Full wwPDB EM Validation Report ⓘ

Apr 10, 2022 – 04:17 am BST

PDB ID	:	7R04
EMDB ID	:	EMD-14219
Title	:	Neurofibromin in open conformation
Authors	:	Chaker-Margot, M.; Scheffzek, K.; Maier, T.
Deposited on	:	2022-02-01
Resolution	:	3.70 Å(reported)
Based on initial models	:	6V65, 2E2X

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:

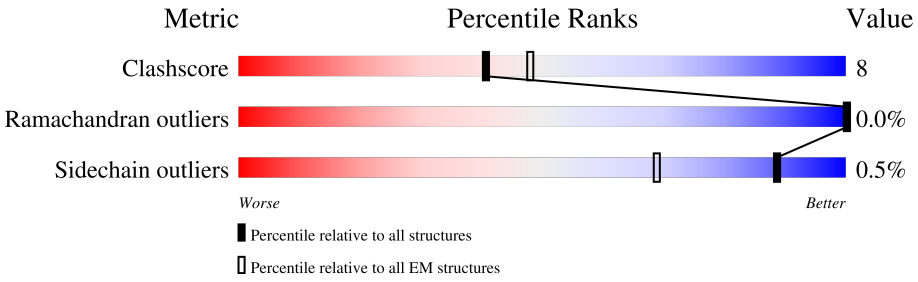
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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	2818	67% 15% 17%
1	B	2818	18% 64% 15% 21%

2 Entry composition

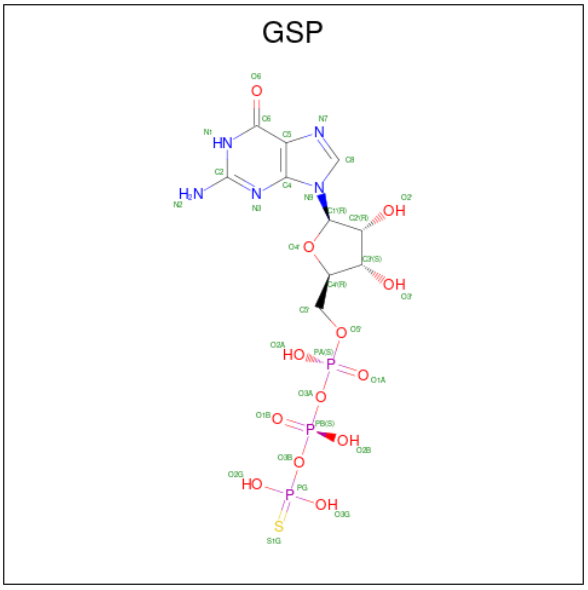
There are 2 unique types of molecules in this entry. The entry contains 36262 atoms, of which 12 are hydrogens and 0 are deuteriums.

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 Isoform I of Neurofibromin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2326	Total 18523	C 11890	N 3124	O 3390	S 119	0	0
1	B	2229	Total 17695	C 11363	N 2980	O 3236	S 116	0	0

- Molecule 2 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$) (labeled as "Ligand of Interest" by depositor).



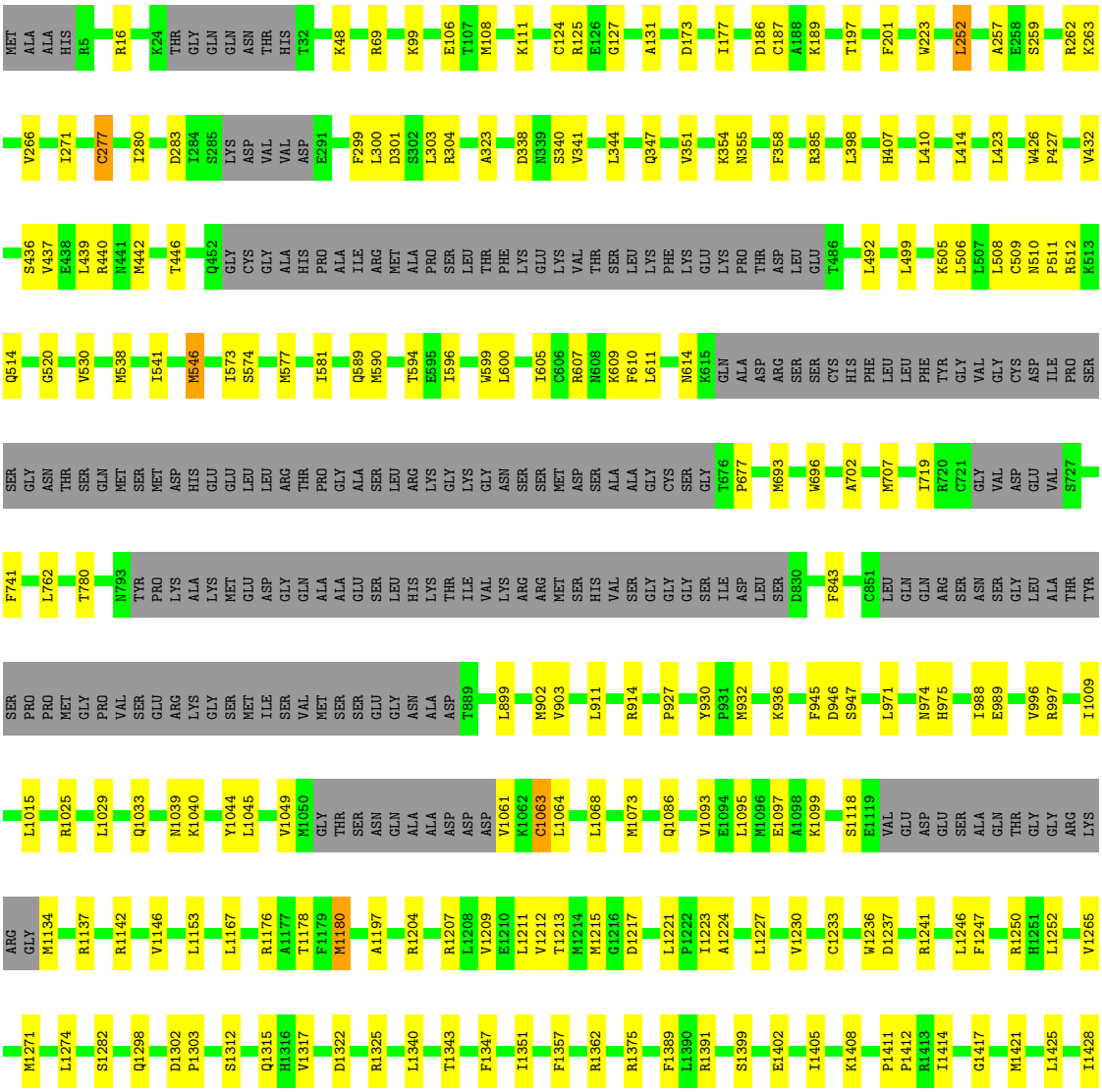
Mol	Chain	Residues	Atoms							AltConf
2	A	1	Total 44	C 10	H 12	N 5	O 13	P 3	S 1	0

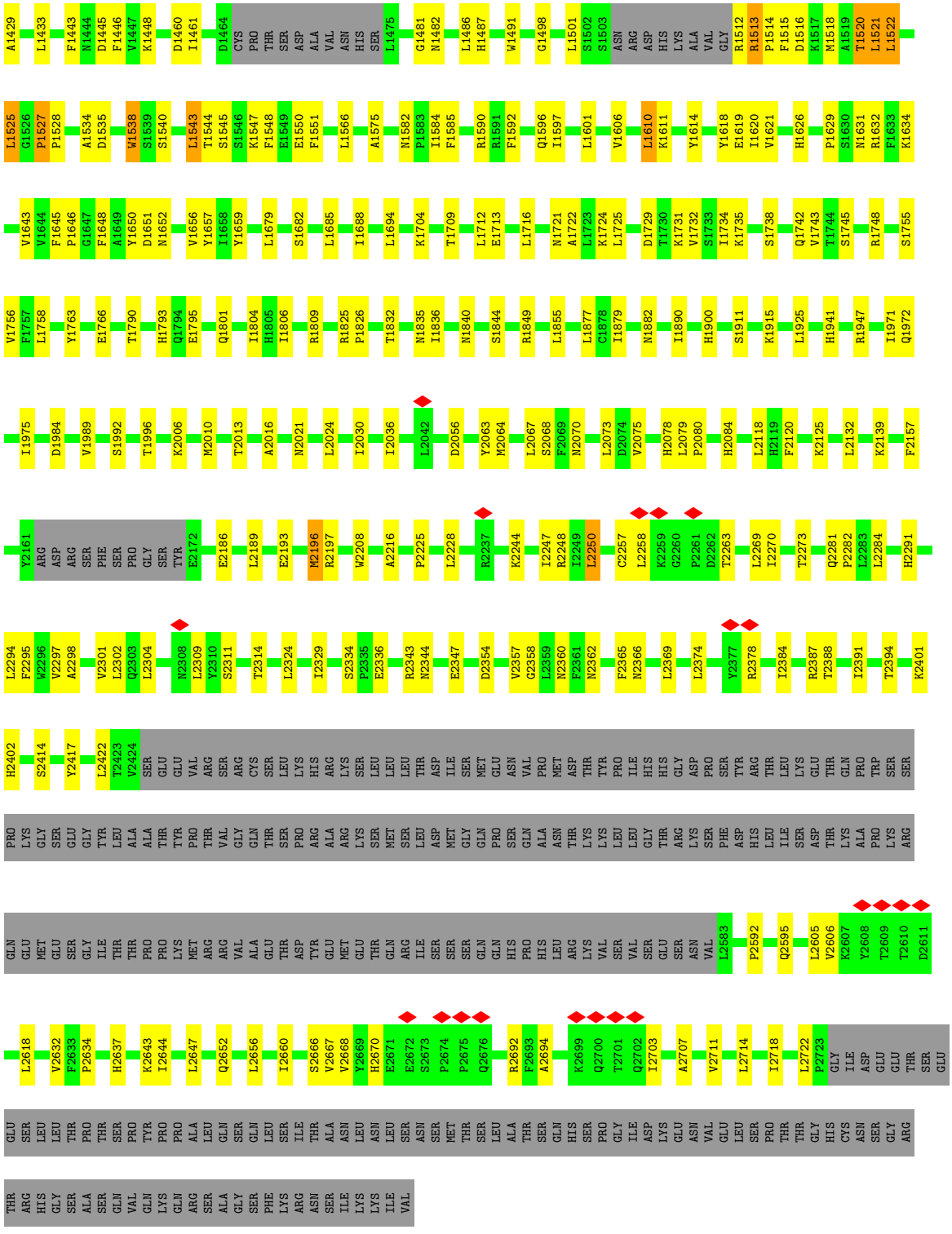
3 Residue-property plots (i)

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: Isoform I of Neurofibromin

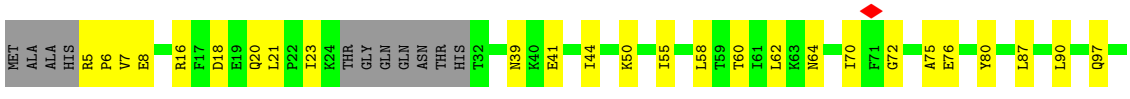
Chain A:

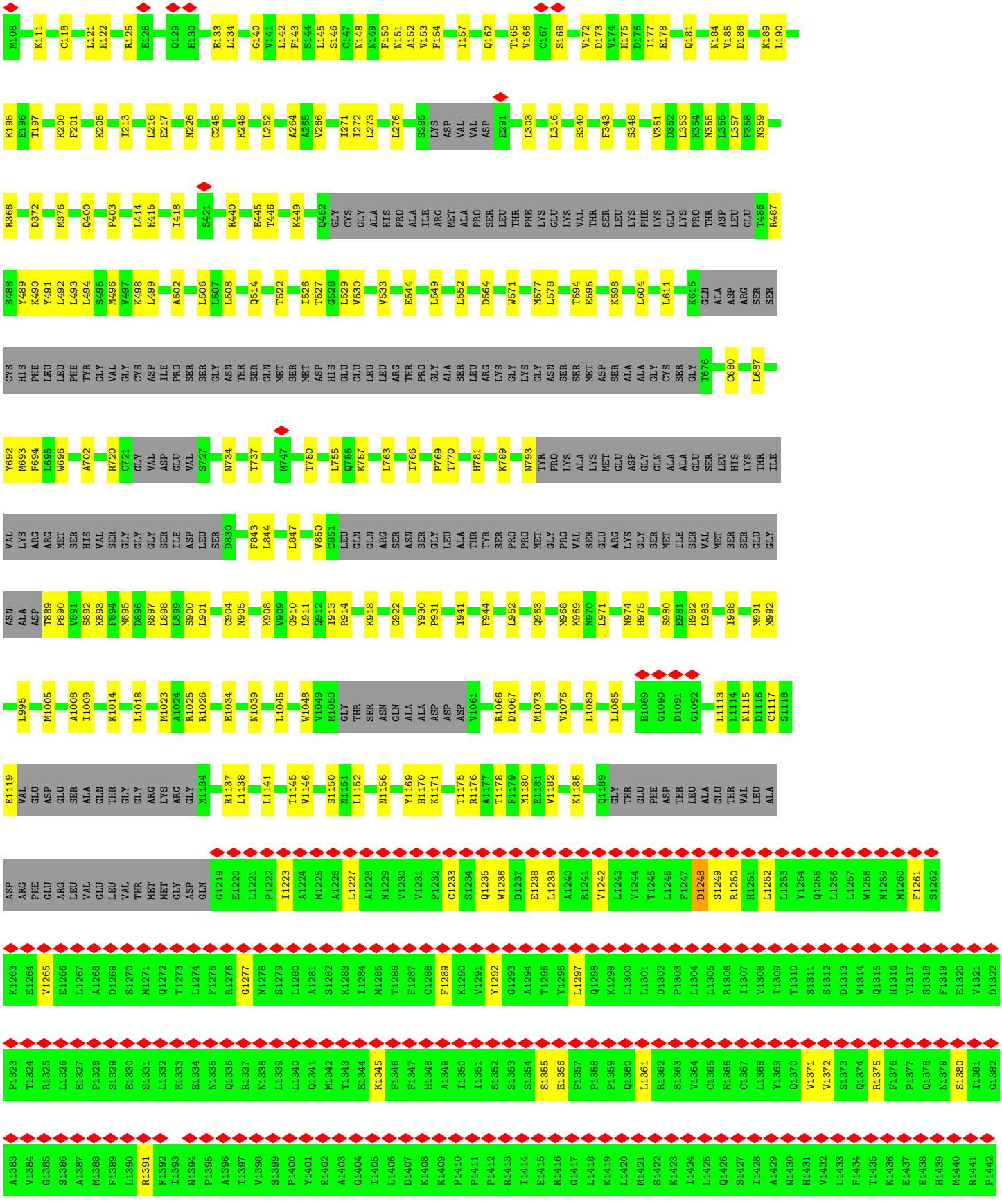


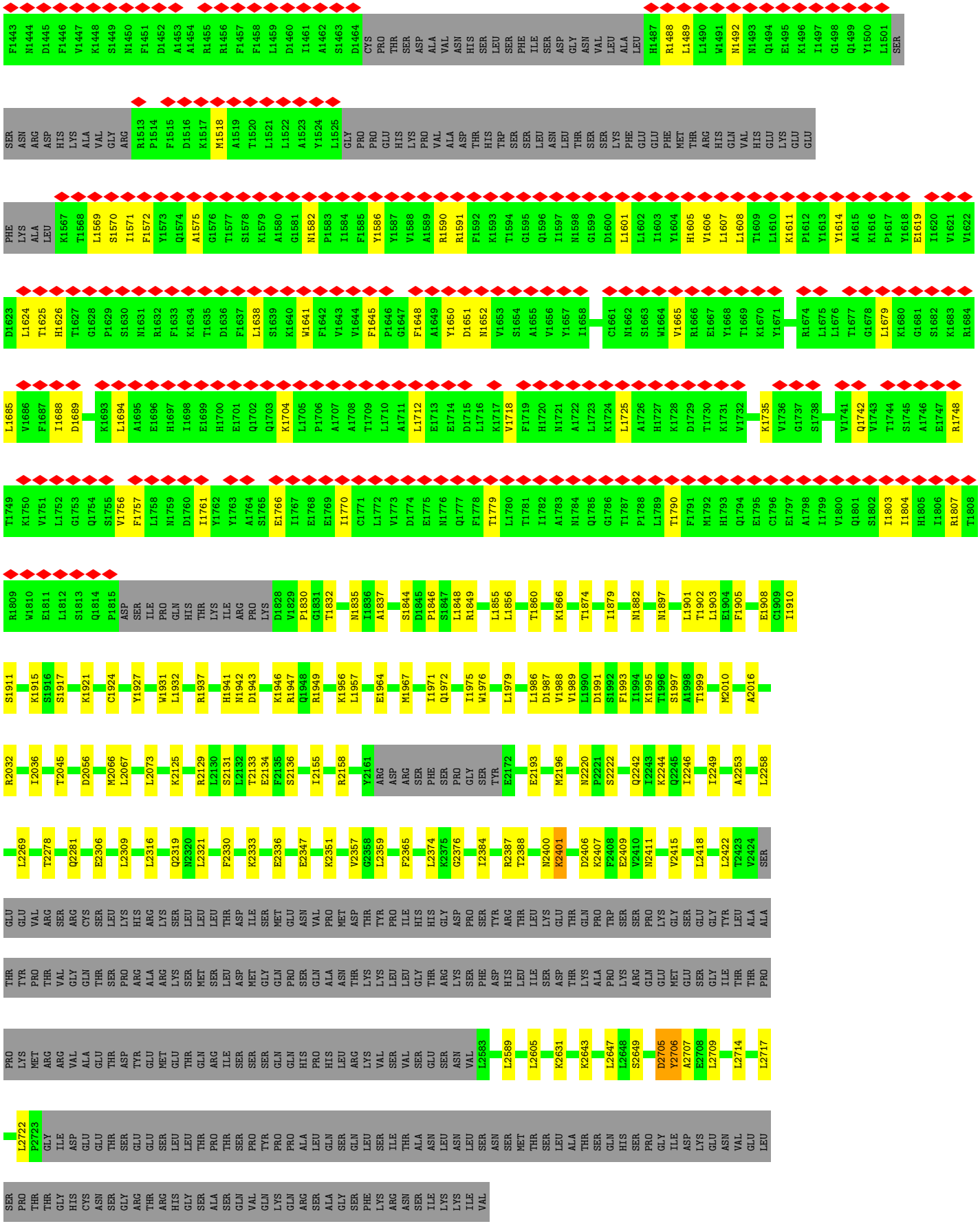


• Molecule 1: Isoform I of Neurofibromin

Chain B:




M108 K111 C118 L121 H122 R125 E126 Q129 H130 E133 L134 G140 V141 L142 F143 S144 L145 S146 C147 N148 N149 F150 N151 A152 V153 F154 I157 Q162 T165 V166 C167 S168 V172 D173 V174 H175 D176 I177 E178 Q181 N184 V185 D186 K189 L190
K195 E196 T197 K200 F201 K205 I213 L216 E217 N226 C245 K248 L252 A264 A265 V266 I271 I272 I273 L276 S285 LYS ASP VAL VAL ASP E291 L303 L316 S340 F343 S348 V351 D352 L353 K354 N355 L356 L357 F358 N359
R366 D372 M376 Q400 P403 L414 H415 I418 S421 R440 E445 T446 K449 Q452 GLY CYS GLY ALA HIS PRO ALA ILE ARG MET ALA PRO SER LEU THR PHE LYS GLU LYS VAL THR SER LEU LYS PHE LYS GLU LYS PRO THR ASP LEU GLU T486 R487
S488 Y489 K490 Y491 L492 L493 L494 S495 M496 V497 K498 L499 A502 L506 L507 L508 Q514 T522 I526 T527 G528 L529 V530 V533 E544 L549 L552 D564 W571 M577 L578 T594 E595 K598 L604 L611 K615 GLN ALA ASP ARG SER 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 SER GLY T676 C680 L687
Y692 M693 F694 L695 W696 A702 R720 C721 GLY VAL ASP GLU VAL S727 N734 T737 M747 T750 L755 Q756 K757 L763 I766 P769 T770 H781 K789 N793 TYR PRO LYS ALA LYS MET GLU ASP GLY GLN ALA ALA GLU SER LEU HIS LYS THR ILE
VAL LYS ARG ARG MET SER HIS VAL SER GLY GLY GLY SER ILE ASP LEU SER D830 F843 L844 L847 V850 C851 LEU GLN GLN ARG SER ASN SER GLY LEU ALA THR TYR SER PRO PRO MET GLY PRO VAL SER GLU ARG LYS GLY SER MET ILE SER VAL MET SER SER GLU GLY
ASN ALA ASP T889 P890 V891 S892 K893 F894 M895 D896 R897 L898 L899 S900 L901 C904 N905 K908 V909 G910 L911 Q912 I913 R914 K918 G922 Y930 P931 I941 F944 L962 Q963 M968 K969 N970 L971 N974 H975 S980 E981 H982 L983 I988 M991 M992
L995 M1005 A1008 I1009 K1014 L1018 M1023 A1024 R1025 R1026 E1034 N1039 L1045 W1048 V1049 M1050 GLY THR SER ASN GLN ALA ALA ASP ASP V1061 R1066 D1067 M1073 V1076 L1080 L1085 E1089 G1090 D1091 G1092 L1113 L1114 N1115 D1116 C1117 S1118
E1119 VAL GLU ASP GLU SER ALA GLN THR GLY GLY ARG LYS ARG GLY M1134 R1137 L1138 L1141 T1145 V1146 S1150 N1151 L1152 N1156 Y1169 H1170 K1171 T1175 R1176 A1177 T1178 F1179 M1180 E1181 V1182 K1185 Q1189 GLY THR GLU PHE ASP THR LEU ALA GLU THR VAL LEU ALA
ASP ARG PHE GLU ARG LEU VAL GLU LEU VAL THR MET MET GLY ASP GLN G1219 E1220 L1221 P1222 I1223 A1224 M1225 A1226 L1227 A1228 N1229 V1230 V1231 P1232 C1233 S1234 Q1235 W1236 D1237 E1238 L1239 A1240 R1241 V1242 L1243 V1244 T1245 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 A1281 S1282 K1283 I1284 M1285 T1286 F1287 C1288 F1289 K1290 V1291 Y1292 G1293 A1294 T1295 Y1296 L1297 Q1298 K1299 L1300 L1301 D1302 P1303 L1304 L1305 R1306 I1307 V1308 I1309 T1310 S1311 S1312 D1313 W1314 Q1315 H1316 V1317 S1318 F1319 E1320 V1321 D1322
P1323 T1324 R1325 L1326 E1327 P1328 S1329 E1330 S1331 L1332 E1333 E1334 N1335 Q1336 R1337 N1338 L1339 L1340 Q1341 M1342 T1343 E1344 K1345 F1346 F1347 H1348 A1349 I1350 I1351 S1352 S1353 S1354 S1355 E1356 F1357 P1358 P1359 Q1360 L1361 R1362 S1363 V1364 C1365 H1366 C1367 I1368 Y1369 Q1370 V1371 V1372 S1373 Q1374 R1375 F1376 P1377 Q1378 N1379 S1380 I1381 G1382
A1383 V1384 G1385 S1386 A1387 M1388 F1389 L1390 R1391 F1392 I1393 N1394 P1395 A1396 I1397 V1398 S1399 P1400 Y1401 E1402 A1403 G1404 I1405 L1406 D1407 K1408 K1409 P1410 P1411 P1412 R1413 I1414 E1415 R1416 G1417 L1418 K1419 L1420 M1421 S1422 K1423 I1424 L1425 Q1426 S1427 I1428 A1429 N1430 H1431 V1432 L1433 F1434 T1435 K1436 E1437 E1438 H1439 M1440 R1441 P1442


F1443 N1444 D1445 F1446 V1447 K1448 S1449 N1450 F1451 D1452 A1453 A1454 R1455 R1456 F1457 F1458 L1459 D1460 I1461 A1462 S1463 D1464 CYS PRO THR SER ASP ALA VAL ASN HIS SER LEU SER PHE ILE SER ASP GLY ASN VAL LEU ALA LEU H1487 R1488 L1489 L1490 W1491 N1492 N1493 Q1494 E1495 K1496 I1497 G1498 Q1499 Y1500 L1501 SER
SER ASN ARG ASP HIS LYS ALA VAL GLY ARG R1513 P1514 F1515 D1516 K1517 M1518 A1519 T1520 L1521 L1522 A1523 Y1524 L1525 GLY PRO PRO GLU HIS LYS PRO VAL ALA ASP THR HIS TRP SER SER LEU ASN LEU THR SER SER LYS PHE GLU GLU PHE MET THR ARG HIS GLN VAL HIS GLU LYS GLU GLU
PHE LYS ALA LEU K1567 T1568 L1569 S1570 I1571 F1572 Y1573 Q1574 A1575 G1576 T1577 S1578 K1579 A1580 G1581 N1582 P1583 I1584 F1585 Y1586 Y1587 V1588 A1589 R1590 R1591 F1592 K1593 T1594 G1595 Q1596 I1597 N1598 G1599 D1600 L1601 L1602 L1603 Y1604 H1605 V1606 L1607 L1608 T1609 L1610 K1611 P1612 Y1613 Y1614 A1615 K1616 P1617 Y1618 E1619 I1620 V1621 V1622
D1623 L1624 T1625 H1626 T1627 G1628 P1629 S1630 N1631 R1632 F1633 K1634 T1635 D1636 F1637 L1638 S1639 K1640 W1641 F1642 V1643 V1644 F1645 P1646 G1647 F1648 A1649 Y1650 D1651 N1652 V1653 S1654 A1655 V1656 Y1657 I1658 C1661 N1662 S1663 W1664 V1665 R1666 E1667 Y1668 T1669 K1670 Y1671 R1674 L1675 L1676 T1677 G1678 L1679 K1680 G1681 S1682 K1683 R1684
L1685 V1686 F1687 I1688 D1689 K1693 L1694 A1695 E1696 H1697 I1698 E1699 H1700 E1701 Q1702 Q1703 K1704 L1705 P1706 A1707 A1708 T1709 L1710 A1711 L1712 E1713 E1714 D1715 L1716 K1717 V1718 F1719 H1720 N1721 A1722 L1723 K1724 L1725 A1726 H1727 K1728 D1729 T1730 K1731 V1732 K1735 V1736 G1737 S1738 V1741 Q1742 V1743 T1744 S1745 A1746 E1747 R1748
T1749 K1750 V1751 L1752 G1753 Q1754 S1755 V1756 F1757 L1758 N1759 D1760 I1761 Y1762 Y1763 A1764 S1765 E1766 I1767 E1768 E1769 I1770 C1771 L1772 V1773 D1774 E1775 N1776 Q1777 F1778 T1779 L1780 T1781 I1782 A1783 N1784 Q1785 G1786 T1787 P1788 L1789 T1790 F1791 M1792 H1793 Q1794 E1795 C1796 E1797 A1798 I1799 V1800 Q1801 S1802 I1803 I1804 H1805 I1806 R1807 T1808
R1809 W1810 E1811 L1812 S1813 Q1814 P1815 ASP SER ILE PRO GLN HIS THR LYS ILE ARG PRO LYS D1828 V1829 P1830 G1831 T1832 N1835 I1836 A1837 S1844 D1845 P1846 S1847 L1848 R1849 L1855 L1856 T1860 K1866 T1874 I1879 N1882 N1897 L1901 T1902 L1903 E1904 F1905 E1908 C1909 I1910
S1911 K1915 S1916 S1917 K1921 C1924 Y1927 W1931 L1932 R1937 H1941 N1942 D1943 K1946 R1947 Q1948 R1949 K1956 L1957 E1964 M1967 I1971 Q1972 I1975 W1976 L1979 L1986 D1987 V1988 V1989 L1990 D1991 S1992 F1993 I1994 K1995 T1996 S1997 A1998 T1999 M2010 A2016
R2032 I2036 T2045 D2056 M2066 L2067 L2073 K2125 R2129 L2130 S2131 L2132 T2133 E2134 F2135 S2136 I2155 R2158 Y2161 ARG ASP ARG SER PHE SER PRO GLY SER TYR E2172 E2193 M2196 N2220 P2221 S2222 Q2242 I2243 K2244 Q2245 I2246 I2249 A2253 L2258
L2269 T2278 Q2281 E2306 L2309 L2316 Q2319 W2320 L2321 F2330 K2333 E2336 E2347 K2351 V2357 G2358 L2359 F2365 L2374 K2375 G2376 I2384 R2387 T2388 N2400 K2401 D2406 K2407 F2408 E2409 V2410 W2411 V2415 L2418 L2422 T2423 V2424 SER
GLU GLU VAL ARG SER ARG CYS SER LEU LYS HIS ARG 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 LYS GLU THR GLN PRO TRP SER SER PRO LYS GLY SER GLU GLY TYR LEU ALA 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 ASN THR LYS LYS LEU LEU GLY THR ARG LYS SER PHE ASP HIS LEU ILE SER ASP THR LYS ALA 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 LYS VAL SER VAL SER GLU SER ASN VAL L2583 L2589 L2605 K2631 K2643 L2647 L2648 S2649 D2705 Y2706 A2707 E2708 L2709 L2714 L2717
L2722 P2723 GLY 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 LEU SER ILE THR ALA ASN LEU LEU ASN LEU SER LEU SER ASN SER MET THR SER LEU ALA THR SER GLN HIS SER PRO GLY ILE ASP LYS GLU ASN LEU
SER PRO THR THR GLY HIS CYS ASN SER GLY ARG THR ARG HIS GLY 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	300000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	52.847	Depositor
Minimum map value	-20.737	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.998	Depositor
Recommended contour level	6.0	Depositor
Map size (Å)	541.696, 541.696, 541.696	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.35	0/18902	0.61	10/25620 (0.0%)
1	B	0.30	0/18052	0.56	5/24473 (0.0%)
All	All	0.32	0/36954	0.59	15/50093 (0.0%)

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	B	0	2

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1984	ASP	CB-CG-OD1	8.51	125.96	118.30
1	B	1608	LEU	CA-CB-CG	6.22	129.61	115.30
1	A	1180	MET	CA-CB-CG	6.01	123.51	113.30
1	A	1610	LEU	CA-CB-CG	5.92	128.93	115.30
1	B	1023	MET	CG-SD-CE	5.53	109.04	100.20
1	A	1217	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	2706	TYR	N-CA-CB	5.45	120.40	110.60
1	A	1167	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	1527	PRO	N-CA-C	-5.37	98.15	112.10
1	A	252	LEU	CB-CG-CD2	5.29	120.00	111.00
1	A	2196	MET	CB-CG-SD	5.14	127.81	112.40
1	A	546	MET	CG-SD-CE	-5.13	91.99	100.20
1	A	2250	LEU	CA-CB-CG	5.08	126.99	115.30
1	B	2010	MET	CG-SD-CE	5.05	108.28	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2705	ASP	C-N-CA	5.04	134.29	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1248	ASP	Peptide
1	B	2705	ASP	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	18523	0	18780	295	0
1	B	17695	0	17898	261	0
2	A	32	12	12	3	0
All	All	36250	12	36690	547	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 8.

All (547) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:THR:O	1:A:201:PHE:HB2	1.52	1.08
1:A:1535:ASP:HA	1:A:1596:GLN:HG3	1.36	1.06
1:A:1491:TRP:CD1	1:A:1528:PRO:HD3	1.94	1.03
1:A:1544:THR:HB	1:A:1547:LYS:HG2	1.48	0.95
1:A:1204:ARG:HD2	1:A:1525:LEU:HD13	1.56	0.87
1:A:1501:LEU:HD23	1:A:1515:PHE:HB2	1.56	0.87
1:A:1748:ARG:HA	1:A:1756:VAL:O	1.77	0.84
1:A:277:CYS:HB2	1:A:280:ILE:HG12	1.60	0.82
1:A:1176:ARG:O	1:A:1180:MET:HB2	1.81	0.79
1:B:173:ASP:O	1:B:177:ILE:HB	1.83	0.78
1:A:1204:ARG:HG2	1:A:1525:LEU:HD22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:908:LYS:O	1:B:911:LEU:HB2	1.86	0.75
1:A:1282:SER:HB3	1:A:1391:ARG:HH12	1.52	0.75
1:A:975:HIS:HB2	1:A:1025:ARG:HH21	1.53	0.73
1:A:1513:ARG:N	1:A:1514:PRO:HD2	2.04	0.73
1:A:1540:SER:HB3	1:A:1543:LEU:HD12	1.69	0.73
1:A:385:ARG:NH2	1:A:423:LEU:O	2.22	0.72
1:B:941:ILE:HD11	1:B:991:MET:HB2	1.71	0.72
1:B:487:ARG:HE	1:B:490:LYS:HZ3	1.39	0.70
1:A:2193:GLU:HA	1:A:2196:MET:HG2	1.74	0.69
1:A:538:MET:HB2	1:A:541:ILE:HD13	1.75	0.67
1:A:2250:LEU:HD23	1:A:2273:THR:HG21	1.76	0.67
1:A:1972:GLN:OE1	1:B:1882:ASN:ND2	2.27	0.67
1:B:62:LEU:HD11	1:B:90:LEU:HD11	1.75	0.67
1:A:1527:PRO:HB2	1:A:1528:PRO:HD2	1.77	0.66
1:A:1515:PHE:O	1:A:1518:MET:HG3	1.94	0.66
1:B:154:PHE:O	1:B:157:ILE:HB	1.95	0.66
1:A:903:VAL:HA	1:A:914:ARG:HH12	1.58	0.66
1:A:1547:LYS:O	1:A:1550:GLU:HG3	1.96	0.66
1:B:1971:ILE:HG23	1:B:1975:ILE:HD12	1.76	0.66
1:B:2278:THR:HG23	1:B:2319:GLN:HG2	1.77	0.66
1:A:1039:ASN:ND2	1:A:1086:GLN:O	2.29	0.65
1:A:932:MET:HB3	1:A:936:LYS:HZ3	1.59	0.65
1:B:2036:ILE:HD13	1:B:2056:ASP:HB3	1.79	0.65
1:A:1535:ASP:HA	1:A:1596:GLN:CG	2.22	0.65
1:A:2592:PRO:HA	1:A:2595:GLN:HE21	1.62	0.64
1:B:1223:ILE:O	1:B:1227:LEU:HB2	1.98	0.64
1:A:1487:HIS:NE2	1:A:1528:PRO:HA	2.13	0.64
1:B:357:LEU:HB3	1:B:376:MET:HG3	1.79	0.64
1:A:1584:ILE:HA	1:A:1619:GLU:O	1.98	0.64
1:A:2193:GLU:O	1:A:2197:ARG:NH1	2.30	0.64
1:A:300:LEU:O	1:A:303:LEU:HB3	1.98	0.64
1:B:2155:ILE:HA	1:B:2158:ARG:HB2	1.80	0.64
1:B:911:LEU:HD13	1:B:914:ARG:HH12	1.63	0.63
1:B:499:LEU:HD21	1:B:506:LEU:HD23	1.81	0.63
1:A:1538:TRP:CZ3	1:A:1548:PHE:HA	2.33	0.63
1:B:1718:VAL:HG13	1:B:1735:LYS:HG2	1.79	0.63
1:A:1996:THR:O	1:A:2006:LYS:NZ	2.31	0.63
1:A:1298:GLN:HG2	1:A:1405:ILE:HG23	1.82	0.62
1:B:1372:VAL:HG13	1:B:1380:SER:HB2	1.81	0.62
1:A:2343:ARG:NH2	1:A:2354:ASP:OD2	2.31	0.62
1:B:201:PHE:HB3	1:B:252:LEU:HD13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ILE:HD12	1:B:75:ALA:HB1	1.82	0.62
1:A:440:ARG:HH21	1:A:508:LEU:HA	1.65	0.62
1:B:1748:ARG:HA	1:B:1756:VAL:O	1.99	0.62
1:A:1513:ARG:HE	1:A:1516:ASP:HB2	1.65	0.62
1:A:2343:ARG:NH1	1:A:2362:ASN:OD1	2.31	0.62
1:A:1849:ARG:NH1	1:A:1879:ILE:O	2.34	0.61
1:A:2336:GLU:OE2	1:A:2366:ASN:ND2	2.34	0.61
1:A:436:SER:HA	1:A:439:LEU:HD13	1.82	0.60
1:B:1911:SER:O	1:B:1915:LYS:NZ	2.34	0.60
1:B:1849:ARG:NH1	1:B:1879:ILE:O	2.34	0.60
1:B:2281:GLN:OE1	1:B:2319:GLN:NE2	2.34	0.60
1:A:902:MET:O	1:A:914:ARG:NH1	2.34	0.60
1:A:1911:SER:O	1:A:1915:LYS:NZ	2.34	0.60
1:A:996:VAL:HG12	1:A:1015:LEU:HD21	1.84	0.60
1:A:1061:VAL:N	1:A:1063:CYS:HG	1.99	0.60
1:A:1825:ARG:HD2	1:A:1826:PRO:HD2	1.82	0.60
1:A:1738:SER:OG	1:A:1809:ARG:NH2	2.35	0.60
1:A:574:SER:OG	1:A:607:ARG:NH1	2.35	0.60
1:A:2021:ASN:HD21	1:A:2024:LEU:HD12	1.67	0.59
1:B:910:GLY:HA2	1:B:913:ILE:HB	1.84	0.59
1:B:1250:ARG:HD2	1:B:1611:LYS:HE2	1.84	0.59
1:A:446:THR:HG21	1:A:492:LEU:HD22	1.85	0.59
1:A:2075:VAL:O	1:A:2079:LEU:HB2	2.02	0.59
1:A:259:SER:HA	1:A:263:LYS:HD2	1.84	0.59
1:A:989:GLU:OE2	1:A:1033:GLN:NE2	2.36	0.59
1:B:490:LYS:HA	1:B:493:LEU:HD12	1.84	0.59
1:A:299:PHE:O	1:A:303:LEU:N	2.34	0.58
1:A:510:ASN:O	1:A:512:ARG:NH1	2.32	0.58
1:B:2384:ILE:HG13	1:B:2387:ARG:HH12	1.69	0.58
1:A:2064:MET:O	1:A:2068:SER:OG	2.21	0.58
1:A:2247:ILE:HD12	1:A:2714:LEU:HD22	1.84	0.58
1:A:1722:ALA:HB3	1:A:1732:VAL:O	2.04	0.58
1:A:2711:VAL:HA	1:A:2714:LEU:HD12	1.86	0.58
1:B:440:ARG:HH21	1:B:508:LEU:HA	1.67	0.58
1:A:124:CYS:SG	1:A:125:ARG:N	2.76	0.58
1:A:16:ARG:NH2	1:B:2649:SER:OG	2.36	0.58
1:A:2216:ALA:HB1	1:A:2228:LEU:HD23	1.86	0.57
1:A:1590:ARG:NH1	1:A:1763:TYR:OH	2.37	0.57
1:A:589:GLN:NE2	1:A:590:MET:O	2.37	0.57
1:B:2374:LEU:HD11	1:B:2605:LEU:HD11	1.86	0.57
1:A:338:ASP:HA	1:A:341:VAL:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1312:SER:HA	1:A:1315:GLN:HB2	1.87	0.57
1:B:1679:LEU:HB3	1:B:1685:LEU:HD11	1.84	0.57
1:A:2301:VAL:HG13	1:A:2309:LEU:HB3	1.87	0.57
1:B:348:SER:HA	1:B:353:LEU:HD13	1.87	0.57
1:B:890:PRO:HA	1:B:893:LYS:HE2	1.87	0.57
1:B:1169:TYR:HA	1:B:1176:ARG:HH21	1.69	0.56
1:A:2668:VAL:HG13	1:B:50:LYS:HE3	1.88	0.56
1:A:1679:LEU:HB3	1:A:1685:LEU:HD11	1.87	0.56
1:B:1150:SER:HA	1:B:1182:VAL:HG13	1.88	0.56
1:A:1543:LEU:HD13	1:A:1643:VAL:HG21	1.88	0.56
1:A:1362:ARG:NH1	1:A:1460:ASP:O	2.33	0.56
1:A:2314:THR:HG1	1:A:2387:ARG:HH11	1.53	0.56
1:A:988:ILE:HD11	1:A:1029:LEU:HD13	1.87	0.55
1:B:185:VAL:O	1:B:226:ASN:ND2	2.40	0.55
1:B:1937:ARG:O	1:B:1941:HIS:NE2	2.39	0.55
1:B:1903:LEU:HG	1:B:1949:ARG:HD2	1.88	0.55
1:B:2376:GLY:HA3	1:B:2388:THR:HG21	1.87	0.55
1:A:2284:LEU:HD13	1:A:2291:HIS:CE1	2.41	0.55
1:A:407:HIS:ND1	1:A:442:MET:SD	2.61	0.55
1:A:1941:HIS:O	1:A:1947:ARG:NH2	2.25	0.55
1:B:1689:ASP:HB3	1:B:1757:PHE:HB2	1.88	0.55
1:A:2010:MET:O	1:A:2013:THR:OG1	2.20	0.55
1:A:2311:SER:O	1:A:2387:ARG:NH1	2.40	0.55
1:A:2718:ILE:HA	1:A:2722:LEU:HD13	1.89	0.55
1:A:2666:SER:O	1:A:2670:HIS:ND1	2.36	0.55
1:B:1488:ARG:O	1:B:1492:ASN:HB2	2.07	0.55
1:A:610:PHE:O	1:A:614:ASN:ND2	2.32	0.55
1:A:1215:MET:HG2	1:A:1221:LEU:HB2	1.89	0.55
1:B:1026:ARG:HH21	1:B:1034:GLU:HG3	1.70	0.55
1:B:2067:LEU:O	1:B:2073:LEU:N	2.40	0.55
1:A:1732:VAL:HG12	1:A:1745:SER:HA	1.88	0.55
1:B:1265:VAL:HG12	1:B:1375:ARG:HD3	1.88	0.55
1:A:106:GLU:HG3	1:A:108:MET:HG3	1.87	0.55
1:A:1748:ARG:HB3	1:A:1755:SER:HB3	1.89	0.54
1:B:217:GLU:HG2	1:B:272:ILE:HG13	1.88	0.54
1:B:1590:ARG:NH1	1:B:1625:THR:OG1	2.40	0.54
1:A:499:LEU:HD21	1:A:506:LEU:HD23	1.89	0.54
1:B:498:LYS:O	1:B:502:ALA:N	2.40	0.54
1:A:530:VAL:HG21	1:A:577:MET:HG3	1.89	0.54
1:A:1176:ARG:NH2	1:A:1840:ASN:OD1	2.32	0.54
1:B:154:PHE:HA	1:B:157:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2244:LYS:HG3	1:B:2722:LEU:HD13	1.89	0.54
1:B:2706:TYR:HB2	1:B:2709:LEU:HD12	1.90	0.54
1:B:1582:ASN:ND2	1:B:1619:GLU:OE2	2.35	0.54
1:B:905:ASN:HB2	1:B:914:ARG:HH11	1.73	0.54
1:A:304:ARG:HG2	1:A:347:GLN:HE21	1.72	0.53
1:A:1118:SER:HA	1:A:1142:ARG:HH22	1.73	0.53
1:B:2155:ILE:HG22	1:B:2158:ARG:HD2	1.88	0.53
1:A:1227:LEU:HA	1:A:1230:VAL:HG12	1.90	0.53
1:B:991:MET:N	1:B:991:MET:SD	2.78	0.53
1:B:734:ASN:OD1	1:B:770:THR:OG1	2.27	0.53
1:B:1987:ASP:OD1	1:B:1988:VAL:N	2.40	0.53
1:A:1582:ASN:ND2	1:A:1619:GLU:OE2	2.37	0.53
1:B:1277:GLY:O	1:B:1391:ARG:NH2	2.41	0.53
1:B:2258:LEU:HD21	1:B:2707:ALA:HB3	1.89	0.53
1:A:1204:ARG:CG	1:A:1525:LEU:HD22	2.37	0.53
1:A:340:SER:O	1:A:344:LEU:N	2.34	0.53
1:A:1221:LEU:HD23	1:A:1224:ALA:H	1.72	0.53
1:A:437:VAL:HA	1:A:510:ASN:HD21	1.73	0.53
1:A:2080:PRO:HB3	1:A:2208:TRP:HB2	1.91	0.53
1:A:280:ILE:HA	1:A:283:ASP:HB2	1.89	0.53
1:A:1271:MET:HA	1:A:1274:LEU:HD12	1.91	0.53
1:A:1734:ILE:HG12	1:A:1743:VAL:HG12	1.91	0.53
1:B:1261:PHE:HB3	1:B:1371:VAL:HG11	1.91	0.53
1:B:264:ALA:HB2	1:B:316:LEU:HD23	1.90	0.53
1:A:1806:ILE:HA	1:A:1809:ARG:HG2	1.91	0.53
1:A:2244:LYS:HD2	1:A:2248:ARG:HH21	1.73	0.53
1:B:897:ARG:NH1	1:B:900:SER:OG	2.42	0.52
1:B:1941:HIS:O	1:B:1947:ARG:NH2	2.35	0.52
1:B:1645:PHE:HB2	1:B:1650:TYR:CZ	2.45	0.52
1:A:1745:SER:OG	1:A:1758:LEU:N	2.42	0.52
1:A:2291:HIS:HB3	1:A:2324:LEU:HD11	1.91	0.52
1:B:737:THR:HG21	1:B:766:ILE:HA	1.90	0.52
1:B:1045:LEU:HA	1:B:1048:TRP:HB2	1.91	0.52
1:A:1411:PRO:HD2	1:A:1414:ILE:HD12	1.91	0.52
1:A:899:LEU:HD22	1:A:902:MET:HE1	1.91	0.52
1:A:1211:LEU:HD11	1:A:1518:MET:HB3	1.92	0.52
1:A:1538:TRP:HZ3	1:A:1548:PHE:HA	1.71	0.52
1:A:2595:GLN:HE22	1:A:2632:VAL:HG21	1.75	0.52
1:A:2374:LEU:O	1:A:2378:ARG:NH2	2.43	0.52
1:B:908:LYS:HA	1:B:911:LEU:HD23	1.92	0.52
1:A:1425:LEU:HD13	1:A:1428:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:692:TYR:HB3	1:B:843:PHE:HZ	1.75	0.52
1:B:1942:ASN:OD1	1:B:1943:ASP:N	2.43	0.52
1:A:301:ASP:HA	1:A:304:ARG:HD3	1.91	0.52
1:A:414:LEU:HD11	1:A:432:VAL:HG11	1.92	0.52
1:A:1712:LEU:O	1:A:1742:GLN:NE2	2.31	0.52
1:A:1925:LEU:HG	1:A:1975:ILE:HD11	1.92	0.52
1:B:41:GLU:HA	1:B:44:ILE:HD12	1.92	0.52
1:B:2400:ASN:ND2	1:B:2406:ASP:O	2.43	0.52
1:A:594:THR:HG22	1:A:702:ALA:HB2	1.92	0.51
1:A:1659:TYR:OH	1:A:1713:GLU:OE2	2.27	0.51
1:A:1688:ILE:HG21	1:A:1694:LEU:HB2	1.92	0.51
1:A:351:VAL:HB	1:A:355:ASN:HB2	1.92	0.51
1:B:72:GLY:O	1:B:76:GLU:N	2.40	0.51
1:B:366:ARG:NH2	1:B:372:ASP:OD2	2.43	0.51
1:B:988:ILE:HG13	1:B:992:MET:HE2	1.92	0.51
1:A:2030:ILE:HD13	1:A:2078:HIS:HB3	1.91	0.51
1:A:780:THR:HG21	1:A:843:PHE:HD2	1.75	0.51
1:A:2357:VAL:O	1:A:2692:ARG:NH1	2.43	0.51
1:B:680:CYS:SG	1:B:720:ARG:NH2	2.83	0.51
1:A:1212:VAL:HA	1:A:1223:ILE:HG13	1.93	0.51
1:B:1005:MET:O	1:B:1009:ILE:N	2.40	0.51
1:B:2306:GLU:HB3	1:B:2309:LEU:HB2	1.93	0.51
1:A:971:LEU:O	1:A:974:ASN:ND2	2.43	0.51
1:A:1212:VAL:HG21	1:A:1486:LEU:HD21	1.92	0.51
1:B:1235:GLN:O	1:B:1239:LEU:N	2.44	0.51
1:B:1972:GLN:HA	1:B:1976:TRP:HD1	1.74	0.51
1:A:2186:GLU:HA	1:A:2189:LEU:HB2	1.93	0.51
1:B:1835:ASN:HD22	1:B:1908:GLU:HB2	1.74	0.51
1:B:1924:CYS:HA	1:B:1927:TYR:CE1	2.45	0.51
1:A:2388:THR:HA	1:A:2391:ILE:HG22	1.93	0.51
1:A:514:GLN:HA	1:A:520:GLY:HA2	1.92	0.51
1:A:2354:ASP:HB3	1:A:2360:ASN:HA	1.93	0.51
1:B:165:THR:HG23	1:B:166:VAL:HG23	1.93	0.51
1:B:1995:LYS:O	1:B:1999:THR:N	2.43	0.51
1:A:927:PRO:O	1:A:930:TYR:HB2	2.11	0.50
1:A:1806:ILE:HG22	1:A:1809:ARG:HE	1.77	0.50
1:A:2384:ILE:HG13	1:A:2387:ARG:HH22	1.75	0.50
1:A:1241:ARG:NH2	1:A:1482:ASN:OD1	2.45	0.50
1:B:186:ASP:O	1:B:190:LEU:N	2.33	0.50
1:A:1204:ARG:CD	1:A:1525:LEU:HD22	2.42	0.50
1:A:1724:LYS:O	1:A:1729:ASP:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:CYS:HG	1:A:223:TRP:HE1	1.56	0.50
1:A:2324:LEU:HG	1:A:2329:ILE:HD13	1.94	0.50
1:B:789:LYS:NZ	1:B:793:ASN:OD1	2.36	0.50
1:B:1742:GLN:HG2	1:B:1761:ILE:HG12	1.93	0.50
1:A:1204:ARG:HG2	1:A:1525:LEU:CD2	2.40	0.50
1:A:1213:THR:HG21	1:A:1250:ARG:HG3	1.94	0.50
1:A:1322:ASP:HB3	1:A:1325:ARG:HB2	1.93	0.50
1:B:118:CYS:O	1:B:122:HIS:ND1	2.42	0.49
1:B:1803:ILE:HG22	1:B:1807:ARG:HE	1.76	0.49
1:B:2409:GLU:OE1	1:B:2411:ASN:ND2	2.32	0.49
1:A:1971:ILE:HG23	1:A:1975:ILE:HD13	1.95	0.49
1:A:2250:LEU:HB2	1:A:2270:ILE:HG12	1.93	0.49
1:B:172:VAL:HA	1:B:175:HIS:HB2	1.93	0.49
1:A:1501:LEU:HD23	1:A:1515:PHE:CB	2.35	0.49
1:A:2606:VAL:HB	1:A:2618:LEU:HD23	1.92	0.49
1:A:945:PHE:HE2	1:A:997:ARG:HD2	1.78	0.49
1:B:1250:ARG:HB3	1:B:1252:LEU:HG	1.93	0.49
1:B:2045:THR:O	1:B:2222:SER:OG	2.29	0.49
1:B:97:GLN:OE1	1:B:148:ASN:ND2	2.45	0.49
1:B:151:ASN:O	1:B:154:PHE:HB3	2.13	0.49
1:A:505:LYS:O	1:A:509:CYS:N	2.34	0.49
1:A:1648:PHE:HA	1:A:1651:ASP:HB2	1.95	0.49
1:B:271:ILE:HD11	1:B:303:LEU:HD22	1.94	0.49
1:B:763:LEU:HD22	1:B:847:LEU:HD21	1.95	0.49
1:A:1040:LYS:HE2	1:A:1044:TYR:CZ	2.48	0.49
1:B:195:LYS:NZ	1:B:245:CYS:SG	2.79	0.49
1:A:2354:ASP:O	1:A:2358:GLY:N	2.36	0.49
1:B:1626:HIS:NE2	1:B:1766:GLU:OE1	2.45	0.49
1:B:1066:ARG:HB3	1:B:1137:ARG:HD3	1.95	0.49
1:A:1049:VAL:HG22	1:A:1073:MET:HE1	1.96	0.48
1:A:1095:LEU:HG	1:A:1099:LYS:HE2	1.95	0.48
1:A:1197:ALA:HB2	1:A:1597:ILE:HD11	1.95	0.48
1:B:1993:PHE:O	1:B:1997:SER:N	2.41	0.48
1:B:1115:ASN:O	1:B:1119:GLU:N	2.45	0.48
1:A:1621:VAL:HG22	1:A:1657:TYR:HB2	1.96	0.48
1:B:5:ARG:HB3	1:B:8:GLU:HG2	1.96	0.48
1:A:271:ILE:HG13	1:A:323:ALA:HB1	1.96	0.48
1:A:1237:ASP:OD1	1:A:1237:ASP:N	2.46	0.48
1:A:1445:ASP:HA	1:A:1448:LYS:HE3	1.95	0.48
1:B:1570:SER:O	1:B:1591:ARG:NH1	2.37	0.48
1:B:489:TYR:O	1:B:492:LEU:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1964:GLU:OE1	1:B:1967:MET:N	2.44	0.48
1:A:1209:VAL:HG13	1:A:1246:LEU:HD11	1.95	0.48
1:B:1606:VAL:HG11	1:B:1641:TRP:HZ3	1.78	0.48
1:B:1830:PRO:HB2	1:B:1901:LEU:HD21	1.95	0.48
1:A:1575:ALA:HB1	1:A:1704:LYS:HD3	1.95	0.47
1:A:2391:ILE:HA	1:A:2394:THR:HG22	1.96	0.47
1:A:1709:THR:HA	1:A:1712:LEU:HD12	1.96	0.47
1:A:2647:LEU:HD13	1:A:2656:LEU:HD21	1.94	0.47
1:A:2295:PHE:HZ	1:A:2369:LEU:HD21	1.79	0.47
1:B:750:THR:H	1:B:755:LEU:HD11	1.78	0.47
1:A:1645:PHE:HB2	1:A:1650:TYR:CZ	2.49	0.47
1:A:1682:SER:HB3	1:A:1685:LEU:HG	1.96	0.47
1:A:2378:ARG:NH2	1:A:2694:ALA:O	2.48	0.47
1:A:2667:VAL:HG11	1:B:6:PRO:HG2	1.96	0.47
1:B:527:THR:HA	1:B:530:VAL:HG12	1.96	0.47
1:B:1902:THR:HG22	1:B:1931:TRP:HE3	1.79	0.47
1:A:1614:TYR:O	1:A:1652:ASN:ND2	2.42	0.47
1:A:2414:SER:HA	1:A:2417:TYR:HD2	1.79	0.47
1:B:498:LYS:HD2	1:B:544:GLU:OE1	2.14	0.47
1:A:1211:LEU:HD22	1:A:1521:LEU:HD22	1.95	0.47
1:A:1540:SER:CB	1:A:1543:LEU:HD12	2.42	0.47
1:A:2157:PHE:HB2	1:B:1846:PRO:HG3	1.96	0.47
1:B:351:VAL:HB	1:B:355:ASN:HB2	1.95	0.47
1:B:594:THR:HG22	1:B:702:ALA:HB2	1.96	0.47
1:B:905:ASN:HD22	1:B:914:ARG:HD3	1.80	0.47
1:B:930:TYR:HE1	1:B:971:LEU:HD22	1.80	0.47
1:B:1866:LYS:O	1:B:1897:ASN:ND2	2.46	0.47
1:B:1910:ILE:HG21	1:B:1956:LYS:HB3	1.96	0.47
1:B:142:LEU:HD23	1:B:145:LEU:HD12	1.97	0.47
1:B:1085:LEU:HD23	1:B:1156:ASN:HD21	1.80	0.47
1:A:1551:PHE:HE2	2:A:2901:GSP:O3'	1.97	0.47
1:A:1247:PHE:O	1:A:1252:LEU:N	2.44	0.47
1:A:1513:ARG:N	1:A:1514:PRO:CD	2.75	0.47
1:A:1721:ASN:HB3	1:A:1793:HIS:CE1	2.50	0.47
1:A:2084:HIS:HB2	1:A:2208:TRP:HZ3	1.79	0.47
1:B:1067:ASP:OD1	1:B:1137:ARG:NH1	2.40	0.47
1:B:197:THR:HG21	1:B:216:LEU:HD21	1.96	0.46
1:B:2193:GLU:HA	1:B:2196:MET:HG2	1.96	0.46
1:B:60:THR:O	1:B:64:ASN:ND2	2.48	0.46
1:B:895:MET:HE3	1:B:898:LEU:HD12	1.97	0.46
1:B:1250:ARG:N	1:B:1611:LYS:HD3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:ILE:HG22	1:A:609:LYS:HE3	1.97	0.46
1:B:1712:LEU:O	1:B:1742:GLN:NE2	2.42	0.46
1:B:2336:GLU:HG3	1:B:2365:PHE:CD2	2.50	0.46
1:B:2347:GLU:O	1:B:2351:LYS:N	2.48	0.46
1:B:2400:ASN:HD22	1:B:2407:LYS:HA	1.80	0.46
1:B:1238:GLU:O	1:B:1242:VAL:N	2.46	0.46
1:B:1770:ILE:HG21	1:B:1804:ILE:HD11	1.96	0.46
1:A:2225:PRO:HB3	1:A:2269:LEU:HD23	1.98	0.46
1:A:2304:LEU:HD22	1:A:2703:ILE:HG23	1.98	0.46
1:A:2314:THR:OG1	1:A:2387:ARG:NH1	2.36	0.46
1:B:1005:MET:H	1:B:1008:ALA:HB3	1.80	0.46
1:B:1080:LEU:HD23	1:B:1152:LEU:HD13	1.98	0.46
1:B:1943:ASP:HB3	1:B:1946:LYS:NZ	2.30	0.46
1:A:2132:LEU:HD21	1:B:1874:THR:HG23	1.97	0.46
1:B:1117:CYS:HA	1:B:1138:LEU:HD22	1.97	0.46
1:B:162:GLN:OE1	1:B:200:LYS:HD3	2.16	0.46
1:B:769:PRO:HA	1:B:850:VAL:HG12	1.97	0.46
1:B:1932:LEU:HD23	1:B:1979:LEU:HD21	1.98	0.46
1:B:2244:LYS:HE3	1:B:2722:LEU:HB2	1.96	0.46
1:A:2374:LEU:HD22	1:A:2605:LEU:HD21	1.97	0.46
1:B:918:LYS:O	1:B:922:GLY:N	2.49	0.46
1:A:1045:LEU:HD23	1:A:1045:LEU:HA	1.81	0.46
1:A:1582:ASN:HB3	1:A:1618:TYR:HA	1.98	0.46
1:A:1207:ARG:HG3	1:A:1521:LEU:HD21	1.98	0.46
1:A:2644:ILE:HG23	1:A:2660:ILE:HG23	1.97	0.46
1:B:248:LYS:HB2	1:B:248:LYS:HE3	1.83	0.46
1:A:186:ASP:HB3	1:A:189:LYS:HG3	1.98	0.45
1:A:707:MET:HG3	1:A:741:PHE:HD1	1.81	0.45
1:A:1399:SER:HB3	1:A:1402:GLU:HB2	1.97	0.45
1:B:121:LEU:HB3	1:B:134:LEU:HD21	1.97	0.45
1:B:1355:SER:OG	1:B:1356:GLU:OE1	2.31	0.45
1:A:1597:ILE:HG23	1:A:1601:LEU:HD23	1.98	0.45
1:A:596:ILE:O	1:A:599:TRP:HB3	2.16	0.45
1:A:1538:TRP:HZ3	1:A:1548:PHE:CA	2.29	0.45
1:B:2316:LEU:HD12	1:B:2319:GLN:HE21	1.81	0.45
1:A:1538:TRP:CZ2	2:A:2901:GSP:C8	3.05	0.45
1:B:359:ASN:HD22	1:B:403:PRO:HD2	1.81	0.45
1:B:1779:THR:HG22	1:B:1790:THR:HG22	1.98	0.45
1:A:1443:PHE:HA	1:A:1446:PHE:HD2	1.81	0.45
1:B:491:TYR:O	1:B:494:LEU:HB3	2.16	0.45
1:B:944:PHE:HA	1:B:952:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1417:GLY:O	1:A:1421:MET:HG2	2.17	0.45
1:A:1724:LYS:HG3	1:A:1732:VAL:HG21	1.97	0.45
1:A:2634:PRO:HA	1:A:2637:HIS:HD1	1.82	0.45
1:B:168:SER:HA	1:B:205:LYS:HE2	1.99	0.45
1:B:974:ASN:OD1	1:B:1025:ARG:NH2	2.48	0.45
1:A:1611:LYS:HA	1:A:1614:TYR:CE2	2.51	0.45
1:A:2067:LEU:O	1:A:2073:LEU:HG	2.17	0.45
1:A:2281:GLN:HG3	1:A:2282:PRO:HD3	1.98	0.45
1:A:2643:LYS:HE3	1:A:2647:LEU:HD11	1.99	0.45
1:B:80:TYR:OH	1:B:133:GLU:OE2	2.25	0.45
1:A:48:LYS:HG3	1:A:99:LYS:HD3	1.98	0.45
1:A:546:MET:HE1	1:A:599:TRP:HB2	1.97	0.45
1:A:1347:PHE:O	1:A:1351:ILE:HG12	2.17	0.45
1:B:571:TRP:HZ2	1:B:611:LEU:HB2	1.82	0.45
1:B:918:LYS:HB2	1:B:963:GLN:NE2	2.31	0.45
1:B:992:MET:HA	1:B:995:LEU:HB2	1.98	0.45
1:B:1227:LEU:HD11	1:B:1489:LEU:HG	1.99	0.45
1:B:1569:LEU:HA	1:B:1605:HIS:CE1	2.52	0.45
1:A:1233:CYS:HA	1:A:1236:TRP:CD2	2.52	0.45
1:B:2643:LYS:HE3	1:B:2647:LEU:HD11	1.97	0.45
1:A:201:PHE:CE2	1:A:252:LEU:HD22	2.51	0.45
1:A:581:ILE:HG21	1:A:600:LEU:HD21	1.99	0.45
1:B:1572:PHE:O	1:B:1605:HIS:NE2	2.48	0.45
1:A:1009:ILE:HG21	1:A:1064:LEU:HB3	1.99	0.44
1:B:1688:ILE:HG21	1:B:1694:LEU:HB2	1.99	0.44
1:B:1176:ARG:HB3	1:B:1848:LEU:HD21	1.99	0.44
1:B:2253:ALA:HB2	1:B:2269:LEU:HD22	1.98	0.44
1:A:762:LEU:HD23	1:A:762:LEU:HA	1.82	0.44
1:A:1315:GLN:HB3	1:A:1317:VAL:HG13	1.99	0.44
1:A:1989:VAL:O	1:A:1992:SER:OG	2.30	0.44
1:B:400:GLN:NE2	1:B:445:GLU:OE1	2.48	0.44
1:B:490:LYS:H	1:B:490:LYS:HD2	1.82	0.44
1:B:1986:LEU:O	1:B:1989:VAL:HB	2.17	0.44
1:A:1512:ARG:HE	1:A:1512:ARG:HA	1.83	0.44
1:B:87:LEU:HD23	1:B:90:LEU:HD12	1.99	0.44
1:A:127:GLY:O	1:A:131:ALA:N	2.37	0.44
1:B:595:GLU:HA	1:B:598:LYS:HE3	1.99	0.44
1:B:1832:THR:HB	1:B:1908:GLU:HG2	2.00	0.44
1:A:197:THR:O	1:A:201:PHE:CB	2.43	0.44
1:B:2415:VAL:HG21	1:B:2589:LEU:HD11	1.98	0.44
1:A:1302:ASP:OD1	1:A:1303:PRO:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:781:HIS:HA	1:B:844:LEU:HD11	2.00	0.44
1:B:2066:MET:SD	1:B:2066:MET:N	2.91	0.44
1:A:354:LYS:O	1:A:358:PHE:N	2.50	0.44
1:A:1265:VAL:O	1:A:1375:ARG:NE	2.51	0.44
1:B:1688:ILE:HG13	1:B:1694:LEU:HD12	2.00	0.44
1:B:2242:GLN:O	1:B:2246:ILE:HG13	2.18	0.44
1:A:1357:PHE:CD2	1:A:1461:ILE:HD13	2.53	0.43
1:A:1433:LEU:HD21	1:A:1448:LYS:HB3	1.99	0.43
1:A:1634:LYS:HD2	1:A:1634:LYS:HA	1.80	0.43
1:A:2036:ILE:HD13	1:A:2056:ASP:HB3	2.00	0.43
1:B:694:PHE:HD2	1:B:702:ALA:HB1	1.82	0.43
1:B:1005:MET:O	1:B:1009:ILE:HG12	2.18	0.43
1:B:1073:MET:HA	1:B:1076:VAL:HB	1.99	0.43
1:B:1917:SER:O	1:B:1921:LYS:N	2.50	0.43
1:B:1957:LEU:HD12	1:B:1975:ILE:HD13	1.99	0.43
1:B:2133:THR:O	1:B:2136:SER:OG	2.29	0.43
1:A:1340:LEU:O	1:A:1343:THR:OG1	2.23	0.43
1:A:1566:LEU:HD13	1:A:1601:LEU:HB3	1.99	0.43
1:A:1629:PRO:O	1:A:1632:ARG:NH1	2.47	0.43
1:B:415:HIS:HD2	1:B:498:LYS:HB3	1.84	0.43
1:B:514:GLN:OE1	1:B:522:THR:OG1	2.31	0.43
1:B:549:LEU:HD23	1:B:552:LEU:HD12	2.00	0.43
1:B:975:HIS:H	1:B:1025:ARG:HH21	1.65	0.43
1:B:1902:THR:HG22	1:B:1931:TRP:CE3	2.53	0.43
1:A:2294:LEU:HA	1:A:2297:VAL:HG22	2.01	0.43
1:B:577:MET:HE3	1:B:577:MET:HB3	1.87	0.43
1:B:931:PRO:HG3	1:B:982:HIS:HA	1.99	0.43
1:B:273:LEU:HD23	1:B:276:LEU:HD12	2.01	0.43
1:B:969:LYS:HE3	1:B:1014:LYS:HD2	2.00	0.43
1:B:1073:MET:HG2	1:B:1113:LEU:HD11	2.01	0.43
1:A:1512:ARG:HA	1:A:1512:ARG:NE	2.34	0.43
1:A:2016:ALA:HB2	1:B:1882:ASN:ND2	2.34	0.43
1:B:1248:ASP:OD1	1:B:1292:TYR:OH	2.26	0.43
1:B:1297:LEU:HD23	1:B:1297:LEU:HA	1.86	0.43
1:B:2631:LYS:HD3	1:B:2631:LYS:HA	1.81	0.43
1:A:693:MET:HG3	1:A:696:TRP:HE1	1.84	0.43
1:A:945:PHE:CE2	1:A:997:ARG:HD2	2.54	0.43
1:A:1512:ARG:C	1:A:1514:PRO:HD2	2.38	0.43
1:A:1534:ALA:C	1:A:1596:GLN:HE21	2.22	0.43
1:A:1725:LEU:HB2	1:A:1790:THR:HB	2.01	0.43
1:A:1801:GLN:HA	1:A:1804:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1844:SER:O	1:A:1849:ARG:NH2	2.52	0.43
1:B:2129:ARG:HE	1:B:2129:ARG:HB2	1.70	0.43
1:B:2333:LYS:HA	1:B:2333:LYS:HD3	1.66	0.43
1:A:1544:THR:HB	1:A:1547:LYS:CG	2.33	0.42
1:B:143:PHE:HD1	1:B:184:ASN:HD21	1.67	0.42
1:B:968:MET:HB2	1:B:1018:LEU:HD11	2.01	0.42
1:A:263:LYS:O	1:A:266:VAL:HB	2.19	0.42
1:A:1793:HIS:CD2	1:A:1795:GLU:H	2.37	0.42
1:A:2634:PRO:HA	1:A:2637:HIS:ND1	2.34	0.42
1:B:111:LYS:HE2	1:B:152:ALA:HB3	2.01	0.42
1:B:2357:VAL:HG23	1:B:2359:LEU:H	1.84	0.42
1:A:573:ILE:HD12	1:A:573:ILE:HA	1.88	0.42
1:A:1481:GLY:HA3	1:A:1900:HIS:ND1	2.34	0.42
1:A:1540:SER:HA	1:A:1543:LEU:HG	2.01	0.42
1:B:414:LEU:O	1:B:418:ILE:HG12	2.19	0.42
1:B:1835:ASN:ND2	1:B:1905:PHE:O	2.40	0.42
1:A:1176:ARG:HE	1:A:1840:ASN:ND2	2.17	0.42
1:B:1146:VAL:HG22	1:B:1178:THR:HG23	2.01	0.42
1:B:1249:SER:HB2	1:B:1607:LEU:HD11	2.02	0.42
1:B:1345:LYS:HA	1:B:1345:LYS:HD3	1.80	0.42
1:B:1572:PHE:HA	1:B:1586:TYR:O	2.18	0.42
1:A:257:ALA:HB2	1:A:266:VAL:HG21	2.00	0.42
1:B:2714:LEU:HD23	1:B:2717:LEU:HD12	2.01	0.42
1:A:1596:GLN:HG2	1:A:1597:ILE:H	1.85	0.42
1:B:529:LEU:O	1:B:533:VAL:HG13	2.20	0.42
1:B:693:MET:HA	1:B:696:TRP:CD1	2.55	0.42
1:B:1837:ALA:HB2	1:B:1855:LEU:HD22	2.00	0.42
1:A:1491:TRP:CE3	1:A:1522:LEU:HD12	2.55	0.42
1:B:564:ASP:N	1:B:564:ASP:OD1	2.51	0.42
1:B:1638:LEU:HA	1:B:1641:TRP:HD1	1.85	0.42
1:A:2063:TYR:O	1:A:2067:LEU:HB2	2.19	0.42
1:A:2120:PHE:O	1:A:2125:LYS:NZ	2.49	0.42
1:A:2422:LEU:HD23	1:A:2422:LEU:HA	1.91	0.42
1:A:426:TRP:CD1	1:A:427:PRO:HD3	2.55	0.42
1:A:1153:LEU:HD12	1:A:1153:LEU:HA	1.85	0.42
1:A:1527:PRO:HB2	1:A:1528:PRO:CD	2.49	0.42
1:A:1596:GLN:HG2	1:A:1597:ILE:N	2.35	0.42
1:B:1141:LEU:O	1:B:1145:THR:OG1	2.31	0.42
1:B:1844:SER:O	1:B:1849:ARG:NH2	2.52	0.42
1:A:2118:LEU:HD23	1:A:2118:LEU:HA	1.87	0.42
1:B:901:LEU:HA	1:B:904:CYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1721:ASN:O	1:A:1793:HIS:ND1	2.52	0.41
1:A:1832:THR:O	1:A:1836:ILE:HG13	2.20	0.41
1:A:2257:CYS:HA	1:A:2263:THR:HG21	2.01	0.41
1:B:1725:LEU:HB2	1:B:1790:THR:OG1	2.20	0.41
1:A:398:LEU:HG	1:A:410:LEU:HD13	2.03	0.41
1:A:2336:GLU:HG3	1:A:2365:PHE:CD2	2.55	0.41
1:B:18:ASP:HA	1:B:21:LEU:HD12	2.01	0.41
1:B:140:GLY:O	1:B:143:PHE:HB3	2.19	0.41
1:B:490:LYS:O	1:B:493:LEU:HB2	2.19	0.41
1:B:1233:CYS:O	1:B:1236:TRP:HB2	2.19	0.41
1:B:1575:ALA:HB1	1:B:1704:LYS:HD2	2.01	0.41
1:A:1525:LEU:HD13	1:A:1525:LEU:HA	1.73	0.41
1:A:1585:PHE:HB2	1:A:1620:ILE:HG22	2.01	0.41
1:A:1626:HIS:NE2	1:A:1766:GLU:OE1	2.54	0.41
1:A:1721:ASN:HA	1:A:1731:LYS:HE2	2.03	0.41
1:B:146:SER:HA	1:B:150:PHE:HB3	2.02	0.41
1:B:578:LEU:HD21	1:B:687:LEU:HD12	2.03	0.41
1:B:2125:LYS:HB3	1:B:2129:ARG:HH21	1.83	0.41
1:B:2131:SER:HA	1:B:2134:GLU:HG2	2.03	0.41
1:A:173:ASP:HA	1:A:177:ILE:HG12	2.02	0.41
1:A:1592:PHE:O	1:A:1631:ASN:ND2	2.34	0.41
1:A:1855:LEU:HD23	1:A:1855:LEU:HA	1.91	0.41
1:B:150:PHE:O	1:B:153:VAL:HB	2.21	0.41
1:B:178:GLU:O	1:B:181:GLN:HG2	2.20	0.41
1:B:980:SER:HA	1:B:983:LEU:HB3	2.02	0.41
1:B:1176:ARG:O	1:B:1180:MET:HG2	2.21	0.41
1:B:1614:TYR:O	1:B:1652:ASN:ND2	2.49	0.41
1:B:1624:LEU:HD13	1:B:1665:VAL:HG11	2.02	0.41
1:A:1411:PRO:HA	1:A:1412:PRO:HD3	1.92	0.41
1:A:1716:LEU:HB3	1:A:1735:LYS:HB3	2.03	0.41
1:A:1890:ILE:HD13	1:A:1890:ILE:HA	1.89	0.41
1:B:20:GLN:HA	1:B:23:ILE:HD12	2.03	0.41
1:B:446:THR:HA	1:B:449:LYS:HD2	2.03	0.41
1:B:493:LEU:O	1:B:496:MET:HB2	2.20	0.41
1:B:1601:LEU:HD23	1:B:1601:LEU:HA	1.84	0.41
1:B:1150:SER:HB2	1:B:1185:LYS:HD2	2.01	0.41
1:A:1389:PHE:CD2	1:A:1429:ALA:HB2	2.56	0.41
1:A:1501:LEU:HD12	1:A:1501:LEU:HA	1.92	0.41
1:A:1516:ASP:O	1:A:1520:THR:HG23	2.21	0.41
1:A:2298:ALA:O	1:A:2302:LEU:N	2.52	0.41
1:A:946:ASP:OD1	1:A:947:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1146:VAL:HG13	1:A:1178:THR:HG23	2.02	0.41
1:A:1656:VAL:HB	1:A:1685:LEU:HD23	2.03	0.41
1:A:1721:ASN:HB3	1:A:1793:HIS:HE1	1.86	0.41
1:A:2344:ASN:HA	1:A:2347:GLU:HG2	2.03	0.41
1:B:5:ARG:HG3	1:B:7:VAL:H	1.86	0.41
1:B:213:ILE:HD13	1:B:266:VAL:HG12	2.03	0.41
1:B:340:SER:HA	1:B:343:PHE:HB3	2.03	0.41
1:B:604:LEU:HD11	1:B:687:LEU:HD11	2.03	0.41
1:B:1045:LEU:HA	1:B:1045:LEU:HD23	1.82	0.41
1:B:1856:LEU:O	1:B:1860:THR:HG23	2.21	0.41
1:B:2418:LEU:O	1:B:2422:LEU:HB2	2.21	0.41
1:A:911:LEU:O	1:A:914:ARG:HG2	2.20	0.41
1:A:1009:ILE:HG23	1:A:1068:LEU:HD12	2.02	0.41
1:A:1498:GLY:HA2	1:A:1515:PHE:CE1	2.55	0.41
1:A:1606:VAL:O	1:A:1610:LEU:HB3	2.21	0.41
1:A:1877:LEU:HD12	1:A:1877:LEU:HA	1.95	0.41
1:B:757:LYS:HD3	1:B:757:LYS:HA	1.75	0.41
1:B:2321:LEU:HD23	1:B:2321:LEU:HA	1.89	0.41
1:A:1093:VAL:HB	1:A:1097:GLU:HG2	2.03	0.40
1:A:1134:MET:HG3	1:A:1137:ARG:HD2	2.03	0.40
1:A:1614:TYR:CE1	1:A:1646:PRO:HG2	2.56	0.40
1:A:2334:SER:HB3	1:A:2402:HIS:CE1	2.56	0.40
1:B:1289:PHE:HD1	1:B:1361:LEU:HD22	1.86	0.40
1:B:2330:PHE:O	1:B:2401:LYS:NZ	2.45	0.40
1:A:510:ASN:OD1	1:A:511:PRO:HD2	2.21	0.40
1:B:526:ILE:HG22	1:B:577:MET:SD	2.61	0.40
1:A:108:MET:HA	1:A:111:LYS:HB3	2.03	0.40
1:A:611:LEU:HD22	1:A:719:ILE:HG22	2.01	0.40
1:A:1538:TRP:HE1	2:A:2901:GSP:H2'	1.86	0.40
1:B:1991:ASP:OD1	1:B:2032:ARG:NH1	2.54	0.40
1:B:2249:ILE:HG22	1:B:2269:LEU:HD21	2.03	0.40
1:A:1882:ASN:ND2	1:B:2016:ALA:HB2	2.37	0.40
1:A:2070:ASN:OD1	1:A:2070:ASN:N	2.55	0.40
1:A:2652:GLN:HE22	1:B:16:ARG:HH12	1.69	0.40
1:B:186:ASP:H	1:B:189:LYS:HB2	1.84	0.40
1:B:910:GLY:O	1:B:914:ARG:N	2.46	0.40
1:B:1571:ILE:HG12	1:B:1591:ARG:HB3	2.03	0.40
1:B:1648:PHE:HA	1:B:1651:ASP:HB2	2.03	0.40
1:A:1402:GLU:OE1	1:A:1402:GLU:N	2.53	0.40
1:A:2258:LEU:HD21	1:A:2707:ALA:HB3	2.03	0.40
1:B:55:ILE:HD13	1:B:58:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:889:THR:O	1:B:892:SER:OG	2.35	0.40
1:B:1170:HIS:HD1	1:B:1175:THR:HG1	1.67	0.40
1:B:1171:LYS:HE3	1:B:1171:LYS:HB2	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2298/2818 (82%)	2209 (96%)	88 (4%)	1 (0%)	100	100
1	B	2195/2818 (78%)	2128 (97%)	67 (3%)	0	100	100
All	All	4493/5636 (80%)	4337 (96%)	155 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	677	PRO

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	2085/2512 (83%)	2069 (99%)	16 (1%)	81	89
1	B	1982/2512 (79%)	1976 (100%)	6 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4067/5024 (81%)	4045 (100%)	22 (0%)	89 94

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ARG
1	A	262	ARG
1	A	277	CYS
1	A	1063	CYS
1	A	1408	LYS
1	A	1513	ARG
1	A	1520	THR
1	A	1521	LEU
1	A	1522	LEU
1	A	1525	LEU
1	A	1538	TRP
1	A	1543	LEU
1	A	1545	SER
1	A	1835	ASN
1	A	2139	LYS
1	A	2401	LYS
1	B	39	ASN
1	B	125	ARG
1	B	1039	ASN
1	B	1518	MET
1	B	2220	ASN
1	B	2401	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	GLN
1	A	553	HIS
1	A	2021	ASN
1	A	2400	ASN
1	A	2595	GLN
1	B	64	ASN
1	B	148	ASN
1	B	963	GLN
1	B	1394	ASN
1	B	1426	GLN

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Mol	Chain	Res	Type
1	B	1882	ASN
1	B	2050	GLN
1	B	2220	ASN

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)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GSP	A	2901	-	26,34,34	1.12	1 (3%)	28,54,54	2.33	4 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GSP	A	2901	-	-	2/17/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2901	GSP	C6-N1	3.72	1.39	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2901	GSP	C5-C6-N1	-9.03	111.08	123.43
2	A	2901	GSP	C2-N1-C6	6.04	125.53	115.93
2	A	2901	GSP	C2-N3-C4	-3.16	111.74	115.36
2	A	2901	GSP	N3-C2-N1	-2.70	123.62	127.22

There are no chirality outliers.

All (2) torsion outliers are listed below:

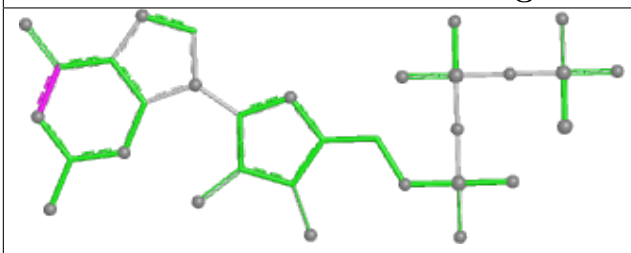
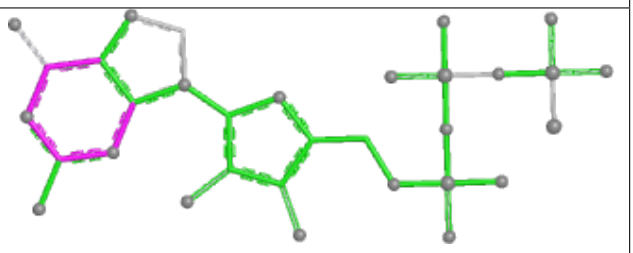
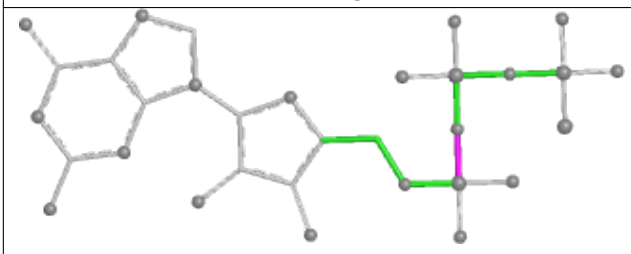
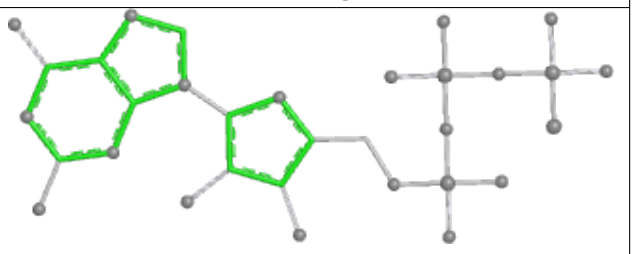
Mol	Chain	Res	Type	Atoms
2	A	2901	GSP	PB-O3A-PA-O2A
2	A	2901	GSP	PB-O3A-PA-O1A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2901	GSP	3	0

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

Ligand GSP A 2901	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

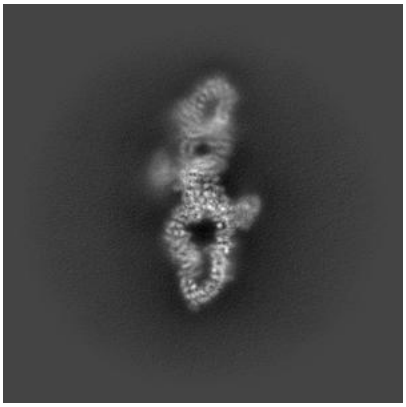
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14219. These allow visual inspection of the internal detail of the map and identification of artifacts.

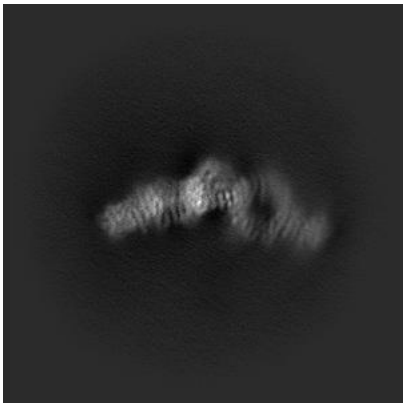
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

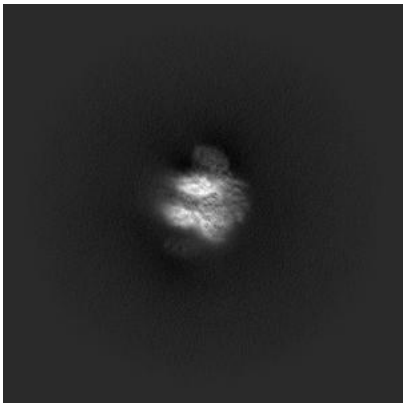
6.1.1 Primary map



X



Y

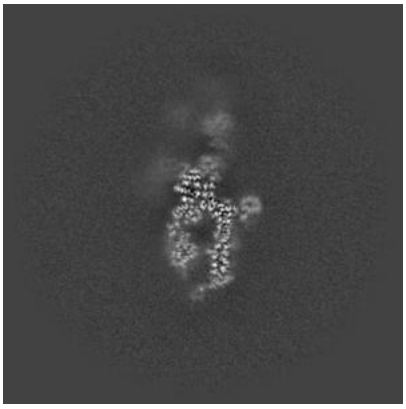


Z

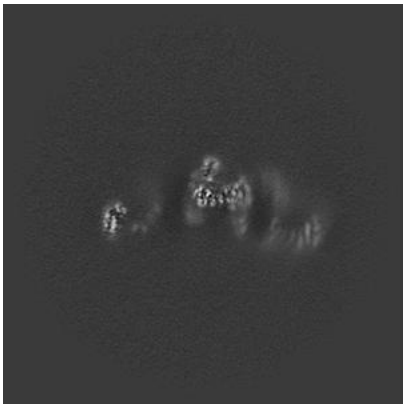
The images above show the map projected in three orthogonal directions.

6.2 Central slices

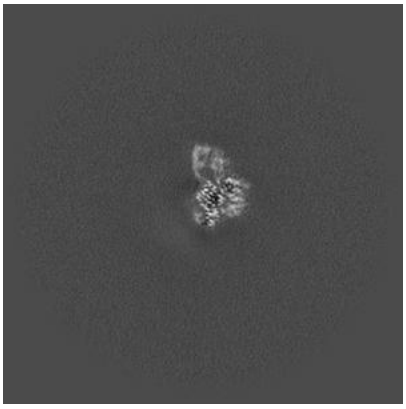
6.2.1 Primary map



X Index: 256



Y Index: 256

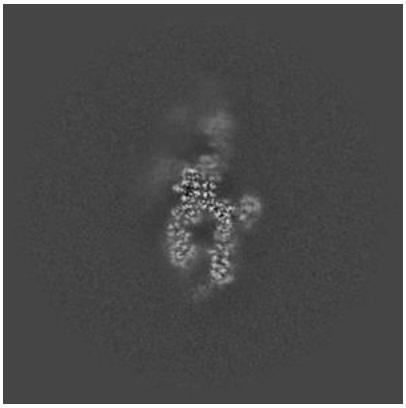


Z Index: 256

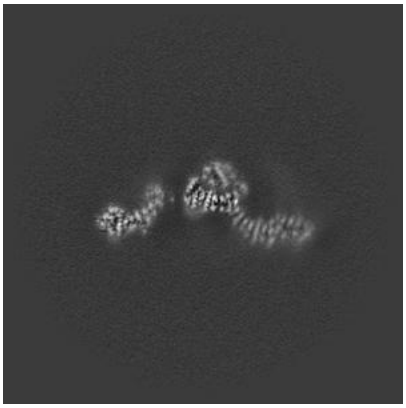
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

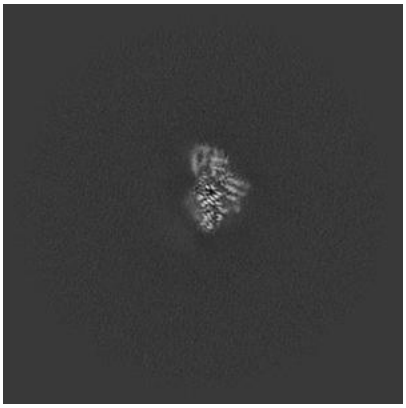
6.3.1 Primary map



X Index: 258



Y Index: 242



Z Index: 252

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

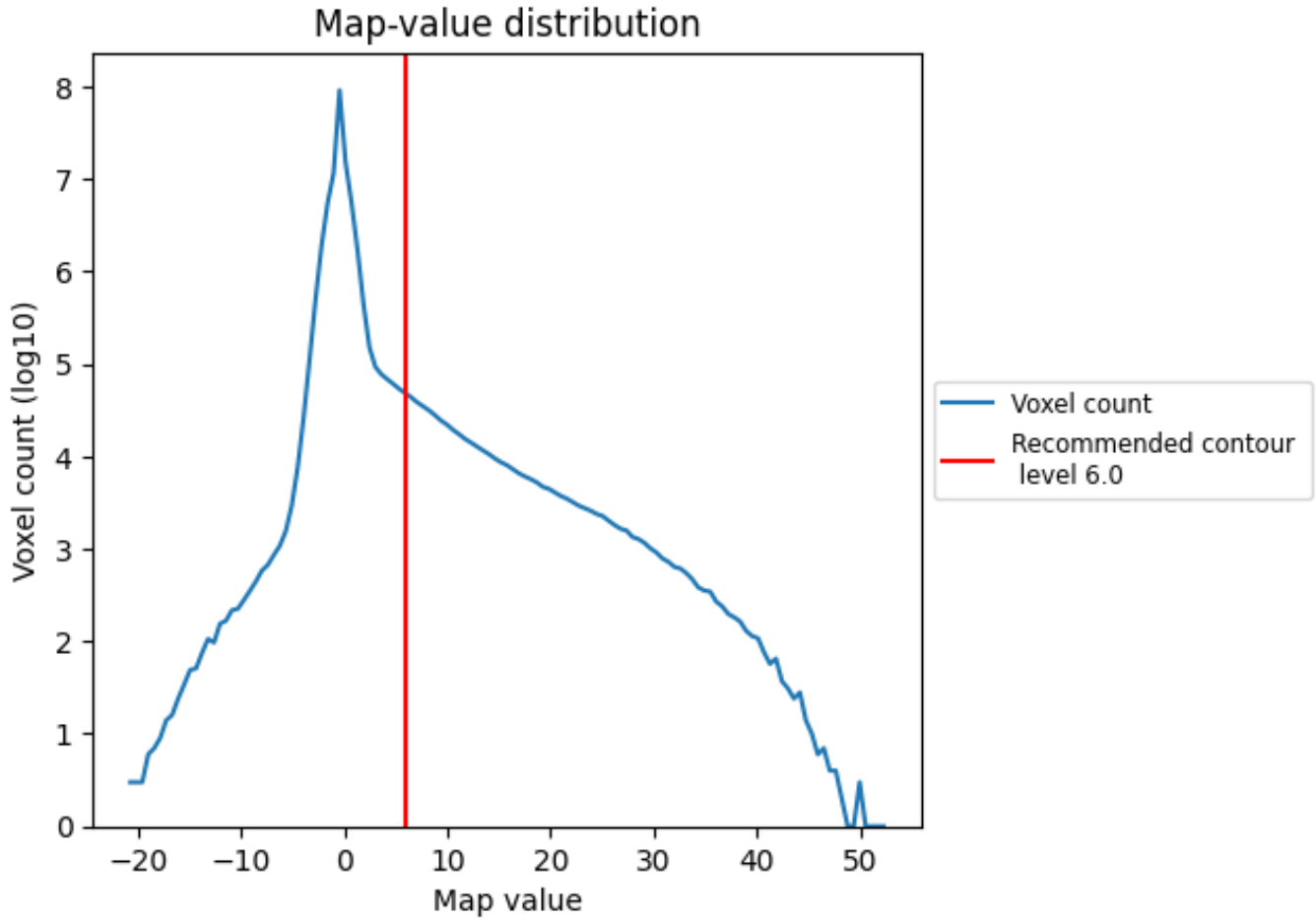
6.5 Mask visualisation (i)

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

7 Map analysis

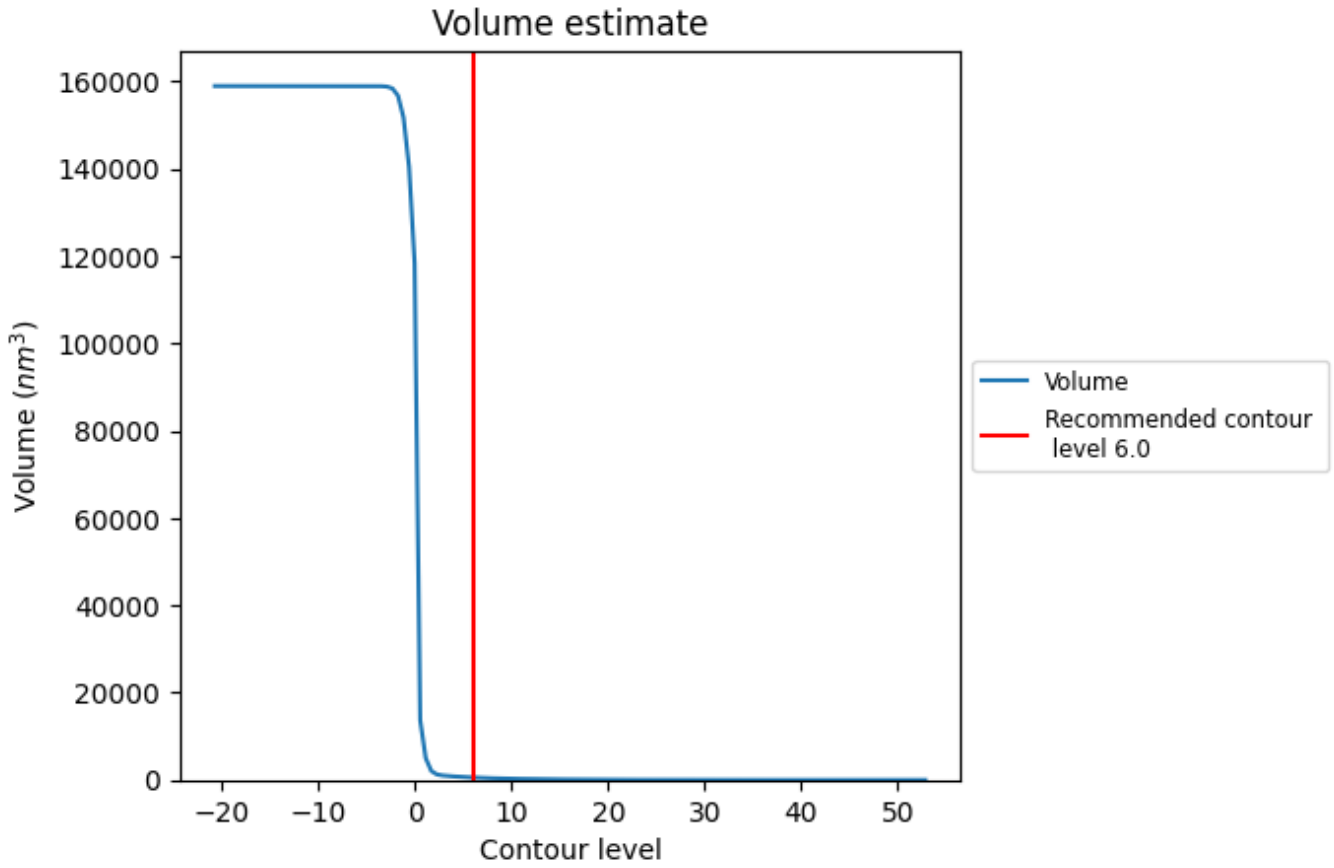
This section contains the results of statistical analysis of the map.

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.

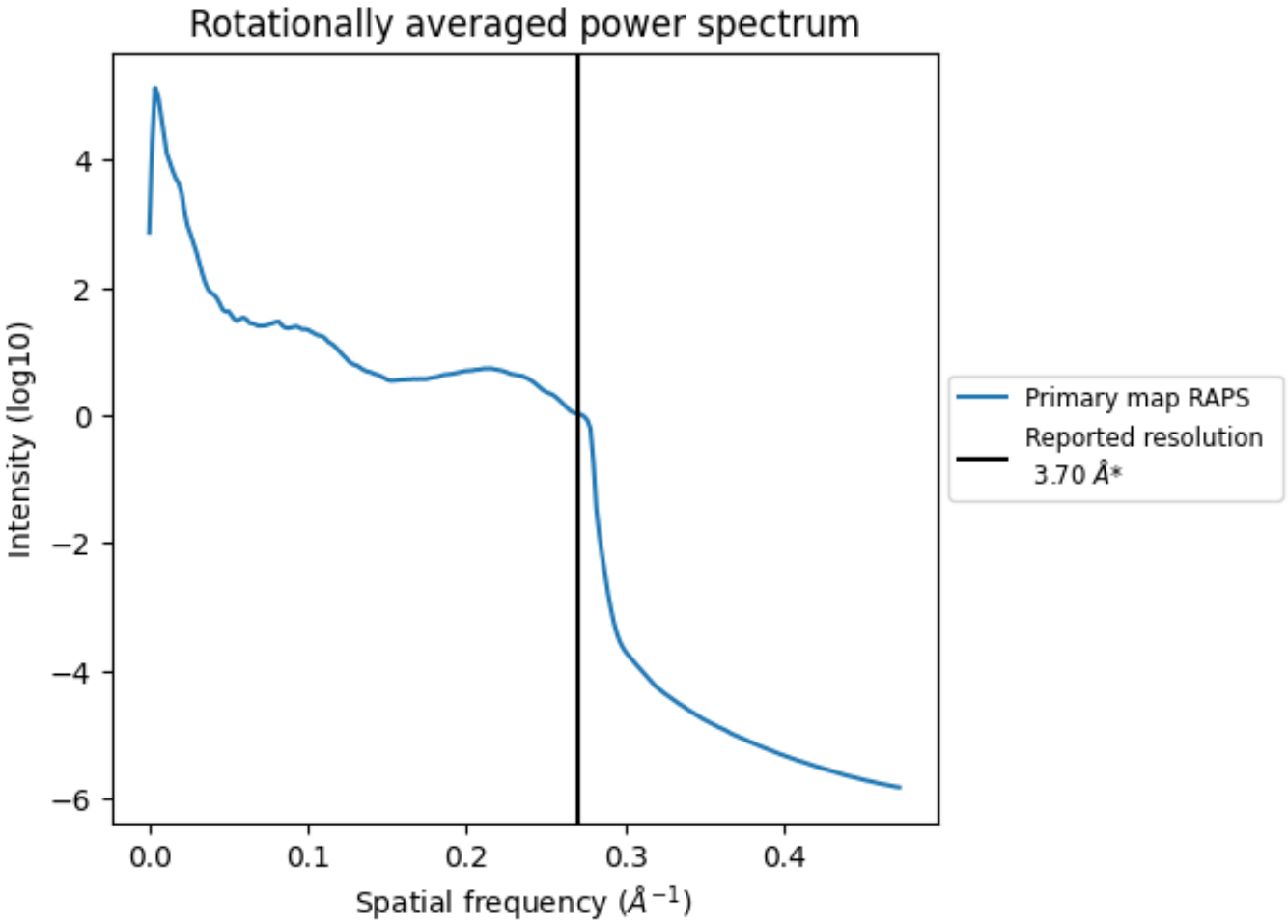
7.2 Volume estimate



The volume at the recommended contour level is 564 nm^3; this corresponds to an approximate mass of 510 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 0.270 Å^{-1}

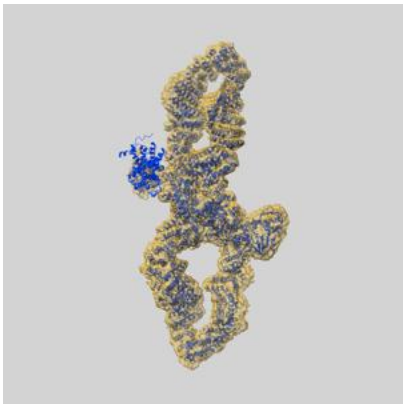
8 Fourier-Shell correlation (i)

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

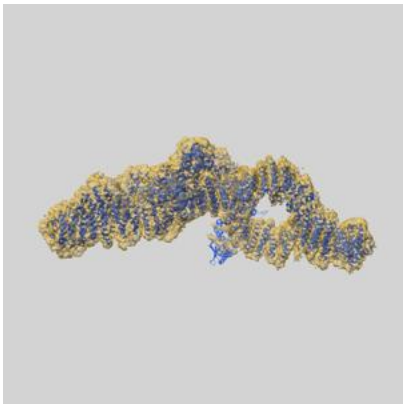
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14219 and PDB model 7R04. Per-residue inclusion information can be found in section 3 on page 4.

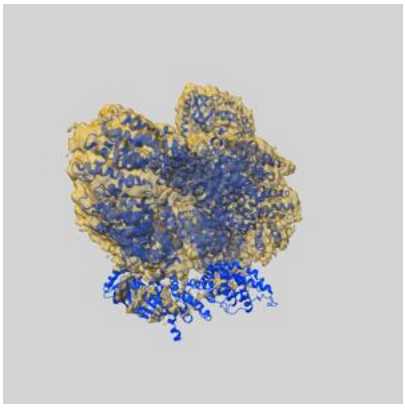
9.1 Map-model overlay



X



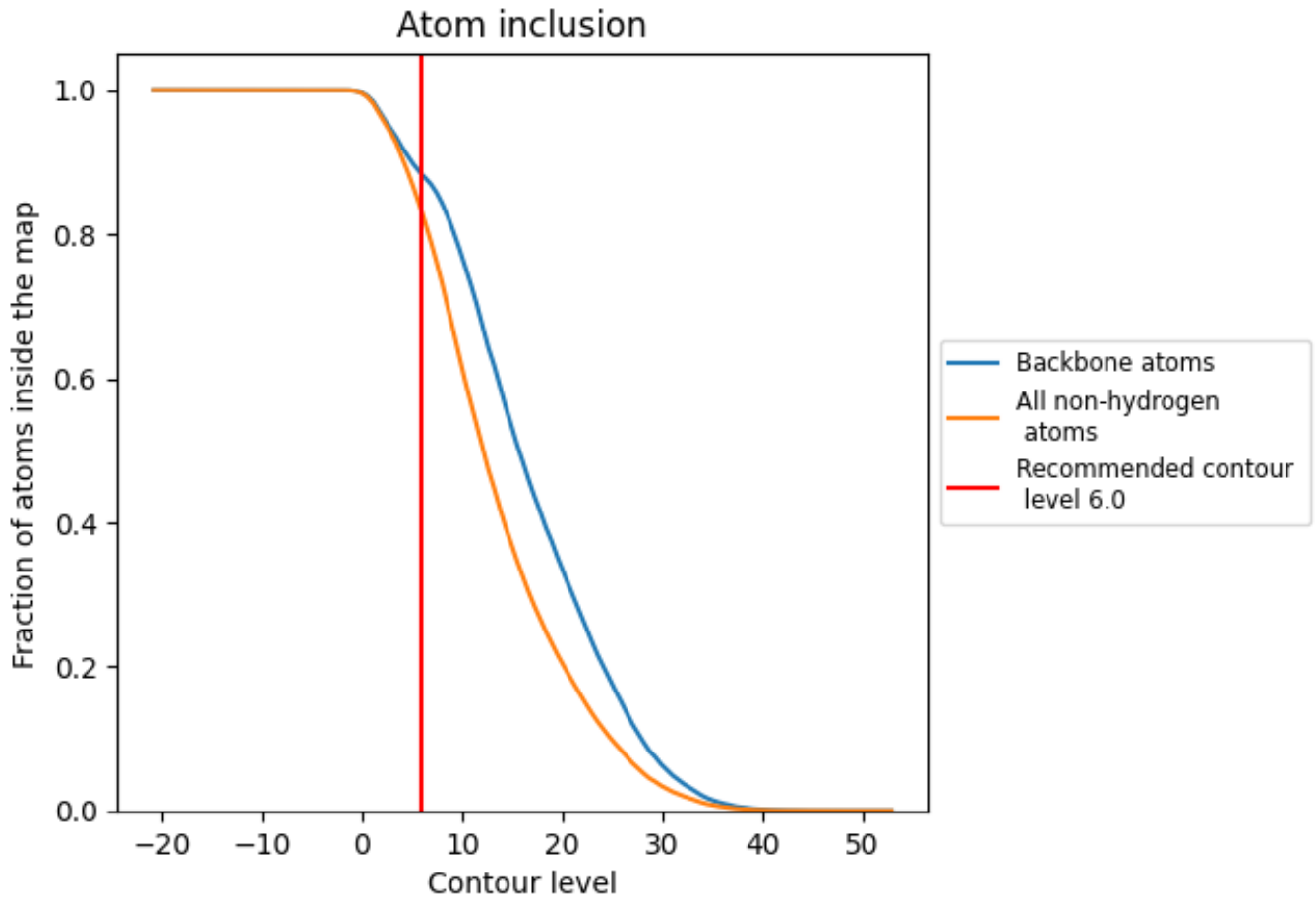
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0 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, 88% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.