wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 08:25 am GMT

PDB ID	:	5LKH
EMDB ID	:	EMD-4068
Title	:	Cryo-EM structure of the Tc toxin TcdA1 in its pore state (obtained by flexible fitting)
Authors	:	Gatsogiannis, C.; Merino, F.; Prumbaum, D.; Roderer, D.; Leidreiter, F.; Meusch, D.; Raunser, S.
Deposited on	:	2016-07-22
Resolution	:	3.46 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

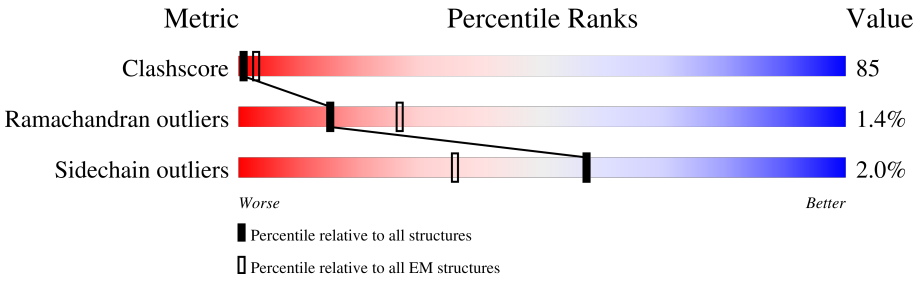
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.46 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	2516	22% 12% 24% · 62%
1	B	2516	22% 12% 24% · 62%
1	C	2516	24% 12% 24% · 62%
1	D	2516	25% 12% 24% · 62%
1	E	2516	24% 12% 24% · 62%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 37345 atoms, of which 0 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.

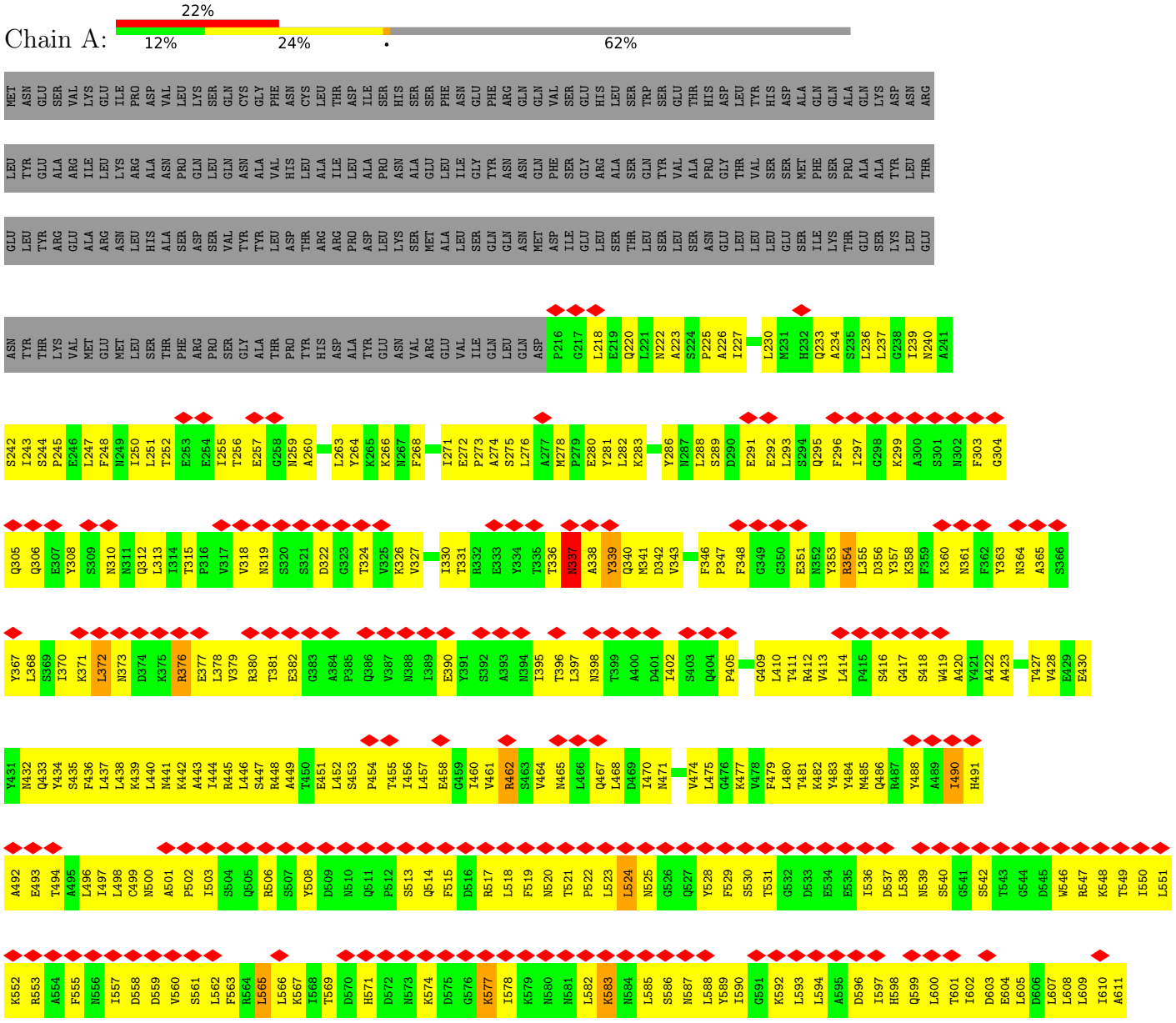
- Molecule 1 is a protein called TcdA1.

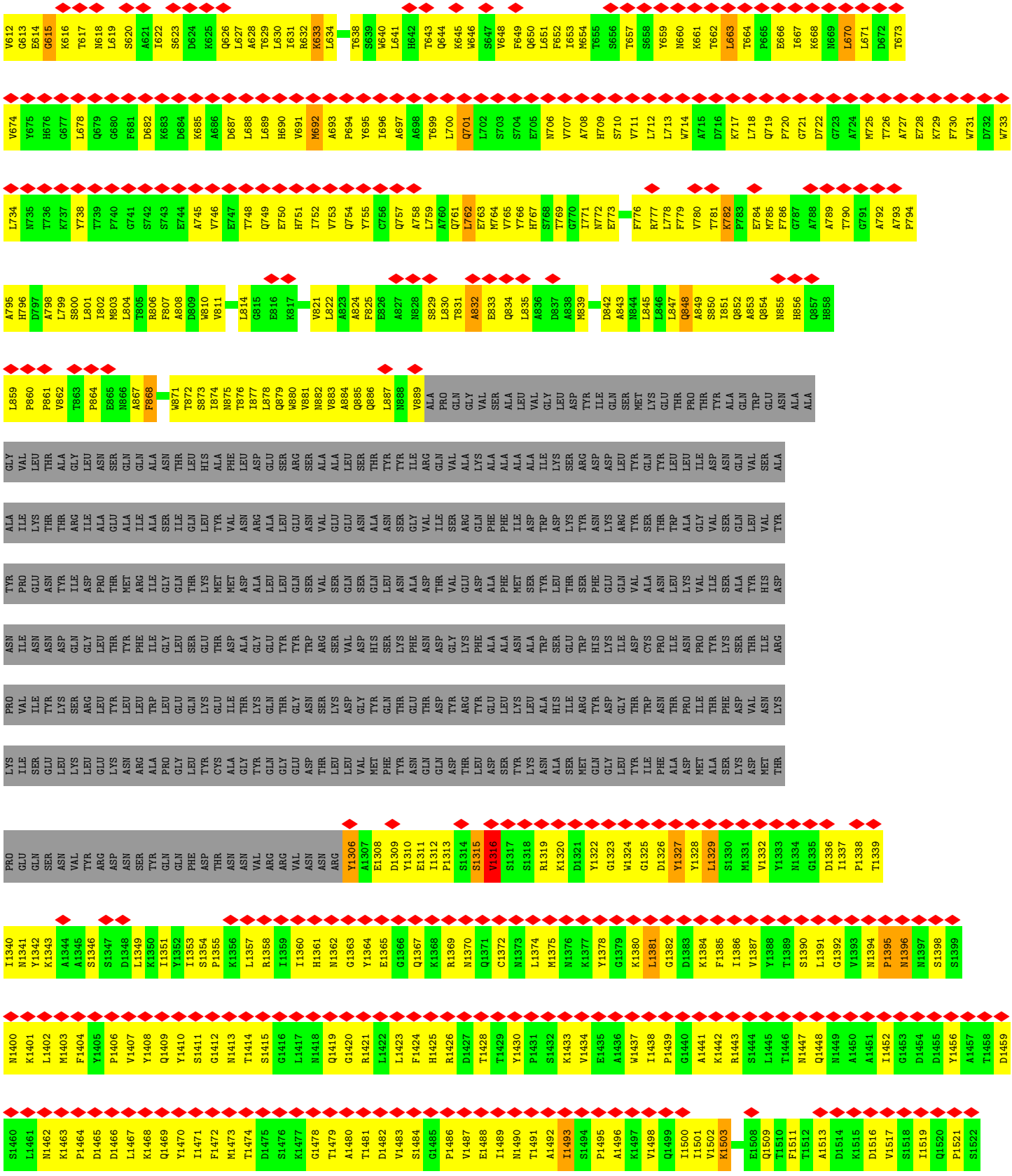
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	948	Total	C	N	O	S	0	0
			7469	4751	1240	1458	20		
1	B	948	Total	C	N	O	S	0	0
			7469	4751	1240	1458	20		
1	C	948	Total	C	N	O	S	0	0
			7469	4751	1240	1458	20		
1	D	948	Total	C	N	O	S	0	0
			7469	4751	1240	1458	20		
1	E	948	Total	C	N	O	S	0	0
			7469	4751	1240	1458	20		

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: TcdA1

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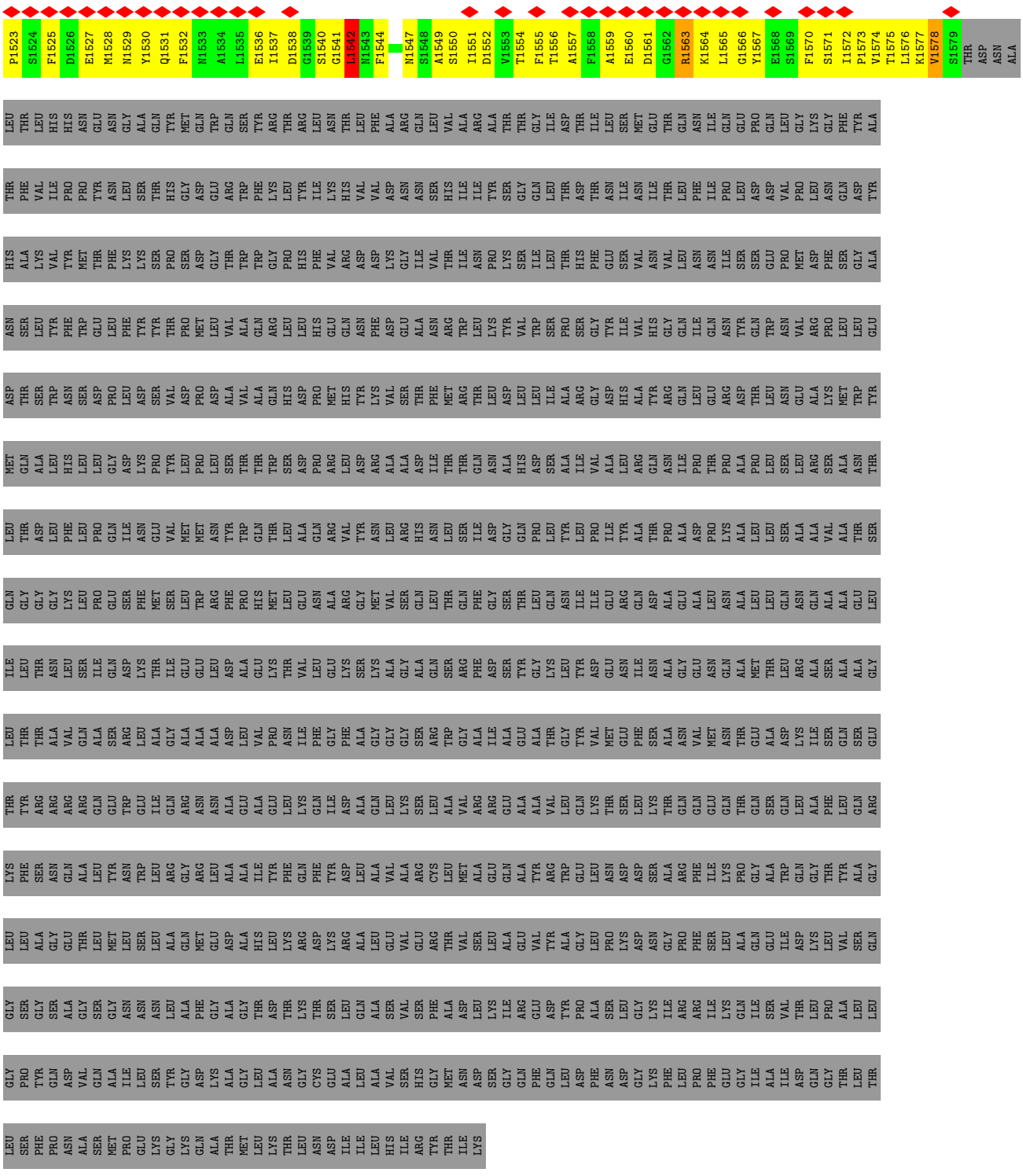
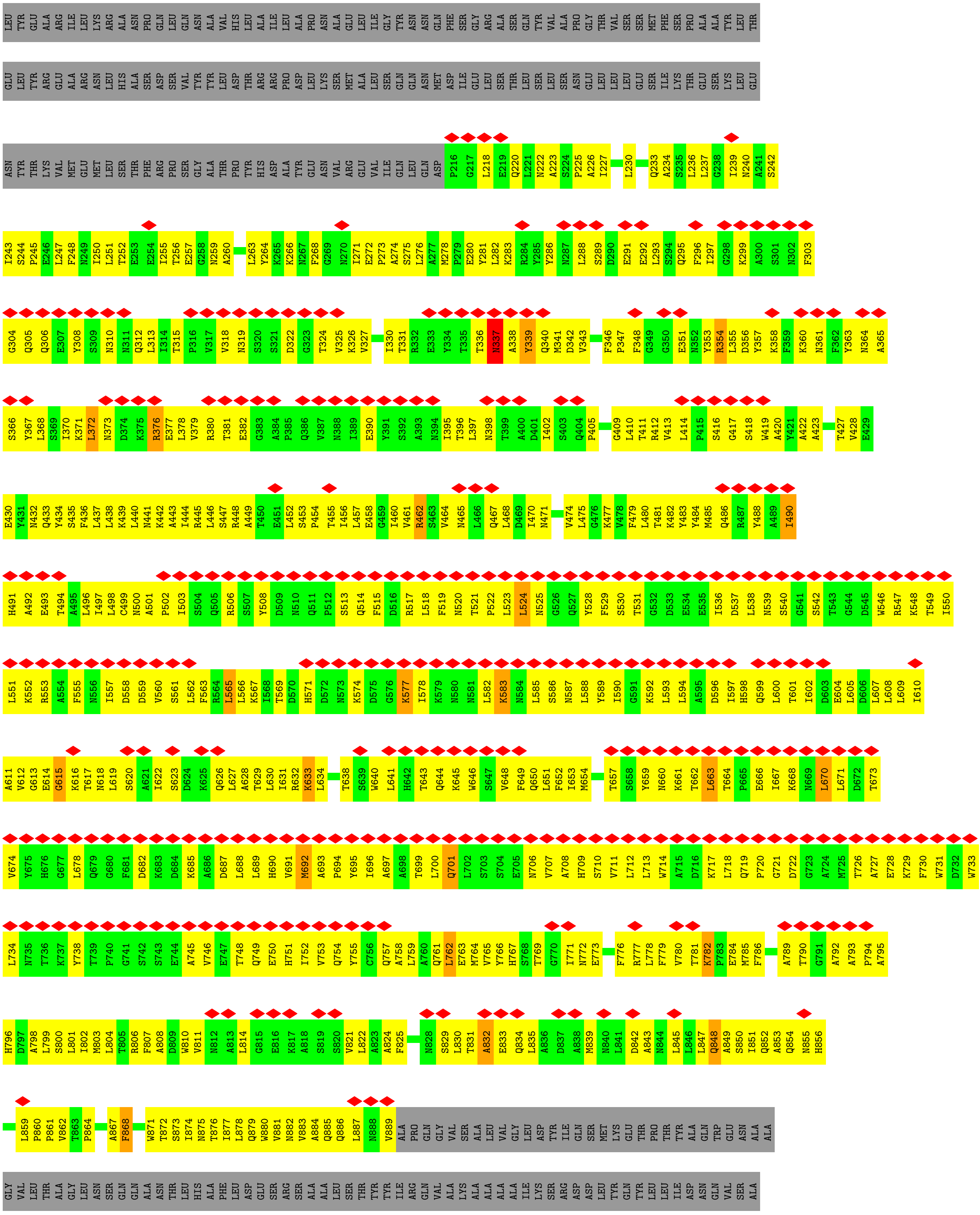
V674 Y675 H676 G677 L678 Q679 G680 F681 D682 K683 D684 K685 A686 D687 L688 L689 H690 V691 M692 A693 P694 Y695 I696 A697 A698 T699 L700 Q701 L702 S703 S704 E705 N706 V707 A708 H709 S710 V711 L712 L713 W714 A715 D716 K717 L718 Q719 P720 G721 D722 G723 A724 M725 T726 A727 E728 K729 F730 W731 D732 W733
L734 N735 T736 K737 Y738 T739 P740 G741 S742 S743 E744 A745 V746 E747 T748 Q749 E750 H751 I752 V753 Q754 Y755 C756 Q757 A758 L759 A760 Q761 L762 E763 M764 V765 Y766 H767 S768 T769 G770 T771 N772 E773 F776 R777 L778 F779 V780 T781 K782 P783 E784 M785 F786 G787 A788 A789 T790 G791 A792 A793 P794
A795 H796 D797 A798 L799 S800 L801 I802 M803 L804 T805 R806 F807 A808 D809 W810 V811 L814 G815 E816 K817 V821 L822 A823 A824 F825 E826 A827 N828 S829 L830 T831 A832 E833 Q834 L835 A836 D837 A838 M839 D842 A843 N844 L845 L846 L847 Q848 A849 S850 I851 Q852 A853 Q854 N855 H856 Q857 H858
L859 P860 P861 V862 T863 P864 E865 N866 A867 F868 W871 T872 S873 I874 N875 T876 I877 L878 Q879 W880 V881 N882 V883 A884 Q885 Q886 L887 N888 V889 ALA PRO GLN GLY VAL SER ALA LEU VAL GLY LEU ASP TYR ILE GLN SER MET LYS GLU THR PRO THR TYR ALA GLN TRP GLU ASN ALA ALA
GLY VAL LEU THR ALA GLY LEU ASN SER GLN GLN ALA ASN THR LEU HIS ALA PHE LEU ASP GLU SER ARG SER ALA ALA LEU SER THR TYR TYR ILE ARG GLN VAL ALA LYS ALA ALA ALA ALA ILE LYS SER ARG ASP ASP LEU TYR GLN TYR LEU LEU ILE ASP ASN GLN VAL SER ALA
ALA ILE LYS THR THR ARG ILE ALA GLU ALA ILE ILE ALA SER ILE GLN LEU TYR VAL ASN ARG ALA LEU LEU GLU GLU ASN VAL GLU GLU GLU ASN ALA ASN SER GLY VAL ILE SER ARG GLN PHE PHE ILE ASP TRP ASP LYS TYR ASN LYS ARG TYR SER THR TRP ALA GLY VAL SER GLN LEU VAL TYR
TYR PRO GLU ASN TYR ILE ASP PRO THR MET ARG ILE GLY GLN THR LYS MET MET MET ASP ALA LEU LEU GLN SER VAL SER GLN SER GLN LEU ASN ALA ASP THR VAL GLU ASP ALA PHE MET SER TYR LEU THR SER PHE GLU GLN VAL ALA ASN LEU LYS VAL ILE SER ALA TYR HIS ASP
ASN ILE ASN ASP GLN GLY LEU THR TYR PHE ILE GLY LEU SER GLU THR ASP ALA GLY GLU TYR TYR TRP ARG SER VAL ASP HIS SER LYS PHE ASN ASP GLY LYS PHE ALA ALA ASN ALA TRP SER GLU TRP HIS LYS ILE ASP CYS PRO ILE ASN PRO TYR LYS SER THR ILE ARG
PRO VAL ILE TYR LYS SER ARG LEU LEU TYR LEU LEU TRP LEU GLU GLN LYS GLU ILE THR LYS GLN THR GLY ASN SER LYS ASP GLY TYR GLN THR GLU THR ASP TYR ARG TYR GLU GLU LEU LYS LEU ALA HIS ILE ARG TYR ASP GLY THR TRP ASN PHE ILE THR PHE ASP VAL ASN LYS
LYS ILE SER GLU LEU LYS LEU GLU LYS ASN ARG ALA PRO GLY LEU TYR CYS ALA GLY TYR GLN GLY GLU ASP THR LEU LEU VAL MET PHE TYR ASN GLN GLN ARG ASP THR LEU ASP SER TYR LYS ASN ALA SER MET GLN GLY LEU TYR ILE PHE ALA ASP MET ALA SER LYS ASP MET THR
PRO GLU GLN SER ASN VAL TYR ARG ASP ASN SER TYR GLN GLN PHE ASP THR ASN ASN VAL ARG ARG VAL ASN ASN ARG Y1306 A1307 E1308 D1309 Y1310 E1311 I1312 P1313 S1314 S1315 V1316 S1317 S1318 R1319 K1320 D1321 Y1322 G1323 W1324 G1325 D1326 Y1327 Y1328 L1329 S1330 M1331 V1332 Y1333 N1334 G1335 D1336 I1337 P1338 T1339
I1340 N1341 Y1342 K1343 A1344 A1345 S1346 S1347 D1348 L1349 K1350 I1351 Y1352 I1353 S1354 P1355 K1356 L1357 R1358 I1359 I1360 H1361 N1362 G1363 Y1364 E1365 G1366 Q1367 K1368 R1369 N1370 Q1371 C1372 N1373 L1374 M1375 N1376 K1377 Y1378 G1379 K1380 L1381 G1382 D1383 K1384 F1385 I1386 V1387 Y1388 T1389 S1390 L1391 G1392 V1393 N1394 P1395 N1396 N1397 S1398 S1399
N1400 K1401 L1402 M1403 F1404 Y1405 P1406 V1407 Y1408 Q1409 Y1410 S1411 G1412 N1413 T1414 S1415 G1416 L1417 N1418 Q1419 G1420 R1421 L1422 L1423 F1424 H1425 R1426 D1427 T1428 T1429 Y1430 P1431 S1432 K1433 V1434 E1435 A1436 W1437 I1438 P1439 G1440 A1441 K1442 R1443 S1444 L1445 T1446 N1447 Q1448 N1449 A1450 A1451 I1452 G1453 D1454 D1455 Y1456 A1457 T1458 D1459
S1460 L1461 N1462 K1463 P1464 D1465 D1466 L1467 K1468 Q1469 Y1470 I1471 F1472 M1473 T1474 D1475 S1476 K1477 G1478 T1479 A1480 T1481 D1482 V1483 S1484 G1485 P1486 V1487 E1488 I1489 N1490 T1491 A1492 I1493 S1494 P1495 A1496 K1497 V1498 Q1499 I1500 I1501 V1502 K1503 E1508 Q1509 T1510 F1511 T1512 A1513 D1514 K1515 D1516 V1517 S1518 I1519 Q1520 P1521 S1522



• Molecule 1: TcdA1

Chain B: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GLU LEU TYR ARG GLU ALA ARG ASN LEU HIS ALA SER ASP SER VAL TYR TYR LEU ASP THR ARG ARG PRO ASP LEU LYS SER MET ALA LEU SER GLN GLN ASN MET ASP ILE GLU LEU SER THR LEU SER LEU SER ASN GLU LEU LEU LEU GLU SER ILE LYS THR GLU SER LYS LEU GLU
ASN TYR THR LYS VAL MET GLU MET LEU SER THR PHE ARG PRO SER GLY ALA THR PRO TYR HIS ASP ALA TYR GLU ASN VAL ARG GLU VAL ILE GLN LEU GLN ASP P216 G217 L218 E219 Q220 L221 N222 A223 S224 P225 A226 I227 L230 Q233 A234 S235 L236 L237 G238 I239 N240 A241 S242
I243 S244 P245 E246 L247 F248 N249 I250 L251 T252 E253 E254 I255 T256 E257 G258 N259 A260 L263 Y264 K265 K266 N267 F268 G269 N270 I271 E272 P273 A274 S275 L276 A277 M278 P279 E280 Y281 L282 K283 R284 Y285 Y286 N287 L288 S289 D290 E291 E292 L293 S294 Q295 F296 I297 G298 K299 A300 S301 N302 F303
G304 Q305 Q306 E307 Y308 S309 N310 N311 Q312 L313 I314 T315 P316 V317 V318 N319 S320 S321 D322 G323 T324 V325 K326 V327 I330 T331 R332 E333 Y334 T335 T336 N337 A338 Y339 Q340 M341 D342 V343 F346 P347 F348 G349 G350 E351 N352 Y353 R354 L355 D356 Y357 K358 F359 K360 N361 F362 Y363 N364 A365
S366 Y367 L368 S369 I370 K371 L372 N373 D374 K375 R376 E377 L378 V379 R380 T381 E382 G383 A384 P385 Q386 V387 N388 I389 E390 Y391 S392 A393 N394 I395 T396 L397 N398 T399 A400 D401 I402 S403 Q404 P405 G409 L410 T411 R412 V413 L414 P415 S416 G417 S418 W419 A420 Y421 A422 A423 T427 V428 E429
E430 Y431 N432 Q433 Y434 S435 F436 L437 L438 K439 L440 N441 K442 A443 I444 R445 L446 S447 R448 A449 T450 E451 L452 S453 P454 T455 I456 L457 E458 G459 I460 V461 R462 S463 V464 N465 L466 Q467 L468 D469 I470 N471 V474 L475 G476 K477 V478 F479 L480 T481 K482 Y483 Y484 M485 Q486 R487 Y488 A489 I490
H491 A492 E493 T494 A495 L496 I497 L498 C499 N500 A501 P502 I503 S504 Q505 R506 S507 Y508 D509 N510 Q511 P512 S513 Q514 F515 D516 R517 L518 F519 N520 T521 P522 L523 L524 N525 G526 Q527 Y528 F529 S530 T531 G532 D533 E534 E535 I536 D537 L538 N539 S540 G541 S542 T543 G544 D545 W546 R547 K548 T549 I550
L551 K552 R553 A554 F555 N556 I557 D558 D559 V560 S561 L562 F563 R564 L565 L566 K567 I568 T569 D570 H571 D572 N573 K574 D575 G576 K577 I578 K579 N580 N581 L582 K583 N584 L585 S586 N587 L588 Y589 I590 G591 K592 L593 L594 A595 D596 I597 H598 Q599 L600 T601 I602 D603 E604 L605 D606 L607 L608 L609 I610
A611 V612 G613 E614 G615 K616 T617 N618 L619 S620 A621 I622 S623 D624 K625 Q626 L627 A628 T629 L630 I631 R632 K633 L634 T638 S639 W640 L641 H642 T643 Q644 K645 W646 S647 V648 F649 Q650 L651 F652 I653 M654 T657 S658 Y659 N660 K661 T662 L663 T664 P665 E666 I667 K668 N669 L670 L671 D672 T673
V674 Y675 H676 G677 L678 Q679 G680 F681 D682 K683 D684 K685 A686 D687 L688 L689 H690 V691 M692 A693 P694 Y695 I696 A697 A698 T699 L700 Q701 L702 S703 S704 E705 N706 V707 A708 H709 S710 V711 L712 L713 W714 A715 D716 K717 L718 Q719 P720 G721 D722 G723 A724 M725 T726 A727 E728 K729 F730 W731 D732 W733
L734 N735 T736 K737 Y738 T739 P740 G741 S742 S743 E744 A745 V746 E747 T748 Q749 E750 H751 I752 V753 Q754 Y755 C756 Q757 A758 L759 A760 Q761 L762 E763 M764 V765 Y766 H767 S768 T769 G770 I771 N772 E773 F776 R777 L778 F779 V780 T781 K782 P783 E784 M785 F786 A789 T790 G791 A792 A793 P794 A795
H796 D797 A798 L799 S800 L801 I802 M803 L804 T805 R806 F807 A808 D809 W810 V811 N812 A813 L814 G815 E816 K817 A818 S819 S820 V821 L822 A823 A824 F825 N828 S829 L830 T831 A832 E833 Q834 L835 A836 D837 A838 M839 N840 L841 D842 A843 N844 L845 L846 L847 Q848 A849 S850 I851 Q852 A853 Q854 N855 H856
L859 P860 P861 V862 T863 P864 A867 F868 W871 T872 S873 I874 N875 T876 I877 L878 Q879 W880 V881 N882 V883 A884 Q885 Q886 L887 N888 V889 ALA PRO GLN GLY VAL SER ALA LEU VAL GLY LEU ASP TYR ILE GLN SER MET LYS GLU THR PRO THR TYR ALA GLN TRP GLU ASN ALA ALA
GLY VAL LEU THR ALA GLY LEU ASN SER GLN GLN ALA ASN THR LEU HIS ALA PHE LEU ASP GLU SER ARG SER ALA ALA LEU SER THR TYR TYR ILE ARG GLN VAL ALA LYS ALA ALA ALA ALA ILE LYS SER ARG ASP ASP LEU TYR GLN TYR LEU LEU ILE ASP ASN GLN VAL SER ALA

ALA ILE LYS THR THR ARG ILE ALA GLU ALA ILE ALA SER ILE GLN LEU TYR VAL ASN ARG ALA LEU GLU ASN VAL GLU GLU ASN ALA ASN SER GLY VAL ILE SER ARG GLN PHE PHE ILE ASP TRP ASP LYS TYR ASN LYS ARG TYR SER THR TRP ALA GLY VAL SER GLN LEU VAL TYR

TYR PRO GLU ASN TYR ILE ASP PRO THR MET ARG ILE GLY GLN THR LYS MET MET ASP ALA LEU LEU GLN SER VAL SER GLN SER GLN LEU ASN ALA ASP THR VAL GLU ASP ALA PHE MET SER TYR LEU THR SER PHE GLU GLN VAL ALA ASN LEU LYS VAL ILE SER ALA TYR HIS ASP

ASN ILE ASN ASN ASP GLN GLY LEU THR TYR PHE ILE GLY LEU SER GLU THR ASP ALA GLY GLU TYR TYR TRP ARG SER VAL ASP HIS SER LYS PHE ASN ASP GLY LYS PHE ALA ALA ASN ALA TRP SER GLU TRP HIS LYS ILE ASP CYS PRO ILE ASN PRO TYR LYS SER THR ILE ARG

PRO VAL ILE TYR LYS SER ARG LEU TYR LEU LEU TRP LEU GLU GLN LYS GLU ILE THR LYS GLN THR GLY ASN SER LYS ASP GLY TYR GLN THR GLU THR ASP TYR ARG TYR GLU LEU LYS LEU ALA HIS ILE ARG TYR ASP GLY THR TRP ASN THR PRO ILE THR PHE ASP VAL ASN LYS

LYS ILE SER GLU LEU LYS LEU GLU LYS ASN ARG ALA PRO GLY LEU TYR CYS ALA GLY TYR GLN GLY GLU ASP THR LEU LEU VAL MET PHE TYR ASN GLN GLN ASP THR LEU ASP SER TYR LYS ASN ALA SER MET GLN GLY LEU TYR ILE PHE ALA ASP MET ALA SER LYS ASP MET THR

PRO GLU GLN SER ASN VAL TYR ARG ASP ASN SER TYR GLN GLN PHE ASP THR ASN ASN VAL ARG ARG VAL ASN ASN ARG Y1306 A1307 E1308 D1309 Y1310 E1311 I1312 P1313 S1314 S1315 V1316 S1317 S1318 R1319 K1320 D1321 Y1322 G1323 W1324 G1325 D1326 Y1327 Y1328 L1329 S1330 M1331 V1332 Y1333 N1334 G1335 D1336 I1337 P1338 T1339

I1340 N1341 Y1342 K1343 A1344 A1345 S1346 S1347 D1348 L1349 K1350 I1351 Y1352 I1353 S1354 P1355 K1356 L1357 R1358 I1359 I1360 H1361 N1362 G1363 Y1364 E1365 G1366 Q1367 K1368 R1369 N1370 Q1371 C1372 N1373 L1374 M1375 N1376 K1377 Y1378 G1379 K1380 L1381 G1382 D1383 K1384 F1385 I1386 V1387 Y1388 T1389 S1390 L1391 G1392 V1393 N1394 P1395 N1396 N1397 S1398 S1399

N1400 K1401 L1402 M1403 F1404 Y1405 P1406 V1407 Y1408 Q1409 Y1410 S1411 G1412 N1413 T1414 S1415 G1416 L1417 N1418 Q1419 G1420 R1421 L1422 L1423 F1424 H1425 R1426 D1427 T1428 T1429 Y1430 P1431 S1432 K1433 V1434 E1435 A1436 W1437 I1438 P1439 G1440 A1441 K1442 R1443 S1444 L1445 T1446 N1447 Q1448 N1449 A1450 A1451 I1452 G1453 D1454 D1455 Y1456 A1457 T1458 D1459

S1460 L1461 N1462 K1463 P1464 D1465 D1466 L1467 K1468 Q1469 Y1470 I1471 F1472 M1473 T1474 D1475 S1476 K1477 G1478 T1479 A1480 T1481 D1482 V1483 S1484 G1485 P1486 V1487 E1488 I1489 N1490 T1491 A1492 I1493 S1494 P1495 A1496 K1497 V1498 Q1499 I1500 I1501 V1502 K1503 A1504 Q1509 T1510 F1511 T1512 A1513 D1514 K1515 D1516 V1517 S1518 I1519 Q1520 P1521 S1522

P1523 S1524 F1525 D1526 E1527 M1528 N1529 Y1530 Q1531 F1532 N1533 A1534 L1535 E1536 I1537 D1538 G1539 S1540 G1541 L1542 N1543 F1544 N1547 S1548 A1549 S1550 I1551 D1552 V1553 T1554 F1555 T1556 A1557 F1558 A1559 E1560 D1561 G1562 R1563 K1564 L1565 G1566 Y1567 E1568 S1569 F1570 S1571 I1572 P1573 V1574 T1575 L1576 K1577 V1578 S1579 THR ASP ASN ALA

LEU THR LEU HIS HIS ASN GLU ASN GLY ALA GLN TYR MET GLN TRP GLN SER TYR ARG THR ARG LEU ASN THR LEU PHE ALA ARG GLN LEU VAL ALA ARG ALA THR THR GLY ILE ASP THR ILE LEU SER MET GLU THR GLN ASN ILE GLN GLU PRO GLN LEU GLY LYS GLY PHE TYR ALA

THR PHE VAL ILE PRO PRO TYR ASN LEU SER THR HIS GLY ASP GLU ARG TRP PHE LYS LEU TYR ILE LYS HIS VAL VAL ASP ASN ASN SER HIS ILE ILE TYR SER GLY GLN LEU THR ASP THR ASN ILE ASN ILE THR LEU PHE ILE PRO LEU ASP ASP VAL PRO LEU ASN GLN ASP TYR

HIS ALA LYS VAL TYR MET THR PHE LYS LYS SER PRO SER ASP GLY THR TRP TRP GLY PRO HIS PHE VAL ARG ASP ASP LYS GLY ILE VAL THR ILE ASN PRO LYS SER ILE LEU THR HIS PHE GLU SER VAL ASN VAL LEU ASN ASN ILE SER SER GLU PRO MET ASP PHE SER GLY ALA

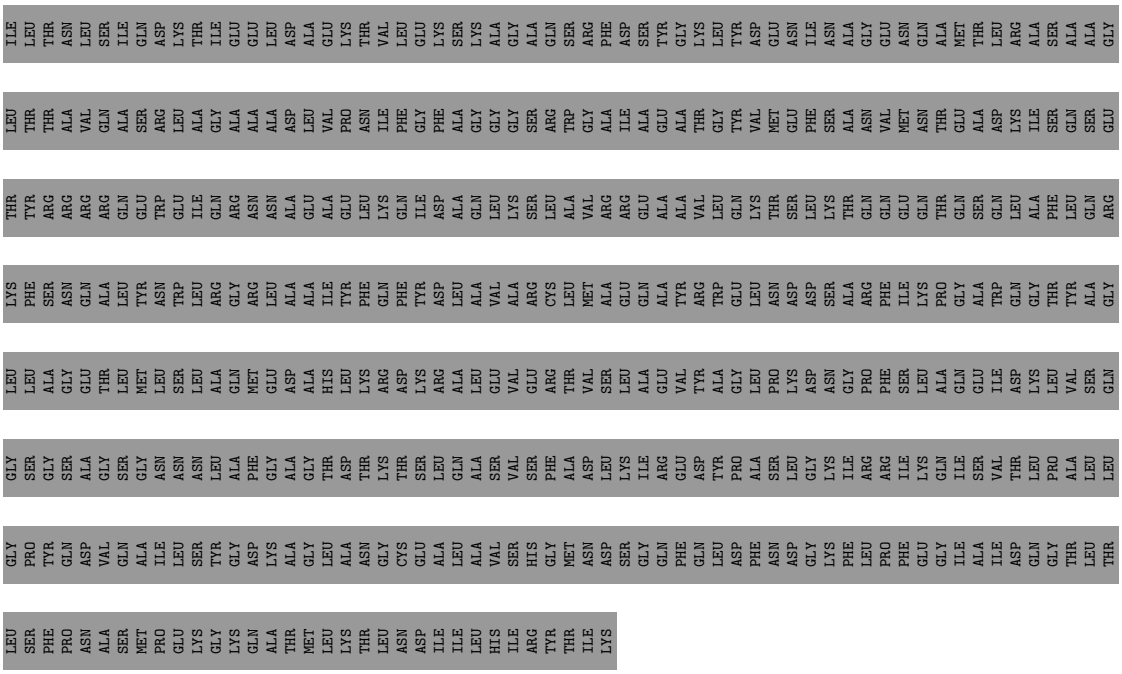
ASN SER LEU TYR PHE TRP GLU LEU PHE TYR TYR THR PRO MET LEU VAL ALA GLN ARG LEU LEU HIS GLU GLN ASN PHE ASP GLU ALA ASN ARG TRP LEU LYS TYR VAL TRP SER PRO SER GLY TYR ILE VAL HIS GLY GLN ILE GLN ASN TYR GLN TRP ASN VAL ARG PRO LEU LEU GLU

ASP THR SER TRP ASN SER ASP PRO LEU ASP SER VAL ASP PRO ASP ALA VAL ALA GLN HIS ASP PRO MET HIS TYR LYS VAL SER THR PHE MET ARG THR LEU ASP LEU LEU ILE ALA ARG GLY ASP HIS ALA TYR ARG GLN LEU GLU ARG ASP THR LEU ASN GLU ALA LYS MET TRP TYR

MET GLN ALA LEU HIS LEU LEU GLY ASP LYS PRO TYR LEU PRO LEU SER THR THR TRP SER ASP PRO ARG LEU ASP ARG ALA ALA ASP ILE THR THR GLN ASN ALA HIS ASP SER ALA ILE VAL ALA LEU ARG GLN ASN ILE PRO THR PRO ALA PRO LEU SER LEU ARG SER ALA ASN THR

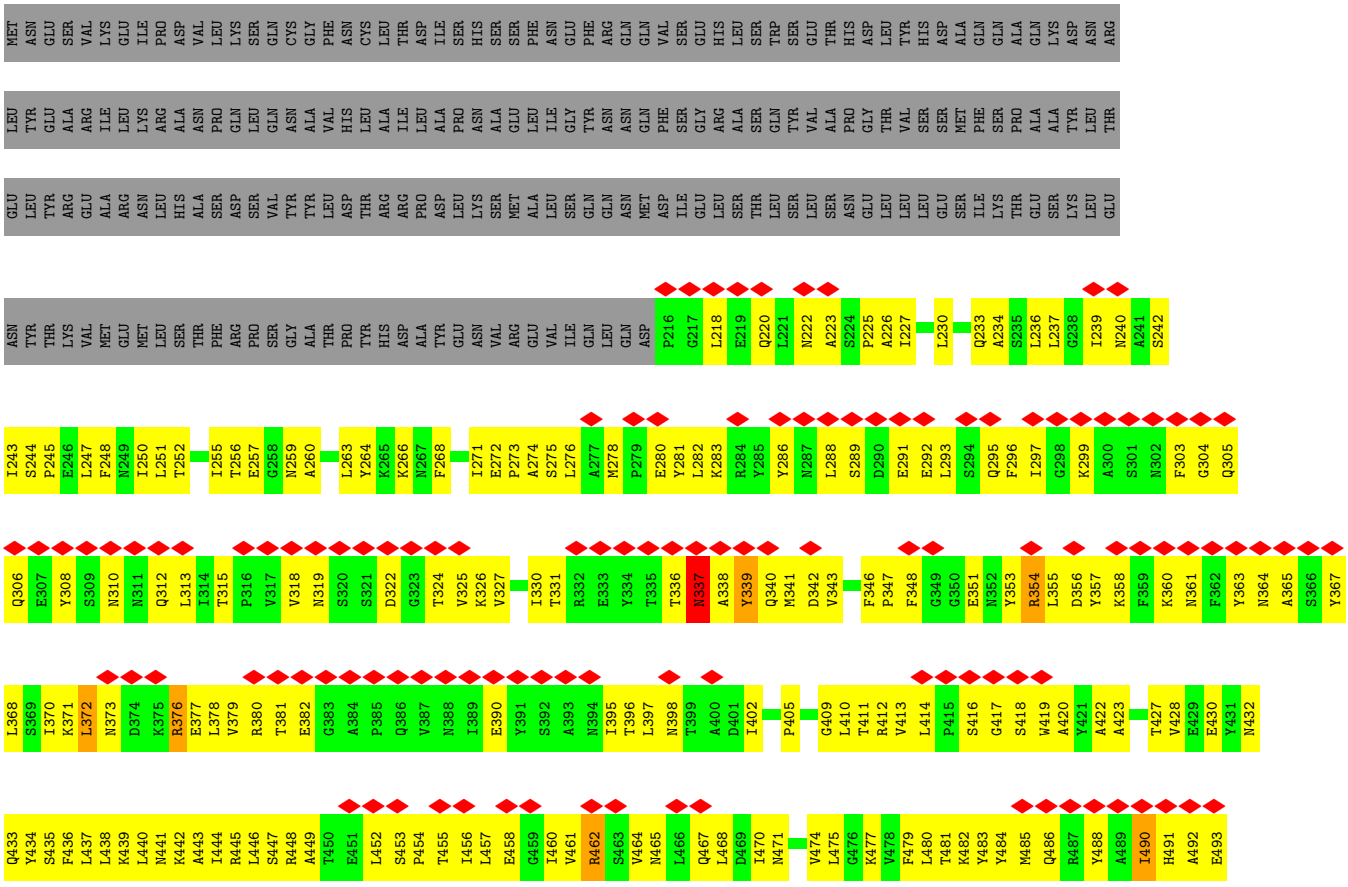
LEU THR ASP LEU PHE LEU PRO GLN ILE ASN GLU VAL MET MET ASN TYR TRP GLN THR LEU ALA GLN ARG VAL TYR ASN LEU ARG HIS ASN LEU SER ILE ASP GLY GLN PRO LEU TYR LEU PRO ILE TYR ALA THR PRO ALA ASP PRO LYS ALA LEU LEU SER ALA ALA VAL ALA THR SER

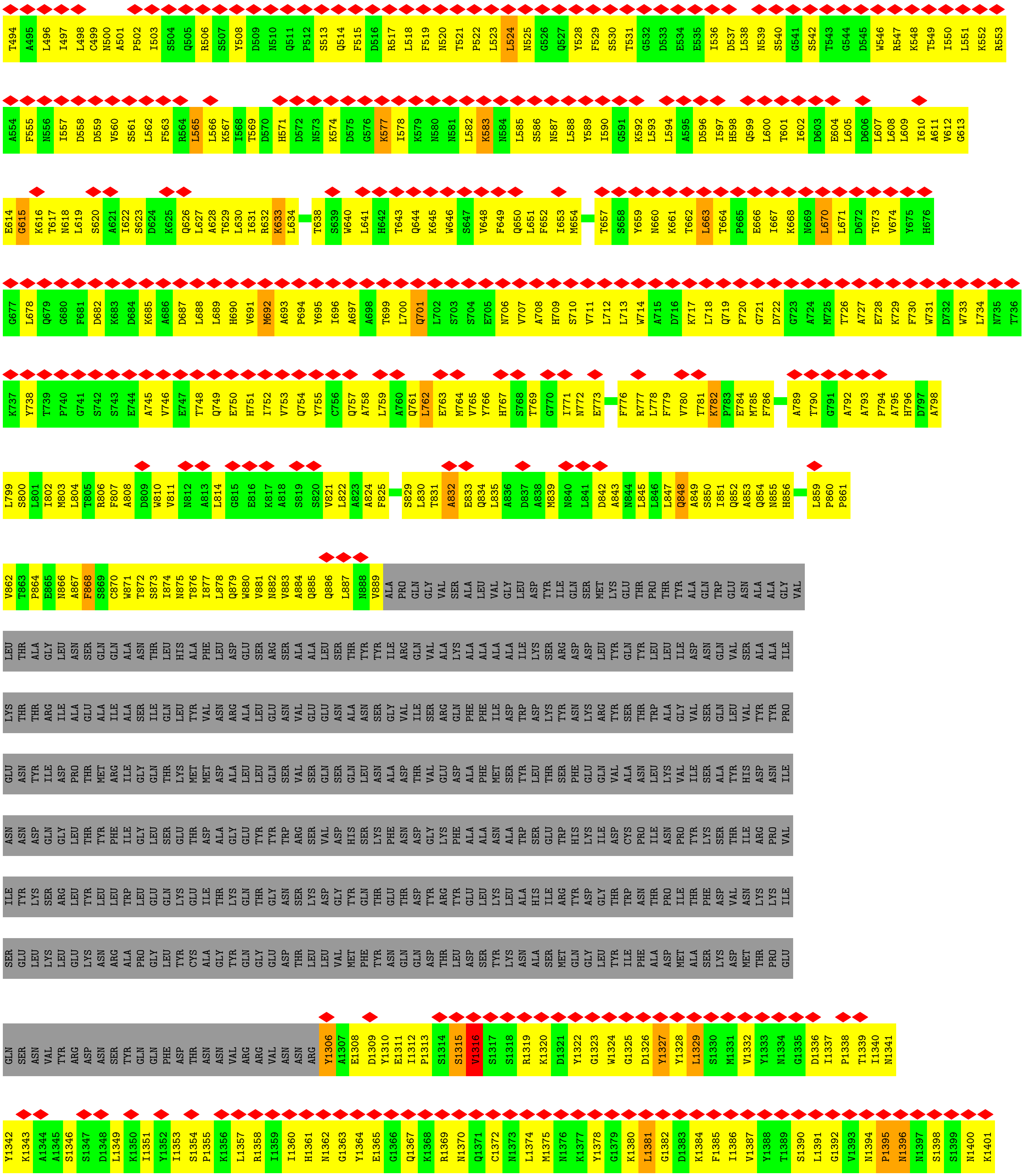
GLN GLY GLY GLY LYS LEU PRO GLU SER PHE MET SER LEU TRP ARG PHE PRO HIS MET LEU GLU ASN ALA ARG GLY MET VAL SER GLN LEU THR GLN PHE GLY SER THR LEU GLN ASN ILE ILE GLU ARG GLN ASP ALA GLU ALA LEU ASN ALA LEU LEU GLN ASN GLN ALA ALA GLU LEU



• Molecule 1: TcdA1

Chain C:

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A554 F555 N556 I557 D558 D559 V560 S561 L562 F563 R564 L565 L566 K567 I568 T569 D570 H571 D572 N573 K574 D575 G576 K577 I578 K579 N580 N581 L582 K583 N584 L585 S586 N587 L588 Y589 I590 G591 K592 L593 L594 A595 D596 I597 H598 Q599 L600 T601 I602 D603 E604 L605 D606 L607 L608 L609 I610 A611 V612 G613
E614 G615 K616 T617 N618 L619 S620 A621 I622 S623 D624 K625 Q626 L627 A628 T629 L630 I631 R632 K633 L634 T638 S639 W640 L641 H642 T643 Q644 K645 W646 S647 V648 F649 Q650 L651 F652 I653 M654 T657 S658 Y659 N660 K661 T662 L663 T664 P665 E666 I667 K668 N669 L670 L671 D672 T673 V674 Y675 H676
G677 L678 Q679 G680 F681 D682 K683 D684 K685 A686 D687 L688 L689 H690 V691 M692 A693 P694 Y695 I696 A697 A698 T699 L700 Q701 L702 S703 S704 E705 N706 V707 A708 H709 S710 V711 L712 L713 W714 A715 D716 K717 L718 Q719 P720 G721 D722 G723 A724 M725 T726 A727 E728 K729 F730 W731 D732 W733 L734 N735 T736
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L799 S800 L801 I802 M803 L804 T805 R806 F807 A808 D809 W810 V811 N812 A813 L814 G815 E816 K817 A818 S819 S820 V821 L822 A823 A824 F825 S829 L830 T831 A832 E833 Q834 L835 A836 D837 A838 M839 N840 L841 D842 A843 N844 L845 L846 L847 Q848 A849 S850 I851 Q852 A853 Q854 N855 H856 L859 P860 P861
V862 T863 P864 E865 N866 A867 F868 S869 C870 W871 T872 S873 I874 N875 T876 I877 L878 Q879 W880 V881 N882 V883 A884 Q885 Q886 L887 N888 V889 ALA PRO GLN GLY VAL SER ALA LEU VAL GLY LEU ASP TYR ILE GLN SER MET LYS GLU THR PRO THR TYR ALA GLN TRP GLU ASN ALA ALA GLY VAL
LEU THR ALA GLY LEU ASN SER GLN GLN ALA ASN THR LEU HIS ALA PHE LEU ASP GLU SER ARG SER ALA ALA LEU SER THR TYR ILE ARG GLN VAL ALA LYS ALA ALA ALA ALA ILE LYS SER ARG ASP ASP LEU TYR GLN TYR LEU LEU ILE ASP ASN GLN VAL SER ALA ALA ILE
LYS THR THR ARG ILE ALA GLU ALA ILE ALA SER ILE GLN LEU TYR VAL ASN ARG ALA LEU GLU ASN VAL GLU GLU ASN ALA ASN SER GLY VAL ILE SER ARG GLN PHE PHE ILE ASP TRP ASP LYS TYR ASN LYS ARG TYR SER THR TRP ALA GLY VAL SER GLN LEU VAL TYR TYR PRO
GLU ASN TYR ILE ASP PRO THR MET ARG ILE GLY GLN THR LYS MET MET ASP ALA LEU LEU GLN SER VAL SER GLN SER GLN LEU ASN ALA ASP THR VAL GLU ASP ALA PHE MET SER TYR LEU THR SER PHE GLU GLN VAL ALA ASN LEU LYS VAL ILE SER ALA TYR HIS ASP ASN ILE
ASN ASN ASP GLN GLY LEU THR TYR PHE ILE GLY LEU SER GLU THR ASP ALA GLY GLU TYR TYR TRP ARG SER VAL ASP HIS SER LYS PHE ASN ASP GLY LYS PHE ALA ALA ASN ALA TRP SER GLU TRP HIS LYS ILE ASP CYS PRO ILE ASN PRO TYR LYS SER THR ILE ARG PRO VAL
ILE TYR LYS SER ARG LEU TYR LEU LEU TRP LEU GLU GLN LYS GLU ILE THR LYS GLN THR GLY ASN SER LYS ASP GLY TYR GLN THR GLU THR ASP TYR ARG TYR GLU LEU LYS LEU ALA HIS ILE ARG TYR ASP GLY THR TRP ASN THR PRO ILE THR PHE ASP VAL ASN LYS LYS ILE
SER GLU LEU LYS LEU GLU LYS ASN ARG ALA PRO GLY LEU TYR CYS ALA GLY TYR GLN GLY GLU ASP THR LEU LEU VAL MET PHE TYR ASN GLN GLN ASP THR LEU ASP SER TYR LYS ASN ALA SER MET GLN GLY LEU TYR ILE PHE ALA ASP MET ALA SER LYS ASP MET THR PRO GLU
GLN SER ASN VAL TYR ARG ASP ASN SER TYR GLN GLN PHE ASP THR ASN ASN VAL ARG ARG VAL ASN ASN ARG Y1306 A1307 E1308 D1309 Y1310 E1311 I1312 P1313 S1314 S1315 V1316 S1317 S1318 R1319 K1320 D1321 Y1322 G1323 W1324 G1325 D1326 Y1327 Y1328 L1329 S1330 M1331 V1332 Y1333 N1334 G1335 D1336 I1337 P1338 T1339 I1340 N1341
Y1342 K1343 A1344 A1345 S1346 S1347 D1348 L1349 K1350 I1351 Y1352 I1353 S1354 P1355 K1356 L1357 R1358 I1359 I1360 H1361 N1362 G1363 Y1364 E1365 G1366 Q1367 K1368 R1369 N1370 Q1371 C1372 N1373 L1374 M1375 N1376 K1377 Y1378 G1379 K1380 L1381 G1382 D1383 K1384 F1385 I1386 V1387 Y1388 T1389 S1390 L1391 G1392 V1393 N1394 P1395 N1396 N1397 S1398 S1399 N1400 K1401

L1402 M1403 F1404 Y1405 P1406 V1407 Y1408 Q1409 Y1410 S1411 G1412 N1413 T1414 S1415 G1416 L1417 N1418 Q1419 G1420 R1421 L1422 L1423 F1424 H1425 R1426 D1427 T1428 T1429 Y1430 P1431 S1432 K1433 V1434 E1435 A1436 W1437 I1438 P1439 G1440 A1441 K1442 R1443 S1444 L1445 T1446 N1447 Q1448 N1449 A1450 A1451 I1452 G1453 D1454 D1455 Y1456 A1457 T1458 D1459 S1460 L1461

N1462 K1463 P1464 D1465 D1466 L1467 K1468 Q1469 Y1470 I1471 F1472 M1473 T1474 D1475 S1476 K1477 G1478 T1479 A1480 T1481 D1482 V1483 S1484 G1485 P1486 V1487 E1488 I1489 N1490 T1491 A1492 I1493 S1494 P1495 A1496 K1497 V1498 Q1499 I1500 I1501 V1502 K1503 A1504 K1507 E1508 Q1509 T1510 F1511 T1512 A1513 D1514 K1515 D1516 V1517 S1518 I1519 Q1520 P1521 S1522

P1523 S1524 F1525 D1526 E1527 M1528 N1529 Y1530 Q1531 F1532 N1533 A1534 L1535 E1536 I1537 D1538 G1539 S1540 G1541 L1542 N1543 F1544 N1547 S1548 A1549 S1550 I1551 D1552 V1553 T1554 F1555 T1556 A1557 F1558 A1559 E1560 D1561 G1562 R1563 K1564 L1565 G1566 Y1567 E1568 S1569 F1570 S1571 I1572 P1573 V1574 T1575 L1576 K1577 V1578 S1579 THR ASP ASN ALA

LEU THR LEU HIS HIS ASN GLU ASN GLY ALA GLN TYR MET GLN TRP GLN SER TYR ARG THR ARG LEU ASN THR LEU PHE ALA ARG GLN LEU VAL ALA ARG ALA THR THR GLY ILE ASP THR ILE LEU SER MET GLU THR GLN ASN ILE GLN GLU PRO GLN LEU GLY LYS GLY PHE TYR ALA

THR PHE VAL ILE PRO PRO TYR ASN LEU SER THR HIS GLY ASP GLU ARG TRP PHE LYS LEU TYR ILE LYS HIS VAL VAL ASP ASN ASN SER HIS ILE ILE TYR SER GLY GLN LEU THR ASP THR ASN ILE ASN ILE THR LEU PHE ILE PRO LEU ASP ASP VAL PRO LEU ASN GLN ASP TYR

HIS ALA LYS VAL TYR MET THR PHE LYS LYS SER PRO SER ASP GLY THR TRP TRP GLY PRO HIS PHE VAL ARG ASP ASP LYS GLY ILE VAL THR ILE ASN PRO LYS SER ILE LEU THR HIS PHE GLU SER VAL ASN VAL LEU ASN ASN ILE SER SER GLU PRO MET ASP PHE SER GLY ALA

ASN SER LEU TYR PHE TRP GLU LEU PHE TYR TYR THR PRO MET LEU VAL ALA GLN ARG LEU LEU HIS GLU GLN ASN PHE ASP GLU ALA ASN ARG TRP LEU LYS TYR VAL TRP SER PRO SER GLY TYR ILE VAL HIS GLY GLN ILE GLN ASN TYR GLN TRP ASN VAL ARG PRO LEU LEU GLU

ASP THR SER TRP ASN SER ASP PRO LEU ASP SER VAL ASP PRO ASP ALA VAL ALA GLN HIS ASP PRO MET HIS TYR LYS VAL SER THR PHE MET ARG THR LEU ASP LEU LEU ILE ALA ARG GLY ASP HIS ALA TYR ARG GLN LEU GLU ARG ASP THR LEU ASN GLU ALA LYS MET TRP TYR

MET GLN ALA LEU HIS LEU LEU GLY ASP LYS PRO TYR LEU PRO LEU SER THR THR TRP SER ASP PRO ARG LEU ASP ARG ALA ALA ASP ILE THR THR GLN ASN ALA HIS ASP SER ALA ILE VAL ALA LEU ARG GLN ASN ILE PRO THR PRO ALA PRO LEU SER LEU ARG SER ALA ASN THR

LEU THR ASP LEU PHE LEU PRO GLN ILE ASN GLU VAL MET MET ASN TYR TRP GLN THR LEU ALA GLN ARG VAL TYR ASN LEU ARG HIS ASN LEU SER ILE ASP GLY GLN PRO LEU TYR LEU PRO ILE TYR ALA THR PRO ALA ASP PRO LYS ALA LEU LEU SER ALA ALA VAL ALA THR SER

GLN GLY GLY GLY LYS LEU PRO GLU SER PHE MET SER LEU TRP ARG PHE PRO HIS MET LEU GLU ASN ALA ARG GLY MET VAL SER GLN LEU THR GLN PHE GLY SER THR LEU GLN ASN ILE ILE GLU ARG GLN ASP ALA GLU ALA LEU ASN ALA LEU LEU GLN ASN GLN ALA ALA GLU LEU

ILE LEU THR ASN LEU SER ILE GLN ASP LYS THR ILE GLU GLU LEU ASP ALA GLU LYS THR VAL LEU GLU LYS SER LYS ALA GLY ALA GLN SER ARG PHE ASP SER TYR GLY LYS LEU TYR ASP GLU ASN ILE ASN ALA GLY GLU ASN GLN ALA MET THR LEU ARG ALA SER ALA ALA GLY

LEU THR THR ALA VAL GLN ALA SER ARG LEU ALA GLY ALA ALA ALA ASP LEU VAL PRO ASN ILE PHE GLY PHE ALA GLY GLY GLY SER ARG TRP GLY ALA ILE ALA GLU ALA THR GLY TYR VAL MET GLU PHE SER ALA ASN VAL MET ASN THR GLU ALA ASP LYS ILE SER GLN SER GLU

THR TYR ARG ARG ARG ARG GLN GLU TRP GLU ILE GLN ARG ASN ASN ALA GLU ALA GLU LEU LYS GLN ILE ASP ALA GLN LEU LYS SER LEU ALA VAL ARG ARG GLU ALA ALA VAL LEU GLN LYS THR SER LEU LYS THR GLN GLN GLU GLN THR GLN SER GLN LEU ALA PHE LEU GLN ARG

LYS PHE SER ASN GLN ALA LEU TYR ASN TRP LEU ARG GLY ARG LEU ALA ALA ILE TYR PHE GLN PHE TYR ASP LEU ALA VAL ALA ARG CYS LEU MET ALA GLU GLN ALA TYR ARG TRP GLU LEU ASN ASP ASP SER ALA ARG PHE ILE LYS PRO GLY ALA TRP GLN GLY THR TYR ALA GLY

LEU LEU ALA GLY GLU THR LEU MET LEU SER LEU ALA GLN MET GLU ASP ALA HIS LEU LYS ARG ASP LYS ARG ALA LEU GLU VAL GLU ARG THR VAL SER LEU ALA GLU VAL TYR ALA GLY LEU PRO LYS ASP ASN GLY PRO PHE SER LEU ALA GLN GLU ILE ASP LYS LEU VAL SER GLN

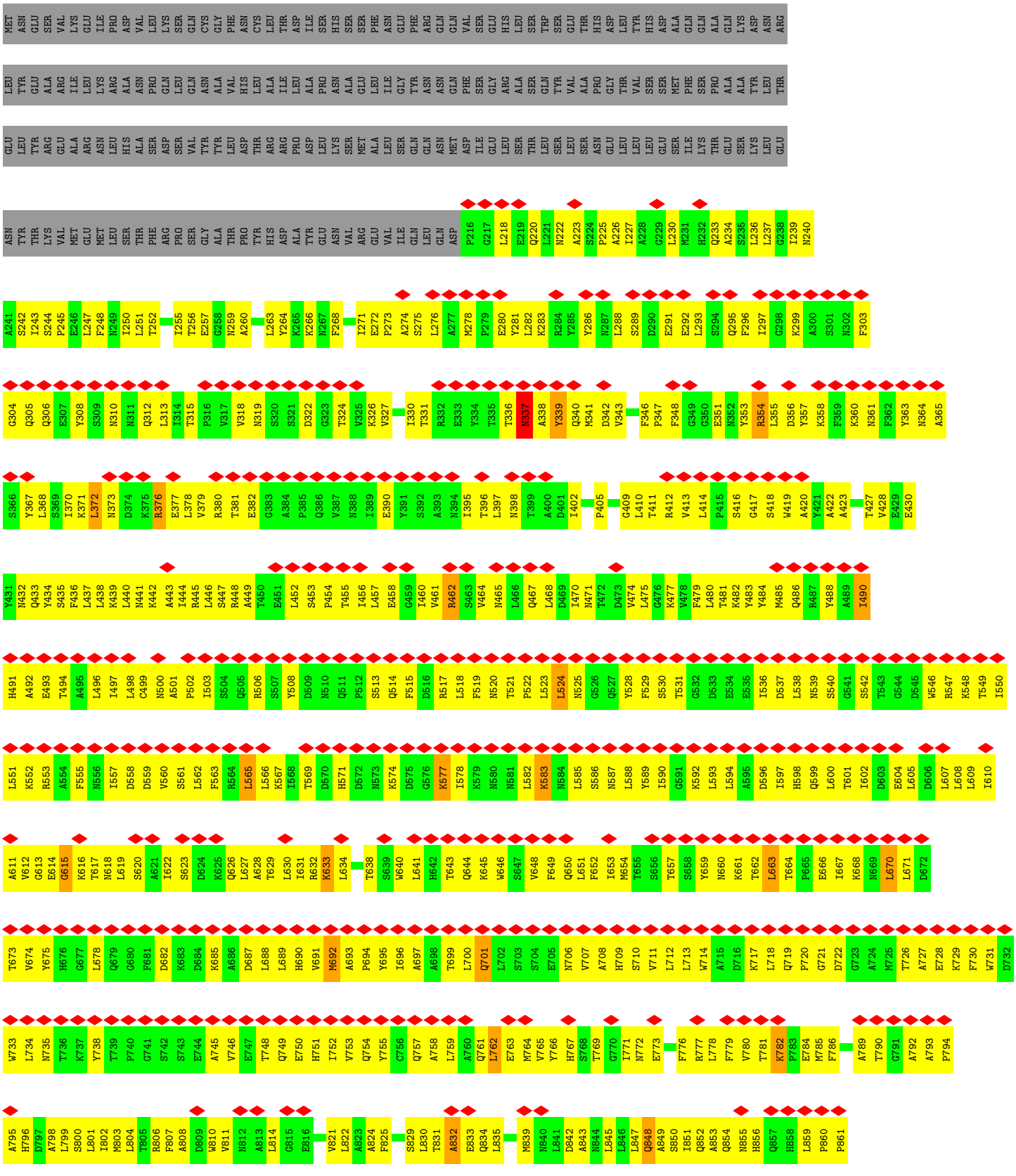
GLY SER GLY SER ALA GLY SER GLY ASN ASN LEU ALA PHE GLY ALA GLY THR ASP THR LYS THR SER LEU GLN ALA SER VAL SER PHE ALA ASP LEU LYS ILE ARG GLU ASP TYR PRO ALA SER LEU GLY LYS ILE ARG ARG ILE LYS GLN ILE SER VAL THR LEU PRO ALA LEU LEU

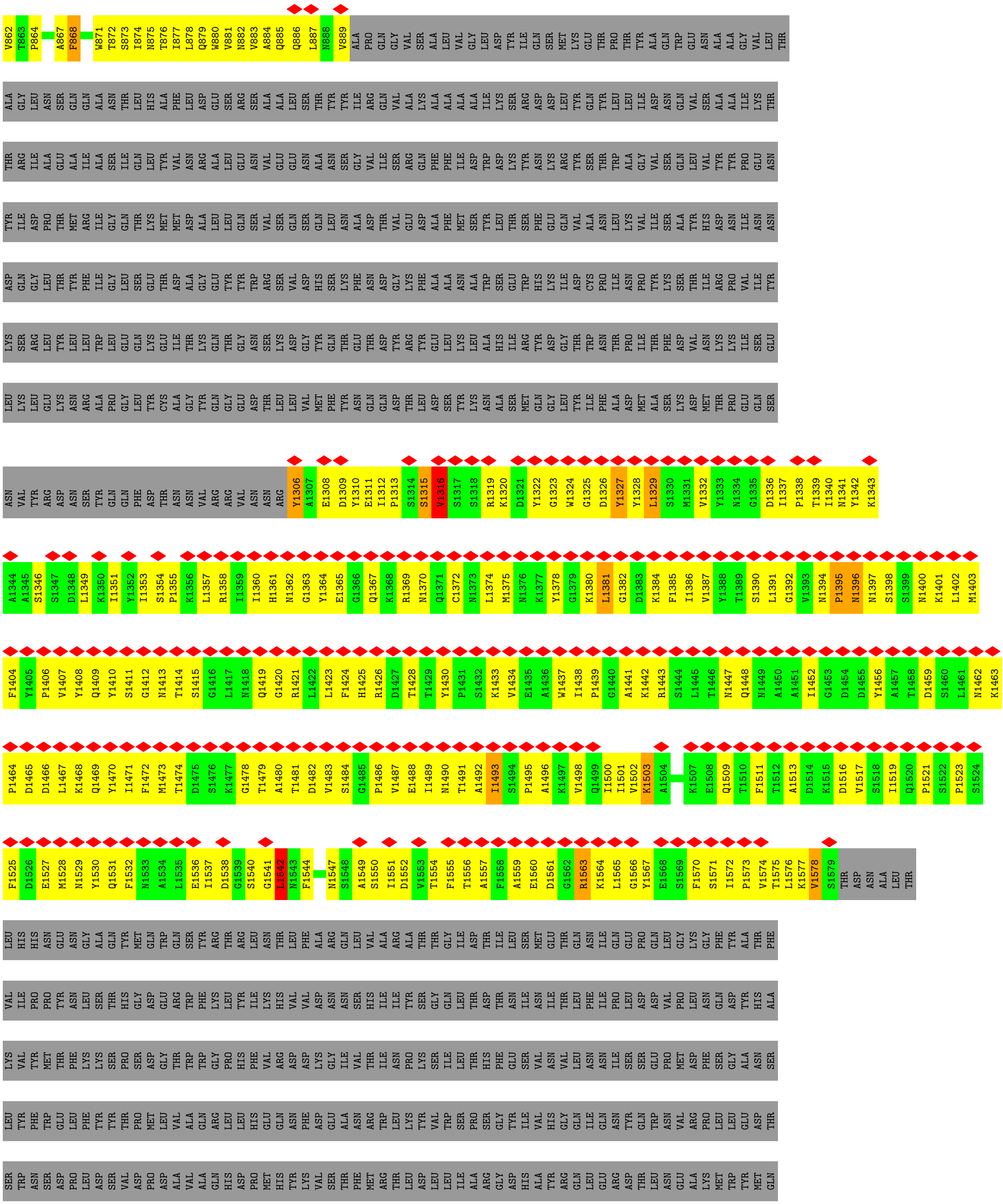
GLY PRO TYR GLN ASP VAL GLN ALA ILE LEU SER TYR GLY ASP LYS ALA GLY LEU ALA ASN GLY CYS GLU ALA LEU ALA VAL SER HIS GLY MET ASN ASP SER GLY GLN PHE GLN LEU ASP PHE ASN ASP GLY LYS PHE LEU PRO PHE GLU GLY ILE ALA ILE ASP GLN GLY THR LEU THR

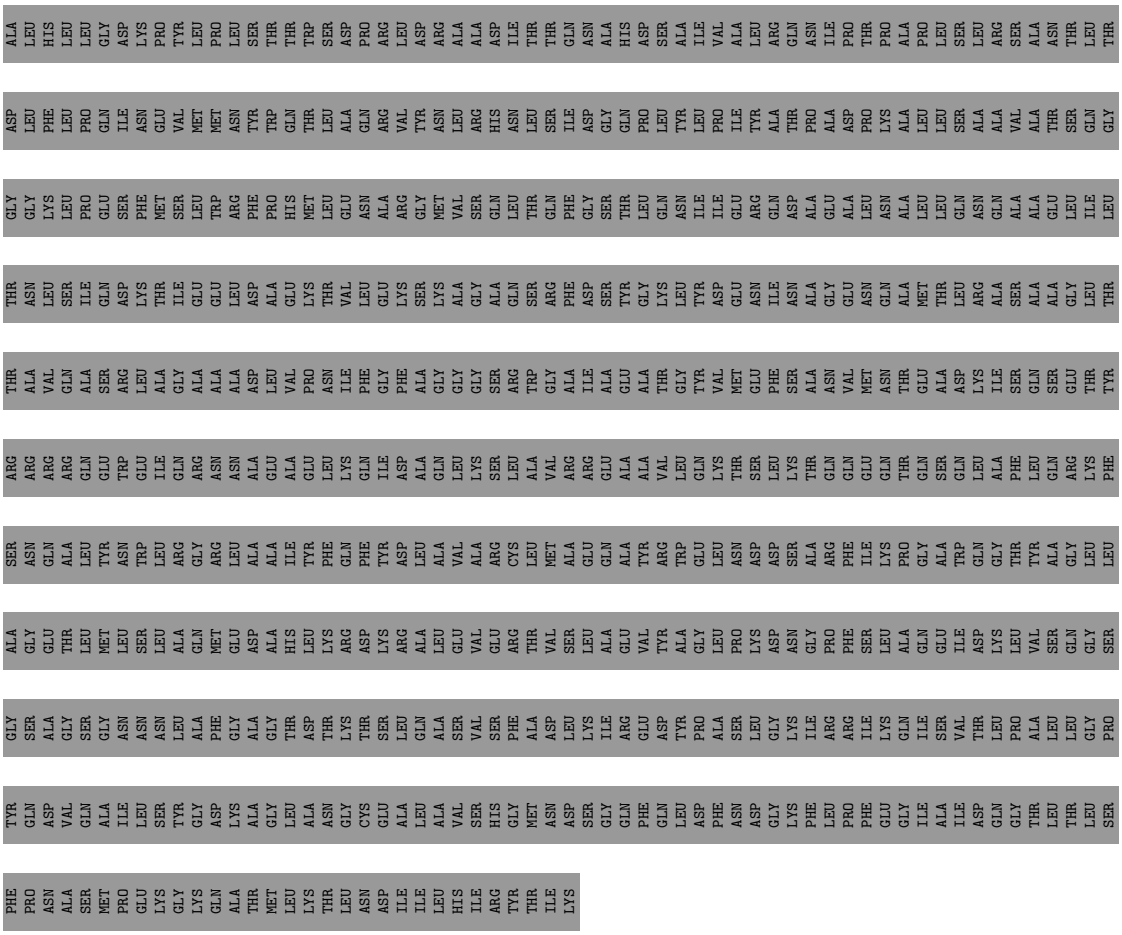
LEU SER PHE PRO ASN ALA SER MET PRO GLU LYS GLY LYS GLN ALA THR MET LEU LYS THR LEU ASN ASP ILE ILE LEU HIS ILE ARG TYR THR ILE LYS

• Molecule 1: TcdA1

Chain D:

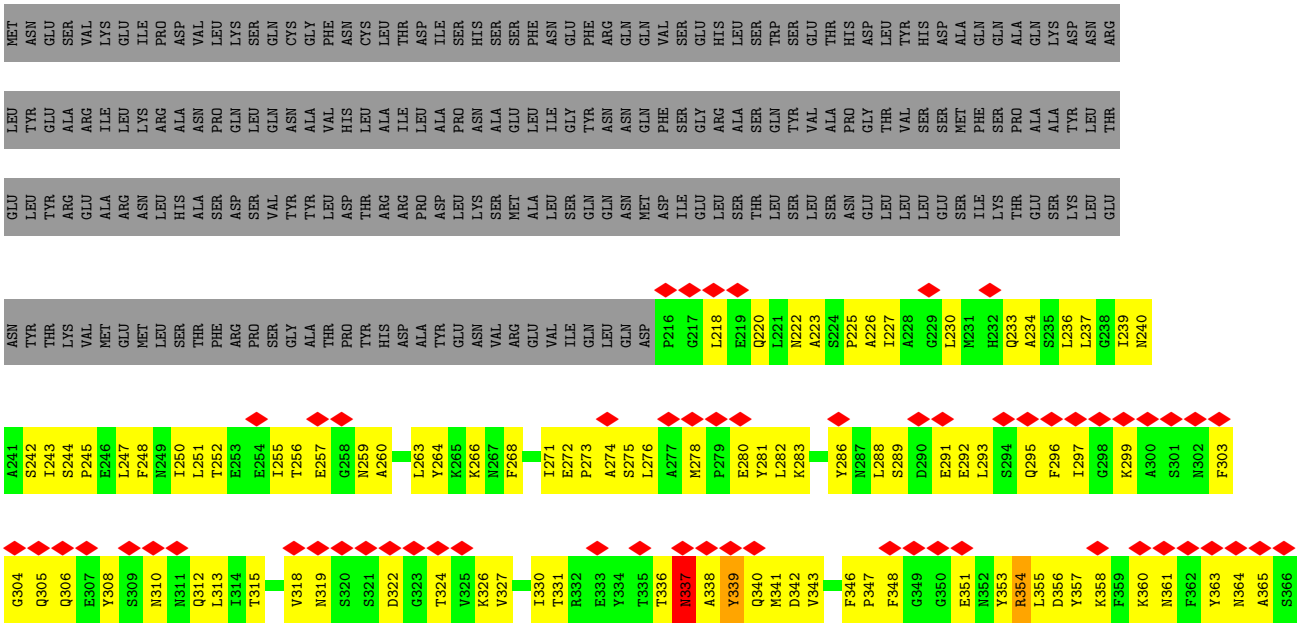


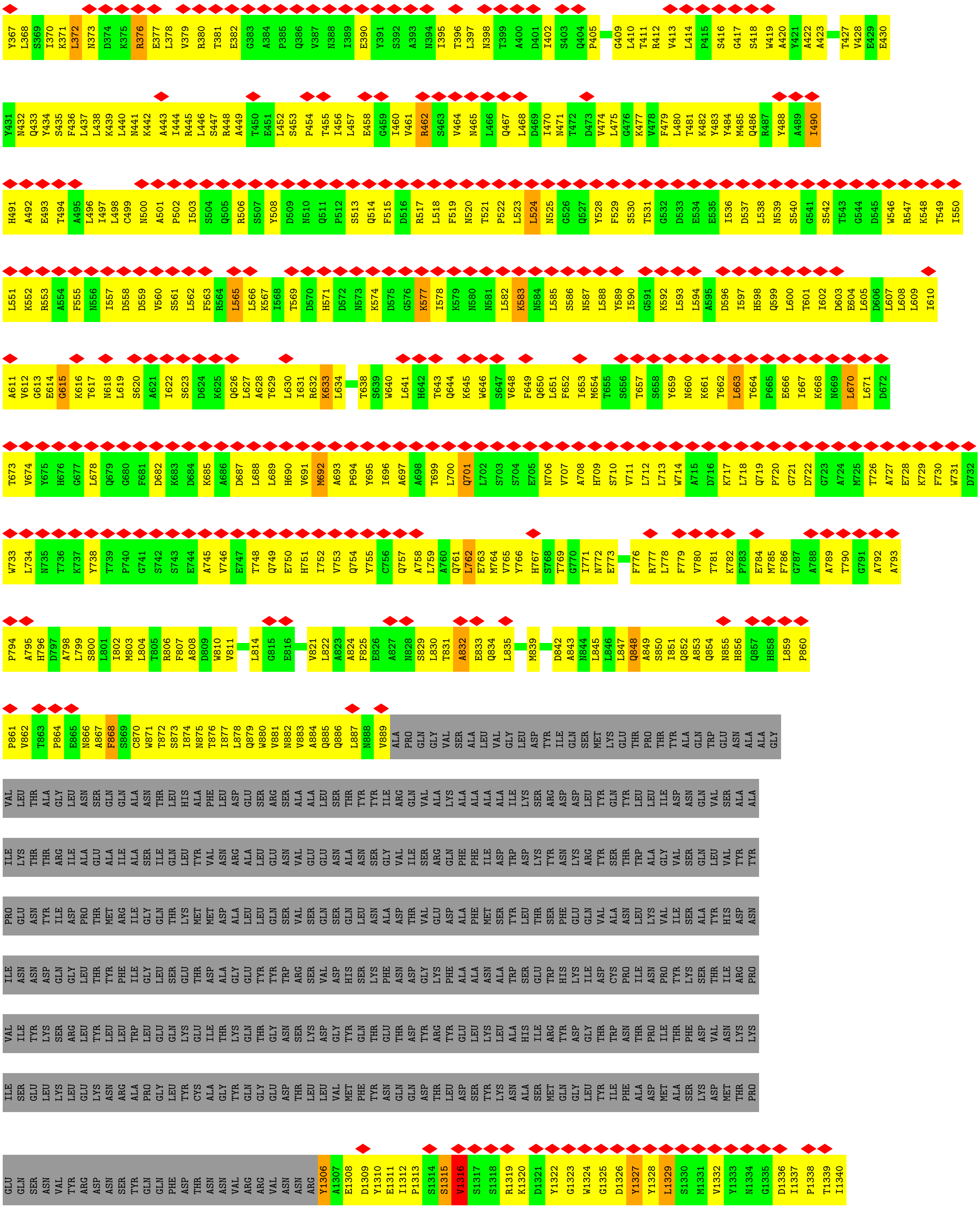

V862 T863 P864 A867 F868 W871 T872 S873 I874 N875 T876 I877 L878 Q879 W880 V881 N882 V883 A884 Q885 Q886 L887 N888 V889 ALA PRO GLN GLY VAL SER ALA LEU VAL GLY LEU ASP TYR ILE GLN SER MET LYS GLU THR PRO THR TYR ALA GLN TRP GLU ASN ALA ALA GLY VAL LEU THR
ALA GLY LEU ASN SER GLN GLN ALA ASN THR LEU HIS ALA PHE LEU ASP GLU SER ARG SER ALA ALA LEU SER THR TYR TYR ILE ARG GLN VAL ALA LYS ALA ALA ALA ALA ILE LYS SER ARG ASP ASP LEU TYR GLN TYR LEU LEU ILE ASP ASN GLN VAL SER ALA ALA ILE LYS THR
THR ARG ILE ALA GLU ALA ILE ALA SER ILE GLN LEU TYR VAL ASN ARG ALA LEU GLU ASN VAL GLU GLU ASN ALA ASN SER GLY VAL ILE SER ARG GLN PHE PHE ILE ASP TRP ASP LYS TYR ASN LYS ARG TYR SER THR TRP ALA GLY VAL SER GLN LEU VAL TYR TYR PRO GLU ASN
TYR ILE ASP PRO THR MET ARG ILE GLY GLN THR LYS MET MET ASP ALA LEU LEU GLN SER VAL SER GLN SER GLN LEU ASN ALA ASP THR VAL GLU ASP ALA PHE MET SER TYR LEU THR SER PHE GLU GLN VAL ALA ASN LEU LYS VAL ILE SER ALA TYR HIS ASP ASN ILE ASN ASN
ASP GLN GLY LEU THR TYR PHE ILE GLY LEU SER GLU THR ASP ALA GLY GLU TYR TYR TRP ARG SER VAL ASP HIS SER LYS PHE ASN ASP GLY LYS PHE ALA ALA ASN ALA TRP SER GLU TRP HIS LYS ILE ASP CYS PRO ILE ASN PRO TYR LYS SER THR ILE ARG PRO VAL ILE TYR
LYS SER ARG LEU TYR LEU LEU TRP LEU GLU GLN LYS GLU ILE THR LYS GLN THR GLY ASN SER LYS ASP GLY TYR GLN THR GLU THR ASP TYR ARG TYR GLU LEU LYS LEU ALA HIS ILE ARG TYR ASP GLY THR TRP ASN THR PRO ILE THR PHE ASP VAL ASN LYS LYS ILE SER GLU
LEU LYS LEU GLU LYS ASN ARG ALA PRO GLY LEU TYR CYS ALA GLY TYR GLN GLY GLU ASP THR LEU LEU VAL MET PHE TYR ASN GLN GLN ASP THR LEU ASP SER TYR LYS ASN ALA SER MET GLN GLY LEU TYR ILE PHE ALA ASP MET ALA SER LYS ASP MET THR PRO GLU GLN SER
ASN VAL TYR ARG ASP ASN SER TYR GLN GLN PHE ASP THR ASN ASN VAL ARG ARG VAL ASN ASN ARG Y1306 A1307 E1308 D1309 Y1310 E1311 I1312 P1313 S1314 S1315 V1316 S1317 S1318 R1319 K1320 D1321 Y1322 G1323 W1324 G1325 D1326 Y1327 Y1328 L1329 S1330 M1331 V1332 Y1333 N1334 G1335 D1336 I1337 P1338 T1339 I1340 N1341 Y1342 K1343
A1344 A1345 S1346 S1347 D1348 L1349 K1350 I1351 Y1352 I1353 S1354 P1355 K1356 L1357 R1358 I1359 I1360 H1361 N1362 G1363 Y1364 E1365 G1366 Q1367 K1368 R1369 N1370 Q1371 C1372 N1373 L1374 M1375 N1376 K1377 Y1378 G1379 K1380 L1381 G1382 D1383 K1384 F1385 I1386 V1387 Y1388 T1389 S1390 L1391 G1392 V1393 N1394 P1395 N1396 N1397 S1398 S1399 N1400 K1401 L1402 M1403
F1404 Y1405 P1406 V1407 Y1408 Q1409 Y1410 S1411 G1412 N1413 T1414 S1415 G1416 L1417 N1418 Q1419 G1420 R1421 L1422 L1423 F1424 H1425 R1426 D1427 T1428 T1429 Y1430 P1431 S1432 K1433 V1434 E1435 A1436 W1437 I1438 P1439 G1440 A1441 K1442 R1443 S1444 L1445 T1446 N1447 Q1448 N1449 A1450 A1451 I1452 G1453 D1454 D1455 Y1456 A1457 T1458 D1459 S1460 L1461 N1462 K1463
P1464 D1465 D1466 L1467 K1468 Q1469 Y1470 I1471 F1472 M1473 T1474 D1475 S1476 K1477 G1478 T1479 A1480 T1481 D1482 V1483 S1484 G1485 P1486 V1487 E1488 I1489 N1490 T1491 A1492 I1493 S1494 P1495 A1496 K1497 V1498 Q1499 I1500 I1501 V1502 K1503 A1504 K1507 E1508 Q1509 T1510 F1511 T1512 A1513 D1514 K1515 D1516 V1517 S1518 I1519 Q1520 P1521 S1522 P1523 S1524
F1525 D1526 E1527 M1528 N1529 Y1530 Q1531 F1532 N1533 A1534 L1535 E1536 I1537 D1538 G1539 S1540 G1541 L1542 N1543 F1544 N1547 S1548 A1549 S1550 I1551 D1552 V1553 T1554 F1555 T1556 A1557 F1558 A1559 E1560 D1561 G1562 R1563 K1564 L1565 G1566 Y1567 E1568 S1569 F1570 S1571 I1572 P1573 V1574 T1575 L1576 K1577 V1578 S1579 THR ASP ASN ALA LEU THR
LEU HIS HIS ASN GLU ASN GLY ALA GLN TYR MET GLN TRP GLN SER TYR ARG THR ARG LEU ASN THR LEU PHE ALA ARG GLN LEU VAL ALA ARG ALA THR THR GLY ILE ASP THR ILE LEU SER MET GLU THR GLN ASN ILE GLN GLU PRO GLN LEU GLY LYS GLY PHE TYR ALA THR PHE
VAL ILE PRO PRO TYR ASN LEU SER THR HIS GLY ASP GLU ARG TRP PHE LYS LEU TYR ILE LYS HIS VAL VAL ASP ASN ASN SER HIS ILE ILE TYR SER GLY GLN LEU THR ASP THR ASN ILE ASN ILE THR LEU PHE ILE PRO LEU ASP ASP VAL PRO LEU ASN GLN ASP TYR HIS ALA
LYS VAL TYR MET THR PHE LYS LYS SER PRO SER ASP GLY THR TRP TRP GLY PRO HIS PHE VAL ARG ASP ASP LYS GLY ILE VAL THR ILE ASN PRO LYS SER ILE LEU THR HIS PHE GLU SER VAL ASN VAL LEU ASN ASN ILE SER SER GLU PRO MET ASP PHE SER GLY ALA ASN SER
LEU TYR PHE TRP GLU LEU PHE TYR TYR THR PRO MET LEU VAL ALA GLN ARG LEU LEU HIS GLU GLN ASN PHE ASP GLU ALA ASN ARG TRP LEU LYS TYR VAL TRP SER PRO SER GLY TYR ILE VAL HIS GLY GLN ILE GLN ASN TYR GLN TRP ASN VAL ARG PRO LEU LEU GLU ASP THR
SER TRP ASN SER ASP PRO LEU ASP SER VAL ASP PRO ASP ALA VAL ALA GLN HIS ASP PRO MET HIS TYR LYS VAL SER THR PHE MET ARG THR LEU ASP LEU LEU ILE ALA ARG GLY ASP HIS ALA TYR ARG GLN LEU GLU ARG ASP THR LEU ASN GLU ALA LYS MET TRP TYR MET GLN



- Molecule 1: TcdA1

Chain E:

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Y431 N432 Q433 Y434 S435 F436 L437 L438 K439 L440 N441 K442 A443 I444 R445 L446 S447 R448 A449 T450 E451 L452 S453 P454 T455 I456 L457 E458 G459 I460 V461 R462 S463 V464 N465 L466 Q467 L468 D469 I470 N471 T472 D473 V474 L475 G476 K477 V478 F479 L480 T481 K482 Y483 Y484 M485 Q486 R487 Y488 A489 I490
H491 A492 E493 T494 A495 L496 I497 L498 C499 N500 A501 P502 I503 S504 Q505 R506 S507 Y508 D509 N510 Q511 P512 S513 Q514 F515 D516 R517 L518 F519 N520 T521 P522 L523 L524 N525 G526 Q527 Y528 F529 S530 T531 G532 D533 E534 E535 I536 D537 L538 N539 S540 G541 S542 T543 G544 D545 W546 R547 K548 T549 I550
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A611 V612 G613 E614 G615 K616 T617 N618 L619 S620 A621 I622 S623 D624 K625 Q626 L627 A628 T629 L630 I631 R632 K633 L634 T638 S639 W640 L641 H642 T643 Q644 K645 W646 S647 V648 F649 Q650 L651 F652 I653 M654 T655 S656 T657 S658 Y659 N660 K661 T662 L663 T664 P665 E666 I667 K668 N669 L670 L671 D672
T673 V674 Y675 H676 G677 L678 Q679 G680 F681 D682 K683 D684 K685 A686 D687 L688 L689 H690 V691 M692 A693 P694 Y695 I696 A697 A698 T699 L700 Q701 L702 S703 S704 E705 N706 V707 A708 H709 S710 V711 L712 L713 W714 A715 D716 K717 L718 Q719 P720 G721 D722 G723 A724 M725 T726 A727 E728 K729 F730 W731 D732
W733 L734 N735 T736 K737 Y738 T739 P740 G741 S742 S743 E744 A745 V746 E747 T748 Q749 E750 H751 I752 V753 Q754 Y755 C756 Q757 A758 L759 A760 Q761 L762 E763 M764 V765 Y766 H767 S768 T769 G770 I771 N772 E773 F776 R777 L778 F779 V780 T781 K782 P783 E784 M785 F786 G787 A788 A789 T790 G791 A792 A793
P794 A795 H796 D797 A798 L799 S800 L801 I802 M803 L804 T805 R806 F807 A808 D809 W810 V811 L814 G815 E816 V821 L822 A823 A824 F825 E826 A827 N828 S829 L830 T831 A832 E833 Q834 L835 M839 D842 A843 N844 L845 L846 L847 Q848 A849 S850 I851 Q852 A853 Q854 N855 H856 Q857 H858 L859 P860
P861 V862 T863 P864 E865 N866 A867 F868 S869 C870 W871 T872 S873 I874 N875 T876 I877 L878 Q879 W880 V881 N882 V883 A884 Q885 Q886 L887 N888 V889 ALA PRO GLN GLY VAL SER ALA LEU VAL GLY LEU ASP TYR ILE GLN SER MET LYS GLU THR PRO THR TYR ALA GLN TRP GLU ASN ALA ALA GLY
VAL LEU THR ALA GLY LEU ASN SER GLN GLN ALA ASN THR LEU HIS ALA PHE LEU ASP GLU SER ARG SER ALA ALA LEU SER THR TYR TYR ILE ARG GLN VAL ALA LYS ALA ALA ALA ALA ILE LYS SER ARG ASP ASP LEU TYR GLN TYR LEU LEU ILE ASP ASN GLN VAL SER ALA ALA
ILE LYS THR THR ARG ILE ALA GLU ALA ILE ALA SER ILE GLN LEU TYR VAL ASN ARG ALA LEU GLU ASN VAL GLU GLU ASN ALA ASN SER GLY VAL ILE SER ARG GLN PHE PHE ILE ASP TRP ASP LYS TYR ASN LYS ARG TYR SER THR TRP ALA GLY VAL SER GLN LEU VAL TYR TYR
PRO GLU ASN TYR ILE ASP PRO THR MET ARG ILE GLY GLN THR LYS MET MET ASP ALA LEU LEU GLN SER VAL SER GLN SER GLN LEU ASN ALA ASP THR VAL GLU ASP ALA PHE MET SER TYR LEU THR SER PHE GLU GLN VAL ALA ASN LEU LYS VAL ILE SER ALA TYR HIS ASP ASN
ILE ASN ASN ASP GLN GLY LEU THR TYR PHE ILE GLY LEU SER GLU THR ASP ALA GLY GLU TYR TYR ARG SER VAL ASP HIS SER LYS PHE ASN ASP GLY LYS PHE ALA ALA ASN ALA TRP SER GLU TRP HIS LYS ILE ASP CYS PRO ILE ASN PRO TYR LYS SER THR ILE ARG PRO
VAL ILE TYR LYS SER ARG LEU TYR LEU LEU TRP LEU GLU GLN LYS GLU ILE THR LYS GLN THR GLY ASN SER LYS ASP GLY TYR GLN THR GLU THR ASP TYR ARG TYR GLU LEU LYS LEU ALA HIS ILE ARG TYR ASP GLY THR TRP ASN THR PRO ILE THR PHE ASP VAL ASN LYS LYS
ILE SER GLU LEU LYS LEU GLU LYS ASN ARG ALA PRO GLY LEU TYR CYS ALA GLY TYR GLN GLY GLU ASP THR LEU LEU VAL MET PHE TYR ASN GLN GLN ASP THR LEU ASP SER TYR LYS ASN ALA SER MET GLN GLY LEU TYR ILE PHE ALA ASP MET ALA SER LYS ASP MET THR PRO
GLU GLN SER ASN VAL TYR ARG ASP ASN SER TYR GLN GLN PHE ASP THR ASN ASN VAL ARG ARG VAL ASN ASN ARG Y1306 A1307 E1308 D1309 Y1310 E1311 I1312 P1313 S1314 S1315 V1316 S1317 S1318 R1319 K1320 D1321 Y1322 G1323 W1324 G1325 D1326 Y1327 Y1328 L1329 S1330 M1331 V1332 Y1333 N1334 G1335 D1336 I1337 P1338 T1339 I1340

N1341 Y1342 K1343 A1344 A1345 S1346 S1347 D1348 L1349 K1350 I1351 Y1352 I1353 S1354 P1355 K1356 L1357 R1358 I1359 I1360 H1361 N1362 G1363 Y1364 E1365 G1366 Q1367 K1368 R1369 N1370 Q1371 C1372 N1373 L1374 M1375 N1376 K1377 Y1378 G1379 K1380 L1381 G1382 D1383 K1384 F1385 I1386 V1387 Y1388 T1389 S1390 L1391 G1392 V1393 N1394 P1395 N1396 N1397 S1398 S1399 N1400

K1401 L1402 M1403 F1404 Y1405 P1406 V1407 Y1408 Q1409 Y1410 S1411 G1412 N1413 T1414 S1415 G1416 L1417 N1418 Q1419 G1420 R1421 L1422 L1423 F1424 H1425 R1426 D1427 T1428 T1429 Y1430 P1431 S1432 K1433 V1434 E1435 A1436 W1437 I1438 P1439 G1440 A1441 K1442 R1443 S1444 L1445 T1446 N1447 Q1448 N1449 A1450 A1451 I1452 G1453 D1454 D1455 Y1456 A1457 T1458 D1459 S1460

L1461 N1462 K1463 P1464 D1465 D1466 L1467 K1468 Q1469 Y1470 I1471 F1472 M1473 T1474 D1475 S1476 K1477 G1478 T1479 A1480 T1481 D1482 V1483 S1484 G1485 P1486 V1487 E1488 I1489 N1490 T1491 A1492 I1493 S1494 P1495 A1496 K1497 V1498 Q1499 I1500 I1501 V1502 K1503 A1504 K1507 E1508 Q1509 T1510 F1511 T1512 A1513 D1514 K1515 D1516 V1517 S1518 I1519 Q1520 P1521

S1522 P1523 S1524 F1525 D1526 E1527 M1528 N1529 Y1530 Q1531 F1532 N1533 A1534 L1535 E1536 I1537 D1538 G1539 S1540 G1541 L1542 N1543 F1544 N1547 S1548 A1549 S1550 I1551 D1552 V1553 T1554 F1555 T1556 A1557 F1558 A1559 E1560 D1561 G1562 R1563 K1564 L1565 G1566 Y1567 E1568 S1569 F1570 S1571 I1572 P1573 V1574 T1575 L1576 K1577 V1578 S1579 THR ASP ASN

ALA LEU THR LEU HIS HIS ASN GLU ASN GLY ALA GLN TYR MET GLN TRP GLN SER TYR ARG THR ARG LEU ASN THR LEU PHE ALA ARG GLN LEU VAL ALA ARG ALA THR THR GLY ILE ASP THR ILE LEU SER MET GLU THR GLN ASN ILE GLN GLU PRO GLN LEU GLY LYS GLY PHE TYR

ALA THR PHE VAL ILE PRO PRO TYR ASN LEU SER THR HIS GLY ASP GLU ARG TRP PHE LYS LEU TYR ILE LYS HIS VAL VAL ASP ASN ASN SER HIS ILE ILE TYR SER GLY GLN LEU THR ASP THR ASN ILE ASN ILE THR LEU PHE ILE PRO LEU ASP ASP VAL PRO LEU ASN GLN ASP

TYR HIS ALA LYS VAL TYR MET THR PHE LYS LYS SER PRO SER ASP GLY THR TRP TRP GLY PRO HIS PHE VAL ARG ASP ASP LYS GLY ILE VAL THR ILE ASN PRO LYS SER ILE LEU THR HIS PHE GLU SER VAL ASN VAL LEU ASN ASN ILE SER SER GLU PRO MET ASP PHE SER GLY

ALA ASN SER LEU TYR PHE TRP GLU LEU PHE TYR TYR THR PRO MET LEU VAL ALA GLN ARG LEU LEU HIS GLU GLN ASN PHE ASP GLU ALA ASN ARG TRP LEU LYS TYR VAL TRP SER PRO SER GLY TYR ILE VAL HIS GLY GLN ILE GLN ASN TYR GLN TRP ASN VAL ARG PRO LEU LEU

GLU ASP THR SER TRP ASN SER ASP PRO LEU ASP SER VAL ASP PRO ASP ALA VAL ALA GLN HIS ASP PRO MET HIS TYR LYS VAL SER THR PHE MET ARG THR LEU ASP LEU LEU ILE ALA ARG GLY ASP HIS ALA TYR ARG GLN LEU GLU ARG ASP THR LEU ASN GLU ALA LYS MET TRP

TYR MET GLN ALA LEU HIS LEU LEU GLY ASP LYS PRO TYR LEU PRO LEU SER THR THR TRP SER ASP PRO ARG LEU ASP ARG ALA ALA ASP ILE THR THR GLN ASN ALA HIS ASP SER ALA ILE VAL ALA LEU ARG GLN ASN ILE PRO THR PRO ALA PRO LEU SER LEU ARG SER ALA ASN

THR LEU THR ASP LEU PHE LEU PRO GLN ILE ASN GLU VAL MET MET ASN TYR TRP GLN THR LEU ALA GLN ARG VAL TYR ASN LEU ARG HIS ASN LEU SER ILE ASP GLY GLN PRO LEU TYR LEU PRO ILE TYR ALA THR PRO ALA ASP PRO LYS ALA LEU LEU SER ALA ALA VAL ALA THR

SER GLN GLY GLY GLY LYS LEU PRO GLU SER PHE MET SER LEU TRP ARG PHE PRO HIS MET LEU GLU ASN ALA ARG GLY MET VAL SER GLN LEU THR GLN PHE GLY SER THR LEU GLN ASN ILE ILE GLU ARG GLN ASP ALA GLU ALA LEU ASN ALA LEU LEU GLN ASN GLN ALA ALA GLU

LEU ILE LEU THR ASN LEU SER ILE GLN ASP LYS THR ILE GLU GLU LEU ASP ALA GLU LYS THR VAL LEU GLU LYS SER LYS ALA GLY ALA GLN SER ARG PHE ASP SER TYR GLY LYS LEU TYR ASP GLU ASN ILE ASN ALA GLY GLU ASN GLN ALA MET THR LEU ARG ALA SER ALA ALA

GLY LEU THR THR ALA VAL GLN ALA SER ARG LEU ALA GLY ALA ALA ALA ASP LEU VAL PRO ASN ILE PHE GLY PHE ALA GLY GLY GLY SER ARG TRP GLY ALA ILE ALA GLU ALA THR GLY TYR VAL MET GLU PHE SER ALA ASN VAL MET ASN THR GLU ALA ASP LYS ILE SER GLN SER

GLU THR TYR ARG ARG ARG ARG GLN GLU TRP GLU ILE GLN ARG ASN ASN ALA GLU ALA GLU LEU LYS GLN ILE ASP ALA GLN LEU LYS SER LEU ALA VAL ARG ARG GLU ALA ALA VAL LEU GLN LYS THR SER LEU LYS THR GLN GLN GLU GLN THR GLN SER GLN LEU ALA PHE LEU GLN

ARG LYS PHE SER ASN GLN ALA LEU TYR ASN TRP LEU ARG GLY ARG LEU ALA ALA ILE TYR PHE GLN PHE TYR ASP LEU ALA VAL ALA ARG CYS LEU MET ALA GLU GLN ALA TYR ARG TRP GLU LEU ASN ASP ASP SER ALA ARG PHE ILE LYS PRO GLY ALA TRP GLN GLY THR TYR ALA

GLY LEU LEU ALA GLY GLU THR LEU MET LEU SER LEU ALA GLN MET GLU ASP ALA HIS LEU LYS ARG ASP LYS ARG ALA LEU GLU VAL GLU ARG THR VAL SER LEU ALA GLU VAL TYR ALA GLY LEU PRO LYS ASP ASN GLY PRO PHE SER LEU ALA GLN GLU ILE ASP LYS LEU VAL SER

GLN GLY SER GLY SER ALA GLY SER GLY ASN ASN LEU ALA PHE GLY ALA GLY THR ASP THR LYS THR SER LEU GLN ALA SER VAL SER PHE ALA ASP LEU LYS ILE ARG GLU ASP TYR PRO ALA SER LEU GLY LYS ILE ARG ARG ILE LYS GLN ILE SER VAL THR LEU PRO ALA LEU


LEU GLY PRO TYR GLN ASP VAL GLN ALA ILE LEU SER TYR GLY ASP LYS ALA GLY LEU ALA ASN GLY CYS GLU ALA LEU ALA VAL SER HIS GLY MET ASN ASP SER GLY GLN PHE GLN LEU ASP PHE ASN ASP GLY LYS PHE LEU PRO PHE GLU GLY ILE ALA ILE ASP GLN GLY THR LEU


THR LEU SER PHE PRO ASN ALA SER MET PRO GLU LYS GLY LYS GLN ALA THR MET LEU LYS THR LEU ASN ASP ILE ILE LEU HIS ILE ARG TYR THR ILE LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	13000	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 ($e^-/Å^2$)	15.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	29.239	Depositor
Minimum map value	-15.199	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.75	Depositor
Map size (Å)	442.74002, 442.74002, 442.74002	wwPDB
Map dimensions	282, 282, 282	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.57, 1.57, 1.57	Depositor

5 Model quality

5.1 Standard geometry

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	0.89	0/7627	1.14	20/10362 (0.2%)
1	B	0.89	0/7627	1.14	20/10362 (0.2%)
1	C	0.89	0/7627	1.14	20/10362 (0.2%)
1	D	0.89	0/7627	1.14	20/10362 (0.2%)
1	E	0.89	0/7627	1.14	20/10362 (0.2%)
All	All	0.89	0/38135	1.14	100/51810 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1541	GLY	C-N-CA	9.54	145.55	121.70
1	B	1541	GLY	C-N-CA	9.53	145.53	121.70
1	E	1541	GLY	C-N-CA	9.52	145.49	121.70
1	A	1541	GLY	C-N-CA	9.51	145.49	121.70
1	D	1541	GLY	C-N-CA	9.51	145.47	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	615	GLY	Peptide
1	B	615	GLY	Peptide
1	C	615	GLY	Peptide
1	D	615	GLY	Peptide
1	E	615	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7469	0	7341	1262	0
1	B	7469	0	7341	1262	0
1	C	7469	0	7341	1271	0
1	D	7469	0	7341	1254	0
1	E	7469	0	7341	1268	0
All	All	37345	0	36705	6317	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 85.

The worst 5 of 6317 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:C:557:ILE:HD11	1:C:592:LYS:HD2	1.21	1.21
1:C:218:LEU:HD21	1:C:239:ILE:HG21	1.19	1.18
1:A:1406:PRO:HG3	1:A:1473:MET:HE1	1.22	1.17
1:A:557:ILE:HD11	1:A:592:LYS:HD2	1.21	1.17
1:E:227:ILE:HD13	1:E:883:VAL:HB	1.26	1.16

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	944/2516 (38%)	899 (95%)	32 (3%)	13 (1%)	11	44
1	B	944/2516 (38%)	899 (95%)	32 (3%)	13 (1%)	11	44
1	C	944/2516 (38%)	899 (95%)	32 (3%)	13 (1%)	11	44
1	D	944/2516 (38%)	899 (95%)	32 (3%)	13 (1%)	11	44
1	E	944/2516 (38%)	899 (95%)	32 (3%)	13 (1%)	11	44
All	All	4720/12580 (38%)	4495 (95%)	160 (3%)	65 (1%)	15	44

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ARG
1	A	525	ASN
1	A	1346	SER
1	A	1381	LEU
1	A	1542	LEU

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	817/2157 (38%)	801 (98%)	16 (2%)	55	79
1	B	817/2157 (38%)	801 (98%)	16 (2%)	55	79
1	C	817/2157 (38%)	801 (98%)	16 (2%)	55	79
1	D	817/2157 (38%)	801 (98%)	16 (2%)	55	79
1	E	817/2157 (38%)	801 (98%)	16 (2%)	55	79
All	All	4085/10785 (38%)	4005 (98%)	80 (2%)	57	79

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	762	LEU
1	E	692	MET
1	D	796	HIS
1	E	372	LEU
1	E	796	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	340	GLN
1	E	310	ASN
1	D	486	GLN
1	D	885	GLN
1	E	505	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

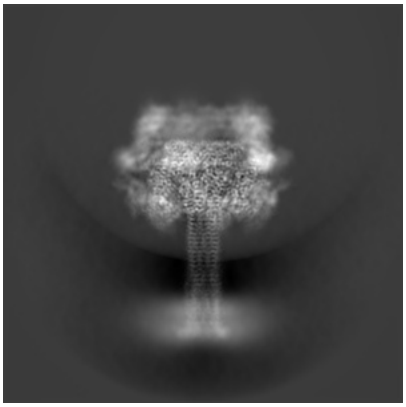
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4068. These allow visual inspection of the internal detail of the map and identification of artifacts.

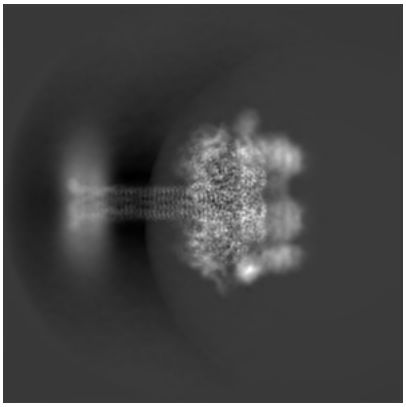
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

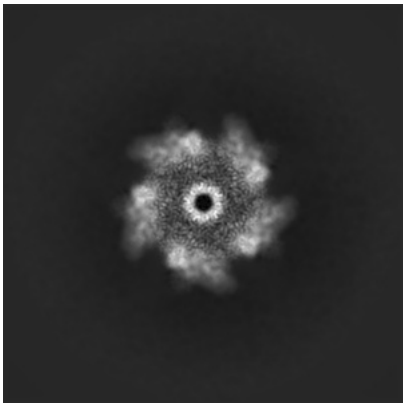
6.1.1 Primary map



X



Y



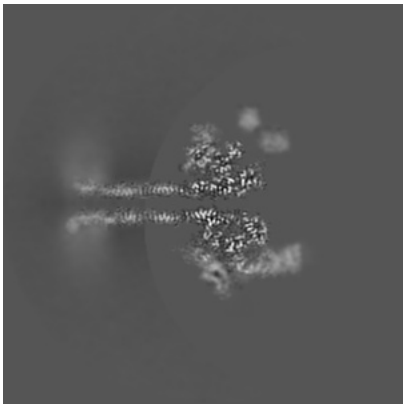
Z

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

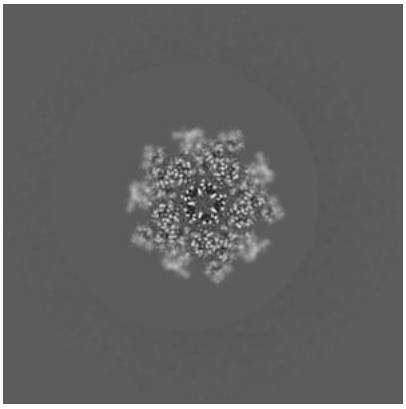
6.2 Central slices

6.2.1 Primary map

X Index: 141



Y Index: 141

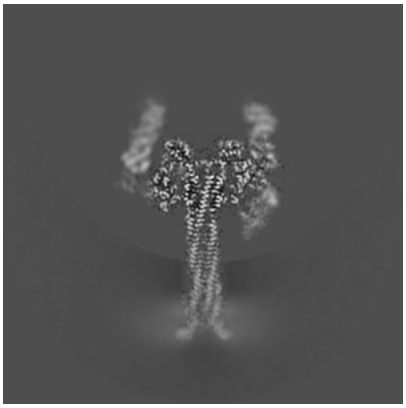


Z Index: 141

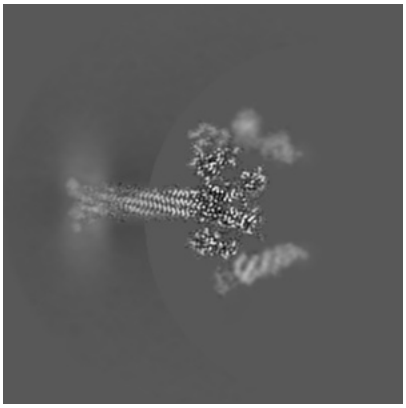
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

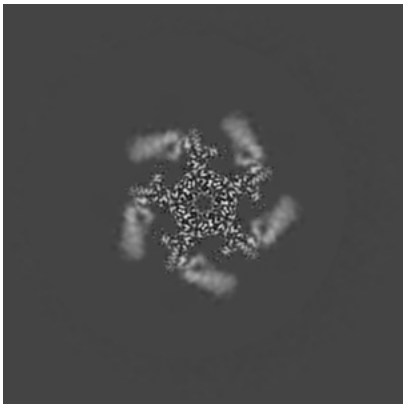
6.3.1 Primary map



X Index: 134



Y Index: 132



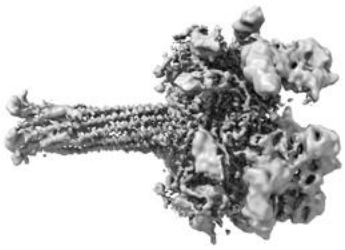
Z Index: 169

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

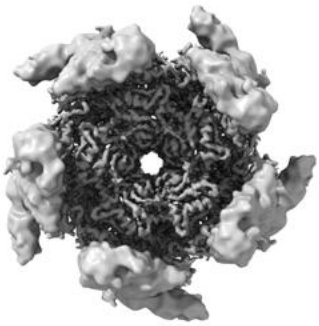
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

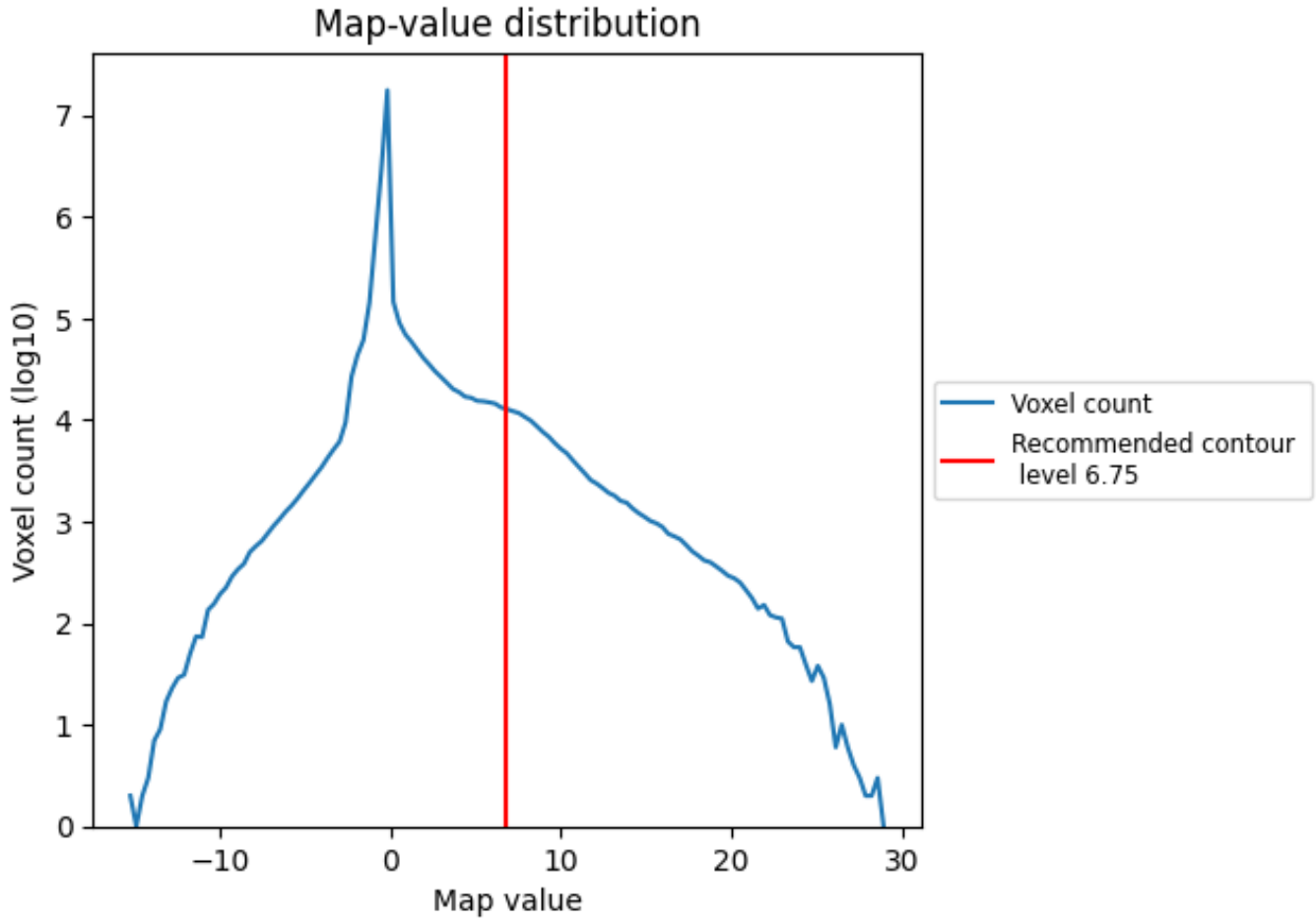
6.5 Mask visualisation (i)

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

7 Map analysis

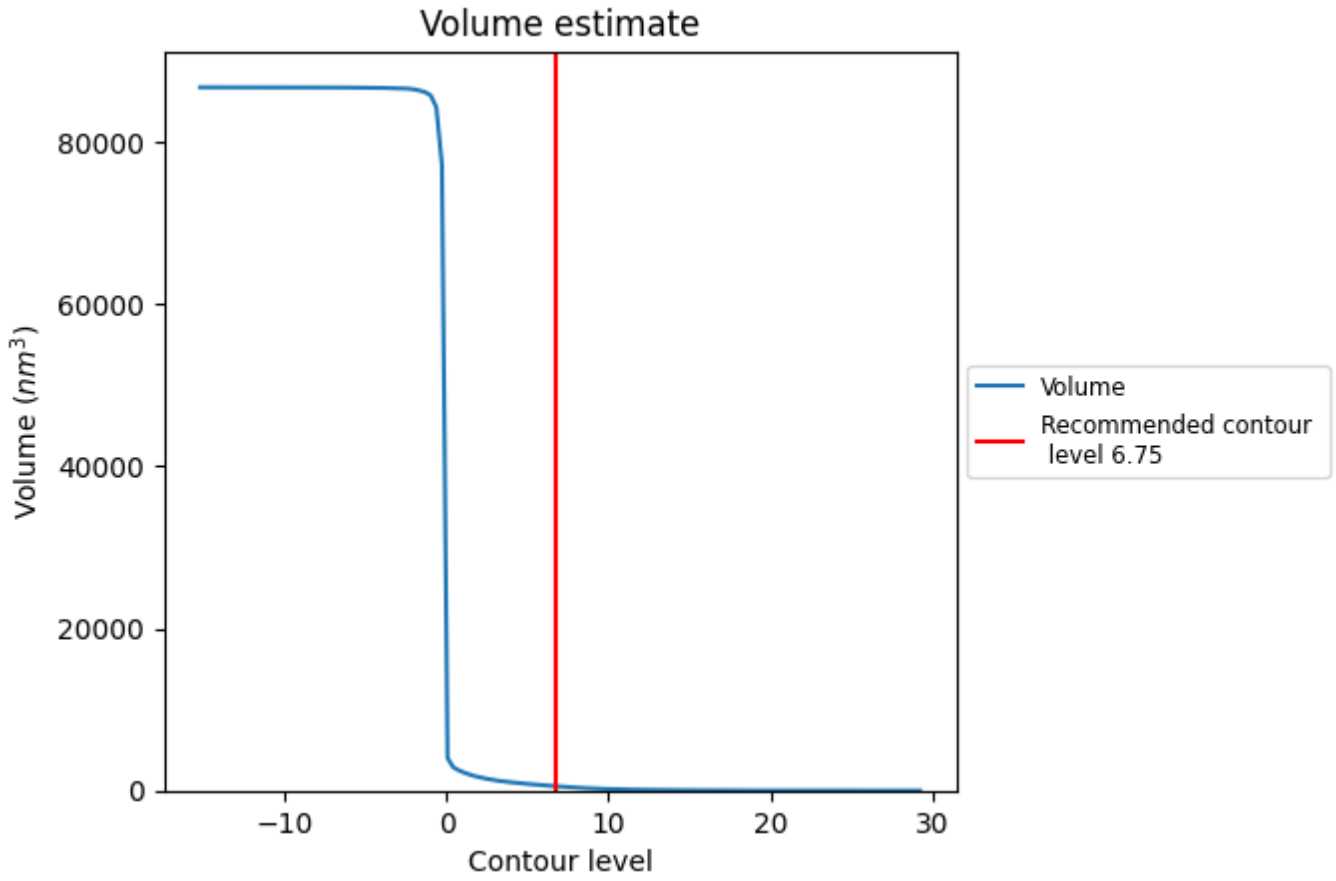
This section contains the results of statistical analysis of the map.

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.

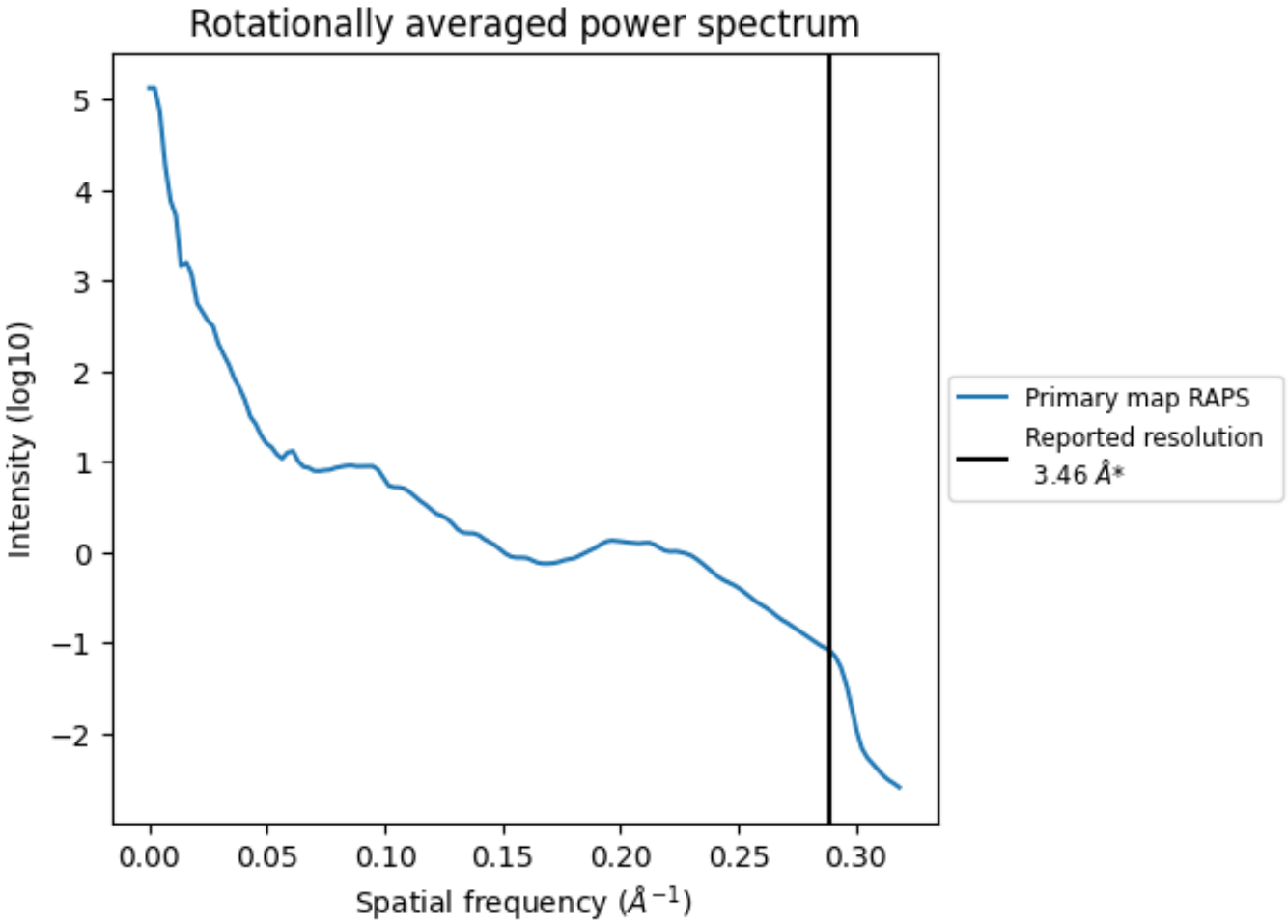
7.2 Volume estimate (i)



The volume at the recommended contour level is 535 nm^3; this corresponds to an approximate mass of 483 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 0.289 Å^{-1}

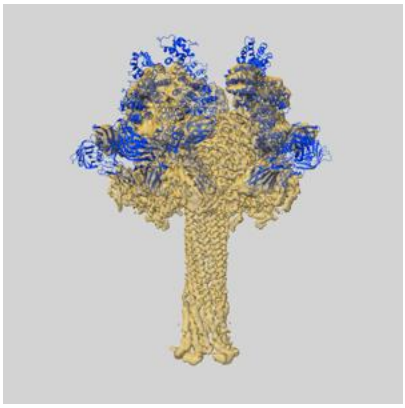
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

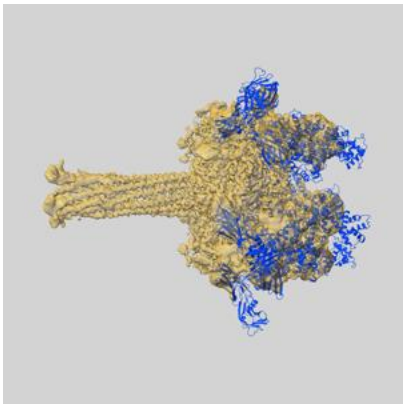
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4068 and PDB model 5LKH. Per-residue inclusion information can be found in section 3 on page 4.

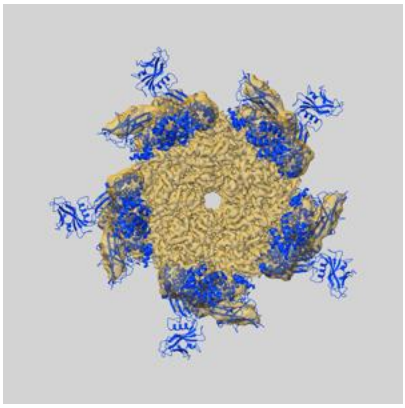
9.1 Map-model overlay



X



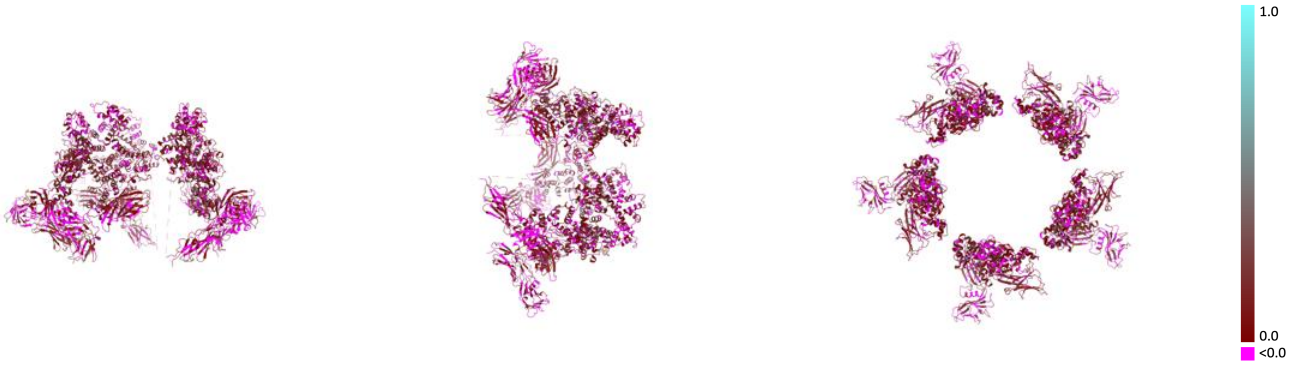
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.75 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.

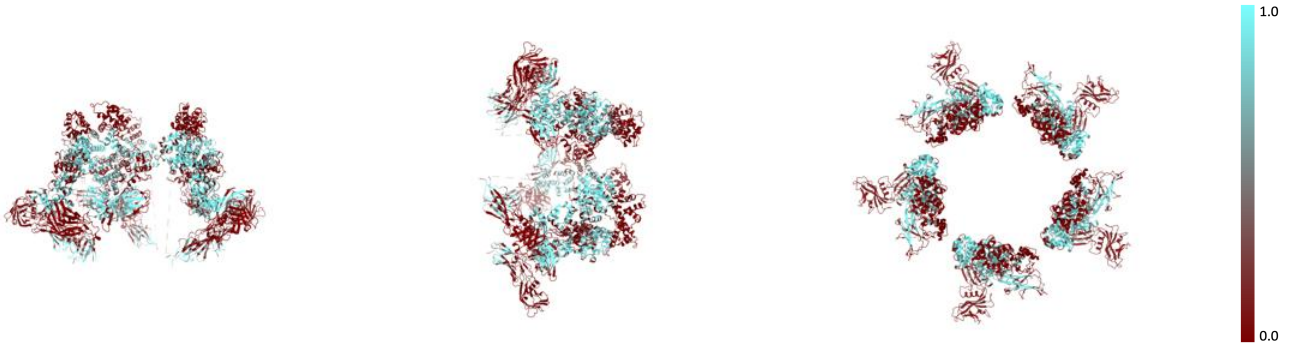
9.2 Q-score mapped to coordinate model



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.

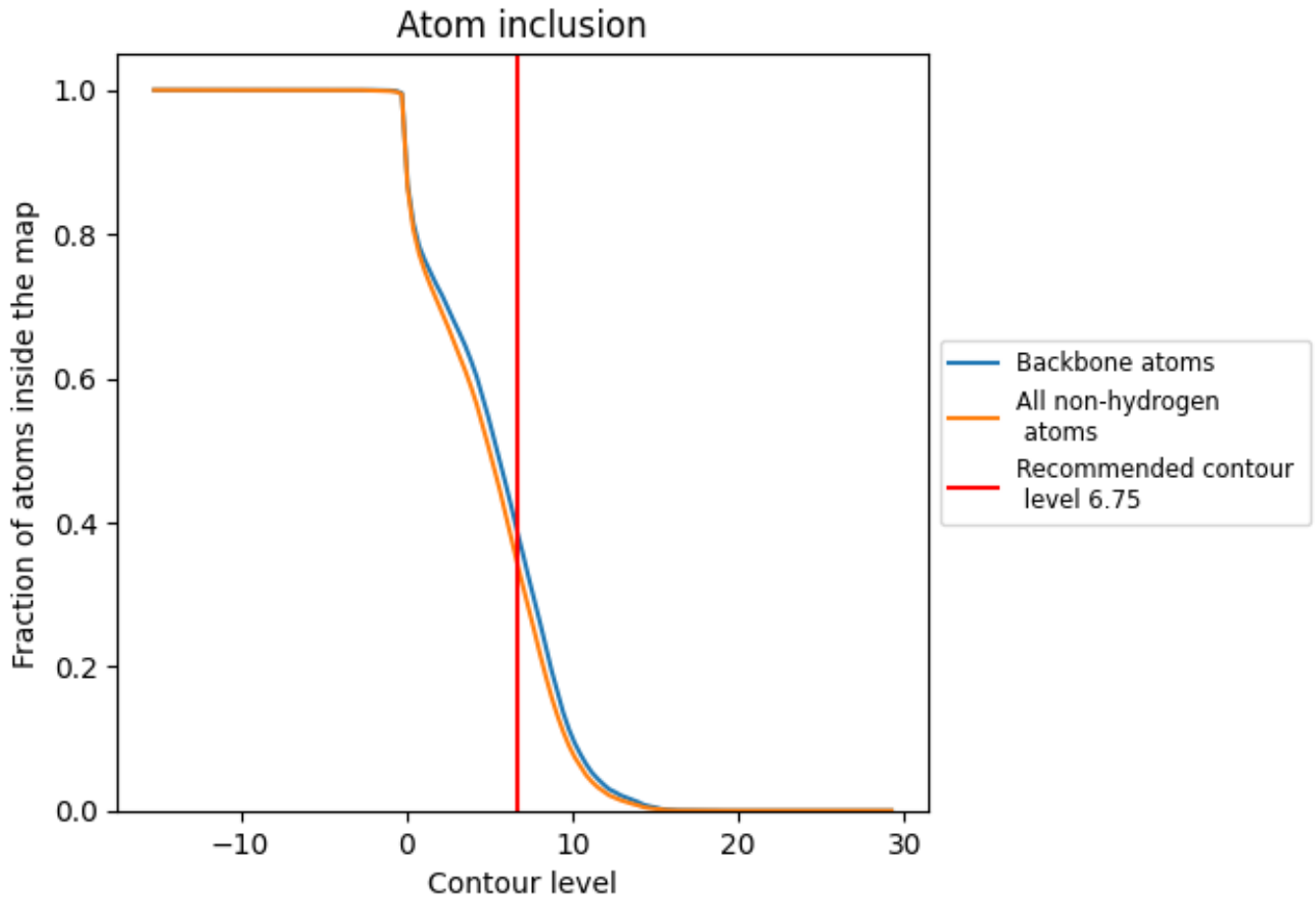
9.3 Atom inclusion mapped to coordinate model



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 (6.75).

9.4 Atom inclusion (i)



At the recommended contour level, 38% of all backbone atoms, 34% 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 (6.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3369	0.0670
A	0.3577	0.0800
B	0.3591	0.0780
C	0.3250	0.0580
D	0.3118	0.0520
E	0.3309	0.0660