | 29  | GLY  | O-C-N      | -7.52 | 114.11      | 122.84   |
| 1   | A     | 290 | ILE  | CB-CA-C    | 7.52  | 119.21      | 110.93   |
| 1   | A     | 387 | ARG  | CA-C-O     | 7.52  | 129.93      | 121.51   |
| 1   | B     | 209 | ARG  | CD-NE-CZ   | -7.50 | 113.90      | 124.40   |
| 1   | B     | 470 | GLN  | CA-C-O     | -7.50 | 113.39      | 121.56   |
| 1   | A     | 169 | ARG  | NE-CZ-NH1  | 7.49  | 128.99      | 121.50   |
| 1   | B     | 414 | GLN  | CB-CA-C    | 7.49  | 120.17      | 110.13   |
| 1   | A     | 344 | PRO  | CA-C-O     | -7.49 | 112.72      | 121.86   |
| 1   | A     | 134 | LYS  | CA-C-O     | -7.48 | 112.78      | 120.71   |
| 1   | A     | 174 | HIS  | CA-CB-CG   | 7.48  | 121.28      | 113.80   |
| 1   | A     | 432 | ASN  | CA-C-O     | -7.47 | 113.37      | 121.44   |
| 1   | A     | 230 | TYR  | CA-C-O     | -7.46 | 112.56      | 121.66   |
| 1   | B     | 381 | ARG  | NE-CZ-NH1  | -7.46 | 114.04      | 121.50   |
| 1   | B     | 337 | ASN  | CA-C-O     | -7.43 | 113.82      | 122.37   |
| 1   | B     | 177 | ASP  | CA-C-N     | 7.43  | 128.06      | 120.04   |
| 1   | B     | 177 | ASP  | C-N-CA     | 7.43  | 128.06      | 120.04   |
| 1   | B     | 304 | HIS  | CA-CB-CG   | 7.43  | 121.23      | 113.80   |
| 1   | A     | 103 | GLY  | N-CA-C     | -7.41 | 105.88      | 114.69   |
| 1   | A     | 405 | PRO  | N-CD-CG    | -7.39 | 94.93       | 103.80   |
| 1   | A     | 393 | MET  | CB-CA-C    | -7.37 | 99.26       | 110.90   |
| 1   | A     | 10  | GLN  | CA-C-O     | -7.36 | 113.28      | 121.00   |
| 1   | B     | 126 | ARG  | CA-CB-CG   | 7.36  | 128.81      | 114.10   |
| 1   | B     | 407 | SER  | CA-C-O     | -7.36 | 109.99      | 120.51   |
| 1   | B     | 239 | GLN  | OE1-CD-NE2 | -7.35 | 115.25      | 122.60   |
| 1   | A     | 399 | GLY  | CA-C-N     | 7.34  | 130.50      | 120.67   |
| 1   | A     | 399 | GLY  | C-N-CA     | 7.34  | 130.50      | 120.67   |
| 1   | A     | 262 | ARG  | O-C-N      | 7.33  | 129.93      | 122.08   |
| 1   | B     | 343 | GLU  | CG-CD-OE1  | 7.33  | 135.25      | 118.40   |
| 1   | B     | 453 | GLU  | CA-C-N     | 7.32  | 130.09      | 120.28   |
| 1   | B     | 453 | GLU  | C-N-CA     | 7.32  | 130.09      | 120.28   |
| 1   | A     | 451 | ASN  | CA-CB-CG   | 7.32  | 119.92      | 112.60   |
| 1   | A     | 30  | GLY  | N-CA-C     | -7.31 | 104.26      | 115.66   |
| 1   | A     | 368 | ASN  | CA-C-O     | -7.30 | 110.07      | 120.51   |
| 1   | A     | 425 | SER  | CB-CA-C    | -7.29 | 99.61       | 110.62   |
| 1   | B     | 129 | ARG  | NE-CZ-NH2  | 7.29  | 125.76      | 119.20   |
| 1   | B     | 457 | ARG  | CD-NE-CZ   | 7.28  | 134.60      | 124.40   |
| 1   | A     | 416 | SER  | CA-C-N     | -7.28 | 111.62      | 122.83   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 416 | SER  | C-N-CA     | -7.28 | 111.62      | 122.83   |
| 1   | A     | 89  | ASP  | CA-CB-CG   | -7.28 | 105.32      | 112.60   |
| 1   | B     | 193 | HIS  | CA-C-O     | -7.26 | 113.37      | 121.00   |
| 1   | A     | 386 | GLN  | OE1-CD-NE2 | -7.26 | 115.34      | 122.60   |
| 1   | B     | 480 | ASN  | OD1-CG-ND2 | 7.26  | 129.86      | 122.60   |
| 1   | A     | 176 | LYS  | CA-C-O     | -7.26 | 112.77      | 121.05   |
| 1   | A     | 343 | GLU  | CB-CA-C    | 7.25  | 124.46      | 110.17   |
| 1   | B     | 494 | ALA  | CA-C-N     | 7.25  | 130.00      | 120.28   |
| 1   | B     | 494 | ALA  | C-N-CA     | 7.25  | 130.00      | 120.28   |
| 1   | A     | 239 | GLN  | CB-CG-CD   | 7.25  | 124.92      | 112.60   |
| 1   | B     | 433 | SER  | N-CA-C     | -7.24 | 101.55      | 113.50   |
| 1   | B     | 158 | LEU  | CA-C-N     | 7.23  | 134.47      | 122.54   |
| 1   | B     | 158 | LEU  | C-N-CA     | 7.23  | 134.47      | 122.54   |
| 1   | A     | 163 | PHE  | CA-C-N     | 7.23  | 129.67      | 120.56   |
| 1   | A     | 163 | PHE  | C-N-CA     | 7.23  | 129.67      | 120.56   |
| 1   | B     | 111 | ARG  | N-CA-C     | -7.22 | 97.63       | 109.40   |
| 1   | B     | 450 | LEU  | N-CA-CB    | -7.20 | 98.77       | 111.08   |
| 1   | B     | 381 | ARG  | CD-NE-CZ   | -7.20 | 114.32      | 124.40   |
| 1   | B     | 443 | ARG  | CD-NE-CZ   | 7.20  | 134.47      | 124.40   |
| 1   | B     | 178 | PRO  | CA-C-N     | 7.19  | 130.22      | 120.44   |
| 1   | B     | 178 | PRO  | C-N-CA     | 7.19  | 130.22      | 120.44   |
| 1   | A     | 102 | ILE  | O-C-N      | 7.19  | 131.56      | 122.57   |
| 1   | A     | 172 | GLN  | CA-CB-CG   | -7.18 | 99.74       | 114.10   |
| 1   | A     | 111 | ARG  | NE-CZ-NH1  | 7.17  | 128.67      | 121.50   |
| 1   | B     | 9   | ASP  | CA-CB-CG   | 7.17  | 119.77      | 112.60   |
| 1   | A     | 218 | THR  | CA-C-N     | -7.16 | 109.97      | 122.64   |
| 1   | A     | 218 | THR  | C-N-CA     | -7.16 | 109.97      | 122.64   |
| 1   | B     | 414 | GLN  | OE1-CD-NE2 | 7.14  | 129.74      | 122.60   |
| 1   | B     | 436 | ASP  | CA-CB-CG   | 7.13  | 119.73      | 112.60   |
| 1   | B     | 145 | VAL  | CA-C-N     | -7.11 | 114.97      | 122.30   |
| 1   | B     | 145 | VAL  | C-N-CA     | -7.11 | 114.97      | 122.30   |
| 1   | B     | 375 | ASN  | OD1-CG-ND2 | -7.09 | 115.51      | 122.60   |
| 1   | B     | 343 | GLU  | N-CA-CB    | -7.09 | 97.75       | 110.37   |
| 1   | B     | 113 | SER  | O-C-N      | 7.08  | 130.47      | 123.46   |
| 1   | B     | 270 | THR  | CA-CB-OG1  | -7.08 | 98.97       | 109.60   |
| 1   | A     | 77  | GLY  | CA-C-O     | 7.07  | 128.35      | 121.63   |
| 1   | B     | 183 | ASP  | CA-CB-CG   | -7.05 | 105.55      | 112.60   |
| 1   | A     | 69  | PRO  | CA-C-O     | -7.04 | 113.31      | 121.34   |
| 1   | B     | 225 | ASP  | CA-C-O     | -7.02 | 110.82      | 119.18   |
| 1   | A     | 93  | TYR  | O-C-N      | 7.01  | 129.29      | 122.07   |
| 1   | A     | 328 | VAL  | CA-C-N     | -7.01 | 110.34      | 120.29   |
| 1   | A     | 328 | VAL  | C-N-CA     | -7.01 | 110.34      | 120.29   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 319 | ARG  | CD-NE-CZ   | -7.00 | 114.59      | 124.40   |
| 1   | A     | 332 | ALA  | CA-C-N     | 7.00  | 131.75      | 122.30   |
| 1   | A     | 332 | ALA  | C-N-CA     | 7.00  | 131.75      | 122.30   |
| 1   | B     | 386 | GLN  | OE1-CD-NE2 | -6.99 | 115.61      | 122.60   |
| 1   | B     | 475 | LYS  | O-C-N      | 6.99  | 130.15      | 122.11   |
| 1   | A     | 94  | SER  | O-C-N      | -6.98 | 114.75      | 123.27   |
| 1   | A     | 259 | TYR  | CA-C-N     | 6.98  | 128.87      | 120.14   |
| 1   | A     | 259 | TYR  | C-N-CA     | 6.98  | 128.87      | 120.14   |
| 1   | B     | 465 | HIS  | CA-CB-CG   | 6.98  | 120.78      | 113.80   |
| 1   | A     | 366 | GLY  | O-C-N      | 6.96  | 128.73      | 121.77   |
| 1   | B     | 94  | SER  | N-CA-C     | 6.94  | 120.49      | 108.76   |
| 1   | A     | 413 | HIS  | N-CA-CB    | 6.93  | 120.28      | 110.36   |
| 1   | B     | 360 | THR  | CA-C-O     | 6.93  | 127.06      | 119.15   |
| 1   | B     | 88  | HIS  | CA-C-N     | -6.93 | 112.88      | 122.93   |
| 1   | B     | 88  | HIS  | C-N-CA     | -6.93 | 112.88      | 122.93   |
| 1   | B     | 269 | ALA  | CA-C-O     | 6.93  | 127.97      | 119.79   |
| 1   | B     | 413 | HIS  | N-CA-CB    | 6.93  | 120.82      | 110.29   |
| 1   | B     | 70  | GLU  | CA-C-N     | 6.92  | 130.57      | 120.82   |
| 1   | B     | 70  | GLU  | C-N-CA     | 6.92  | 130.57      | 120.82   |
| 1   | A     | 335 | PRO  | CA-CB-CG   | -6.91 | 91.37       | 104.50   |
| 1   | B     | 363 | HIS  | CA-C-N     | 6.91  | 130.40      | 120.79   |
| 1   | B     | 363 | HIS  | C-N-CA     | 6.91  | 130.40      | 120.79   |
| 1   | A     | 106 | THR  | O-C-N      | 6.89  | 128.26      | 121.57   |
| 1   | A     | 67  | ARG  | CG-CD-NE   | 6.89  | 127.16      | 112.00   |
| 1   | A     | 153 | PHE  | CA-C-O     | -6.89 | 111.66      | 119.79   |
| 1   | B     | 102 | ILE  | O-C-N      | 6.89  | 130.12      | 122.75   |
| 1   | B     | 32  | ASN  | CA-CB-CG   | 6.88  | 119.48      | 112.60   |
| 1   | B     | 302 | TRP  | N-CA-CB    | 6.88  | 120.05      | 110.01   |
| 1   | B     | 425 | SER  | CA-C-N     | -6.87 | 111.43      | 120.91   |
| 1   | B     | 425 | SER  | C-N-CA     | -6.87 | 111.43      | 120.91   |
| 1   | B     | 65  | ARG  | CA-C-N     | 6.87  | 130.75      | 120.31   |
| 1   | B     | 65  | ARG  | C-N-CA     | 6.87  | 130.75      | 120.31   |
| 1   | B     | 112 | PHE  | CA-C-O     | -6.86 | 113.28      | 121.66   |
| 1   | B     | 96  | ALA  | CA-C-N     | 6.86  | 131.10      | 120.82   |
| 1   | B     | 96  | ALA  | C-N-CA     | 6.86  | 131.10      | 120.82   |
| 1   | A     | 143 | ASP  | CA-C-O     | -6.85 | 113.04      | 120.92   |
| 1   | B     | 457 | ARG  | NE-CZ-NH2  | -6.82 | 113.06      | 119.20   |
| 1   | B     | 200 | SER  | CA-C-N     | 6.82  | 130.33      | 120.38   |
| 1   | B     | 200 | SER  | C-N-CA     | 6.82  | 130.33      | 120.38   |
| 1   | B     | 325 | PHE  | CA-C-O     | -6.78 | 113.65      | 120.90   |
| 1   | B     | 193 | HIS  | CA-C-N     | 6.77  | 132.19      | 120.68   |
| 1   | B     | 193 | HIS  | C-N-CA     | 6.77  | 132.19      | 120.68   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 302 | TRP  | CA-CB-CG   | 6.77  | 126.45      | 113.60   |
| 1   | B     | 263 | ASP  | CB-CA-C    | 6.76  | 121.37      | 110.96   |
| 1   | A     | 111 | ARG  | N-CA-CB    | 6.75  | 122.48      | 110.80   |
| 1   | A     | 266 | ASN  | CB-CA-C    | 6.75  | 121.41      | 110.95   |
| 1   | A     | 9   | ASP  | CB-CA-C    | 6.74  | 122.07      | 110.94   |
| 1   | A     | 121 | SER  | CA-C-N     | -6.74 | 112.60      | 122.65   |
| 1   | A     | 121 | SER  | C-N-CA     | -6.74 | 112.60      | 122.65   |
| 1   | B     | 46  | ARG  | O-C-N      | 6.74  | 131.22      | 122.19   |
| 1   | A     | 396 | ASN  | OD1-CG-ND2 | -6.74 | 115.86      | 122.60   |
| 1   | B     | 242 | LYS  | CA-C-O     | -6.74 | 110.88      | 120.51   |
| 1   | B     | 494 | ALA  | CB-CA-C    | 6.73  | 122.01      | 110.84   |
| 1   | A     | 52  | GLN  | N-CA-CB    | 6.72  | 120.22      | 110.47   |
| 1   | A     | 291 | PHE  | CB-CA-C    | 6.71  | 120.16      | 109.62   |
| 1   | B     | 250 | ALA  | CA-C-N     | 6.71  | 130.12      | 120.79   |
| 1   | B     | 250 | ALA  | C-N-CA     | 6.71  | 130.12      | 120.79   |
| 1   | B     | 147 | ASN  | CA-C-O     | -6.71 | 113.80      | 121.58   |
| 1   | A     | 360 | THR  | CA-C-N     | 6.71  | 130.51      | 120.31   |
| 1   | A     | 360 | THR  | C-N-CA     | 6.71  | 130.51      | 120.31   |
| 1   | A     | 179 | ASP  | N-CA-C     | -6.71 | 103.13      | 112.45   |
| 1   | B     | 318 | ASN  | CA-C-O     | 6.70  | 126.12      | 119.08   |
| 1   | A     | 207 | GLY  | N-CA-C     | -6.70 | 102.89      | 112.81   |
| 1   | B     | 89  | ASP  | CB-CG-OD1  | -6.70 | 103.00      | 118.40   |
| 1   | A     | 482 | SER  | O-C-N      | 6.69  | 129.22      | 122.12   |
| 1   | B     | 336 | SER  | CA-C-O     | 6.69  | 127.89      | 119.12   |
| 1   | B     | 299 | THR  | CA-CB-OG1  | -6.69 | 99.57       | 109.60   |
| 1   | A     | 246 | VAL  | CA-C-N     | 6.69  | 129.53      | 120.44   |
| 1   | A     | 246 | VAL  | C-N-CA     | 6.69  | 129.53      | 120.44   |
| 1   | A     | 40  | SER  | CA-C-N     | 6.68  | 131.41      | 121.72   |
| 1   | A     | 40  | SER  | C-N-CA     | 6.68  | 131.41      | 121.72   |
| 1   | A     | 270 | THR  | N-CA-CB    | 6.68  | 120.66      | 110.44   |
| 1   | A     | 384 | ASN  | CB-CG-ND2  | -6.68 | 106.38      | 116.40   |
| 1   | A     | 19  | ALA  | CA-C-O     | 6.66  | 126.94      | 119.41   |
| 1   | A     | 475 | LYS  | N-CA-CB    | 6.65  | 119.93      | 109.82   |
| 1   | B     | 89  | ASP  | OD1-CG-OD2 | 6.64  | 138.84      | 122.90   |
| 1   | B     | 433 | SER  | CA-C-O     | 6.64  | 125.76      | 118.65   |
| 1   | A     | 284 | THR  | N-CA-CB    | -6.62 | 100.79      | 110.26   |
| 1   | A     | 270 | THR  | N-CA-C     | -6.62 | 104.95      | 113.16   |
| 1   | B     | 126 | ARG  | O-C-N      | 6.62  | 131.30      | 122.96   |
| 1   | A     | 387 | ARG  | CD-NE-CZ   | -6.62 | 115.14      | 124.40   |
| 1   | A     | 382 | VAL  | O-C-N      | 6.61  | 130.24      | 122.83   |
| 1   | B     | 445 | PHE  | CA-C-O     | -6.61 | 113.51      | 120.92   |
| 1   | A     | 299 | THR  | CA-CB-OG1  | -6.61 | 99.68       | 109.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 111 | ARG  | CD-NE-CZ   | 6.61  | 133.65      | 124.40   |
| 1   | B     | 435 | ASN  | CB-CA-C    | 6.60  | 121.71      | 110.56   |
| 1   | B     | 48  | PRO  | O-C-N      | -6.59 | 114.97      | 123.00   |
| 1   | B     | 33  | PRO  | CA-C-N     | 6.58  | 132.32      | 122.91   |
| 1   | B     | 33  | PRO  | C-N-CA     | 6.58  | 132.32      | 122.91   |
| 1   | B     | 19  | ALA  | CA-C-O     | 6.58  | 126.38      | 119.14   |
| 1   | A     | 73  | VAL  | CA-C-O     | -6.58 | 114.31      | 121.28   |
| 1   | B     | 65  | ARG  | NE-CZ-NH2  | 6.57  | 125.11      | 119.20   |
| 1   | A     | 444 | THR  | OG1-CB-CG2 | 6.57  | 122.44      | 109.30   |
| 1   | B     | 262 | ARG  | NH1-CZ-NH2 | 6.57  | 127.84      | 119.30   |
| 1   | B     | 62  | HIS  | CA-CB-CG   | -6.56 | 107.24      | 113.80   |
| 1   | B     | 237 | THR  | CA-C-O     | -6.55 | 113.58      | 121.05   |
| 1   | A     | 360 | THR  | N-CA-CB    | -6.55 | 99.41       | 110.41   |
| 1   | B     | 261 | LEU  | N-CA-C     | -6.54 | 104.07      | 111.14   |
| 1   | B     | 70  | GLU  | CB-CG-CD   | 6.54  | 123.71      | 112.60   |
| 1   | B     | 223 | ASN  | O-C-N      | 6.54  | 130.92      | 122.23   |
| 1   | B     | 281 | GLN  | N-CA-C     | -6.53 | 99.05       | 109.76   |
| 1   | B     | 431 | PHE  | CA-CB-CG   | -6.53 | 107.27      | 113.80   |
| 1   | B     | 182 | TRP  | CB-CA-C    | 6.52  | 123.20      | 110.67   |
| 1   | B     | 187 | LEU  | N-CA-CB    | -6.52 | 100.22      | 110.46   |
| 1   | B     | 343 | GLU  | CA-C-N     | 6.52  | 126.43      | 119.85   |
| 1   | B     | 343 | GLU  | C-N-CA     | 6.52  | 126.43      | 119.85   |
| 1   | B     | 449 | VAL  | CB-CA-C    | 6.51  | 116.79      | 111.06   |
| 1   | A     | 153 | PHE  | O-C-N      | 6.51  | 131.05      | 122.33   |
| 1   | B     | 219 | PHE  | CA-C-O     | -6.51 | 113.35      | 121.55   |
| 1   | B     | 381 | ARG  | NE-CZ-NH2  | 6.50  | 125.05      | 119.20   |
| 1   | A     | 424 | PHE  | CA-C-N     | 6.50  | 132.08      | 122.86   |
| 1   | A     | 424 | PHE  | C-N-CA     | 6.50  | 132.08      | 122.86   |
| 1   | B     | 16  | GLU  | CB-CG-CD   | 6.49  | 123.64      | 112.60   |
| 1   | A     | 212 | ASP  | CA-CB-CG   | 6.46  | 119.06      | 112.60   |
| 1   | A     | 49  | LEU  | CA-C-N     | 6.46  | 130.66      | 121.42   |
| 1   | A     | 49  | LEU  | C-N-CA     | 6.46  | 130.66      | 121.42   |
| 1   | A     | 122 | ALA  | CB-CA-C    | 6.46  | 120.34      | 109.48   |
| 1   | A     | 429 | GLN  | CA-CB-CG   | 6.46  | 127.02      | 114.10   |
| 1   | B     | 483 | ASP  | CA-C-O     | -6.46 | 112.96      | 120.20   |
| 1   | A     | 13  | HIS  | CA-C-N     | 6.46  | 129.58      | 120.28   |
| 1   | A     | 13  | HIS  | C-N-CA     | 6.46  | 129.58      | 120.28   |
| 1   | B     | 330 | GLN  | OE1-CD-NE2 | -6.45 | 116.15      | 122.60   |
| 1   | B     | 499 | TYR  | CA-C-N     | 6.45  | 133.30      | 121.70   |
| 1   | B     | 499 | TYR  | C-N-CA     | 6.45  | 133.30      | 121.70   |
| 1   | A     | 80  | ALA  | CB-CA-C    | 6.44  | 121.11      | 110.03   |
| 1   | A     | 207 | GLY  | CA-C-O     | -6.44 | 116.64      | 122.57   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 71  | ARG  | CB-CG-CD   | 6.44  | 126.11      | 111.30   |
| 1   | A     | 372 | ILE  | CA-CB-CG1  | 6.43  | 121.33      | 110.40   |
| 1   | A     | 499 | TYR  | CA-C-N     | 6.42  | 133.26      | 121.70   |
| 1   | A     | 499 | TYR  | C-N-CA     | 6.42  | 133.26      | 121.70   |
| 1   | B     | 32  | ASN  | CA-C-O     | -6.42 | 112.42      | 119.61   |
| 1   | B     | 263 | ASP  | CA-CB-CG   | 6.42  | 119.02      | 112.60   |
| 1   | B     | 457 | ARG  | NE-CZ-NH1  | 6.42  | 127.92      | 121.50   |
| 1   | B     | 374 | VAL  | O-C-N      | 6.41  | 130.44      | 122.05   |
| 1   | A     | 440 | THR  | CA-CB-CG2  | 6.41  | 121.39      | 110.50   |
| 1   | A     | 353 | ARG  | CD-NE-CZ   | 6.40  | 133.36      | 124.40   |
| 1   | A     | 96  | ALA  | O-C-N      | 6.40  | 130.80      | 122.93   |
| 1   | B     | 266 | ASN  | CA-CB-CG   | -6.40 | 106.20      | 112.60   |
| 1   | B     | 320 | ASN  | O-C-N      | 6.40  | 129.66      | 121.34   |
| 1   | A     | 190 | GLU  | N-CA-C     | -6.40 | 105.33      | 113.01   |
| 1   | A     | 454 | GLN  | CB-CG-CD   | 6.39  | 123.47      | 112.60   |
| 1   | A     | 465 | HIS  | CA-C-N     | 6.39  | 130.03      | 120.31   |
| 1   | A     | 465 | HIS  | C-N-CA     | 6.39  | 130.03      | 120.31   |
| 1   | A     | 55  | VAL  | N-CA-C     | -6.39 | 106.31      | 111.81   |
| 1   | A     | 164 | ILE  | CB-CG1-CD1 | 6.39  | 127.22      | 113.80   |
| 1   | A     | 113 | SER  | O-C-N      | 6.39  | 129.27      | 123.26   |
| 1   | A     | 405 | PRO  | CA-N-CD    | -6.39 | 102.56      | 111.50   |
| 1   | B     | 30  | GLY  | N-CA-C     | -6.38 | 105.70      | 115.66   |
| 1   | B     | 5   | ASP  | CA-CB-CG   | -6.38 | 106.22      | 112.60   |
| 1   | A     | 89  | ASP  | CA-C-O     | 6.38  | 128.32      | 121.11   |
| 1   | B     | 338 | MET  | N-CA-C     | -6.38 | 99.20       | 109.40   |
| 1   | B     | 182 | TRP  | N-CA-CB    | -6.37 | 100.41      | 110.28   |
| 1   | A     | 323 | ASN  | CB-CG-ND2  | 6.36  | 125.94      | 116.40   |
| 1   | A     | 379 | ARG  | CA-CB-CG   | 6.36  | 126.82      | 114.10   |
| 1   | B     | 114 | THR  | CA-C-O     | -6.36 | 113.83      | 120.89   |
| 1   | A     | 496 | LEU  | N-CA-C     | -6.35 | 104.40      | 111.71   |
| 1   | B     | 87  | THR  | O-C-N      | 6.35  | 128.66      | 121.93   |
| 1   | B     | 461 | ASN  | N-CA-C     | -6.35 | 104.05      | 110.97   |
| 1   | B     | 127 | ASP  | CA-C-O     | -6.35 | 114.67      | 120.13   |
| 1   | B     | 434 | ALA  | CA-C-N     | -6.35 | 112.49      | 122.65   |
| 1   | B     | 434 | ALA  | C-N-CA     | -6.35 | 112.49      | 122.65   |
| 1   | B     | 265 | PHE  | N-CA-CB    | 6.34  | 119.20      | 110.01   |
| 1   | B     | 381 | ARG  | CA-C-N     | 6.33  | 130.67      | 121.18   |
| 1   | B     | 381 | ARG  | C-N-CA     | 6.33  | 130.67      | 121.18   |
| 1   | A     | 336 | SER  | CA-CB-OG   | 6.32  | 123.74      | 111.10   |
| 1   | B     | 111 | ARG  | CA-C-O     | -6.31 | 113.89      | 120.70   |
| 1   | A     | 59  | GLU  | CA-C-O     | 6.31  | 127.10      | 120.42   |
| 1   | B     | 478 | VAL  | N-CA-C     | 6.30  | 117.05      | 110.62   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 126 | ARG  | CA-CB-CG   | 6.30  | 126.70      | 114.10   |
| 1   | B     | 294 | ASN  | CB-CA-C    | 6.30  | 119.99      | 109.85   |
| 1   | A     | 323 | ASN  | OD1-CG-ND2 | -6.29 | 116.31      | 122.60   |
| 1   | B     | 242 | LYS  | O-C-N      | 6.29  | 130.95      | 122.59   |
| 1   | A     | 456 | LYS  | N-CA-C     | -6.28 | 103.96      | 111.69   |
| 1   | B     | 60  | MET  | CA-CB-CG   | 6.28  | 126.66      | 114.10   |
| 1   | B     | 466 | LEU  | O-C-N      | 6.28  | 129.99      | 122.27   |
| 1   | A     | 199 | PHE  | CA-CB-CG   | -6.27 | 107.53      | 113.80   |
| 1   | B     | 239 | GLN  | CG-CD-OE1  | 6.27  | 133.34      | 120.80   |
| 1   | B     | 270 | THR  | CA-C-O     | -6.27 | 112.22      | 119.56   |
| 1   | B     | 163 | PHE  | O-C-N      | 6.26  | 128.78      | 122.08   |
| 1   | B     | 175 | LEU  | CA-C-N     | 6.26  | 129.76      | 120.87   |
| 1   | B     | 175 | LEU  | C-N-CA     | 6.26  | 129.76      | 120.87   |
| 1   | A     | 265 | PHE  | O-C-N      | 6.25  | 128.59      | 122.09   |
| 1   | A     | 175 | LEU  | CA-C-N     | 6.24  | 130.34      | 121.42   |
| 1   | A     | 175 | LEU  | C-N-CA     | 6.24  | 130.34      | 121.42   |
| 1   | B     | 193 | HIS  | CA-CB-CG   | -6.23 | 107.57      | 113.80   |
| 1   | B     | 7   | ALA  | CA-C-N     | 6.23  | 129.25      | 120.28   |
| 1   | B     | 7   | ALA  | C-N-CA     | 6.23  | 129.25      | 120.28   |
| 1   | B     | 199 | PHE  | CA-C-O     | -6.21 | 112.39      | 119.78   |
| 1   | B     | 312 | VAL  | CA-CB-CG2  | 6.21  | 120.96      | 110.40   |
| 1   | A     | 193 | HIS  | CA-C-N     | 6.21  | 131.20      | 120.58   |
| 1   | A     | 193 | HIS  | C-N-CA     | 6.21  | 131.20      | 120.58   |
| 1   | A     | 416 | SER  | N-CA-C     | -6.20 | 105.81      | 113.19   |
| 1   | B     | 101 | HIS  | CA-CB-CG   | 6.20  | 120.00      | 113.80   |
| 1   | A     | 402 | ASN  | CB-CG-ND2  | 6.19  | 125.69      | 116.40   |
| 1   | A     | 188 | ARG  | NE-CZ-NH1  | -6.19 | 115.31      | 121.50   |
| 1   | B     | 49  | LEU  | CA-C-O     | 6.19  | 127.67      | 120.49   |
| 1   | A     | 347 | ASP  | CA-C-N     | 6.17  | 128.87      | 120.54   |
| 1   | A     | 347 | ASP  | C-N-CA     | 6.17  | 128.87      | 120.54   |
| 1   | B     | 353 | ARG  | CA-C-O     | -6.17 | 114.01      | 120.55   |
| 1   | B     | 488 | TYR  | N-CA-C     | -6.17 | 104.48      | 111.14   |
| 1   | A     | 225 | ASP  | CA-C-O     | -6.17 | 111.84      | 119.18   |
| 1   | B     | 346 | PRO  | CB-CA-C    | 6.16  | 118.90      | 110.52   |
| 1   | B     | 289 | GLU  | CB-CG-CD   | 6.15  | 123.06      | 112.60   |
| 1   | B     | 95  | LYS  | CG-CD-CE   | 6.15  | 125.44      | 111.30   |
| 1   | A     | 400 | ALA  | N-CA-C     | 6.15  | 118.54      | 109.50   |
| 1   | B     | 278 | LEU  | CA-C-N     | 6.15  | 132.21      | 122.62   |
| 1   | B     | 278 | LEU  | C-N-CA     | 6.15  | 132.21      | 122.62   |
| 1   | A     | 351 | GLN  | OE1-CD-NE2 | 6.14  | 128.74      | 122.60   |
| 1   | A     | 223 | ASN  | OD1-CG-ND2 | 6.13  | 128.73      | 122.60   |
| 1   | B     | 48  | PRO  | N-CA-CB    | -6.13 | 96.94       | 103.38   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 376 | CYS  | CB-CA-C    | 6.13  | 118.28      | 109.26   |
| 1   | A     | 461 | ASN  | CA-C-O     | -6.12 | 114.58      | 121.00   |
| 1   | B     | 408 | PHE  | O-C-N      | -6.11 | 113.89      | 122.26   |
| 1   | B     | 364 | ARG  | NE-CZ-NH2  | -6.11 | 113.70      | 119.20   |
| 1   | B     | 492 | ILE  | CA-C-O     | -6.10 | 114.10      | 121.18   |
| 1   | A     | 472 | PHE  | N-CA-C     | -6.09 | 104.27      | 111.03   |
| 1   | A     | 429 | GLN  | N-CA-CB    | -6.09 | 101.04      | 111.21   |
| 1   | B     | 397 | GLN  | OE1-CD-NE2 | -6.08 | 116.52      | 122.60   |
| 1   | B     | 81  | PHE  | N-CA-CB    | -6.08 | 101.49      | 110.85   |
| 1   | A     | 294 | ASN  | OD1-CG-ND2 | -6.08 | 116.52      | 122.60   |
| 1   | B     | 129 | ARG  | CB-CG-CD   | 6.08  | 125.28      | 111.30   |
| 1   | B     | 454 | GLN  | OE1-CD-NE2 | 6.08  | 128.68      | 122.60   |
| 1   | B     | 474 | GLN  | O-C-N      | 6.08  | 128.33      | 122.07   |
| 1   | B     | 365 | LEU  | O-C-N      | -6.07 | 115.07      | 122.11   |
| 1   | B     | 111 | ARG  | NE-CZ-NH2  | -6.06 | 113.74      | 119.20   |
| 1   | A     | 381 | ARG  | N-CA-CB    | 6.06  | 120.05      | 110.84   |
| 1   | A     | 424 | PHE  | O-C-N      | 6.06  | 130.75      | 123.36   |
| 1   | B     | 480 | ASN  | CA-CB-CG   | -6.05 | 106.55      | 112.60   |
| 1   | A     | 471 | LEU  | CB-CA-C    | 6.05  | 122.96      | 110.31   |
| 1   | A     | 102 | ILE  | CB-CA-C    | -6.05 | 101.37      | 111.29   |
| 1   | B     | 368 | ASN  | CA-CB-CG   | 6.05  | 118.65      | 112.60   |
| 1   | A     | 281 | GLN  | CB-CG-CD   | 6.05  | 122.88      | 112.60   |
| 1   | A     | 364 | ARG  | NH1-CZ-NH2 | 6.05  | 127.16      | 119.30   |
| 1   | B     | 134 | LYS  | CD-CE-NZ   | -6.05 | 92.54       | 111.90   |
| 1   | A     | 52  | GLN  | CA-CB-CG   | 6.05  | 126.19      | 114.10   |
| 1   | B     | 219 | PHE  | N-CA-C     | -6.04 | 100.45      | 109.94   |
| 1   | B     | 289 | GLU  | CA-CB-CG   | 6.04  | 126.19      | 114.10   |
| 1   | B     | 193 | HIS  | CB-CG-CD2  | -6.04 | 123.35      | 131.20   |
| 1   | A     | 281 | GLN  | N-CA-C     | -6.04 | 100.45      | 110.17   |
| 1   | B     | 168 | LYS  | N-CA-CB    | 6.03  | 120.68      | 110.49   |
| 1   | B     | 281 | GLN  | O-C-N      | 6.03  | 130.25      | 123.19   |
| 1   | A     | 107 | PRO  | CB-CA-C    | 6.03  | 118.88      | 110.98   |
| 1   | B     | 215 | GLY  | N-CA-C     | -6.03 | 107.19      | 114.66   |
| 1   | B     | 124 | THR  | CA-CB-OG1  | -6.02 | 100.56      | 109.60   |
| 1   | B     | 476 | LYS  | CB-CG-CD   | 6.02  | 125.15      | 111.30   |
| 1   | B     | 291 | PHE  | N-CA-C     | -6.02 | 102.68      | 109.60   |
| 1   | A     | 102 | ILE  | CA-C-N     | -6.02 | 114.07      | 122.86   |
| 1   | A     | 102 | ILE  | C-N-CA     | -6.02 | 114.07      | 122.86   |
| 1   | A     | 185 | TRP  | N-CA-C     | 6.01  | 118.61      | 111.33   |
| 1   | A     | 344 | PRO  | O-C-N      | 6.01  | 130.70      | 123.13   |
| 1   | B     | 109 | ALA  | CA-C-O     | -6.01 | 114.29      | 121.56   |
| 1   | B     | 137 | THR  | CA-CB-OG1  | -6.00 | 100.60      | 109.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 89  | ASP  | CB-CA-C   | 6.00  | 121.14      | 109.33   |
| 1   | B     | 108 | ILE  | CA-C-O    | -5.99 | 114.93      | 121.28   |
| 1   | A     | 239 | GLN  | CG-CD-NE2 | 5.99  | 125.39      | 116.40   |
| 1   | A     | 96  | ALA  | CA-C-O    | -5.98 | 113.93      | 120.81   |
| 1   | A     | 323 | ASN  | CA-C-N    | 5.98  | 128.54      | 120.65   |
| 1   | A     | 323 | ASN  | C-N-CA    | 5.98  | 128.54      | 120.65   |
| 1   | A     | 297 | ASP  | CA-CB-CG  | 5.97  | 118.57      | 112.60   |
| 1   | A     | 177 | ASP  | N-CA-CB   | -5.96 | 99.76       | 110.37   |
| 1   | A     | 119 | SER  | N-CA-C    | 5.96  | 119.38      | 111.75   |
| 1   | A     | 282 | VAL  | CA-CB-CG1 | 5.96  | 120.53      | 110.40   |
| 1   | B     | 362 | ARG  | CA-C-N    | 5.96  | 129.99      | 121.71   |
| 1   | B     | 362 | ARG  | C-N-CA    | 5.96  | 129.99      | 121.71   |
| 1   | B     | 29  | GLY  | CA-C-O    | 5.96  | 128.84      | 119.31   |
| 1   | B     | 37  | LYS  | CB-CG-CD  | 5.95  | 124.99      | 111.30   |
| 1   | A     | 289 | GLU  | CB-CG-CD  | 5.95  | 122.71      | 112.60   |
| 1   | B     | 71  | ARG  | CA-CB-CG  | 5.94  | 125.99      | 114.10   |
| 1   | A     | 67  | ARG  | CA-C-N    | 5.94  | 130.97      | 122.24   |
| 1   | A     | 67  | ARG  | C-N-CA    | 5.94  | 130.97      | 122.24   |
| 1   | A     | 388 | ASP  | CA-CB-CG  | -5.94 | 106.66      | 112.60   |
| 1   | B     | 54  | VAL  | CA-CB-CG1 | 5.93  | 120.49      | 110.40   |
| 1   | B     | 259 | TYR  | CA-C-N    | 5.93  | 126.56      | 119.98   |
| 1   | B     | 259 | TYR  | C-N-CA    | 5.93  | 126.56      | 119.98   |
| 1   | A     | 480 | ASN  | CA-CB-CG  | 5.92  | 118.52      | 112.60   |
| 1   | B     | 88  | HIS  | CA-C-O    | 5.92  | 127.72      | 121.33   |
| 1   | B     | 143 | ASP  | CA-CB-CG  | 5.91  | 118.51      | 112.60   |
| 1   | B     | 215 | GLY  | CA-C-N    | 5.91  | 132.82      | 121.54   |
| 1   | B     | 215 | GLY  | C-N-CA    | 5.91  | 132.82      | 121.54   |
| 1   | B     | 59  | GLU  | CB-CG-CD  | 5.90  | 122.62      | 112.60   |
| 1   | B     | 137 | THR  | CA-CB-CG2 | 5.90  | 120.52      | 110.50   |
| 1   | B     | 213 | GLY  | N-CA-C    | -5.89 | 100.61      | 111.04   |
| 1   | A     | 472 | PHE  | CB-CA-C   | 5.89  | 120.08      | 110.95   |
| 1   | B     | 261 | LEU  | CA-C-O    | -5.89 | 114.64      | 120.70   |
| 1   | B     | 169 | ARG  | NE-CZ-NH1 | -5.88 | 115.62      | 121.50   |
| 1   | B     | 309 | LEU  | O-C-N     | 5.88  | 129.92      | 123.04   |
| 1   | A     | 468 | ASP  | O-C-N     | 5.88  | 129.40      | 122.34   |
| 1   | B     | 229 | VAL  | N-CA-CB   | -5.88 | 102.41      | 111.05   |
| 1   | A     | 54  | VAL  | CA-C-N    | 5.88  | 129.28      | 122.35   |
| 1   | A     | 54  | VAL  | C-N-CA    | 5.88  | 129.28      | 122.35   |
| 1   | B     | 162 | SER  | CA-C-N    | 5.88  | 128.96      | 120.79   |
| 1   | B     | 162 | SER  | C-N-CA    | 5.88  | 128.96      | 120.79   |
| 1   | A     | 263 | ASP  | CB-CA-C   | 5.87  | 122.11      | 110.42   |
| 1   | B     | 262 | ARG  | NE-CZ-NH1 | -5.87 | 115.63      | 121.50   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 129 | ARG  | CA-C-N     | 5.86  | 127.34      | 120.71   |
| 1   | B     | 129 | ARG  | C-N-CA     | 5.86  | 127.34      | 120.71   |
| 1   | B     | 219 | PHE  | O-C-N      | 5.86  | 129.64      | 122.14   |
| 1   | A     | 463 | ALA  | CA-C-O     | 5.86  | 126.57      | 119.31   |
| 1   | A     | 228 | ALA  | CA-C-N     | 5.85  | 130.18      | 122.51   |
| 1   | A     | 228 | ALA  | C-N-CA     | 5.85  | 130.18      | 122.51   |
| 1   | B     | 359 | ASP  | CA-CB-CG   | 5.85  | 118.45      | 112.60   |
| 1   | A     | 304 | HIS  | N-CA-CB    | 5.84  | 120.23      | 110.41   |
| 1   | A     | 496 | LEU  | CB-CA-C    | 5.84  | 121.44      | 110.63   |
| 1   | B     | 95  | LYS  | CB-CA-C    | -5.84 | 100.70      | 110.81   |
| 1   | B     | 419 | GLU  | CB-CG-CD   | 5.84  | 122.53      | 112.60   |
| 1   | A     | 379 | ARG  | NE-CZ-NH1  | 5.84  | 127.34      | 121.50   |
| 1   | A     | 149 | THR  | CA-CB-OG1  | -5.84 | 100.84      | 109.60   |
| 1   | A     | 282 | VAL  | O-C-N      | 5.83  | 129.34      | 123.10   |
| 1   | A     | 418 | LEU  | CB-CA-C    | 5.83  | 120.27      | 109.54   |
| 1   | B     | 10  | GLN  | N-CA-C     | 5.83  | 117.32      | 110.97   |
| 1   | A     | 353 | ARG  | O-C-N      | -5.83 | 115.56      | 122.20   |
| 1   | B     | 249 | ALA  | CA-C-O     | 5.83  | 126.67      | 119.79   |
| 1   | B     | 307 | TYR  | O-C-N      | 5.82  | 128.01      | 121.32   |
| 1   | A     | 320 | ASN  | OD1-CG-ND2 | 5.81  | 128.41      | 122.60   |
| 1   | A     | 270 | THR  | CA-CB-CG2  | 5.81  | 120.38      | 110.50   |
| 1   | B     | 68  | ILE  | CA-C-O     | -5.81 | 112.17      | 119.95   |
| 1   | A     | 179 | ASP  | CA-C-N     | 5.80  | 128.31      | 120.65   |
| 1   | A     | 179 | ASP  | C-N-CA     | 5.80  | 128.31      | 120.65   |
| 1   | B     | 325 | PHE  | N-CA-C     | -5.80 | 104.15      | 111.11   |
| 1   | A     | 206 | ASP  | O-C-N      | 5.79  | 130.67      | 122.68   |
| 1   | A     | 429 | GLN  | O-C-N      | -5.78 | 116.16      | 122.92   |
| 1   | A     | 357 | TYR  | O-C-N      | 5.78  | 124.94      | 120.38   |
| 1   | A     | 338 | MET  | CB-CA-C    | 5.77  | 116.79      | 110.15   |
| 1   | B     | 251 | ARG  | CD-NE-CZ   | -5.77 | 116.32      | 124.40   |
| 1   | B     | 206 | ASP  | CA-C-O     | -5.77 | 115.38      | 122.36   |
| 1   | B     | 413 | HIS  | O-C-N      | 5.77  | 129.48      | 122.96   |
| 1   | B     | 325 | PHE  | N-CA-CB    | 5.76  | 118.52      | 109.94   |
| 1   | A     | 349 | MET  | O-C-N      | -5.75 | 116.03      | 122.12   |
| 1   | A     | 291 | PHE  | N-CA-C     | -5.75 | 101.21      | 109.48   |
| 1   | B     | 54  | VAL  | CA-C-N     | 5.74  | 132.31      | 121.97   |
| 1   | B     | 54  | VAL  | C-N-CA     | 5.74  | 132.31      | 121.97   |
| 1   | A     | 225 | ASP  | CA-CB-CG   | -5.74 | 106.86      | 112.60   |
| 1   | A     | 27  | THR  | CA-C-O     | 5.74  | 129.47      | 121.73   |
| 1   | A     | 186 | SER  | CA-C-O     | 5.73  | 125.98      | 119.27   |
| 1   | A     | 311 | PRO  | N-CA-CB    | -5.72 | 98.21       | 103.25   |
| 1   | A     | 330 | GLN  | CA-C-N     | 5.72  | 128.96      | 120.95   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 330 | GLN  | C-N-CA     | 5.72  | 128.96      | 120.95   |
| 1   | A     | 412 | GLU  | CA-C-O     | -5.72 | 114.42      | 121.11   |
| 1   | B     | 217 | HIS  | N-CA-CB    | 5.72  | 118.62      | 110.44   |
| 1   | A     | 92  | ARG  | N-CA-C     | -5.71 | 104.97      | 111.14   |
| 1   | B     | 105 | ARG  | CD-NE-CZ   | -5.71 | 116.41      | 124.40   |
| 1   | B     | 321 | PRO  | CA-C-N     | 5.71  | 128.90      | 120.74   |
| 1   | B     | 321 | PRO  | C-N-CA     | 5.71  | 128.90      | 120.74   |
| 1   | B     | 363 | HIS  | CG-CD2-NE2 | 5.71  | 112.91      | 107.20   |
| 1   | B     | 441 | GLN  | OE1-CD-NE2 | -5.71 | 116.89      | 122.60   |
| 1   | A     | 36  | ASP  | CA-C-O     | -5.70 | 113.25      | 120.20   |
| 1   | A     | 361 | HIS  | CA-CB-CG   | -5.69 | 108.11      | 113.80   |
| 1   | A     | 33  | PRO  | CB-CA-C    | 5.69  | 118.88      | 110.85   |
| 1   | B     | 421 | ARG  | CA-C-O     | 5.69  | 127.18      | 120.58   |
| 1   | B     | 110 | VAL  | CA-C-O     | -5.69 | 114.56      | 120.64   |
| 1   | B     | 446 | TYR  | CA-CB-CG   | 5.69  | 124.14      | 113.90   |
| 1   | B     | 177 | ASP  | N-CA-CB    | -5.68 | 100.25      | 110.37   |
| 1   | B     | 429 | GLN  | CA-C-N     | 5.68  | 131.55      | 123.14   |
| 1   | B     | 429 | GLN  | C-N-CA     | 5.68  | 131.55      | 123.14   |
| 1   | A     | 241 | ILE  | CA-C-N     | 5.68  | 132.39      | 121.54   |
| 1   | A     | 241 | ILE  | C-N-CA     | 5.68  | 132.39      | 121.54   |
| 1   | B     | 322 | VAL  | CA-CB-CG1  | 5.67  | 120.04      | 110.40   |
| 1   | A     | 71  | ARG  | O-C-N      | -5.66 | 115.91      | 122.87   |
| 1   | A     | 210 | HIS  | CB-CA-C    | -5.65 | 101.73      | 111.45   |
| 1   | B     | 108 | ILE  | CB-CG1-CD1 | 5.65  | 125.67      | 113.80   |
| 1   | B     | 332 | ALA  | CA-C-O     | -5.65 | 114.23      | 120.33   |
| 1   | A     | 124 | THR  | CA-C-N     | 5.65  | 131.67      | 122.69   |
| 1   | A     | 124 | THR  | C-N-CA     | 5.65  | 131.67      | 122.69   |
| 1   | B     | 98  | VAL  | CA-C-O     | -5.64 | 113.72      | 120.78   |
| 1   | B     | 169 | ARG  | CB-CA-C    | -5.64 | 100.31      | 110.36   |
| 1   | A     | 470 | GLN  | CA-C-O     | -5.64 | 115.56      | 121.99   |
| 1   | A     | 22  | LYS  | N-CA-C     | -5.64 | 97.35       | 109.81   |
| 1   | B     | 118 | GLU  | N-CA-C     | -5.64 | 102.57      | 110.35   |
| 1   | A     | 206 | ASP  | CA-C-O     | -5.63 | 113.98      | 122.38   |
| 1   | B     | 464 | GLY  | CA-C-O     | -5.63 | 114.70      | 120.45   |
| 1   | B     | 322 | VAL  | CB-CA-C    | 5.63  | 119.42      | 112.04   |
| 1   | A     | 117 | GLY  | O-C-N      | 5.63  | 129.83      | 122.91   |
| 1   | B     | 141 | ASN  | O-C-N      | 5.63  | 129.50      | 122.86   |
| 1   | B     | 58  | ASP  | CA-C-O     | 5.62  | 126.90      | 121.00   |
| 1   | A     | 115 | VAL  | CA-C-O     | -5.62 | 115.23      | 120.34   |
| 1   | B     | 67  | ARG  | NE-CZ-NH2  | 5.61  | 124.25      | 119.20   |
| 1   | B     | 293 | PHE  | CA-C-N     | -5.61 | 109.45      | 121.63   |
| 1   | B     | 293 | PHE  | C-N-CA     | -5.61 | 109.45      | 121.63   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 461 | ASN  | CB-CA-C    | 5.60  | 119.59      | 110.96   |
| 1   | A     | 282 | VAL  | N-CA-CB    | 5.60  | 120.63      | 111.44   |
| 1   | B     | 272 | ASN  | CA-CB-CG   | -5.60 | 107.00      | 112.60   |
| 1   | A     | 461 | ASN  | N-CA-C     | -5.60 | 104.87      | 110.97   |
| 1   | A     | 481 | PHE  | CA-C-N     | 5.59  | 127.77      | 120.28   |
| 1   | A     | 481 | PHE  | C-N-CA     | 5.59  | 127.77      | 120.28   |
| 1   | B     | 218 | THR  | O-C-N      | 5.59  | 129.59      | 123.22   |
| 1   | A     | 302 | TRP  | CB-CA-C    | 5.58  | 116.21      | 109.85   |
| 1   | A     | 43  | VAL  | O-C-N      | 5.58  | 130.43      | 122.62   |
| 1   | B     | 295 | PRO  | CA-C-N     | 5.58  | 131.72      | 122.73   |
| 1   | B     | 295 | PRO  | C-N-CA     | 5.58  | 131.72      | 122.73   |
| 1   | B     | 22  | LYS  | N-CA-C     | -5.58 | 97.48       | 109.81   |
| 1   | B     | 115 | VAL  | CA-CB-CG1  | 5.58  | 119.88      | 110.40   |
| 1   | B     | 290 | ILE  | N-CA-C     | 5.58  | 119.00      | 113.53   |
| 1   | A     | 4   | ARG  | CD-NE-CZ   | 5.57  | 132.20      | 124.40   |
| 1   | A     | 422 | THR  | CA-C-O     | -5.57 | 115.27      | 121.23   |
| 1   | B     | 202 | ARG  | CG-CD-NE   | -5.57 | 99.74       | 112.00   |
| 1   | B     | 204 | ILE  | CA-CB-CG1  | 5.57  | 119.87      | 110.40   |
| 1   | B     | 262 | ARG  | CD-NE-CZ   | -5.57 | 116.60      | 124.40   |
| 1   | B     | 225 | ASP  | CA-CB-CG   | 5.57  | 118.17      | 112.60   |
| 1   | B     | 312 | VAL  | CA-C-O     | -5.56 | 115.28      | 120.34   |
| 1   | A     | 481 | PHE  | O-C-N      | 5.56  | 128.01      | 122.12   |
| 1   | B     | 281 | GLN  | OE1-CD-NE2 | -5.56 | 117.04      | 122.60   |
| 1   | B     | 368 | ASN  | O-C-N      | 5.56  | 129.22      | 121.83   |
| 1   | B     | 366 | GLY  | CA-C-N     | 5.55  | 125.91      | 119.47   |
| 1   | B     | 366 | GLY  | C-N-CA     | 5.55  | 125.91      | 119.47   |
| 1   | B     | 63  | PHE  | CA-CB-CG   | 5.55  | 119.35      | 113.80   |
| 1   | B     | 263 | ASP  | CA-C-O     | -5.55 | 115.17      | 121.00   |
| 1   | B     | 436 | ASP  | CA-C-N     | 5.55  | 129.24      | 121.02   |
| 1   | B     | 436 | ASP  | C-N-CA     | 5.55  | 129.24      | 121.02   |
| 1   | A     | 49  | LEU  | CB-CA-C    | 5.55  | 119.48      | 110.22   |
| 1   | A     | 247 | GLU  | CG-CD-OE1  | 5.55  | 131.16      | 118.40   |
| 1   | B     | 93  | TYR  | CA-C-O     | -5.54 | 114.62      | 120.55   |
| 1   | B     | 482 | SER  | N-CA-CB    | 5.54  | 118.05      | 110.01   |
| 1   | A     | 334 | ASP  | CA-CB-CG   | 5.54  | 118.14      | 112.60   |
| 1   | B     | 122 | ALA  | CB-CA-C    | 5.54  | 118.98      | 109.51   |
| 1   | A     | 76  | LYS  | CA-C-O     | -5.53 | 114.39      | 120.36   |
| 1   | A     | 351 | GLN  | CA-C-O     | -5.53 | 114.01      | 120.20   |
| 1   | B     | 310 | ILE  | N-CA-CB    | -5.53 | 104.43      | 111.39   |
| 1   | A     | 247 | GLU  | CA-CB-CG   | 5.52  | 125.15      | 114.10   |
| 1   | A     | 370 | LEU  | CA-C-N     | 5.52  | 131.81      | 122.26   |
| 1   | A     | 370 | LEU  | C-N-CA     | 5.52  | 131.81      | 122.26   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 247 | GLU  | CG-CD-OE2  | -5.52 | 105.70      | 118.40   |
| 1   | B     | 440 | THR  | O-C-N      | 5.52  | 129.94      | 122.59   |
| 1   | A     | 172 | GLN  | N-CA-CB    | 5.52  | 118.74      | 110.19   |
| 1   | A     | 384 | ASN  | CA-C-O     | -5.51 | 115.01      | 120.80   |
| 1   | A     | 184 | PHE  | CA-CB-CG   | -5.51 | 108.29      | 113.80   |
| 1   | B     | 432 | ASN  | CA-CB-CG   | 5.51  | 118.11      | 112.60   |
| 1   | B     | 52  | GLN  | CB-CA-C    | -5.50 | 98.81       | 110.31   |
| 1   | A     | 281 | GLN  | CG-CD-OE1  | 5.50  | 131.80      | 120.80   |
| 1   | A     | 322 | VAL  | CB-CA-C    | 5.50  | 118.87      | 111.94   |
| 1   | B     | 372 | ILE  | CA-CB-CG1  | 5.50  | 119.75      | 110.40   |
| 1   | B     | 11  | MET  | O-C-N      | 5.50  | 128.65      | 122.22   |
| 1   | A     | 385 | TYR  | CB-CA-C    | 5.49  | 120.09      | 110.64   |
| 1   | B     | 242 | LYS  | N-CA-C     | -5.49 | 99.10       | 110.80   |
| 1   | B     | 109 | ALA  | O-C-N      | -5.48 | 116.03      | 123.10   |
| 1   | A     | 71  | ARG  | CD-NE-CZ   | 5.48  | 132.07      | 124.40   |
| 1   | B     | 257 | PRO  | O-C-N      | 5.48  | 130.04      | 122.64   |
| 1   | A     | 230 | TYR  | O-C-N      | 5.48  | 129.22      | 123.03   |
| 1   | A     | 126 | ARG  | N-CA-CB    | 5.47  | 118.13      | 109.71   |
| 1   | A     | 366 | GLY  | CA-C-N     | 5.47  | 126.67      | 119.84   |
| 1   | A     | 366 | GLY  | C-N-CA     | 5.47  | 126.67      | 119.84   |
| 1   | B     | 65  | ARG  | NE-CZ-NH1  | -5.46 | 116.04      | 121.50   |
| 1   | B     | 94  | SER  | CA-C-O     | -5.46 | 114.26      | 120.32   |
| 1   | B     | 459 | CYS  | CB-CA-C    | 5.46  | 119.87      | 110.86   |
| 1   | A     | 155 | ARG  | NE-CZ-NH2  | 5.46  | 124.11      | 119.20   |
| 1   | B     | 150 | PRO  | CA-C-N     | -5.45 | 112.16      | 121.97   |
| 1   | B     | 150 | PRO  | C-N-CA     | -5.45 | 112.16      | 121.97   |
| 1   | A     | 27  | THR  | N-CA-C     | 5.45  | 117.80      | 109.95   |
| 1   | A     | 176 | LYS  | CB-CA-C    | 5.45  | 118.74      | 109.53   |
| 1   | B     | 105 | ARG  | CB-CA-C    | -5.44 | 99.76       | 109.71   |
| 1   | B     | 444 | THR  | CA-CB-OG1  | -5.43 | 101.45      | 109.60   |
| 1   | B     | 32  | ASN  | O-C-N      | 5.43  | 130.50      | 121.59   |
| 1   | A     | 130 | GLY  | N-CA-C     | -5.43 | 105.69      | 111.93   |
| 1   | B     | 371 | GLN  | N-CA-C     | -5.43 | 106.02      | 113.30   |
| 1   | A     | 236 | LYS  | CA-C-O     | -5.42 | 114.85      | 121.36   |
| 1   | A     | 320 | ASN  | O-C-N      | 5.42  | 128.53      | 121.64   |
| 1   | A     | 406 | ASN  | CA-CB-CG   | -5.42 | 107.18      | 112.60   |
| 1   | A     | 345 | SER  | O-C-N      | 5.42  | 127.55      | 121.32   |
| 1   | A     | 105 | ARG  | CB-CA-C    | -5.41 | 101.48      | 110.14   |
| 1   | A     | 58  | ASP  | CA-C-O     | 5.41  | 126.98      | 120.92   |
| 1   | B     | 167 | GLN  | OE1-CD-NE2 | -5.40 | 117.20      | 122.60   |
| 1   | A     | 73  | VAL  | CA-CB-CG1  | 5.39  | 119.56      | 110.40   |
| 1   | B     | 358 | PRO  | N-CA-C     | -5.39 | 106.38      | 113.65   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 397 | GLN  | CA-C-N     | 5.39  | 130.58      | 120.07   |
| 1   | B     | 397 | GLN  | C-N-CA     | 5.39  | 130.58      | 120.07   |
| 1   | A     | 139 | ASP  | N-CA-C     | -5.38 | 106.90      | 112.93   |
| 1   | A     | 250 | ALA  | CA-C-N     | 5.38  | 127.75      | 120.44   |
| 1   | A     | 250 | ALA  | C-N-CA     | 5.38  | 127.75      | 120.44   |
| 1   | A     | 202 | ARG  | CB-CG-CD   | 5.37  | 123.66      | 111.30   |
| 1   | A     | 305 | GLY  | N-CA-C     | -5.37 | 106.29      | 112.73   |
| 1   | B     | 158 | LEU  | N-CA-C     | 5.37  | 118.62      | 111.75   |
| 1   | A     | 377 | PRO  | N-CA-C     | -5.36 | 101.42      | 112.47   |
| 1   | B     | 48  | PRO  | N-CA-C     | 5.36  | 119.45      | 111.41   |
| 1   | B     | 183 | ASP  | N-CA-CB    | 5.36  | 119.55      | 110.49   |
| 1   | A     | 287 | GLU  | N-CA-C     | -5.36 | 105.44      | 111.28   |
| 1   | A     | 330 | GLN  | N-CA-C     | 5.35  | 119.68      | 113.20   |
| 1   | B     | 25  | VAL  | N-CA-CB    | -5.35 | 104.69      | 110.53   |
| 1   | B     | 326 | ALA  | CA-C-O     | -5.35 | 113.47      | 119.79   |
| 1   | A     | 358 | PRO  | CB-CA-C    | 5.35  | 119.49      | 111.68   |
| 1   | A     | 67  | ARG  | CB-CG-CD   | 5.35  | 123.60      | 111.30   |
| 1   | A     | 329 | GLU  | CG-CD-OE2  | -5.35 | 106.10      | 118.40   |
| 1   | A     | 226 | GLY  | CA-C-O     | 5.34  | 124.29      | 118.95   |
| 1   | A     | 235 | TYR  | N-CA-CB    | 5.34  | 119.08      | 110.65   |
| 1   | A     | 414 | GLN  | CA-CB-CG   | 5.34  | 124.78      | 114.10   |
| 1   | B     | 370 | LEU  | N-CA-CB    | 5.34  | 118.35      | 110.56   |
| 1   | A     | 39  | ASN  | CB-CG-ND2  | 5.34  | 124.41      | 116.40   |
| 1   | B     | 408 | PHE  | N-CA-C     | 5.34  | 119.56      | 112.30   |
| 1   | B     | 431 | PHE  | N-CA-C     | 5.34  | 117.42      | 109.25   |
| 1   | B     | 169 | ARG  | NE-CZ-NH2  | 5.33  | 124.00      | 119.20   |
| 1   | A     | 281 | GLN  | CA-CB-CG   | 5.33  | 124.76      | 114.10   |
| 1   | A     | 43  | VAL  | CA-C-N     | -5.33 | 113.50      | 121.87   |
| 1   | A     | 43  | VAL  | C-N-CA     | -5.33 | 113.50      | 121.87   |
| 1   | A     | 329 | GLU  | N-CA-C     | -5.33 | 105.56      | 111.36   |
| 1   | A     | 134 | LYS  | CB-CG-CD   | -5.32 | 99.06       | 111.30   |
| 1   | B     | 138 | GLU  | OE1-CD-OE2 | -5.32 | 110.13      | 122.90   |
| 1   | A     | 72  | VAL  | CA-CB-CG1  | 5.32  | 119.44      | 110.40   |
| 1   | B     | 265 | PHE  | O-C-N      | 5.31  | 127.54      | 122.07   |
| 1   | A     | 137 | THR  | O-C-N      | 5.31  | 128.78      | 122.20   |
| 1   | B     | 482 | SER  | O-C-N      | 5.31  | 127.53      | 122.07   |
| 1   | B     | 452 | GLU  | N-CA-C     | -5.30 | 107.36      | 113.88   |
| 1   | A     | 363 | HIS  | CA-C-N     | 5.30  | 127.64      | 120.65   |
| 1   | A     | 363 | HIS  | C-N-CA     | 5.30  | 127.64      | 120.65   |
| 1   | B     | 24  | ASP  | N-CA-CB    | 5.30  | 117.94      | 110.36   |
| 1   | A     | 390 | PRO  | CA-C-O     | -5.30 | 115.33      | 121.95   |
| 1   | A     | 250 | ALA  | CB-CA-C    | 5.29  | 119.57      | 110.79   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 497 | ASP  | CA-CB-CG   | 5.29  | 117.89      | 112.60   |
| 1   | B     | 192 | LEU  | N-CA-CB    | -5.28 | 102.33      | 110.20   |
| 1   | A     | 378 | TYR  | CB-CA-C    | 5.28  | 120.27      | 109.67   |
| 1   | A     | 406 | ASN  | CB-CG-ND2  | -5.27 | 108.49      | 116.40   |
| 1   | A     | 293 | PHE  | CA-CB-CG   | 5.27  | 119.07      | 113.80   |
| 1   | B     | 427 | ASP  | O-C-N      | 5.27  | 129.28      | 123.16   |
| 1   | A     | 303 | PRO  | CB-CA-C    | 5.27  | 118.28      | 111.64   |
| 1   | B     | 108 | ILE  | N-CA-C     | 5.27  | 117.34      | 108.81   |
| 1   | B     | 414 | GLN  | CB-CG-CD   | -5.27 | 103.65      | 112.60   |
| 1   | A     | 464 | GLY  | O-C-N      | 5.26  | 128.33      | 122.54   |
| 1   | B     | 135 | PHE  | O-C-N      | 5.26  | 129.50      | 123.29   |
| 1   | B     | 386 | GLN  | CB-CA-C    | 5.26  | 118.43      | 109.80   |
| 1   | A     | 383 | ALA  | CA-C-N     | -5.26 | 112.39      | 122.08   |
| 1   | A     | 383 | ALA  | C-N-CA     | -5.26 | 112.39      | 122.08   |
| 1   | A     | 154 | ILE  | N-CA-C     | 5.26  | 117.33      | 108.81   |
| 1   | A     | 218 | THR  | CA-CB-CG2  | 5.26  | 119.44      | 110.50   |
| 1   | B     | 282 | VAL  | CA-C-O     | 5.26  | 126.71      | 120.72   |
| 1   | A     | 318 | ASN  | CB-CG-OD1  | 5.25  | 131.30      | 120.80   |
| 1   | A     | 219 | PHE  | CB-CA-C    | 5.25  | 122.09      | 111.60   |
| 1   | B     | 477 | ALA  | CA-C-O     | -5.24 | 114.89      | 121.02   |
| 1   | B     | 47  | GLY  | O-C-N      | 5.24  | 127.00      | 121.77   |
| 1   | B     | 272 | ASN  | CB-CA-C    | -5.24 | 104.27      | 112.12   |
| 1   | B     | 39  | ASN  | CB-CG-ND2  | -5.23 | 108.55      | 116.40   |
| 1   | B     | 474 | GLN  | N-CA-CB    | 5.23  | 117.60      | 110.01   |
| 1   | A     | 9   | ASP  | N-CA-C     | -5.23 | 106.76      | 112.72   |
| 1   | B     | 282 | VAL  | CA-CB-CG1  | 5.23  | 119.29      | 110.40   |
| 1   | A     | 333 | PHE  | CA-CB-CG   | 5.23  | 119.03      | 113.80   |
| 1   | B     | 60  | MET  | CA-C-N     | 5.23  | 127.29      | 120.28   |
| 1   | B     | 60  | MET  | C-N-CA     | 5.23  | 127.29      | 120.28   |
| 1   | B     | 165 | HIS  | CA-C-O     | -5.22 | 115.32      | 121.07   |
| 1   | A     | 438 | ASN  | CA-C-O     | -5.22 | 113.11      | 119.32   |
| 1   | B     | 207 | GLY  | CA-C-N     | 5.22  | 130.28      | 121.14   |
| 1   | B     | 207 | GLY  | C-N-CA     | 5.22  | 130.28      | 121.14   |
| 1   | B     | 472 | PHE  | CA-C-N     | 5.22  | 127.33      | 120.60   |
| 1   | B     | 472 | PHE  | C-N-CA     | 5.22  | 127.33      | 120.60   |
| 1   | B     | 340 | PRO  | O-C-N      | -5.22 | 115.59      | 122.64   |
| 1   | A     | 488 | TYR  | N-CA-C     | -5.22 | 104.85      | 111.11   |
| 1   | B     | 126 | ARG  | NH1-CZ-NH2 | -5.22 | 112.52      | 119.30   |
| 1   | B     | 100 | GLU  | CA-C-O     | -5.21 | 113.46      | 119.61   |
| 1   | A     | 485 | HIS  | CA-CB-CG   | -5.21 | 108.59      | 113.80   |
| 1   | B     | 342 | ILE  | CA-CB-CG2  | 5.21  | 119.35      | 110.50   |
| 1   | A     | 329 | GLU  | N-CA-CB    | 5.20  | 117.86      | 110.16   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 87  | THR  | CA-C-N     | 5.20  | 130.40      | 121.87   |
| 1   | A     | 87  | THR  | C-N-CA     | 5.20  | 130.40      | 121.87   |
| 1   | B     | 310 | ILE  | CA-C-O     | -5.20 | 114.63      | 119.62   |
| 1   | B     | 477 | ALA  | N-CA-CB    | 5.20  | 118.56      | 109.72   |
| 1   | A     | 159 | LEU  | CA-C-O     | -5.19 | 113.00      | 119.18   |
| 1   | A     | 168 | LYS  | CA-CB-CG   | 5.19  | 124.48      | 114.10   |
| 1   | A     | 368 | ASN  | OD1-CG-ND2 | -5.19 | 117.41      | 122.60   |
| 1   | B     | 334 | ASP  | OD1-CG-OD2 | -5.19 | 110.44      | 122.90   |
| 1   | B     | 36  | ASP  | CA-C-O     | -5.18 | 113.01      | 120.11   |
| 1   | B     | 129 | ARG  | CG-CD-NE   | 5.18  | 123.41      | 112.00   |
| 1   | B     | 258 | ASP  | N-CA-CB    | -5.18 | 102.70      | 110.73   |
| 1   | A     | 397 | GLN  | N-CA-C     | -5.18 | 106.91      | 113.23   |
| 1   | B     | 436 | ASP  | CB-CA-C    | 5.18  | 120.73      | 110.42   |
| 1   | A     | 51  | VAL  | CA-C-O     | -5.18 | 112.75      | 119.53   |
| 1   | B     | 213 | GLY  | O-C-N      | 5.17  | 128.34      | 123.48   |
| 1   | B     | 461 | ASN  | O-C-N      | 5.16  | 127.40      | 122.03   |
| 1   | A     | 489 | GLY  | N-CA-C     | 5.16  | 118.74      | 112.49   |
| 1   | B     | 111 | ARG  | NE-CZ-NH1  | 5.16  | 126.66      | 121.50   |
| 1   | A     | 343 | GLU  | CA-C-N     | 5.16  | 125.61      | 120.14   |
| 1   | A     | 343 | GLU  | C-N-CA     | 5.16  | 125.61      | 120.14   |
| 1   | B     | 231 | CYS  | O-C-N      | 5.16  | 129.03      | 123.10   |
| 1   | B     | 247 | GLU  | N-CA-C     | -5.16 | 105.35      | 111.69   |
| 1   | A     | 41  | LEU  | CA-C-O     | -5.16 | 114.51      | 120.49   |
| 1   | A     | 324 | TYR  | N-CA-CB    | 5.15  | 117.44      | 109.91   |
| 1   | A     | 484 | VAL  | CA-CB-CG1  | 5.15  | 119.16      | 110.40   |
| 1   | A     | 292 | PRO  | CA-C-N     | 5.15  | 130.60      | 122.36   |
| 1   | A     | 292 | PRO  | C-N-CA     | 5.15  | 130.60      | 122.36   |
| 1   | A     | 100 | GLU  | CG-CD-OE2  | -5.15 | 106.56      | 118.40   |
| 1   | A     | 393 | MET  | CA-C-O     | -5.15 | 115.40      | 120.70   |
| 1   | B     | 297 | ASP  | CB-CA-C    | 5.15  | 118.63      | 110.19   |
| 1   | A     | 320 | ASN  | CA-C-O     | -5.15 | 115.34      | 120.64   |
| 1   | B     | 111 | ARG  | CB-CG-CD   | 5.14  | 123.12      | 111.30   |
| 1   | A     | 290 | ILE  | N-CA-CB    | -5.14 | 105.68      | 112.36   |
| 1   | A     | 129 | ARG  | O-C-N      | -5.14 | 116.46      | 123.24   |
| 1   | A     | 277 | THR  | N-CA-CB    | 5.14  | 118.80      | 110.43   |
| 1   | B     | 99  | PHE  | CA-C-O     | 5.14  | 125.54      | 119.48   |
| 1   | B     | 145 | VAL  | CB-CA-C    | 5.14  | 119.71      | 111.29   |
| 1   | A     | 92  | ARG  | NE-CZ-NH2  | 5.13  | 123.82      | 119.20   |
| 1   | A     | 115 | VAL  | N-CA-C     | 5.13  | 116.43      | 112.12   |
| 1   | B     | 320 | ASN  | OD1-CG-ND2 | -5.13 | 117.47      | 122.60   |
| 1   | A     | 68  | ILE  | CA-C-O     | -5.13 | 114.38      | 120.90   |
| 1   | B     | 322 | VAL  | CA-C-N     | 5.13  | 130.01      | 122.77   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 322 | VAL  | C-N-CA     | 5.13  | 130.01      | 122.77   |
| 1   | B     | 82  | GLY  | O-C-N      | -5.13 | 119.54      | 123.80   |
| 1   | B     | 207 | GLY  | CA-C-O     | -5.13 | 116.63      | 122.78   |
| 1   | A     | 318 | ASN  | N-CA-CB    | -5.12 | 101.40      | 111.60   |
| 1   | A     | 238 | ASP  | N-CA-C     | -5.12 | 106.98      | 113.18   |
| 1   | B     | 241 | ILE  | CA-C-O     | -5.12 | 114.38      | 120.78   |
| 1   | A     | 316 | VAL  | O-C-N      | 5.12  | 128.56      | 123.18   |
| 1   | A     | 108 | ILE  | CA-C-N     | 5.12  | 130.85      | 122.81   |
| 1   | A     | 108 | ILE  | C-N-CA     | 5.12  | 130.85      | 122.81   |
| 1   | A     | 375 | ASN  | OD1-CG-ND2 | -5.11 | 117.49      | 122.60   |
| 1   | B     | 43  | VAL  | O-C-N      | 5.11  | 130.28      | 122.76   |
| 1   | A     | 386 | GLN  | N-CA-CB    | 5.11  | 117.78      | 110.06   |
| 1   | B     | 106 | THR  | N-CA-C     | -5.11 | 102.43      | 110.14   |
| 1   | B     | 309 | LEU  | CA-C-O     | -5.11 | 114.87      | 120.69   |
| 1   | A     | 256 | ASP  | O-C-N      | 5.10  | 124.91      | 121.19   |
| 1   | A     | 396 | ASN  | CA-CB-CG   | 5.10  | 117.70      | 112.60   |
| 1   | B     | 225 | ASP  | CB-CG-OD1  | 5.10  | 130.12      | 118.40   |
| 1   | A     | 441 | GLN  | CG-CD-NE2  | 5.09  | 124.04      | 116.40   |
| 1   | B     | 251 | ARG  | NE-CZ-NH2  | 5.09  | 123.79      | 119.20   |
| 1   | A     | 461 | ASN  | N-CA-CB    | 5.09  | 117.34      | 109.91   |
| 1   | B     | 349 | MET  | CA-C-N     | 5.09  | 129.29      | 120.58   |
| 1   | B     | 349 | MET  | C-N-CA     | 5.09  | 129.29      | 120.58   |
| 1   | A     | 133 | VAL  | N-CA-CB    | -5.09 | 104.39      | 111.41   |
| 1   | B     | 243 | ASN  | CA-C-N     | -5.09 | 115.70      | 122.72   |
| 1   | B     | 243 | ASN  | C-N-CA     | -5.09 | 115.70      | 122.72   |
| 1   | B     | 175 | LEU  | CA-CB-CG   | 5.07  | 134.04      | 116.30   |
| 1   | B     | 429 | GLN  | CG-CD-NE2  | -5.07 | 108.80      | 116.40   |
| 1   | A     | 172 | GLN  | OE1-CD-NE2 | -5.07 | 117.53      | 122.60   |
| 1   | B     | 446 | TYR  | CA-C-O     | -5.07 | 112.46      | 119.05   |
| 1   | A     | 10  | GLN  | CA-C-N     | -5.07 | 112.61      | 120.31   |
| 1   | A     | 10  | GLN  | C-N-CA     | -5.07 | 112.61      | 120.31   |
| 1   | A     | 92  | ARG  | CD-NE-CZ   | -5.07 | 117.31      | 124.40   |
| 1   | B     | 450 | LEU  | CA-CB-CG   | 5.06  | 134.02      | 116.30   |
| 1   | A     | 381 | ARG  | CD-NE-CZ   | -5.06 | 117.32      | 124.40   |
| 1   | B     | 55  | VAL  | CA-CB-CG1  | 5.05  | 118.99      | 110.40   |
| 1   | B     | 72  | VAL  | CB-CA-C    | 5.05  | 121.43      | 111.79   |
| 1   | B     | 155 | ARG  | NE-CZ-NH1  | 5.05  | 126.55      | 121.50   |
| 1   | B     | 468 | ASP  | OD1-CG-OD2 | -5.04 | 110.79      | 122.90   |
| 1   | B     | 488 | TYR  | CA-C-O     | 5.04  | 125.90      | 120.70   |
| 1   | A     | 81  | PHE  | N-CA-CB    | -5.04 | 103.04      | 111.20   |
| 1   | A     | 386 | GLN  | O-C-N      | 5.03  | 128.95      | 123.01   |
| 1   | B     | 410 | ALA  | CB-CA-C    | 5.03  | 118.82      | 109.51   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 329 | GLU  | OE1-CD-OE2 | 5.03  | 134.96      | 122.90   |
| 1   | A     | 339 | PRO  | CB-CA-C    | 5.02  | 117.05      | 110.92   |
| 1   | B     | 126 | ARG  | NE-CZ-NH1  | -5.02 | 116.48      | 121.50   |
| 1   | B     | 481 | PHE  | O-C-N      | 5.02  | 127.44      | 122.12   |
| 1   | B     | 470 | GLN  | CB-CG-CD   | -5.02 | 104.07      | 112.60   |
| 1   | B     | 310 | ILE  | CA-C-N     | 5.01  | 124.78      | 119.76   |
| 1   | B     | 310 | ILE  | C-N-CA     | 5.01  | 124.78      | 119.76   |
| 1   | A     | 172 | GLN  | CB-CA-C    | -5.01 | 101.39      | 110.56   |
| 1   | A     | 321 | PRO  | O-C-N      | 5.01  | 129.22      | 123.01   |
| 1   | B     | 331 | LEU  | CA-C-O     | -5.01 | 115.05      | 120.81   |
| 1   | A     | 70  | GLU  | CA-C-O     | -5.01 | 116.18      | 121.94   |
| 1   | B     | 129 | ARG  | CD-NE-CZ   | -5.01 | 117.39      | 124.40   |
| 1   | B     | 328 | VAL  | CA-C-O     | -5.01 | 116.34      | 120.80   |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 353 | ARG  | Sidechain |
| 1   | A     | 362 | ARG  | Sidechain |
| 1   | A     | 430 | ARG  | Sidechain |
| 1   | A     | 71  | ARG  | Sidechain |
| 1   | B     | 105 | ARG  | Sidechain |
| 1   | B     | 310 | ILE  | Mainchain |

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4008  | 0        | 3833     | 344     | 3            |
| 1   | B     | 4008  | 0        | 3833     | 309     | 2            |
| 2   | A     | 43    | 0        | 30       | 16      | 0            |
| 2   | B     | 43    | 0        | 30       | 11      | 0            |
| 3   | A     | 48    | 0        | 24       | 0       | 0            |
| 3   | B     | 48    | 0        | 24       | 3       | 0            |
| 4   | A     | 48    | 0        | 0        | 4       | 1            |
| 4   | B     | 50    | 0        | 0        | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All   | 8296  | 0        | 7774     | 629     | 3            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (629) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:155:ARG:NH2  | 1:A:438:ASN:HD21 | 1.19                     | 1.38              |
| 1:A:155:ARG:HH22 | 1:A:438:ASN:ND2  | 1.28                     | 1.31              |
| 1:B:155:ARG:HH22 | 1:B:438:ASN:ND2  | 1.27                     | 1.29              |
| 1:B:155:ARG:NH2  | 1:B:438:ASN:HD21 | 1.34                     | 1.26              |
| 1:A:367:PRO:HG2  | 1:A:390:PRO:HG2  | 1.19                     | 1.14              |
| 1:A:177:ASP:HB3  | 1:A:180:MET:HE2  | 1.33                     | 1.10              |
| 1:A:322:VAL:HA   | 1:B:172:GLN:NE2  | 1.66                     | 1.10              |
| 1:A:487:GLU:O    | 1:A:491:ARG:HG3  | 1.52                     | 1.10              |
| 1:A:173:THR:CG2  | 1:A:175:LEU:HD12 | 1.84                     | 1.08              |
| 1:A:384:ASN:C    | 1:A:384:ASN:HD22 | 1.56                     | 1.04              |
| 1:B:444:THR:O    | 1:B:448:LYS:HG2  | 1.62                     | 1.00              |
| 1:A:444:THR:HA   | 1:A:448:LYS:HD3  | 1.42                     | 1.00              |
| 1:A:220:LYS:HE3  | 1:A:420:HIS:CD2  | 1.97                     | 0.98              |
| 1:A:189:PRO:O    | 1:A:192:LEU:HD12 | 1.63                     | 0.97              |
| 2:A:507:HEM:HMB1 | 2:A:507:HEM:HBB2 | 1.44                     | 0.97              |
| 1:B:170:ASN:HD22 | 1:B:172:GLN:H    | 1.12                     | 0.96              |
| 1:A:471:LEU:HD22 | 1:A:474:GLN:NE2  | 1.79                     | 0.96              |
| 1:A:371:GLN:HE21 | 1:A:393:MET:HB2  | 1.30                     | 0.94              |
| 1:A:148:ASN:HD22 | 1:A:148:ASN:H    | 0.99                     | 0.93              |
| 1:A:383:ALA:HB1  | 1:A:411:PRO:HG3  | 1.51                     | 0.93              |
| 1:A:173:THR:HG21 | 1:A:175:LEU:HD12 | 1.46                     | 0.93              |
| 1:B:173:THR:HG22 | 1:B:175:LEU:HG   | 1.49                     | 0.93              |
| 1:A:367:PRO:HG2  | 1:A:390:PRO:CG   | 1.99                     | 0.92              |
| 1:B:451:ASN:O    | 1:B:455:ARG:HG3  | 1.69                     | 0.92              |
| 1:B:142:TRP:HB2  | 1:B:339:PRO:HD3  | 1.52                     | 0.92              |
| 1:B:406:ASN:HD22 | 1:B:408:PHE:H    | 1.18                     | 0.91              |
| 1:A:322:VAL:HA   | 1:B:172:GLN:HE22 | 1.30                     | 0.91              |
| 1:B:229:VAL:HG13 | 1:B:282:VAL:HG23 | 1.52                     | 0.91              |
| 1:B:298:LEU:HD12 | 1:B:349:MET:HG3  | 1.53                     | 0.91              |
| 1:B:177:ASP:HB3  | 1:B:180:MET:HE2  | 1.51                     | 0.90              |
| 1:B:189:PRO:O    | 1:B:192:LEU:HD12 | 1.72                     | 0.88              |
| 1:B:229:VAL:CG1  | 1:B:282:VAL:HG23 | 2.03                     | 0.88              |
| 1:B:177:ASP:HB3  | 1:B:180:MET:CE   | 2.04                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:92:ARG:HH11  | 1:A:92:ARG:HB2   | 1.40                     | 0.87              |
| 1:A:384:ASN:HD22 | 1:A:385:TYR:N    | 1.72                     | 0.87              |
| 1:A:406:ASN:C    | 1:A:406:ASN:HD22 | 1.83                     | 0.87              |
| 1:A:220:LYS:HE3  | 1:A:420:HIS:HD2  | 1.37                     | 0.87              |
| 1:A:384:ASN:C    | 1:A:384:ASN:ND2  | 2.30                     | 0.86              |
| 1:B:284:THR:HG22 | 1:B:286:SER:H    | 1.40                     | 0.85              |
| 1:B:179:ASP:O    | 1:B:183:ASP:HB2  | 1.75                     | 0.85              |
| 1:A:406:ASN:ND2  | 1:A:408:PHE:H    | 1.75                     | 0.85              |
| 1:B:450:LEU:HD23 | 1:B:455:ARG:HG2  | 1.58                     | 0.85              |
| 1:B:406:ASN:ND2  | 1:B:408:PHE:H    | 1.74                     | 0.84              |
| 1:A:223:ASN:C    | 1:A:223:ASN:HD22 | 1.82                     | 0.84              |
| 1:B:90:ILE:HD13  | 1:B:312:VAL:HG13 | 1.60                     | 0.84              |
| 1:B:251:ARG:O    | 1:B:255:GLU:HB2  | 1.77                     | 0.84              |
| 1:A:485:HIS:CD2  | 1:A:486:PRO:HD2  | 2.14                     | 0.83              |
| 1:A:458:LEU:O    | 1:A:462:ILE:HG13 | 1.76                     | 0.83              |
| 1:B:74:HIS:O     | 1:B:111:ARG:NH2  | 2.11                     | 0.82              |
| 1:A:458:LEU:O    | 1:A:458:LEU:HD12 | 1.80                     | 0.82              |
| 1:A:149:THR:OG1  | 1:A:150:PRO:HD2  | 1.79                     | 0.81              |
| 1:B:394:MET:HE3  | 1:B:394:MET:HA   | 1.61                     | 0.81              |
| 1:A:148:ASN:HD22 | 1:A:148:ASN:N    | 1.78                     | 0.81              |
| 1:B:384:ASN:C    | 1:B:384:ASN:HD22 | 1.87                     | 0.81              |
| 1:A:100:GLU:O    | 1:A:101:HIS:HB3  | 1.80                     | 0.80              |
| 1:B:170:ASN:ND2  | 1:B:172:GLN:H    | 1.78                     | 0.80              |
| 1:B:297:ASP:OD1  | 1:B:300:LYS:HE2  | 1.81                     | 0.80              |
| 1:A:149:THR:OG1  | 1:A:150:PRO:CD   | 2.30                     | 0.79              |
| 2:A:507:HEM:HBB2 | 2:A:507:HEM:CMB  | 2.11                     | 0.79              |
| 1:B:496:LEU:O    | 1:B:500:ASN:HB2  | 1.81                     | 0.79              |
| 1:A:98:VAL:HG23  | 1:A:137:THR:CG2  | 2.12                     | 0.79              |
| 1:B:394:MET:HA   | 1:B:394:MET:CE   | 2.13                     | 0.78              |
| 1:A:134:LYS:HE3  | 1:A:331:LEU:CD2  | 2.13                     | 0.78              |
| 1:A:444:THR:O    | 1:A:448:LYS:HG2  | 1.83                     | 0.78              |
| 1:B:177:ASP:CB   | 1:B:180:MET:HE2  | 2.12                     | 0.78              |
| 1:A:98:VAL:CG2   | 1:A:137:THR:HG22 | 2.14                     | 0.77              |
| 1:B:160:PHE:HB3  | 1:B:161:PRO:HD3  | 1.66                     | 0.77              |
| 1:A:321:PRO:O    | 1:B:172:GLN:NE2  | 2.17                     | 0.77              |
| 1:B:284:THR:HB   | 1:B:287:GLU:HG3  | 1.66                     | 0.77              |
| 1:B:158:LEU:HD12 | 1:B:158:LEU:O    | 1.85                     | 0.77              |
| 1:B:43:VAL:HG13  | 1:B:48:PRO:HD2   | 1.67                     | 0.76              |
| 1:A:92:ARG:HB2   | 1:A:92:ARG:NH1   | 2.00                     | 0.76              |
| 1:A:406:ASN:C    | 1:A:406:ASN:ND2  | 2.39                     | 0.76              |
| 1:B:356:ALA:O    | 1:B:360:THR:HG22 | 1.85                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:374:VAL:O    | 1:A:374:VAL:HG22 | 1.83                     | 0.76              |
| 1:A:108:ILE:HD13 | 1:A:315:LEU:HD12 | 1.65                     | 0.75              |
| 1:B:147:ASN:HB2  | 2:B:507:HEM:HAC  | 1.68                     | 0.75              |
| 1:A:229:VAL:HG13 | 1:A:282:VAL:HG23 | 1.67                     | 0.75              |
| 1:A:294:ASN:ND2  | 1:A:296:PHE:H    | 1.85                     | 0.75              |
| 1:A:148:ASN:H    | 1:A:148:ASN:ND2  | 1.79                     | 0.75              |
| 1:A:238:ASP:OD1  | 1:A:314:LYS:NZ   | 2.13                     | 0.74              |
| 1:A:223:ASN:ND2  | 1:A:225:ASP:H    | 1.84                     | 0.74              |
| 1:B:79:GLY:O     | 1:B:80:ALA:HB2   | 1.88                     | 0.74              |
| 1:A:405:PRO:HD2  | 1:A:405:PRO:O    | 1.85                     | 0.74              |
| 1:B:98:VAL:HG23  | 1:B:137:THR:CG2  | 2.17                     | 0.74              |
| 1:A:446:TYR:HA   | 1:A:450:LEU:HD21 | 1.70                     | 0.73              |
| 1:B:279:TYR:CE1  | 1:B:311:PRO:HG3  | 2.22                     | 0.73              |
| 1:A:297:ASP:OD1  | 1:A:300:LYS:HE2  | 1.88                     | 0.73              |
| 1:A:79:GLY:O     | 1:A:80:ALA:HB2   | 1.88                     | 0.73              |
| 1:A:263:ASP:O    | 1:A:264:LEU:C    | 2.32                     | 0.73              |
| 1:A:173:THR:HG23 | 1:A:175:LEU:HD12 | 1.69                     | 0.72              |
| 1:B:371:GLN:HE22 | 1:B:393:MET:H    | 1.37                     | 0.72              |
| 2:B:507:HEM:HAD1 | 4:B:518:HOH:O    | 1.89                     | 0.72              |
| 1:B:450:LEU:CD2  | 1:B:455:ARG:HG2  | 2.19                     | 0.72              |
| 1:B:223:ASN:ND2  | 1:B:225:ASP:H    | 1.88                     | 0.72              |
| 1:A:446:TYR:HA   | 1:A:450:LEU:CD2  | 2.19                     | 0.72              |
| 1:B:476:LYS:O    | 1:B:477:ALA:C    | 2.31                     | 0.72              |
| 1:A:92:ARG:O     | 1:A:223:ASN:HB3  | 1.90                     | 0.72              |
| 1:B:220:LYS:HE3  | 1:B:420:HIS:CD2  | 2.25                     | 0.72              |
| 1:B:189:PRO:C    | 1:B:191:SER:H    | 1.95                     | 0.72              |
| 1:A:77:GLY:O     | 1:A:324:TYR:OH   | 2.06                     | 0.71              |
| 1:B:173:THR:CG2  | 1:B:175:LEU:HG   | 2.20                     | 0.71              |
| 1:A:371:GLN:NE2  | 1:A:393:MET:HB2  | 2.05                     | 0.71              |
| 1:B:410:ALA:HB1  | 1:B:411:PRO:HD2  | 1.72                     | 0.71              |
| 1:A:361:HIS:NE2  | 2:A:507:HEM:O2A  | 2.24                     | 0.71              |
| 1:B:360:THR:HG21 | 2:B:507:HEM:HMA3 | 1.73                     | 0.70              |
| 1:B:18:ARG:O     | 1:B:21:GLN:NE2   | 2.24                     | 0.70              |
| 1:A:220:LYS:CE   | 1:A:420:HIS:CD2  | 2.74                     | 0.70              |
| 1:A:170:ASN:HD22 | 1:A:173:THR:H    | 1.40                     | 0.70              |
| 1:A:358:PRO:O    | 1:A:362:ARG:HD2  | 1.91                     | 0.70              |
| 1:A:209:ARG:HG2  | 1:A:274:PRO:HB3  | 1.73                     | 0.70              |
| 1:A:173:THR:CG2  | 1:A:175:LEU:CD1  | 2.66                     | 0.69              |
| 1:B:63:PHE:C     | 1:B:65:ARG:H     | 1.99                     | 0.69              |
| 1:A:466:LEU:HD12 | 1:A:466:LEU:O    | 1.92                     | 0.69              |
| 1:A:60:MET:HE1   | 1:A:63:PHE:HD2   | 1.55                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:98:VAL:CG2   | 1:B:137:THR:CG2  | 2.70                     | 0.69              |
| 1:B:456:LYS:HB3  | 1:B:491:ARG:HH12 | 1.58                     | 0.69              |
| 1:A:173:THR:HG22 | 1:A:175:LEU:H    | 1.57                     | 0.69              |
| 1:B:169:ARG:NH1  | 1:B:174:HIS:O    | 2.26                     | 0.69              |
| 1:B:90:ILE:CD1   | 1:B:312:VAL:HG13 | 2.23                     | 0.68              |
| 1:B:306:ASP:HB3  | 1:B:307:TYR:CE2  | 2.27                     | 0.68              |
| 1:A:94:SER:HB2   | 1:A:221:LEU:HD22 | 1.74                     | 0.68              |
| 1:A:152:PHE:CB   | 1:A:298:LEU:HD13 | 2.23                     | 0.68              |
| 1:A:496:LEU:O    | 1:A:500:ASN:HB2  | 1.93                     | 0.68              |
| 1:B:384:ASN:ND2  | 1:B:386:GLN:H    | 1.91                     | 0.68              |
| 1:A:90:ILE:O     | 1:A:93:TYR:HB2   | 1.93                     | 0.68              |
| 1:A:453:GLU:OE1  | 1:A:456:LYS:HE2  | 1.92                     | 0.68              |
| 1:B:402:ASN:C    | 1:B:402:ASN:HD22 | 2.00                     | 0.68              |
| 1:A:85:GLU:HA    | 1:A:104:LYS:O    | 1.94                     | 0.68              |
| 1:B:65:ARG:HG3   | 1:B:65:ARG:HH11  | 1.59                     | 0.68              |
| 1:B:279:TYR:HE1  | 1:B:311:PRO:HG3  | 1.59                     | 0.68              |
| 1:A:383:ALA:HB1  | 1:A:411:PRO:CG   | 2.24                     | 0.67              |
| 1:B:223:ASN:C    | 1:B:223:ASN:HD22 | 2.01                     | 0.67              |
| 1:A:406:ASN:HD22 | 1:A:408:PHE:H    | 1.39                     | 0.67              |
| 1:B:189:PRO:C    | 1:B:191:SER:N    | 2.50                     | 0.67              |
| 1:B:447:LEU:HB2  | 1:B:448:LYS:HD3  | 1.75                     | 0.67              |
| 1:A:36:ASP:HB3   | 1:B:430:ARG:HD3  | 1.75                     | 0.67              |
| 1:B:18:ARG:HD3   | 1:B:21:GLN:HG3   | 1.77                     | 0.67              |
| 1:B:104:LYS:NZ   | 1:B:138:GLU:OE1  | 2.23                     | 0.67              |
| 1:A:322:VAL:CA   | 1:B:172:GLN:NE2  | 2.52                     | 0.67              |
| 1:B:179:ASP:O    | 1:B:183:ASP:CB   | 2.42                     | 0.67              |
| 1:A:281:GLN:HG2  | 1:A:307:TYR:O    | 1.95                     | 0.67              |
| 1:B:98:VAL:HG23  | 1:B:137:THR:HB   | 1.76                     | 0.67              |
| 1:A:131:PHE:C    | 1:A:131:PHE:HD1  | 2.03                     | 0.66              |
| 1:B:15:LYS:HE2   | 4:B:522:HOH:O    | 1.95                     | 0.66              |
| 1:B:95:LYS:HG2   | 1:B:222:VAL:O    | 1.94                     | 0.66              |
| 1:B:275:SER:HA   | 1:B:315:LEU:O    | 1.94                     | 0.66              |
| 1:A:118:GLU:OE2  | 1:A:169:ARG:NE   | 2.21                     | 0.66              |
| 1:A:90:ILE:HD13  | 1:A:312:VAL:HG13 | 1.77                     | 0.66              |
| 1:A:484:VAL:CG2  | 1:A:488:TYR:HD1  | 2.09                     | 0.66              |
| 1:A:183:ASP:O    | 1:A:187:LEU:HB2  | 1.95                     | 0.65              |
| 1:B:374:VAL:HG22 | 1:B:374:VAL:O    | 1.94                     | 0.65              |
| 1:A:126:ARG:O    | 1:A:127:ASP:HB2  | 1.96                     | 0.65              |
| 1:A:458:LEU:HD11 | 1:A:462:ILE:HD11 | 1.79                     | 0.65              |
| 1:A:43:VAL:HG13  | 1:A:48:PRO:HD2   | 1.78                     | 0.65              |
| 1:A:463:ALA:O    | 1:A:467:LYS:HB3  | 1.97                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:17:GLN:O     | 1:A:17:GLN:HG2   | 1.96                     | 0.65              |
| 1:B:445:PHE:O    | 1:B:449:VAL:HB   | 1.97                     | 0.65              |
| 1:A:428:VAL:HG13 | 1:B:50:LEU:CD1   | 2.26                     | 0.64              |
| 1:B:142:TRP:HB2  | 1:B:339:PRO:CD   | 2.27                     | 0.64              |
| 1:A:172:GLN:NE2  | 1:B:322:VAL:HA   | 2.12                     | 0.64              |
| 1:A:360:THR:HB   | 1:B:64:ASP:HB3   | 1.79                     | 0.64              |
| 1:A:179:ASP:O    | 1:A:183:ASP:HB2  | 1.96                     | 0.64              |
| 1:A:342:ILE:O    | 1:A:343:GLU:HB2  | 1.97                     | 0.64              |
| 1:A:98:VAL:CG2   | 1:A:137:THR:CG2  | 2.74                     | 0.63              |
| 1:A:147:ASN:CG   | 2:A:507:HEM:HAC  | 2.23                     | 0.63              |
| 1:B:173:THR:HG22 | 1:B:175:LEU:CG   | 2.24                     | 0.63              |
| 1:A:238:ASP:CG   | 1:A:314:LYS:HZ2  | 2.05                     | 0.63              |
| 1:A:236:LYS:HG3  | 1:A:279:TYR:CE2  | 2.33                     | 0.63              |
| 1:A:304:HIS:HD2  | 1:A:309:LEU:HD21 | 1.62                     | 0.63              |
| 1:B:170:ASN:HD22 | 1:B:172:GLN:N    | 1.90                     | 0.63              |
| 1:B:284:THR:HG22 | 1:B:286:SER:HB2  | 1.81                     | 0.63              |
| 1:A:220:LYS:CE   | 1:A:420:HIS:HD2  | 2.09                     | 0.63              |
| 1:A:131:PHE:C    | 1:A:131:PHE:CD1  | 2.75                     | 0.63              |
| 1:A:172:GLN:HE21 | 1:B:322:VAL:HA   | 1.63                     | 0.63              |
| 1:A:110:VAL:HA   | 1:A:132:ALA:O    | 1.99                     | 0.62              |
| 1:A:471:LEU:HD22 | 1:A:474:GLN:CD   | 2.23                     | 0.62              |
| 1:A:172:GLN:HG3  | 1:B:322:VAL:O    | 1.98                     | 0.62              |
| 1:B:173:THR:HG21 | 1:B:175:LEU:HD12 | 1.82                     | 0.62              |
| 1:B:43:VAL:O     | 1:B:47:GLY:HA3   | 1.99                     | 0.62              |
| 1:B:191:SER:O    | 1:B:195:VAL:HG23 | 2.00                     | 0.62              |
| 1:B:98:VAL:CG2   | 1:B:137:THR:HG22 | 2.29                     | 0.62              |
| 1:B:74:HIS:CE1   | 1:B:115:VAL:HG22 | 2.35                     | 0.61              |
| 1:A:300:LYS:NZ   | 4:A:530:HOH:O    | 2.29                     | 0.61              |
| 1:A:453:GLU:OE1  | 1:A:456:LYS:CE   | 2.48                     | 0.61              |
| 1:B:51:VAL:O     | 1:B:51:VAL:CG1   | 2.47                     | 0.61              |
| 1:A:100:GLU:O    | 1:A:100:GLU:CG   | 2.48                     | 0.61              |
| 1:A:100:GLU:O    | 1:A:100:GLU:HG3  | 2.01                     | 0.61              |
| 1:B:17:GLN:O     | 1:B:17:GLN:HG2   | 2.00                     | 0.61              |
| 1:B:406:ASN:HD22 | 1:B:408:PHE:N    | 1.93                     | 0.60              |
| 1:B:458:LEU:CD1  | 1:B:462:ILE:CD1  | 2.79                     | 0.60              |
| 1:B:478:VAL:HG11 | 1:B:493:GLN:OE1  | 2.01                     | 0.60              |
| 1:B:192:LEU:HD22 | 1:B:484:VAL:HG11 | 1.82                     | 0.60              |
| 1:A:147:ASN:CB   | 2:A:507:HEM:HAC  | 2.31                     | 0.60              |
| 1:A:435:ASN:C    | 1:A:436:ASP:O    | 2.42                     | 0.60              |
| 1:A:471:LEU:HD21 | 1:A:500:ASN:OD1  | 2.01                     | 0.60              |
| 1:B:470:GLN:OE1  | 1:B:472:PHE:HE2  | 1.85                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:160:PHE:HB3  | 1:A:161:PRO:HD3  | 1.84                     | 0.60              |
| 1:A:484:VAL:HG22 | 1:A:488:TYR:HD1  | 1.66                     | 0.59              |
| 1:B:307:TYR:N    | 1:B:307:TYR:CD2  | 2.68                     | 0.59              |
| 1:B:385:TYR:OH   | 1:B:411:PRO:O    | 2.20                     | 0.59              |
| 1:A:95:LYS:HG2   | 1:A:222:VAL:O    | 2.02                     | 0.59              |
| 1:A:155:ARG:NH2  | 1:A:438:ASN:ND2  | 2.05                     | 0.59              |
| 1:A:284:THR:HG22 | 1:A:286:SER:H    | 1.66                     | 0.59              |
| 1:A:152:PHE:HB3  | 1:A:298:LEU:HD13 | 1.84                     | 0.59              |
| 1:B:371:GLN:NE2  | 1:B:393:MET:H    | 2.01                     | 0.59              |
| 1:B:458:LEU:CD1  | 1:B:462:ILE:HD11 | 2.32                     | 0.59              |
| 1:A:9:ASP:HB3    | 1:A:13:HIS:CE1   | 2.38                     | 0.59              |
| 1:B:192:LEU:HD22 | 1:B:484:VAL:CG1  | 2.33                     | 0.59              |
| 1:A:152:PHE:HB2  | 1:A:298:LEU:HD13 | 1.83                     | 0.59              |
| 1:A:275:SER:HA   | 1:A:315:LEU:O    | 2.02                     | 0.58              |
| 1:B:384:ASN:C    | 1:B:384:ASN:ND2  | 2.61                     | 0.58              |
| 1:B:177:ASP:HB3  | 1:B:180:MET:HE3  | 1.85                     | 0.58              |
| 1:B:89:ASP:C     | 1:B:89:ASP:OD1   | 2.39                     | 0.58              |
| 1:B:131:PHE:HD1  | 1:B:131:PHE:C    | 2.09                     | 0.58              |
| 1:B:156:ASP:OD2  | 1:B:158:LEU:HB2  | 2.02                     | 0.58              |
| 1:A:4:ARG:HD3    | 1:A:9:ASP:OD1    | 2.03                     | 0.58              |
| 1:A:268:ILE:HG23 | 1:A:318:ASN:HA   | 1.85                     | 0.58              |
| 1:B:372:ILE:O    | 1:B:373:PRO:C    | 2.45                     | 0.58              |
| 1:B:458:LEU:HD12 | 1:B:462:ILE:CD1  | 2.33                     | 0.58              |
| 1:A:74:HIS:O     | 1:A:111:ARG:NH2  | 2.32                     | 0.58              |
| 1:A:98:VAL:HG23  | 1:A:137:THR:HG22 | 1.81                     | 0.58              |
| 1:A:189:PRO:C    | 1:A:191:SER:H    | 2.10                     | 0.58              |
| 1:A:236:LYS:HG3  | 1:A:279:TYR:HE2  | 1.67                     | 0.57              |
| 1:A:385:TYR:OH   | 1:A:411:PRO:O    | 2.18                     | 0.57              |
| 1:B:21:GLN:O     | 1:B:22:LYS:CB    | 2.53                     | 0.57              |
| 1:B:51:VAL:O     | 1:B:51:VAL:HG13  | 2.03                     | 0.57              |
| 1:B:63:PHE:C     | 1:B:65:ARG:N     | 2.61                     | 0.57              |
| 1:A:371:GLN:NE2  | 1:A:393:MET:H    | 2.01                     | 0.57              |
| 1:A:400:ALA:O    | 1:A:401:PRO:C    | 2.47                     | 0.57              |
| 1:A:428:VAL:HG13 | 1:B:50:LEU:HD12  | 1.85                     | 0.57              |
| 1:A:439:VAL:O    | 1:A:442:VAL:N    | 2.38                     | 0.57              |
| 1:B:439:VAL:O    | 1:B:440:THR:C    | 2.48                     | 0.57              |
| 1:B:453:GLU:O    | 1:B:456:LYS:HG2  | 2.05                     | 0.57              |
| 1:A:453:GLU:OE1  | 1:A:456:LYS:NZ   | 2.38                     | 0.57              |
| 1:B:125:VAL:O    | 1:B:129:ARG:NH2  | 2.35                     | 0.57              |
| 1:A:147:ASN:HB2  | 2:A:507:HEM:HAC  | 1.87                     | 0.56              |
| 1:A:173:THR:HG23 | 1:A:175:LEU:CD1  | 2.34                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:175:LEU:HD22 | 1:B:262:ARG:NH2  | 2.20                     | 0.56              |
| 1:A:374:VAL:O    | 1:A:374:VAL:CG2  | 2.53                     | 0.56              |
| 1:B:284:THR:CG2  | 1:B:286:SER:HB2  | 2.35                     | 0.56              |
| 1:A:154:ILE:HG13 | 1:A:349:MET:CE   | 2.34                     | 0.56              |
| 1:A:367:PRO:CG   | 1:A:390:PRO:HG2  | 2.12                     | 0.56              |
| 1:B:456:LYS:CB   | 1:B:491:ARG:HH12 | 2.18                     | 0.56              |
| 1:B:466:LEU:HD12 | 1:B:466:LEU:O    | 2.04                     | 0.56              |
| 1:A:60:MET:CE    | 1:A:63:PHE:HD2   | 2.19                     | 0.56              |
| 1:A:348:LYS:CE   | 4:A:549:HOH:O    | 2.53                     | 0.56              |
| 1:A:201:ASP:C    | 1:A:203:GLY:H    | 2.14                     | 0.56              |
| 1:A:356:ALA:O    | 1:A:360:THR:HG22 | 2.06                     | 0.56              |
| 1:A:60:MET:HE1   | 1:A:63:PHE:CD2   | 2.40                     | 0.56              |
| 1:A:98:VAL:HG23  | 1:A:137:THR:HB   | 1.86                     | 0.56              |
| 1:B:301:VAL:HG22 | 1:B:441:GLN:OE1  | 2.05                     | 0.56              |
| 1:B:63:PHE:O     | 1:B:65:ARG:N     | 2.39                     | 0.56              |
| 1:B:415:PRO:C    | 1:B:417:ALA:H    | 2.14                     | 0.56              |
| 1:A:487:GLU:HG2  | 1:A:491:ARG:HD2  | 1.88                     | 0.55              |
| 1:A:229:VAL:HG13 | 1:A:282:VAL:CG2  | 2.36                     | 0.55              |
| 1:A:266:ASN:O    | 1:A:267:ALA:O    | 2.25                     | 0.55              |
| 1:B:334:ASP:O    | 1:B:337:ASN:HB2  | 2.06                     | 0.55              |
| 1:A:177:ASP:HB3  | 1:A:180:MET:CE   | 2.23                     | 0.55              |
| 1:A:471:LEU:HD22 | 1:A:474:GLN:HE22 | 1.63                     | 0.55              |
| 1:B:60:MET:HE1   | 1:B:63:PHE:HD2   | 1.70                     | 0.55              |
| 1:B:304:HIS:HE1  | 3:B:508:NDP:O3B  | 1.89                     | 0.55              |
| 1:B:229:VAL:CG1  | 1:B:282:VAL:CG2  | 2.82                     | 0.55              |
| 1:B:493:GLN:O    | 1:B:494:ALA:C    | 2.48                     | 0.55              |
| 2:B:507:HEM:HMB1 | 2:B:507:HEM:HBB2 | 1.88                     | 0.55              |
| 1:A:345:SER:HB2  | 1:A:346:PRO:CD   | 2.37                     | 0.55              |
| 1:B:274:PRO:HB2  | 1:B:276:TRP:CZ3  | 2.41                     | 0.55              |
| 1:A:239:GLN:NE2  | 1:A:239:GLN:H    | 2.05                     | 0.55              |
| 1:B:98:VAL:HG23  | 1:B:137:THR:HG21 | 1.87                     | 0.55              |
| 1:A:245:SER:OG   | 1:A:248:ASP:HB2  | 2.07                     | 0.55              |
| 1:B:65:ARG:HG3   | 1:B:65:ARG:NH1   | 2.21                     | 0.55              |
| 1:B:73:VAL:O     | 1:B:74:HIS:HB2   | 2.06                     | 0.55              |
| 1:B:131:PHE:C    | 1:B:131:PHE:CD1  | 2.84                     | 0.55              |
| 1:A:157:ALA:CB   | 2:A:507:HEM:HBB1 | 2.37                     | 0.55              |
| 1:A:179:ASP:O    | 1:A:183:ASP:N    | 2.33                     | 0.55              |
| 1:A:447:LEU:CB   | 1:A:448:LYS:HD2  | 2.37                     | 0.55              |
| 1:B:157:ALA:HB2  | 2:B:507:HEM:HBB1 | 1.89                     | 0.55              |
| 1:A:237:THR:HG21 | 1:A:240:GLY:O    | 2.07                     | 0.54              |
| 1:A:154:ILE:HG13 | 1:A:349:MET:HE2  | 1.88                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:188:ARG:O    | 1:B:191:SER:HB3  | 2.07                     | 0.54              |
| 1:B:410:ALA:HB1  | 1:B:411:PRO:CD   | 2.36                     | 0.54              |
| 1:B:391:MET:HE3  | 1:B:393:MET:CE   | 2.38                     | 0.54              |
| 1:B:485:HIS:CD2  | 1:B:486:PRO:HD2  | 2.42                     | 0.54              |
| 1:B:406:ASN:ND2  | 1:B:406:ASN:C    | 2.65                     | 0.54              |
| 1:B:147:ASN:CB   | 2:B:507:HEM:HAC  | 2.38                     | 0.54              |
| 1:A:294:ASN:C    | 1:A:294:ASN:HD22 | 2.15                     | 0.54              |
| 1:B:394:MET:HE3  | 1:B:394:MET:CA   | 2.36                     | 0.54              |
| 1:A:178:PRO:O    | 1:A:182:TRP:HB2  | 2.08                     | 0.54              |
| 1:A:189:PRO:C    | 1:A:191:SER:N    | 2.66                     | 0.54              |
| 1:B:402:ASN:C    | 1:B:402:ASN:ND2  | 2.64                     | 0.54              |
| 1:B:453:GLU:HA   | 1:B:453:GLU:OE2  | 2.06                     | 0.54              |
| 1:A:74:HIS:HA    | 1:A:114:THR:O    | 2.08                     | 0.54              |
| 1:B:19:ALA:C     | 1:B:21:GLN:H     | 2.16                     | 0.54              |
| 1:A:487:GLU:CG   | 1:A:491:ARG:HD2  | 2.37                     | 0.53              |
| 1:B:57:THR:O     | 1:B:61:ALA:HB2   | 2.09                     | 0.53              |
| 1:A:82:GLY:HA3   | 1:A:316:VAL:O    | 2.08                     | 0.53              |
| 1:A:125:VAL:O    | 1:A:129:ARG:NH1  | 2.32                     | 0.53              |
| 1:B:189:PRO:HB2  | 1:B:192:LEU:CD1  | 2.39                     | 0.53              |
| 1:B:212:ASP:OD1  | 1:B:237:THR:HG22 | 2.08                     | 0.53              |
| 1:B:291:PHE:CE1  | 1:B:293:PHE:HB2  | 2.44                     | 0.53              |
| 1:A:73:VAL:O     | 1:A:74:HIS:HB2   | 2.07                     | 0.53              |
| 1:B:331:LEU:HD13 | 1:B:333:PHE:CZ   | 2.44                     | 0.53              |
| 1:A:4:ARG:CD     | 1:A:9:ASP:OD1    | 2.56                     | 0.53              |
| 1:A:371:GLN:HE22 | 1:A:393:MET:H    | 1.57                     | 0.53              |
| 1:B:229:VAL:HG11 | 1:B:282:VAL:HG23 | 1.89                     | 0.53              |
| 1:B:383:ALA:HB1  | 1:B:411:PRO:HG3  | 1.90                     | 0.53              |
| 1:A:276:TRP:HZ3  | 1:A:317:LEU:HD22 | 1.74                     | 0.53              |
| 1:A:406:ASN:ND2  | 1:A:406:ASN:O    | 2.42                     | 0.52              |
| 1:A:322:VAL:HA   | 1:B:172:GLN:HE21 | 1.68                     | 0.52              |
| 1:B:155:ARG:NH2  | 1:B:438:ASN:ND2  | 2.13                     | 0.52              |
| 1:A:294:ASN:HD22 | 1:A:295:PRO:N    | 2.07                     | 0.52              |
| 1:B:54:VAL:HG23  | 1:B:54:VAL:O     | 2.10                     | 0.52              |
| 1:A:142:TRP:HA   | 1:A:337:ASN:O    | 2.09                     | 0.52              |
| 1:A:92:ARG:O     | 1:A:223:ASN:CB   | 2.57                     | 0.52              |
| 1:A:405:PRO:O    | 1:A:405:PRO:CD   | 2.55                     | 0.52              |
| 1:A:177:ASP:CB   | 1:A:180:MET:HE2  | 2.23                     | 0.52              |
| 1:A:200:SER:O    | 1:A:203:GLY:N    | 2.40                     | 0.52              |
| 1:B:18:ARG:HG2   | 1:B:18:ARG:HH11  | 1.75                     | 0.52              |
| 1:B:245:SER:OG   | 1:B:248:ASP:HB2  | 2.10                     | 0.52              |
| 1:A:342:ILE:O    | 1:A:343:GLU:CB   | 2.56                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:458:LEU:HD12 | 1:A:462:ILE:HG13 | 1.92                     | 0.52              |
| 1:B:21:GLN:O     | 1:B:22:LYS:HB3   | 2.10                     | 0.52              |
| 1:B:60:MET:CE    | 1:B:64:ASP:OD2   | 2.58                     | 0.52              |
| 1:B:136:TYR:HB3  | 4:B:531:HOH:O    | 2.09                     | 0.52              |
| 1:A:38:LEU:HA    | 1:B:159:LEU:HD22 | 1.91                     | 0.51              |
| 1:A:54:VAL:HA    | 1:A:57:THR:HG23  | 1.93                     | 0.51              |
| 1:B:148:ASN:H    | 1:B:148:ASN:HD22 | 1.58                     | 0.51              |
| 1:B:392:CYS:SG   | 1:B:396:ASN:HB2  | 2.51                     | 0.51              |
| 1:B:458:LEU:HD11 | 1:B:462:ILE:CD1  | 2.40                     | 0.51              |
| 1:A:391:MET:HE3  | 1:A:393:MET:CE   | 2.40                     | 0.51              |
| 1:B:236:LYS:O    | 1:B:276:TRP:HA   | 2.10                     | 0.51              |
| 1:A:430:ARG:HD3  | 1:B:36:ASP:HB3   | 1.92                     | 0.51              |
| 1:B:400:ALA:O    | 1:B:401:PRO:C    | 2.54                     | 0.51              |
| 1:A:46:ARG:HD3   | 1:B:294:ASN:ND2  | 2.26                     | 0.51              |
| 1:A:324:TYR:O    | 1:A:325:PHE:C    | 2.54                     | 0.51              |
| 1:B:110:VAL:HG21 | 1:B:317:LEU:HD11 | 1.92                     | 0.51              |
| 1:B:84:PHE:O     | 1:B:105:ARG:HA   | 2.11                     | 0.51              |
| 1:B:129:ARG:H    | 1:B:148:ASN:ND2  | 2.09                     | 0.51              |
| 1:B:447:LEU:HB2  | 1:B:448:LYS:CD   | 2.39                     | 0.51              |
| 1:B:406:ASN:HD22 | 1:B:406:ASN:C    | 2.18                     | 0.51              |
| 1:A:150:PRO:HD2  | 1:A:151:ILE:H    | 1.76                     | 0.50              |
| 1:B:19:ALA:C     | 1:B:21:GLN:N     | 2.69                     | 0.50              |
| 1:B:90:ILE:CD1   | 1:B:312:VAL:CG1  | 2.89                     | 0.50              |
| 1:A:142:TRP:HB2  | 1:A:339:PRO:HD3  | 1.93                     | 0.50              |
| 1:A:372:ILE:O    | 1:A:373:PRO:C    | 2.54                     | 0.50              |
| 1:A:406:ASN:OD1  | 1:A:410:ALA:HB3  | 2.10                     | 0.50              |
| 1:A:74:HIS:CE1   | 1:A:115:VAL:HG22 | 2.46                     | 0.50              |
| 1:A:223:ASN:C    | 1:A:223:ASN:ND2  | 2.56                     | 0.50              |
| 1:A:276:TRP:CZ3  | 1:A:317:LEU:HD22 | 2.45                     | 0.50              |
| 1:B:152:PHE:HB3  | 1:B:298:LEU:HD13 | 1.94                     | 0.50              |
| 1:B:236:LYS:HG3  | 1:B:279:TYR:CE2  | 2.47                     | 0.50              |
| 1:B:470:GLN:OE1  | 1:B:472:PHE:CE2  | 2.65                     | 0.50              |
| 1:A:266:ASN:O    | 1:A:267:ALA:C    | 2.54                     | 0.50              |
| 1:B:173:THR:CG2  | 1:B:175:LEU:CG   | 2.86                     | 0.50              |
| 1:B:394:MET:CE   | 1:B:394:MET:CA   | 2.84                     | 0.50              |
| 1:B:437:ASP:OD2  | 1:B:437:ASP:C    | 2.55                     | 0.50              |
| 1:B:9:ASP:OD1    | 1:B:12:LYS:NZ    | 2.45                     | 0.50              |
| 1:B:127:ASP:C    | 1:B:128:PRO:O    | 2.52                     | 0.50              |
| 1:B:384:ASN:HD22 | 1:B:385:TYR:N    | 2.08                     | 0.50              |
| 1:A:90:ILE:HG21  | 1:A:312:VAL:HG22 | 1.94                     | 0.50              |
| 1:A:170:ASN:ND2  | 1:A:172:GLN:H    | 2.10                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:458:LEU:CD1  | 1:A:462:ILE:HD11 | 2.41                     | 0.50              |
| 1:B:189:PRO:HB2  | 1:B:192:LEU:HD12 | 1.93                     | 0.50              |
| 1:B:300:LYS:NZ   | 1:B:437:ASP:O    | 2.43                     | 0.50              |
| 1:A:449:VAL:O    | 1:A:449:VAL:HG12 | 2.12                     | 0.49              |
| 1:A:430:ARG:NH2  | 1:B:53:ASP:OD2   | 2.45                     | 0.49              |
| 1:B:283:MET:HE2  | 1:B:307:TYR:CZ   | 2.47                     | 0.49              |
| 1:A:118:GLU:HG3  | 1:B:120:GLY:CA   | 2.43                     | 0.49              |
| 1:A:309:LEU:HD12 | 4:A:517:HOH:O    | 2.11                     | 0.49              |
| 1:A:406:ASN:HD22 | 1:A:408:PHE:N    | 2.09                     | 0.49              |
| 1:A:235:TYR:HA   | 1:A:277:THR:O    | 2.12                     | 0.49              |
| 1:B:57:THR:O     | 1:B:61:ALA:CB    | 2.60                     | 0.49              |
| 1:A:81:PHE:CD1   | 1:A:81:PHE:N     | 2.80                     | 0.49              |
| 1:B:299:THR:C    | 1:B:300:LYS:HG2  | 2.37                     | 0.49              |
| 1:B:306:ASP:O    | 1:B:308:PRO:HD3  | 2.13                     | 0.49              |
| 1:A:487:GLU:HG2  | 1:A:491:ARG:CD   | 2.42                     | 0.49              |
| 1:B:178:PRO:O    | 1:B:182:TRP:HB2  | 2.12                     | 0.49              |
| 1:A:53:ASP:C     | 1:A:55:VAL:H     | 2.19                     | 0.49              |
| 1:B:458:LEU:CD1  | 1:B:462:ILE:HD12 | 2.42                     | 0.49              |
| 1:A:93:TYR:HB3   | 1:A:221:LEU:HD13 | 1.94                     | 0.49              |
| 1:A:223:ASN:ND2  | 1:A:225:ASP:N    | 2.57                     | 0.49              |
| 1:B:182:TRP:O    | 1:B:183:ASP:C    | 2.55                     | 0.49              |
| 1:B:294:ASN:HD21 | 1:B:296:PHE:HD2  | 1.61                     | 0.49              |
| 1:A:127:ASP:C    | 1:A:128:PRO:O    | 2.52                     | 0.48              |
| 1:A:371:GLN:HE22 | 1:A:393:MET:N    | 2.11                     | 0.48              |
| 1:A:18:ARG:O     | 1:A:21:GLN:NE2   | 2.47                     | 0.48              |
| 1:A:134:LYS:HE3  | 1:A:331:LEU:HD23 | 1.94                     | 0.48              |
| 1:A:471:LEU:CD2  | 1:A:474:GLN:HE22 | 2.25                     | 0.48              |
| 1:A:471:LEU:CD2  | 1:A:474:GLN:NE2  | 2.64                     | 0.48              |
| 1:A:294:ASN:ND2  | 1:A:294:ASN:C    | 2.69                     | 0.48              |
| 1:A:463:ALA:HA   | 1:A:466:LEU:HB3  | 1.94                     | 0.48              |
| 1:A:487:GLU:O    | 1:A:491:ARG:CG   | 2.44                     | 0.48              |
| 1:B:229:VAL:HG11 | 1:B:282:VAL:CG2  | 2.43                     | 0.48              |
| 1:B:361:HIS:NE2  | 2:B:507:HEM:O2A  | 2.46                     | 0.48              |
| 1:A:86:VAL:N     | 1:A:104:LYS:O    | 2.43                     | 0.48              |
| 1:A:98:VAL:HG21  | 1:A:137:THR:HG22 | 1.94                     | 0.48              |
| 1:B:135:PHE:CD1  | 1:B:142:TRP:CE3  | 3.02                     | 0.48              |
| 1:A:435:ASN:O    | 1:A:436:ASP:O    | 2.31                     | 0.48              |
| 1:A:458:LEU:HD12 | 1:A:458:LEU:C    | 2.38                     | 0.48              |
| 1:A:444:THR:O    | 1:A:445:PHE:C    | 2.57                     | 0.48              |
| 1:A:447:LEU:HB2  | 1:A:448:LYS:CD   | 2.44                     | 0.48              |
| 1:B:223:ASN:ND2  | 1:B:225:ASP:N    | 2.59                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:384:ASN:HD22 | 1:B:386:GLN:H    | 1.62                     | 0.48              |
| 1:A:155:ARG:NE   | 1:A:433:SER:O    | 2.29                     | 0.48              |
| 1:A:177:ASP:CG   | 1:A:180:MET:HG3  | 2.38                     | 0.48              |
| 1:B:129:ARG:HG2  | 4:B:542:HOH:O    | 2.13                     | 0.48              |
| 1:A:59:GLU:HB2   | 4:A:515:HOH:O    | 2.14                     | 0.47              |
| 1:A:236:LYS:O    | 1:A:276:TRP:HA   | 2.14                     | 0.47              |
| 1:B:441:GLN:O    | 1:B:444:THR:HG23 | 2.14                     | 0.47              |
| 1:A:84:PHE:O     | 1:A:105:ARG:HA   | 2.13                     | 0.47              |
| 1:B:487:GLU:O    | 1:B:491:ARG:HG3  | 2.14                     | 0.47              |
| 1:A:283:MET:HB3  | 1:A:302:TRP:CH2  | 2.49                     | 0.47              |
| 1:A:357:TYR:CZ   | 2:A:507:HEM:NA   | 2.82                     | 0.47              |
| 1:B:72:VAL:HG13  | 1:B:73:VAL:HG22  | 1.95                     | 0.47              |
| 1:B:429:GLN:HE21 | 1:B:429:GLN:HB2  | 1.34                     | 0.47              |
| 1:A:478:VAL:O    | 1:A:482:SER:HB2  | 2.14                     | 0.47              |
| 1:A:40:SER:HB3   | 1:A:49:LEU:HD13  | 1.97                     | 0.47              |
| 1:B:386:GLN:O    | 1:B:387:ARG:NH1  | 2.47                     | 0.47              |
| 1:A:64:ASP:HB3   | 1:B:360:THR:HB   | 1.97                     | 0.47              |
| 1:A:172:GLN:NE2  | 1:B:321:PRO:O    | 2.46                     | 0.47              |
| 1:B:293:PHE:O    | 1:B:295:PRO:HD3  | 2.15                     | 0.47              |
| 1:B:297:ASP:OD2  | 1:B:299:THR:OG1  | 2.31                     | 0.47              |
| 1:B:98:VAL:CG2   | 1:B:137:THR:HG21 | 2.44                     | 0.47              |
| 1:B:159:LEU:HD11 | 1:B:188:ARG:CZ   | 2.44                     | 0.47              |
| 1:B:284:THR:HG22 | 1:B:286:SER:N    | 2.21                     | 0.47              |
| 1:B:471:LEU:O    | 1:B:472:PHE:C    | 2.58                     | 0.47              |
| 1:A:5:ASP:OD2    | 1:A:7:ALA:HB3    | 2.15                     | 0.47              |
| 1:A:217:HIS:HB2  | 1:A:219:PHE:CZ   | 2.50                     | 0.47              |
| 1:A:93:TYR:CZ    | 1:A:282:VAL:HG11 | 2.50                     | 0.46              |
| 1:B:351:GLN:HA   | 1:B:354:LEU:HD22 | 1.97                     | 0.46              |
| 1:A:98:VAL:HG23  | 1:A:137:THR:CB   | 2.45                     | 0.46              |
| 1:B:149:THR:HG23 | 1:B:151:ILE:O    | 2.15                     | 0.46              |
| 1:B:298:LEU:HD12 | 1:B:349:MET:CG   | 2.37                     | 0.46              |
| 1:A:439:VAL:O    | 1:A:440:THR:C    | 2.58                     | 0.46              |
| 1:B:134:LYS:HE3  | 1:B:331:LEU:CD2  | 2.46                     | 0.46              |
| 1:B:89:ASP:OD1   | 1:B:89:ASP:O     | 2.32                     | 0.46              |
| 1:B:145:VAL:HG22 | 1:B:333:PHE:HB3  | 1.97                     | 0.46              |
| 1:B:209:ARG:HB2  | 4:B:541:HOH:O    | 2.14                     | 0.46              |
| 1:B:209:ARG:HH11 | 1:B:209:ARG:HD3  | 1.45                     | 0.46              |
| 1:B:236:LYS:HE2  | 1:B:236:LYS:HB3  | 1.70                     | 0.46              |
| 1:A:43:VAL:O     | 1:A:47:GLY:HA3   | 2.16                     | 0.46              |
| 1:B:435:ASN:O    | 1:B:436:ASP:C    | 2.59                     | 0.46              |
| 1:A:19:ALA:C     | 1:A:21:GLN:H     | 2.24                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:157:ALA:HB2  | 2:A:507:HEM:HBB1 | 1.98                     | 0.46              |
| 1:A:444:THR:CA   | 1:A:448:LYS:HD3  | 2.28                     | 0.46              |
| 1:A:239:GLN:N    | 1:A:239:GLN:CD   | 2.74                     | 0.46              |
| 1:A:384:ASN:ND2  | 1:A:386:GLN:H    | 2.14                     | 0.46              |
| 1:B:218:THR:HA   | 1:B:231:CYS:O    | 2.15                     | 0.46              |
| 1:B:444:THR:HB   | 1:B:448:LYS:HZ3  | 1.81                     | 0.46              |
| 1:B:447:LEU:O    | 1:B:455:ARG:NH2  | 2.49                     | 0.46              |
| 1:B:138:GLU:OE2  | 1:B:138:GLU:N    | 2.44                     | 0.46              |
| 1:A:77:GLY:HA3   | 1:A:112:PHE:O    | 2.15                     | 0.46              |
| 1:A:79:GLY:O     | 1:A:80:ALA:CB    | 2.59                     | 0.46              |
| 1:A:293:PHE:O    | 1:A:295:PRO:HD3  | 2.16                     | 0.46              |
| 1:A:168:LYS:HE3  | 1:B:67:ARG:NH2   | 2.30                     | 0.45              |
| 1:B:239:GLN:HE21 | 1:B:239:GLN:HB2  | 1.53                     | 0.45              |
| 1:A:112:PHE:CD2  | 1:A:208:HIS:HB3  | 2.51                     | 0.45              |
| 1:B:110:VAL:HA   | 1:B:132:ALA:O    | 2.17                     | 0.45              |
| 1:B:294:ASN:HA   | 1:B:295:PRO:HD2  | 1.75                     | 0.45              |
| 1:B:458:LEU:HD11 | 1:B:462:ILE:HD11 | 1.97                     | 0.45              |
| 1:A:147:ASN:ND2  | 2:A:507:HEM:C3C  | 2.84                     | 0.45              |
| 1:A:173:THR:HG22 | 1:A:175:LEU:N    | 2.28                     | 0.45              |
| 1:A:360:THR:HG21 | 2:A:507:HEM:HMA3 | 1.98                     | 0.45              |
| 1:A:418:LEU:HD23 | 1:A:418:LEU:HA   | 1.78                     | 0.45              |
| 1:B:22:LYS:HA    | 1:B:22:LYS:HD3   | 1.61                     | 0.45              |
| 1:B:220:LYS:HD2  | 1:B:228:ALA:HB1  | 1.99                     | 0.45              |
| 1:A:141:ASN:OD1  | 1:A:377:PRO:HA   | 2.16                     | 0.45              |
| 1:A:147:ASN:HB2  | 2:A:507:HEM:CAC  | 2.46                     | 0.45              |
| 1:B:177:ASP:OD1  | 1:B:179:ASP:HB2  | 2.17                     | 0.45              |
| 1:A:326:ALA:HA   | 1:A:330:GLN:HE21 | 1.81                     | 0.45              |
| 1:A:406:ASN:HD22 | 1:A:407:SER:N    | 2.14                     | 0.45              |
| 1:B:71:ARG:HD2   | 1:B:111:ARG:NH2  | 2.30                     | 0.45              |
| 1:B:450:LEU:HD11 | 1:B:458:LEU:HD22 | 1.99                     | 0.45              |
| 1:B:467:LYS:HE2  | 1:B:468:ASP:OD2  | 2.17                     | 0.45              |
| 1:A:267:ALA:O    | 1:A:268:ILE:C    | 2.59                     | 0.45              |
| 1:A:322:VAL:CA   | 1:B:172:GLN:HE21 | 2.28                     | 0.45              |
| 1:B:239:GLN:OE1  | 1:B:274:PRO:HA   | 2.17                     | 0.45              |
| 1:A:3:ASN:C      | 1:A:4:ARG:HG3    | 2.42                     | 0.45              |
| 1:A:282:VAL:HG23 | 1:A:283:MET:N    | 2.31                     | 0.45              |
| 1:B:65:ARG:NH1   | 1:B:65:ARG:CG    | 2.76                     | 0.45              |
| 1:B:177:ASP:HA   | 1:B:178:PRO:HD3  | 1.70                     | 0.45              |
| 1:A:51:VAL:O     | 1:A:51:VAL:CG1   | 2.65                     | 0.44              |
| 1:A:97:LYS:O     | 1:A:100:GLU:HB3  | 2.16                     | 0.44              |
| 1:A:118:GLU:OE2  | 1:A:169:ARG:NH2  | 2.50                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:435:ASN:C    | 1:B:436:ASP:O    | 2.60                     | 0.44              |
| 1:A:9:ASP:O      | 1:A:12:LYS:HB3   | 2.17                     | 0.44              |
| 1:A:155:ARG:HH11 | 1:A:155:ARG:HD3  | 1.40                     | 0.44              |
| 1:A:172:GLN:HE21 | 1:B:322:VAL:CA   | 2.29                     | 0.44              |
| 1:A:251:ARG:O    | 1:A:255:GLU:HB2  | 2.17                     | 0.44              |
| 1:A:414:GLN:HA   | 1:A:415:PRO:HD2  | 1.89                     | 0.44              |
| 1:B:223:ASN:ND2  | 1:B:223:ASN:C    | 2.69                     | 0.44              |
| 1:B:293:PHE:O    | 1:B:295:PRO:CD   | 2.65                     | 0.44              |
| 1:A:342:ILE:HG22 | 1:A:343:GLU:H    | 1.82                     | 0.44              |
| 1:A:471:LEU:HD11 | 1:A:500:ASN:OD1  | 2.18                     | 0.44              |
| 1:A:353:ARG:O    | 1:A:354:LEU:C    | 2.56                     | 0.44              |
| 1:A:357:TYR:CB   | 1:A:358:PRO:CD   | 2.96                     | 0.44              |
| 1:B:191:SER:O    | 1:B:195:VAL:CG2  | 2.63                     | 0.44              |
| 1:B:354:LEU:HD12 | 1:B:354:LEU:HA   | 1.68                     | 0.44              |
| 1:B:487:GLU:CG   | 1:B:491:ARG:HD2  | 2.46                     | 0.44              |
| 1:A:439:VAL:CG2  | 1:A:443:ARG:NH1  | 2.81                     | 0.44              |
| 1:B:134:LYS:HE2  | 1:B:134:LYS:HB2  | 1.65                     | 0.44              |
| 1:B:135:PHE:CE1  | 1:B:142:TRP:CZ3  | 3.05                     | 0.44              |
| 1:A:439:VAL:HG23 | 1:A:443:ARG:HH11 | 1.82                     | 0.44              |
| 1:B:206:ASP:HA   | 1:B:244:LEU:HG   | 1.99                     | 0.44              |
| 1:A:108:ILE:CD1  | 1:A:315:LEU:HD12 | 2.42                     | 0.44              |
| 1:A:447:LEU:HB2  | 1:A:448:LYS:HD2  | 2.00                     | 0.44              |
| 2:A:507:HEM:CMB  | 2:A:507:HEM:CBB  | 2.92                     | 0.44              |
| 1:B:262:ARG:HH11 | 1:B:262:ARG:HD3  | 1.58                     | 0.44              |
| 1:B:381:ARG:HH11 | 1:B:381:ARG:HD3  | 1.46                     | 0.44              |
| 1:A:72:VAL:HG12  | 2:A:507:HEM:HMA1 | 1.99                     | 0.44              |
| 1:A:84:PHE:HA    | 1:A:314:LYS:O    | 2.18                     | 0.44              |
| 1:A:449:VAL:O    | 1:A:449:VAL:CG1  | 2.64                     | 0.44              |
| 1:B:229:VAL:HG13 | 1:B:282:VAL:CG2  | 2.37                     | 0.44              |
| 1:B:186:SER:O    | 1:B:476:LYS:NZ   | 2.35                     | 0.43              |
| 1:B:194:GLN:O    | 1:B:198:LEU:N    | 2.44                     | 0.43              |
| 1:A:79:GLY:HA2   | 1:A:110:VAL:O    | 2.18                     | 0.43              |
| 1:A:39:ASN:ND2   | 1:B:432:ASN:HA   | 2.33                     | 0.43              |
| 1:A:282:VAL:CG2  | 1:A:283:MET:N    | 2.78                     | 0.43              |
| 1:A:343:GLU:HA   | 1:A:344:PRO:HD3  | 1.94                     | 0.43              |
| 1:A:99:PHE:CE1   | 1:A:312:VAL:HG11 | 2.53                     | 0.43              |
| 1:A:170:ASN:HA   | 1:A:171:PRO:HD3  | 1.85                     | 0.43              |
| 1:A:298:LEU:HD23 | 1:A:298:LEU:HA   | 1.66                     | 0.43              |
| 1:B:98:VAL:HG23  | 1:B:137:THR:CB   | 2.45                     | 0.43              |
| 1:B:157:ALA:CB   | 2:B:507:HEM:CBB  | 2.95                     | 0.43              |
| 1:B:290:ILE:O    | 1:B:291:PHE:C    | 2.59                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:91:THR:HA    | 1:A:94:SER:O     | 2.19                     | 0.43              |
| 1:A:461:ASN:O    | 1:A:462:ILE:C    | 2.61                     | 0.43              |
| 1:B:15:LYS:C     | 1:B:17:GLN:N     | 2.75                     | 0.43              |
| 1:A:50:LEU:HD12  | 1:B:428:VAL:HG13 | 2.00                     | 0.43              |
| 1:A:354:LEU:HD12 | 1:A:354:LEU:HA   | 1.71                     | 0.43              |
| 1:B:78:ALA:O     | 1:B:111:ARG:HA   | 2.19                     | 0.43              |
| 1:B:221:LEU:O    | 1:B:228:ALA:HA   | 2.19                     | 0.43              |
| 1:B:238:ASP:OD1  | 1:B:275:SER:OG   | 2.34                     | 0.43              |
| 1:A:182:TRP:HB3  | 1:A:473:ILE:CG2  | 2.48                     | 0.43              |
| 1:A:201:ASP:C    | 1:A:203:GLY:N    | 2.74                     | 0.43              |
| 1:A:435:ASN:O    | 1:A:436:ASP:C    | 2.62                     | 0.43              |
| 1:B:92:ARG:HD2   | 1:B:93:TYR:CE1   | 2.54                     | 0.43              |
| 1:B:449:VAL:HG21 | 3:B:508:NDP:C4D  | 2.49                     | 0.43              |
| 1:A:187:LEU:HA   | 1:A:187:LEU:HD12 | 1.72                     | 0.42              |
| 1:A:118:GLU:H    | 1:A:118:GLU:HG2  | 1.16                     | 0.42              |
| 1:A:170:ASN:HD21 | 1:B:10:GLN:NE2   | 2.17                     | 0.42              |
| 1:A:150:PRO:CD   | 1:A:151:ILE:H    | 2.31                     | 0.42              |
| 1:A:172:GLN:HG3  | 1:B:322:VAL:C    | 2.44                     | 0.42              |
| 1:A:337:ASN:HD22 | 1:A:337:ASN:HA   | 1.57                     | 0.42              |
| 1:A:342:ILE:HG22 | 1:A:343:GLU:N    | 2.34                     | 0.42              |
| 1:B:474:GLN:O    | 1:B:475:LYS:C    | 2.61                     | 0.42              |
| 1:B:484:VAL:HG22 | 1:B:488:TYR:HD1  | 1.84                     | 0.42              |
| 1:A:394:MET:HE2  | 1:A:394:MET:HB3  | 1.92                     | 0.42              |
| 1:A:89:ASP:OD1   | 1:A:89:ASP:C     | 2.57                     | 0.42              |
| 1:A:134:LYS:CE   | 1:A:331:LEU:CD2  | 2.92                     | 0.42              |
| 1:A:471:LEU:HD21 | 1:A:500:ASN:CG   | 2.44                     | 0.42              |
| 1:B:157:ALA:HB2  | 2:B:507:HEM:CBB  | 2.49                     | 0.42              |
| 1:B:304:HIS:CE1  | 3:B:508:NDP:O3B  | 2.71                     | 0.42              |
| 1:B:394:MET:HA   | 1:B:394:MET:HE2  | 1.97                     | 0.42              |
| 1:B:453:GLU:OE2  | 1:B:453:GLU:CA   | 2.66                     | 0.42              |
| 1:A:135:PHE:CD1  | 1:A:142:TRP:CE3  | 3.08                     | 0.42              |
| 1:B:364:ARG:HH21 | 1:B:364:ARG:HD2  | 1.35                     | 0.42              |
| 1:A:87:THR:OG1   | 1:A:88:HIS:ND1   | 2.51                     | 0.42              |
| 1:A:90:ILE:HD13  | 1:A:312:VAL:CG1  | 2.48                     | 0.42              |
| 1:A:238:ASP:CG   | 1:A:314:LYS:NZ   | 2.73                     | 0.42              |
| 1:B:43:VAL:C     | 1:B:44:GLY:O     | 2.62                     | 0.42              |
| 1:B:332:ALA:HB1  | 1:B:361:HIS:CE1  | 2.55                     | 0.42              |
| 1:B:393:MET:C    | 1:B:394:MET:O    | 2.58                     | 0.42              |
| 1:A:92:ARG:H     | 1:A:92:ARG:HG3   | 1.56                     | 0.42              |
| 1:A:453:GLU:OE2  | 1:A:456:LYS:HG2  | 2.20                     | 0.42              |
| 1:B:402:ASN:HD22 | 1:B:403:TYR:N    | 2.18                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:304:HIS:CD2  | 1:A:309:LEU:HD21 | 2.47                     | 0.42              |
| 1:B:5:ASP:OD1    | 1:B:5:ASP:N      | 2.53                     | 0.42              |
| 1:B:236:LYS:H    | 1:B:236:LYS:HG2  | 1.67                     | 0.42              |
| 1:B:479:LYS:HE2  | 1:B:479:LYS:HB3  | 1.46                     | 0.42              |
| 1:B:485:HIS:HA   | 1:B:486:PRO:HD2  | 1.73                     | 0.42              |
| 1:A:147:ASN:ND2  | 2:A:507:HEM:CAC  | 2.83                     | 0.41              |
| 1:B:324:TYR:C    | 1:B:324:TYR:CD2  | 2.98                     | 0.41              |
| 1:B:387:ARG:HA   | 1:B:396:ASN:HD21 | 1.84                     | 0.41              |
| 1:B:441:GLN:C    | 1:B:444:THR:HG23 | 2.45                     | 0.41              |
| 1:A:329:GLU:OE2  | 1:A:329:GLU:HA   | 2.20                     | 0.41              |
| 1:A:410:ALA:O    | 1:A:411:PRO:C    | 2.62                     | 0.41              |
| 1:A:496:LEU:HD23 | 1:A:496:LEU:HA   | 1.99                     | 0.41              |
| 1:B:415:PRO:C    | 1:B:417:ALA:N    | 2.78                     | 0.41              |
| 1:A:415:PRO:C    | 1:A:417:ALA:N    | 2.77                     | 0.41              |
| 1:A:456:LYS:HG3  | 1:A:460:GLU:OE1  | 2.20                     | 0.41              |
| 1:A:77:GLY:CA    | 1:A:112:PHE:O    | 2.69                     | 0.41              |
| 1:A:237:THR:CG2  | 1:A:240:GLY:O    | 2.68                     | 0.41              |
| 1:A:388:ASP:H    | 1:A:396:ASN:HD21 | 1.68                     | 0.41              |
| 1:B:360:THR:HG21 | 2:B:507:HEM:CMA  | 2.47                     | 0.41              |
| 1:A:188:ARG:O    | 1:A:191:SER:HB3  | 2.21                     | 0.41              |
| 1:A:339:PRO:O    | 1:A:340:PRO:C    | 2.63                     | 0.41              |
| 1:B:439:VAL:O    | 1:B:440:THR:O    | 2.38                     | 0.41              |
| 1:A:400:ALA:HA   | 1:A:401:PRO:HD3  | 1.98                     | 0.41              |
| 1:B:189:PRO:O    | 1:B:192:LEU:HB2  | 2.21                     | 0.41              |
| 1:A:345:SER:CB   | 1:A:346:PRO:CD   | 2.98                     | 0.41              |
| 1:A:170:ASN:HD22 | 1:A:172:GLN:H    | 1.69                     | 0.41              |
| 1:A:206:ASP:HA   | 1:A:244:LEU:HG   | 2.01                     | 0.41              |
| 1:A:284:THR:CG2  | 1:A:286:SER:H    | 2.30                     | 0.41              |
| 1:A:145:VAL:HG22 | 1:A:333:PHE:HB3  | 2.02                     | 0.41              |
| 1:A:294:ASN:HA   | 1:A:295:PRO:HD2  | 1.84                     | 0.41              |
| 1:A:471:LEU:HD21 | 1:A:500:ASN:ND2  | 2.36                     | 0.41              |
| 1:B:50:LEU:HD23  | 1:B:50:LEU:HA    | 1.85                     | 0.41              |
| 1:B:118:GLU:H    | 1:B:118:GLU:HG2  | 1.02                     | 0.41              |
| 1:B:148:ASN:C    | 1:B:214:TYR:HD2  | 2.29                     | 0.41              |
| 1:B:280:ILE:O    | 1:B:280:ILE:HG13 | 2.21                     | 0.41              |
| 1:B:369:TYR:CD1  | 1:B:369:TYR:C    | 2.98                     | 0.41              |
| 1:B:448:LYS:HG2  | 1:B:448:LYS:H    | 1.50                     | 0.41              |
| 1:A:221:LEU:HG   | 1:A:231:CYS:SG   | 2.61                     | 0.41              |
| 1:B:9:ASP:HB3    | 1:B:13:HIS:CE1   | 2.56                     | 0.41              |
| 1:B:446:TYR:HA   | 1:B:450:LEU:HD22 | 2.03                     | 0.41              |
| 1:A:14:TRP:CH2   | 1:A:18:ARG:HD2   | 2.56                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:65:ARG:HH12  | 1:B:359:ASP:CG   | 2.28                     | 0.40              |
| 1:A:147:ASN:CG   | 2:A:507:HEM:CAC  | 2.93                     | 0.40              |
| 1:A:273:TYR:N    | 1:A:273:TYR:CD2  | 2.83                     | 0.40              |
| 1:B:84:PHE:HA    | 1:B:314:LYS:O    | 2.21                     | 0.40              |
| 1:B:275:SER:HB3  | 1:B:316:VAL:HG22 | 2.02                     | 0.40              |
| 2:B:507:HEM:HHA  | 2:B:507:HEM:HAA1 | 1.92                     | 0.40              |
| 1:A:14:TRP:CZ3   | 1:A:18:ARG:HD2   | 2.57                     | 0.40              |
| 1:A:439:VAL:CG2  | 1:A:443:ARG:HH11 | 2.34                     | 0.40              |
| 1:B:258:ASP:O    | 1:B:259:TYR:C    | 2.63                     | 0.40              |
| 1:A:120:GLY:HA2  | 1:B:118:GLU:HG3  | 2.03                     | 0.40              |
| 1:A:274:PRO:HG2  | 1:A:317:LEU:HB2  | 2.02                     | 0.40              |
| 1:A:440:THR:O    | 1:A:443:ARG:N    | 2.54                     | 0.40              |
| 1:B:18:ARG:HH11  | 1:B:18:ARG:CG    | 2.32                     | 0.40              |
| 1:B:158:LEU:HD13 | 1:B:158:LEU:HA   | 1.70                     | 0.40              |
| 1:A:262:ARG:CZ   | 1:B:175:LEU:HD13 | 2.51                     | 0.40              |
| 1:A:357:TYR:HB2  | 1:A:358:PRO:CD   | 2.51                     | 0.40              |
| 1:A:22:LYS:HA    | 1:A:23:PRO:HD3   | 1.89                     | 0.40              |
| 1:A:440:THR:O    | 1:A:441:GLN:C    | 2.64                     | 0.40              |
| 1:A:471:LEU:HD21 | 1:A:500:ASN:HD21 | 1.87                     | 0.40              |
| 1:A:472:PHE:O    | 1:A:475:LYS:N    | 2.55                     | 0.40              |
| 1:B:71:ARG:C     | 1:B:73:VAL:N     | 2.79                     | 0.40              |
| 1:B:369:TYR:HA   | 1:B:372:ILE:HD13 | 2.04                     | 0.40              |

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:419:GLU:OE2 | 1:B:430:ARG:NH1[6_556] | 1.78                     | 0.42              |
| 1:A:10:GLN:NE2  | 4:A:541:HOH:O[6_556]   | 1.86                     | 0.34              |
| 1:A:183:ASP:OD1 | 1:B:407:SER:OG[6_556]  | 2.12                     | 0.08              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed       | Favoured  | Allowed   | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|-----------|----------|-------------|----|
| 1   | A     | 496/506 (98%)  | 418 (84%) | 64 (13%)  | 14 (3%)  | 4           | 6  |
| 1   | B     | 496/506 (98%)  | 425 (86%) | 63 (13%)  | 8 (2%)   | 7           | 14 |
| All | All   | 992/1012 (98%) | 843 (85%) | 127 (13%) | 22 (2%)  | 5           | 9  |

All (22) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 242 | LYS  |
| 1   | A     | 267 | ALA  |
| 1   | A     | 373 | PRO  |
| 1   | A     | 440 | THR  |
| 1   | A     | 451 | ASN  |
| 1   | A     | 54  | VAL  |
| 1   | A     | 101 | HIS  |
| 1   | A     | 268 | ILE  |
| 1   | B     | 54  | VAL  |
| 1   | B     | 64  | ASP  |
| 1   | B     | 242 | LYS  |
| 1   | B     | 440 | THR  |
| 1   | A     | 128 | PRO  |
| 1   | A     | 340 | PRO  |
| 1   | B     | 267 | ALA  |
| 1   | A     | 22  | LYS  |
| 1   | A     | 64  | ASP  |
| 1   | B     | 80  | ALA  |
| 1   | A     | 436 | ASP  |
| 1   | B     | 22  | LYS  |
| 1   | B     | 401 | PRO  |
| 1   | A     | 485 | HIS  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Rotameric | Outliers  | Percentiles |   |
|-----|-------|---------------|-----------|-----------|-------------|---|
| 1   | A     | 430/437 (98%) | 346 (80%) | 84 (20%)  | 1           | 2 |
| 1   | B     | 430/437 (98%) | 355 (83%) | 75 (17%)  | 2           | 3 |
| All | All   | 860/874 (98%) | 701 (82%) | 159 (18%) | 1           | 3 |

All (159) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | ARG  |
| 1   | A     | 11  | MET  |
| 1   | A     | 18  | ARG  |
| 1   | A     | 21  | GLN  |
| 1   | A     | 26  | LEU  |
| 1   | A     | 37  | LYS  |
| 1   | A     | 38  | LEU  |
| 1   | A     | 40  | SER  |
| 1   | A     | 43  | VAL  |
| 1   | A     | 51  | VAL  |
| 1   | A     | 55  | VAL  |
| 1   | A     | 57  | THR  |
| 1   | A     | 67  | ARG  |
| 1   | A     | 72  | VAL  |
| 1   | A     | 76  | LYS  |
| 1   | A     | 89  | ASP  |
| 1   | A     | 92  | ARG  |
| 1   | A     | 98  | VAL  |
| 1   | A     | 100 | GLU  |
| 1   | A     | 102 | ILE  |
| 1   | A     | 118 | GLU  |
| 1   | A     | 125 | VAL  |
| 1   | A     | 129 | ARG  |
| 1   | A     | 137 | THR  |
| 1   | A     | 144 | LEU  |
| 1   | A     | 148 | ASN  |
| 1   | A     | 155 | ARG  |
| 1   | A     | 158 | LEU  |
| 1   | A     | 159 | LEU  |
| 1   | A     | 195 | VAL  |
| 1   | A     | 204 | ILE  |
| 1   | A     | 220 | LYS  |
| 1   | A     | 223 | ASN  |
| 1   | A     | 229 | VAL  |
| 1   | A     | 235 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 236 | LYS  |
| 1   | A     | 239 | GLN  |
| 1   | A     | 242 | LYS  |
| 1   | A     | 246 | VAL  |
| 1   | A     | 255 | GLU  |
| 1   | A     | 261 | LEU  |
| 1   | A     | 263 | ASP  |
| 1   | A     | 264 | LEU  |
| 1   | A     | 268 | ILE  |
| 1   | A     | 282 | VAL  |
| 1   | A     | 284 | THR  |
| 1   | A     | 286 | SER  |
| 1   | A     | 290 | ILE  |
| 1   | A     | 298 | LEU  |
| 1   | A     | 304 | HIS  |
| 1   | A     | 311 | PRO  |
| 1   | A     | 315 | LEU  |
| 1   | A     | 317 | LEU  |
| 1   | A     | 331 | LEU  |
| 1   | A     | 335 | PRO  |
| 1   | A     | 337 | ASN  |
| 1   | A     | 339 | PRO  |
| 1   | A     | 354 | LEU  |
| 1   | A     | 365 | LEU  |
| 1   | A     | 372 | ILE  |
| 1   | A     | 373 | PRO  |
| 1   | A     | 384 | ASN  |
| 1   | A     | 386 | GLN  |
| 1   | A     | 393 | MET  |
| 1   | A     | 394 | MET  |
| 1   | A     | 402 | ASN  |
| 1   | A     | 406 | ASN  |
| 1   | A     | 414 | GLN  |
| 1   | A     | 429 | GLN  |
| 1   | A     | 439 | VAL  |
| 1   | A     | 443 | ARG  |
| 1   | A     | 444 | THR  |
| 1   | A     | 448 | LYS  |
| 1   | A     | 450 | LEU  |
| 1   | A     | 452 | GLU  |
| 1   | A     | 453 | GLU  |
| 1   | A     | 456 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 458 | LEU  |
| 1   | A     | 471 | LEU  |
| 1   | A     | 475 | LYS  |
| 1   | A     | 482 | SER  |
| 1   | A     | 484 | VAL  |
| 1   | A     | 498 | LYS  |
| 1   | A     | 500 | ASN  |
| 1   | B     | 4   | ARG  |
| 1   | B     | 10  | GLN  |
| 1   | B     | 18  | ARG  |
| 1   | B     | 21  | GLN  |
| 1   | B     | 37  | LYS  |
| 1   | B     | 40  | SER  |
| 1   | B     | 43  | VAL  |
| 1   | B     | 48  | PRO  |
| 1   | B     | 51  | VAL  |
| 1   | B     | 57  | THR  |
| 1   | B     | 71  | ARG  |
| 1   | B     | 73  | VAL  |
| 1   | B     | 76  | LYS  |
| 1   | B     | 89  | ASP  |
| 1   | B     | 90  | ILE  |
| 1   | B     | 91  | THR  |
| 1   | B     | 92  | ARG  |
| 1   | B     | 95  | LYS  |
| 1   | B     | 102 | ILE  |
| 1   | B     | 118 | GLU  |
| 1   | B     | 137 | THR  |
| 1   | B     | 138 | GLU  |
| 1   | B     | 148 | ASN  |
| 1   | B     | 150 | PRO  |
| 1   | B     | 154 | ILE  |
| 1   | B     | 155 | ARG  |
| 1   | B     | 158 | LEU  |
| 1   | B     | 159 | LEU  |
| 1   | B     | 172 | GLN  |
| 1   | B     | 192 | LEU  |
| 1   | B     | 220 | LYS  |
| 1   | B     | 223 | ASN  |
| 1   | B     | 229 | VAL  |
| 1   | B     | 235 | TYR  |
| 1   | B     | 236 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 242 | LYS  |
| 1   | B     | 244 | LEU  |
| 1   | B     | 246 | VAL  |
| 1   | B     | 247 | GLU  |
| 1   | B     | 261 | LEU  |
| 1   | B     | 264 | LEU  |
| 1   | B     | 284 | THR  |
| 1   | B     | 290 | ILE  |
| 1   | B     | 298 | LEU  |
| 1   | B     | 315 | LEU  |
| 1   | B     | 317 | LEU  |
| 1   | B     | 318 | ASN  |
| 1   | B     | 331 | LEU  |
| 1   | B     | 335 | PRO  |
| 1   | B     | 337 | ASN  |
| 1   | B     | 339 | PRO  |
| 1   | B     | 354 | LEU  |
| 1   | B     | 355 | PHE  |
| 1   | B     | 365 | LEU  |
| 1   | B     | 372 | ILE  |
| 1   | B     | 384 | ASN  |
| 1   | B     | 386 | GLN  |
| 1   | B     | 394 | MET  |
| 1   | B     | 402 | ASN  |
| 1   | B     | 405 | PRO  |
| 1   | B     | 406 | ASN  |
| 1   | B     | 407 | SER  |
| 1   | B     | 414 | GLN  |
| 1   | B     | 415 | PRO  |
| 1   | B     | 443 | ARG  |
| 1   | B     | 444 | THR  |
| 1   | B     | 448 | LYS  |
| 1   | B     | 450 | LEU  |
| 1   | B     | 458 | LEU  |
| 1   | B     | 471 | LEU  |
| 1   | B     | 475 | LYS  |
| 1   | B     | 479 | LYS  |
| 1   | B     | 484 | VAL  |
| 1   | B     | 498 | LYS  |
| 1   | B     | 500 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | ASN  |
| 1   | A     | 10  | GLN  |
| 1   | A     | 13  | HIS  |
| 1   | A     | 39  | ASN  |
| 1   | A     | 148 | ASN  |
| 1   | A     | 167 | GLN  |
| 1   | A     | 170 | ASN  |
| 1   | A     | 172 | GLN  |
| 1   | A     | 223 | ASN  |
| 1   | A     | 234 | HIS  |
| 1   | A     | 243 | ASN  |
| 1   | A     | 272 | ASN  |
| 1   | A     | 281 | GLN  |
| 1   | A     | 294 | ASN  |
| 1   | A     | 304 | HIS  |
| 1   | A     | 330 | GLN  |
| 1   | A     | 337 | ASN  |
| 1   | A     | 368 | ASN  |
| 1   | A     | 371 | GLN  |
| 1   | A     | 384 | ASN  |
| 1   | A     | 396 | ASN  |
| 1   | A     | 397 | GLN  |
| 1   | A     | 406 | ASN  |
| 1   | A     | 414 | GLN  |
| 1   | A     | 420 | HIS  |
| 1   | A     | 429 | GLN  |
| 1   | A     | 438 | ASN  |
| 1   | A     | 474 | GLN  |
| 1   | A     | 480 | ASN  |
| 1   | A     | 485 | HIS  |
| 1   | B     | 10  | GLN  |
| 1   | B     | 13  | HIS  |
| 1   | B     | 17  | GLN  |
| 1   | B     | 39  | ASN  |
| 1   | B     | 101 | HIS  |
| 1   | B     | 148 | ASN  |
| 1   | B     | 167 | GLN  |
| 1   | B     | 170 | ASN  |
| 1   | B     | 172 | GLN  |
| 1   | B     | 223 | ASN  |
| 1   | B     | 234 | HIS  |
| 1   | B     | 272 | ASN  |
| 1   | B     | 281 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 294 | ASN  |
| 1   | B     | 304 | HIS  |
| 1   | B     | 337 | ASN  |
| 1   | B     | 368 | ASN  |
| 1   | B     | 371 | GLN  |
| 1   | B     | 384 | ASN  |
| 1   | B     | 396 | ASN  |
| 1   | B     | 397 | GLN  |
| 1   | B     | 402 | ASN  |
| 1   | B     | 406 | ASN  |
| 1   | B     | 414 | GLN  |
| 1   | B     | 420 | HIS  |
| 1   | B     | 429 | GLN  |
| 1   | B     | 438 | ASN  |
| 1   | B     | 474 | GLN  |
| 1   | B     | 485 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | NDP  | A     | 508 | -    | 51,52,52     | 2.21 | 11 (21%) | 71,80,80    | 2.55 | 16 (22%) |
| 2   | HEM  | A     | 507 | 1    | 50,50,50     | 2.24 | 11 (22%) | 67,82,82    | 3.31 | 21 (31%) |
| 3   | NDP  | B     | 508 | -    | 51,52,52     | 2.23 | 11 (21%) | 71,80,80    | 2.55 | 16 (22%) |
| 2   | HEM  | B     | 507 | 1    | 50,50,50     | 2.08 | 13 (26%) | 67,82,82    | 3.04 | 20 (29%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals   | Torsions   | Rings   |
|-----|------|-------|-----|------|-----------|------------|---------|
| 3   | NDP  | A     | 508 | -    | 1/1/14/17 | 5/34/77/77 | 0/5/5/5 |
| 2   | HEM  | A     | 507 | 1    | -         | 1/14/54/54 | -       |
| 3   | NDP  | B     | 508 | -    | 1/1/14/17 | 5/34/77/77 | 0/5/5/5 |
| 2   | HEM  | B     | 507 | 1    | -         | 2/14/54/54 | -       |

All (46) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | B     | 508 | NDP  | P2B-O2B | 9.26  | 1.75        | 1.59     |
| 3   | A     | 508 | NDP  | P2B-O2B | 9.15  | 1.75        | 1.59     |
| 2   | A     | 507 | HEM  | CHC-C1C | 7.82  | 1.53        | 1.38     |
| 2   | B     | 507 | HEM  | CHC-C1C | 6.99  | 1.52        | 1.38     |
| 2   | A     | 507 | HEM  | C4C-NC  | 5.72  | 1.50        | 1.39     |
| 2   | A     | 507 | HEM  | FE-NC   | 5.45  | 2.13        | 1.95     |
| 3   | B     | 508 | NDP  | O4B-C1B | 5.44  | 1.54        | 1.42     |
| 3   | A     | 508 | NDP  | O4B-C1B | 5.41  | 1.54        | 1.42     |
| 2   | A     | 507 | HEM  | C1C-NC  | -5.20 | 1.29        | 1.39     |
| 2   | B     | 507 | HEM  | FE-NC   | 5.05  | 2.11        | 1.95     |
| 3   | B     | 508 | NDP  | O3B-C3B | -4.84 | 1.31        | 1.43     |
| 3   | A     | 508 | NDP  | O3B-C3B | -4.79 | 1.31        | 1.43     |
| 2   | B     | 507 | HEM  | C1C-NC  | -4.76 | 1.30        | 1.39     |
| 3   | B     | 508 | NDP  | C4N-C3N | -4.69 | 1.41        | 1.50     |
| 3   | A     | 508 | NDP  | C4N-C3N | -4.65 | 1.41        | 1.50     |
| 2   | B     | 507 | HEM  | C4C-NC  | 4.59  | 1.48        | 1.39     |
| 2   | A     | 507 | HEM  | C1C-C2C | -4.23 | 1.37        | 1.45     |
| 3   | B     | 508 | NDP  | PN-O3   | -3.98 | 1.55        | 1.59     |
| 3   | A     | 508 | NDP  | PN-O3   | -3.93 | 1.55        | 1.59     |
| 3   | B     | 508 | NDP  | C4N-C5N | -3.90 | 1.38        | 1.49     |
| 3   | A     | 508 | NDP  | C4N-C5N | -3.87 | 1.39        | 1.49     |
| 3   | B     | 508 | NDP  | C7N-C3N | 3.53  | 1.56        | 1.48     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | A     | 508 | NDP  | C7N-C3N | 3.48  | 1.56        | 1.48     |
| 2   | B     | 507 | HEM  | C3C-C4C | 3.32  | 1.51        | 1.46     |
| 2   | B     | 507 | HEM  | CMA-C3A | 3.05  | 1.57        | 1.50     |
| 2   | B     | 507 | HEM  | O1A-CGA | 2.96  | 1.31        | 1.22     |
| 2   | A     | 507 | HEM  | CAC-C3C | 2.96  | 1.55        | 1.47     |
| 2   | B     | 507 | HEM  | C1C-C2C | -2.90 | 1.39        | 1.45     |
| 2   | A     | 507 | HEM  | CMA-C3A | 2.86  | 1.56        | 1.50     |
| 2   | B     | 507 | HEM  | C2A-C3A | -2.86 | 1.31        | 1.38     |
| 2   | A     | 507 | HEM  | CMB-C2B | 2.74  | 1.56        | 1.50     |
| 2   | A     | 507 | HEM  | CHC-C4B | 2.70  | 1.45        | 1.39     |
| 2   | B     | 507 | HEM  | CBD-CGD | 2.63  | 1.56        | 1.50     |
| 2   | B     | 507 | HEM  | FE-NB   | 2.51  | 2.02        | 1.94     |
| 2   | A     | 507 | HEM  | CAB-C3B | 2.40  | 1.53        | 1.47     |
| 2   | A     | 507 | HEM  | FE-NB   | 2.32  | 2.02        | 1.94     |
| 3   | A     | 508 | NDP  | O2B-C2B | 2.27  | 1.51        | 1.44     |
| 3   | B     | 508 | NDP  | C2A-N1A | 2.24  | 1.37        | 1.33     |
| 3   | A     | 508 | NDP  | C2A-N1A | 2.23  | 1.37        | 1.33     |
| 3   | B     | 508 | NDP  | O2B-C2B | 2.21  | 1.51        | 1.44     |
| 3   | B     | 508 | NDP  | PA-O2A  | -2.11 | 1.45        | 1.55     |
| 3   | A     | 508 | NDP  | PA-O2A  | -2.11 | 1.45        | 1.55     |
| 3   | A     | 508 | NDP  | PN-O2N  | -2.09 | 1.45        | 1.55     |
| 3   | B     | 508 | NDP  | PN-O2N  | -2.08 | 1.45        | 1.55     |
| 2   | B     | 507 | HEM  | CAB-C3B | 2.05  | 1.52        | 1.47     |
| 2   | B     | 507 | HEM  | CAA-C2A | 2.04  | 1.56        | 1.51     |

All (73) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2   | A     | 507 | HEM  | CHC-C1C-NC  | -20.70 | 101.92      | 124.45   |
| 2   | B     | 507 | HEM  | CHC-C1C-NC  | -17.82 | 105.05      | 124.45   |
| 3   | B     | 508 | NDP  | C2B-C1B-N9A | 12.15  | 133.75      | 113.75   |
| 3   | A     | 508 | NDP  | C2B-C1B-N9A | 12.12  | 133.69      | 113.75   |
| 3   | A     | 508 | NDP  | O3B-C3B-C4B | 9.53   | 138.46      | 111.08   |
| 3   | B     | 508 | NDP  | O3B-C3B-C4B | 9.51   | 138.40      | 111.08   |
| 2   | A     | 507 | HEM  | C2C-C1C-NC  | 7.12   | 122.80      | 109.64   |
| 2   | B     | 507 | HEM  | C2C-C1C-NC  | 6.79   | 122.20      | 109.64   |
| 3   | A     | 508 | NDP  | O4B-C1B-C2B | -6.41  | 95.55       | 106.59   |
| 3   | B     | 508 | NDP  | O4B-C1B-C2B | -6.38  | 95.61       | 106.59   |
| 2   | A     | 507 | HEM  | CAA-CBA-CGA | 5.51   | 128.27      | 113.67   |
| 3   | B     | 508 | NDP  | O2X-P2B-O2B | 5.48   | 127.21      | 105.85   |
| 3   | A     | 508 | NDP  | O2X-P2B-O2B | 5.47   | 127.16      | 105.85   |
| 2   | A     | 507 | HEM  | C3C-C2C-C1C | -5.27  | 102.06      | 107.05   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 507 | HEM  | C4C-NC-C1C  | -5.27 | 97.23       | 105.82   |
| 3   | A     | 508 | NDP  | O4B-C1B-N9A | -4.96 | 98.56       | 108.09   |
| 2   | B     | 507 | HEM  | C3C-C2C-C1C | -4.96 | 102.35      | 107.05   |
| 3   | B     | 508 | NDP  | O4B-C1B-N9A | -4.94 | 98.60       | 108.09   |
| 2   | B     | 507 | HEM  | O2D-CGD-O1D | 4.74  | 135.51      | 123.33   |
| 2   | A     | 507 | HEM  | O2A-CGA-O1A | -4.24 | 112.42      | 123.33   |
| 2   | B     | 507 | HEM  | CAA-C2A-C1A | -4.24 | 116.65      | 124.94   |
| 2   | B     | 507 | HEM  | C4C-NC-C1C  | -4.10 | 99.13       | 105.82   |
| 3   | A     | 508 | NDP  | O3X-P2B-O2B | -3.98 | 90.34       | 105.85   |
| 3   | B     | 508 | NDP  | O3X-P2B-O2B | -3.96 | 90.41       | 105.85   |
| 2   | A     | 507 | HEM  | CHD-C4C-NC  | 3.77  | 128.56      | 124.45   |
| 2   | A     | 507 | HEM  | O2D-CGD-O1D | 3.76  | 133.00      | 123.33   |
| 2   | B     | 507 | HEM  | CHD-C4C-NC  | 3.76  | 128.55      | 124.45   |
| 2   | B     | 507 | HEM  | O1A-CGA-CBA | -3.59 | 111.69      | 123.09   |
| 2   | A     | 507 | HEM  | O1D-CGD-CBD | -3.57 | 111.77      | 123.09   |
| 3   | B     | 508 | NDP  | O2N-PN-O3   | 3.55  | 116.87      | 107.27   |
| 3   | A     | 508 | NDP  | O2N-PN-O3   | 3.53  | 116.83      | 107.27   |
| 2   | B     | 507 | HEM  | CMC-C2C-C3C | 3.41  | 136.67      | 128.43   |
| 2   | B     | 507 | HEM  | CAA-C2A-C3A | 3.30  | 134.47      | 127.07   |
| 2   | B     | 507 | HEM  | CHA-C1A-NA  | 3.23  | 129.72      | 123.86   |
| 3   | B     | 508 | NDP  | O3B-C3B-C2B | 3.22  | 120.20      | 111.19   |
| 3   | B     | 508 | NDP  | C6N-N1N-C2N | 3.21  | 122.76      | 119.32   |
| 3   | A     | 508 | NDP  | O3B-C3B-C2B | 3.20  | 120.13      | 111.19   |
| 3   | A     | 508 | NDP  | C6N-N1N-C2N | 3.18  | 122.73      | 119.32   |
| 2   | B     | 507 | HEM  | O1D-CGD-CBD | -3.17 | 113.03      | 123.09   |
| 2   | A     | 507 | HEM  | O2A-CGA-CBA | 3.06  | 123.68      | 114.00   |
| 2   | B     | 507 | HEM  | C3B-C4B-NB  | -2.87 | 107.41      | 109.47   |
| 2   | B     | 507 | HEM  | O2A-CGA-O1A | 2.81  | 130.57      | 123.33   |
| 2   | A     | 507 | HEM  | C3B-C4B-NB  | -2.81 | 107.45      | 109.47   |
| 2   | B     | 507 | HEM  | CHB-C4A-NA  | -2.78 | 118.82      | 123.86   |
| 2   | B     | 507 | HEM  | C1A-CHA-C4D | -2.72 | 119.86      | 126.25   |
| 3   | A     | 508 | NDP  | O2A-PA-O3   | 2.70  | 114.57      | 107.27   |
| 3   | B     | 508 | NDP  | O2A-PA-O3   | 2.69  | 114.56      | 107.27   |
| 2   | A     | 507 | HEM  | CHD-C1D-ND  | -2.64 | 121.58      | 124.42   |
| 3   | A     | 508 | NDP  | O2B-C2B-C3B | -2.64 | 102.22      | 111.68   |
| 3   | B     | 508 | NDP  | O2B-C2B-C3B | -2.64 | 102.22      | 111.68   |
| 3   | B     | 508 | NDP  | C3N-C2N-N1N | -2.63 | 119.34      | 123.20   |
| 3   | A     | 508 | NDP  | C3N-C2N-N1N | -2.57 | 119.43      | 123.20   |
| 2   | A     | 507 | HEM  | CHC-C1C-C2C | 2.57  | 130.82      | 125.49   |
| 2   | A     | 507 | HEM  | CHA-C4D-ND  | 2.52  | 127.48      | 124.37   |
| 3   | B     | 508 | NDP  | C3D-C2D-C1D | 2.52  | 106.23      | 101.46   |
| 3   | A     | 508 | NDP  | C3D-C2D-C1D | 2.50  | 106.19      | 101.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | A     | 508 | NDP  | C1D-N1N-C2N | -2.49 | 117.04      | 121.14   |
| 2   | A     | 507 | HEM  | CBA-CAA-C2A | 2.48  | 119.40      | 112.53   |
| 3   | B     | 508 | NDP  | C1D-N1N-C2N | -2.47 | 117.06      | 121.14   |
| 2   | A     | 507 | HEM  | CMC-C2C-C3C | 2.47  | 134.40      | 128.43   |
| 2   | A     | 507 | HEM  | C1C-CHC-C4B | 2.44  | 131.21      | 126.02   |
| 2   | B     | 507 | HEM  | CHA-C4D-ND  | 2.40  | 127.34      | 124.37   |
| 2   | A     | 507 | HEM  | CBB-CAB-C3B | -2.37 | 115.68      | 127.53   |
| 3   | A     | 508 | NDP  | O2B-C2B-C1B | -2.26 | 102.10      | 110.05   |
| 2   | B     | 507 | HEM  | C2A-C1A-NA  | -2.25 | 107.65      | 110.15   |
| 3   | B     | 508 | NDP  | O2B-C2B-C1B | -2.24 | 102.18      | 110.05   |
| 2   | B     | 507 | HEM  | CMC-C2C-C1C | -2.19 | 120.87      | 124.73   |
| 3   | B     | 508 | NDP  | O3D-C3D-C4D | -2.18 | 104.83      | 111.08   |
| 3   | A     | 508 | NDP  | O3D-C3D-C4D | -2.14 | 104.92      | 111.08   |
| 2   | A     | 507 | HEM  | C1A-CHA-C4D | -2.13 | 121.25      | 126.25   |
| 2   | A     | 507 | HEM  | CMB-C2B-C1B | -2.12 | 121.73      | 125.03   |
| 2   | A     | 507 | HEM  | CBC-CAC-C3C | -2.10 | 117.04      | 127.53   |
| 2   | B     | 507 | HEM  | CMA-C3A-C4A | 2.05  | 128.54      | 125.42   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 3   | A     | 508 | NDP  | C3B  |
| 3   | B     | 508 | NDP  | C3B  |

All (13) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | B     | 507 | HEM  | C2C-C3C-CAC-CBC |
| 2   | B     | 507 | HEM  | C4C-C3C-CAC-CBC |
| 3   | A     | 508 | NDP  | O4B-C4B-C5B-O5B |
| 3   | B     | 508 | NDP  | O4B-C4B-C5B-O5B |
| 3   | A     | 508 | NDP  | C2B-C1B-N9A-C8A |
| 3   | B     | 508 | NDP  | C2B-C1B-N9A-C8A |
| 3   | A     | 508 | NDP  | PN-O3-PA-O2A    |
| 3   | B     | 508 | NDP  | PN-O3-PA-O2A    |
| 3   | A     | 508 | NDP  | C2B-C1B-N9A-C4A |
| 3   | B     | 508 | NDP  | C2B-C1B-N9A-C4A |
| 3   | A     | 508 | NDP  | O4D-C1D-N1N-C6N |
| 3   | B     | 508 | NDP  | O4D-C1D-N1N-C6N |
| 2   | A     | 507 | HEM  | C4C-C3C-CAC-CBC |

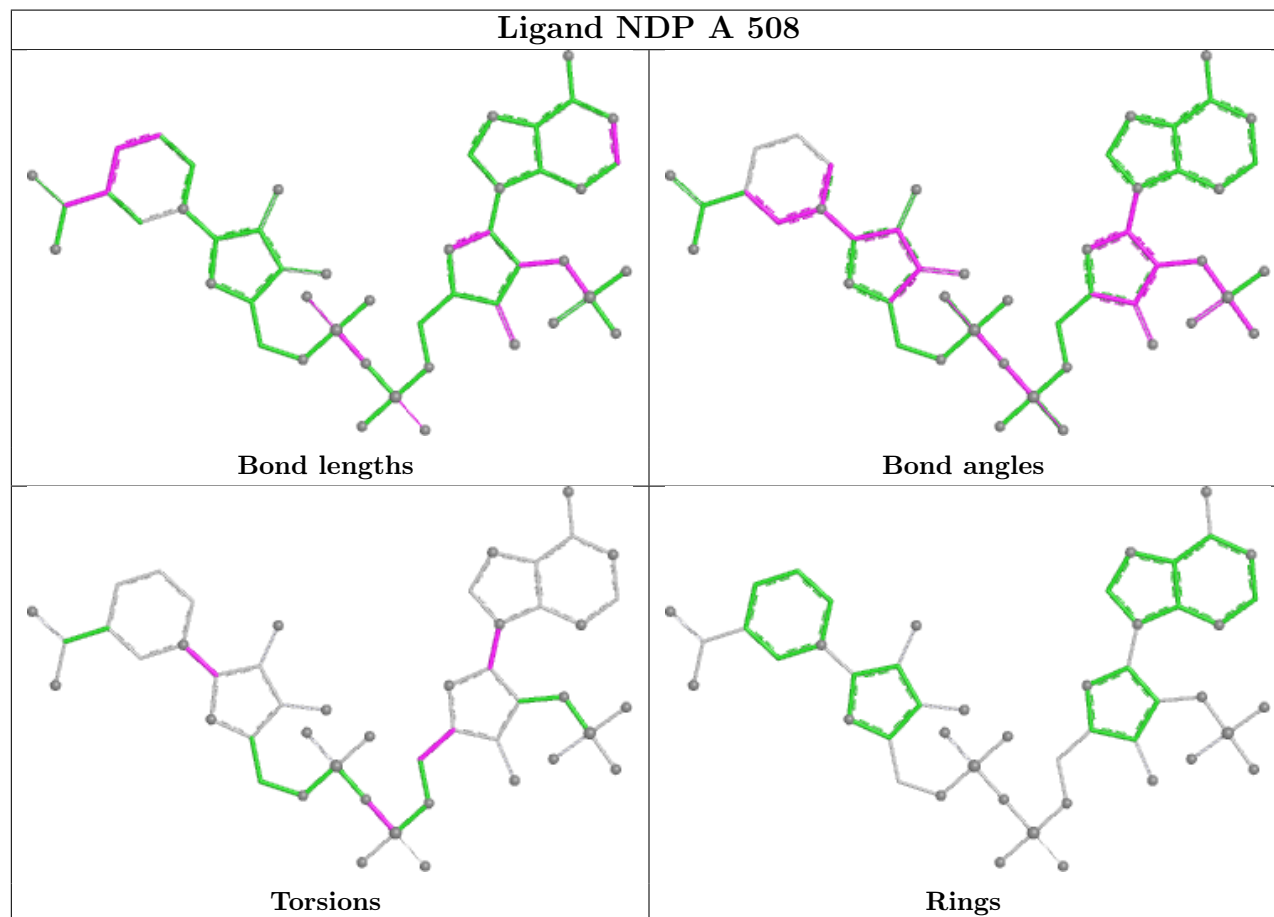
There are no ring outliers.

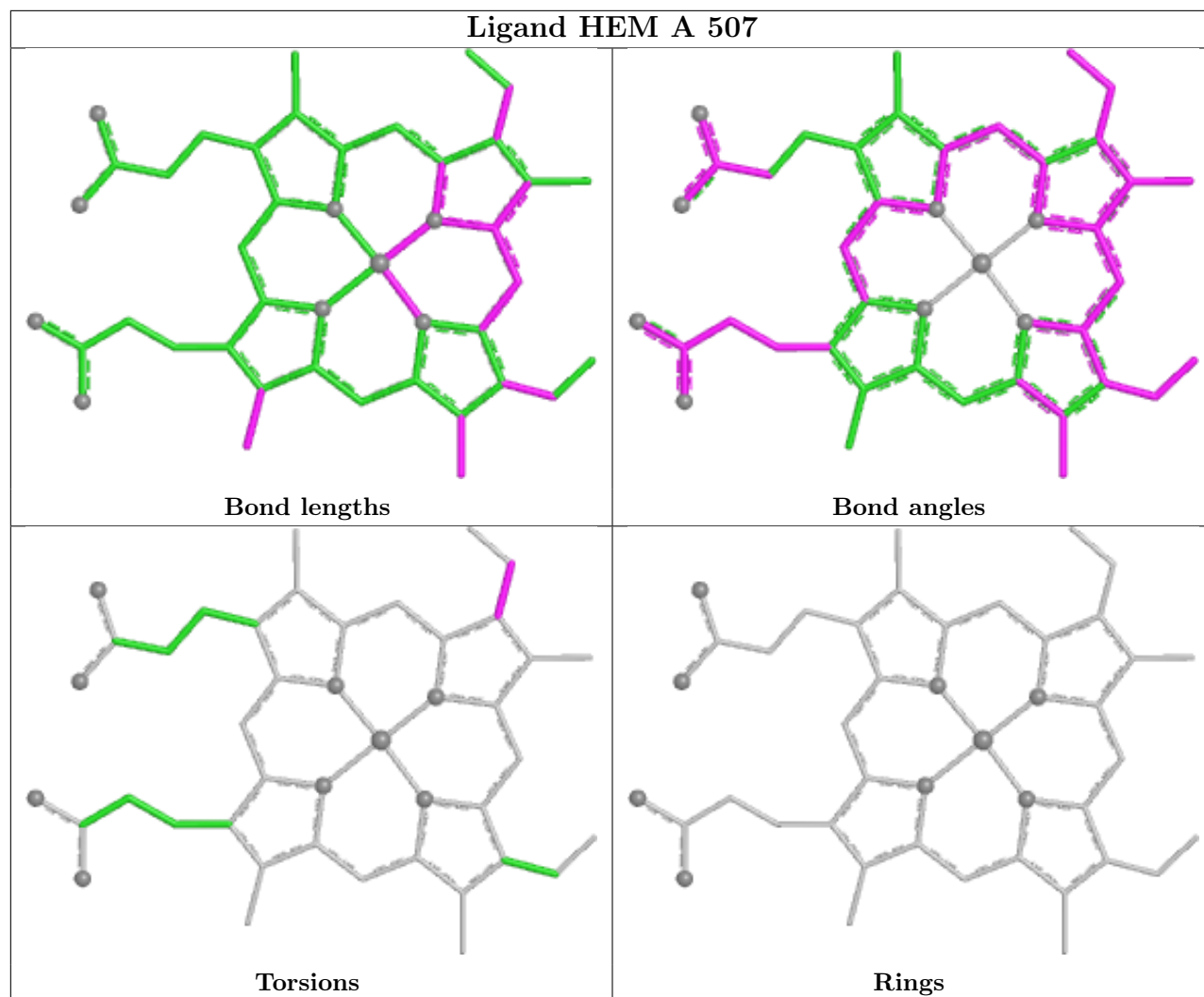


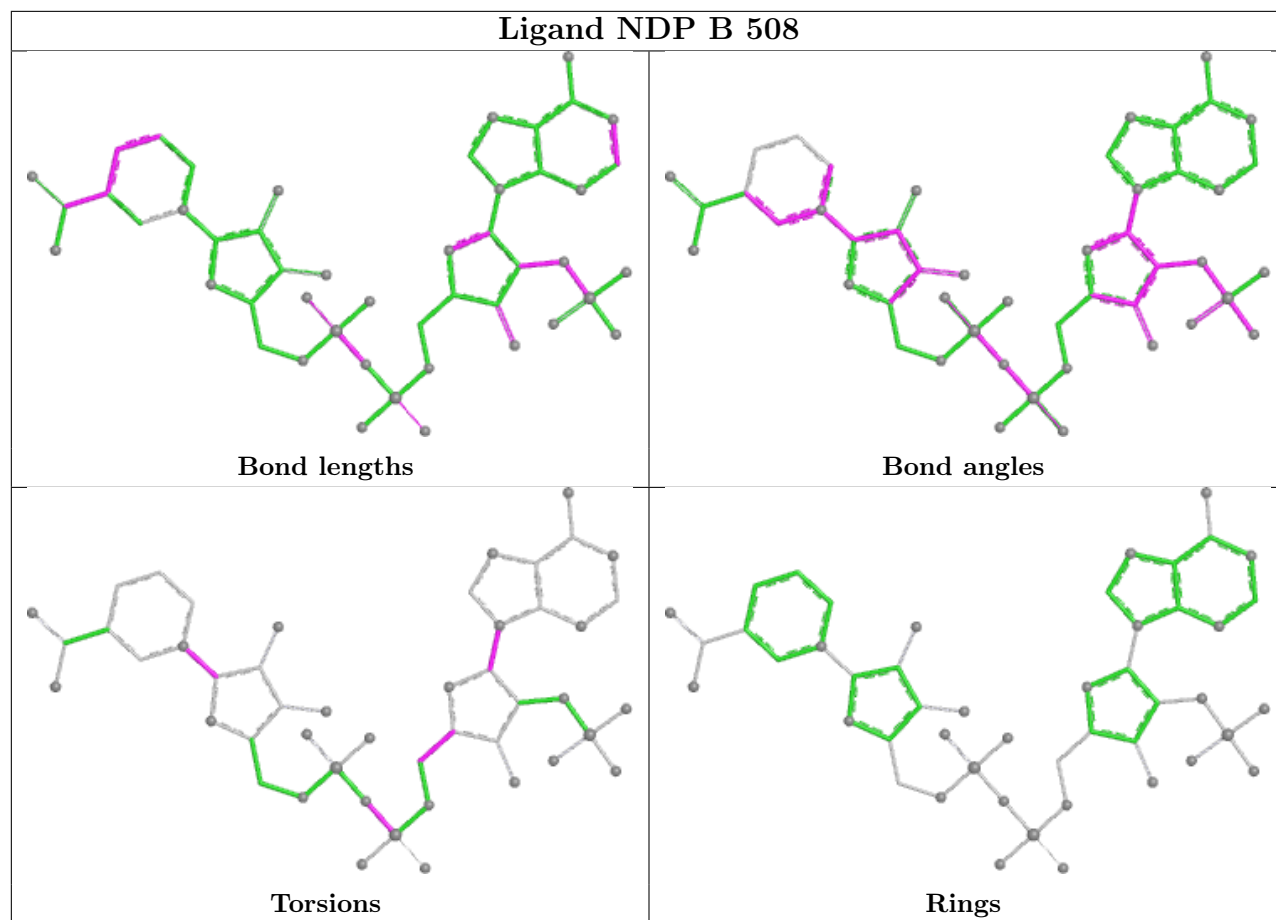
3 monomers are involved in 30 short contacts:

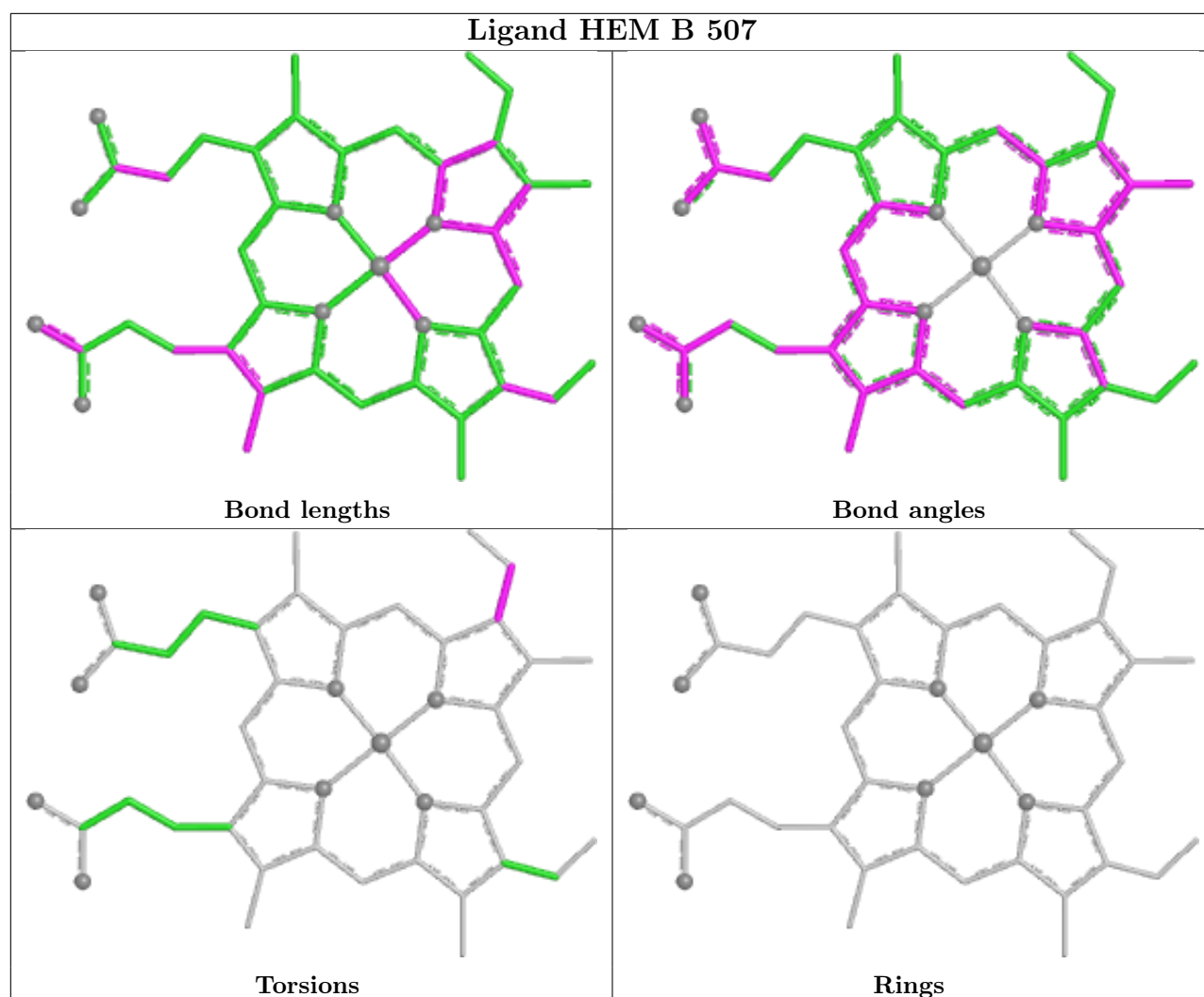
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 507 | HEM  | 16      | 0            |
| 3   | B     | 508 | NDP  | 3       | 0            |
| 2   | B     | 507 | HEM  | 11      | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.