Full wwPDB EM Validation Report ⓘ

Oct 30, 2023 – 03:20 PM EDT

PDB ID	:	8TLA
EMDB ID	:	EMD-41366
Title	:	Human Type 3 IP3 Receptor - Higher-Order Inhibited State - Symmetry Mate 1
Authors	:	Paknejad, N.; Sapuru, V.; Hite, R.K.
Deposited on	:	2023-07-26
Resolution	:	3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
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.

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

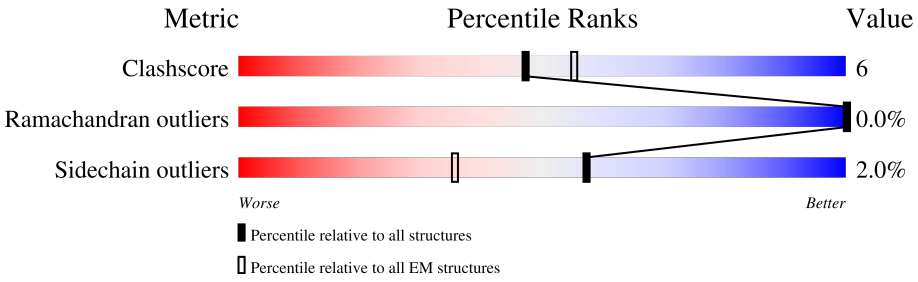
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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 (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2671	30% 61% 13% · 26%
1	B	2671	34% 61% 13% · 26%
1	C	2671	17% 65% 10% 25%
1	D	2671	14% 65% 11% 24%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 130502 atoms, of which 65433 are hydrogens and 0 are deuteriums.

In the tables below, 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.

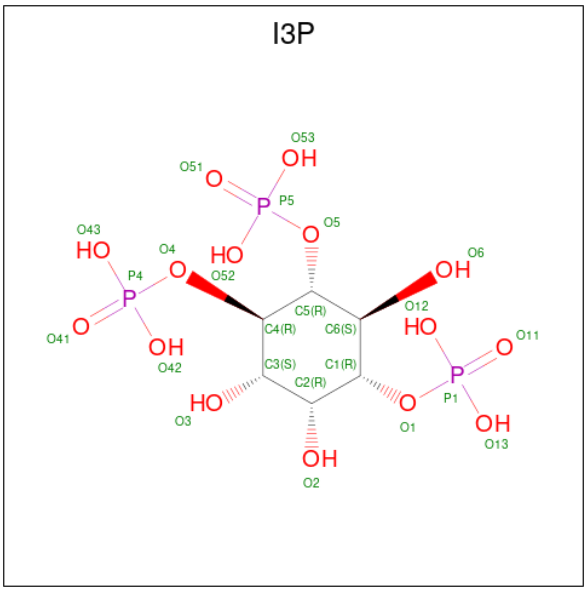
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1989	Total	C	H	N	O	S	0	0
			32350	10293	16244	2749	2960	104		
1	B	1987	Total	C	H	N	O	S	0	0
			32312	10283	16225	2743	2957	104		
1	C	2004	Total	C	H	N	O	S	0	0
			32571	10370	16344	2767	2986	104		
1	D	2034	Total	C	H	N	O	S	0	0
			32957	10480	16536	2807	3029	105		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).

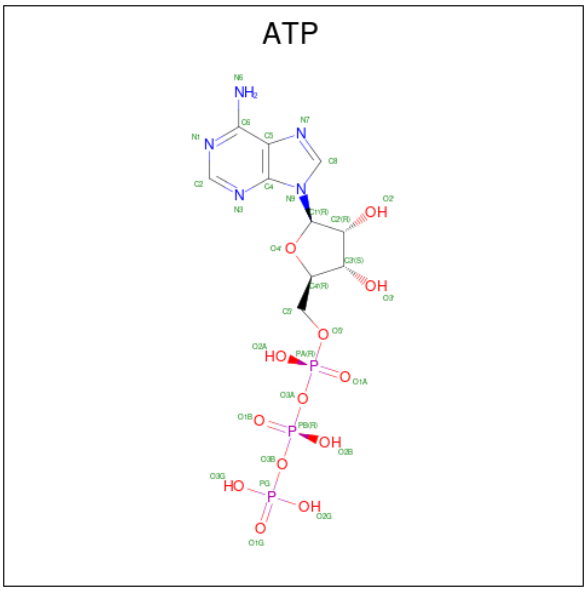


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



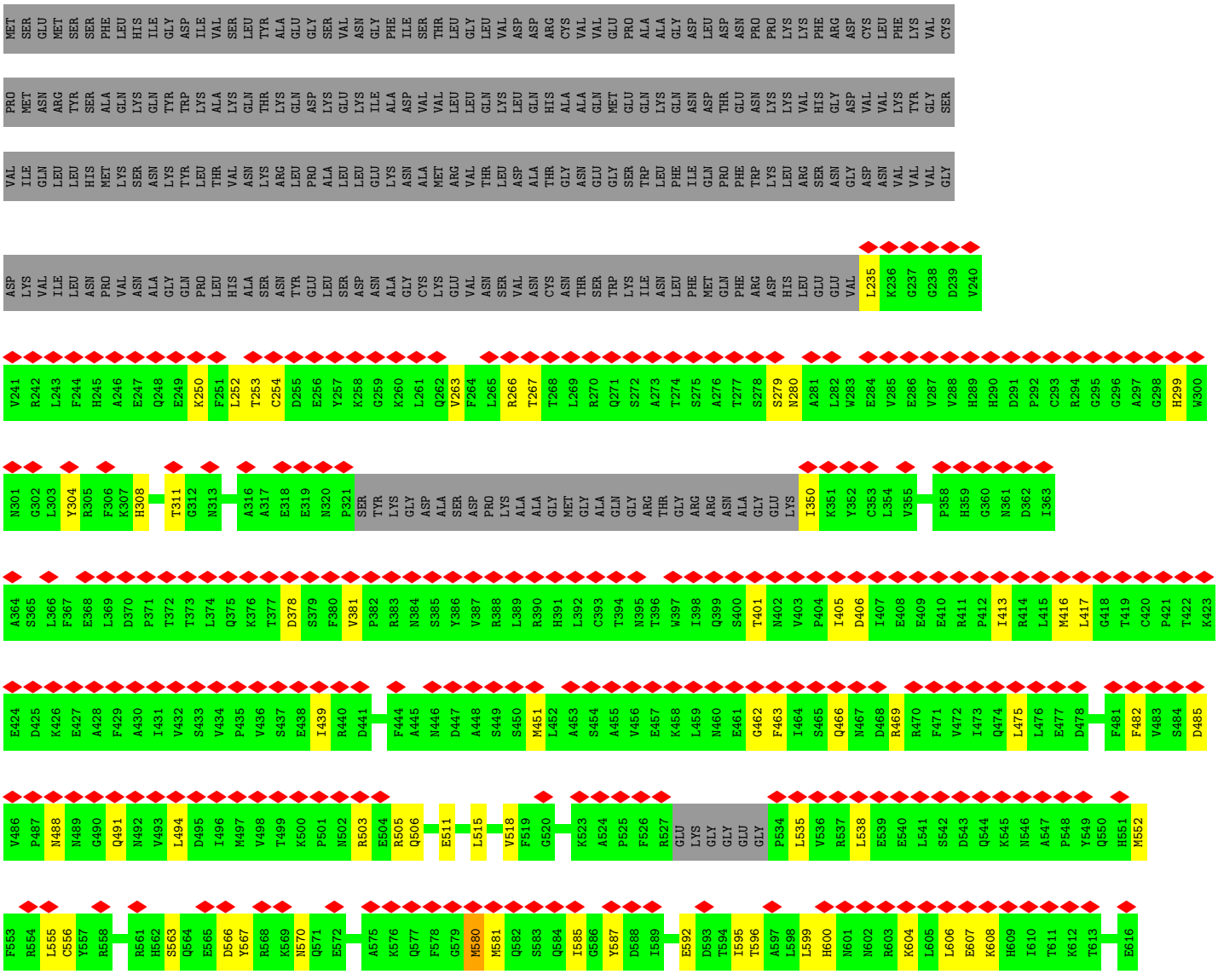
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

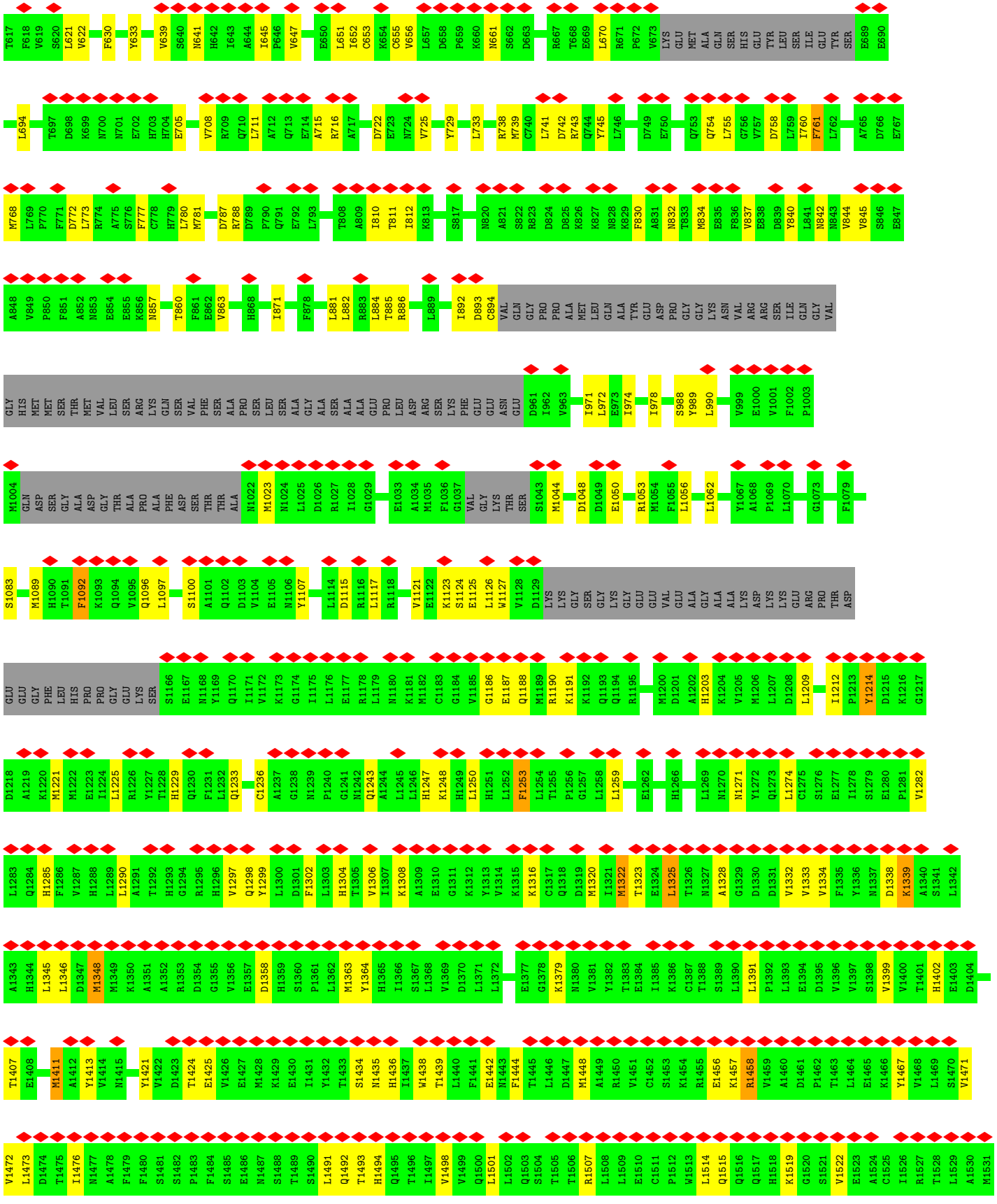
3 Residue-property plots (i)

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

Chain A:

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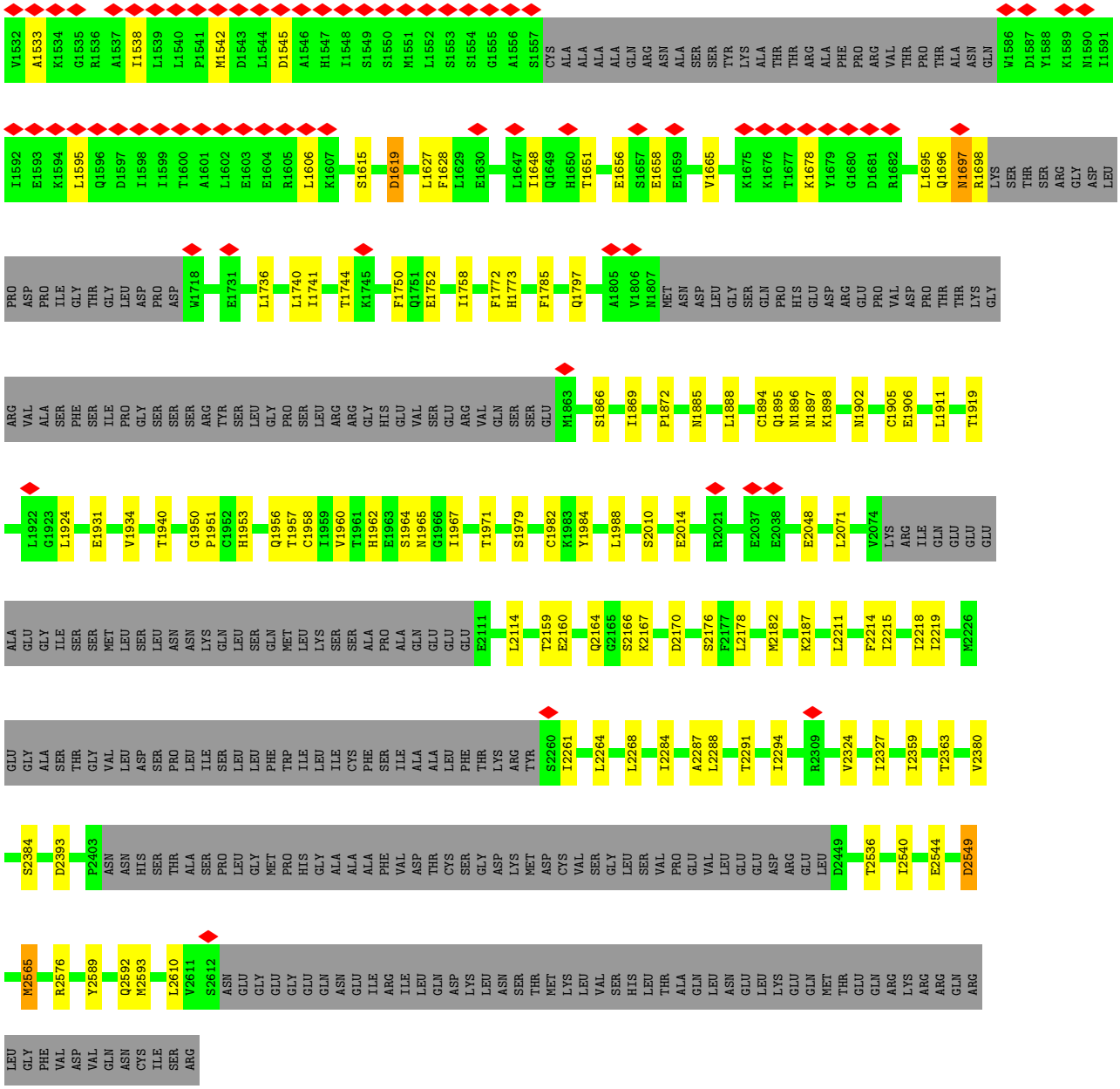
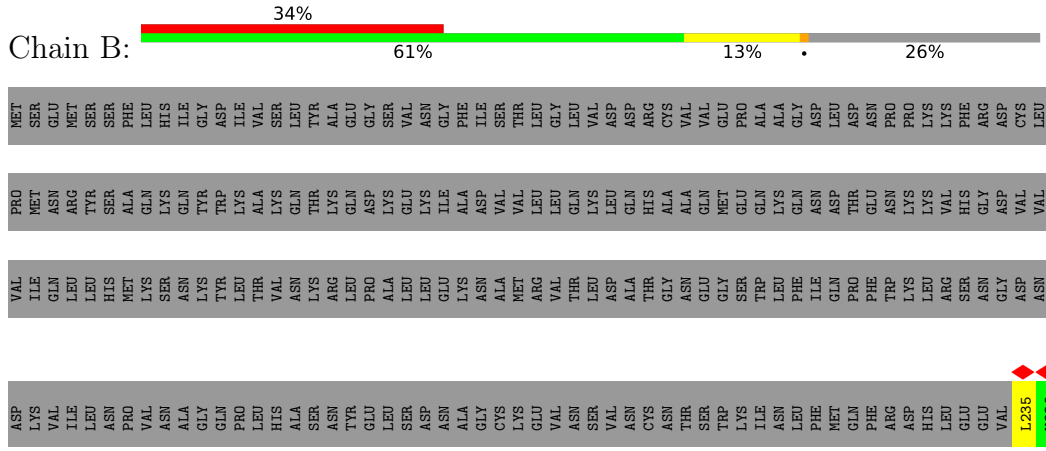
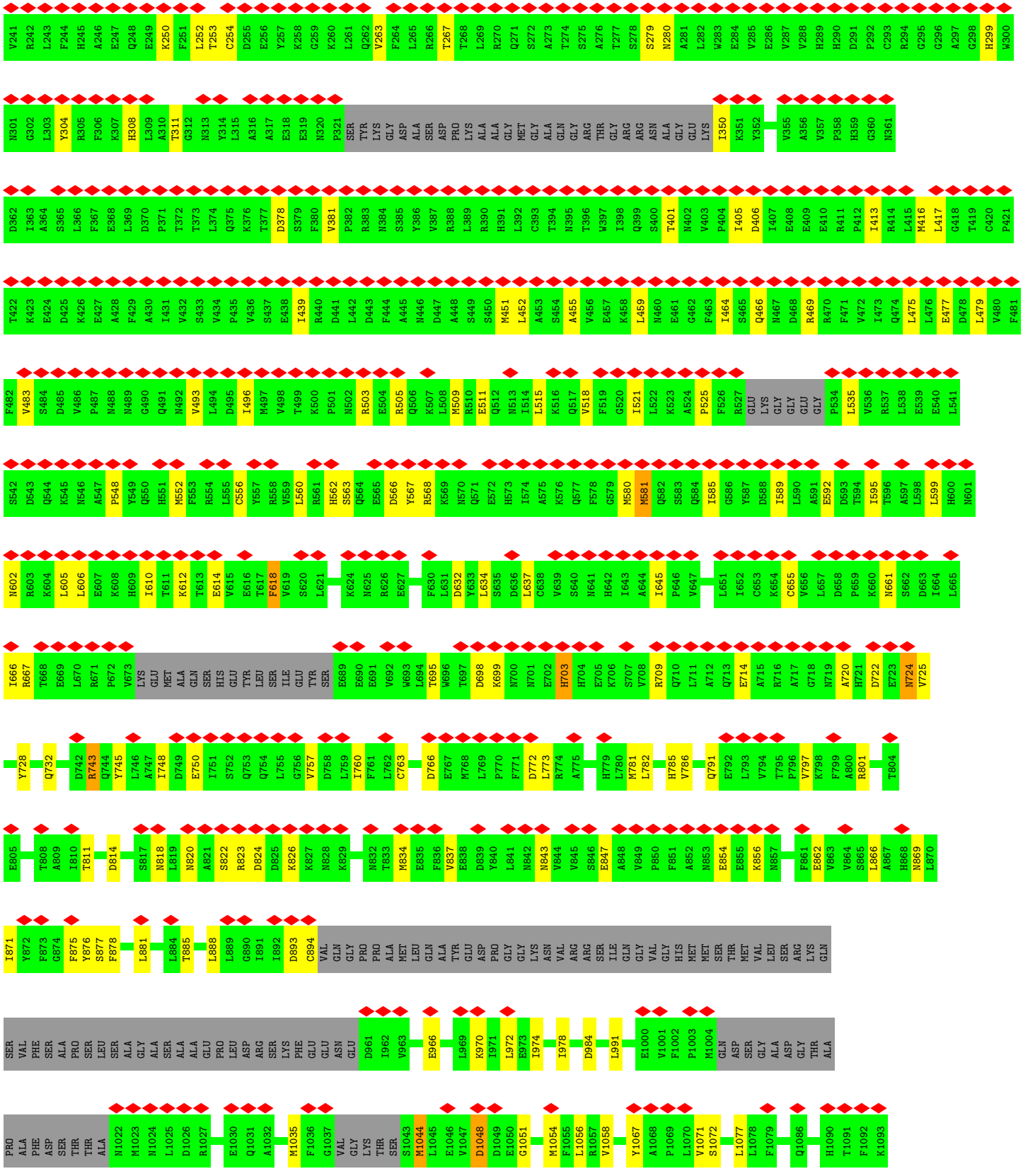
L694 T697 D698 K699 N700 N701 E702 H703 H704 E705 V708 R709 Q710 L711 A712 Q713 E714 A715 R716 A717 D722 E723 N724 V725 Y729 L733 R738 M739 C740 L741 D742 R743 Q744 Y745 L746 D749 E750 Q753 Q754 L755 G756 V757 D758 L759 I760 F761 L762 A765 D766 E767
M768 L769 P770 F771 D772 L773 R774 A775 S776 F777 C778 H779 L780 M781 D787 R788 D789 P790 Q791 E792 L793 T808 A809 I810 T811 I812 K813 S817 N820 A821 S822 R823 D824 D825 K826 K827 N828 K829 F830 A831 N832 T833 M834 E835 F836 V837 E838 D839 Y840 L841 N842 N843 V844 V845 S846 E847
A848 V849 P850 F851 A852 N853 E854 E855 K856 N857 T860 F861 E862 V863 H868 I871 F878 L881 L882 R883 L884 T885 R886 L889 I892 D893 C894 VAL GLN GLY PRO PRO ALA MET LEU GLN ALA TYR GLU ASP PRO GLY GLY LYS ASN VAL ARG ARG SER ILE GLN GLY VAL
GLY HIS MET MET SER THR MET VAL LEU SER ARG LYS GLN SER VAL PHE SER ALA PRO SER LEU SER ALA ALA GLY ALA SER ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961 I962 V963 I971 L972 E973 I974 I978 S988 Y989 L990 V999 E1000 V1001 F1002 P1003
M1004 GLN ASP SER GLY ALA ASP GLY THR ALA PRO ALA PHE ASP SER THR THR ALA N1022 M1023 N1024 L1025 D1026 R1027 I1028 G1029 E1033 A1034 M1035 F1036 G1037 VAL GLY LYS THR SER S1043 M1044 D1048 D1049 E1050 R1053 M1054 F1055 L1056 L1062 Y1067 A1068 P1069 L1070 G1073 F1079
S1083 M1089 H1090 T1091 F1092 K1093 Q1094 V1095 Q1096 L1097 S1100 A1101 Q1102 D1103 V1104 E1105 N1106 Y1107 L1114 D1115 R1116 L1117 R1118 V1121 E1122 K1123 S1124 E1125 L1126 W1127 V1128 D1129 LYS LYS GLY SER GLY LYS LYS GLY GLU GLU VAL GLU ALA GLY ALA ALA LYS ASP LYS LYS GLU ARG PRO THR ASP
GLU GLU GLY PHE LEU HIS PRO PRO GLY GLU LYS SER S1166 E1167 N1168 Y1169 Q1170 I1171 V1172 K1173 G1174 I1175 L1176 E1177 R1178 L1179 N1180 K1181 M1182 C1183 G1184 V1185 G1186 E1187 Q1188 M1189 R1190 K1191 K1192 Q1193 Q1194 R1195 M1200 D1201 A1202 H1203 K1204 V1205 M1206 L1207 D1208 L1209 I1212 P1213 Y1214 D1215 K1216 G1217
D1218 A1219 K1220 M1221 M1222 E1223 I1224 L1225 R1226 Y1227 T1228 H1229 Q1230 F1231 L1232 Q1233 C1236 A1237 G1238 N1239 P1240 G1241 N1242 Q1243 A1244 L1245 L1246 H1247 K1248 H1249 L1250 H1251 L1252 F1253 L1254 T1255 P1256 G1257 L1258 L1259 E1262 H1266 L1269 N1270 N1271 Y1272 Q1273 L1274 C1275 S1276 E1277 I1278 S1279 E1280 P1281 V1282
L1283 Q1284 H1285 F1286 V1287 H1288 L1289 L1290 A1291 T1292 H1293 G1294 R1295 H1296 V1297 Q1298 Y1299 L1300 D1301 F1302 L1303 H1304 T1305 V1306 I1307 K1308 A1309 E1310 G1311 K1312 Y1313 V1314 K1315 K1316 C1317 Q1318 D1319 M1320 I1321 M1322 T1323 E1324 L1325 T1326 N1327 A1328 G1329 D1330 D1331 V1332 V1333 V1334 F1335 Y1336 N1337 D1338 K1339 A1340 S1341 L1342
A1343 H1344 L1345 L1346 D1347 M1348 M1349 K1350 A1351 A1352 R1353 D1354 G1355 V1356 E1357 D1358 H1359 S1360 P1361 L1362 M1363 Y1364 H1365 I1366 S1367 L1368 V1369 D1370 L1371 L1372 E1377 G1378 K1379 N1380 V1381 Y1382 T1383 E1384 I1385 K1386 C1387 T1388 S1389 L1390 L1391 P1392 L1393 E1394 D1395 V1396 V1397 S1398 V1399 V1400 T1401 H1402 E1403 D1404
T1407 E1408 M1411 A1412 Y1413 V1414 N1415 Y1421 V1422 D1423 T1424 E1425 V1426 E1427 M1428 K1429 E1430 I1431 Y1432 T1433 S1434 N1435 H1436 I1437 W1438 T1439 L1440 F1441 E1442 N1443 F1444 T1445 L1446 D1447 M1448 A1449 R1450 V1451 C1452 S1453 K1454 R1455 E1456 K1457 R1458 V1459 A1460 D1461 P1462 T1463 L1464 E1465 K1466 Y1467 V1468 L1469 S1470 V1471
V1472 L1473 D1474 T1475 I1476 N1477 A1478 F1479 F1480 S1481 S1482 P1483 F1484 S1485 E1486 N1487 S1488 T1489 S1490 L1491 Q1492 T1493 H1494 Q1495 T1496 I1497 V1498 V1499 Q1500 L1501 L1502 Q1503 S1504 T1505 T1506 R1507 L1508 L1509 E1510 C1511 P1512 W1513 L1514 Q1515 Q1516 Q1517 H1518 K1519 G1520 S1521 V1522 E1523 A1524 C1525 I1526 R1527 T1528 L1529 A1530 M1531



• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

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N301 G302 L303 Y304 R305 F306 K307 H308 L309 A310 T311 G312 N313 Y314 L315 A316 A317 E318 E319 N320 P321 SER TYR LYS GLY ASP ALA SER ASP PRO LYS ALA ALA GLY MET GLY ALA GLN GLY ARG THR GLY ARG ARG ASN ALA GLY GLU LYS I350 K351 Y352 V355 A356 V357 P358 H359 G360 N361
D362 I363 A364 S365 L366 F367 E368 L369 D370 P371 T372 T373 L374 Q375 K376 T377 D378 S379 F380 V381 P382 R383 N384 S385 Y386 V387 R388 L389 R390 H391 L392 C393 T394 N395 T396 W397 I398 Q399 S400 T401 N402 V403 P404 I405 D406 I407 E408 E409 E410 R411 P412 I413 R414 L415 M416 L417 G418 T419 C420 P421
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F482 V483 S484 D485 V486 P487 N488 N489 G490 Q491 N492 V493 L494 D495 I496 M497 V498 T499 K500 P501 N502 R503 E504 R505 Q506 K507 L508 M509 R510 E511 Q512 N513 I514 L515 K516 Q517 V518 F519 G520 I521 L522 K523 A524 P525 F526 R527 GLU LYS GLY GLU GLY P534 L535 V536 R537 L538 E539 E540 L541
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N602 R603 K604 L605 L606 E607 K608 H609 I610 T611 K612 T613 E614 V615 E616 T617 F618 V619 S620 L621 K624 N625 R626 E627 F630 L631 D632 Y633 L634 S635 D636 L637 C638 V639 S640 N641 H642 I643 A644 I645 P646 V647 L651 I652 C653 K654 C655 V656 L657 D658 P659 K660 N661 S662 D663 I664 L665
I666 R667 T668 E669 L670 R671 P672 V673 LYS GLU MET ALA GLN SER HIS GLU TYR LEU SER ILE GLU TYR SER E689 E690 E691 V692 W693 L694 T695 W696 T697 D698 K699 N700 N701 E702 H703 H704 E705 K706 S707 V708 R709 Q710 L711 A712 Q713 E714 A715 R716 A717 G718 N719 A720 H721 D722 E723 N724 V725
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E805 T808 A809 I810 T811 D814 S817 N818 L819 N820 A821 S822 R823 D824 D825 K826 K827 N828 K829 N832 T833 M834 E835 F836 V837 E838 D839 Y840 L841 N842 N843 V844 V845 S846 E847 A848 V849 P850 F851 A852 N853 E854 E855 K856 N857 F861 E862 V863 V864 S865 L866 A867 H868 N869 L870
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SER VAL PHE SER ALA PRO SER LEU SER ALA GLY ALA SER ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961 I962 V963 E966 L969 K970 I971 L972 E973 I974 I978 D984 L991 E1000 V1001 F1002 P1003 M1004 GLN ASP SER GLY ALA ASP GLY THR ALA
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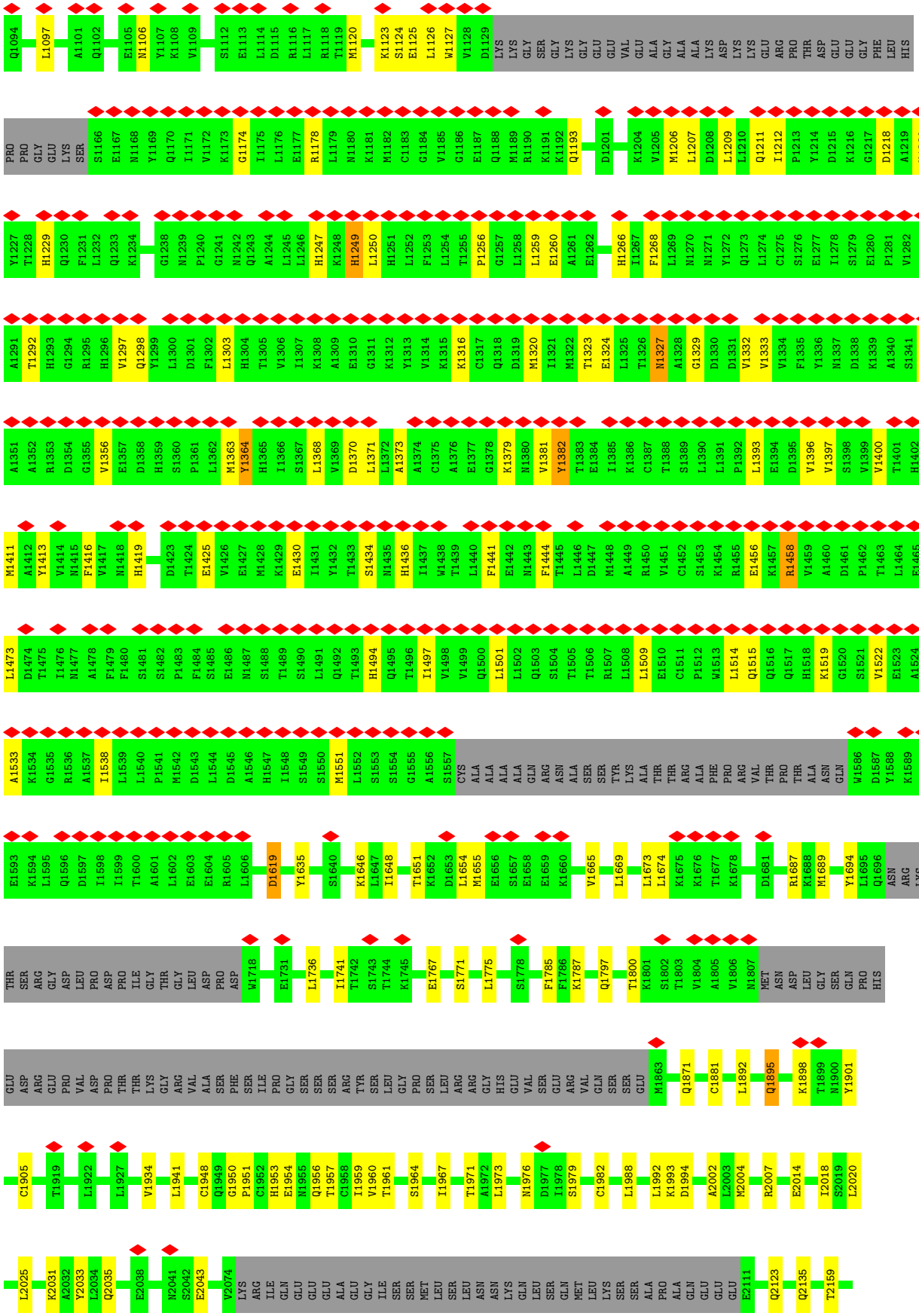
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PRO PRO GLY GLU LYS SER S1166 E1167 N1168 Y1169 Q1170 I1171 V1172 K1173 G1174 I1175 L1176 E1177 R1178 L1179 N1180 K1181 M1182 C1183 G1184 V1185 G1186 E1187 Q1188 M1189 R1190 K1191 K1192 Q1193 D1201 K1204 V1205 M1206 L1207 D1208 L1209 L1210 Q1211 I1212 P1213 Y1214 D1215 K1216 G1217 D1218 A1219 K1220 M1221 M1222 E1223 I1224 L1225 R1226
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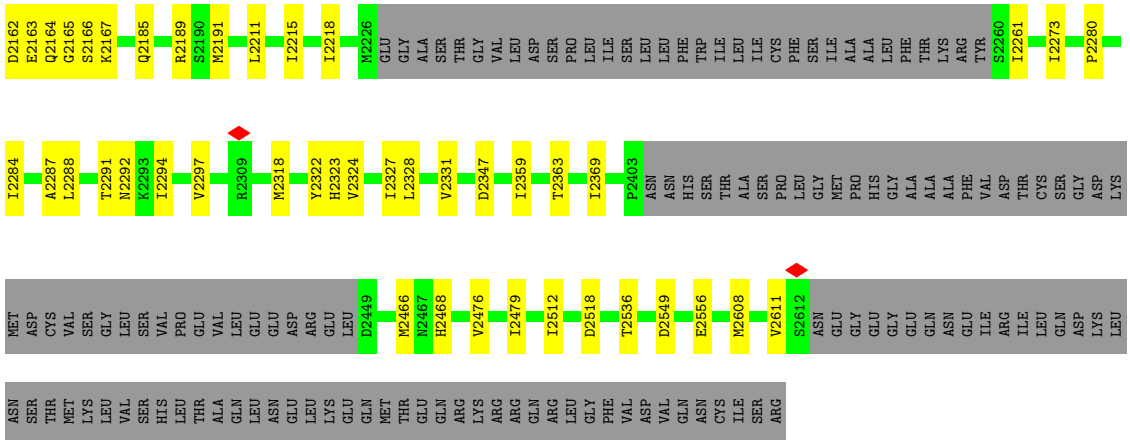
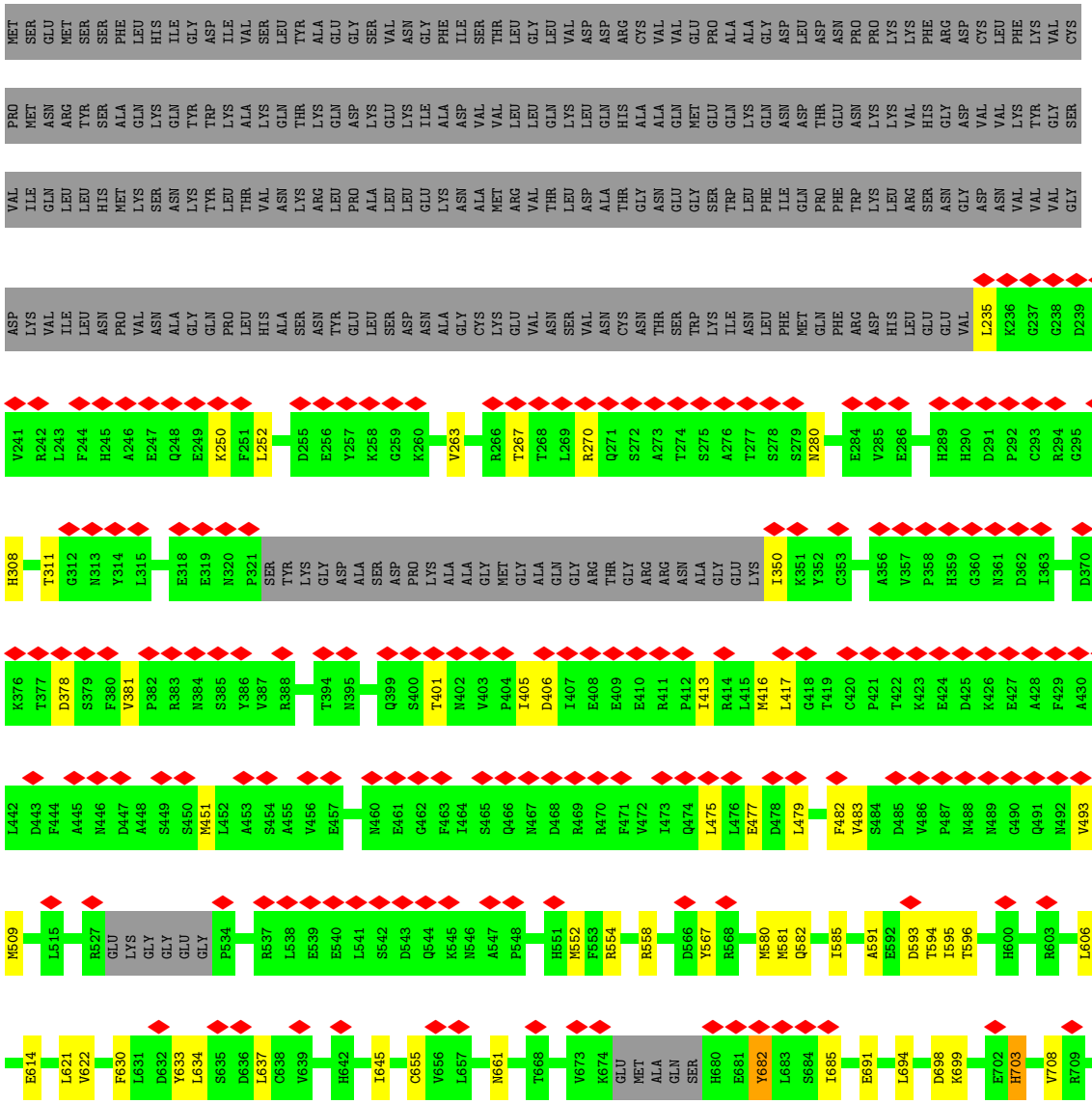
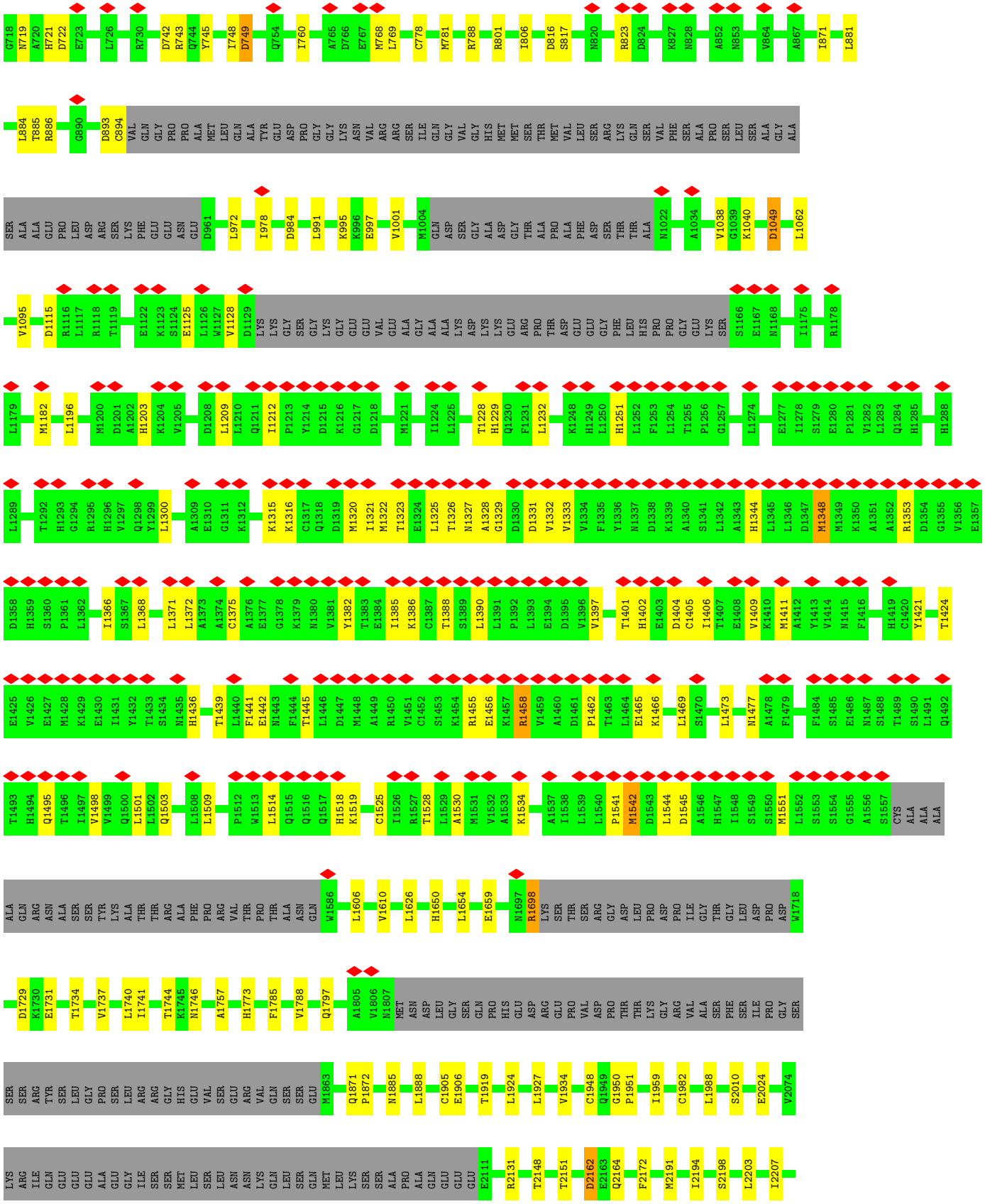
L1473 D1474 T1475 I1476 N1477 A1478 F1479 F1480 S1481 S1482 P1483 F1484 S1485 E1486 N1487 S1488 T1489 S1490 L1491 Q1492 T1493 H1494 Q1495 T1496 I1497 V1498 V1499 Q1500 L1501 L1502 Q1503 S1504 T1505 T1506 R1507 L1508 L1509 E1510 C1511 P1512 W1513 L1514 Q1515 Q1516 Q1517 H1518 K1519 G1520 S1521 V1522 E1523 A1524 C1525 I1526 R1527 T1528 L1529 A1530 M1531 V1532
A1533 K1534 G1535 R1536 A1537 I1538 L1539 L1540 P1541 M1542 D1543 L1544 D1545 A1546 H1547 I1548 S1549 S1550 M1551 L1552 S1553 S1554 G1555 A1556 S1557 CYS ALA ALA ALA ALA GLN ARG ASN ALA SER SER TYR LYS ALA THR THR ARG ALA PHE PRO ARG VAL THR PRO THR ALA ASN GLN W1586 D1587 Y1588 K1589 N1590 I1591 I1592
E1593 K1594 L1595 Q1596 D1597 I1598 I1599 T1600 A1601 L1602 E1603 E1604 R1605 L1606 D1619 Y1635 S1640 K1646 L1647 I1648 T1651 K1652 D1653 L1654 M1655 E1656 S1657 E1658 E1659 K1660 V1665 L1669 L1673 L1674 K1675 K1676 T1677 K1678 D1681 R1687 K1688 M1689 Y1694 L1695 Q1696 ASN ARG LYS SER
THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO ASP W1718 E1731 L1736 I1741 T1742 S1743 T1744 K1745 E1767 S1771 L1775 S1778 F1785 F1786 K1787 Q1797 T1800 K1801 S1802 T1803 V1804 A1805 V1806 N1807 MET ASN ASP LEU GLY SER GLN PRO HIS
GLU ASP ARG GLU PRO VAL ASP PRO THR THR LYS GLY ARG VAL ALA SER PHE SER ILE PRO GLY SER SER SER ARG TYR SER LEU GLY PRO SER LEU ARG ARG GLY HIS GLU VAL SER GLU ARG VAL GLN SER SER GLU M1863 Q1871 C1881 L1892 Q1895 K1898 T1899 N1900 Y1901
C1905 T1919 L1922 L1927 V1934 L1941 C1948 Q1949 G1950 P1951 C1952 H1953 E1954 N1955 Q1956 T1957 C1958 I1959 V1960 T1961 S1964 I1967 T1971 A1972 L1973 N1976 D1977 I1978 S1979 C1982 L1988 L1992 K1993 D1994 A2002 L2003 M2004 R2007 E2014 I2018 S2019 L2020
L2025 K2031 A2032 Y2033 L2034 Q2035 E2038 N2041 S2042 E2043 V2074 LYS ARG ILE GLN GLU GLU GLU ALA GLU GLY ILE SER SER MET LEU SER LEU ASN ASN LYS GLN LEU SER GLN MET LEU LYS SER SER ALA PRO ALA GLN GLU GLU GLU E2111 Q2123 Q2135 T2159



• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

Chain C:

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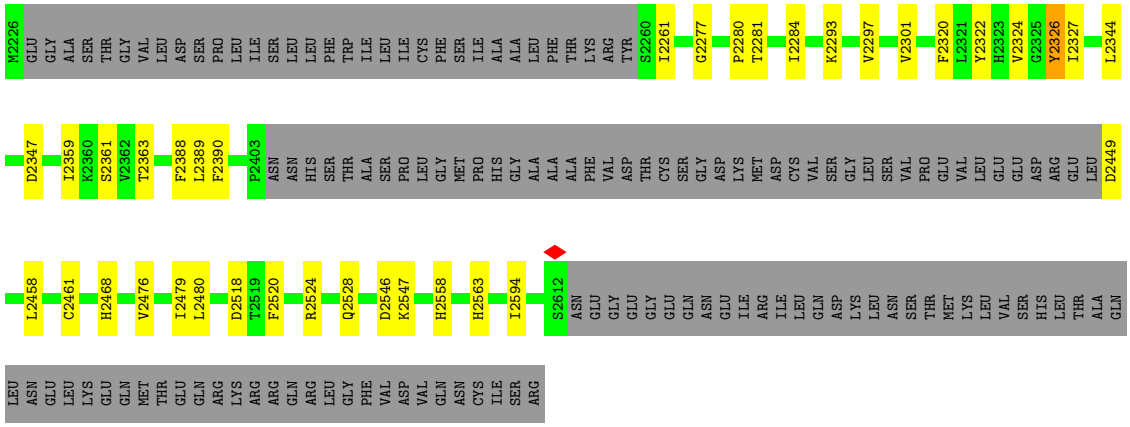
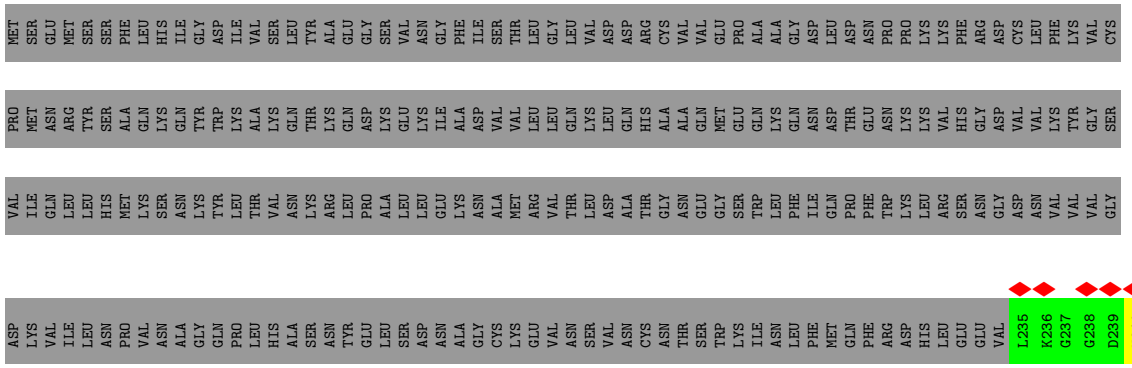
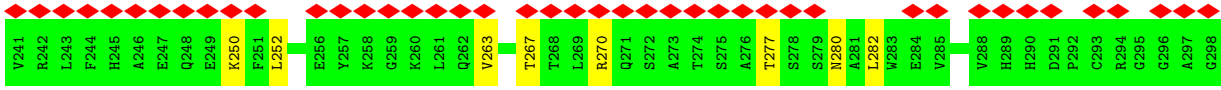
L884 T885 R886 G890 D893 C894 VAL GLN GLY PRO PRO ALA MET LEU GLN ALA TYR GLU ASP PRO GLY GLY LYS ASN VAL ARG ARG SER ILE GLN GLN GLY VAL GLY HIS MET MET SER THR MET VAL LEU SER ARG LYS GLN SER VAL PHE SER ALA PRO SER LEU SER ALA GLY ALA
SER ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961 L972 I978 D984 L991 K995 K996 E997 V1001 M1004 GLN ASP SER GLY ALA ASP GLY THR ALA PRO ALA PHE ASP SER THR THR ALA N1022 A1034 V1038 G1039 K1040 D1049 L1062
V1095 D1115 R1116 L1117 R1118 T1119 E1122 K1123 S1124 E1125 L1126 W1127 V1128 D1129 LYS LYS GLY SER GLY LYS GLY GLU GLU VAL GLU ALA GLY ALA ALA LYS ASP LYS LYS GLU ARG PRO THR ASP GLU GLU GLY PHE LEU HIS PRO PRO GLY GLU LYS SER S1166 E1167 N1168 I1175 R1178
L1179 M1182 L1196 M1200 D1201 A1202 H1203 K1204 V1205 D1208 L1209 L1210 Q1211 I1212 P1213 Y1214 D1215 K1216 G1217 D1218 M1221 I1224 L1225 T1228 H1229 Q1230 F1231 L1232 K1248 H1249 L1250 H1251 L1252 F1253 L1254 T1255 P1256 G1257 L1274 E1277 I1278 S1279 E1280 P1281 V1282 L1283 Q1284 H1285 H1288
L1289 T1292 H1293 G1294 R1295 H1296 V1297 Q1298 Y1299 L1300 A1309 E1310 G1311 K1312 K1315 K1316 C1317 Q1318 D1319 M1320 I1321 M1322 T1323 E1324 L1325 T1326 N1327 A1328 G1329 D1330 D1331 V1332 V1333 V1334 F1335 Y1336 N1337 D1338 K1339 A1340 S1341 L1342 A1343 H1344 L1345 L1346 D1347 M1348 M1349 K1350 A1351 A1352 R1353 D1354 G1355 V1356 E1357
D1358 H1359 S1360 P1361 L1362 I1366 S1367 L1368 L1371 L1372 A1373 A1374 C1375 A1376 E1377 G1378 K1379 N1380 V1381 Y1382 T1383 E1384 I1385 K1386 C1387 T1388 S1389 L1390 L1391 P1392 L1393 E1394 D1395 V1396 V1397 T1401 H1402 E1403 D1404 C1405 I1406 T1407 E1408 V1409 K1410 M1411 A1412 Y1413 V1414 N1415 F1416 H1419 C1420 Y1421 T1424
E1425 V1426 E1427 M1428 K1429 E1430 I1431 Y1432 T1433 S1434 N1435 H1436 T1439 L1440 F1441 E1442 N1443 F1444 T1445 L1446 D1447 M1448 A1449 R1450 V1451 C1452 S1453 K1454 R1455 E1456 K1457 R1458 V1459 A1460 D1461 P1462 T1463 L1464 E1465 K1466 L1469 S1470 L1473 N1477 A1478 F1479 F1484 S1485 E1486 N1487 S1488 T1489 S1490 L1491 Q1492
T1493 H1494 Q1495 T1496 I1497 V1498 V1499 Q1500 L1501 L1502 Q1503 L1508 L1509 P1512 W1513 L1514 Q1515 Q1516 Q1517 H1518 K1519 C1525 I1526 R1527 T1528 L1529 A1530 M1531 V1532 A1533 K1534 A1537 I1538 L1539 L1540 P1541 M1542 D1543 L1544 D1545 A1546 H1547 I1548 S1549 S1550 M1551 L1552 S1553 S1554 G1555 A1556 S1557 CYS ALA ALA ALA
ALA GLN ARG ASN ALA SER SER TYR LYS ALA THR THR ARG ALA PHE PRO ARG VAL THR PRO THR ALA ASN GLN W1586 L1606 V1610 L1626 H1650 L1654 E1659 N1697 R1698 LYS SER THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO ASP W1718
D1729 K1730 E1731 T1734 V1737 L1740 I1741 T1744 K1745 N1746 A1757 H1773 F1785 V1788 Q1797 A1805 V1806 N1807 MET ASN ASP LEU GLY SER GLN PRO HIS GLU ASP ARG GLU PRO VAL ASP PRO THR THR LYS GLY ARG VAL ALA SER PHE SER ILE PRO GLY SER
SER SER ARG TYR SER LEU GLY PRO SER LEU ARG ARG GLY HIS GLU VAL SER GLU ARG VAL GLN SER SER GLU M1863 Q1871 P1872 N1885 L1888 C1905 E1906 T1919 L1924 L1927 V1934 C1948 Q1949 G1950 P1951 I1959 C1982 L1988 S2010 E2024 V2074
LYS ARG ILE GLN GLU GLU GLU ALA GLU GLY ILE SER SER MET LEU SER LEU ASN ASN LYS GLN LEU SER GLN MET LEU LYS SER SER ALA PRO ALA GLN GLU GLU GLU E2111 R2131 T2148 T2151 D2162 E2163 Q2164 F2172 M2191 I2194 S2198 L2203 I2207

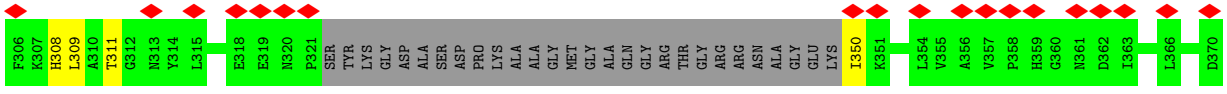


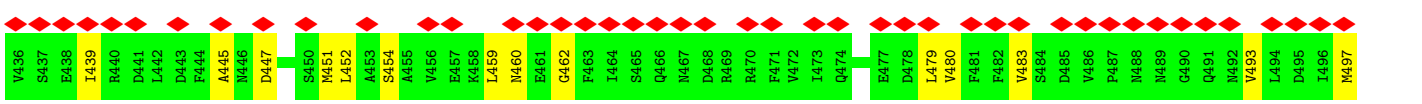
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

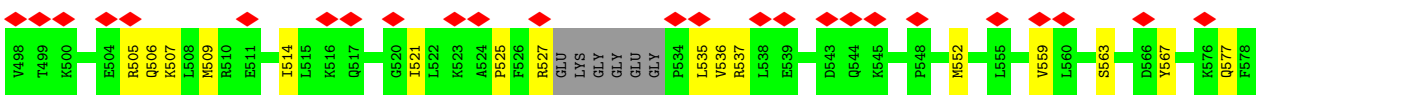
Chain D:

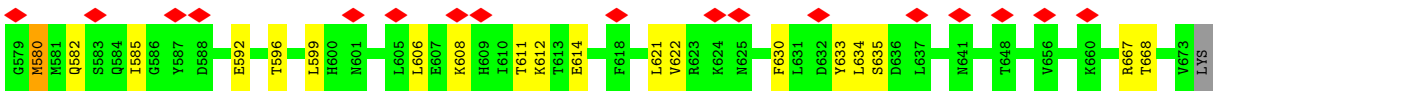


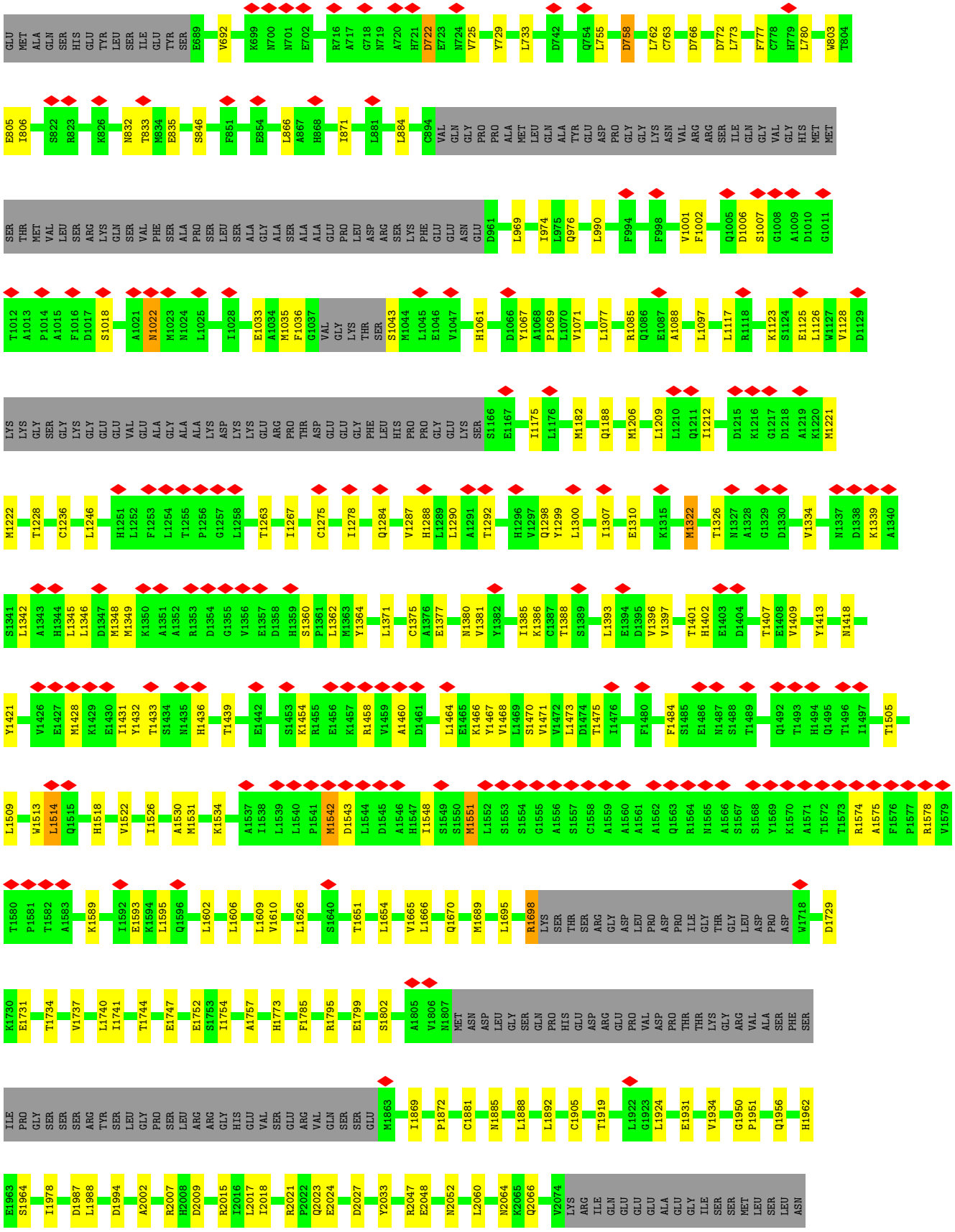








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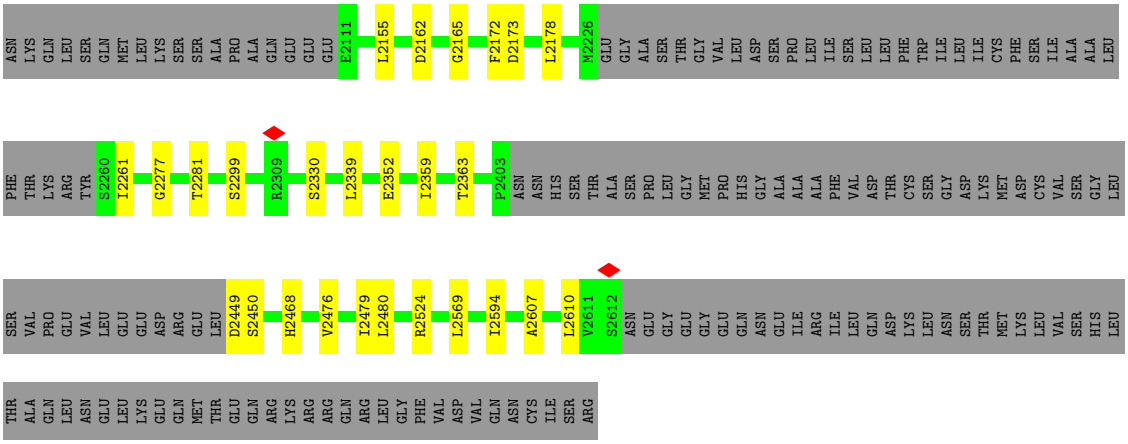
E805 I806 S822 R823 K826 N832 T833 H834 E835 S846 F851 E854 L866 A867 H868 I871 L881 L884 C894 VAL GLN GLY PRO PRO ALA MET LEU GLN ALA TYR GLU ASP PRO GLY GLY LYS ASN VAL ARG ARG SER ILE GLN GLY VAL GLY HIS MET MET
SER THR MET VAL LEU SER ARG LYS GLN SER VAL PHE SER ALA PRO SER LEU SER ALA GLY ALA SER ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961 L969 I974 L975 Q976 L990 F994 F998 V1001 F1002 Q1005 D1006 S1007 G1008 A1009 D1010 G1011
T1012 A1013 P1014 A1015 F1016 D1017 S1018 A1021 N1022 M1023 N1024 L1025 I1028 E1033 A1034 M1035 F1036 G1037 VAL GLY LYS THR SER S1043 M1044 L1045 E1046 V1047 H1061 D1066 Y1067 A1068 P1069 L1070 V1071 L1077 R1085 Q1086 E1087 A1088 L1097 L1117 R1118 K1123 S1124 E1125 L1126 W1127 V1128 D1129
LYS LYS GLY SER GLY LYS GLY GLU GLU VAL GLU ALA GLY ALA ALA LYS ASP LYS LYS GLU ARG PRO THR ASP GLU GLU GLY PHE LEU HIS PRO PRO GLY GLU LYS SER S1166 E1167 I1175 L1176 M1182 Q1188 M1206 L1209 L1210 Q1211 I1212 D1215 K1216 G1217 D1218 A1219 K1220 M1221
M1222 T1228 C1236 L1246 H1251 L1252 F1253 L1254 T1255 P1256 G1257 L1258 T1263 I1267 C1275 I1278 Q1284 V1287 H1288 L1289 L1290 A1291 T1292 H1296 V1297 Q1298 Y1299 L1300 I1307 E1310 K1315 M1322 T1326 N1327 A1328 G1329 D1330 V1334 N1337 D1338 K1339 A1340
S1341 L1342 A1343 H1344 L1345 L1346 D1347 M1348 M1349 K1350 A1351 A1352 R1353 D1354 G1355 V1356 E1357 D1358 H1359 S1360 P1361 L1362 M1363 Y1364 L1371 C1375 A1376 E1377 N1380 V1381 Y1382 I1385 K1386 C1387 T1388 S1389 L1393 E1394 D1395 V1396 V1397 T1401 H1402 E1403 D1404 T1407 E1408 V1409 Y1413 N1418
Y1421 V1426 E1427 M1428 K1429 E1430 I1431 Y1432 T1433 S1434 N1435 H1436 T1439 E1442 S1453 K1454 R1455 E1456 K1457 R1458 V1459 A1460 D1461 L1464 E1465 K1466 Y1467 V1468 L1469 S1470 V1471 V1472 L1473 D1474 T1475 I1476 F1480 F1484 S1485 E1486 N1487 S1488 T1489 Q1492 T1493 H1494 Q1495 T1496 I1497 T1505
L1509 W1513 L1514 Q1515 H1518 V1522 I1526 A1530 M1531 K1534 A1537 I1538 L1539 L1540 P1541 M1542 D1543 L1544 D1545 A1546 H1547 I1548 S1549 S1550 M1551 L1552 S1553 S1554 G1555 A1556 S1557 C1558 A1559 A1560 A1561 A1562 Q1563 R1564 N1565 A1566 S1567 S1568 Y1569 K1570 A1571 T1572 T1573 R1574 A1575 F1576 P1577 R1578 V1579
T1580 P1581 T1582 A1583 K1589 I1592 E1593 K1594 L1595 Q1596 L1602 L1606 L1609 V1610 L1626 S1640 T1651 L1654 V1665 L1666 Q1670 M1689 L1695 R1698 LYS SER THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO ASP W1718 D1729
K1730 E1731 T1734 V1737 L1740 I1741 T1744 E1747 E1752 S1753 I1754 A1757 H1773 F1785 R1795 E1799 S1802 A1805 V1806 N1807 MET ASN ASP LEU GLY SER GLN PRO HIS GLU ASP ARG GLU PRO VAL ASP PRO THR THR LYS GLY ARG VAL ALA SER PHE SER
ILE PRO GLY SER SER SER ARG TYR SER LEU GLY PRO SER LEU ARG ARG GLY HIS GLU VAL SER GLU ARG VAL GLN SER SER GLU M1863 I1869 P1872 C1881 N1885 L1888 L1892 C1905 T1919 L1922 G1923 L1924 E1931 V1934 G1950 P1951 Q1956 H1962
E1963 S1964 I1978 D1987 L1988 D1994 A2002 R2007 H2008 D2009 R2015 I2016 L2017 I2018 R2021 P2022 Q2023 E2024 D2027 Y2033 R2047 E2048 N2052 L2060 N2064 K2065 Q2066 V2074 LYS ARG ILE GLN GLU GLU GLU ALA GLU GLY ILE SER SER MET LEU SER LEU ASN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PHE THR LYS ARG TYR S2260 I2261 G2277 T2281 S2299 R2309 S2330 L2339 E2352 I2359 T2363 P2403 ASN ASN HIS SER THR ALA SER PRO LEU GLY MET PRO HIS GLY ALA ALA ALA PHE VAL ASP THR CYS SER GLY ASP LYS MET ASP CYS VAL SER GLY LEU
SER VAL PRO GLU VAL LEU GLU GLU ASP ARG GLU LEU D2449 S2450 H2468 V2476 I2479 L2480 R2524 L2569 I2594 A2607 L2610 V2611 S2612 ASN GLU GLY GLU GLY GLU GLN ASN GLU ILE ARG ILE LEU GLN ASP LYS LEU ASN SER THR MET LYS LEU VAL SER HIS LEU
THR ALA GLN LEU ASN GLU LEU LEU LYS GLU GLN MET THR GLU GLN ARG LYS ARG ARG GLN ARG LEU GLY PHE VAL ASP VAL GLN ASN CYS ILE SER ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85139	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	66	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4300	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.885	Depositor
Minimum map value	-0.441	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	422.912, 422.912, 422.912	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ATP, I3P, CA

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	0.25	0/16403	0.46	0/22156
1	B	0.25	0/16384	0.46	0/22131
1	C	0.24	0/16528	0.45	0/22327
1	D	0.25	0/16726	0.46	0/22603
All	All	0.25	0/66041	0.46	0/89217

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	16106	16244	16243	235	0
1	B	16087	16225	16224	236	0
1	C	16227	16344	16353	178	0
1	D	16421	16536	16535	194	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	9	9	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	9	9	1	0
3	C	24	9	9	1	0
3	D	24	9	9	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	12	12	0	0
5	B	31	12	12	0	0
5	C	31	12	12	0	0
5	D	31	12	12	0	0
All	All	65069	65433	65439	837	0

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 6.

All (837) 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:D:1962:HIS:HD1	1:D:1964:SER:HG	1.08	0.99
1:A:1962:HIS:HD1	1:A:1964:SER:HG	1.06	0.96
1:C:885:THR:HG22	1:C:978:ILE:HD13	1.48	0.93
1:A:729:TYR:CE1	1:A:733:LEU:HD21	2.04	0.92
1:C:2203:LEU:O	1:C:2207:ILE:HD12	1.73	0.89
1:D:445:ALA:HB1	1:D:514:ILE:HD11	1.56	0.86
1:B:885:THR:HG22	1:B:978:ILE:HD13	1.58	0.84
1:A:503:ARG:NH2	1:A:566:ASP:O	2.11	0.83
1:D:1729:ASP:OD1	1:D:1734:THR:OG1	1.96	0.83
1:B:2163:GLU:OE2	1:B:2163:GLU:N	2.13	0.82
1:C:611:THR:OG1	1:C:614:GLU:OE1	1.96	0.82
1:B:1767:GLU:N	1:B:1767:GLU:OE1	2.13	0.80
1:A:1740:LEU:O	1:A:1744:THR:HG22	1.81	0.80
1:C:593:ASP:OD2	1:C:594:THR:N	2.15	0.80
1:A:1658:GLU:N	1:A:1658:GLU:OE1	2.15	0.79
1:B:1895:GLN:NE2	1:B:1901:TYR:O	2.16	0.78
1:A:655:CYS:O	1:A:661:ASN:ND2	2.17	0.78
1:C:698:ASP:OD1	1:C:699:LYS:N	2.16	0.78
1:A:1302:PHE:O	1:A:1306:VAL:HG23	1.84	0.77
1:C:2518:ASP:O	1:D:2524:ARG:NH2	2.18	0.77
1:C:2518:ASP:OD1	1:D:2524:ARG:NH2	2.17	0.77
1:D:1288:HIS:O	1:D:1292:THR:HG23	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ARG:NH2	3:C:3002:I3P:O51	2.19	0.76
1:C:691:GLU:N	1:C:691:GLU:OE1	2.18	0.76
1:D:2048:GLU:N	1:D:2048:GLU:OE1	2.18	0.76
1:B:503:ARG:NH2	1:B:566:ASP:O	2.19	0.75
1:B:2287:ALA:O	1:B:2291:THR:HG23	1.86	0.75
1:A:1056:LEU:HD22	1:A:1627:LEU:HD13	1.69	0.75
1:B:2043:GLU:N	1:B:2043:GLU:OE2	2.19	0.74
1:C:2322:TYR:OH	1:C:2347:ASP:OD1	2.04	0.74
1:D:1418:ASN:OD1	1:D:1475:THR:OG1	2.03	0.74
1:A:2164:GLN:NE2	1:B:2556:GLU:OE2	2.19	0.74
1:A:694:LEU:HD21	1:A:729:TYR:CD2	2.23	0.74
1:B:1954:GLU:OE2	1:B:1954:GLU:N	2.19	0.74
1:B:881:LEU:O	1:B:885:THR:HG23	1.88	0.74
1:B:479:LEU:O	1:B:483:VAL:HG23	1.89	0.73
1:B:2518:ASP:OD1	1:C:2524:ARG:NE	2.19	0.73
1:C:881:LEU:O	1:C:885:THR:HG23	1.88	0.73
1:A:2287:ALA:O	1:A:2291:THR:HG23	1.88	0.73
1:A:451:MET:HG3	1:A:475:LEU:HD22	1.71	0.73
1:B:666:ILE:N	1:B:732:GLN:OE1	2.22	0.73
1:D:2021:ARG:NH1	1:D:2024:GLU:OE2	2.22	0.73
1:C:1397:VAL:HG21	1:C:1436:HIS:CD2	2.23	0.72
1:C:1402:HIS:ND1	1:C:1404:ASP:O	2.22	0.72
1:D:1747:GLU:N	1:D:1747:GLU:OE1	2.22	0.72
1:C:2326:TYR:CE1	1:C:2344:LEU:HD22	2.25	0.72
1:C:2024:GLU:OE2	1:C:2024:GLU:N	2.23	0.71
1:D:1466:LYS:O	1:D:1470:SER:OG	2.06	0.71
1:C:2162:ASP:OD2	1:C:2164:GLN:N	2.23	0.71
1:D:1188:GLN:N	1:D:1188:GLN:OE1	2.24	0.71
1:A:1097:LEU:HD12	1:A:1595:LEU:HD22	1.73	0.70
1:A:2544:GLU:N	1:A:2544:GLU:OE2	2.23	0.70
1:D:1322:MET:O	1:D:1326:THR:HG23	1.90	0.70
1:A:1282:VAL:O	1:A:1285:HIS:ND1	2.24	0.70
1:A:1895:GLN:O	1:A:1896:ASN:ND2	2.25	0.69
1:D:1526:ILE:HG23	1:D:1551:MET:CE	2.21	0.69
1:A:990:LEU:HD23	1:A:1092:PHE:CD1	2.28	0.69
1:A:1297:VAL:HG21	1:A:1363:MET:HE3	1.73	0.69
1:B:1456:GLU:O	1:B:1458:ARG:NH1	2.26	0.68
1:B:1953:HIS:O	1:B:1957:THR:HG23	1.94	0.68
1:A:580:MET:SD	1:A:581:MET:N	2.67	0.67
1:D:299:HIS:ND1	1:D:378:ASP:O	2.27	0.67
1:A:641:ASN:OD1	1:A:641:ASN:O	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:HIS:ND1	1:B:378:ASP:O	2.27	0.67
1:B:2359:ILE:O	1:B:2363:THR:HG23	1.93	0.67
1:A:299:HIS:ND1	1:A:378:ASP:O	2.28	0.66
1:A:621:LEU:HD13	1:A:630:PHE:CE1	2.31	0.66
1:D:277:THR:O	1:D:507:LYS:NZ	2.27	0.66
1:A:299:HIS:O	1:A:304:TYR:OH	2.13	0.66
1:C:299:HIS:ND1	1:C:378:ASP:O	2.28	0.66
1:D:1737:VAL:HG11	1:D:1757:ALA:HB2	1.78	0.66
1:C:608:LYS:HE3	1:C:608:LYS:HA	1.77	0.66
1:B:1648:ILE:HG23	1:B:1736:LEU:HD22	1.77	0.66
1:D:1236:CYS:HB3	1:D:1246:LEU:HD12	1.77	0.65
1:A:1934:VAL:HG11	1:A:1988:LEU:HD13	1.78	0.65
1:A:773:LEU:HD11	1:A:777:PHE:CE2	2.31	0.65
1:C:1445:THR:HG22	1:C:1501:LEU:HA	1.79	0.65
1:A:972:LEU:HD11	1:A:1062:LEU:HD13	1.79	0.65
1:B:299:HIS:O	1:B:304:TYR:OH	2.12	0.65
1:A:716:ARG:NH1	1:A:768:MET:O	2.30	0.65
1:D:479:LEU:O	1:D:483:VAL:HG23	1.97	0.65
1:C:2320:PHE:O	1:C:2324:VAL:HG13	1.98	0.64
1:C:596:THR:HG21	1:C:633:TYR:HD1	1.62	0.64
1:C:2326:TYR:CD1	1:C:2344:LEU:HD22	2.33	0.64
1:A:1186:GLY:O	1:A:1190:ARG:N	2.30	0.64
1:D:1962:HIS:ND1	1:D:1964:SER:OG	2.16	0.63
1:C:886:ARG:NE	1:C:1049:ASP:OD2	2.32	0.63
1:A:538:LEU:HD13	1:A:587:TYR:CE2	2.33	0.63
1:B:451:MET:HB2	1:B:475:LEU:HD22	1.81	0.63
1:D:1022:ASN:C	1:D:1022:ASN:HD22	2.01	0.63
1:A:1247:HIS:CD2	1:A:1274:LEU:HD22	2.34	0.63
1:A:1467:TYR:O	1:A:1471:VAL:HG22	1.99	0.63
1:D:299:HIS:O	1:D:304:TYR:OH	2.13	0.62
1:B:1044:MET:SD	1:B:1044:MET:N	2.68	0.62
1:C:1441:PHE:O	1:C:1445:THR:HG23	1.98	0.62
1:B:618:PHE:CE2	1:B:637:LEU:HD11	2.34	0.61
1:D:2155:LEU:CD2	1:D:2178:LEU:HD11	2.30	0.61
1:C:299:HIS:O	1:C:304:TYR:OH	2.13	0.61
1:C:893:ASP:OD1	1:C:894:CYS:N	2.33	0.61
1:A:621:LEU:HD12	1:A:622:VAL:N	2.15	0.61
1:A:972:LEU:HD11	1:A:1062:LEU:CD1	2.30	0.61
1:B:811:THR:N	1:B:814:ASP:OD1	2.33	0.61
1:B:1124:SER:HB2	1:B:1212:ILE:HD11	1.81	0.61
1:C:479:LEU:O	1:C:483:VAL:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:LEU:HD21	1:A:729:TYR:CE2	2.36	0.60
1:A:1953:HIS:O	1:A:1957:THR:HG23	2.00	0.60
1:D:460:ASN:OD1	1:D:527:ARG:NH2	2.33	0.60
1:B:1207:LEU:HD13	1:B:1249:HIS:HD2	1.65	0.60
1:D:1300:LEU:HD22	1:D:1371:LEU:HD23	1.83	0.60
1:D:480:VAL:HG11	1:D:493:VAL:HB	1.83	0.60
1:B:515:LEU:HD23	1:B:560:LEU:HD23	1.84	0.60
1:B:695:THR:HG23	1:B:703:HIS:CE1	2.37	0.60
1:A:811:THR:HG22	1:A:812:ILE:H	1.66	0.60
1:B:782:LEU:HD11	1:B:869:ASN:OD1	2.01	0.60
1:B:1207:LEU:HD13	1:B:1249:HIS:CD2	2.36	0.60
1:A:1898:LYS:HA	1:A:1898:LYS:HE3	1.83	0.59
1:A:2536:THR:O	1:A:2536:THR:HG22	2.01	0.59
1:B:2211:LEU:O	1:B:2215:ILE:HD12	2.02	0.59
1:C:1329:GLY:O	1:C:1333:VAL:HG22	2.00	0.59
1:B:2324:VAL:HA	1:B:2327:ILE:HD12	1.83	0.59
1:C:991:LEU:HD11	1:C:1095:VAL:HG21	1.84	0.59
1:B:801:ARG:NH2	1:B:984:ASP:OD1	2.36	0.59
1:B:589:ILE:O	1:B:589:ILE:HG22	2.01	0.59
1:B:1651:THR:OG1	1:B:1665:VAL:HG11	2.02	0.59
1:C:1541:PRO:O	1:C:1545:ASP:N	2.31	0.59
1:D:1978:ILE:HG22	1:D:1978:ILE:O	2.03	0.59
1:B:1260:GLU:N	1:B:1260:GLU:OE1	2.35	0.58
1:D:252:LEU:HD11	1:D:263:VAL:HG12	1.85	0.58
1:A:252:LEU:HD11	1:A:263:VAL:HG12	1.85	0.58
1:A:743:ARG:NE	1:A:787:ASP:OD1	2.36	0.58
1:B:1473:LEU:HD11	1:B:1522:VAL:CG2	2.32	0.58
1:D:596:THR:HG21	1:D:633:TYR:HB3	1.86	0.58
1:B:252:LEU:HD11	1:B:263:VAL:HG12	1.85	0.58
1:C:614:GLU:OE1	1:C:614:GLU:N	2.36	0.58
1:C:1551:MET:SD	1:C:1551:MET:N	2.76	0.58
1:D:1307:ILE:HD11	1:D:1375:CYS:SG	2.43	0.58
1:C:1333:VAL:HG23	1:C:1333:VAL:O	2.03	0.58
1:C:596:THR:HG21	1:C:633:TYR:CD1	2.39	0.58
1:A:812:ILE:HD12	1:A:1044:MET:SD	2.44	0.58
1:B:760:ILE:HG21	1:B:781:MET:HB2	1.85	0.58
1:B:2031:LYS:NZ	1:B:2035:GLN:OE1	2.36	0.58
1:C:1182:MET:HE3	1:C:1182:MET:O	2.04	0.58
1:C:1322:MET:SD	1:C:1322:MET:N	2.76	0.58
1:A:1338:ASP:OD2	1:A:1339:LYS:N	2.37	0.58
1:B:2162:ASP:OD1	1:B:2165:GLY:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2280:PRO:O	1:B:2284:ILE:HG13	2.04	0.58
1:C:252:LEU:HD11	1:C:263:VAL:HG12	1.84	0.58
1:D:1346:LEU:HD21	1:D:1402:HIS:NE2	2.18	0.58
1:A:1089:MET:CE	1:A:1606:LEU:HD12	2.33	0.58
1:A:1325:LEU:HD22	1:A:1333:VAL:CG1	2.33	0.58
1:B:1473:LEU:HD11	1:B:1522:VAL:HG22	1.86	0.57
1:B:1669:LEU:O	1:B:1673:LEU:HD12	2.04	0.57
1:D:435:PRO:O	1:D:439:ILE:HD12	2.04	0.57
1:A:506:GLN:NE2	1:A:563:SER:O	2.37	0.57
1:A:1298:GLN:N	1:A:1298:GLN:OE1	2.38	0.57
1:B:1531:MET:SD	1:B:1531:MET:N	2.76	0.57
1:C:621:LEU:HD12	1:C:622:VAL:N	2.19	0.57
1:D:1209:LEU:O	1:D:1212:ILE:HG22	2.04	0.57
1:A:1325:LEU:HD22	1:A:1333:VAL:HG12	1.87	0.57
1:B:2536:THR:HG22	1:B:2536:THR:O	2.05	0.57
1:D:2172:PHE:HZ	1:D:2594:ILE:HG23	1.69	0.57
1:B:709:ARG:NH1	1:B:766:ASP:OD2	2.37	0.56
1:A:1243:GLN:OE1	1:A:1271:ASN:ND2	2.38	0.56
1:B:811:THR:OG1	1:B:814:ASP:OD1	2.21	0.56
1:C:760:ILE:HG21	1:C:781:MET:HB2	1.87	0.56
1:A:266:ARG:NH2	3:A:3002:I3P:O43	2.38	0.56
1:B:847:GLU:OE2	1:B:856:LYS:NZ	2.38	0.56
1:C:1542:MET:SD	1:C:1542:MET:N	2.74	0.56
1:A:252:LEU:HD11	1:A:263:VAL:CG1	2.36	0.56
1:B:509:MET:SD	1:B:563:SER:OG	2.63	0.56
1:D:1526:ILE:HG23	1:D:1551:MET:HE2	1.88	0.56
1:A:585:ILE:HD11	1:A:592:GLU:HG3	1.88	0.55
1:C:2207:ILE:HD12	1:C:2207:ILE:H	1.71	0.55
1:B:1960:VAL:HG13	1:B:1961:THR:HG23	1.88	0.55
1:C:1729:ASP:OD2	1:C:1734:THR:OG1	2.19	0.55
1:B:252:LEU:HD11	1:B:263:VAL:CG1	2.36	0.55
1:A:1123:LYS:HD2	1:A:1126:LEU:HD22	1.89	0.55
1:D:1298:GLN:OE1	1:D:1298:GLN:N	2.40	0.55
1:A:1752:GLU:OE1	1:A:1752:GLU:HA	2.06	0.55
1:B:655:CYS:O	1:B:661:ASN:ND2	2.39	0.55
1:B:820:ASN:O	1:B:824:ASP:N	2.35	0.55
1:B:1316:LYS:O	1:B:1320:MET:HE3	2.06	0.55
1:D:1275:CYS:O	1:D:1278:ILE:HG22	2.07	0.55
1:B:1515:GLN:O	1:B:1519:LYS:N	2.36	0.55
1:C:2359:ILE:O	1:C:2363:THR:HG23	2.06	0.55
1:A:1444:PHE:O	1:A:1448:MET:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1456:GLU:O	1:A:1458:ARG:NH1	2.38	0.54
1:C:2277:GLY:O	1:C:2281:THR:OG1	2.23	0.54
1:A:1290:LEU:HD21	1:A:1299:TYR:HB2	1.89	0.54
1:A:2215:ILE:O	1:A:2219:ILE:HG13	2.06	0.54
1:C:1445:THR:HG22	1:C:1501:LEU:CA	2.36	0.54
1:D:252:LEU:HD11	1:D:263:VAL:CG1	2.37	0.54
1:D:1206:MET:SD	1:D:1228:THR:HG23	2.47	0.54
1:A:705:GLU:N	1:A:705:GLU:OE2	2.40	0.54
1:C:252:LEU:HD11	1:C:263:VAL:CG1	2.36	0.54
1:D:1433:THR:HG22	1:D:1433:THR:O	2.06	0.54
1:B:1123:LYS:HD3	1:B:1126:LEU:HD13	1.89	0.54
1:D:1464:LEU:O	1:D:1468:VAL:HG23	2.07	0.54
1:D:1934:VAL:HG11	1:D:1988:LEU:HD13	1.88	0.54
1:A:1056:LEU:HD23	1:A:1056:LEU:O	2.08	0.54
1:A:1648:ILE:HG23	1:A:1736:LEU:HD22	1.89	0.54
1:D:1097:LEU:HD12	1:D:1595:LEU:HD22	1.90	0.54
1:B:1225:LEU:O	1:B:1229:HIS:ND1	2.41	0.54
1:C:596:THR:HG22	1:C:637:LEU:HD21	1.88	0.54
1:D:1123:LYS:HD2	1:D:1126:LEU:HD13	1.89	0.54
1:D:1407:THR:HG21	1:D:1464:LEU:HA	1.90	0.54
1:A:1089:MET:HE2	1:A:1606:LEU:HD12	1.88	0.54
1:D:1467:TYR:O	1:D:1471:VAL:HG22	2.08	0.54
1:C:1125:GLU:OE2	1:C:1125:GLU:N	2.36	0.53
1:D:1731:GLU:OE1	1:D:1731:GLU:HA	2.08	0.53
1:A:647:VAL:O	1:A:651:LEU:HD23	2.09	0.53
1:C:1737:VAL:HG11	1:C:1757:ALA:HB2	1.89	0.53
1:D:1670:GLN:NE2	1:D:1752:GLU:OE1	2.40	0.53
1:A:599:LEU:HB3	1:A:606:LEU:HD13	1.90	0.53
1:A:990:LEU:HD23	1:A:1092:PHE:HD1	1.72	0.53
1:B:452:LEU:HD22	1:B:521:ILE:CD1	2.38	0.53
1:D:1001:VAL:HG12	1:D:1002:PHE:CD2	2.42	0.53
1:C:1919:THR:HG22	1:C:1924:LEU:HD23	1.89	0.53
1:B:2218:ILE:HD11	1:B:2273:ILE:HD11	1.90	0.53
1:A:1491:LEU:CD2	1:A:1498:VAL:HG11	2.39	0.53
1:B:452:LEU:HD22	1:B:521:ILE:HD11	1.90	0.53
1:B:1247:HIS:O	1:B:1250:LEU:HD22	2.08	0.53
1:D:1397:VAL:O	1:D:1401:THR:HG23	2.09	0.53
1:B:1303:LEU:HD12	1:B:1371:LEU:HD21	1.91	0.53
1:B:1332:VAL:O	1:B:1368:LEU:HD11	2.07	0.53
1:B:1342:LEU:O	1:B:1346:LEU:HD13	2.08	0.53
1:D:1036:PHE:HZ	1:D:1088:ALA:HB3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:990:LEU:HD23	1:A:1092:PHE:CE1	2.44	0.53
1:D:2023:GLN:NE2	1:D:2027:ASP:OD1	2.42	0.53
1:A:2540:ILE:HD11	1:A:2565:MET:HB3	1.90	0.53
1:B:1067:TYR:O	1:B:1071:VAL:HG23	2.09	0.53
1:B:1125:GLU:HG2	1:B:1126:LEU:HD12	1.90	0.53
1:B:2123:GLN:OE1	1:B:2135:GLN:NE2	2.42	0.53
1:A:760:ILE:HG21	1:A:781:MET:HB2	1.90	0.52
1:B:1407:THR:O	1:B:1411:MET:HG3	2.09	0.52
1:B:1298:GLN:OE1	1:B:1298:GLN:N	2.41	0.52
1:D:833:THR:CG2	1:D:866:LEU:HD21	2.39	0.52
1:A:1332:VAL:HG23	1:A:1333:VAL:HG13	1.91	0.52
1:B:451:MET:N	1:B:451:MET:SD	2.83	0.52
1:B:772:ASP:OD1	1:B:773:LEU:N	2.42	0.52
1:D:2449:ASP:OD1	1:D:2450:SER:N	2.42	0.52
1:B:1393:LEU:O	1:B:1393:LEU:HD12	2.10	0.52
1:C:745:TYR:O	1:C:749:ASP:OD2	2.27	0.52
1:C:816:ASP:O	1:C:823:ARG:NH2	2.42	0.52
1:D:1342:LEU:O	1:D:1346:LEU:HD13	2.09	0.52
1:C:1934:VAL:HG11	1:C:1988:LEU:HD13	1.91	0.52
1:A:871:ILE:HD11	1:A:884:LEU:CD2	2.39	0.52
1:A:1491:LEU:HD23	1:A:1498:VAL:HG11	1.91	0.52
1:C:1196:LEU:HD12	1:C:1196:LEU:O	2.09	0.52
1:A:482:PHE:O	1:A:505:ARG:NH1	2.43	0.52
1:A:1533:ALA:HA	1:A:1538:ILE:HD11	1.91	0.52
1:B:599:LEU:HB3	1:B:606:LEU:HD13	1.92	0.52
1:B:1323:THR:O	1:B:1327:ASN:OD1	2.28	0.52
1:C:1316:LYS:O	1:C:1320:MET:HG3	2.08	0.52
1:D:805:GLU:OE1	1:D:805:GLU:HA	2.09	0.52
1:C:1606:LEU:O	1:C:1610:VAL:HG23	2.10	0.52
1:C:655:CYS:O	1:C:661:ASN:ND2	2.40	0.52
1:C:885:THR:HG21	1:C:978:ILE:HG21	1.91	0.52
1:D:1513:TRP:O	1:D:1514:LEU:CB	2.58	0.52
1:B:477:GLU:OE1	1:B:493:VAL:HG11	2.10	0.52
1:D:2476:VAL:HG22	1:D:2480:LEU:HD13	1.92	0.52
1:C:1469:LEU:HD22	1:C:1518:HIS:CG	2.45	0.51
1:A:2178:LEU:O	1:A:2182:MET:HG3	2.10	0.51
1:B:1206:MET:HA	1:B:1206:MET:CE	2.40	0.51
1:B:1287:VAL:HG11	1:B:1324:GLU:HB3	1.92	0.51
1:D:1542:MET:H	1:D:1542:MET:CE	2.23	0.51
1:C:719:ASN:OD1	1:C:721:HIS:N	2.43	0.51
1:D:350:ILE:HD11	1:D:401:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:LEU:HD12	1:A:780:LEU:O	2.11	0.51
1:C:1421:TYR:HA	1:C:1424:THR:HG23	1.92	0.51
1:A:350:ILE:HD11	1:A:401:THR:HG21	1.93	0.51
1:A:1083:SER:O	1:A:1083:SER:OG	2.29	0.51
1:B:667:ARG:NE	1:B:667:ARG:HA	2.26	0.51
1:B:1379:LYS:NZ	1:B:1425:GLU:OE1	2.43	0.51
1:C:885:THR:CG2	1:C:978:ILE:HD13	2.33	0.51
1:D:506:GLN:NE2	1:D:563:SER:O	2.43	0.51
1:A:772:ASP:OD1	1:A:773:LEU:N	2.44	0.51
1:C:2172:PHE:HZ	1:C:2594:ILE:HG23	1.76	0.51
1:B:606:LEU:HD23	1:B:645:ILE:HD11	1.92	0.51
1:B:568:ARG:NH2	3:B:3002:I3P:O3	2.43	0.51
1:D:832:ASN:HA	1:D:835:GLU:OE1	2.10	0.51
1:B:614:GLU:OE1	1:B:614:GLU:N	2.43	0.51
1:C:708:VAL:HG11	1:C:769:LEU:HD21	1.93	0.51
1:C:1948:CYS:SG	1:C:1959:ILE:HD12	2.51	0.51
1:B:518:VAL:HG11	1:B:560:LEU:HG	1.93	0.51
1:B:279:SER:OG	1:B:511:GLU:OE2	2.19	0.50
1:C:2191:MET:CE	1:C:2194:ILE:HD12	2.40	0.50
1:B:862:GLU:HA	1:B:862:GLU:OE1	2.12	0.50
1:C:1659:GLU:OE1	1:C:1746:ASN:ND2	2.44	0.50
1:A:788:ARG:HG3	1:A:788:ARG:HH11	1.76	0.50
1:B:1533:ALA:HA	1:B:1538:ILE:HD11	1.93	0.50
1:B:2014:GLU:HA	1:B:2014:GLU:OE2	2.10	0.50
1:C:350:ILE:HD11	1:C:401:THR:HG21	1.92	0.50
1:A:656:VAL:HG21	1:A:739:MET:HE1	1.94	0.50
1:A:2264:LEU:O	1:A:2268:LEU:HG	2.11	0.50
1:B:1209:LEU:O	1:B:1212:ILE:HG22	2.11	0.50
1:A:1316:LYS:O	1:A:1320:MET:HG3	2.12	0.50
1:B:1441:PHE:CG	1:B:1501:LEU:HD11	2.46	0.50
1:C:1344:HIS:O	1:C:1348:MET:HG2	2.12	0.50
1:C:2388:PHE:HD2	1:C:2458:LEU:HD13	1.77	0.50
1:B:2536:THR:O	1:B:2536:THR:CG2	2.59	0.50
1:D:622:VAL:HG23	1:D:630:PHE:HB2	1.94	0.50
1:B:1106:ASN:ND2	1:B:1193:GLN:OE1	2.45	0.50
1:A:1407:THR:O	1:A:1411:MET:HG3	2.12	0.50
1:B:757:VAL:HG22	1:B:785:HIS:CG	2.46	0.50
1:B:2322:TYR:OH	1:B:2347:ASP:OD1	2.19	0.50
1:A:1514:LEU:HD23	1:A:1519:LYS:HD2	1.93	0.50
1:C:1229:HIS:HA	1:C:1232:LEU:HD12	1.93	0.50
1:D:871:ILE:HD13	1:D:974:ILE:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2294:ILE:HD13	1:A:2327:ILE:HD11	1.92	0.49
1:B:350:ILE:HD11	1:B:401:THR:HG21	1.92	0.49
1:B:893:ASP:OD1	1:B:894:CYS:N	2.45	0.49
1:B:2218:ILE:HD11	1:B:2273:ILE:CD1	2.41	0.49
1:A:1097:LEU:CD1	1:A:1595:LEU:HD22	2.42	0.49
1:A:1472:VAL:HG12	1:A:1476:ILE:HD12	1.94	0.49
1:A:1956:GLN:O	1:A:1960:VAL:HG23	2.12	0.49
1:D:1799:GLU:C	1:D:1799:GLU:OE1	2.50	0.49
1:A:485:ASP:OD2	1:A:505:ARG:NH1	2.45	0.49
1:A:1050:GLU:OE1	1:A:1053:ARG:NE	2.46	0.49
1:A:2010:SER:O	1:A:2014:GLU:OE1	2.30	0.49
1:C:1323:THR:O	1:C:1326:THR:OG1	2.24	0.49
1:D:599:LEU:HB3	1:D:606:LEU:HD13	1.95	0.49
1:D:976:GLN:HG2	1:D:1077:LEU:HD21	1.93	0.49
1:C:1372:LEU:HA	1:C:1375:CYS:SG	2.52	0.49
1:B:1048:ASP:OD1	1:B:1048:ASP:C	2.50	0.49
1:C:1323:THR:O	1:C:1327:ASN:OD1	2.30	0.49
1:C:1473:LEU:O	1:C:1477:ASN:ND2	2.46	0.49
1:D:1542:MET:SD	1:D:1543:ASP:OD2	2.70	0.49
1:A:811:THR:HG22	1:A:812:ILE:N	2.27	0.49
1:A:1297:VAL:HG12	1:A:1364:TYR:HA	1.94	0.49
1:B:602:ASN:HD22	1:B:605:LEU:HD12	1.78	0.49
1:B:1206:MET:HA	1:B:1206:MET:HE2	1.95	0.49
1:B:1960:VAL:CG1	1:B:1961:THR:HG23	2.41	0.49
1:A:1117:LEU:HD12	1:A:1117:LEU:O	2.13	0.49
1:A:1979:SER:HA	1:A:1982:CYS:SG	2.53	0.49
1:B:1396:VAL:O	1:B:1400:VAL:HG12	2.13	0.49
1:B:1509:LEU:HD21	1:B:1551:MET:CE	2.43	0.49
1:C:405:ILE:HD11	1:C:416:MET:HA	1.95	0.49
1:C:1455:ARG:NH1	1:C:1465:GLU:OE2	2.45	0.49
1:D:871:ILE:HD11	1:D:884:LEU:CD2	2.43	0.49
1:A:1627:LEU:HD21	1:A:1695:LEU:HD23	1.94	0.49
1:B:834:MET:O	1:B:837:VAL:HG12	2.13	0.49
1:B:2261:ILE:O	1:B:2261:ILE:HG22	2.13	0.49
1:C:1731:GLU:HA	1:C:1731:GLU:OE1	2.12	0.49
1:C:1919:THR:CG2	1:C:1924:LEU:HD23	2.43	0.49
1:C:2476:VAL:HG22	1:C:2480:LEU:HD13	1.95	0.49
1:D:577:GLN:O	1:D:580:MET:SD	2.71	0.49
1:D:1128:VAL:HG23	1:D:1221:MET:HE1	1.95	0.49
1:C:267:THR:HG23	1:C:413:ILE:O	2.13	0.49
1:C:2261:ILE:HG22	1:C:2261:ILE:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:621:LEU:HD12	1:D:622:VAL:N	2.26	0.49
1:A:308:HIS:ND1	1:A:311:THR:OG1	2.30	0.48
1:A:1117:LEU:HD12	1:A:1121:VAL:HG23	1.95	0.48
1:B:1256:PRO:HA	1:B:1289:LEU:HD11	1.95	0.48
1:B:2468:HIS:HB2	1:B:2479:ILE:HD13	1.95	0.48
1:A:267:THR:HG23	1:A:413:ILE:O	2.13	0.48
1:A:871:ILE:HD11	1:A:884:LEU:HD23	1.93	0.48
1:A:1656:GLU:OE2	1:A:1656:GLU:N	2.42	0.48
1:B:1288:HIS:O	1:B:1292:THR:HG23	2.13	0.48
1:D:280:ASN:O	1:D:308:HIS:NE2	2.46	0.48
1:D:405:ILE:HD11	1:D:416:MET:HA	1.95	0.48
1:D:969:LEU:HD11	1:D:1069:PRO:HB2	1.95	0.48
1:D:1001:VAL:HG12	1:D:1002:PHE:CE2	2.48	0.48
1:A:694:LEU:HD13	1:A:708:VAL:CG2	2.43	0.48
1:A:1056:LEU:CD2	1:A:1627:LEU:HD13	2.42	0.48
1:D:1509:LEU:HD23	1:D:1509:LEU:O	2.13	0.48
1:A:1358:ASP:O	1:A:1363:MET:CE	2.61	0.48
1:D:1033:GLU:HG2	1:D:1606:LEU:HD21	1.93	0.48
1:A:893:ASP:OD2	1:A:894:CYS:N	2.46	0.48
1:B:1898:LYS:HD2	1:B:1898:LYS:N	2.28	0.48
1:C:972:LEU:HD11	1:C:1062:LEU:HD13	1.95	0.48
1:D:2162:ASP:OD1	1:D:2165:GLY:N	2.47	0.48
1:A:2048:GLU:OE1	1:A:2048:GLU:N	2.47	0.48
1:A:2536:THR:O	1:A:2536:THR:CG2	2.61	0.48
1:B:405:ILE:HD11	1:B:416:MET:HA	1.95	0.48
1:B:782:LEU:HD13	1:B:866:LEU:HD12	1.96	0.48
1:C:482:PHE:O	1:C:505:ARG:NH1	2.45	0.48
1:C:280:ASN:O	1:C:308:HIS:NE2	2.47	0.48
1:D:452:LEU:HB3	1:D:521:ILE:HD11	1.95	0.48
1:D:1626:LEU:HD13	1:D:1698:ARG:HB2	1.95	0.48
1:A:1473:LEU:HD13	1:A:1522:VAL:HG22	1.96	0.48
1:B:1396:VAL:HG13	1:B:1413:TYR:HB3	1.96	0.48
1:A:250:LYS:HE2	1:A:267:THR:HG22	1.96	0.48
1:B:720:ALA:O	1:B:724:ASN:OD1	2.32	0.48
1:B:1434:SER:HB3	1:B:1436:HIS:ND1	2.29	0.48
1:C:682:TYR:HB2	1:C:685:ILE:HD12	1.96	0.48
1:C:1495:GLN:HA	1:C:1498:VAL:HG22	1.95	0.48
1:D:267:THR:HG23	1:D:413:ILE:O	2.14	0.48
1:A:1866:SER:O	1:A:1869:ILE:HG22	2.14	0.48
1:D:1602:LEU:CD2	1:D:1606:LEU:HD12	2.44	0.48
1:D:1924:LEU:N	1:D:1924:LEU:HD22	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:LEU:HG	1:A:742:ASP:OD1	2.14	0.47
1:A:1123:LYS:HD3	1:A:1126:LEU:HD13	1.95	0.47
1:A:1773:HIS:HB2	1:A:1888:LEU:HD21	1.96	0.47
1:B:280:ASN:O	1:B:308:HIS:NE2	2.46	0.47
1:B:1467:TYR:O	1:B:1471:VAL:HG22	2.14	0.47
1:C:1315:LYS:N	1:C:1315:LYS:HD3	2.29	0.47
1:A:1345:LEU:O	1:A:1348:MET:HG3	2.14	0.47
1:A:1514:LEU:HD23	1:A:1519:LYS:CD	2.43	0.47
1:A:1902:ASN:ND2	1:A:1905:CYS:SG	2.87	0.47
1:B:1741:ILE:HG21	1:B:1785:PHE:CE1	2.49	0.47
1:A:837:VAL:HG23	1:A:863:VAL:HG13	1.95	0.47
1:A:1248:LYS:HE2	1:A:1248:LYS:HA	1.96	0.47
1:B:1979:SER:HA	1:B:1982:CYS:SG	2.54	0.47
1:D:1290:LEU:HD21	1:D:1299:TYR:HB2	1.96	0.47
1:B:505:ARG:O	1:B:509:MET:HG3	2.14	0.47
1:C:1038:VAL:HG22	1:C:1038:VAL:O	2.13	0.47
1:C:1322:MET:HA	1:C:1322:MET:HE3	1.96	0.47
1:C:1514:LEU:HD23	1:C:1519:LYS:CG	2.44	0.47
1:C:2293:LYS:O	1:C:2297:VAL:HG23	2.14	0.47
1:D:250:LYS:HE2	1:D:267:THR:HG22	1.95	0.47
1:D:2277:GLY:O	1:D:2281:THR:OG1	2.29	0.47
1:A:1967:ILE:O	1:A:1971:THR:HG23	2.14	0.47
1:B:1509:LEU:HD21	1:B:1551:MET:HE2	1.96	0.47
1:D:1381:VAL:O	1:D:1385:ILE:HG13	2.14	0.47
1:B:250:LYS:HE2	1:B:267:THR:HG22	1.95	0.47
1:B:267:THR:HG23	1:B:413:ILE:O	2.14	0.47
1:B:1934:VAL:HG11	1:B:1988:LEU:HD13	1.94	0.47
1:C:1456:GLU:O	1:C:1458:ARG:NH1	2.47	0.47
1:D:2468:HIS:HB2	1:D:2479:ILE:HD13	1.96	0.47
1:A:1187:GLU:OE1	1:A:1190:ARG:NH1	2.48	0.47
1:A:1741:ILE:HG21	1:A:1785:PHE:CE1	2.50	0.47
1:B:585:ILE:HD11	1:B:592:GLU:HG3	1.96	0.47
1:B:1973:LEU:CD2	1:B:1992:LEU:HD21	2.44	0.47
1:C:1950:GLY:N	1:C:1951:PRO:HA	2.30	0.47
1:D:1950:GLY:N	1:D:1951:PRO:HA	2.30	0.47
1:A:892:ILE:CG2	1:A:971:ILE:HD13	2.45	0.47
1:B:1373:ALA:O	1:B:1419:HIS:ND1	2.46	0.47
1:B:1430:GLU:O	1:B:1434:SER:OG	2.21	0.47
1:B:2328:LEU:O	1:B:2331:VAL:HG12	2.15	0.47
1:C:1411:MET:HE3	1:C:1466:LYS:HG3	1.97	0.47
1:C:2162:ASP:OD2	1:C:2162:ASP:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:611:THR:HG22	1:D:612:LYS:N	2.30	0.47
1:A:715:ALA:N	1:A:722:ASP:OD2	2.48	0.47
1:A:1615:SER:O	1:A:1619:ASP:OD2	2.32	0.47
1:C:606:LEU:HD23	1:C:645:ILE:HD13	1.97	0.47
1:C:1397:VAL:HG21	1:C:1436:HIS:HD2	1.74	0.47
1:D:1956:GLN:NE2	1:D:2002:ALA:O	2.48	0.47
1:A:1399:VAL:HG21	1:A:1413:TYR:HE2	1.79	0.47
1:A:2380:VAL:O	1:A:2384:SER:OG	2.28	0.47
1:B:464:ILE:HG22	1:B:535:LEU:HD21	1.97	0.47
1:B:1344:HIS:O	1:B:1348:MET:HG2	2.15	0.47
1:C:1773:HIS:HB2	1:C:1888:LEU:HD21	1.97	0.47
1:D:614:GLU:OE1	1:D:614:GLU:N	2.48	0.47
1:C:1386:LYS:O	1:C:1390:LEU:HD13	2.15	0.46
1:D:509:MET:HA	1:D:514:ILE:HD12	1.98	0.46
1:A:1229:HIS:CG	1:A:1259:LEU:HD22	2.51	0.46
1:B:455:ALA:O	1:B:459:LEU:HG	2.14	0.46
1:B:2004:MET:O	1:B:2004:MET:HG2	2.14	0.46
1:D:1125:GLU:HA	1:D:1128:VAL:HG12	1.97	0.46
1:A:1124:SER:HA	1:A:1127:TRP:CD1	2.50	0.46
1:C:716:ARG:NH2	1:C:768:MET:O	2.48	0.46
1:C:2546:ASP:OD2	1:C:2547:LYS:N	2.48	0.46
1:D:582:GLN:O	1:D:585:ILE:HG22	2.16	0.46
1:D:976:GLN:CG	1:D:1077:LEU:HD21	2.45	0.46
1:D:1346:LEU:HD21	1:D:1402:HIS:CD2	2.50	0.46
1:A:405:ILE:HD11	1:A:416:MET:HA	1.95	0.46
1:A:755:LEU:HD12	1:A:780:LEU:HD21	1.97	0.46
1:A:1651:THR:OG1	1:A:1665:VAL:HG11	2.16	0.46
1:C:2468:HIS:HB3	1:C:2479:ILE:HG21	1.96	0.46
1:D:1473:LEU:CD1	1:D:1522:VAL:HG22	2.46	0.46
1:A:670:LEU:HD12	1:A:670:LEU:O	2.15	0.46
1:B:469:ARG:HD2	1:B:548:PRO:HB2	1.97	0.46
1:D:803:TRP:HA	1:D:806:ILE:HD12	1.97	0.46
1:A:1545:ASP:OD1	1:A:1545:ASP:C	2.54	0.46
1:B:1976:ASN:O	1:B:1993:LYS:NZ	2.47	0.46
1:C:2131:ARG:HG2	1:C:2131:ARG:HH11	1.79	0.46
1:A:711:LEU:HG	1:A:722:ASP:OD1	2.16	0.46
1:A:715:ALA:CA	1:A:722:ASP:OD2	2.63	0.46
1:A:1391:LEU:O	1:A:1421:TYR:OH	2.32	0.46
1:B:854:GLU:OE2	1:B:854:GLU:N	2.33	0.46
1:B:1226:ARG:HA	1:B:1259:LEU:HD11	1.98	0.46
1:C:1885:ASN:ND2	1:C:1888:LEU:HD23	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1797:GLN:O	1:B:1800:THR:HG22	2.16	0.46
1:B:2004:MET:O	1:B:2004:MET:CG	2.64	0.46
1:C:250:LYS:HE2	1:C:267:THR:HG22	1.97	0.46
1:D:1919:THR:HG22	1:D:1924:LEU:HD23	1.97	0.46
1:A:2324:VAL:O	1:A:2327:ILE:HG22	2.16	0.46
1:C:1503:GLN:CG	1:C:1544:LEU:HD22	2.45	0.46
1:A:840:TYR:O	1:A:844:VAL:HG23	2.16	0.46
1:B:1396:VAL:HG21	1:B:1416:PHE:CE2	2.50	0.46
1:D:1432:TYR:HE2	1:D:1484:PHE:HB2	1.80	0.46
1:A:2284:ILE:O	1:A:2288:LEU:HD13	2.15	0.45
1:B:745:TYR:HA	1:B:748:ILE:HB	1.98	0.45
1:B:1469:LEU:HA	1:B:1473:LEU:HD12	1.98	0.45
1:B:1654:LEU:HD12	1:B:1654:LEU:O	2.16	0.45
1:C:1321:ILE:HG22	1:C:1325:LEU:HD11	1.98	0.45
1:C:1530:ALA:O	1:C:1534:LYS:HG2	2.17	0.45
1:C:1785:PHE:O	1:C:1788:VAL:HG22	2.15	0.45
1:A:515:LEU:HD11	1:A:570:ASN:ND2	2.31	0.45
1:A:1678:LYS:HA	1:A:1678:LYS:HE3	1.98	0.45
1:A:2261:ILE:HG22	1:A:2261:ILE:O	2.16	0.45
1:B:786:VAL:O	1:B:791:GLN:NE2	2.50	0.45
1:B:2185:GLN:O	1:B:2189:ARG:HG3	2.15	0.45
1:C:406:ASP:OD1	1:C:406:ASP:N	2.50	0.45
1:C:1228:THR:O	1:C:1232:LEU:HG	2.16	0.45
1:D:763:CYS:HB2	1:D:777:PHE:CD2	2.52	0.45
1:D:1326:THR:HG21	1:D:1386:LYS:HE3	1.98	0.45
1:A:406:ASP:OD1	1:A:406:ASP:N	2.50	0.45
1:A:1096:GLN:NE2	1:A:1097:LEU:O	2.49	0.45
1:A:1950:GLY:N	1:A:1951:PRO:HA	2.32	0.45
1:B:972:LEU:HG	1:B:1077:LEU:HD12	1.99	0.45
1:B:1329:GLY:O	1:B:1333:VAL:HG22	2.17	0.45
1:B:1397:VAL:HA	1:B:1400:VAL:HG12	1.99	0.45
1:B:1494:HIS:O	1:B:1497:ILE:N	2.45	0.45
1:B:1881:CYS:SG	1:B:1892:LEU:HD12	2.57	0.45
1:C:1469:LEU:HD21	1:C:1514:LEU:HD12	1.98	0.45
1:B:966:GLU:O	1:B:970:LYS:HG2	2.17	0.45
1:A:604:LYS:HD3	1:A:604:LYS:N	2.32	0.45
1:A:621:LEU:HD13	1:A:630:PHE:CD1	2.50	0.45
1:B:801:ARG:HD2	1:B:991:LEU:HD12	1.98	0.45
1:C:1405:CYS:SG	1:C:1406:ILE:N	2.89	0.45
1:C:2280:PRO:O	1:C:2284:ILE:HG13	2.17	0.45
1:D:252:LEU:HD13	1:D:417:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1741:ILE:HG21	1:A:1785:PHE:HE1	1.82	0.45
1:A:1931:GLU:O	1:A:1934:VAL:HG12	2.17	0.45
1:C:806:ILE:HG22	1:C:995:LYS:HD2	1.99	0.45
1:C:1385:ILE:O	1:C:1388:THR:OG1	2.32	0.45
1:C:1503:GLN:HG3	1:C:1544:LEU:HD22	1.98	0.45
1:A:1056:LEU:HD23	1:A:1056:LEU:C	2.37	0.45
1:A:2214:PHE:O	1:A:2218:ILE:HG12	2.16	0.45
1:B:1994:ASP:OD1	1:B:1994:ASP:C	2.55	0.45
1:D:2359:ILE:O	1:D:2363:THR:HG23	2.17	0.45
1:A:761:PHE:C	1:A:761:PHE:CD2	2.89	0.45
1:B:1303:LEU:HD12	1:B:1371:LEU:CD2	2.46	0.45
1:C:703:HIS:ND1	1:C:703:HIS:N	2.64	0.45
1:D:1396:VAL:HG13	1:D:1413:TYR:HB3	1.97	0.45
1:D:2352:GLU:HA	1:D:2352:GLU:OE1	2.17	0.45
1:B:1950:GLY:N	1:B:1951:PRO:HA	2.32	0.45
1:C:252:LEU:HD13	1:C:417:LEU:HD12	1.99	0.45
1:C:483:VAL:HG22	1:C:509:MET:SD	2.57	0.45
1:C:997:GLU:HA	1:C:997:GLU:OE1	2.17	0.45
1:C:1924:LEU:HD12	1:C:1927:LEU:HD12	1.99	0.45
1:C:2297:VAL:HG21	1:C:2327:ILE:CD1	2.47	0.45
1:D:2064:ASN:OD1	1:D:2066:GLN:N	2.50	0.45
1:A:1048:ASP:C	1:A:1048:ASP:OD1	2.55	0.45
1:A:1444:PHE:CD2	1:A:1472:VAL:HG13	2.52	0.45
1:D:1432:TYR:N	1:D:1432:TYR:CD1	2.84	0.45
1:D:1436:HIS:O	1:D:1439:THR:OG1	2.30	0.45
1:D:2009:ASP:OD1	1:D:2009:ASP:C	2.55	0.45
1:A:974:ILE:O	1:A:978:ILE:HG12	2.17	0.44
1:A:1434:SER:HB2	1:A:1436:HIS:CE1	2.52	0.44
1:B:871:ILE:HD13	1:B:974:ILE:HG23	1.98	0.44
1:B:1957:THR:HG22	1:B:2007:ARG:HH22	1.82	0.44
1:C:1514:LEU:HD23	1:C:1519:LYS:HG3	1.98	0.44
1:D:240:VAL:HG11	1:D:309:LEU:HD13	1.98	0.44
1:D:758:ASP:O	1:D:762:LEU:HD23	2.17	0.44
1:D:1393:LEU:HD11	1:D:1431:ILE:HG12	1.99	0.44
1:A:280:ASN:O	1:A:308:HIS:NE2	2.47	0.44
1:B:1220:LYS:HD3	1:B:1220:LYS:N	2.32	0.44
1:D:1931:GLU:O	1:D:1934:VAL:HG12	2.17	0.44
1:D:2178:LEU:HD13	1:D:2569:LEU:HD22	1.99	0.44
1:A:518:VAL:HG13	1:A:556:CYS:HB3	1.99	0.44
1:A:2159:THR:HG21	1:A:2167:LYS:HB3	1.99	0.44
1:B:1619:ASP:OD1	1:B:1687:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1333:VAL:HA	1:C:1368:LEU:HD21	1.99	0.44
1:A:252:LEU:HD13	1:A:417:LEU:HD12	1.99	0.44
1:A:729:TYR:O	1:A:733:LEU:HG	2.17	0.44
1:A:1696:GLN:O	1:A:1697:ASN:CB	2.65	0.44
1:B:406:ASP:OD1	1:B:406:ASP:N	2.50	0.44
1:B:2014:GLU:O	1:B:2018:ILE:HG13	2.18	0.44
1:C:621:LEU:HD13	1:C:630:PHE:CD1	2.52	0.44
1:D:1589:LYS:O	1:D:1593:GLU:OE1	2.36	0.44
1:A:607:GLU:OE2	1:A:608:LYS:NZ	2.45	0.44
1:A:1346:LEU:HD21	1:A:1402:HIS:CD2	2.52	0.44
1:C:451:MET:CE	1:C:451:MET:O	2.65	0.44
1:C:477:GLU:OE2	1:C:493:VAL:HG11	2.17	0.44
1:C:1924:LEU:HD22	1:C:1924:LEU:N	2.32	0.44
1:A:1250:LEU:HD23	1:A:1253:PHE:HB2	2.00	0.44
1:B:581:MET:N	1:B:581:MET:HE2	2.33	0.44
1:B:1286:PHE:O	1:B:1290:LEU:HG	2.18	0.44
1:B:1509:LEU:HD11	1:B:1551:MET:HE3	2.00	0.44
1:B:2284:ILE:HG22	1:B:2288:LEU:CD1	2.47	0.44
1:C:1741:ILE:HG21	1:C:1785:PHE:CE1	2.53	0.44
1:D:505:ARG:O	1:D:509:MET:HG3	2.16	0.44
1:D:1885:ASN:ND2	1:D:1888:LEU:HD23	2.33	0.44
1:A:745:TYR:N	1:A:1125:GLU:OE2	2.51	0.44
1:A:761:PHE:CE1	1:A:832:ASN:HB3	2.53	0.44
1:B:2323:HIS:O	1:B:2327:ILE:HG13	2.18	0.44
1:D:406:ASP:OD1	1:D:406:ASP:N	2.50	0.44
1:D:1345:LEU:O	1:D:1349:MET:HG3	2.18	0.44
1:A:1696:GLN:O	1:A:1697:ASN:HB3	2.17	0.44
1:C:1740:LEU:O	1:C:1744:THR:HG22	2.17	0.44
1:D:1334:VAL:HG23	1:D:1334:VAL:O	2.17	0.44
1:A:494:LEU:HD11	1:A:555:LEU:HG	1.99	0.43
1:A:2589:TYR:O	1:A:2593:MET:HG2	2.18	0.43
1:B:252:LEU:HD13	1:B:417:LEU:HD12	1.98	0.43
1:B:826:LYS:HD3	1:B:875:PHE:CD1	2.53	0.43
1:B:1967:ILE:O	1:B:1971:THR:HG23	2.18	0.43
1:D:772:ASP:OD1	1:D:773:LEU:N	2.49	0.43
1:D:1433:THR:O	1:D:1433:THR:CG2	2.66	0.43
1:D:1654:LEU:HD12	1:D:1654:LEU:O	2.17	0.43
1:D:1754:ILE:HG21	1:D:1872:PRO:HB2	2.00	0.43
1:A:834:MET:O	1:A:837:VAL:HG12	2.18	0.43
1:D:1006:ASP:OD2	1:D:1007:SER:N	2.51	0.43
1:D:1773:HIS:HB2	1:D:1888:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:LYS:CD	1:A:1126:LEU:HD13	2.48	0.43
1:A:1435:ASN:HA	1:A:1438:TRP:CD1	2.53	0.43
1:B:1444:PHE:CD2	1:B:1472:VAL:HG13	2.53	0.43
1:A:652:ILE:O	1:A:656:VAL:HG23	2.18	0.43
1:A:1247:HIS:HD2	1:A:1274:LEU:HD22	1.81	0.43
1:A:1379:LYS:NZ	1:A:1425:GLU:OE1	2.49	0.43
1:A:1911:LEU:HB2	1:A:1940:THR:HG21	2.00	0.43
1:B:580:MET:N	1:B:580:MET:CE	2.81	0.43
1:D:252:LEU:HD13	1:D:417:LEU:CD1	2.48	0.43
1:D:1377:GLU:O	1:D:1380:ASN:ND2	2.52	0.43
1:D:1530:ALA:O	1:D:1534:LYS:HG2	2.19	0.43
1:D:2015:ARG:HA	1:D:2018:ILE:HD12	2.00	0.43
1:A:1438:TRP:CD1	1:A:1494:HIS:CE1	3.07	0.43
1:A:1542:MET:SD	1:A:1542:MET:C	2.97	0.43
1:B:459:LEU:HD13	1:B:525:PRO:HD3	2.00	0.43
1:B:466:GLN:OE1	1:B:469:ARG:NH2	2.51	0.43
1:B:493:VAL:O	1:B:496:ILE:HG22	2.19	0.43
1:C:252:LEU:HD13	1:C:417:LEU:CD1	2.48	0.43
1:D:833:THR:HG21	1:D:866:LEU:HD21	2.01	0.43
1:D:1310:GLU:HG2	1:D:1310:GLU:O	2.18	0.43
1:B:698:ASP:OD1	1:B:699:LYS:N	2.51	0.43
1:B:1409:VAL:HG13	1:B:1413:TYR:CZ	2.54	0.43
1:C:801:ARG:NH2	1:C:984:ASP:OD1	2.52	0.43
1:C:816:ASP:OD1	1:C:817:SER:N	2.52	0.43
1:D:1454:LYS:HB3	1:D:1460:ALA:HA	2.00	0.43
1:D:1518:HIS:O	1:D:1522:VAL:HG23	2.19	0.43
1:A:639:VAL:HG12	1:A:738:ARG:HH21	1.84	0.43
1:A:857:ASN:HA	1:A:860:THR:HG22	2.00	0.43
1:B:743:ARG:NH1	1:B:745:TYR:OH	2.52	0.43
1:B:1514:LEU:HD23	1:B:1519:LYS:HG2	2.00	0.43
1:C:1509:LEU:HA	1:C:1514:LEU:HD22	2.00	0.43
1:A:252:LEU:HD13	1:A:417:LEU:CD1	2.49	0.43
1:A:580:MET:C	1:A:580:MET:HE2	2.38	0.43
1:A:585:ILE:HD13	1:A:595:ILE:HD12	1.99	0.43
1:A:1188:GLN:HA	1:A:1191:LYS:HG2	2.01	0.43
1:A:1885:ASN:ND2	1:A:1888:LEU:HD23	2.33	0.43
1:A:2294:ILE:CD1	1:A:2327:ILE:HD11	2.49	0.43
1:C:1366:ILE:HD11	1:C:1409:VAL:HG23	2.00	0.43
1:D:497:MET:SD	1:D:497:MET:C	2.97	0.43
1:D:1522:VAL:O	1:D:1526:ILE:HG22	2.19	0.43
1:A:882:LEU:O	1:A:886:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LEU:HD13	1:B:417:LEU:CD1	2.48	0.43
1:B:750:GLU:C	1:B:750:GLU:OE2	2.58	0.43
1:B:782:LEU:HD13	1:B:866:LEU:HA	2.00	0.43
1:B:1356:VAL:HG23	1:B:1363:MET:HE2	2.01	0.43
1:C:308:HIS:ND1	1:C:311:THR:OG1	2.30	0.43
1:D:1994:ASP:OD1	1:D:2052:ASN:ND2	2.52	0.43
1:A:1758:ILE:HD11	1:A:1872:PRO:O	2.18	0.43
1:B:974:ILE:HG22	1:B:978:ILE:HD11	2.00	0.43
1:B:1941:LEU:HD12	1:B:1992:LEU:HD12	2.01	0.43
1:C:580:MET:N	1:C:580:MET:CE	2.82	0.43
1:C:1501:LEU:HD23	1:C:1501:LEU:O	2.19	0.43
1:C:2131:ARG:HG2	1:C:2131:ARG:NH1	2.34	0.43
1:D:462:GLY:O	1:D:535:LEU:HD13	2.18	0.43
1:D:1388:THR:HG22	1:D:1421:TYR:CE1	2.54	0.43
1:D:1574:ARG:O	1:D:1575:ALA:HB3	2.19	0.43
1:D:1651:THR:OG1	1:D:1665:VAL:HG11	2.18	0.43
1:B:2159:THR:HG21	1:B:2167:LYS:HB3	2.01	0.42
1:C:2148:THR:OG1	1:C:2151:THR:OG1	2.34	0.42
1:D:1602:LEU:HD23	1:D:1602:LEU:O	2.19	0.42
1:A:842:ASN:O	1:A:845:VAL:HG12	2.19	0.42
1:A:1334:VAL:HG23	1:A:1334:VAL:O	2.19	0.42
1:B:496:ILE:HG23	1:B:562:HIS:NE2	2.35	0.42
1:B:834:MET:HE2	1:B:876:TYR:CE1	2.53	0.42
1:D:1505:THR:HG21	1:D:1526:ILE:HB	2.00	0.42
1:D:2017:LEU:HG	1:D:2060:LEU:HD22	2.01	0.42
1:A:1797:GLN:NE2	1:A:1906:GLU:O	2.52	0.42
1:B:1473:LEU:HD11	1:B:1522:VAL:HG23	2.01	0.42
1:C:1797:GLN:NE2	1:C:1906:GLU:OE2	2.49	0.42
1:D:592:GLU:O	1:D:596:THR:HG23	2.19	0.42
1:D:2261:ILE:O	1:D:2261:ILE:HG22	2.20	0.42
1:A:279:SER:OG	1:A:511:GLU:OE2	2.36	0.42
1:B:1948:CYS:SG	1:B:1959:ILE:HD12	2.60	0.42
1:A:1209:LEU:O	1:A:1212:ILE:HG22	2.19	0.42
1:D:729:TYR:O	1:D:733:LEU:HG	2.20	0.42
1:D:2607:ALA:HB3	1:D:2610:LEU:HD12	2.00	0.42
1:A:488:ASN:OD1	1:A:491:GLN:NE2	2.53	0.42
1:B:797:VAL:HG22	1:B:984:ASP:HB2	2.02	0.42
1:B:1956:GLN:NE2	1:B:2002:ALA:O	2.53	0.42
1:C:1382:TYR:O	1:C:1386:LYS:HG3	2.19	0.42
1:D:270:ARG:NH2	3:D:3002:I3P:O51	2.46	0.42
1:D:990:LEU:HD13	1:D:1035:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1339:LYS:O	1:D:1339:LYS:HD3	2.20	0.42
1:B:581:MET:HB3	1:B:595:ILE:HD11	2.01	0.42
1:B:760:ILE:HA	1:B:763:CYS:SG	2.59	0.42
1:D:1128:VAL:HG23	1:D:1221:MET:CE	2.50	0.42
1:D:1428:MET:HB3	1:D:1431:ILE:HD12	2.02	0.42
1:D:1513:TRP:O	1:D:1514:LEU:HB3	2.20	0.42
1:D:1666:LEU:HD11	1:D:1740:LEU:HD13	2.01	0.42
1:A:881:LEU:HD22	1:A:978:ILE:CD1	2.50	0.42
1:A:1328:ALA:HB3	1:A:1332:VAL:HG21	2.01	0.42
1:B:1124:SER:HA	1:B:1127:TRP:CE2	2.54	0.42
1:B:1411:MET:HG2	1:B:1467:TYR:HB2	2.01	0.42
1:C:1650:HIS:O	1:C:1654:LEU:HD23	2.19	0.42
1:D:755:LEU:HD13	1:D:780:LEU:HD21	2.01	0.42
1:D:1345:LEU:O	1:D:1348:MET:HG2	2.20	0.42
1:A:882:LEU:O	1:A:885:THR:OG1	2.37	0.42
1:A:1619:ASP:OD2	1:A:1619:ASP:N	2.53	0.42
1:A:2211:LEU:O	1:A:2215:ILE:HD12	2.20	0.42
1:A:2359:ILE:O	1:A:2363:THR:HG23	2.20	0.42
1:B:308:HIS:ND1	1:B:311:THR:OG1	2.30	0.42
1:B:518:VAL:HG13	1:B:556:CYS:SG	2.59	0.42
1:C:581:MET:HB3	1:C:595:ILE:HD11	2.01	0.42
1:C:630:PHE:O	1:C:634:LEU:HD13	2.20	0.42
1:C:1300:LEU:HB3	1:C:1371:LEU:HD22	2.02	0.42
1:D:630:PHE:O	1:D:634:LEU:HG	2.19	0.42
1:B:634:LEU:HA	1:B:637:LEU:HD12	2.02	0.42
1:B:1123:LYS:CD	1:B:1126:LEU:HD13	2.50	0.42
1:B:2369:ILE:HG23	1:B:2512:ILE:HG23	2.02	0.42
1:C:745:TYR:HA	1:C:748:ILE:HB	2.02	0.42
1:A:1023:MET:N	1:A:1023:MET:HE2	2.35	0.41
1:B:1054:MET:O	1:B:1058:VAL:HG22	2.19	0.41
1:B:1941:LEU:HD11	1:B:1973:LEU:HD13	2.02	0.41
1:B:2476:VAL:O	1:B:2479:ILE:HG13	2.20	0.41
1:A:1290:LEU:HD21	1:A:1299:TYR:CB	2.50	0.41
1:A:1457:LYS:O	1:A:1458:ARG:HB2	2.20	0.41
1:B:2294:ILE:O	1:B:2297:VAL:HG12	2.21	0.41
1:C:997:GLU:O	1:C:1001:VAL:HG23	2.20	0.41
1:C:1328:ALA:HB3	1:C:1332:VAL:HG21	2.02	0.41
1:D:1548:ILE:HA	1:D:1551:MET:HG2	2.02	0.41
1:A:653:CYS:SG	1:A:739:MET:HG2	2.60	0.41
1:B:515:LEU:HD21	1:B:563:SER:HB2	2.01	0.41
1:B:1218:ASP:O	1:B:1222:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2608:MET:HA	1:B:2611:VAL:HG12	2.02	0.41
1:C:1525:CYS:O	1:C:1528:THR:OG1	2.32	0.41
1:C:2390:PHE:N	1:C:2390:PHE:CD1	2.89	0.41
1:D:1881:CYS:SG	1:D:1892:LEU:HD12	2.61	0.41
1:A:1492:GLN:OE1	1:A:1492:GLN:N	2.54	0.41
1:A:1515:GLN:O	1:A:1519:LYS:N	2.46	0.41
1:B:991:LEU:HD11	1:B:1097:LEU:HD21	2.02	0.41
1:B:1048:ASP:OD1	1:B:1051:GLY:N	2.47	0.41
1:B:2020:LEU:HD21	1:B:2025:LEU:HD22	2.02	0.41
1:B:2164:GLN:N	1:B:2164:GLN:OE1	2.53	0.41
1:C:694:LEU:HD13	1:C:708:VAL:HG22	2.03	0.41
1:D:1182:MET:HE2	1:D:1182:MET:HA	2.02	0.41
1:B:888:LEU:CD1	1:B:974:ILE:HG21	2.51	0.41
1:C:694:LEU:CD1	1:C:708:VAL:HG22	2.50	0.41
1:D:480:VAL:CG2	1:D:559:VAL:HG23	2.50	0.41
1:D:1117:LEU:HB2	1:D:1175:ILE:HG21	2.02	0.41
1:B:1221:MET:O	1:B:1221:MET:SD	2.78	0.41
1:B:1409:VAL:CG1	1:B:1413:TYR:CZ	3.04	0.41
1:B:1689:MET:HA	1:B:1689:MET:CE	2.50	0.41
1:D:722:ASP:HA	1:D:725:VAL:HG12	2.02	0.41
1:D:1085:ARG:HB2	1:D:1610:VAL:HG22	2.03	0.41
1:D:1626:LEU:HD13	1:D:1698:ARG:CB	2.51	0.41
1:A:466:GLN:OE1	1:A:469:ARG:NH2	2.52	0.41
1:A:1628:PHE:CD1	1:A:1628:PHE:N	2.88	0.41
1:A:2187:LYS:HB2	1:A:2187:LYS:HE3	1.95	0.41
1:A:2549:ASP:OD1	1:A:2549:ASP:N	2.53	0.41
1:C:2389:LEU:HD21	1:D:2339:LEU:CD1	2.51	0.41
1:D:692:VAL:HG21	1:D:763:CYS:SG	2.61	0.41
1:D:1606:LEU:CD2	1:D:1609:LEU:HD12	2.51	0.41
1:D:1869:ILE:O	1:D:1869:ILE:HD12	2.21	0.41
1:A:439:ILE:H	1:A:439:ILE:HD12	1.86	0.41
1:A:1439:THR:HA	1:A:1442:GLU:HG2	2.02	0.41
1:A:1492:GLN:CD	1:A:1493:THR:HG23	2.41	0.41
1:B:722:ASP:HA	1:B:725:VAL:HG12	2.02	0.41
1:B:877:SER:OG	1:B:878:PHE:N	2.53	0.41
1:B:1316:LYS:HD2	1:B:1316:LYS:N	2.36	0.41
1:C:606:LEU:HD23	1:C:645:ILE:CD1	2.50	0.41
1:C:871:ILE:HD11	1:C:884:LEU:CD2	2.51	0.41
1:C:1125:GLU:HA	1:C:1128:VAL:HG12	2.03	0.41
1:C:1316:LYS:HD3	1:C:1316:LYS:H	1.86	0.41
1:D:282:LEU:HD22	1:D:434:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:536:VAL:HG12	1:D:537:ARG:N	2.35	0.41
1:A:253:THR:HG22	1:A:254:CYS:N	2.36	0.41
1:A:596:THR:HG21	1:A:633:TYR:HD1	1.86	0.41
1:A:1501:LEU:HD23	1:A:1501:LEU:O	2.21	0.41
1:A:1919:THR:HG22	1:A:1924:LEU:HD23	2.03	0.41
1:B:581:MET:HE2	1:B:581:MET:H	1.85	0.41
1:B:822:SER:O	1:B:826:LYS:HG2	2.21	0.41
1:B:1551:MET:O	1:B:1551:MET:SD	2.78	0.41
1:B:1771:SER:O	1:B:1775:LEU:HG	2.21	0.41
1:C:1397:VAL:O	1:C:1401:THR:HG23	2.20	0.41
1:C:1439:THR:HA	1:C:1442:GLU:HG2	2.03	0.41
1:C:1469:LEU:HD22	1:C:1518:HIS:CD2	2.55	0.41
1:C:1626:LEU:HD13	1:C:1698:ARG:HB2	2.03	0.41
1:D:459:LEU:HD22	1:D:525:PRO:HG3	2.03	0.41
1:D:1067:TYR:O	1:D:1071:VAL:HG23	2.20	0.41
1:D:1284:GLN:HA	1:D:1287:VAL:HG22	2.03	0.41
1:D:1362:LEU:HD11	1:D:1409:VAL:CG2	2.51	0.41
1:D:1473:LEU:HD11	1:D:1522:VAL:HG22	2.03	0.41
1:D:1740:LEU:O	1:D:1744:THR:HG22	2.21	0.41
1:D:2155:LEU:HD22	1:D:2178:LEU:HD11	2.03	0.41
1:A:235:LEU:N	1:A:381:VAL:O	2.54	0.41
1:A:606:LEU:HD23	1:A:645:ILE:HD13	2.02	0.41
1:A:754:GLN:HA	1:A:754:GLN:OE1	2.21	0.41
1:A:810:ILE:HG21	1:A:989:TYR:HA	2.02	0.41
1:A:1214:TYR:CD2	1:A:1221:MET:HG3	2.56	0.41
1:B:606:LEU:HD12	1:B:610:ILE:HG12	2.02	0.41
1:B:843:ASN:O	1:B:847:GLU:HG3	2.21	0.41
1:B:1674:LEU:HD23	1:B:1674:LEU:HA	1.98	0.41
1:C:1871:GLN:HB3	1:C:1872:PRO:HD3	2.02	0.41
1:C:2297:VAL:O	1:C:2301:VAL:HG22	2.21	0.41
1:C:2558:HIS:CE1	1:C:2563:HIS:ND1	2.89	0.41
1:D:1263:THR:HG22	1:D:1267:ILE:CD1	2.51	0.41
1:D:1626:LEU:HD12	1:D:1695:LEU:HD13	2.03	0.41
1:D:1741:ILE:HG21	1:D:1785:PHE:CE1	2.56	0.41
1:A:722:ASP:HA	1:A:725:VAL:HG12	2.03	0.40
1:A:1221:MET:O	1:A:1221:MET:SD	2.80	0.40
1:A:1221:MET:SD	1:A:1225:LEU:HG	2.61	0.40
1:B:235:LEU:N	1:B:381:VAL:O	2.54	0.40
1:B:1056:LEU:HD12	1:B:1694:TYR:CD2	2.55	0.40
1:B:1120:MET:O	1:B:1127:TRP:NE1	2.47	0.40
1:B:1174:GLY:O	1:B:1178:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1266:HIS:CD2	1:B:1266:HIS:N	2.86	0.40
1:B:1646:LYS:HD2	1:B:1646:LYS:O	2.21	0.40
1:C:451:MET:HG3	1:C:475:LEU:HD22	2.03	0.40
1:D:308:HIS:ND1	1:D:311:THR:OG1	2.31	0.40
1:D:608:LYS:C	1:D:608:LYS:HD3	2.42	0.40
1:D:667:ARG:HD3	1:D:668:THR:N	2.36	0.40
1:D:2007:ARG:HG3	1:D:2007:ARG:HH11	1.86	0.40
1:A:2071:LEU:CD2	1:A:2114:LEU:HD22	2.51	0.40
1:B:1297:VAL:HG12	1:B:1364:TYR:HA	2.03	0.40
1:C:591:ALA:O	1:C:595:ILE:HD12	2.21	0.40
1:C:1209:LEU:O	1:C:1212:ILE:HG22	2.21	0.40
1:D:1288:HIS:CE1	1:D:1292:THR:HG21	2.56	0.40
1:A:694:LEU:O	1:A:705:GLU:HA	2.21	0.40
1:A:1322:MET:HE1	1:A:1323:THR:HA	2.03	0.40
1:B:253:THR:HG22	1:B:254:CYS:N	2.36	0.40
1:B:1124:SER:CB	1:B:1212:ILE:HD11	2.48	0.40
1:B:1333:VAL:HG23	1:B:1333:VAL:O	2.22	0.40
1:C:582:GLN:O	1:C:585:ILE:HG22	2.21	0.40
1:C:2297:VAL:HG21	1:C:2327:ILE:HD11	2.03	0.40
1:D:447:ASP:O	1:D:451:MET:HG2	2.22	0.40
1:D:1626:LEU:HD22	1:D:1698:ARG:CB	2.51	0.40
1:A:462:GLY:O	1:A:535:LEU:HD13	2.21	0.40
1:A:1421:TYR:O	1:A:1424:THR:HG23	2.22	0.40
1:A:1741:ILE:HG23	1:A:1750:PHE:HE2	1.86	0.40
1:B:439:ILE:H	1:B:439:ILE:HD12	1.87	0.40
1:C:235:LEU:N	1:C:381:VAL:O	2.55	0.40
1:C:554:ARG:O	1:C:558:ARG:HG2	2.21	0.40
1:C:743:ARG:NH1	1:C:788:ARG:O	2.55	0.40
1:C:2518:ASP:CG	1:D:2524:ARG:NH2	2.74	0.40
1:D:480:VAL:HG22	1:D:559:VAL:HG23	2.02	0.40
1:A:694:LEU:HD13	1:A:708:VAL:HG22	2.03	0.40
1:A:1304:HIS:CD2	1:A:1304:HIS:C	2.94	0.40
1:A:2610:LEU:HD23	1:A:2610:LEU:HA	1.99	0.40
1:B:823:ARG:HA	1:B:826:LYS:HG2	2.04	0.40
1:B:1381:VAL:HG13	1:B:1382:TYR:N	2.37	0.40
1:C:1462:PRO:O	1:C:1466:LYS:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1961/2671 (73%)	1930 (98%)	30 (2%)	1 (0%)	51 83
1	B	1959/2671 (73%)	1933 (99%)	26 (1%)	0	100 100
1	C	1978/2671 (74%)	1951 (99%)	27 (1%)	0	100 100
1	D	2010/2671 (75%)	1979 (98%)	30 (2%)	1 (0%)	100 100
All	All	7908/10684 (74%)	7793 (98%)	113 (1%)	2 (0%)	100 100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1514	LEU
1	A	1697	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1807/2385 (76%)	1764 (98%)	43 (2%)	49 77
1	B	1805/2385 (76%)	1764 (98%)	41 (2%)	50 78
1	C	1820/2385 (76%)	1790 (98%)	30 (2%)	62 84
1	D	1838/2385 (77%)	1805 (98%)	33 (2%)	59 82
All	All	7270/9540 (76%)	7123 (98%)	147 (2%)	57 80

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	463	PHE
1	A	552	MET
1	A	567	TYR
1	A	580	MET
1	A	600	HIS
1	A	758	ASP
1	A	761	PHE
1	A	830	PHE
1	A	988	SER
1	A	1092	PHE
1	A	1100	SER
1	A	1107	TYR
1	A	1115	ASP
1	A	1203	HIS
1	A	1214	TYR
1	A	1233	GLN
1	A	1236	CYS
1	A	1253	PHE
1	A	1308	LYS
1	A	1322	MET
1	A	1325	LEU
1	A	1339	LYS
1	A	1348	MET
1	A	1411	MET
1	A	1458	ARG
1	A	1507	ARG
1	A	1619	ASP
1	A	1698	ARG
1	A	1772	PHE
1	A	1894	CYS
1	A	1897	ASN
1	A	1958	CYS
1	A	1965	ASN
1	A	1984	TYR
1	A	2160	GLU
1	A	2166	SER
1	A	2170	ASP
1	A	2176	SER
1	A	2393	ASP
1	A	2549	ASP
1	A	2565	MET
1	A	2576	ARG
1	A	2592	GLN

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Mol	Chain	Res	Type
1	B	552	MET
1	B	567	TYR
1	B	581	MET
1	B	612	LYS
1	B	618	PHE
1	B	632	ASP
1	B	703	HIS
1	B	714	GLU
1	B	724	ASN
1	B	728	TYR
1	B	743	ARG
1	B	818	ASN
1	B	1035	MET
1	B	1044	MET
1	B	1048	ASP
1	B	1072	SER
1	B	1211	GLN
1	B	1249	HIS
1	B	1268	PHE
1	B	1288	HIS
1	B	1327	ASN
1	B	1364	TYR
1	B	1370	ASP
1	B	1382	TYR
1	B	1458	ARG
1	B	1467	TYR
1	B	1619	ASP
1	B	1635	TYR
1	B	1655	MET
1	B	1787	LYS
1	B	1871	GLN
1	B	1895	GLN
1	B	1905	CYS
1	B	1964	SER
1	B	2033	TYR
1	B	2166	SER
1	B	2191	MET
1	B	2292	ASN
1	B	2318	MET
1	B	2466	MET
1	B	2549	ASP
1	C	552	MET

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Mol	Chain	Res	Type
1	C	567	TYR
1	C	682	TYR
1	C	703	HIS
1	C	722	ASP
1	C	742	ASP
1	C	749	ASP
1	C	778	CYS
1	C	1040	LYS
1	C	1049	ASP
1	C	1115	ASP
1	C	1203	HIS
1	C	1251	HIS
1	C	1331	ASP
1	C	1348	MET
1	C	1353	ARG
1	C	1458	ARG
1	C	1542	MET
1	C	1698	ARG
1	C	1905	CYS
1	C	1982	CYS
1	C	2010	SER
1	C	2162	ASP
1	C	2198	SER
1	C	2326	TYR
1	C	2361	SER
1	C	2449	ASP
1	C	2461	CYS
1	C	2520	PHE
1	C	2528	GLN
1	D	454	SER
1	D	552	MET
1	D	567	TYR
1	D	580	MET
1	D	635	SER
1	D	722	ASP
1	D	758	ASP
1	D	766	ASP
1	D	846	SER
1	D	1018	SER
1	D	1022	ASN
1	D	1043	SER
1	D	1061	HIS

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Mol	Chain	Res	Type
1	D	1222	MET
1	D	1322	MET
1	D	1360	SER
1	D	1364	TYR
1	D	1458	ARG
1	D	1531	MET
1	D	1542	MET
1	D	1551	MET
1	D	1578	ARG
1	D	1689	MET
1	D	1698	ARG
1	D	1795	ARG
1	D	1802	SER
1	D	1905	CYS
1	D	1987	ASP
1	D	2033	TYR
1	D	2047	ARG
1	D	2173	ASP
1	D	2299	SER
1	D	2330	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	783	HIS
1	A	791	GLN
1	A	1304	HIS
1	B	1065	HIS
1	B	1304	HIS
1	B	1318	GLN
1	B	1418	ASN
1	B	2135	GLN
1	C	573	HIS
1	C	1247	HIS
1	C	1304	HIS
1	D	1229	HIS
1	D	1318	GLN
1	D	1380	ASN
1	D	1622	HIS
1	D	2550	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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	I3P	C	3002	-	24,24,24	2.08	3 (12%)	36,39,39	0.85	0
5	ATP	C	3004	-	26,33,33	0.60	0	31,52,52	1.05	2 (6%)
5	ATP	A	3004	-	26,33,33	0.60	0	31,52,52	1.07	2 (6%)
3	I3P	D	3002	-	24,24,24	2.08	3 (12%)	36,39,39	0.84	0
5	ATP	B	3004	-	26,33,33	0.60	0	31,52,52	1.07	2 (6%)
3	I3P	B	3002	-	24,24,24	2.08	3 (12%)	36,39,39	0.84	0
3	I3P	A	3002	-	24,24,24	2.08	3 (12%)	36,39,39	0.84	0
5	ATP	D	3004	-	26,33,33	0.60	0	31,52,52	1.08	3 (9%)

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	I3P	C	3002	-	-	3/15/39/39	0/1/1/1
5	ATP	C	3004	-	-	8/18/38/38	0/3/3/3
5	ATP	A	3004	-	-	5/18/38/38	0/3/3/3
3	I3P	D	3002	-	-	2/15/39/39	0/1/1/1
5	ATP	B	3004	-	-	7/18/38/38	0/3/3/3
3	I3P	B	3002	-	-	3/15/39/39	0/1/1/1
3	I3P	A	3002	-	-	3/15/39/39	0/1/1/1
5	ATP	D	3004	-	-	3/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3002	I3P	P4-O4	5.74	1.70	1.59
3	B	3002	I3P	P4-O4	5.74	1.70	1.59
3	A	3002	I3P	P4-O4	5.73	1.70	1.59
3	D	3002	I3P	P4-O4	5.73	1.70	1.59
3	D	3002	I3P	P5-O5	5.65	1.70	1.59
3	B	3002	I3P	P5-O5	5.64	1.70	1.59
3	C	3002	I3P	P5-O5	5.64	1.70	1.59
3	A	3002	I3P	P5-O5	5.63	1.69	1.59
3	D	3002	I3P	P1-O1	5.46	1.69	1.59
3	A	3002	I3P	P1-O1	5.45	1.69	1.59
3	B	3002	I3P	P1-O1	5.43	1.69	1.59
3	C	3002	I3P	P1-O1	5.43	1.69	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	3004	ATP	C5-C6-N6	2.32	123.88	120.35
5	B	3004	ATP	C5-C6-N6	2.30	123.85	120.35
5	A	3004	ATP	C5-C6-N6	2.30	123.85	120.35
5	C	3004	ATP	C5-C6-N6	2.30	123.85	120.35
5	D	3004	ATP	O4'-C1'-C2'	-2.09	103.87	106.93
5	C	3004	ATP	PB-O3B-PG	2.05	139.85	132.83
5	D	3004	ATP	PB-O3B-PG	2.05	139.84	132.83
5	A	3004	ATP	PB-O3B-PG	2.05	139.84	132.83
5	B	3004	ATP	PB-O3B-PG	2.04	139.84	132.83

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	3002	I3P	C5-O5-P5-O53
5	A	3004	ATP	C5'-O5'-PA-O2A
5	B	3004	ATP	C5'-O5'-PA-O2A
5	C	3004	ATP	PB-O3B-PG-O2G
5	C	3004	ATP	C5'-O5'-PA-O1A
5	C	3004	ATP	C5'-O5'-PA-O2A
5	D	3004	ATP	PB-O3B-PG-O2G
5	D	3004	ATP	PB-O3B-PG-O3G
5	A	3004	ATP	C3'-C4'-C5'-O5'
5	C	3004	ATP	O4'-C4'-C5'-O5'
5	C	3004	ATP	C3'-C4'-C5'-O5'
5	A	3004	ATP	O4'-C4'-C5'-O5'
5	B	3004	ATP	C3'-C4'-C5'-O5'
5	B	3004	ATP	O4'-C4'-C5'-O5'
3	A	3002	I3P	C4-O4-P4-O42
3	B	3002	I3P	C4-O4-P4-O42
3	C	3002	I3P	C4-O4-P4-O42
3	D	3002	I3P	C6-C1-O1-P1
5	A	3004	ATP	C5'-O5'-PA-O3A
5	C	3004	ATP	C5'-O5'-PA-O3A
5	A	3004	ATP	C5'-O5'-PA-O1A
5	B	3004	ATP	C5'-O5'-PA-O1A
3	A	3002	I3P	C6-C1-O1-P1
3	C	3002	I3P	C6-C1-O1-P1
5	C	3004	ATP	PB-O3A-PA-O2A
3	B	3002	I3P	C6-C1-O1-P1
5	B	3004	ATP	PG-O3B-PB-O2B
5	C	3004	ATP	PG-O3B-PB-O2B
3	A	3002	I3P	C5-O5-P5-O52
3	B	3002	I3P	C5-O5-P5-O52
3	C	3002	I3P	C5-O5-P5-O52
5	B	3004	ATP	C5'-O5'-PA-O3A
5	B	3004	ATP	PG-O3B-PB-O1B
5	D	3004	ATP	PG-O3B-PB-O1B

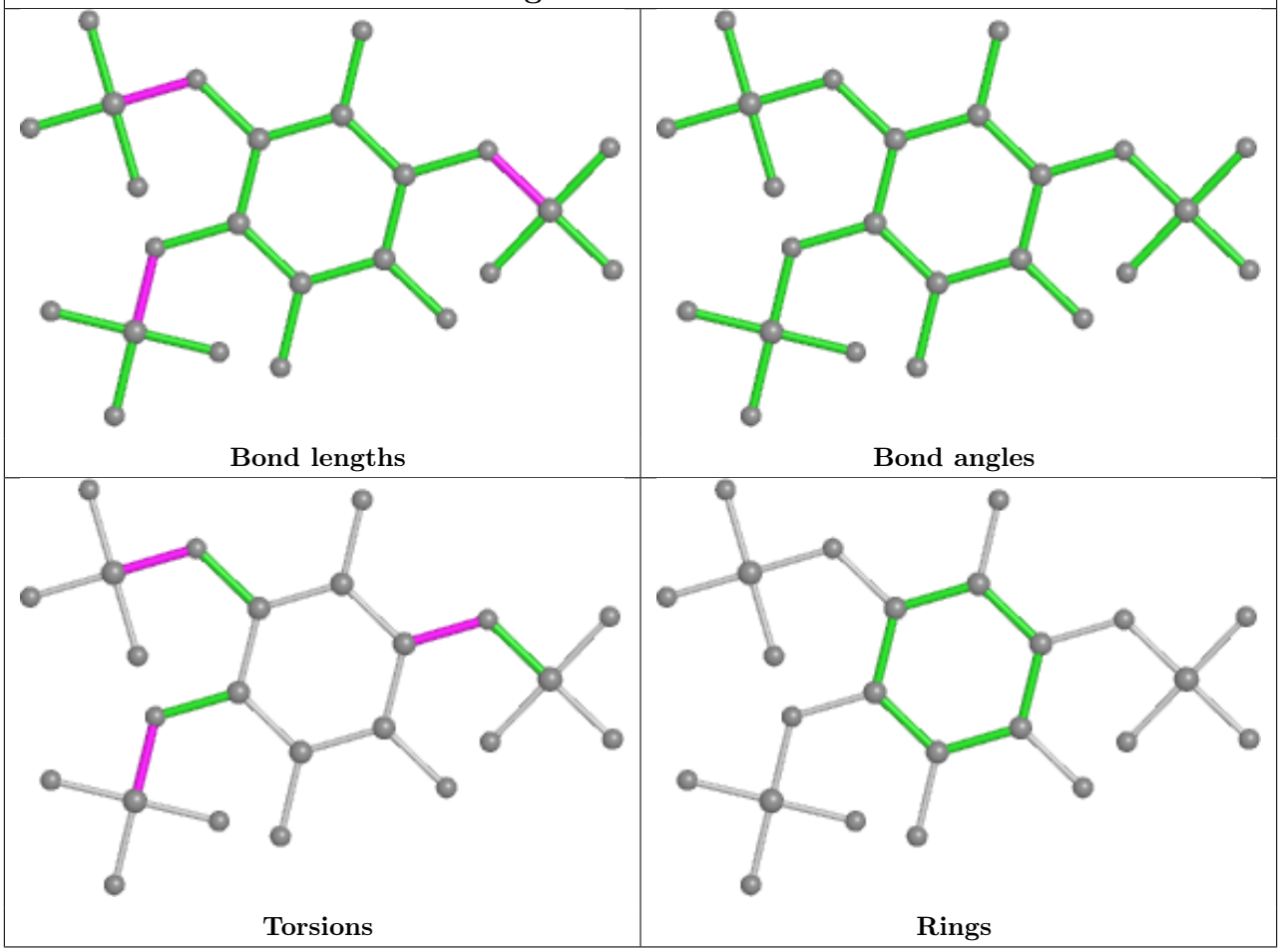
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3002	I3P	1	0
3	D	3002	I3P	1	0
3	B	3002	I3P	1	0
3	A	3002	I3P	1	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 then 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.

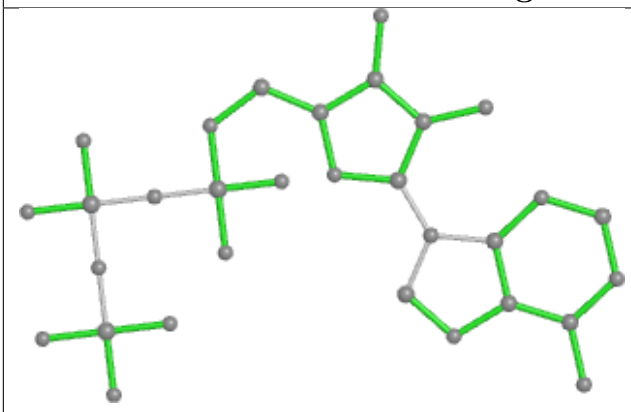
Ligand I3P C 3002



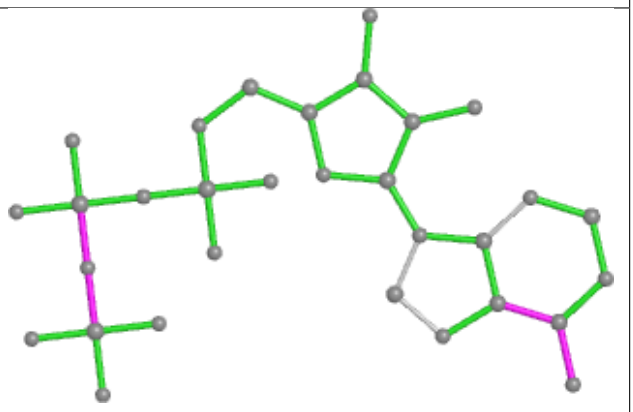
Bond lengths **Bond angles**

Torsions **Rings**

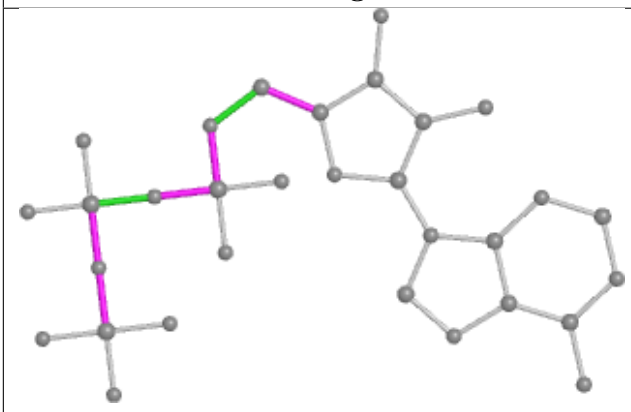
Ligand ATP C 3004



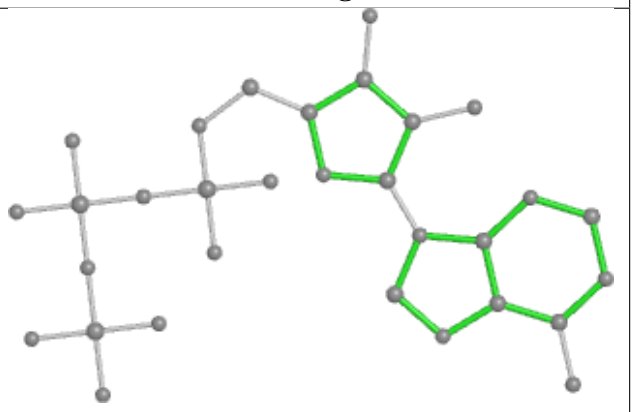
Bond lengths



Bond angles

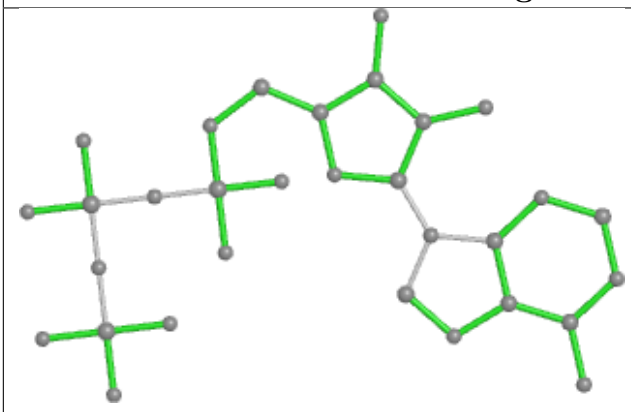


Torsions

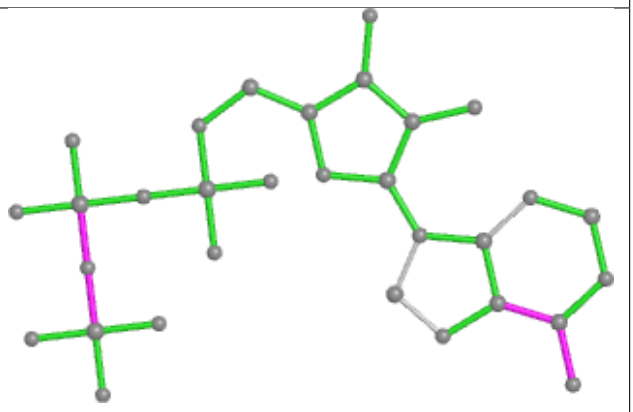


Rings

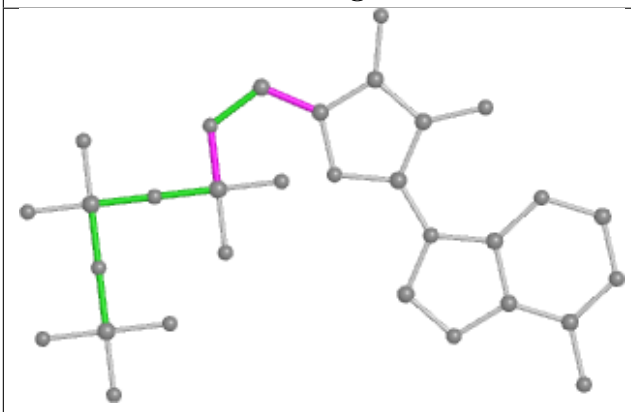
Ligand ATP A 3004



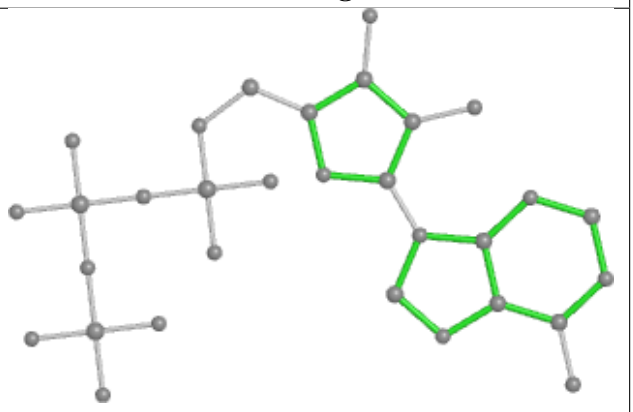
Bond lengths



Bond angles

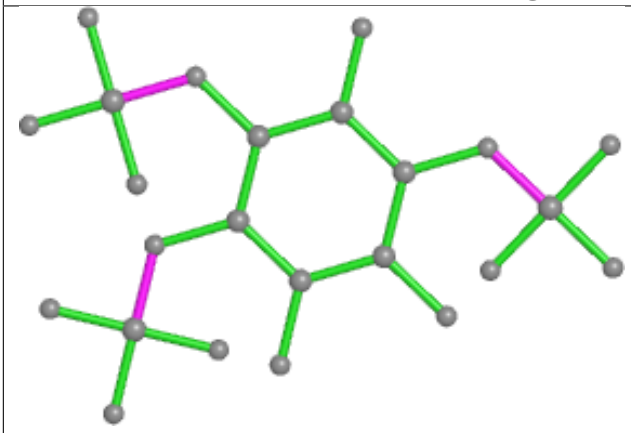


Torsions

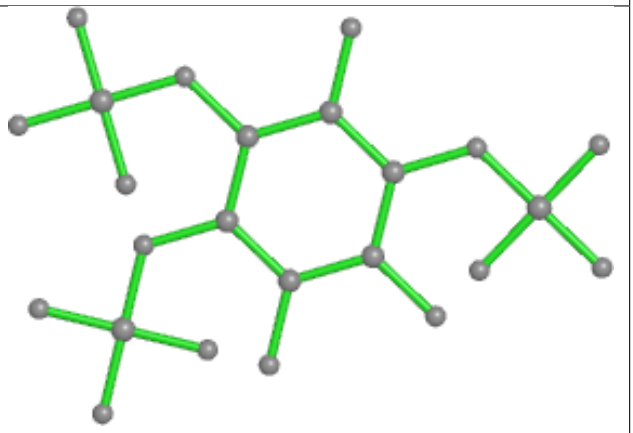


Rings

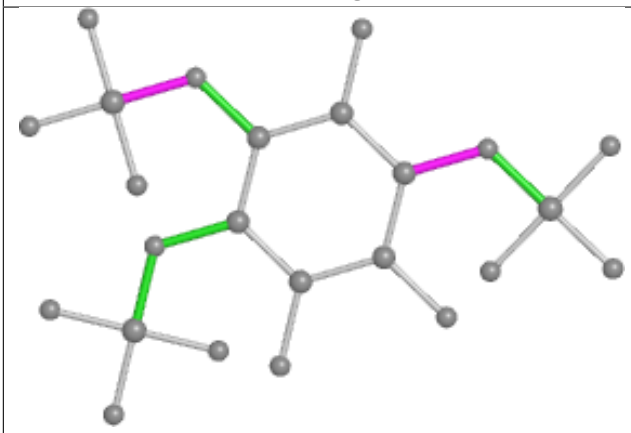
Ligand I3P D 3002



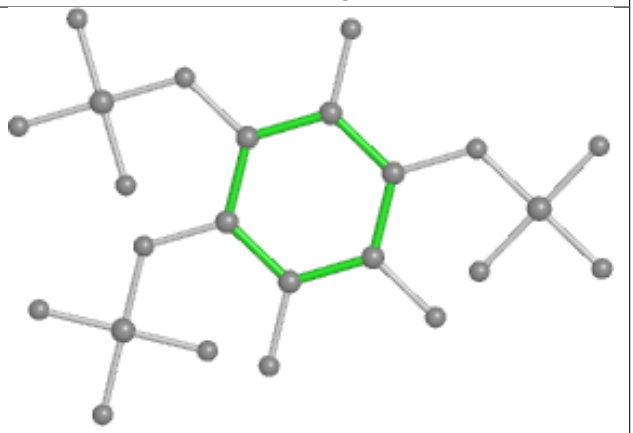
Bond lengths



Bond angles

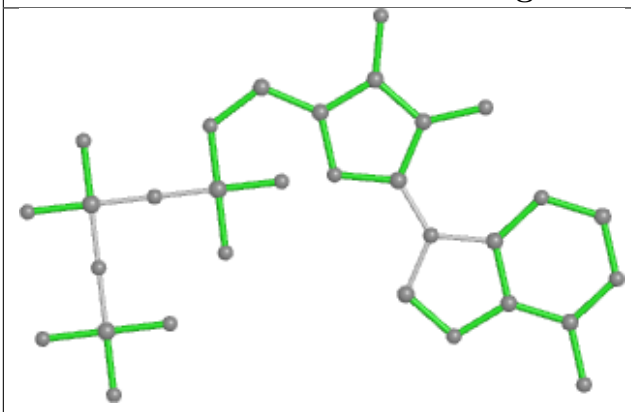


Torsions

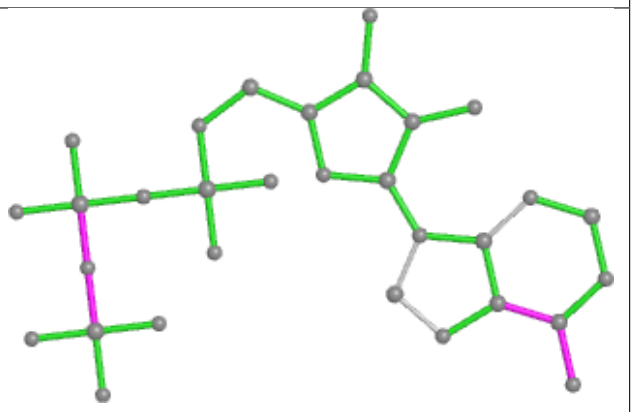


Rings

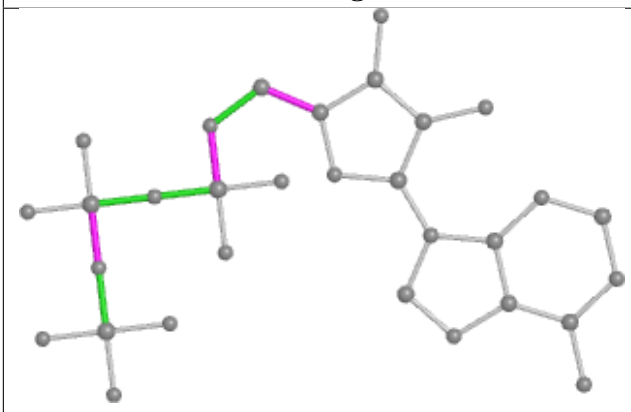
Ligand ATP B 3004



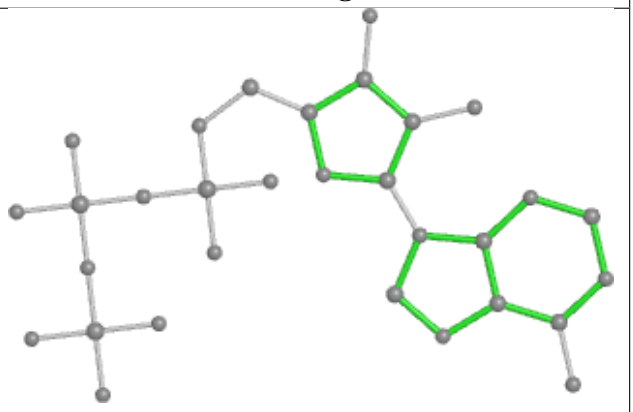
Bond lengths



Bond angles

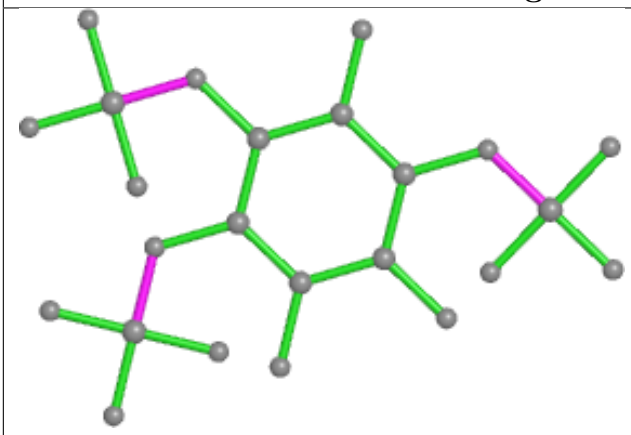


Torsions

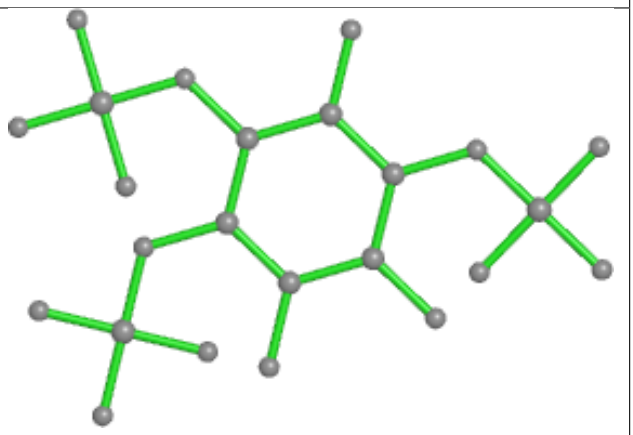


Rings

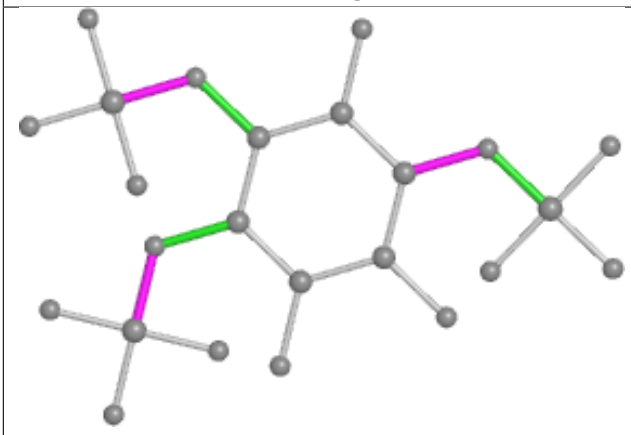
Ligand I3P B 3002



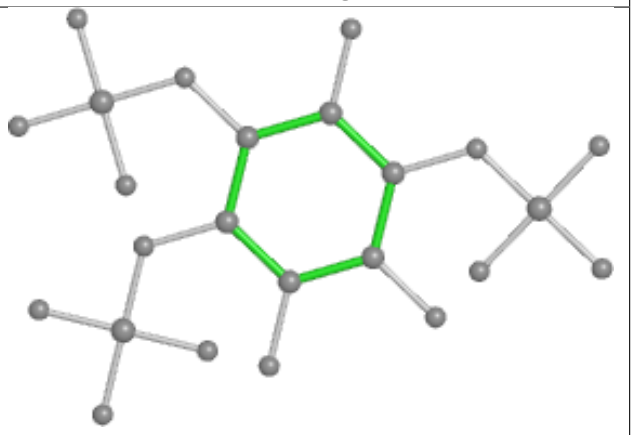
Bond lengths



Bond angles

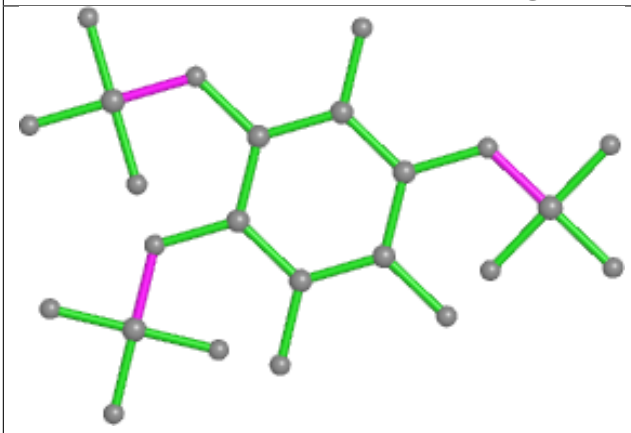


Torsions

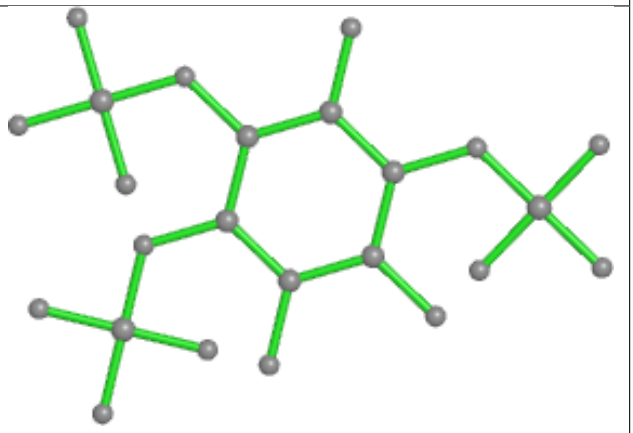


Rings

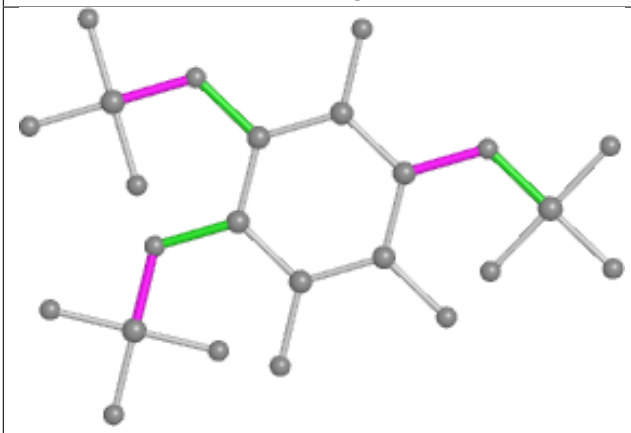
Ligand I3P A 3002



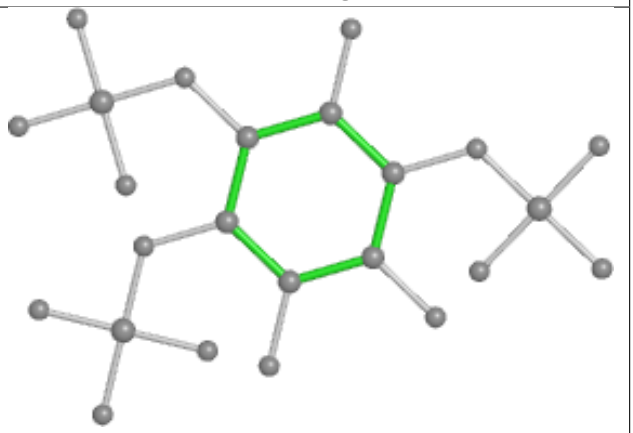
Bond lengths



Bond angles

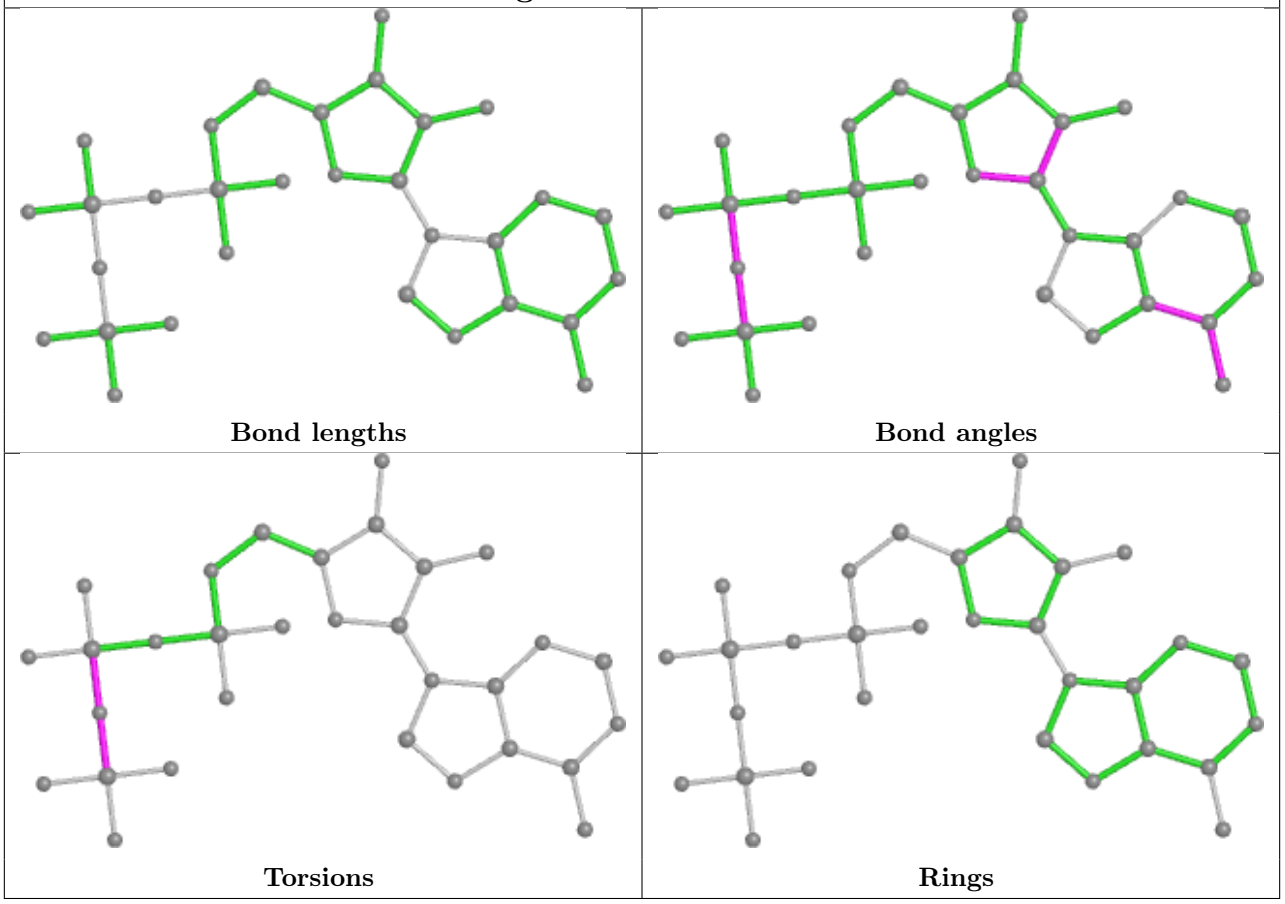


Torsions



Rings

Ligand ATP D 3004



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.

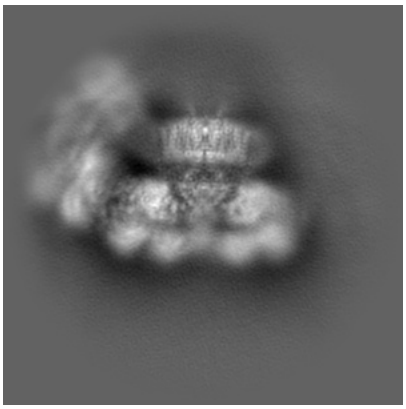
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41366. These allow visual inspection of the internal detail of the map and identification of artifacts.

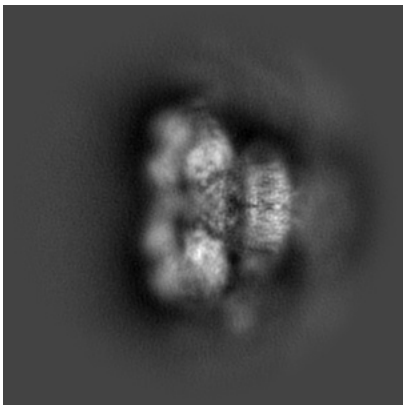
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

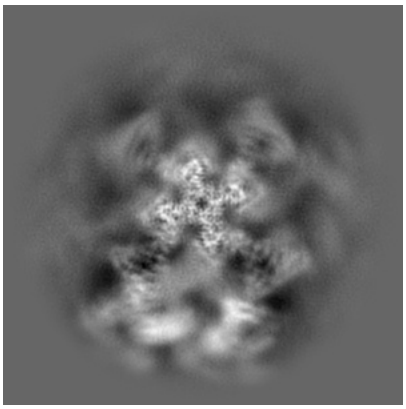
6.1.1 Primary map



X

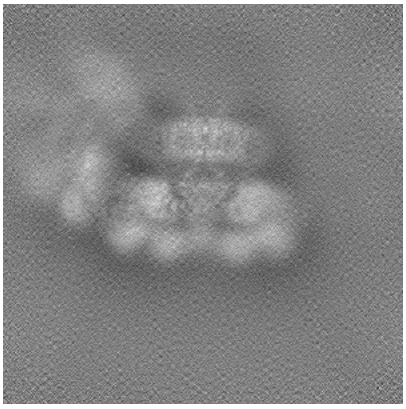


Y

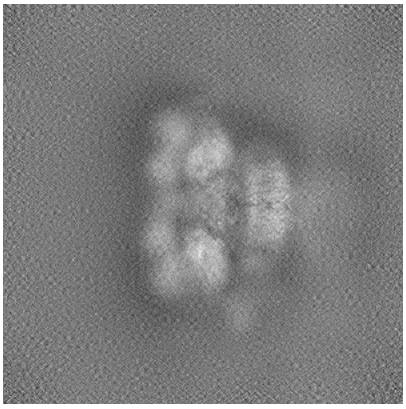


Z

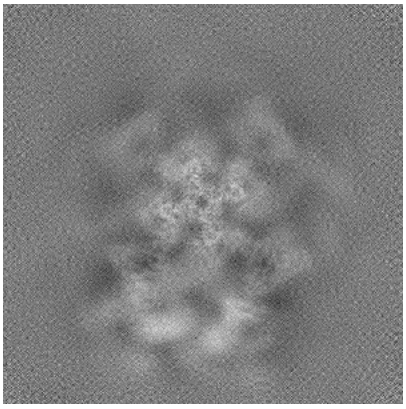
6.1.2 Raw map



X



Y

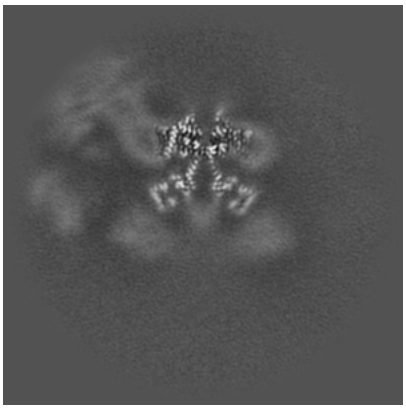


Z

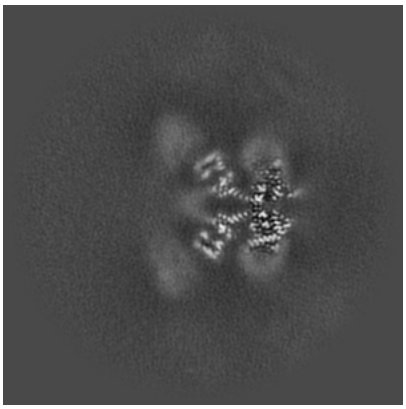
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

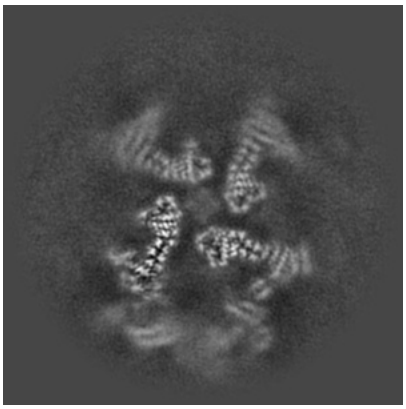
6.2.1 Primary map



X Index: 256

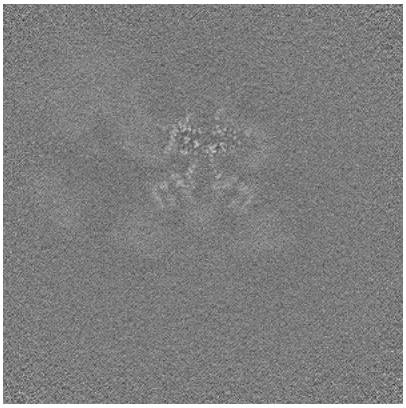


Y Index: 256

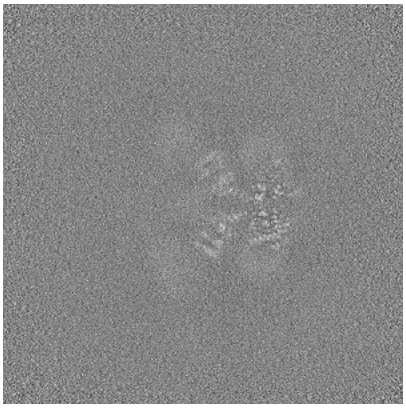


Z Index: 256

6.2.2 Raw map



X Index: 256



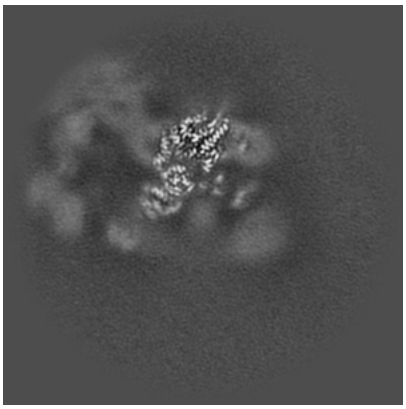
Y Index: 256

Z Index: 256

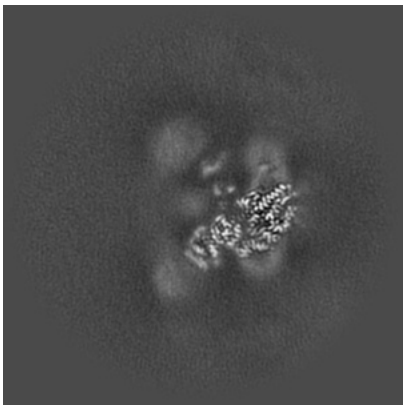
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

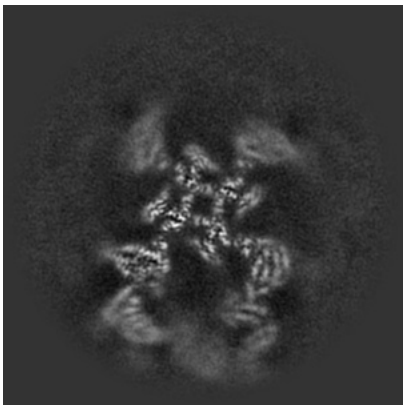
6.3.1 Primary map



X Index: 266

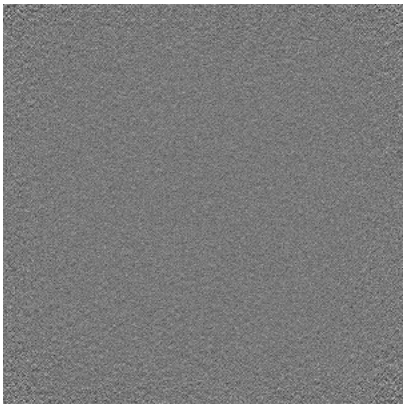


Y Index: 246

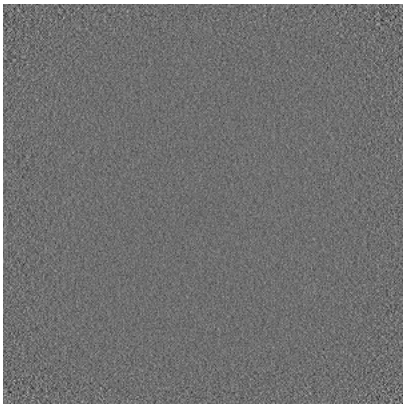


Z Index: 271

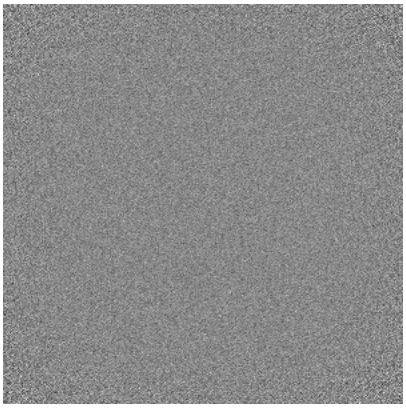
6.3.2 Raw map



X Index: 0



Y Index: 0

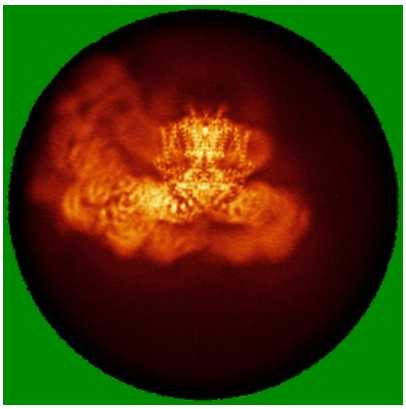


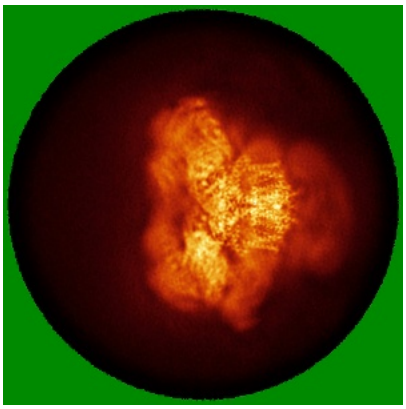
Z Index: 0

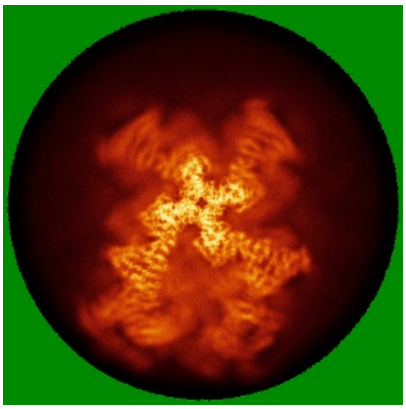
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

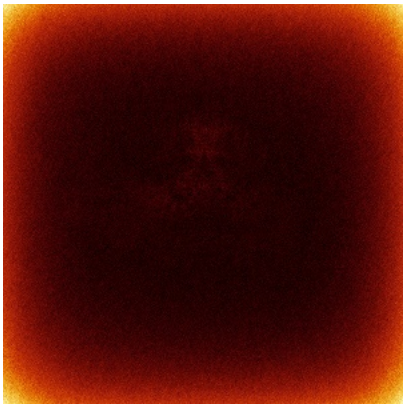
6.4.1 Primary map

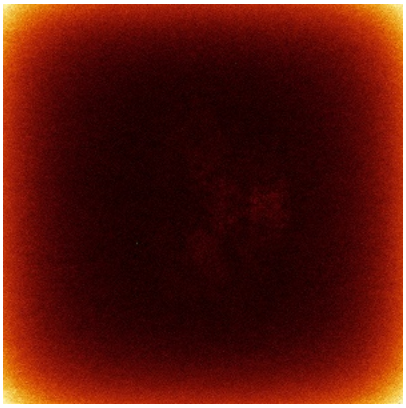

X

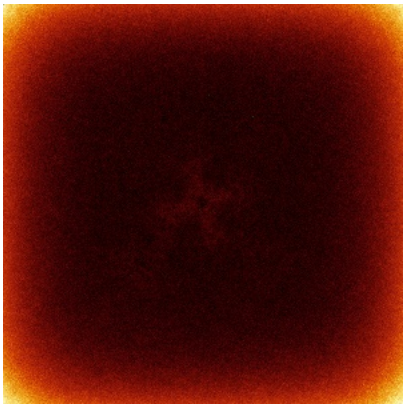

Y


Z

6.4.2 Raw map


X

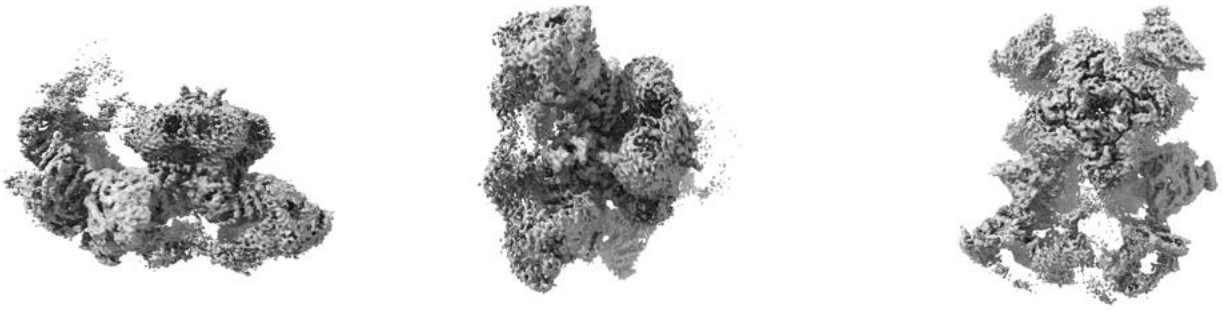

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

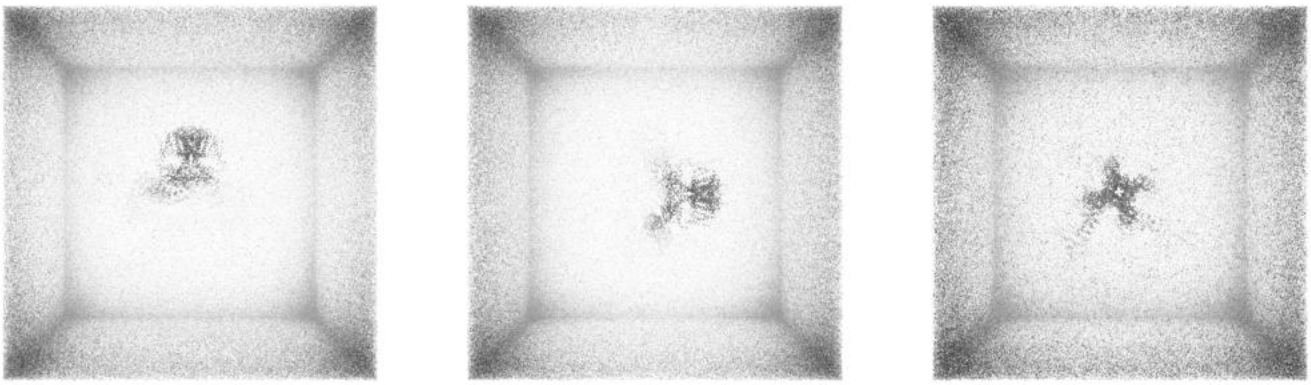
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

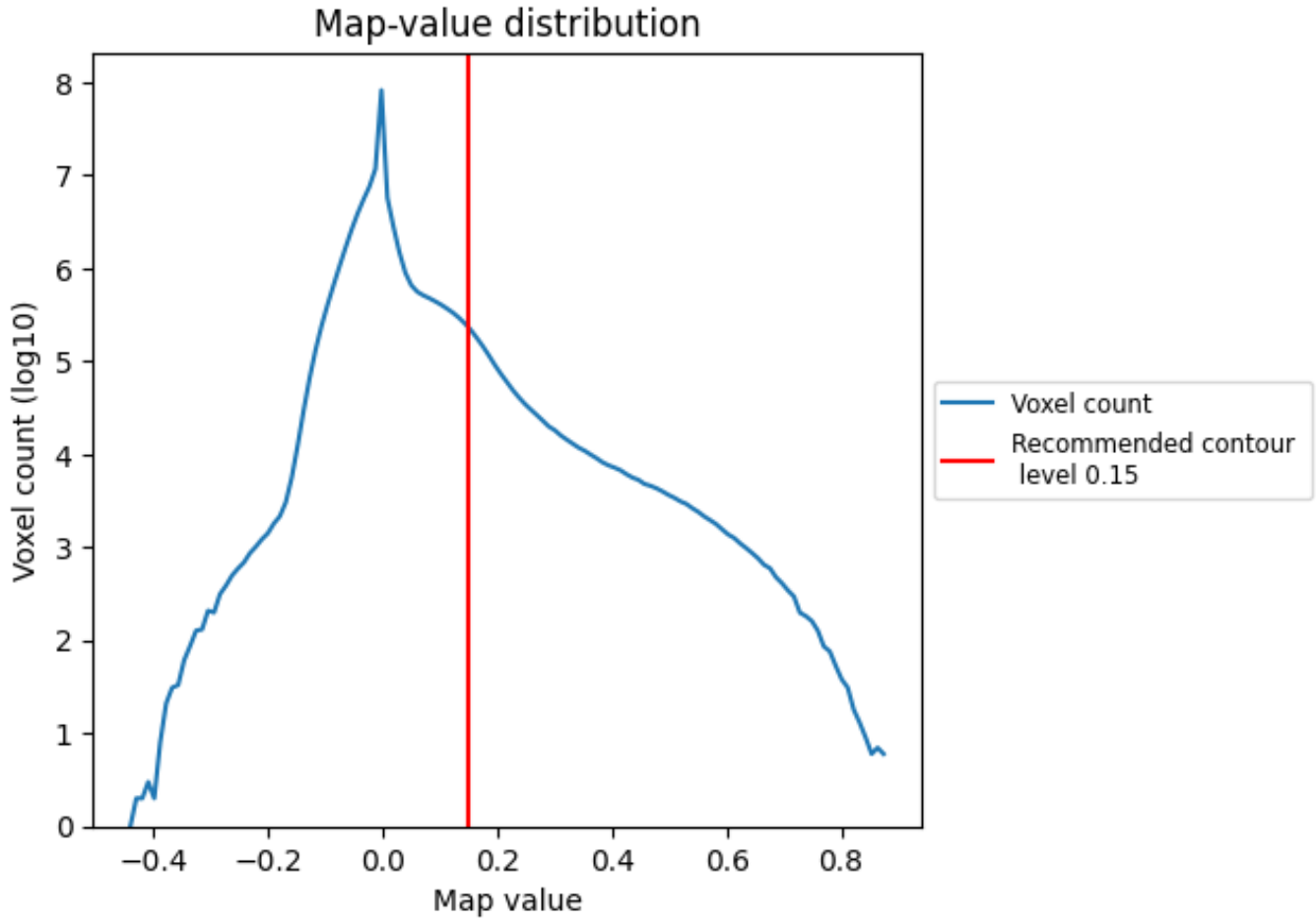
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

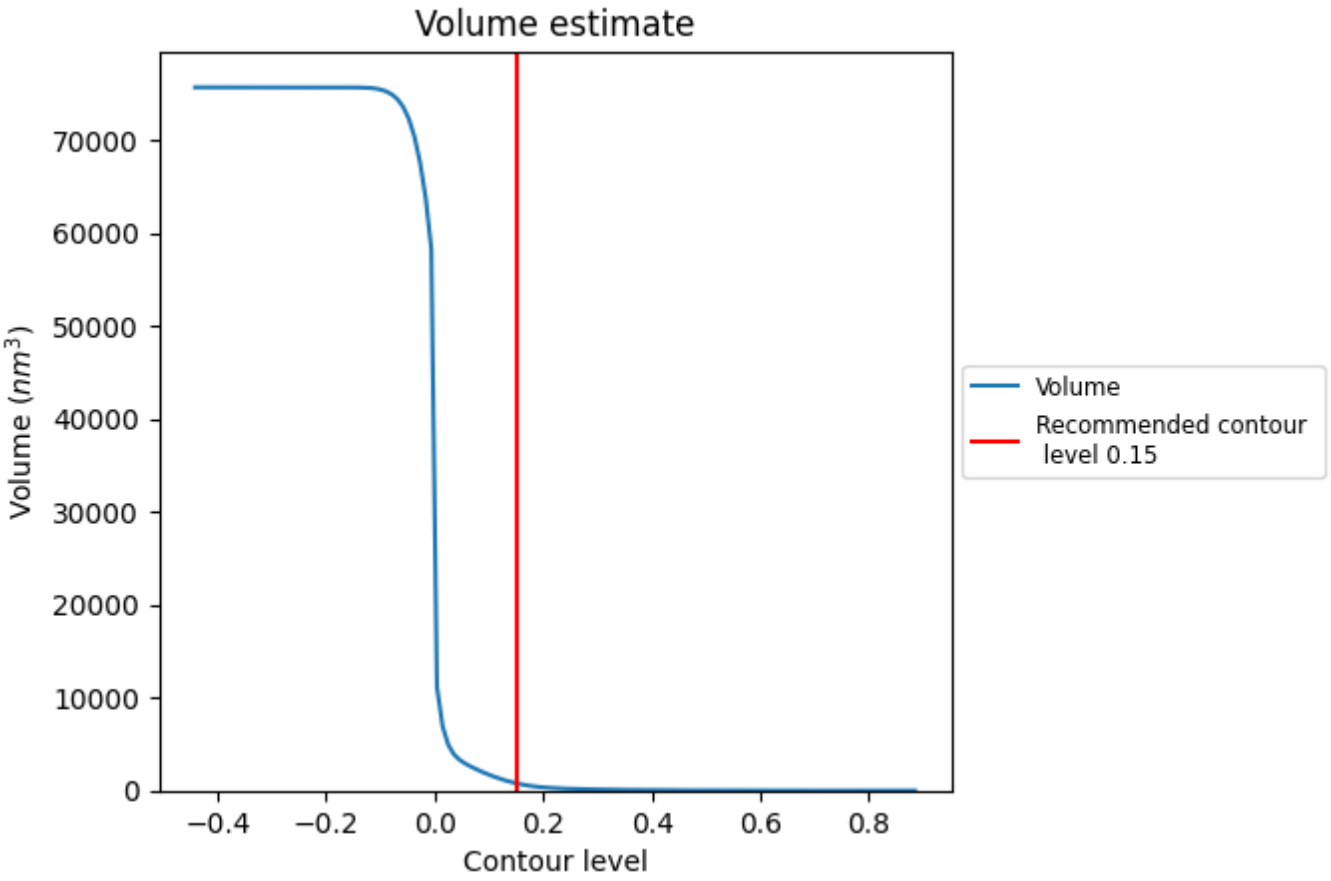
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

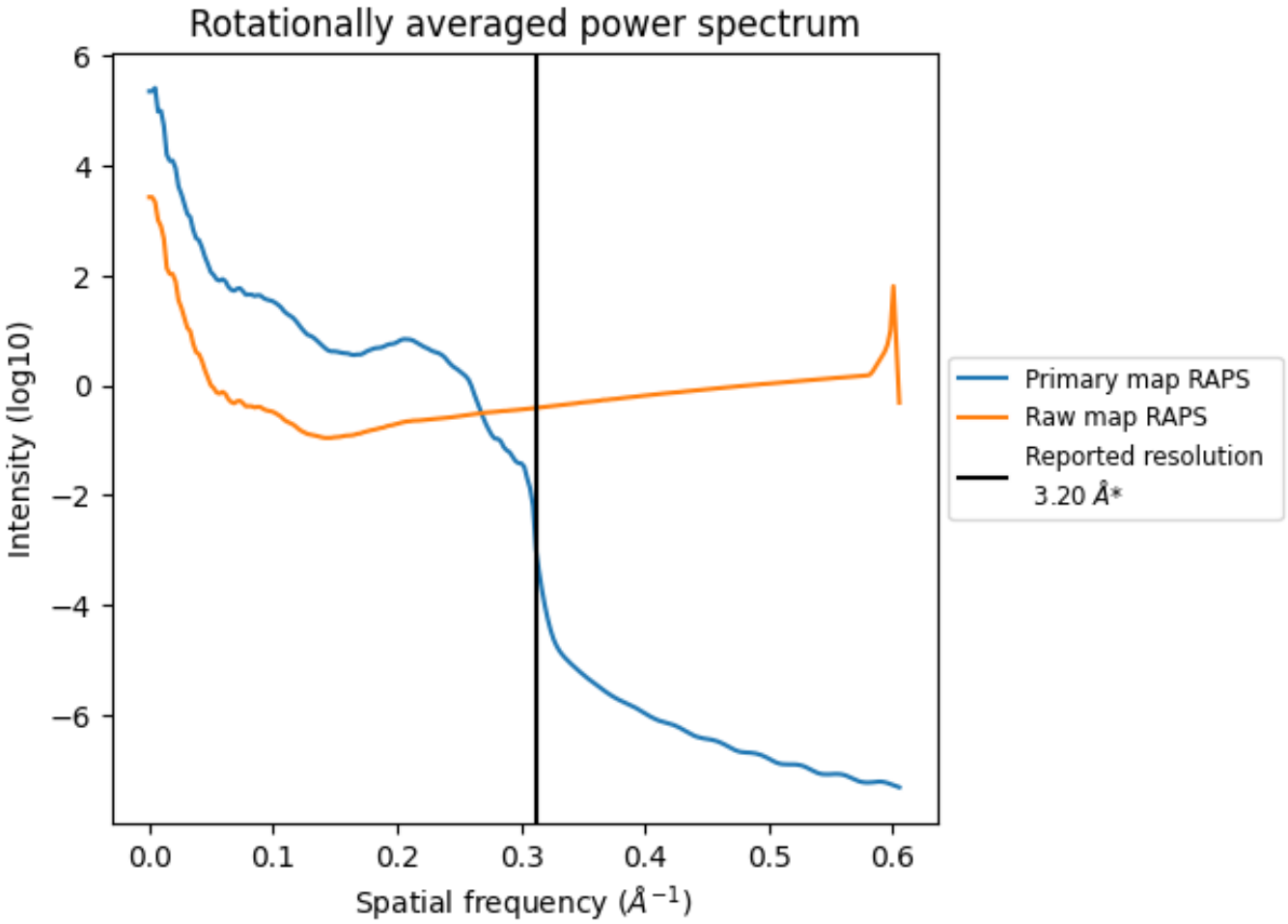
7.2 Volume estimate



The volume at the recommended contour level is 788 nm^3; this corresponds to an approximate mass of 712 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

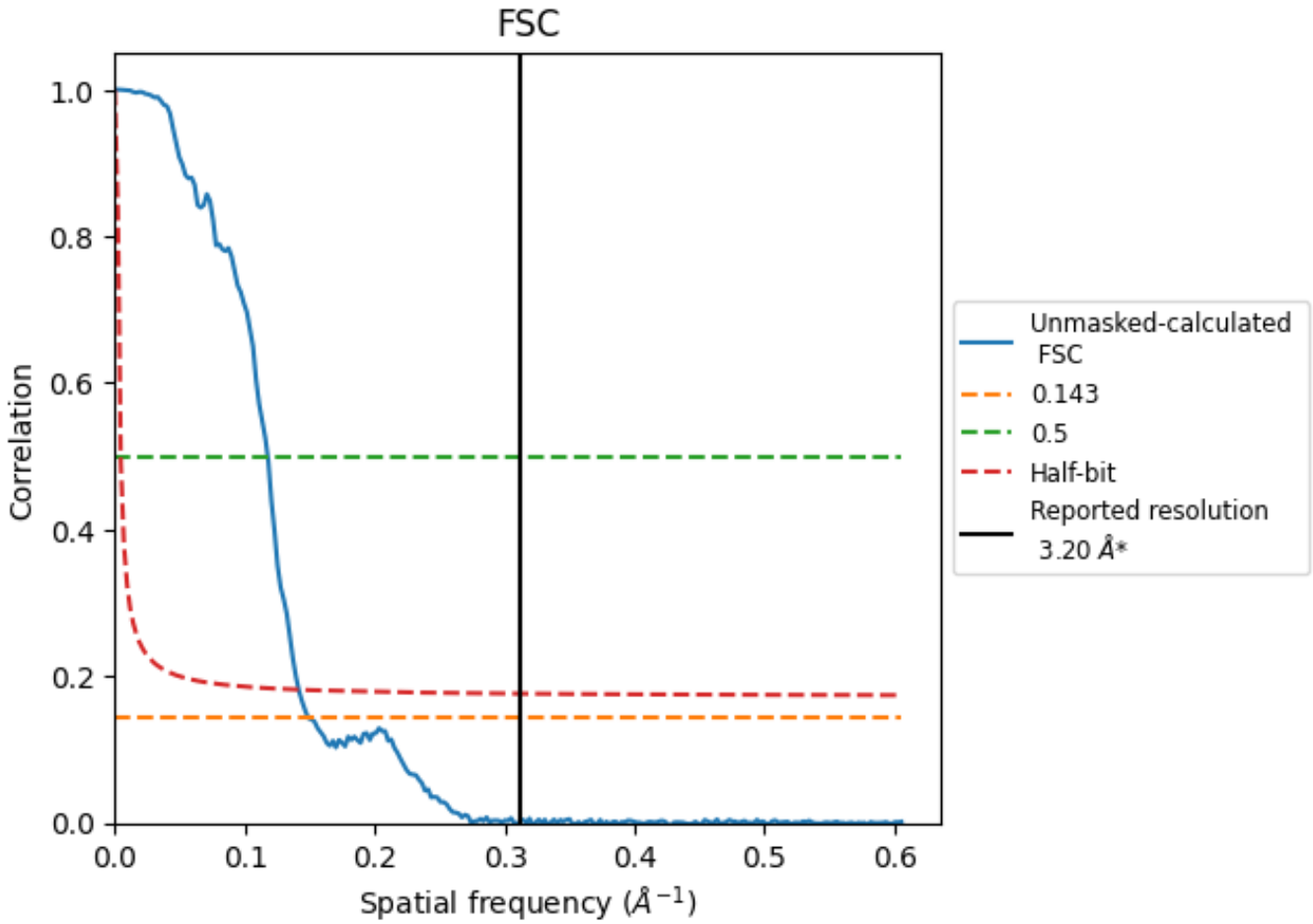


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

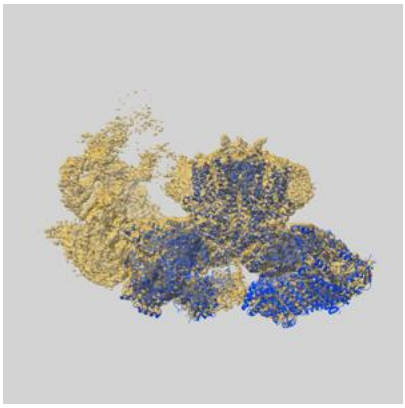
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.72	8.50	7.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.72 differs from the reported value 3.2 by more than 10 %

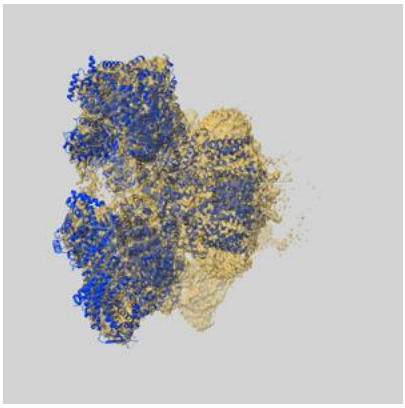
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41366 and PDB model 8TLA. Per-residue inclusion information can be found in section 3 on page 6.

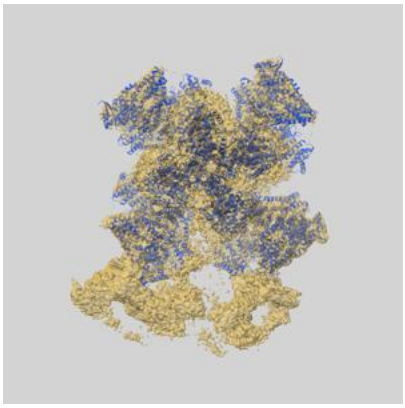
9.1 Map-model overlay



X



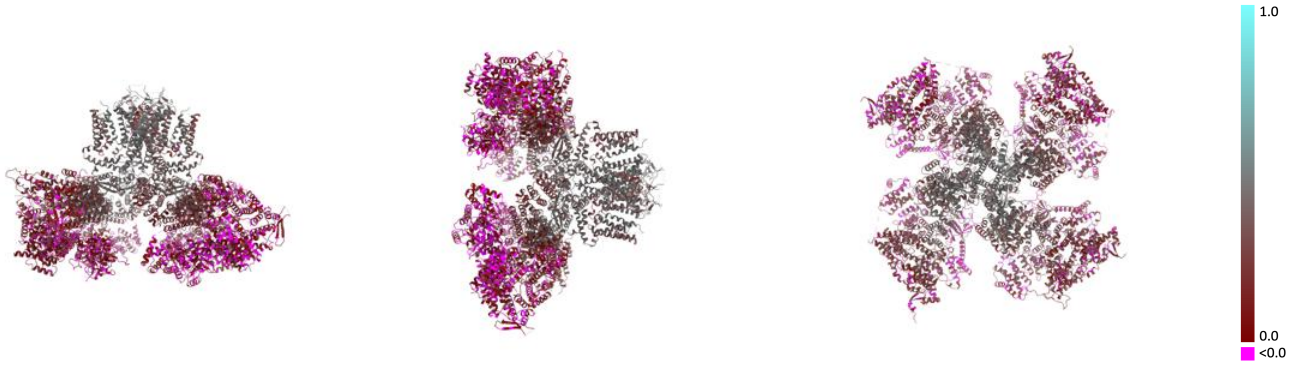
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

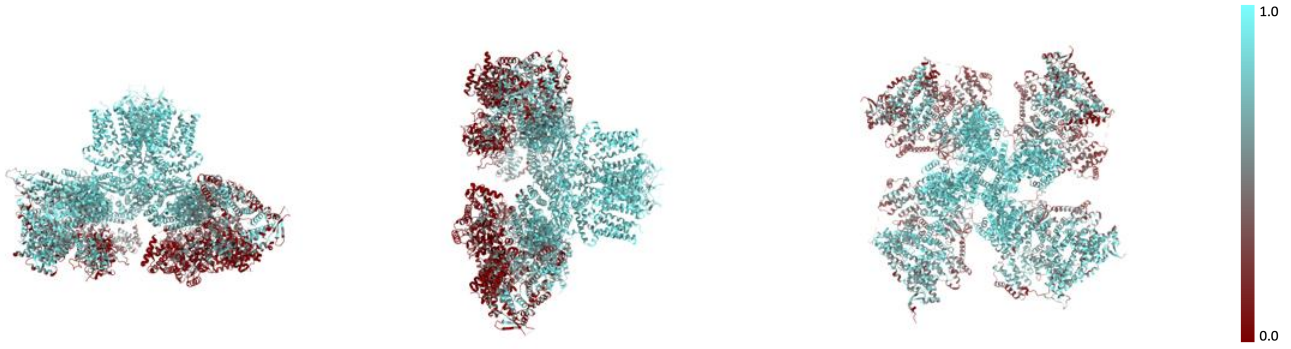
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

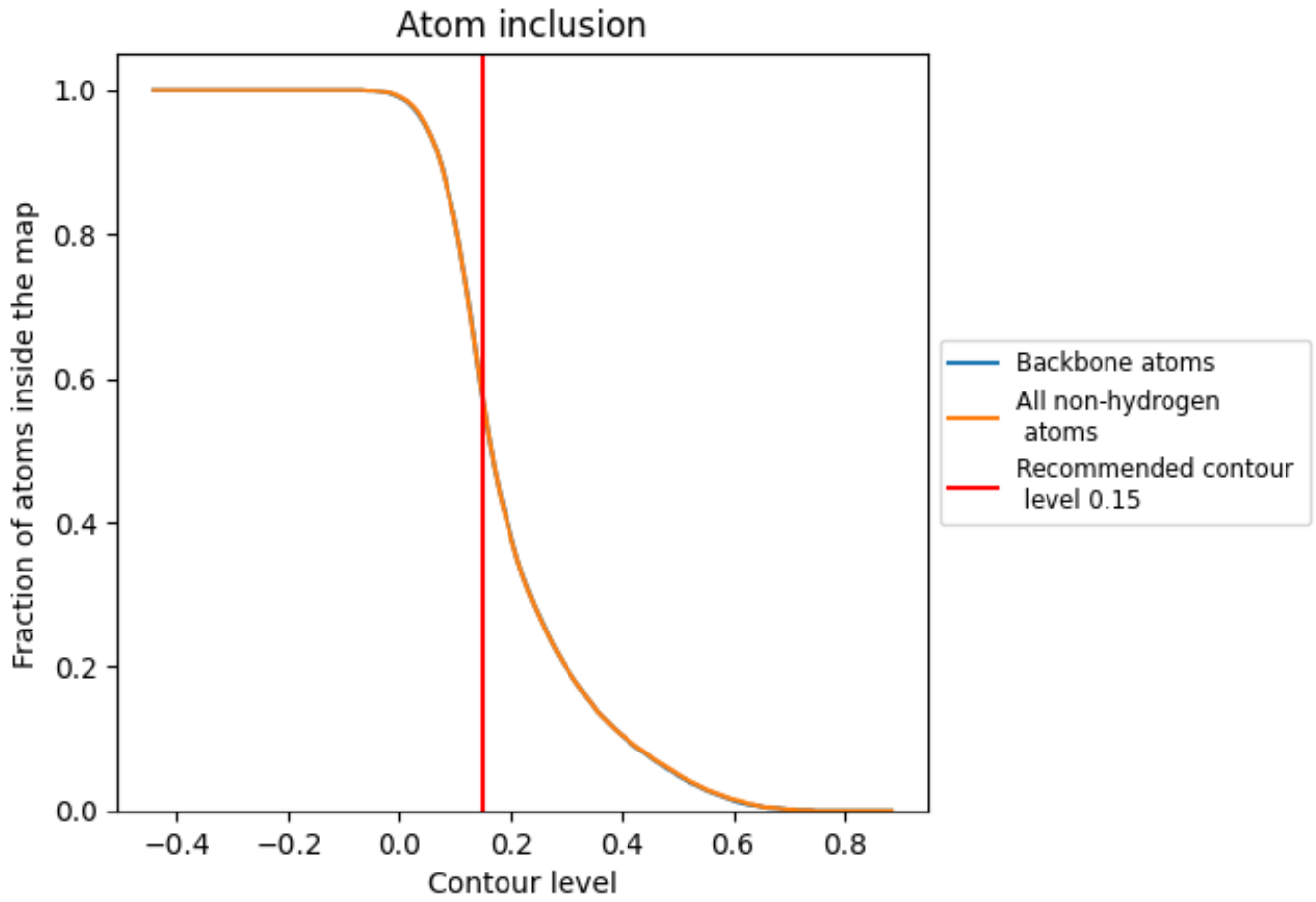
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 57% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5720	0.1980
A	0.5100	0.1710
B	0.4700	0.1640
C	0.6520	0.2320
D	0.6740	0.2250