Full wwPDB EM Validation Report ⓘ

Nov 13, 2021 – 05:16 am GMT

PDB ID	:	7PGU
EMDB ID	:	EMD-13396
Title	:	Autoinhibited structure of human neurofibromin isoform 2 stabilized by Zinc.
Authors	:	Naschberger, A.; Baradaran, R.; Carroni, M.; Rupp, B.
Deposited on	:	2021-08-15
Resolution	:	3.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

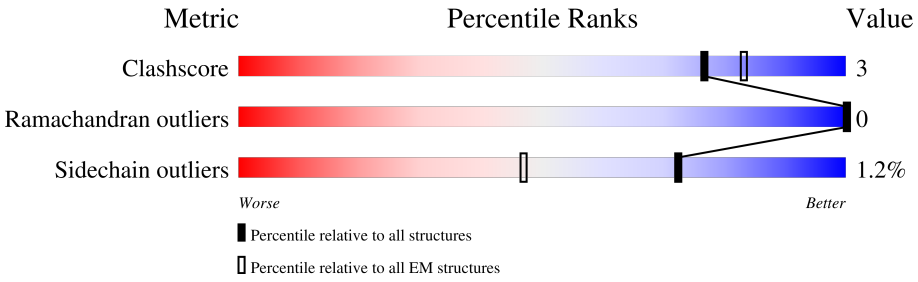
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4 (270009), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.30 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	F	2839	36% 78% 7% 15%
1	N	2839	31% 78% 7% 15%

2 Entry composition

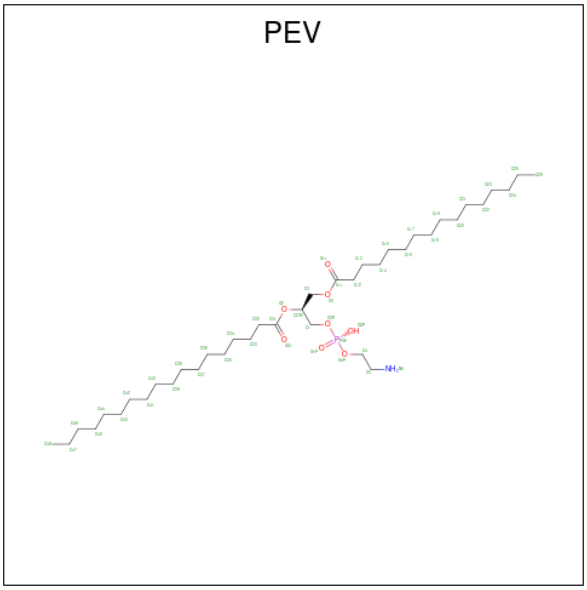
There are 4 unique types of molecules in this entry. The entry contains 77658 atoms, of which 39040 are hydrogens and 0 are deuteriums.

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 Neurofibromin.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	F	2423	Total	C	H	N	O	S	0	0
			38701	12314	19443	3266	3555	123		
1	N	2423	Total	C	H	N	O	S	0	0
			38701	12314	19443	3266	3555	123		

- Molecule 2 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: $C_{39}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
2	F	1	Total	C	H	N	O	P	0
			126	39	77	1	8	1	
2	N	1	Total	C	H	N	O	P	0
			126	39	77	1	8	1	

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
3	F	1	Total Zn 1 1	0
3	N	1	Total Zn 1 1	0

- Molecule 4 is water.

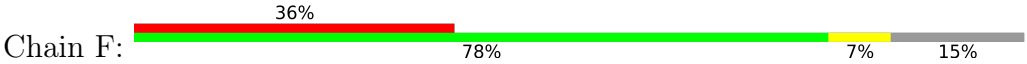
Mol	Chain	Residues	Atoms	AltConf
4	F	1	Total O 1 1	0
4	N	1	Total O 1 1	0

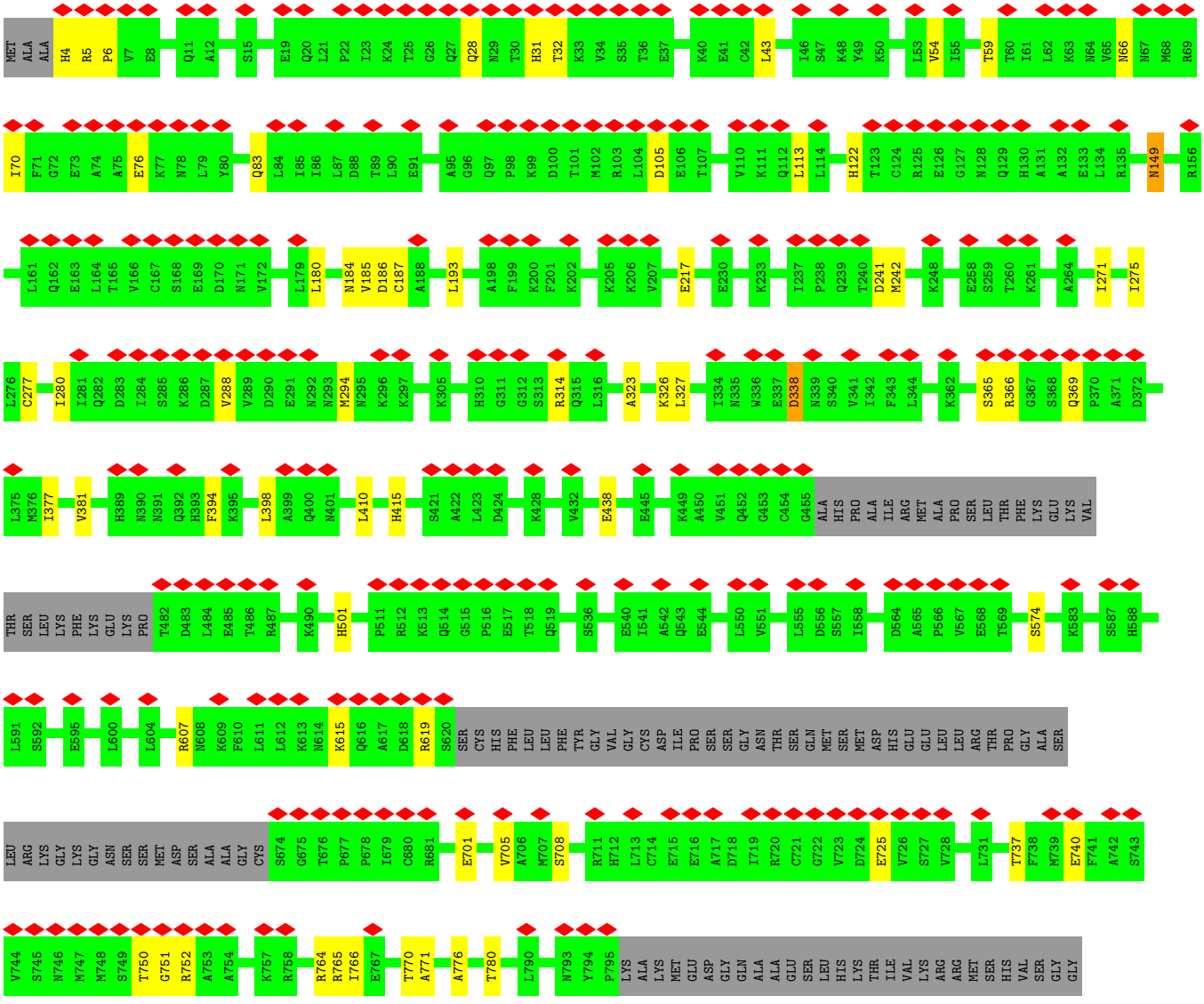
3 Residue-property plots (i)

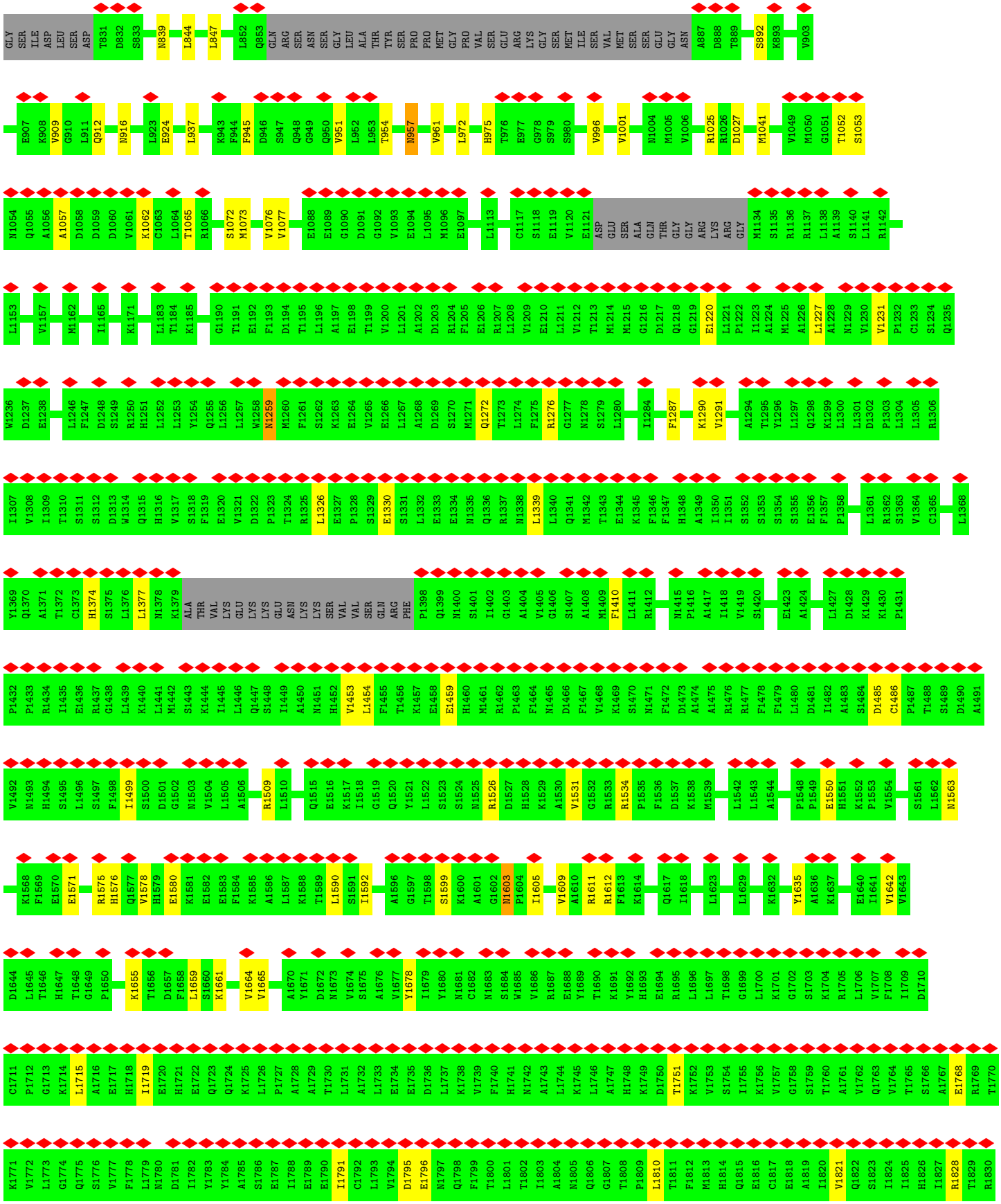
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Neurofibromin

Chain F:



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E907 K908 V909 G910 L911 Q912 N916 L923 E924 L937 K943 F944 F945 D946 S947 Q948 G949 Q950 V951 L952 L953 T954 N957 V961 L972 H975 T976 E977 G978 S979 S980 V996 V1001 N1004 M1005 V1006 R1025 R1026 D1027 M1041 V1049 M1050 G1051 T1052 S1053
N1054 Q1055 A1056 A1057 D1058 D1059 D1060 V1061 K1062 C1063 L1064 T1065 R1066 S1072 M1073 V1076 V1077 E1088 E1089 G1090 D1091 G1092 V1093 E1094 L1095 M1096 E1097 L1113 C1117 S1118 E1119 V1120 E1121 ASP GLU SER ALA GLN THR GLY GLY ARG LYS ARG GLY M1134 S1135 R1136 R1137 L1138 A1139 S1140 L1141 R1142
L1153 V1157 M1162 I1165 K1171 L1183 T1184 K1185 G1190 T1191 E1192 F1193 D1194 T1195 L1196 A1197 E1198 T1199 V1200 L1201 A1202 D1203 R1204 F1205 E1206 R1207 L1208 V1209 E1210 L1211 V1212 T1213 M1214 M1215 G1216 D1217 Q1218 G1219 E1220 L1221 P1222 I1223 A1224 M1225 A1226 L1227 A1228 N1229 V1230 V1231 P1232 C1233 S1234 Q1235
W1236 D1237 E1238 L1246 F1247 D1248 S1249 R1250 H1251 L1252 L1253 Y1254 Q1255 L1256 L1257 W1258 N1259 M1260 F1261 S1262 K1263 E1264 V1265 E1266 L1267 A1268 D1269 S1270 M1271 Q1272 T1273 L1274 F1275 R1276 G1277 N1278 S1279 L1280 I1284 F1287 K1290 V1291 A1294 T1295 Y1296 L1297 Q1298 K1299 L1300 L1301 D1302 P1303 L1304 L1305 R1306
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Y1369 Q1370 A1371 T1372 C1373 H1374 S1375 L1376 L1377 N1378 K1379 ALA THR VAL LYS GLU LYS LYS GLU ASN LYS LYS SER VAL VAL SER GLN ARG PHE P1398 Q1399 N1400 S1401 I1402 G1403 A1404 V1405 G1406 S1407 A1408 M1409 F1410 L1411 R1412 N1415 P1416 A1417 I1418 V1419 S1420 E1423 A1424 L1427 D1428 K1429 K1430 P1431
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V1492 N1493 H1494 S1495 L1496 S1497 F1498 I1499 S1500 D1501 G1502 N1503 V1504 L1505 A1506 R1509 L1510 Q1515 E1516 K1517 I1518 G1519 Q1520 Y1521 L1522 S1523 S1524 N1525 R1526 D1527 H1528 K1529 A1530 V1531 G1532 R1533 R1534 P1535 F1536 D1537 K1538 M1539 L1542 L1543 A1544 P1548 P1549 E1550 H1551 K1552 P1553 V1554 S1561 L1562 N1563
K1568 F1569 E1570 E1571 R1575 H1576 Q1577 V1578 H1579 E1580 K1581 E1582 E1583 F1584 K1585 A1586 L1587 K1588 T1589 L1590 S1591 I1592 A1596 G1597 T1598 S1599 K1600 A1601 G1602 N1603 P1604 I1605 V1609 A1610 R1611 R1612 F1613 K1614 Q1617 I1618 L1623 L1629 K1632 Y1635 A1636 K1637 E1640 I1641 V1642 V1643
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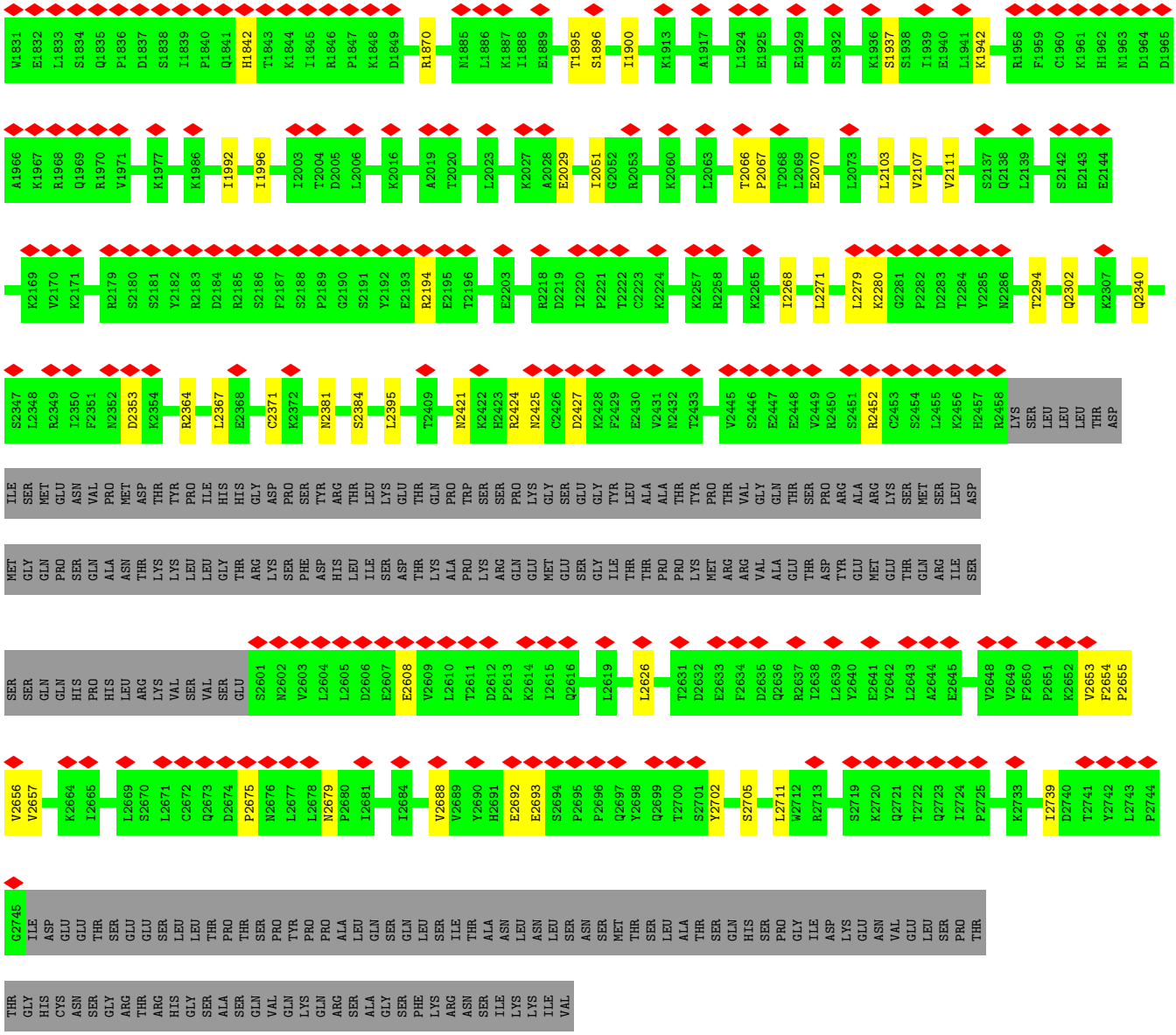
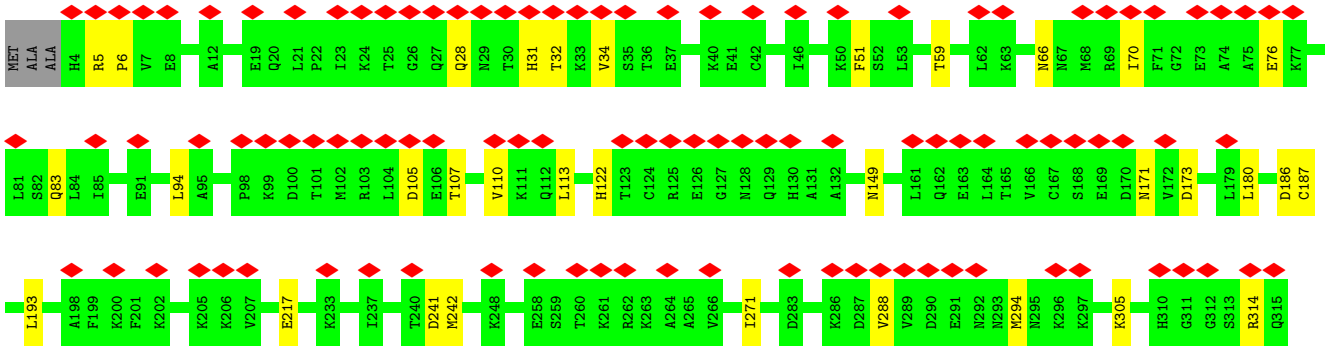
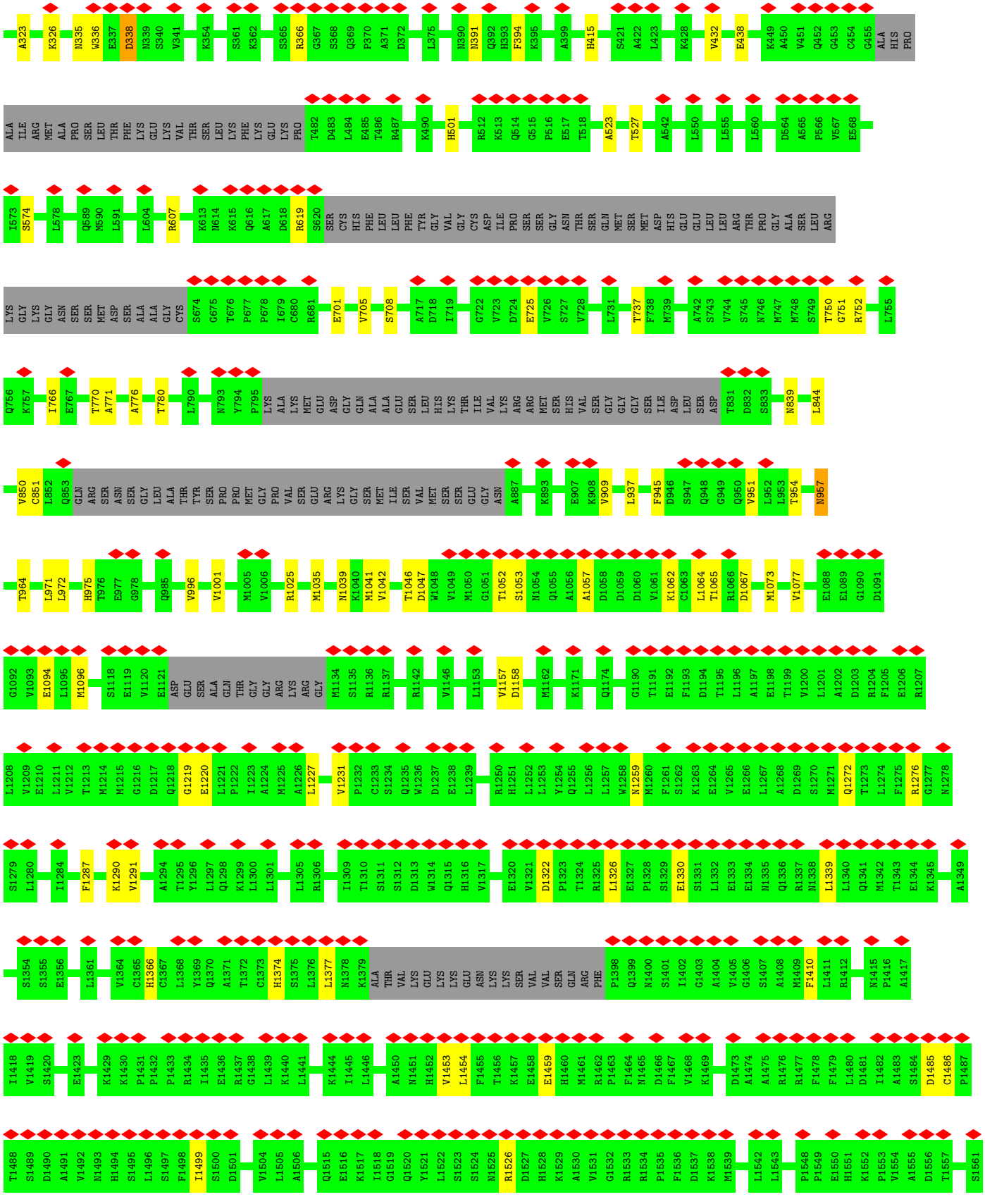
C1711 P1712 G1713 K1714 L1715 A1716 E1717 H1718 I1719 E1720 H1721 E1722 Q1723 Q1724 K1725 L1726 P1727 A1728 A1729 T1730 L1731 A1732 L1733 E1734 E1735 D1736 L1737 K1738 V1739 F1740 H1741 N1742 A1743 L1744 K1745 L1746 A1747 H1748 K1749 D1750 T1751 K1752 V1753 S1754 I1755 K1756 V1757 G1758 S1759 T1760 A1761 V1762 Q1763 V1764 T1765 S1766 A1767 E1768 R1769 T1770
K1771 V1772 L1773 G1774 Q1775 S1776 V1777 F1778 L1779 N1780 D1781 I1782 Y1783 Y1784 A1785 S1786 E1787 I1788 E1789 E1790 I1791 C1792 L1793 V1794 D1795 E1796 N1797 Q1798 F1799 T1800 L1801 T1802 I1803 A1804 N1805 Q1806 G1807 T1808 P1809 L1810 T1811 F1812 M1813 H1814 Q1815 E1816 C1817 E1818 A1819 I1820 V1821 Q1822 S1823 I1824 I1825 H1826 I1827 R1828 T1829 R1830



- Molecule 1: Neurofibromin

Chain N:

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ALA ILE ARG MET ALA PRO SER LEU THR PHE LYS GLU LYS VAL THR SER LEU LYS PHE LYS GLU LYS PRO T482 D483 L484 E485 T486 R487 K490 H501 R512 K513 Q514 Q515 P516 E517 T518 A523 T527 A542 L550 L555 L560 D564 A565 P566 V567 E568
I573 S574 L578 Q589 M590 L591 L604 R607 K613 N614 K615 Q616 A617 D618 R619 S620 SER CYS HIS PHE LEU LEU PHE TYR GLY VAL GLY CYS ASP ILE PRO SER SER GLY ASN THR SER GLN MET SER MET ASP HIS GLU GLU LEU LEU ARG THR PRO GLY ALA SER LEU ARG
LYS GLY LYS GLY ASN SER SER MET ASP SER ALA ALA GLY CYS S674 G675 T676 P677 P678 I679 C680 R681 E701 V705 S708 A717 D718 I719 G722 V723 D724 E725 V726 S727 V728 L731 T737 F738 M739 A742 S743 V744 S745 N746 M747 M748 S749 T750 G751 R752 L755
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S1354 S1355 E1356 L1361 V1364 C1365 H1366 C1367 L1368 Y1369 Q1370 A1371 T1372 C1373 H1374 S1375 L1376 L1377 N1378 K1379 ALA THR VAL LYS GLU LYS LYS GLU ASN LYS LYS SER VAL VAL SER GLN ARG PHE P1398 Q1399 N1400 S1401 I1402 G1403 A1404 V1405 G1406 S1407 A1408 M1409 F1410 L1411 R1412 N1415 P1416 A1417
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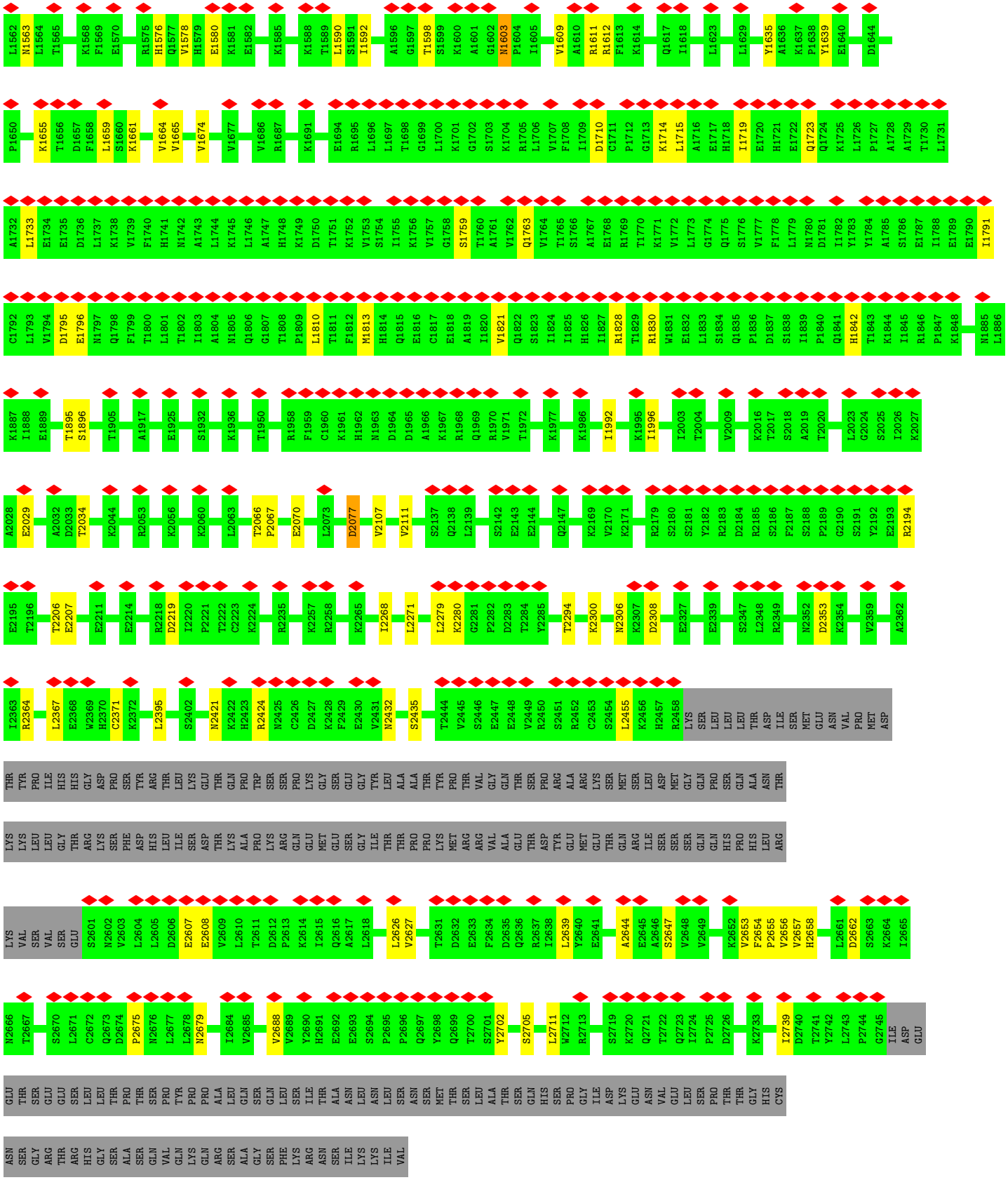
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I2363 R2364 L2367 E2368 W2369 H2370 C2371 K2372 L2395 S2402 N2421 K2422 H2423 R2424 N2425 C2426 D2427 K2428 F2429 E2430 V2431 N2432 S2435 T2444 V2445 S2446 E2447 E2448 V2449 R2450 S2451 R2452 C2453 S2454 L2455 K2456 H2457 R2458 LYS SER LEU LEU LEU THR ASP ILE SER MET GLU ASN VAL PRO MET ASP
THR TYR PRO ILE HIS HIS GLY ASP PRO SER TYR ARG THR LEU LEU LYS GLU THR GLN PRO TRP SER SER PRO PRO LYS GLY SER GLU GLY TYR LEU ALA THR TYR PRO THR VAL GLY GLN THR SER PRO ARG ALA ARG LYS SER MET SER LEU ASP MET GLY GLN PRO SER GLN ALA ALA ASN THR
LYS LYS LEU LEU LEU GLY THR ARG LYS SER PHE ASP HIS LEU ILE SER ASP THR LYS ALA PRO PRO LYS ARG GLN GLU MET GLU SER GLY ILE THR THR PRO PRO LYS MET ARG ARG VAL ALA GLU THR ASP TYR GLU MET GLU THR GLN ARG ILE SER SER SER GLN GLN HIS PRO HIS LEU ARG
LYS VAL SER VAL SER GLU S2601 N2602 V2603 L2604 L2605 D2606 E2607 E2608 V2609 L2610 T2611 D2612 P2613 K2614 I2615 Q2616 A2617 L2618 L2626 V2627 T2631 D2632 E2633 F2634 D2635 Q2636 R2637 I2638 L2639 Y2640 E2641 A2644 E2645 A2646 S2647 V2648 V2649 K2652 V2653 F2654 P2655 V2656 V2657 H2658 L2661 D2662 S2663 K2664 I2665
N2666 T2667 S2670 L2671 C2672 Q2673 D2674 P2675 W2676 L2677 L2678 N2679 I2684 V2685 V2688 V2689 Y2690 H2691 E2692 E2693 S2694 P2695 P2696 Q2697 Y2698 Q2699 T2700 S2701 Y2702 S2705 L2711 W2712 R2713 S2719 K2720 Q2721 T2722 Q2723 I2724 P2725 D2726 K2733 I2739 D2740 T2741 Y2742 L2743 P2744 G2745 ILE ASP GLU
GLU THR SER GLU GLU SER LEU LEU THR PRO THR SER PRO TYR PRO PRO ALA LEU GLN SER GLN LEU SER ILE THR ALA ASN LEU ASN LEU SER ASN SER MET THR SER LEU ALA THR SER GLN HIS SER PRO GLY ILE ASP LYS GLU LEU SER PRO THR THR GLY HIS CYS
ASN SER GLY ARG THR ARG HIS GLY SER ALA SER GLN VAL GLN LYS GLN ARG SER ALA GLY SER PHE LYS ARG ASN SER ILE LYS LYS ILE VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	300087	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 ($e^-/Å^2$)	1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	163.132	Depositor
Minimum map value	-86.089	Depositor
Average map value	0.013	Depositor
Map value standard deviation	1.447	Depositor
Recommended contour level	30.0	Depositor
Map size (Å)	687.98596, 687.98596, 687.98596	wwPDB
Map dimensions	470, 470, 470	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4638, 1.4638, 1.4638	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, PEV

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	F	0.26	0/19654	0.44	0/26645
1	N	0.26	0/19654	0.44	0/26645
All	All	0.26	0/39308	0.44	0/53290

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	F	19258	19443	19458	112	0
1	N	19258	19443	19458	121	0
2	F	49	77	77	0	0
2	N	49	77	77	0	0
3	F	1	0	0	0	0
3	N	1	0	0	0	0
4	F	1	0	0	0	0
4	N	1	0	0	0	0
All	All	38618	39040	39070	231	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 3.

All (231) 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:F:66:ASN:OD1	1:F:83:GLN:NE2	2.04	0.91
1:N:66:ASN:OD1	1:N:83:GLN:NE2	2.04	0.90
1:F:1290:LYS:NZ	1:F:1563:ASN:OD1	2.14	0.81
1:N:2675:PRO:O	1:N:2679:ASN:ND2	2.14	0.80
1:N:217:GLU:OE2	1:N:326:LYS:NZ	2.16	0.79
1:F:2675:PRO:O	1:F:2679:ASN:ND2	2.17	0.78
1:F:217:GLU:OE2	1:F:326:LYS:NZ	2.17	0.76
1:N:2107:VAL:O	1:N:2111:VAL:HG23	1.86	0.75
1:N:1290:LYS:NZ	1:N:1563:ASN:OD1	2.20	0.74
1:N:186:ASP:OD1	1:N:187:CYS:N	2.21	0.74
1:F:1272:GLN:O	1:F:1276:ARG:NH2	2.21	0.74
1:N:752:ARG:NH1	1:N:839:ASN:OD1	2.21	0.73
1:N:2070:GLU:OE1	1:N:2194:ARG:NH1	2.22	0.73
1:N:1272:GLN:O	1:N:1276:ARG:NH2	2.22	0.72
1:F:2107:VAL:O	1:F:2111:VAL:HG23	1.89	0.72
1:N:438:GLU:N	1:N:438:GLU:OE1	2.23	0.71
1:F:438:GLU:N	1:F:438:GLU:OE1	2.23	0.71
1:F:1870:ARG:NH2	1:F:1900:ILE:O	2.24	0.71
1:F:776:ALA:O	1:F:780:THR:HG22	1.91	0.70
1:N:31:HIS:O	1:N:32:THR:OG1	2.09	0.70
1:F:1220:GLU:OE1	1:F:1526:ARG:NH2	2.24	0.70
1:F:912:GLN:O	1:F:916:ASN:ND2	2.26	0.69
1:F:752:ARG:NH1	1:F:839:ASN:OD1	2.26	0.68
1:N:2207:GLU:OE2	1:N:2300:LYS:NZ	2.25	0.68
1:N:1459:GLU:OE1	1:N:1459:GLU:N	2.27	0.67
1:F:1795:ASP:OD1	1:F:1796:GLU:N	2.28	0.66
1:F:186:ASP:OD1	1:F:187:CYS:N	2.27	0.66
1:F:2381:ASN:OD1	1:F:2384:SER:N	2.28	0.66
1:F:1603:ASN:OD1	1:F:1603:ASN:N	2.27	0.66
1:F:149:ASN:N	1:F:149:ASN:OD1	2.27	0.66
1:F:1580:GLU:N	1:F:1580:GLU:OE1	2.29	0.65
1:N:1795:ASP:OD1	1:N:1796:GLU:N	2.28	0.65
1:F:1459:GLU:N	1:F:1459:GLU:OE1	2.29	0.65
1:N:972:LEU:O	1:N:1025:ARG:NH1	2.30	0.65
1:F:2302:GLN:OE1	1:F:2340:GLN:NE2	2.30	0.64
1:N:1759:SER:O	1:N:1830:ARG:NH2	2.31	0.64
1:N:1094:GLU:OE1	1:N:1096:MET:N	2.30	0.64
1:N:1580:GLU:OE1	1:N:1580:GLU:N	2.32	0.63
1:F:1227:LEU:O	1:F:1231:VAL:HG23	1.99	0.62
1:N:1220:GLU:OE1	1:N:1526:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1937:SER:O	1:F:1942:LYS:NZ	2.34	0.61
1:F:2070:GLU:OE1	1:F:2194:ARG:NH1	2.33	0.61
1:F:271:ILE:HD12	1:F:323:ALA:HB1	1.83	0.61
1:F:764:ARG:NH2	1:F:924:GLU:OE1	2.34	0.60
1:N:574:SER:OG	1:N:607:ARG:NH1	2.35	0.60
1:N:1603:ASN:OD1	1:N:1603:ASN:N	2.35	0.60
1:F:415:HIS:ND1	1:F:415:HIS:O	2.34	0.59
1:N:271:ILE:HD12	1:N:323:ALA:HB1	1.83	0.59
1:N:2271:LEU:HB2	1:N:2294:THR:HG21	1.85	0.59
1:N:1227:LEU:O	1:N:1231:VAL:HG23	2.03	0.58
1:N:1001:VAL:O	1:N:1001:VAL:HG12	2.03	0.58
1:F:180:LEU:HD23	1:F:193:LEU:HD23	1.85	0.58
1:F:740:GLU:OE1	1:F:765:ARG:NH1	2.36	0.58
1:N:996:VAL:HG11	1:N:1041:MET:CE	2.34	0.58
1:N:945:PHE:CE1	1:N:951:VAL:HG12	2.38	0.58
1:N:415:HIS:O	1:N:415:HIS:ND1	2.32	0.58
1:F:365:SER:OG	1:F:369:GLN:O	2.20	0.57
1:F:945:PHE:CE1	1:F:951:VAL:HG12	2.39	0.57
1:N:1590:LEU:HD23	1:N:1592:ILE:HD11	1.86	0.57
1:F:705:VAL:O	1:F:708:SER:OG	2.16	0.57
1:F:1576:HIS:O	1:F:1578:VAL:HG13	2.05	0.57
1:F:1001:VAL:HG12	1:F:1001:VAL:O	2.05	0.57
1:F:2271:LEU:HB2	1:F:2294:THR:HG21	1.87	0.56
1:N:725:GLU:OE1	1:N:725:GLU:N	2.37	0.56
1:F:338:ASP:OD1	1:F:338:ASP:N	2.39	0.55
1:N:909:VAL:HG22	1:N:909:VAL:O	2.06	0.55
1:F:1287:PHE:O	1:F:1291:VAL:HG12	2.06	0.55
1:F:2066:THR:HG22	1:F:2067:PRO:HD2	1.88	0.55
1:N:1035:MET:O	1:N:1039:ASN:ND2	2.37	0.55
1:F:1571:GLU:OE2	1:F:1575:ARG:NH1	2.39	0.55
1:N:1287:PHE:O	1:N:1291:VAL:HG12	2.07	0.55
1:N:1576:HIS:O	1:N:1578:VAL:HG13	2.07	0.55
1:F:954:THR:O	1:F:954:THR:HG22	2.07	0.54
1:N:338:ASP:N	1:N:338:ASP:OD1	2.40	0.54
1:F:6:PRO:HB3	1:N:2688:VAL:HG11	1.89	0.54
1:F:770:THR:HG22	1:F:771:ALA:H	1.71	0.54
1:F:909:VAL:HG22	1:F:909:VAL:O	2.08	0.54
1:F:2364:ARG:NE	1:F:2371:CYS:SG	2.80	0.54
1:N:1485:ASP:OD1	1:N:1486:CYS:N	2.41	0.53
1:N:70:ILE:HD11	1:N:76:GLU:HG2	1.89	0.53
1:N:2657:VAL:HG12	1:N:2657:VAL:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:501:HIS:O	1:F:501:HIS:ND1	2.41	0.53
1:N:770:THR:HG22	1:N:771:ALA:H	1.72	0.53
1:N:1053:SER:O	1:N:1057:ALA:N	2.41	0.53
1:F:1073:MET:O	1:F:1077:VAL:HG23	2.08	0.53
1:N:776:ALA:O	1:N:780:THR:HG22	2.09	0.53
1:F:1053:SER:O	1:F:1057:ALA:N	2.42	0.52
1:N:705:VAL:O	1:N:708:SER:OG	2.19	0.52
1:N:954:THR:HG22	1:N:954:THR:O	2.09	0.52
1:N:945:PHE:HE1	1:N:951:VAL:HG12	1.73	0.52
1:N:1715:LEU:HD11	1:N:1719:ILE:HD12	1.92	0.52
1:N:2608:GLU:N	1:N:2608:GLU:OE1	2.41	0.52
1:F:780:THR:HG23	1:F:844:LEU:HD21	1.92	0.52
1:N:780:THR:HG23	1:N:844:LEU:HD21	1.91	0.52
1:F:1485:ASP:OD1	1:F:1486:CYS:N	2.43	0.51
1:F:1509:ARG:NH1	1:F:1550:GLU:O	2.42	0.51
1:N:1062:LYS:O	1:N:1065:THR:HG22	2.11	0.51
1:N:1499:ILE:HD12	1:N:1499:ILE:H	1.74	0.51
1:F:398:LEU:HD13	1:F:410:LEU:HD21	1.93	0.51
1:F:2279:LEU:HD12	1:F:2280:LYS:N	2.26	0.51
1:F:574:SER:OG	1:F:607:ARG:NH1	2.44	0.51
1:N:2353:ASP:N	1:N:2353:ASP:OD1	2.44	0.51
1:N:1339:LEU:HD23	1:N:1339:LEU:O	2.12	0.50
1:N:1664:VAL:O	1:N:1664:VAL:HG22	2.11	0.50
1:N:501:HIS:O	1:N:501:HIS:ND1	2.44	0.50
1:N:59:THR:HG22	1:N:113:LEU:HD13	1.93	0.50
1:N:2077:ASP:N	1:N:2077:ASP:OD1	2.44	0.50
1:F:2051:ILE:HD11	1:F:2103:LEU:HD21	1.94	0.50
1:N:2395:LEU:HD22	1:N:2626:LEU:HD21	1.93	0.49
1:F:2353:ASP:OD1	1:F:2353:ASP:N	2.46	0.49
1:F:1062:LYS:O	1:F:1065:THR:HG22	2.13	0.49
1:F:996:VAL:HG11	1:F:1041:MET:CE	2.43	0.49
1:N:2279:LEU:HD12	1:N:2280:LYS:N	2.26	0.49
1:F:945:PHE:HE1	1:F:951:VAL:HG12	1.77	0.49
1:F:2268:ILE:HG22	1:F:2739:ILE:HD11	1.94	0.49
1:F:184:ASN:OD1	1:F:185:VAL:N	2.46	0.49
1:F:1664:VAL:HG22	1:F:1664:VAL:O	2.12	0.49
1:F:1599:SER:HB3	1:F:1605:ILE:HD11	1.93	0.49
1:F:972:LEU:O	1:F:1025:ARG:NH1	2.46	0.48
1:F:70:ILE:HD11	1:F:76:GLU:HG2	1.94	0.48
1:N:51:PHE:HZ	1:N:94:LEU:HD23	1.79	0.48
1:F:1339:LEU:HD23	1:F:1339:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1499:ILE:HD12	1:F:1499:ILE:H	1.79	0.48
1:F:1590:LEU:HD23	1:F:1592:ILE:HD11	1.96	0.48
1:F:2688:VAL:HG11	1:N:6:PRO:HB3	1.95	0.47
1:N:1639:TYR:CE1	1:N:1674:VAL:HG22	2.49	0.47
1:F:2395:LEU:HD22	1:F:2626:LEU:HD21	1.95	0.47
1:N:1791:ILE:HG22	1:N:1821:VAL:HG13	1.97	0.47
1:F:1655:LYS:O	1:F:1659:LEU:N	2.41	0.47
1:N:937:LEU:HD23	1:N:964:THR:HG23	1.97	0.47
1:F:1453:VAL:HG12	1:F:1454:LEU:N	2.30	0.47
1:N:1655:LYS:O	1:N:1659:LEU:N	2.43	0.47
1:N:107:THR:O	1:N:110:VAL:HG22	2.15	0.47
1:N:1992:ILE:HG23	1:N:1996:ILE:HD12	1.97	0.47
1:N:1453:VAL:HG12	1:N:1454:LEU:N	2.29	0.46
1:F:275:ILE:HD11	1:F:327:LEU:CD1	2.45	0.46
1:N:432:VAL:HG12	1:N:432:VAL:O	2.16	0.46
1:N:1157:VAL:HG23	1:N:1158:ASP:N	2.30	0.46
1:N:2066:THR:HG22	1:N:2067:PRO:HD2	1.96	0.46
1:F:1895:THR:HG22	1:F:1896:SER:N	2.31	0.46
1:N:288:VAL:HG11	1:N:294:MET:HA	1.98	0.46
1:F:2653:VAL:O	1:F:2656:VAL:HG22	2.17	0.45
1:N:1895:THR:HG22	1:N:1896:SER:N	2.31	0.45
1:F:2657:VAL:HG12	1:F:2657:VAL:O	2.15	0.45
1:F:31:HIS:O	1:F:32:THR:OG1	2.14	0.45
1:N:2607:GLU:OE1	1:N:2607:GLU:N	2.44	0.45
1:N:2653:VAL:O	1:N:2656:VAL:HG22	2.17	0.45
1:N:70:ILE:HD11	1:N:76:GLU:CG	2.47	0.45
1:N:1064:LEU:O	1:N:1067:ASP:N	2.49	0.45
1:F:957:ASN:O	1:F:961:VAL:HG13	2.16	0.45
1:F:2608:GLU:OE1	1:F:2608:GLU:N	2.43	0.45
1:F:277:CYS:SG	1:F:280:ILE:HD12	2.57	0.45
1:N:1661:LYS:O	1:N:1665:VAL:HG23	2.17	0.44
1:N:2711:LEU:O	1:N:2711:LEU:HD23	2.16	0.44
1:N:1366:HIS:ND1	1:N:1485:ASP:O	2.50	0.44
1:N:2654:PHE:N	1:N:2655:PRO:HD2	2.31	0.44
1:F:957:ASN:N	1:F:957:ASN:OD1	2.50	0.44
1:N:1609:VAL:HG11	1:N:1612:ARG:HE	1.83	0.44
1:F:1609:VAL:HG11	1:F:1612:ARG:HE	1.82	0.44
1:F:2421:ASN:O	1:F:2425:ASN:N	2.51	0.44
1:N:957:ASN:OD1	1:N:957:ASN:N	2.50	0.44
1:F:1052:THR:HG22	1:F:1052:THR:O	2.17	0.44
1:F:2702:TYR:O	1:F:2705:SER:OG	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:971:LEU:C	1:N:971:LEU:HD23	2.37	0.44
1:N:1047:ASP:N	1:N:1047:ASP:OD1	2.50	0.44
1:N:1733:LEU:O	1:N:1763:GLN:NE2	2.41	0.44
1:N:171:ASN:OD1	1:N:173:ASP:N	2.44	0.44
1:F:1791:ILE:HG22	1:F:1821:VAL:HG13	1.99	0.43
1:N:180:LEU:HD23	1:N:193:LEU:HD23	1.99	0.43
1:F:43:LEU:HD11	1:F:54:VAL:HG13	2.01	0.43
1:N:1073:MET:O	1:N:1077:VAL:HG23	2.18	0.43
1:N:1710:ASP:OD2	1:N:1714:LYS:NZ	2.44	0.43
1:F:725:GLU:OE1	1:F:725:GLU:N	2.49	0.43
1:F:1992:ILE:HG23	1:F:1996:ILE:HD12	2.01	0.43
1:F:737:THR:HG21	1:F:766:ILE:HD13	2.00	0.43
1:F:59:THR:HG22	1:F:113:LEU:HD13	2.01	0.43
1:F:2654:PHE:N	1:F:2655:PRO:HD2	2.33	0.43
1:N:1219:GLY:O	1:N:1259:ASN:ND2	2.52	0.43
1:N:2421:ASN:O	1:N:2424:ARG:N	2.52	0.42
1:N:2627:VAL:HG13	1:N:2639:LEU:HD13	2.01	0.42
1:N:523:ALA:O	1:N:527:THR:HG23	2.19	0.42
1:F:5:ARG:N	1:F:6:PRO:HD2	2.34	0.42
1:F:1326:LEU:HD11	1:F:1330:GLU:HB3	2.01	0.42
1:F:1810:LEU:N	1:F:1810:LEU:HD12	2.34	0.42
1:F:847:LEU:HG	1:F:847:LEU:O	2.18	0.42
1:N:1259:ASN:N	1:N:1259:ASN:OD1	2.52	0.42
1:N:1810:LEU:N	1:N:1810:LEU:HD12	2.35	0.42
1:F:2711:LEU:O	1:F:2711:LEU:HD23	2.20	0.42
1:N:750:THR:OG1	1:N:751:GLY:N	2.52	0.42
1:F:1751:THR:HG23	1:F:1768:GLU:OE1	2.19	0.42
1:N:1326:LEU:HD11	1:N:1330:GLU:HB3	2.01	0.42
1:F:1661:LYS:O	1:F:1665:VAL:HG23	2.20	0.42
1:N:2219:ASP:OD1	1:N:2219:ASP:N	2.52	0.42
1:N:335:ASN:O	1:N:336:TRP:HB3	2.20	0.42
1:N:1052:THR:HG22	1:N:1052:THR:O	2.20	0.42
1:N:70:ILE:HD12	1:N:70:ILE:C	2.40	0.42
1:N:1322:ASP:O	1:N:1326:LEU:N	2.50	0.42
1:F:2427:ASP:OD2	1:F:2452:ARG:NH2	2.52	0.41
1:F:241:ASP:OD1	1:F:242:MET:N	2.53	0.41
1:N:31:HIS:O	1:N:34:VAL:HG12	2.20	0.41
1:N:850:VAL:HG23	1:N:851:CYS:N	2.35	0.41
1:F:377:ILE:O	1:F:381:VAL:HG23	2.20	0.41
1:N:2268:ILE:HG22	1:N:2739:ILE:HD11	2.02	0.41
1:N:1042:VAL:O	1:N:1046:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1598:THR:O	1:N:1723:GLN:NE2	2.54	0.41
1:N:2206:THR:O	1:N:2206:THR:HG22	2.21	0.41
1:F:70:ILE:HD11	1:F:76:GLU:CG	2.50	0.41
1:F:1259:ASN:OD1	1:F:1259:ASN:N	2.53	0.41
1:N:5:ARG:N	1:N:6:PRO:HD2	2.35	0.41
1:N:1377:LEU:HD13	1:N:1377:LEU:C	2.40	0.41
1:F:1377:LEU:HD13	1:F:1377:LEU:C	2.41	0.41
1:N:2644:ALA:O	1:N:2647:SER:OG	2.34	0.41
1:F:288:VAL:HG11	1:F:294:MET:HA	2.01	0.41
1:F:750:THR:OG1	1:F:751:GLY:N	2.54	0.41
1:F:1642:VAL:HG22	1:F:1678:TYR:HD2	1.86	0.41
1:F:2421:ASN:O	1:F:2424:ARG:N	2.54	0.41
1:N:2306:ASN:ND2	1:N:2308:ASP:OD1	2.53	0.41
1:N:2364:ARG:NE	1:N:2371:CYS:SG	2.93	0.41
1:N:2435:SER:O	1:N:2435:SER:OG	2.38	0.41
1:F:2692:GLU:HG2	1:F:2693:GLU:H	1.86	0.41
1:N:996:VAL:HG11	1:N:1041:MET:HE3	2.01	0.41
1:N:2658:HIS:O	1:N:2662:ASP:N	2.54	0.40
1:F:1531:VAL:HA	1:F:1534:ARG:HB2	2.04	0.40
1:F:1715:LEU:HD11	1:F:1719:ILE:HD12	2.04	0.40
1:N:2034:THR:O	1:N:2034:THR:HG22	2.20	0.40
1:N:2702:TYR:O	1:N:2705:SER:OG	2.26	0.40
1:N:241:ASP:OD1	1:N:242:MET:N	2.54	0.40
1:N:1001:VAL:O	1:N:1001:VAL:CG1	2.68	0.40
1:F:615:LYS:O	1:F:619:ARG:NH1	2.54	0.40
1:F:1072:SER:O	1:F:1076:VAL:HG23	2.21	0.40
1:N:737:THR:HG21	1:N:766:ILE:HD13	2.03	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	F	2407/2839 (85%)	2370 (98%)	37 (2%)	0	100	100
1	N	2407/2839 (85%)	2367 (98%)	40 (2%)	0	100	100
All	All	4814/5678 (85%)	4737 (98%)	77 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	F	2170/2531 (86%)	2145 (99%)	25 (1%)	71	83
1	N	2170/2531 (86%)	2143 (99%)	27 (1%)	71	83
All	All	4340/5062 (86%)	4288 (99%)	52 (1%)	72	83

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	4	HIS
1	F	28	GLN
1	F	105	ASP
1	F	122	HIS
1	F	149	ASN
1	F	314	ARG
1	F	338	ASP
1	F	366	ARG
1	F	394	PHE
1	F	701	GLU
1	F	892	SER
1	F	937	LEU
1	F	957	ASN
1	F	975	HIS
1	F	1027	ASP
1	F	1259	ASN
1	F	1374	HIS
1	F	1410	PHE

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Mol	Chain	Res	Type
1	F	1603	ASN
1	F	1611	ARG
1	F	1635	TYR
1	F	1828	ARG
1	F	1842	HIS
1	F	2029	GLU
1	F	2367	LEU
1	N	28	GLN
1	N	105	ASP
1	N	122	HIS
1	N	149	ASN
1	N	305	LYS
1	N	314	ARG
1	N	338	ASP
1	N	366	ARG
1	N	391	ASN
1	N	394	PHE
1	N	619	ARG
1	N	701	GLU
1	N	957	ASN
1	N	975	HIS
1	N	1374	HIS
1	N	1410	PHE
1	N	1603	ASN
1	N	1611	ARG
1	N	1635	TYR
1	N	1813	MET
1	N	1828	ARG
1	N	1842	HIS
1	N	2029	GLU
1	N	2077	ASP
1	N	2367	LEU
1	N	2432	ASN
1	N	2455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	20	GLN
1	F	83	GLN
1	F	97	GLN
1	F	122	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	435	HIS
1	F	1156	ASN
1	F	1235	GLN
1	F	1683	ASN
1	F	1724	GLN
1	F	1943	HIS
1	F	2393	HIS
1	F	2432	ASN
1	F	2434	GLN
1	N	20	GLN
1	N	83	GLN
1	N	97	GLN
1	N	122	HIS
1	N	226	ASN
1	N	435	HIS
1	N	562	ASN
1	N	781	HIS
1	N	905	ASN
1	N	959	GLN
1	N	1156	ASN
1	N	1370	GLN
1	N	1683	ASN
1	N	1723	GLN
1	N	1724	GLN
1	N	1742	ASN
1	N	1856	ASN
1	N	1943	HIS
1	N	2393	HIS
1	N	2432	ASN
1	N	2434	GLN

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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-13396. These allow visual inspection of the internal detail of the map and identification of artifacts.

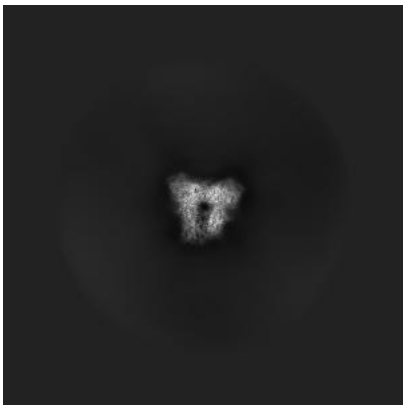
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map

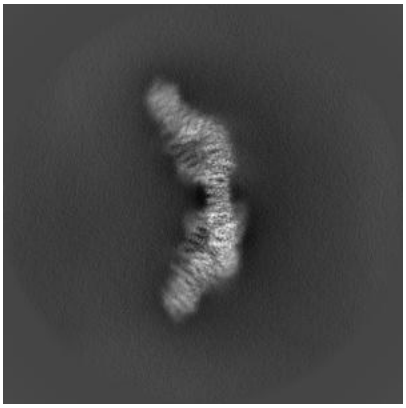
X

Y

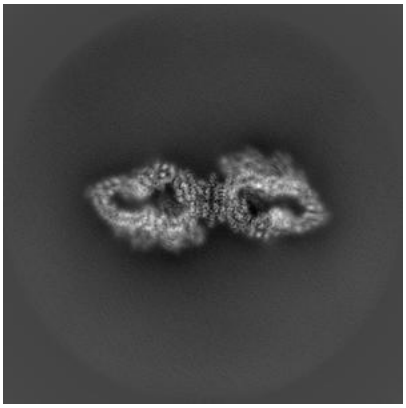


Z

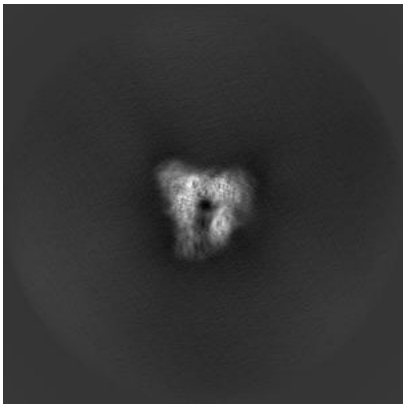
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

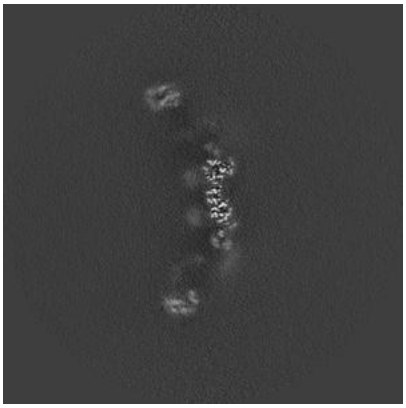
6.2.1 Primary map

X Index: 235

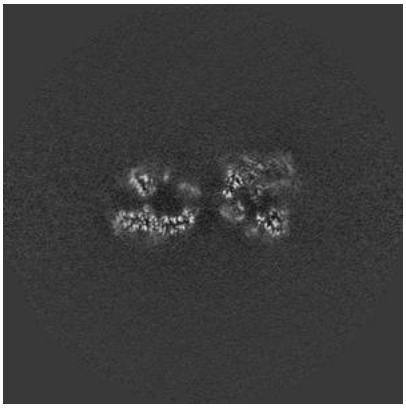
Y Index: 235

Z Index: 235

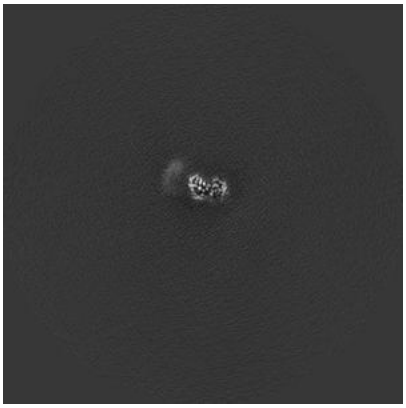
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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

6.3 Largest variance slices (i)

6.3.1 Primary map

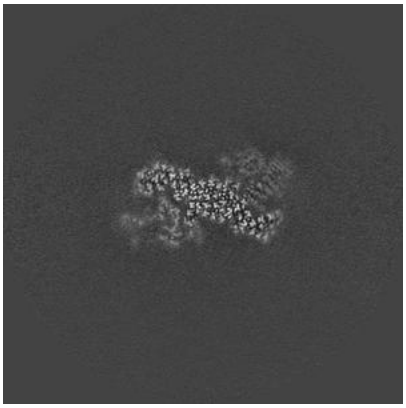
X Index: 251

Y Index: 246

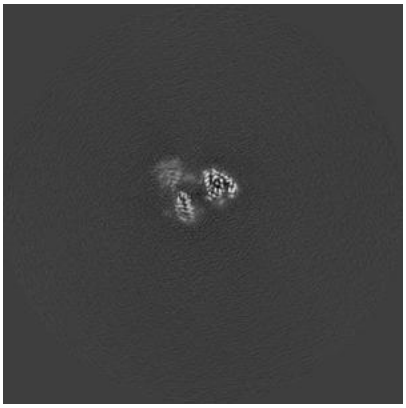
Z Index: 270

6.3.2 Raw map

X Index: 188



Y Index: 213



Z Index: 178

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 30.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

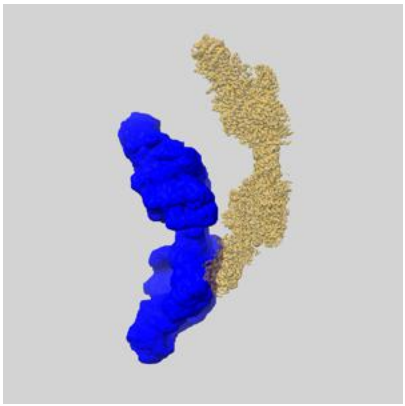
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

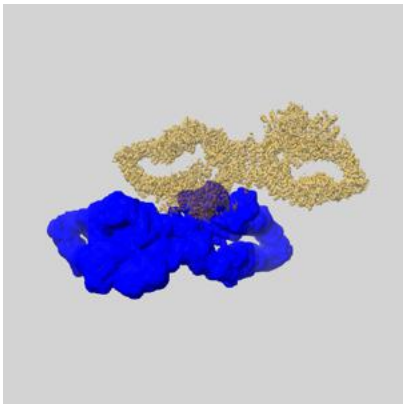
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

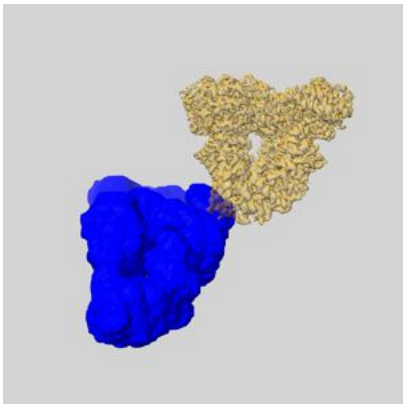
6.5.1 emd_13396_msk_1.map (i)



X



Y

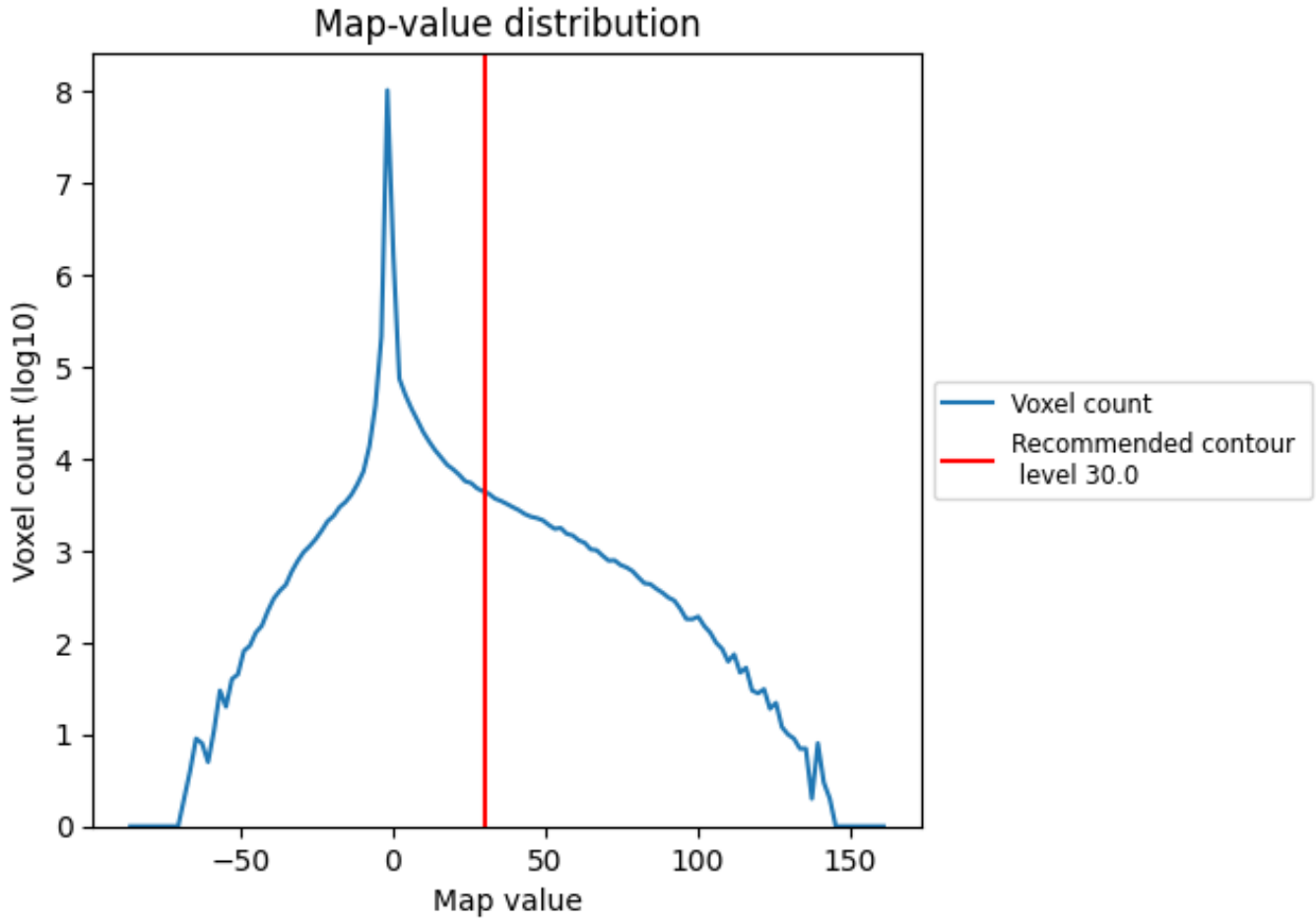


Z

7 Map analysis

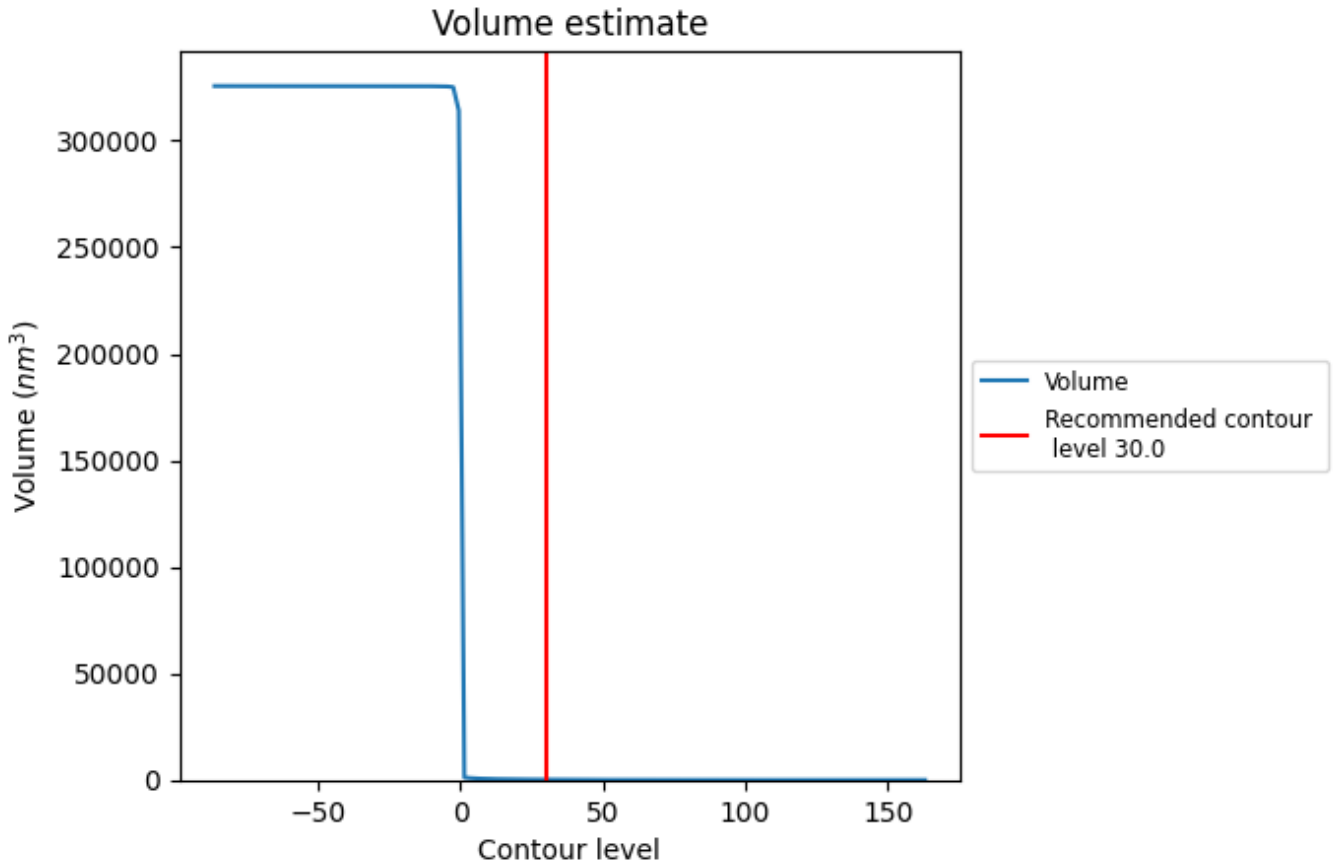
This section contains the results of statistical analysis of the map.

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 172 nm^3; this corresponds to an approximate mass of 155 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.

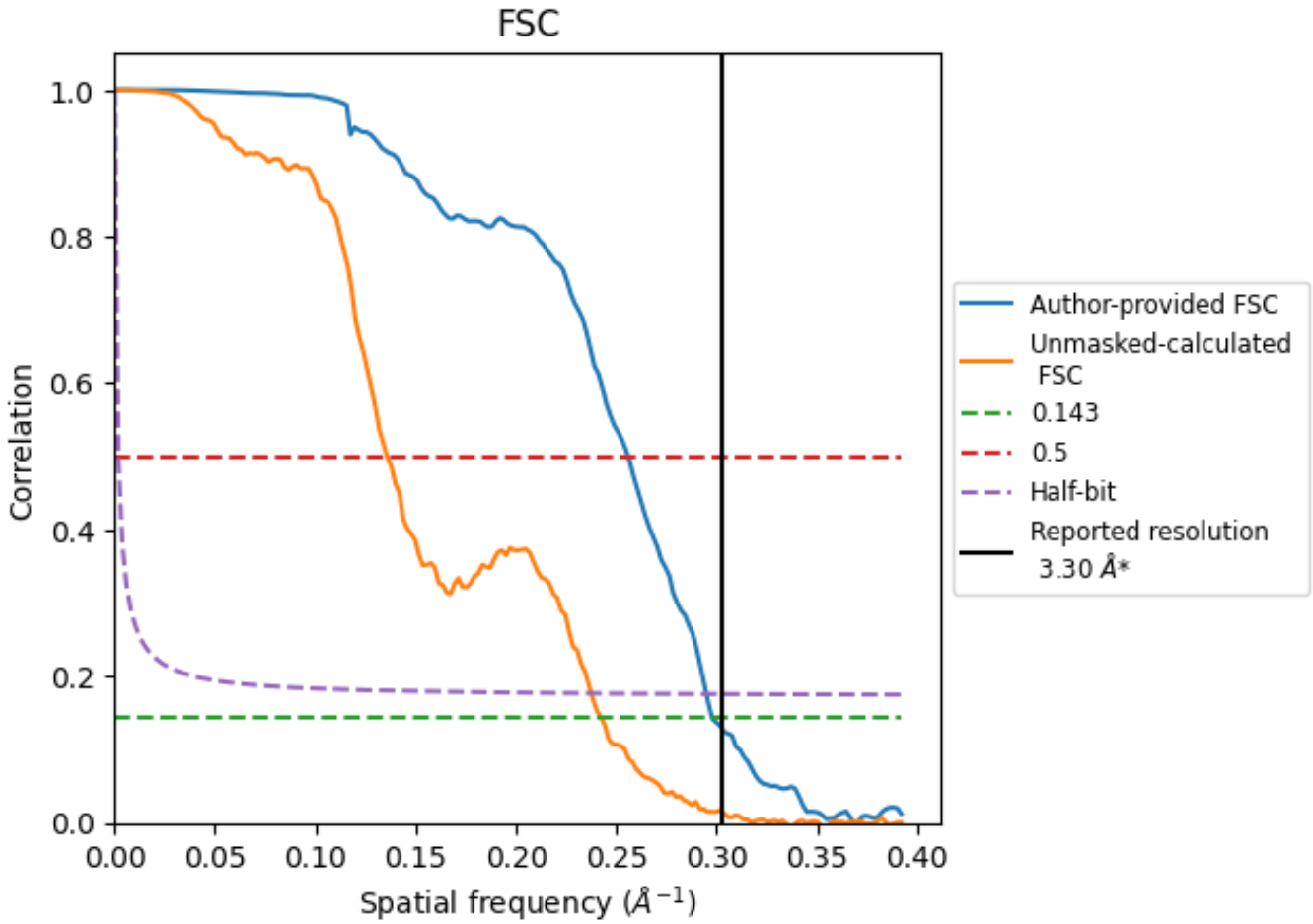
7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

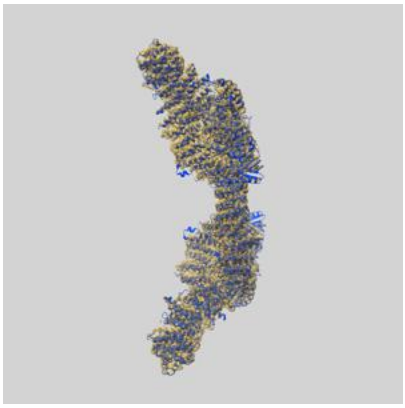
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.36	3.91	3.39
Unmasked-calculated*	4.12	7.36	4.21

*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 4.12 differs from the reported value 3.3 by more than 10 %

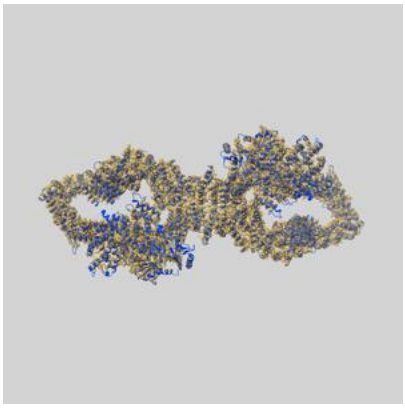
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13396 and PDB model 7PGU. Per-residue inclusion information can be found in section 3 on page 5.

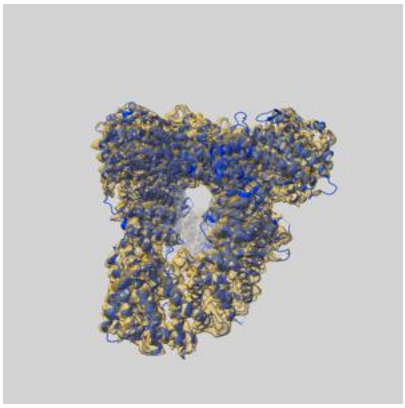
9.1 Map-model overlay



X



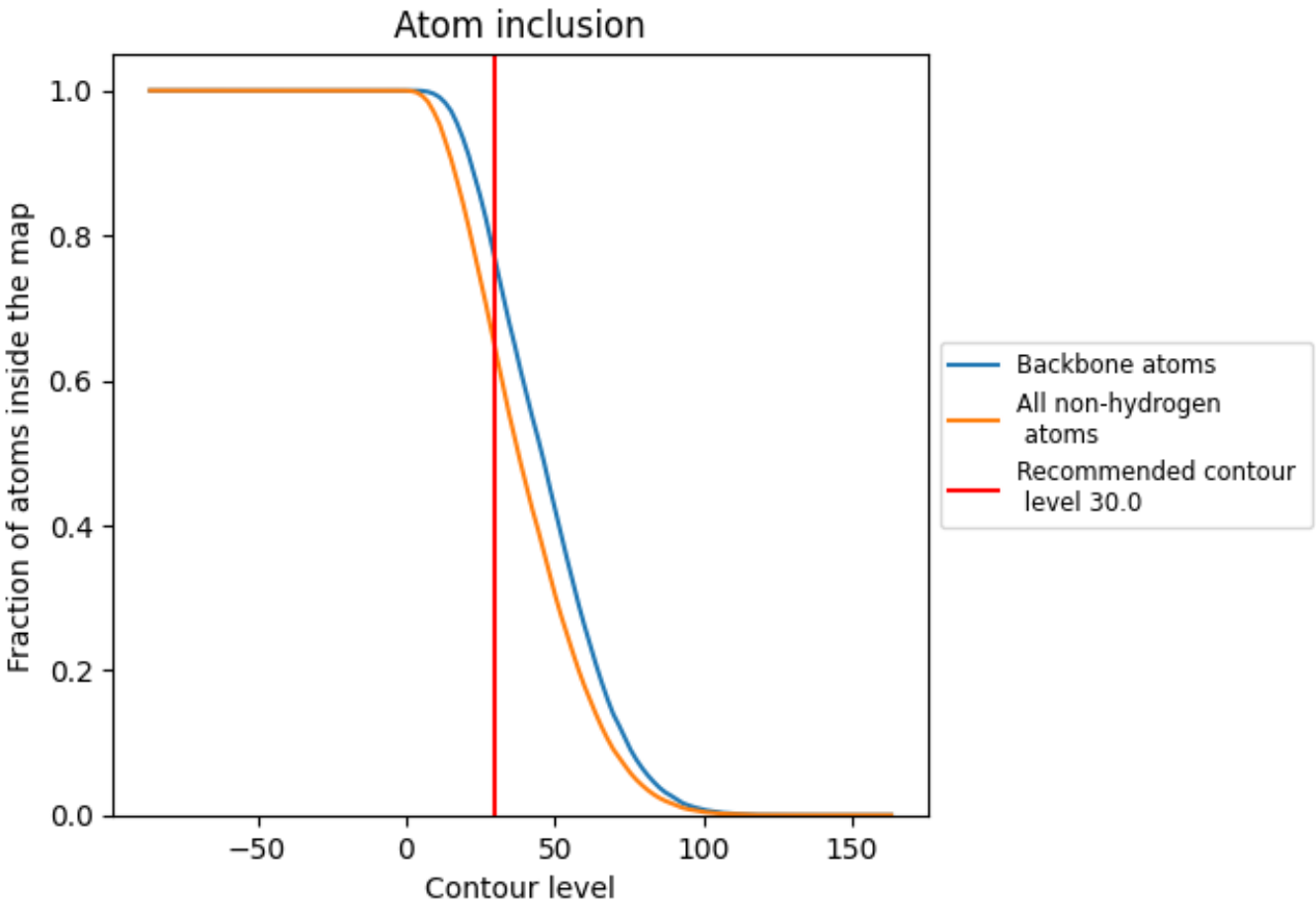
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 30.0 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 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.