Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 05:18 pm GMT

PDB ID	:	6ZH6
EMDB ID	:	EMD-11215
Title	:	Cryo-EM structure of DNA-PKcs:Ku80ct194
Authors	:	Chaplin, A.K.; Hardwick, S.W.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on	:	2020-06-21
Resolution	:	3.93 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

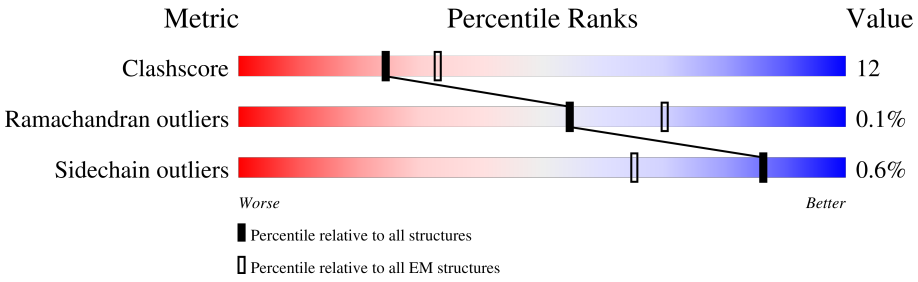
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.93 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	4156	65% 23% 11%
2	B	192	6% 93%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 29201 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-dependent protein kinase catalytic subunit,DNA-PKcs.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3692	29138	18697	4938	5311	192	0	0

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

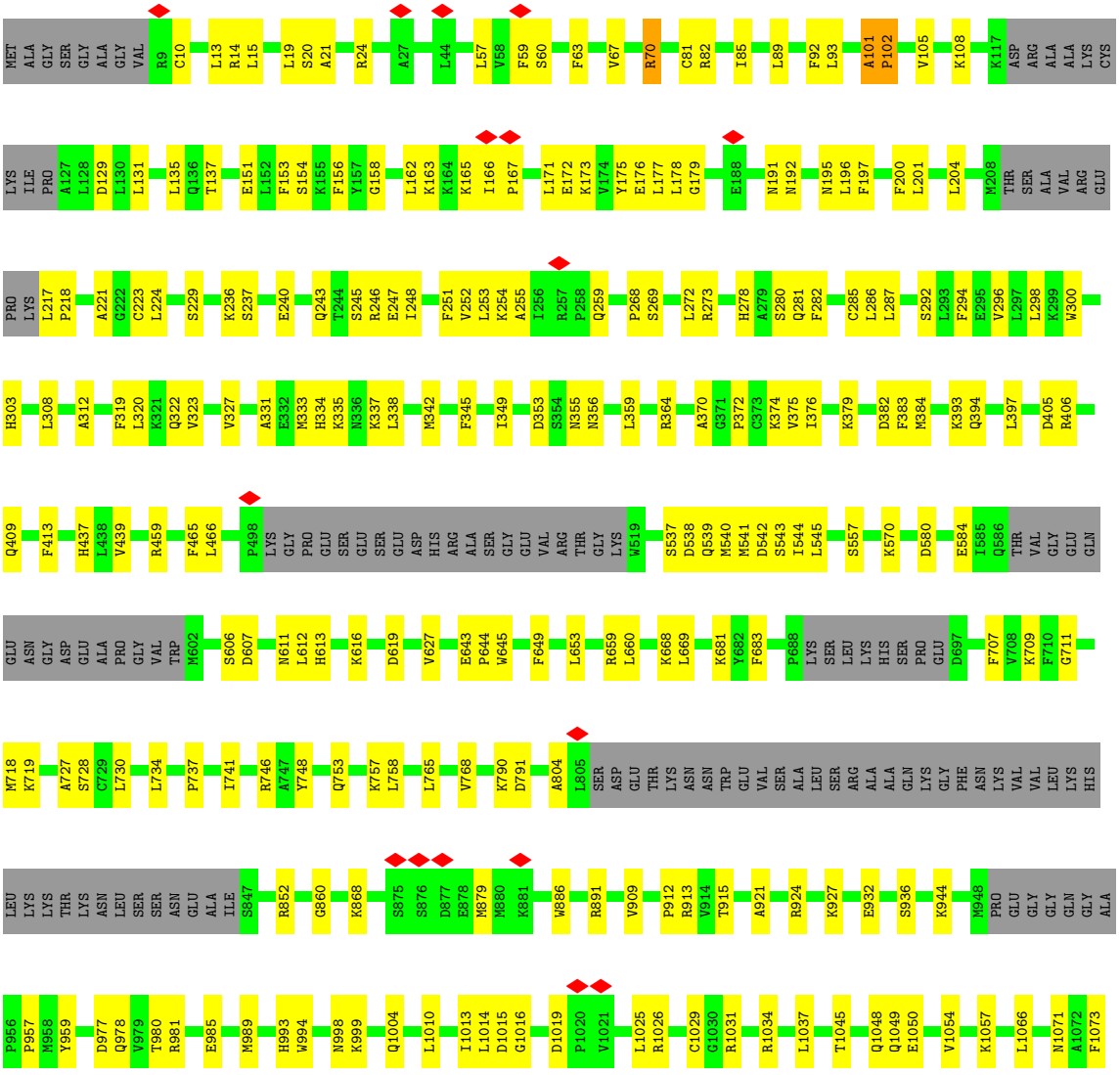
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	13	63	37	13	13	0	0

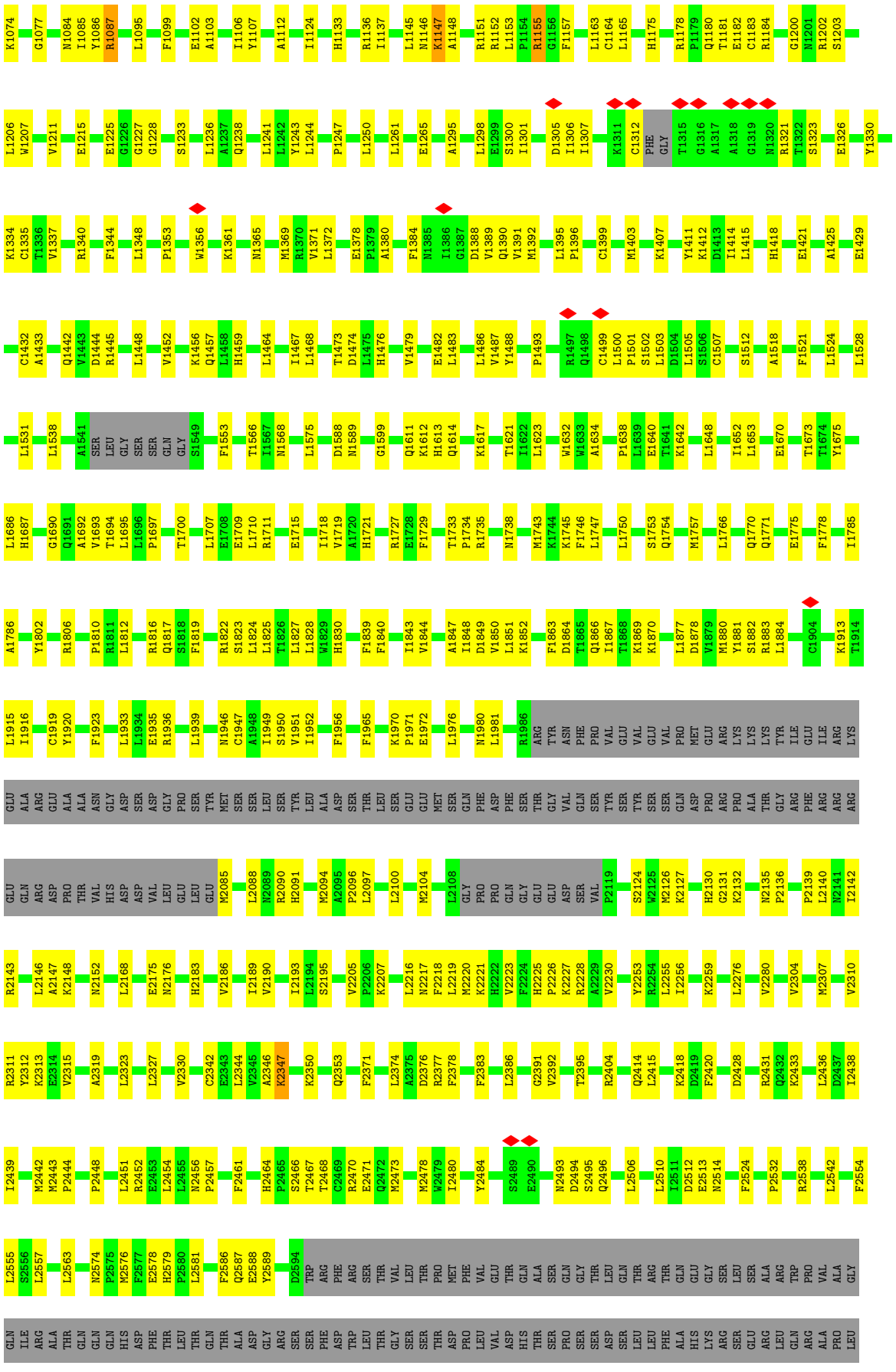
3 Residue-property plots (i)

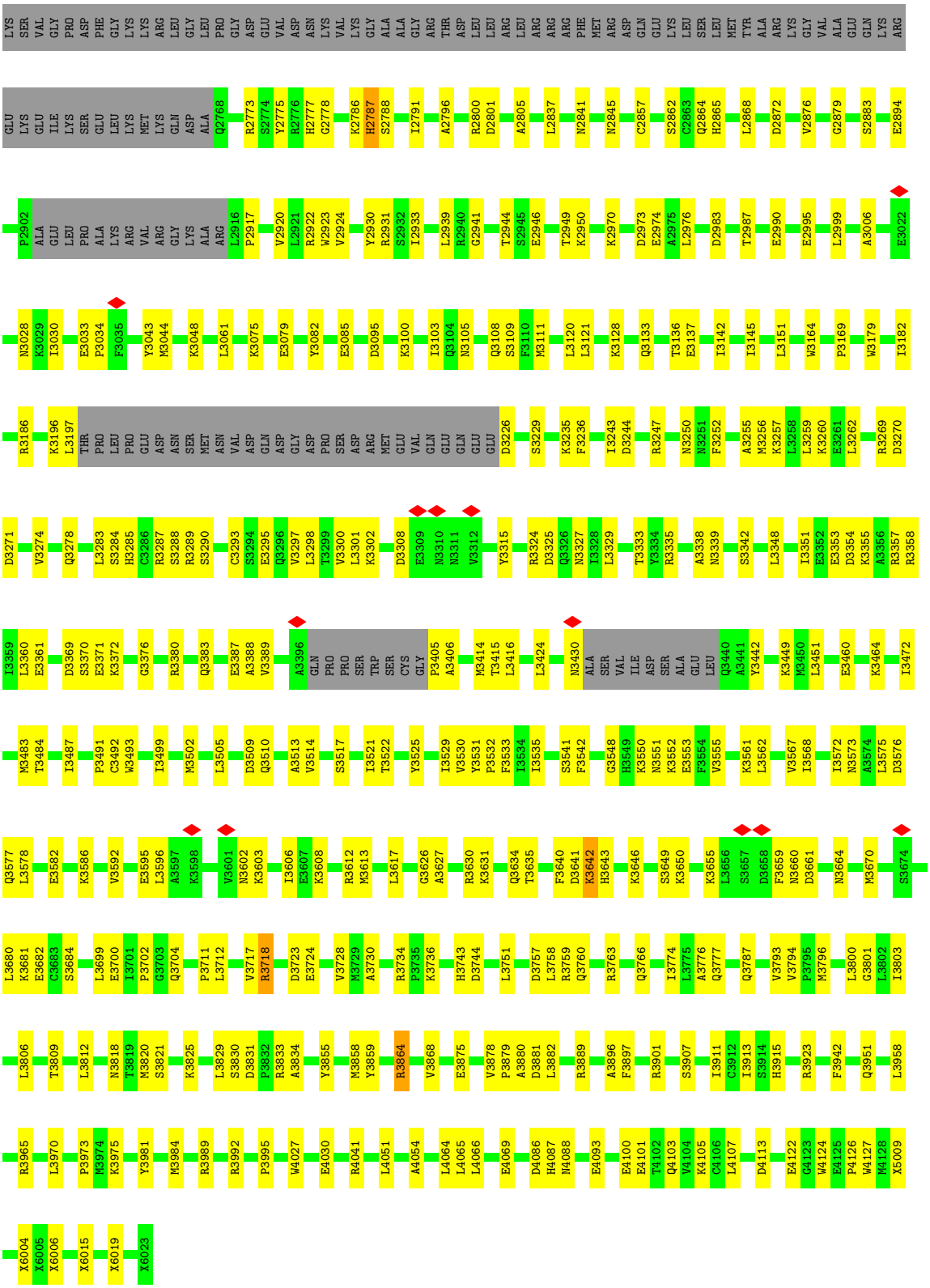
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:

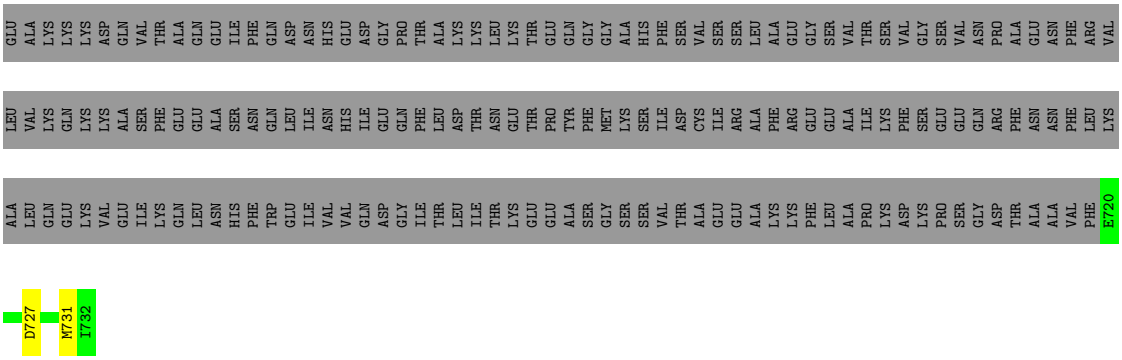



K1074 G1077 N1084 I1085 Y1086 R1087 L1095 F1099 E1102 A1103 I1106 Y1107 A1112 I1124 H1133 R1136 I1137 L1145 N1146 K1147 A1148 R1151 R1152 L1153 P1154 R1155 G1156 F1157 L1163 C1164 L1165 H1175 R1178 P1179 Q1180 T1181 E1182 C1183 R1184 G1200 N1201 R1202 S1203
L1206 W1207 V1211 E1215 E1225 G1226 G1227 G1228 S1233 L1236 A1237 Q1238 L1241 L1242 Y1243 L1244 P1247 L1250 L1261 E1265 A1295 L1298 E1299 S1300 I1301 D1305 I1306 I1307 K1311 C1312 PHE GLY T1315 G1316 A1317 A1318 G1319 N1320 R1321 T1322 S1323 E1326 Y1330
K1334 C1335 T1336 V1337 R1340 F1344 L1348 P1353 W1356 K1361 N1365 M1369 R1370 V1371 L1372 E1378 P1379 A1380 F1384 N1385 I1386 G1387 D1388 V1389 Q1390 V1391 M1392 L1395 P1396 C1399 M1403 K1407 Y1411 K1412 D1413 I1414 L1415 H1418 E1421 A1425 E1429
C1432 A1433 Q1442 V1443 D1444 R1445 L1448 V1452 K1456 Q1457 L1458 H1459 L1464 I1467 L1468 T1473 D1474 L1475 H1476 V1479 E1482 L1483 L1486 V1487 Y1488 P1493 R1497 Q1498 C1499 L1500 P1501 S1502 L1503 D1504 L1505 S1506 C1507 S1512 A1518 F1521 L1524 L1528
L1531 L1538 A1541 SER LEU GLY SER SER GLN GLY S1549 F1553 T1566 I1567 N1568 L1575 D1588 N1589 G1599 Q1611 K1612 H1613 Q1614 K1617 T1621 I1622 L1623 W1632 W1633 A1634 P1638 L1639 E1640 T1641 K1642 L1648 I1652 L1653 E1670 T1673 T1674 Y1675
L1686 H1687 G1690 Q1691 A1692 V1693 T1694 L1695 L1696 P1697 T1700 L1707 E1708 E1709 L1710 R1711 E1715 I1718 V1719 A1720 H1721 R1727 E1728 F1729 T1733 P1734 R1735 N1738 M1743 K1744 K1745 F1746 L1747 L1750 S1753 Q1754 M1757 L1766 Q1770 Q1771 E1775 F1778 I1785
A1786 Y1802 R1806 P1810 R1811 L1812 R1816 Q1817 S1818 F1819 R1822 S1823 L1824 L1825 T1826 L1827 L1828 W1829 H1830 F1839 F1840 I1843 V1844 A1847 I1848 D1849 V1850 L1851 K1852 F1863 D1864 T1865 Q1866 I1867 T1868 K1869 K1870 L1877 D1878 V1879 M1880 Y1881 S1882 R1883 L1884 C1904 K1913 T1914
L1915 I1916 C1919 Y1920 F1923 L1933 L1934 E1935 R1936 L1939 N1946 C1947 A1948 I1949 S1950 V1951 I1952 F1956 F1965 K1970 P1971 E1972 L1976 N1980 L1981 R1986 ARG TYR ASN PHE PRO VAL GLU VAL GLU VAL PRO MET GLU ARG LYS LYS LYS TYR ILE GLU ILE ARG LYS
GLU ALA ARG GLU ALA ALA ASN GLY ASP SER ASP GLY PRO SER TYR MET SER SER LEU SER TYR LEU ALA ASP SER THR LEU SER GLU GLU MET SER GLN PHE ASP PHE SER THR GLY VAL GLN SER TYR SER TYR SER SER GLN ASP PRO ARG PRO ALA THR GLY ARG PHE ARG ARG ARG
GLU GLN ARG ASP PRO THR VAL HIS ASP ASP VAL LEU GLU LEU GLU M2085 L2088 N2089 R2090 H2091 M2094 A2095 P2096 L2097 L2100 M2104 L2108 GLY PRO PRO GLN GLY GLU GLU ASP SER VAL P2119 S2124 W2125 M2126 K2127 H2130 G2131 K2132 N2135 P2136 P2139 L2140 N2141 I2142
R2143 L2146 A2147 K2148 N2152 L2168 E2175 N2176 H2183 V2186 I2189 V2190 I2193 L2194 S2195 V2205 P2206 K2207 L2216 N2217 F2218 L2219 M2220 K2221 H2222 V2223 F2224 H2225 P2226 K2227 R2228 A2229 V2230 Y2253 R2254 L2255 I2256 K2259 L2276 V2280 V2304 M2307 V2310
R2311 Y2312 K2313 E2314 V2315 A2319 L2323 L2327 V2330 C2342 E2343 L2344 V2345 A2346 K2347 K2350 Q2353 F2371 L2374 A2375 D2376 R2377 F2378 F2383 L2386 G2391 V2392 T2395 R2404 Q2414 L2415 K2418 D2419 F2420 D2428 R2431 Q2432 K2433 L2436 D2437 I2438
I2439 M2442 M2443 P2444 P2448 L2451 R2452 E2453 L2454 L2455 N2456 P2457 F2461 H2464 P2465 S2466 T2467 T2468 C2469 R2470 E2471 Q2472 M2473 M2478 W2479 I2480 Y2484 S2489 E2490 N2493 D2494 S2495 Q2496 L2506 L2510 I2511 D2512 E2513 N2514 F2524 P2532 R2538 L2542 F2554
L2555 S2556 L2557 L2563 N2574 P2575 M2576 F2577 E2578 H2579 P2580 L2581 F2586 Q2587 E2588 Y2589 E2594 TRP ARG PHE ARG SER THR VAL LEU THR PRO MET PHE VAL GLU THR GLN ALA SER GLN GLY THR LEU GLN THR ARG THR GLN GLU GLY SER LEU SER ARG GLU ARG LEU GLN ARG ALA PRO LEU
GLN ILE ARG ALA THR GLN GLN HIS ASP PHE THR LEU THR GLN THR ALA ASP GLY ARG SER SER PHE ASP TRP LEU THR GLY SER SER THR ASP PRO LEU VAL ASP HIS THR SER PRO SER SER ASP SER LEU LEU PHE ALA HIS LYS ARG SER GLU ARG LEU GLN ARG ALA PRO LEU



• Molecule 2: X-ray repair cross-complementing protein 5

Chain B: 6% 93%


GLU ALA LYS LYS LYS ASP GLN VAL THR ALA GLN GLU ILE PHE GLN ASP ASN HIS GLU ASP GLY PRO THR ALA LYS LYS LEU LYS THR GLU GLN GLY GLY ALA HIS PHE SER VAL SER SER LEU ALA GLU GLY SER VAL THR SER VAL GLY SER VAL ASN PRO ALA GLU ASN PHE ARG VAL
LEU VAL LYS GLN LYS LYS ALA SER PHE GLU GLU ALA SER ASN GLN LEU ILE ASN HIS ILE GLU GLN PHE LEU ASP THR ASN GLU THR PRO TYR PHE MET LYS SER ILE ASP CYS ILE ARG ALA PHE ARG GLU GLU ALA ILE LYS PHE SER GLU GLU GLN ARG PHE ASN ASN PHE LEU LYS
ALA LEU GLN GLU LYS VAL GLU ILE LYS GLN LEU ASN HIS PHE TRP GLU ILE VAL VAL GLN ASP GLY ILE THR LEU ILE THR LYS GLU GLU ALA SER GLY SER SER VAL THR ALA GLU GLU ALA LYS LYS PHE LEU ALA PRO LYS ASP LYS PRO SER GLY ASP THR ALA ALA VAL PHE E720
D727
M731
I732

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	43995	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 ($e^-/Å^2$)	54.49	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.504	Depositor
Minimum map value	-0.138	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.125	Depositor
Map size (Å)	336.64, 336.64, 336.64	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.27	0/29593	0.44	0/40028
2	B	0.25	0/62	0.36	0/84
All	All	0.27	0/29655	0.44	0/40112

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	29138	0	29130	658	0
2	B	63	0	27	1	0
All	All	29201	0	29157	659	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 12.

All (659) 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:1175:HIS:HB3	1:A:1178:ARG:HH21	1.41	0.85
1:A:1396:PRO:HB3	1:A:1457:GLN:HE22	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1178:ARG:NH1	1:A:1183:CYS:SG	2.55	0.80
1:A:166:ILE:HG13	1:A:167:PRO:HD3	1.64	0.79
1:A:3169:PRO:HG3	1:A:3182:ILE:HD11	1.64	0.79
1:A:3521:ILE:HG22	1:A:3529:ILE:HD11	1.66	0.78
1:A:2578:GLU:OE1	1:A:2579:HIS:ND1	2.17	0.77
1:A:3702:PRO:HB2	1:A:3794:VAL:HG11	1.66	0.76
1:A:251:PHE:HA	1:A:254:LYS:HG2	1.68	0.74
1:A:1151:ARG:NH1	1:A:1163:LEU:O	2.21	0.74
1:A:165:LYS:HB3	1:A:167:PRO:HD2	1.69	0.74
1:A:1445:ARG:HA	1:A:1448:LEU:HB3	1.70	0.73
1:A:3236:PHE:HE1	1:A:3262:LEU:HD21	1.52	0.73
1:A:3288:SER:O	1:A:3289:ARG:NH1	2.22	0.73
1:A:1479:VAL:HA	1:A:1482:GLU:HG3	1.69	0.73
1:A:734:LEU:HD11	1:A:768:VAL:HG12	1.69	0.72
1:A:3592:VAL:HA	1:A:3595:GLU:HG2	1.72	0.72
1:A:3655:LYS:HB2	1:A:3659:PHE:H	1.55	0.72
1:A:3596:LEU:HD22	1:A:3602:ASN:HB2	1.71	0.71
1:A:2148:LYS:HZ3	1:A:2152:ASN:HB3	1.56	0.71
1:A:253:LEU:HD13	1:A:268:PRO:HA	1.72	0.71
1:A:2796:ALA:O	1:A:2800:ARG:NH1	2.24	0.70
1:A:2091:HIS:HB3	1:A:2094:MET:HG2	1.74	0.70
1:A:616:LYS:HD3	1:A:6004:UNK:HA	1.74	0.69
1:A:1010:LEU:HA	1:A:1013:ILE:HG22	1.74	0.69
1:A:1295:ALA:HA	1:A:1298:LEU:HD12	1.76	0.68
1:A:2175:GLU:HG3	1:A:2176:ASN:H	1.57	0.68
1:A:1200:GLY:HA3	1:A:1202:ARG:HH21	1.59	0.68
1:A:3680:LEU:HD23	1:A:3682:GLU:H	1.59	0.68
1:A:2467:THR:HG21	1:A:2514:ASN:HD22	1.57	0.67
1:A:1653:LEU:HD12	1:A:1695:LEU:HD12	1.75	0.67
1:A:2131:GLY:O	1:A:2135:ASN:ND2	2.27	0.67
1:A:668:LYS:NZ	1:A:728:SER:OG	2.24	0.67
1:A:131:LEU:HD11	1:A:171:LEU:HG	1.77	0.67
1:A:236:LYS:O	1:A:246:ARG:NH1	2.28	0.67
1:A:977:ASP:OD1	1:A:978:GLN:N	2.29	0.66
1:A:333:MET:HG3	1:A:334:HIS:CD2	2.30	0.66
1:A:1952:ILE:HG23	1:A:1956:PHE:HB3	1.78	0.66
1:A:3369:ASP:HB3	1:A:3372:LYS:HD3	1.78	0.66
1:A:1864:ASP:HA	1:A:1867:ILE:HG12	1.77	0.66
1:A:2837:LEU:O	1:A:2841:ASN:ND2	2.29	0.65
1:A:3757:ASP:OD1	1:A:3758:LEU:N	2.30	0.65
1:A:1396:PRO:HB3	1:A:1457:GLN:NE2	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ASP:OD1	1:A:539:GLN:NE2	2.29	0.65
1:A:3626:GLY:HA3	1:A:3684:SER:HA	1.78	0.65
1:A:3760:GLN:NE2	1:A:3942:PHE:O	2.30	0.65
1:A:2922:ARG:HH11	1:A:2922:ARG:HG3	1.61	0.65
1:A:3006:ALA:HB3	1:A:3257:LYS:HE2	1.78	0.65
1:A:4086:ASP:OD1	1:A:4087:HIS:N	2.29	0.65
1:A:1049:GLN:OE1	1:A:1057:LYS:NZ	2.29	0.64
1:A:1444:ASP:OD1	1:A:1445:ARG:N	2.29	0.64
1:A:3529:ILE:HG22	1:A:3533:PHE:HB2	1.79	0.64
1:A:3493:TRP:CE2	1:A:3711:PRO:HG3	2.33	0.64
1:A:1568:ASN:ND2	1:A:1599:GLY:O	2.31	0.64
1:A:3776:ALA:HB2	1:A:3787:GLN:HE22	1.63	0.64
1:A:3613:MET:O	1:A:3617:LEU:N	2.27	0.64
1:A:1124:ILE:HD13	1:A:1182:GLU:HG3	1.79	0.63
1:A:1057:LYS:HG3	1:A:1152:ARG:HH22	1.62	0.63
1:A:3525:TYR:HE2	1:A:3712:LEU:HB2	1.63	0.63
1:A:753:GLN:NE2	1:A:791:ASP:O	2.32	0.63
1:A:172:GLU:HG2	1:A:223:CYS:HB3	1.79	0.63
1:A:924:ARG:NH1	1:A:977:ASP:OD2	2.23	0.63
1:A:1414:ILE:O	1:A:1418:HIS:ND1	2.28	0.62
1:A:1202:ARG:HH12	1:A:1207:TRP:HD1	1.47	0.62
1:A:3704:GLN:HE22	1:A:3717:VAL:HB	1.64	0.62
1:A:2391:GLY:O	1:A:2431:ARG:NH2	2.31	0.62
1:A:3164:TRP:O	1:A:3186:ARG:NH1	2.31	0.62
1:A:3923:ARG:O	1:A:4124:TRP:NE1	2.32	0.62
1:A:280:SER:HA	1:A:322:GLN:HE21	1.64	0.62
1:A:10:CYS:SG	1:A:14:ARG:NH1	2.72	0.62
1:A:2100:LEU:O	1:A:2104:MET:HG3	1.99	0.62
1:A:2217:ASN:OD1	1:A:2218:PHE:N	2.33	0.62
1:A:1265:GLU:HG2	1:A:1340:ARG:HH22	1.64	0.61
1:A:2987:THR:HG23	1:A:2990:GLU:H	1.64	0.61
1:A:3576:ASP:HB3	1:A:3800:LEU:HD12	1.82	0.61
1:A:135:LEU:HD11	1:A:176:GLU:HB3	1.81	0.61
1:A:3989:ARG:NH2	1:A:4101:GLU:OE2	2.33	0.61
1:A:254:LYS:HB3	1:A:296:VAL:HG11	1.81	0.61
1:A:1361:LYS:O	1:A:1365:ASN:N	2.32	0.61
1:A:229:SER:O	1:A:278:HIS:NE2	2.33	0.61
1:A:891:ARG:NH1	1:A:957:PRO:O	2.34	0.61
1:A:2135:ASN:O	1:A:2143:ARG:NH1	2.33	0.61
1:A:1840:PHE:HA	1:A:1843:ILE:HG22	1.82	0.61
1:A:2439:ILE:O	1:A:2443:MET:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3108:GLN:NE2	1:A:3111:MET:SD	2.73	0.60
1:A:1014:LEU:HD12	1:A:1025:LEU:HD21	1.84	0.60
1:A:879:MET:SD	1:A:879:MET:N	2.74	0.60
1:A:994:TRP:CE2	1:A:2581:LEU:HD13	2.37	0.60
1:A:1690:GLY:O	1:A:1693:VAL:HG12	2.01	0.60
1:A:1881:TYR:HD2	1:A:1951:VAL:HA	1.66	0.60
1:A:3699:LEU:O	1:A:3718:ARG:HB2	2.01	0.60
1:A:1825:LEU:HA	1:A:1828:LEU:HB2	1.82	0.59
1:A:3424:LEU:HD11	1:A:3442:TYR:HB3	1.85	0.59
1:A:3831:ASP:HB3	1:A:3834:ALA:HB2	1.82	0.59
1:A:1181:THR:HG22	1:A:1184:ARG:HH22	1.66	0.59
1:A:217:LEU:HD23	1:A:218:PRO:HD3	1.84	0.59
1:A:2466:SER:HB2	1:A:2468:THR:HG22	1.85	0.58
1:A:989:MET:O	1:A:993:HIS:ND1	2.29	0.58
1:A:2467:THR:OG1	1:A:2470:ARG:NH2	2.37	0.58
1:A:4088:ASN:ND2	1:A:4113:ASP:OD2	2.35	0.58
1:A:1389:VAL:HG13	1:A:1390:GLN:H	1.67	0.58
1:A:70:ARG:HG2	1:A:82:ARG:HB3	1.85	0.58
1:A:580:ASP:OD2	1:A:616:LYS:NZ	2.37	0.57
1:A:1770:GLN:HG3	1:A:1822:ARG:HH22	1.70	0.57
1:A:2143:ARG:O	1:A:2147:ALA:N	2.34	0.57
1:A:1575:LEU:H	1:A:1575:LEU:HD23	1.70	0.57
1:A:3829:LEU:HD12	1:A:3830:SER:HB3	1.86	0.57
1:A:978:GLN:OE1	1:A:981:ARG:NH2	2.38	0.57
1:A:2931:ARG:HH21	1:A:2939:LEU:HD21	1.69	0.57
1:A:286:LEU:HD23	1:A:319:PHE:HD1	1.70	0.56
1:A:1148:ALA:HB2	1:A:1164:CYS:HB2	1.87	0.56
1:A:1365:ASN:HD22	1:A:1411:TYR:HE1	1.53	0.56
1:A:3256:MET:O	1:A:3260:LYS:N	2.35	0.56
1:A:741:ILE:HG23	1:A:748:TYR:HD2	1.71	0.56
1:A:3525:TYR:CE2	1:A:3712:LEU:HB2	2.40	0.56
1:A:1473:THR:OG1	1:A:1474:ASP:N	2.39	0.56
1:A:1754:GLN:HA	1:A:1785:ILE:HD11	1.85	0.56
1:A:2225:HIS:CD2	1:A:2226:PRO:HD2	2.40	0.56
1:A:1949:ILE:HG23	1:A:2100:LEU:HD22	1.87	0.56
1:A:1976:LEU:HD23	1:A:2142:ILE:HD13	1.87	0.56
1:A:2576:MET:HB3	1:A:2787:HIS:NE2	2.20	0.56
1:A:1802:TYR:CZ	1:A:1806:ARG:HD3	2.41	0.56
1:A:3758:LEU:HD12	1:A:3801:GLY:HA3	1.88	0.56
1:A:3274:VAL:HG11	1:A:3315:TYR:CE2	2.41	0.56
1:A:1819:PHE:O	1:A:1823:SER:OG	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3335:ARG:O	1:A:3339:ASN:ND2	2.37	0.56
1:A:727:ALA:HA	1:A:765:LEU:HD11	1.88	0.55
1:A:1045:THR:HB	1:A:1048:GLN:HG2	1.86	0.55
1:A:1301:ILE:HD12	1:A:1371:VAL:HG21	1.89	0.55
1:A:1817:GLN:OE1	1:A:1936:ARG:NH2	2.36	0.55
1:A:1933:LEU:HB3	1:A:1936:ARG:HB2	1.88	0.55
1:A:248:ILE:HA	1:A:251:PHE:CE2	2.41	0.55
1:A:1203:SER:HB2	1:A:1206:LEU:HD13	1.87	0.55
1:A:3383:GLN:O	1:A:3387:GLU:N	2.36	0.55
1:A:3244:ASP:OD1	1:A:3247:ARG:NH1	2.33	0.55
1:A:131:LEU:HD21	1:A:171:LEU:HA	1.88	0.55
1:A:1512:SER:HB2	1:A:1566:THR:HG21	1.88	0.55
1:A:1882:SER:O	1:A:1883:ARG:HG2	2.06	0.55
1:A:2216:LEU:HA	1:A:2219:LEU:HB2	1.87	0.55
1:A:1634:ALA:O	1:A:1642:LYS:NZ	2.39	0.55
1:A:1623:LEU:HD21	1:A:1652:ILE:HG21	1.88	0.55
1:A:3151:LEU:HD21	1:A:3197:LEU:HB2	1.89	0.55
1:A:3484:THR:HA	1:A:3487:ILE:HG22	1.88	0.55
1:A:3879:PRO:HB2	1:A:3882:LEU:HG	1.89	0.55
1:A:3048:LYS:HE2	1:A:3061:LEU:HD21	1.89	0.55
1:A:3100:LYS:HD3	1:A:3142:ILE:HG21	1.89	0.55
1:A:89:LEU:HA	1:A:92:PHE:HB3	1.88	0.54
1:A:1155:ARG:HG2	1:A:1155:ARG:HH11	1.72	0.54
1:A:2126:MET:O	1:A:2130:HIS:N	2.40	0.54
1:A:3243:ILE:HD13	1:A:3259:LEU:HD13	1.90	0.54
1:A:1479:VAL:HG11	1:A:1518:ALA:HA	1.89	0.54
1:A:3627:ALA:HA	1:A:3630:ARG:HG2	1.90	0.54
1:A:1369:MET:HA	1:A:1372:LEU:HB3	1.89	0.54
1:A:2310:VAL:HG12	1:A:2311:ARG:N	2.23	0.54
1:A:3818:ASN:O	1:A:3889:ARG:NH2	2.38	0.54
1:A:1211:VAL:O	1:A:1215:GLU:HG3	2.08	0.54
1:A:1482:GLU:HA	1:A:1486:LEU:HD23	1.90	0.54
1:A:2999:LEU:HD13	1:A:3043:TYR:HD2	1.72	0.54
1:A:21:ALA:HA	1:A:24:ARG:HD2	1.90	0.54
1:A:281:GLN:N	1:A:281:GLN:OE1	2.41	0.54
1:A:3793:VAL:HG22	1:A:3803:ILE:HG22	1.90	0.54
1:A:3120:LEU:HD12	1:A:3896:ALA:HA	1.89	0.54
1:A:334:HIS:O	1:A:338:LEU:N	2.36	0.54
1:A:1407:LYS:HA	1:A:1412:LYS:HD3	1.90	0.54
1:A:718:MET:SD	1:A:719:LYS:HD3	2.47	0.53
1:A:3530:VAL:HA	1:A:3562:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1733:THR:HG22	1:A:1735:ARG:H	1.72	0.53
1:A:2227:LYS:HB2	1:A:2230:VAL:HG22	1.90	0.53
1:A:3718:ARG:HD3	1:A:3743:HIS:ND1	2.23	0.53
1:A:364:ARG:HG3	1:A:364:ARG:HH11	1.73	0.53
1:A:921:ALA:HB3	1:A:927:LYS:HB2	1.91	0.53
1:A:2786:LYS:O	1:A:2788:SER:N	2.41	0.53
1:A:308:LEU:O	1:A:312:ALA:N	2.38	0.53
1:A:2538:ARG:O	1:A:2542:LEU:N	2.42	0.53
1:A:154:SER:O	1:A:158:GLY:N	2.33	0.53
1:A:1442:GLN:HA	1:A:1445:ARG:NH1	2.23	0.53
1:A:3606:ILE:HD11	1:A:3608:LYS:HB3	1.89	0.53
1:A:397:LEU:HD11	1:A:437:HIS:HB3	1.89	0.53
1:A:542:ASP:OD1	1:A:543:SER:N	2.42	0.53
1:A:653:LEU:HD11	1:A:669:LEU:HG	1.89	0.53
1:A:60:SER:HA	1:A:63:PHE:HD2	1.74	0.53
1:A:466:LEU:HD11	1:A:557:SER:HB3	1.90	0.53
1:A:2168:LEU:HD22	1:A:2189:ILE:HD11	1.89	0.53
1:A:3348:LEU:HD23	1:A:3351:ILE:HD11	1.91	0.53
1:A:3640:PHE:HA	1:A:3643:HIS:HB3	1.89	0.53
1:A:3901:ARG:HG3	1:A:3970:LEU:HD11	1.90	0.53
1:A:1225:GLU:HB3	1:A:1236:LEU:HB2	1.91	0.53
1:A:1227:GLY:N	1:A:1233:SER:O	2.32	0.53
1:A:1575:LEU:HD21	1:A:1617:LYS:HE3	1.91	0.53
1:A:1843:ILE:O	1:A:1847:ALA:N	2.42	0.53
1:A:1972:GLU:HB3	1:A:2142:ILE:HD12	1.90	0.53
1:A:2327:LEU:HA	1:A:2330:VAL:HG12	1.91	0.53
1:A:3567:VAL:HG22	1:A:3699:LEU:HD21	1.91	0.53
1:A:1112:ALA:HB2	1:A:1178:ARG:HH11	1.74	0.52
1:A:3389:VAL:HG11	1:A:3416:LEU:HD22	1.91	0.52
1:A:394:GLN:NE2	1:A:1738:ASN:OD1	2.42	0.52
1:A:1200:GLY:HA3	1:A:1202:ARG:NH2	2.25	0.52
1:A:1686:LEU:O	1:A:1690:GLY:N	2.39	0.52
1:A:320:LEU:HA	1:A:323:VAL:HG12	1.90	0.52
1:A:538:ASP:OD1	1:A:538:ASP:N	2.42	0.52
1:A:3145:ILE:HD11	1:A:3196:LYS:HE2	1.92	0.52
1:A:959:TYR:HB2	1:A:1004:GLN:HG3	1.90	0.52
1:A:1828:LEU:O	1:A:1883:ARG:NH2	2.42	0.52
1:A:162:LEU:HD12	1:A:163:LYS:HG2	1.91	0.52
1:A:345:PHE:O	1:A:349:ILE:HG22	2.09	0.52
1:A:3717:VAL:HA	1:A:3743:HIS:CE1	2.44	0.52
1:A:243:GLN:O	1:A:246:ARG:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:PHE:O	1:A:711:GLY:N	2.39	0.52
1:A:913:ARG:NH1	1:A:2801:ASP:OD2	2.42	0.52
1:A:2470:ARG:NH1	1:A:2512:ASP:OD1	2.42	0.52
1:A:1727:ARG:HG3	1:A:1727:ARG:HH11	1.75	0.52
1:A:201:LEU:HA	1:A:204:LEU:HD12	1.91	0.52
1:A:537:SER:HA	1:A:540:MET:CE	2.40	0.52
1:A:382:ASP:OD1	1:A:383:PHE:N	2.42	0.52
1:A:977:ASP:HB3	1:A:980:THR:HB	1.92	0.51
1:A:192:ASN:HA	1:A:195:ASN:HD21	1.75	0.51
1:A:2439:ILE:HG22	1:A:2443:MET:HB3	1.91	0.51
1:A:3646:LYS:O	1:A:3650:LYS:N	2.40	0.51
1:A:1949:ILE:HD12	1:A:2100:LEU:HD22	1.92	0.51
1:A:3298:LEU:HA	1:A:3301:LEU:HD13	1.92	0.51
1:A:3460:GLU:OE2	1:A:3464:LYS:NZ	2.43	0.51
1:A:57:LEU:O	1:A:60:SER:OG	2.24	0.51
1:A:936:SER:OG	1:A:2773:ARG:NH1	2.44	0.51
1:A:1054:VAL:O	1:A:1054:VAL:HG12	2.10	0.51
1:A:1866:GLN:O	1:A:1870:LYS:N	2.42	0.51
1:A:370:ALA:O	1:A:374:LYS:N	2.40	0.51
1:A:998:ASN:OD1	1:A:999:LYS:N	2.43	0.51
1:A:1840:PHE:O	1:A:1844:VAL:HG13	2.11	0.51
1:A:2464:HIS:CE1	1:A:2466:SER:HB3	2.45	0.51
1:A:2139:PRO:HB2	1:A:2140:LEU:HD12	1.93	0.51
1:A:1675:TYR:OH	1:A:1692:ALA:O	2.20	0.51
1:A:2136:PRO:HA	1:A:2143:ARG:HH12	1.75	0.51
1:A:3370:SER:OG	1:A:3371:GLU:OE1	2.28	0.51
1:A:4093:GLU:OE1	1:A:4093:GLU:N	2.44	0.51
1:A:2415:LEU:HB3	1:A:2420:PHE:HB2	1.93	0.51
1:A:3535:ILE:HG21	1:A:3759:ARG:HD3	1.93	0.50
1:A:3550:LYS:HA	1:A:3553:GLU:HB2	1.93	0.50
1:A:4054:ALA:O	1:A:4103:GLN:NE2	2.41	0.50
1:A:2344:LEU:HD12	1:A:2347:LYS:HE3	1.93	0.50
1:A:1353:PRO:HB2	1:A:1356:TRP:HB3	1.93	0.50
1:A:2555:LEU:HD11	1:A:2857:CYS:SG	2.51	0.50
1:A:3880:ALA:HA	1:A:3965:ARG:HH22	1.77	0.50
1:A:1493:PRO:HD2	1:A:1500:LEU:HD12	1.94	0.50
1:A:1766:LEU:HD13	1:A:1778:PHE:HD2	1.77	0.50
1:A:3285:HIS:NE2	1:A:3333:THR:OG1	2.38	0.50
1:A:3075:LYS:O	1:A:3079:GLU:HG2	2.12	0.50
1:A:3951:GLN:HE22	1:A:4066:LEU:HB3	1.76	0.50
1:A:2148:LYS:O	1:A:2148:LYS:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3256:MET:CE	1:A:3287:ARG:HH21	2.25	0.50
1:A:3509:ASP:OD1	1:A:3509:ASP:N	2.43	0.50
1:A:3681:LYS:HE2	1:A:3681:LYS:HA	1.94	0.50
1:A:1015:ASP:HB2	1:A:1029:CYS:HB3	1.94	0.50
1:A:1016:GLY:HA3	1:A:1077:GLY:HA3	1.93	0.50
1:A:1482:GLU:O	1:A:1486:LEU:N	2.44	0.50
1:A:2513:GLU:OE1	1:A:2513:GLU:N	2.43	0.50
1:A:1670:GLU:O	1:A:1673:THR:OG1	2.29	0.49
1:A:3354:ASP:OD1	1:A:3355:LYS:N	2.45	0.49
1:A:3881:ASP:OD1	1:A:3881:ASP:N	2.45	0.49
1:A:4086:ASP:OD1	1:A:4087:HIS:ND1	2.45	0.49
1:A:1459:HIS:HB2	1:A:1464:LEU:HD22	1.94	0.49
1:A:1638:PRO:HB2	1:A:1640:GLU:HG3	1.93	0.49
1:A:3256:MET:HE3	1:A:3287:ARG:HH21	1.76	0.49
1:A:1389:VAL:HG13	1:A:1390:GLN:N	2.27	0.49
1:A:2862:SER:HB2	1:A:2868:LEU:O	2.12	0.49
1:A:3596:LEU:HD21	1:A:3603:LYS:HB2	1.95	0.49
1:A:3763:ARG:O	1:A:3766:GLN:HG2	2.12	0.49
1:A:1102:GLU:O	1:A:1106:ILE:HG12	2.12	0.49
1:A:1848:ILE:O	1:A:1852:LYS:N	2.45	0.49
1:A:2096:PRO:O	1:A:2100:LEU:N	2.39	0.49
1:A:2428:ASP:HB2	1:A:2431:ARG:HB3	1.94	0.49
1:A:2493:ASN:H	1:A:2496:GLN:HB2	1.76	0.49
1:A:1175:HIS:HD2	1:A:1228:GLY:HA3	1.76	0.49
1:A:2464:HIS:HE1	1:A:2466:SER:HB3	1.77	0.49
1:A:2586:PHE:CD1	1:A:2778:GLY:HA3	2.47	0.49
1:A:2471:GLU:N	1:A:2471:GLU:OE1	2.45	0.49
1:A:3535:ILE:HD11	1:A:3796:MET:O	2.12	0.49
1:A:3821:SER:O	1:A:3825:LYS:N	2.46	0.49
1:A:175:TYR:O	1:A:179:GLY:N	2.33	0.49
1:A:2376:ASP:HB3	1:A:2404:ARG:NH1	2.28	0.49
1:A:3270:ASP:OD1	1:A:3271:ASP:N	2.46	0.49
1:A:191:ASN:O	1:A:195:ASN:ND2	2.46	0.49
1:A:287:LEU:O	1:A:337:LYS:NZ	2.44	0.49
1:A:627:VAL:HG22	1:A:669:LEU:HD22	1.94	0.49
1:A:3269:ARG:HB2	1:A:3269:ARG:NH1	2.28	0.49
1:A:1476:HIS:ND1	1:A:1521:PHE:HB3	2.27	0.48
1:A:2386:LEU:HD23	1:A:2418:LYS:HB3	1.94	0.48
1:A:2494:ASP:OD1	1:A:2495:SER:N	2.45	0.48
1:A:2894:GLU:HB2	1:A:3973:PRO:HG2	1.94	0.48
1:A:3295:GLU:OE1	1:A:3295:GLU:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3499:ILE:HA	1:A:3502:MET:HE2	1.94	0.48
1:A:3913:ILE:HB	1:A:3984:MET:HG2	1.95	0.48
1:A:541:MET:HA	1:A:544:ILE:HG12	1.95	0.48
1:A:606:SER:OG	1:A:1026:ARG:NH1	2.46	0.48
1:A:1429:GLU:O	1:A:1433:ALA:N	2.43	0.48
1:A:3855:TYR:OH	1:A:4122:GLU:HB2	2.13	0.48
1:A:1095:LEU:HD12	1:A:1099:PHE:HE2	1.78	0.48
1:A:3324:ARG:HG3	1:A:3388:ALA:HB1	1.95	0.48
1:A:3483:MET:HE3	1:A:3513:ALA:HB1	1.96	0.48
1:A:6015:UNK:O	1:A:6019:UNK:N	2.46	0.48
1:A:67:VAL:HA	1:A:70:ARG:HH21	1.77	0.48
1:A:93:LEU:HD21	1:A:137:THR:HG22	1.95	0.48
1:A:1164:CYS:SG	1:A:1165:LEU:N	2.87	0.48
1:A:2554:PHE:O	1:A:2555:LEU:HB2	2.14	0.48
1:A:3255:ALA:HB1	1:A:3283:LEU:HD11	1.95	0.48
1:A:1300:SER:HA	1:A:1312:CYS:HB2	1.94	0.48
1:A:2310:VAL:HG12	1:A:2311:ARG:H	1.77	0.48
1:A:758:LEU:HD22	1:A:765:LEU:HD12	1.96	0.48
1:A:2253:TYR:HA	1:A:2256:ILE:HD13	1.96	0.48
1:A:2973:ASP:OD1	1:A:2974:GLU:N	2.47	0.48
1:A:3517:SER:O	1:A:3521:ILE:HG12	2.13	0.48
1:A:3631:LYS:O	1:A:3635:THR:OG1	2.28	0.48
1:A:1133:HIS:O	1:A:1137:ILE:HG12	2.13	0.48
1:A:3226:ASP:N	1:A:3229:SER:HG	2.12	0.48
1:A:3297:VAL:O	1:A:3300:VAL:HG12	2.14	0.48
1:A:282:PHE:HB3	1:A:285:CYS:HB2	1.95	0.48
1:A:2930:TYR:HA	1:A:2933:ILE:HG22	1.95	0.48
1:A:2976:LEU:HD11	1:A:2995:GLU:HB3	1.95	0.48
1:A:3552:LYS:HA	1:A:3555:VAL:HG12	1.94	0.48
1:A:1066:LEU:HD22	1:A:1074:LYS:HD2	1.96	0.47
1:A:1849:ASP:OD1	1:A:1850:VAL:N	2.46	0.47
1:A:3287:ARG:O	1:A:3287:ARG:HG2	2.14	0.47
1:A:3493:TRP:CD2	1:A:3711:PRO:HG3	2.49	0.47
1:A:105:VAL:HA	1:A:108:LYS:HE3	1.95	0.47
1:A:2933:ILE:HD11	1:A:3121:LEU:HD22	1.96	0.47
1:A:355:ASN:OD1	1:A:356:ASN:N	2.47	0.47
1:A:1019:ASP:OD1	1:A:1019:ASP:N	2.47	0.47
1:A:2085:MET:SD	1:A:2088:LEU:HB3	2.54	0.47
1:A:3247:ARG:HD2	1:A:3283:LEU:HA	1.96	0.47
1:A:909:VAL:O	1:A:912:PRO:HD2	2.15	0.47
1:A:2371:PHE:HB3	1:A:2374:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3855:TYR:HA	1:A:3858:MET:HG3	1.96	0.47
1:A:1031:ARG:O	1:A:1034:ARG:HG2	2.15	0.47
1:A:2183:HIS:CE1	1:A:2186:VAL:HG13	2.49	0.47
1:A:2443:MET:N	1:A:2444:PRO:HD2	2.29	0.47
1:A:681:LYS:HE2	1:A:681:LYS:HA	1.97	0.47
1:A:1335:CYS:HB3	1:A:1384:PHE:HD1	1.79	0.47
1:A:1399:CYS:O	1:A:1403:MET:HE3	2.14	0.47
1:A:2220:MET:SD	1:A:2255:LEU:HD23	2.54	0.47
1:A:2941:GLY:HA2	1:A:2944:THR:HG22	1.96	0.47
1:A:151:GLU:HB3	1:A:153:PHE:CZ	2.49	0.47
1:A:327:VAL:HG12	1:A:372:PRO:HB3	1.96	0.47
1:A:3274:VAL:O	1:A:3278:GLN:N	2.41	0.47
1:A:3354:ASP:O	1:A:3358:ARG:N	2.46	0.47
1:A:3472:ILE:HG21	1:A:3483:MET:HE2	1.97	0.47
1:A:3864:ARG:NH1	1:A:3868:VAL:HG21	2.29	0.47
1:A:1524:LEU:O	1:A:1528:LEU:N	2.33	0.47
1:A:1588:ASP:OD1	1:A:1589:ASN:N	2.47	0.47
1:A:1686:LEU:HD13	1:A:1721:HIS:CD2	2.48	0.47
1:A:1920:TYR:HA	1:A:1923:PHE:CE1	2.50	0.47
1:A:2864:GLN:C	1:A:2865:HIS:HD1	2.17	0.47
1:A:3483:MET:CE	1:A:3513:ALA:HB1	2.45	0.47
1:A:3541:SER:OG	1:A:3542:PHE:N	2.47	0.47
1:A:1694:THR:O	1:A:1697:PRO:HD2	2.15	0.47
1:A:1816:ARG:HA	1:A:1819:PHE:CE2	2.49	0.47
1:A:3531:TYR:HB2	1:A:3532:PRO:HD3	1.96	0.47
1:A:3800:LEU:HD23	1:A:3801:GLY:N	2.29	0.47
1:A:757:LYS:HB2	1:A:757:LYS:HE3	1.67	0.47
1:A:1839:PHE:HE1	1:A:1843:ILE:HD12	1.80	0.47
1:A:3911:ILE:HG23	1:A:3915:HIS:CE1	2.50	0.47
1:A:269:SER:O	1:A:273:ARG:HG2	2.15	0.46
1:A:331:ALA:HB2	1:A:375:VAL:HG23	1.97	0.46
1:A:2510:LEU:HB3	1:A:2557:LEU:HD13	1.98	0.46
1:A:2574:ASN:O	1:A:2786:LYS:HA	2.14	0.46
1:A:2920:VAL:O	1:A:2924:VAL:HG23	2.15	0.46
1:A:4126:PRO:HD2	1:A:4127:TRP:CE3	2.50	0.46
1:A:255:ALA:HB3	1:A:296:VAL:HG13	1.98	0.46
1:A:331:ALA:HB1	1:A:376:ILE:HB	1.97	0.46
1:A:1611:GLN:HE21	1:A:1614:GLN:NE2	2.13	0.46
1:A:335:LYS:HA	1:A:338:LEU:HB3	1.97	0.46
1:A:541:MET:HB3	1:A:545:LEU:HD23	1.96	0.46
1:A:570:LYS:HD3	1:A:1505:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1247:PRO:HB2	1:A:1250:LEU:HB3	1.98	0.46
1:A:1323:SER:O	1:A:1326:GLU:N	2.49	0.46
1:A:537:SER:HA	1:A:540:MET:HE1	1.96	0.46
1:A:2578:GLU:CD	1:A:2579:HIS:HD1	2.18	0.46
1:A:1369:MET:HG3	1:A:1372:LEU:HD23	1.96	0.46
1:A:1946:ASN:ND2	1:A:2096:PRO:HG2	2.31	0.46
1:A:4027:TRP:HE3	1:A:4030:GLU:H	1.62	0.46
1:A:3568:ILE:O	1:A:3572:ILE:HG12	2.16	0.46
1:A:709:LYS:O	1:A:709:LYS:HG2	2.15	0.46
1:A:1442:GLN:HA	1:A:1445:ARG:HH12	1.81	0.46
1:A:3875:GLU:HG2	1:A:3965:ARG:HD3	1.97	0.46
1:A:730:LEU:O	1:A:734:LEU:HG	2.16	0.46
1:A:3137:GLU:OE1	1:A:3186:ARG:NE	2.28	0.46
1:A:245:SER:HA	1:A:248:ILE:HB	1.97	0.46
1:A:1947:CYS:O	1:A:1951:VAL:HG23	2.16	0.46
1:A:2841:ASN:O	1:A:2845:ASN:ND2	2.49	0.46
1:A:2970:LYS:HA	1:A:2970:LYS:HD3	1.77	0.46
1:A:3451:LEU:HD11	1:A:3483:MET:HG3	1.97	0.46
1:A:1746:PHE:O	1:A:1750:LEU:N	2.48	0.45
1:A:1771:GLN:HA	1:A:1775:GLU:OE1	2.16	0.45
1:A:2879:GLY:O	1:A:2883:SER:OG	2.21	0.45
1:A:3641:ASP:OD1	1:A:3642:LYS:N	2.48	0.45
1:A:3717:VAL:HA	1:A:3743:HIS:HE1	1.80	0.45
1:A:10:CYS:HA	1:A:13:LEU:HD12	1.98	0.45
1:A:247:GLU:HB2	1:A:282:PHE:CE1	2.51	0.45
1:A:985:GLU:O	1:A:989:MET:HG2	2.15	0.45
1:A:1729:PHE:CE1	1:A:1735:ARG:HG2	2.52	0.45
1:A:2392:VAL:O	1:A:2395:THR:HG22	2.17	0.45
1:A:3033:GLU:HB3	1:A:3034:PRO:HD3	1.98	0.45
1:A:177:LEU:HA	1:A:177:LEU:HD23	1.76	0.45
1:A:659:ARG:HG3	1:A:660:LEU:HG	1.99	0.45
1:A:1965:PHE:H	1:A:1971:PRO:HD2	1.82	0.45
1:A:3751:LEU:HD23	1:A:3803:ILE:HD11	1.98	0.45
1:A:1335:CYS:HB3	1:A:1384:PHE:CD1	2.52	0.45
1:A:1881:TYR:CE2	1:A:1951:VAL:HG22	2.51	0.45
1:A:3376:GLY:O	1:A:3380:ARG:N	2.42	0.45
1:A:319:PHE:CD2	1:A:320:LEU:HD12	2.51	0.45
1:A:439:VAL:HG11	1:A:465:PHE:HE1	1.81	0.45
1:A:2319:ALA:O	1:A:2323:LEU:HG	2.17	0.45
1:A:2587:GLN:HG3	1:A:2588:GLU:O	2.17	0.45
1:A:2917:PRO:O	1:A:2920:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3608:LYS:O	1:A:3612:ARG:HG2	2.17	0.45
1:A:178:LEU:HD21	1:A:196:LEU:HD22	1.99	0.45
1:A:1013:ILE:O	1:A:1013:ILE:HG13	2.17	0.45
1:A:1715:GLU:HA	1:A:1718:ILE:HG12	1.97	0.45
1:A:1770:GLN:HG3	1:A:1822:ARG:HH12	1.82	0.45
1:A:3548:GLY:HA2	1:A:3551:ASN:OD1	2.17	0.45
1:A:3723:ASP:OD1	1:A:3724:GLU:N	2.50	0.45
1:A:3728:VAL:HG22	1:A:3736:LYS:HG3	1.99	0.45
1:A:3825:LYS:HG2	1:A:3829:LEU:HD23	1.99	0.45
1:A:1877:LEU:HD13	1:A:1915:LEU:HD21	1.98	0.45
1:A:3082:TYR:HB3	1:A:3085:GLU:HB2	1.99	0.45
1:A:3133:GLN:O	1:A:3137:GLU:HG3	2.17	0.45
1:A:3287:ARG:HG3	1:A:3287:ARG:HH11	1.81	0.45
1:A:3522:THR:HG21	1:A:3561:LYS:HG3	1.99	0.45
1:A:3878:VAL:HG13	1:A:3965:ARG:HH21	1.82	0.45
1:A:129:ASP:OD1	1:A:129:ASP:N	2.49	0.44
1:A:607:ASP:N	1:A:607:ASP:OD1	2.48	0.44
1:A:619:ASP:OD1	1:A:6006:UNK:N	2.50	0.44
1:A:1153:LEU:HD13	1:A:1163:LEU:HD21	1.98	0.44
1:A:1305:ASP:O	1:A:1330:TYR:OH	2.29	0.44
1:A:1700:THR:HG21	1:A:1753:SER:HB2	1.99	0.44
1:A:1965:PHE:HA	1:A:1970:LYS:HA	1.98	0.44
1:A:2383:PHE:CD2	1:A:2414:GLN:HG2	2.52	0.44
1:A:2480:ILE:O	1:A:2484:TYR:HB2	2.18	0.44
1:A:2506:LEU:HD13	1:A:2524:PHE:HE2	1.82	0.44
1:A:1632:TRP:HZ3	1:A:1648:LEU:HD21	1.81	0.44
1:A:2256:ILE:HA	1:A:2259:LYS:HB2	1.99	0.44
1:A:3858:MET:SD	1:A:3859:TYR:N	2.89	0.44
1:A:3958:LEU:HD21	1:A:4064:LEU:HD11	1.99	0.44
1:A:860:GLY:HA3	1:A:3136:THR:HG21	1.99	0.44
1:A:1034:ARG:HB3	1:A:1084:ASN:HB3	1.99	0.44
1:A:1824:LEU:O	1:A:1828:LEU:N	2.48	0.44
1:A:3105:ASN:O	1:A:3109:SER:N	2.41	0.44
1:A:3284:SER:HB3	1:A:3301:LEU:HD11	1.99	0.44
1:A:3530:VAL:HB	1:A:3562:LEU:HD11	1.99	0.44
1:A:1743:MET:O	1:A:1747:LEU:HG	2.16	0.44
1:A:1830:HIS:O	1:A:1883:ARG:NH2	2.49	0.44
1:A:1881:TYR:HE2	1:A:1951:VAL:HG13	1.81	0.44
1:A:153:PHE:HA	1:A:156:PHE:CD2	2.52	0.44
1:A:237:SER:O	1:A:243:GLN:HG3	2.18	0.44
1:A:1086:TYR:O	1:A:1087:ARG:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3095:ASP:N	1:A:3095:ASP:OD1	2.48	0.44
1:A:3290:SER:HG	1:A:3293:CYS:HG	1.63	0.44
1:A:3700:GLU:HA	1:A:3718:ARG:HA	2.00	0.44
1:A:4065:LEU:O	1:A:4069:GLU:HB3	2.18	0.44
1:A:131:LEU:HA	1:A:173:LYS:HD3	2.00	0.44
1:A:1483:LEU:HA	1:A:1487:VAL:HG12	1.98	0.44
1:A:2923:TRP:CE2	1:A:2946:GLU:HG3	2.53	0.44
1:A:2949:THR:HG23	1:A:2950:LYS:HE3	1.99	0.44
1:A:200:PHE:CE1	1:A:224:LEU:HB3	2.53	0.44
1:A:272:LEU:HD12	1:A:272:LEU:HA	1.89	0.44
1:A:2304:VAL:O	1:A:2307:MET:HG3	2.17	0.44
1:A:3509:ASP:O	1:A:3510:GLN:HG2	2.16	0.44
1:A:3897:PHE:CZ	1:A:3901:ARG:HD3	2.52	0.44
1:A:70:ARG:NH1	1:A:81:CYS:SG	2.91	0.44
1:A:3327:ASN:HB2	1:A:3388:ALA:HB2	2.00	0.44
1:A:3995:PRO:HB3	1:A:4051:LEU:HD13	1.99	0.44
1:A:255:ALA:HB2	1:A:300:TRP:NE1	2.33	0.44
1:A:1388:ASP:HA	1:A:1392:MET:SD	2.58	0.44
1:A:1866:GLN:HA	1:A:1869:LYS:HB3	2.00	0.44
1:A:2461:PHE:HB2	1:A:2473:MET:CE	2.47	0.44
1:A:2478:MET:HG2	1:A:2524:PHE:CE2	2.53	0.44
1:A:3308:ASP:OD1	1:A:3308:ASP:N	2.45	0.44
1:A:3774:ILE:O	1:A:3777:GLN:HG3	2.18	0.44
1:A:259:GLN:OE1	1:A:259:GLN:N	2.43	0.43
1:A:1499:CYS:O	1:A:1501:PRO:HD3	2.18	0.43
1:A:2142:ILE:O	1:A:2146:LEU:N	2.34	0.43
1:A:197:PHE:HA	1:A:200:PHE:HB3	2.00	0.43
1:A:1880:MET:O	1:A:1884:LEU:HD13	2.18	0.43
1:A:3044:MET:HB3	1:A:3048:LYS:HZ3	1.83	0.43
1:A:15:LEU:O	1:A:19:LEU:N	2.39	0.43
1:A:2190:VAL:HA	1:A:2193:ILE:HG12	1.99	0.43
1:A:2946:GLU:OE2	1:A:3975:LYS:NZ	2.41	0.43
1:A:3718:ARG:HD3	1:A:3743:HIS:CE1	2.53	0.43
1:A:393:LYS:HE2	1:A:1687:HIS:CE1	2.53	0.43
1:A:1711:ARG:HD3	1:A:1757:MET:CG	2.48	0.43
1:A:2436:LEU:HD11	1:A:2461:PHE:CD2	2.54	0.43
1:A:2456:ASN:HB2	1:A:2457:PRO:HD3	2.00	0.43
1:A:3169:PRO:HB2	1:A:3179:TRP:NE1	2.33	0.43
1:A:3661:ASP:HA	1:A:3664:ASN:HD21	1.82	0.43
1:A:1718:ILE:HG13	1:A:1719:VAL:N	2.33	0.43
1:A:1878:ASP:OD2	1:A:1950:SER:OG	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2132:LYS:HA	1:A:2135:ASN:HD21	1.83	0.43
1:A:2225:HIS:CG	1:A:2226:PRO:HD2	2.54	0.43
1:A:3472:ILE:HG21	1:A:3483:MET:CE	2.48	0.43
1:A:221:ALA:HA	1:A:224:LEU:HG	1.99	0.43
1:A:459:ARG:NH1	1:A:543:SER:OG	2.50	0.43
1:A:584:GLU:HG3	1:A:613:HIS:O	2.18	0.43
1:A:1050:GLU:OE1	1:A:1050:GLU:N	2.44	0.43
1:A:1335:CYS:SG	1:A:1384:PHE:HA	2.58	0.43
1:A:1476:HIS:CG	1:A:1521:PHE:HB3	2.54	0.43
1:A:2439:ILE:HA	1:A:2442:MET:SD	2.59	0.43
1:A:3568:ILE:HD13	1:A:3699:LEU:HD22	2.00	0.43
1:A:3864:ARG:HH12	1:A:3868:VAL:HG21	1.82	0.43
1:A:1786:ALA:HB2	1:A:1827:LEU:HD23	2.00	0.43
1:A:2195:SER:OG	1:A:5009:UNK:O	2.30	0.43
1:A:3236:PHE:CE1	1:A:3262:LEU:HD21	2.42	0.43
1:A:3502:MET:HG3	1:A:3514:VAL:HG11	2.00	0.43
1:A:3582:GLU:O	1:A:3586:LYS:HG3	2.18	0.43
1:A:746:ARG:HD3	1:A:746:ARG:O	2.19	0.43
1:A:1467:ILE:HG13	1:A:1468:LEU:HG	2.00	0.43
1:A:1538:LEU:HD12	1:A:1553:PHE:CE2	2.54	0.43
1:A:2217:ASN:O	1:A:2221:LYS:HB2	2.19	0.43
1:A:1384:PHE:CE2	1:A:1395:LEU:HD22	2.54	0.43
1:A:1488:TYR:CZ	1:A:1531:LEU:HD11	2.54	0.43
1:A:2438:ILE:O	1:A:2442:MET:HG3	2.19	0.43
1:A:163:LYS:HD3	1:A:163:LYS:HA	1.94	0.43
1:A:294:PHE:O	1:A:298:LEU:HD23	2.19	0.43
1:A:886:TRP:HH2	1:A:915:THR:HG21	1.84	0.43
1:A:20:SER:O	1:A:24:ARG:N	2.51	0.42
1:A:101:ALA:HB3	1:A:102:PRO:HD3	1.99	0.42
1:A:1881:TYR:CD2	1:A:1951:VAL:HA	2.51	0.42
1:A:2454:LEU:O	1:A:2457:PRO:HD2	2.19	0.42
1:A:2555:LEU:O	1:A:2805:ALA:HB1	2.19	0.42
1:A:3338:ALA:O	1:A:3342:SER:N	2.52	0.42
1:A:3670:MET:SD	1:A:3670:MET:N	2.91	0.42
1:A:1344:PHE:CZ	1:A:1348:LEU:HD11	2.54	0.42
1:A:1378:GLU:OE2	1:A:1380:ALA:HB3	2.19	0.42
1:A:1391:VAL:O	1:A:1395:LEU:N	2.49	0.42
1:A:1935:GLU:HG2	1:A:1936:ARG:N	2.33	0.42
1:A:2219:LEU:O	1:A:2223:VAL:HG13	2.19	0.42
1:A:3575:LEU:O	1:A:3578:LEU:HG	2.19	0.42
1:A:3646:LYS:N	1:A:3649:SER:OG	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3806:LEU:HB3	1:A:3809:THR:HG21	2.00	0.42
1:A:3907:SER:O	1:A:3911:ILE:HG12	2.19	0.42
1:A:1418:HIS:O	1:A:1421:GLU:HB2	2.19	0.42
1:A:1946:ASN:HD21	1:A:2096:PRO:HG2	1.85	0.42
1:A:2532:PRO:O	1:A:2538:ARG:NH2	2.52	0.42
1:A:2864:GLN:O	1:A:2865:HIS:ND1	2.52	0.42
1:A:409:GLN:HG3	1:A:413:PHE:HE1	1.84	0.42
1:A:1202:ARG:HG3	1:A:1206:LEU:HB2	2.01	0.42
1:A:1810:PRO:C	1:A:1812:LEU:H	2.23	0.42
1:A:3660:ASN:O	1:A:3664:ASN:ND2	2.53	0.42
1:A:790:LYS:HB2	1:A:790:LYS:HE2	1.73	0.42
1:A:1153:LEU:HD11	1:A:1157:PHE:O	2.20	0.42
1:A:1980:ASN:OD1	1:A:1981:LEU:N	2.48	0.42
1:A:2097:LEU:HA	1:A:2097:LEU:HD23	1.74	0.42
1:A:2872:ASP:O	1:A:2876:VAL:HG23	2.19	0.42
1:A:3250:ASN:HA	1:A:3252:PHE:CE1	2.55	0.42
1:A:85:ILE:HG13	1:A:89:LEU:HD23	2.02	0.42
1:A:300:TRP:HA	1:A:303:HIS:ND1	2.35	0.42
1:A:1261:LEU:HB2	1:A:1337:VAL:HG22	2.01	0.42
1:A:1707:LEU:HA	1:A:1710:LEU:HB3	2.02	0.42
1:A:2554:PHE:HD2	1:A:2555:LEU:HD22	1.84	0.42
1:A:2563:LEU:HD23	1:A:2791:ILE:HG23	2.02	0.42
1:A:3360:LEU:HD12	1:A:3361:GLU:N	2.35	0.42
1:A:3414:MET:SD	1:A:3415:THR:N	2.93	0.42
1:A:3451:LEU:HD23	1:A:3451:LEU:HA	1.84	0.42
1:A:3992:ARG:HD3	1:A:4100:GLU:HG3	2.01	0.42
1:A:1112:ALA:O	1:A:1180:GLN:HG2	2.20	0.42
1:A:1425:ALA:O	1:A:1429:GLU:HG2	2.20	0.42
1:A:1770:GLN:HA	1:A:1822:ARG:NH2	2.35	0.42
1:A:2312:TYR:O	1:A:2315:VAL:HG12	2.19	0.42
1:A:3103:ILE:HD12	1:A:3103:ILE:HA	1.92	0.42
1:A:3405:PRO:HB2	1:A:3406:ALA:H	1.65	0.42
1:A:3734:ARG:HD3	1:A:3734:ARG:HA	1.79	0.42
1:A:2950:LYS:NZ	1:A:2983:ASP:O	2.53	0.42
1:A:13:LEU:HD13	1:A:59:PHE:CE2	2.55	0.41
1:A:353:ASP:OD2	1:A:359:LEU:HB2	2.20	0.41
1:A:1306:ILE:HG23	1:A:1307:ILE:HG12	2.02	0.41
1:A:2350:LYS:HD2	1:A:2353:GLN:HB3	2.02	0.41
1:A:3353:GLU:O	1:A:3357:ARG:N	2.47	0.41
1:A:292:SER:O	1:A:296:VAL:HG23	2.20	0.41
1:A:342:MET:HE1	1:A:384:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1103:ALA:O	1:A:1107:TYR:HD1	2.03	0.41
1:A:1412:LYS:HA	1:A:1415:LEU:HB3	2.02	0.41
1:A:1617:LYS:O	1:A:1621:THR:HG23	2.20	0.41
1:A:1734:PRO:O	1:A:1738:ASN:ND2	2.52	0.41
1:A:3472:ILE:HG13	1:A:3510:GLN:OE1	2.20	0.41
1:A:868:LYS:HB2	1:A:868:LYS:HE3	1.71	0.41
1:A:1414:ILE:HG13	1:A:1418:HIS:CE1	2.55	0.41
1:A:2276:LEU:O	1:A:2280:VAL:HG23	2.19	0.41
1:A:2452:ARG:HA	1:A:2452:ARG:HD2	1.95	0.41
1:A:2589:TYR:HB3	1:A:2775:TYR:O	2.20	0.41
1:A:393:LYS:HA	1:A:397:LEU:HD23	2.02	0.41
1:A:643:GLU:N	1:A:644:PRO:HD2	2.35	0.41
1:A:1244:LEU:HD23	1:A:1244:LEU:HA	1.92	0.41
1:A:240:GLU:HB2	1:A:243:GLN:HG2	2.02	0.41
1:A:932:GLU:HG3	1:A:2775:TYR:OH	2.20	0.41
1:A:3128:LYS:HD3	1:A:3128:LYS:HA	1.80	0.41
1:A:1301:ILE:HG22	1:A:1334:LYS:NZ	2.36	0.41
1:A:1611:GLN:HG2	1:A:1611:GLN:O	2.21	0.41
1:A:2448:PRO:HA	1:A:2451:LEU:HB3	2.02	0.41
1:A:3430:ASN:HA	1:A:4041:ARG:HH11	1.85	0.41
1:A:3492:CYS:HB3	1:A:3521:ILE:HD13	2.01	0.41
1:A:3502:MET:O	1:A:3505:LEU:HG	2.19	0.41
1:A:3820:MET:HB3	1:A:3882:LEU:HD21	2.02	0.41
1:A:3992:ARG:HG2	1:A:4051:LEU:HD22	2.02	0.41
1:A:3028:ASN:C	1:A:3030:ILE:H	2.24	0.41
1:A:3262:LEU:O	1:A:3262:LEU:HD23	2.21	0.41
1:A:3992:ARG:NE	1:A:4051:LEU:O	2.54	0.41
1:A:4107:LEU:HD23	1:A:4107:LEU:HA	1.90	0.41
1:A:645:TRP:O	1:A:649:PHE:N	2.38	0.41
1:A:1146:ASN:OD1	1:A:1147:LYS:N	2.53	0.41
1:A:1611:GLN:HB2	1:A:1613:HIS:CE1	2.56	0.41
1:A:1709:GLU:HA	1:A:1709:GLU:OE1	2.20	0.41
1:A:2342:CYS:O	1:A:2346:ALA:N	2.47	0.41
1:A:2493:ASN:HA	1:A:2496:GLN:HB2	2.01	0.41
1:A:248:ILE:O	1:A:252:VAL:HG23	2.21	0.41
1:A:405:ASP:OD2	1:A:406:ARG:NH1	2.54	0.41
1:A:683:PHE:HD2	1:A:737:PRO:HG3	1.85	0.41
1:A:1071:ASN:OD1	1:A:1073:PHE:N	2.54	0.41
1:A:1432:CYS:HB3	1:A:1486:LEU:HG	2.02	0.41
1:A:2088:LEU:HD12	1:A:2148:LYS:NZ	2.36	0.41
1:A:2931:ARG:HE	1:A:2939:LEU:HD11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3235:LYS:HB2	1:A:3235:LYS:HE3	1.79	0.41
1:A:3257:LYS:HE3	1:A:3257:LYS:HB3	1.94	0.41
1:A:3449:LYS:HD3	1:A:3449:LYS:HA	1.78	0.41
1:A:3491:PRO:HB3	1:A:3493:TRP:CH2	2.56	0.41
1:A:3812:LEU:HD12	1:A:3812:LEU:HA	1.85	0.41
1:A:4066:LEU:HD12	1:A:4066:LEU:HA	1.93	0.41
2:B:727:ASP:O	2:B:731:MET:N	2.40	0.41
1:A:131:LEU:HA	1:A:173:LYS:CD	2.51	0.41
1:A:393:LYS:HE2	1:A:1687:HIS:ND1	2.36	0.41
1:A:611:ASN:O	1:A:612:LEU:HD23	2.21	0.41
1:A:804:ALA:HA	1:A:852:ARG:NH1	2.36	0.41
1:A:1238:GLN:HA	1:A:1243:TYR:OH	2.22	0.41
1:A:1502:SER:O	1:A:1503:LEU:HD22	2.21	0.41
1:A:1718:ILE:HG13	1:A:1719:VAL:H	1.86	0.41
1:A:1913:LYS:HA	1:A:1916:ILE:HD12	2.02	0.41
1:A:2195:SER:O	1:A:5009:UNK:N	2.36	0.41
1:A:1037:LEU:HD23	1:A:1085:ILE:HB	2.04	0.40
1:A:1452:VAL:O	1:A:1456:LYS:HG2	2.22	0.40
1:A:1503:LEU:HA	1:A:1507:CYS:SG	2.61	0.40
1:A:1916:ILE:HA	1:A:1919:CYS:SG	2.61	0.40
1:A:2186:VAL:HA	1:A:2189:ILE:HG22	2.02	0.40
1:A:2205:VAL:HG12	1:A:2207:LYS:H	1.87	0.40
1:A:1145:LEU:HD23	1:A:1151:ARG:HH21	1.87	0.40
1:A:1241:LEU:O	1:A:1244:LEU:HG	2.20	0.40
1:A:1479:VAL:CG1	1:A:1518:ALA:HA	2.52	0.40
1:A:1745:LYS:HD3	1:A:1745:LYS:HA	1.78	0.40
1:A:2777:HIS:CG	1:A:2778:GLY:N	2.90	0.40
1:A:3325:ASP:O	1:A:3329:LEU:HG	2.20	0.40
1:A:3730:ALA:HA	1:A:3734:ARG:NH1	2.36	0.40
1:A:944:LYS:HA	1:A:944:LYS:HD3	1.81	0.40
1:A:3717:VAL:HG22	1:A:3744:ASP:HB3	2.03	0.40
1:A:3981:TYR:OH	1:A:4105:LYS:HE3	2.21	0.40
1:A:1850:VAL:HG13	1:A:1851:LEU:HD23	2.03	0.40
1:A:1863:PHE:O	1:A:1866:GLN:HG2	2.22	0.40
1:A:2443:MET:SD	1:A:2444:PRO:HD3	2.62	0.40
1:A:3630:ARG:O	1:A:3634:GLN:HG2	2.20	0.40
1:A:1867:ILE:HA	1:A:1870:LYS:HB2	2.03	0.40
1:A:1939:LEU:HD23	1:A:1939:LEU:HA	1.91	0.40
1:A:2124:SER:O	1:A:2127:LYS:HB2	2.22	0.40
1:A:2377:ARG:HG3	1:A:2378:PHE:CE2	2.57	0.40
1:A:3573:ASN:O	1:A:3577:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3875:GLU:OE2	1:A:3965:ARG:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	3630/4156 (87%)	3335 (92%)	292 (8%)	3 (0%)	51 83
2	B	11/192 (6%)	11 (100%)	0	0	100 100
All	All	3641/4348 (84%)	3346 (92%)	292 (8%)	3 (0%)	54 83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	PRO
1	A	2787	HIS
1	A	101	ALA

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	3168/3671 (86%)	3150 (99%)	18 (1%)	86 91

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	379	LYS
1	A	1087	ARG
1	A	1136	ARG
1	A	1147	LYS
1	A	1155	ARG
1	A	1321	ARG
1	A	1612	LYS
1	A	2090	ARG
1	A	2228	ARG
1	A	2313	LYS
1	A	2347	LYS
1	A	2433	LYS
1	A	3302	LYS
1	A	3642	LYS
1	A	3718	ARG
1	A	3833	ARG
1	A	3864	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	322	GLN
1	A	1457	GLN
1	A	1614	GLN
1	A	2365	ASN
1	A	2799	GLN
1	A	3664	ASN
1	A	3704	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4128:MET	C	5009:UNK	N	96.24
1	A	5016:UNK	C	6004:UNK	N	50.57

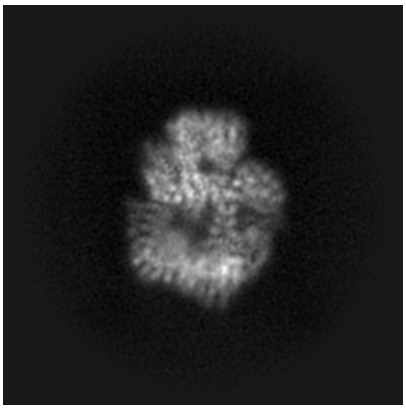
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11215. These allow visual inspection of the internal detail of the map and identification of artifacts.

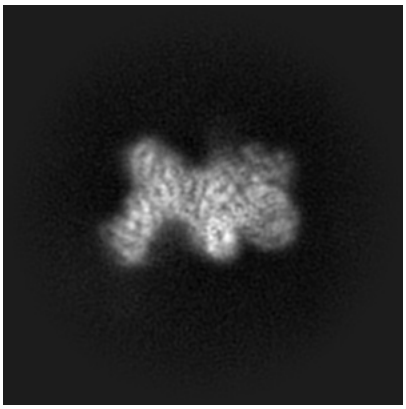
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

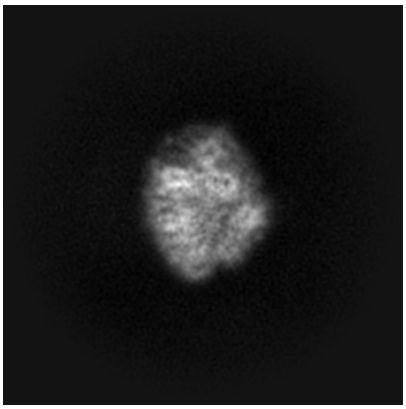
6.1.1 Primary map



X

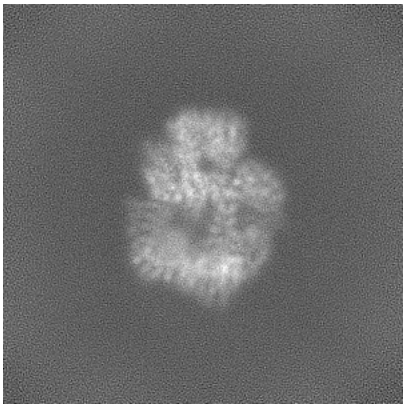


Y

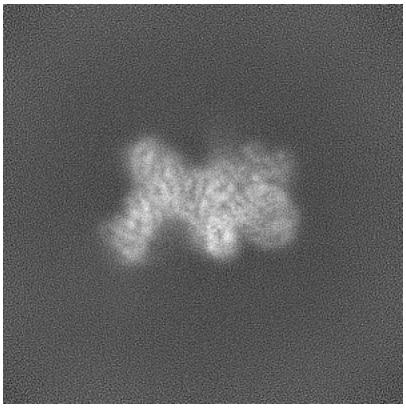


Z

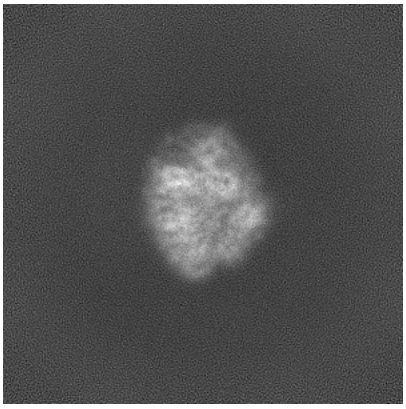
6.1.2 Raw map



X



Y

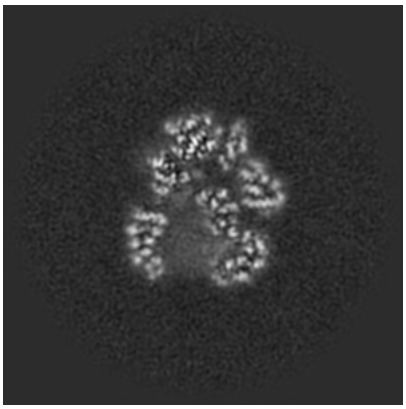


Z

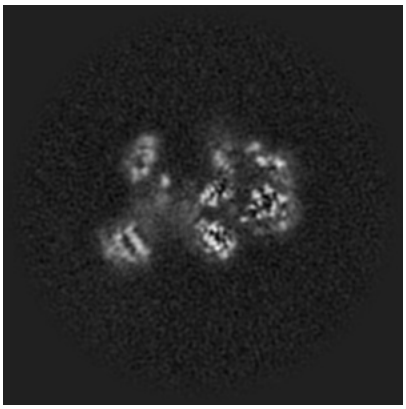
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

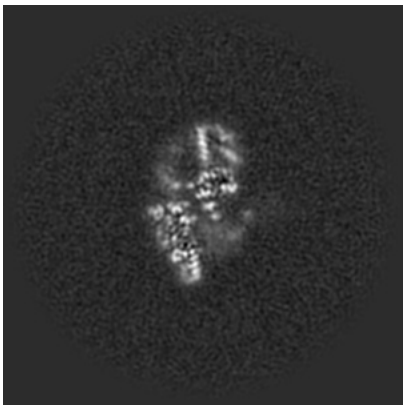
6.2.1 Primary map



X Index: 160

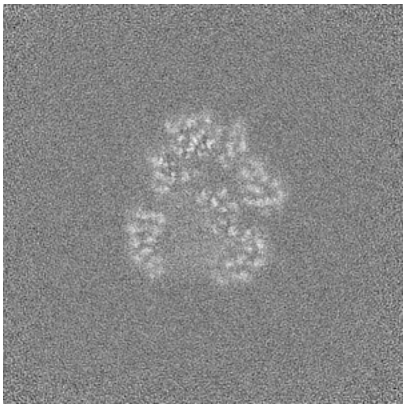


Y Index: 160

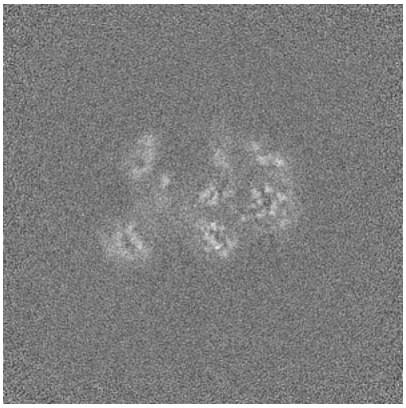


Z Index: 160

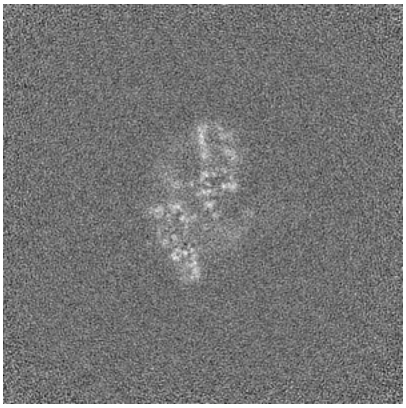
6.2.2 Raw map



X Index: 160



Y Index: 160

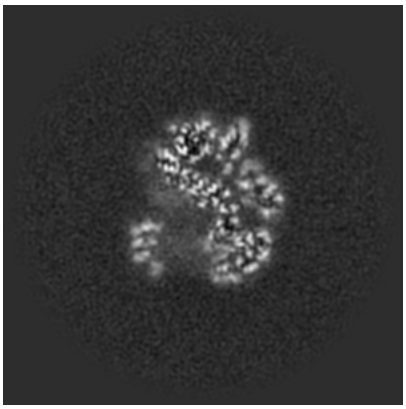


Z Index: 160

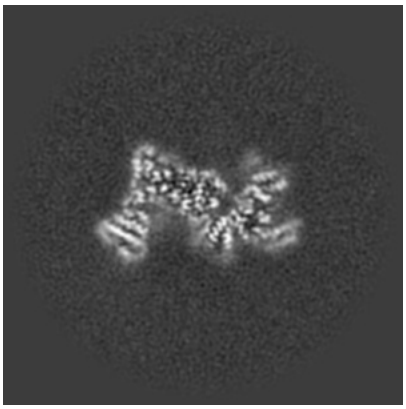
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

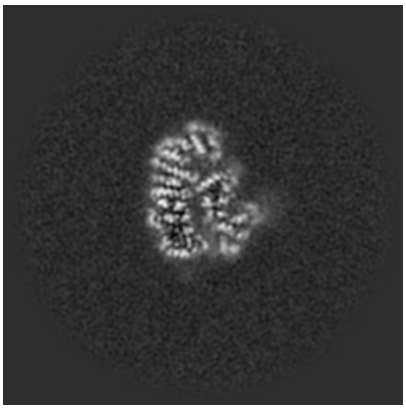
6.3.1 Primary map



X Index: 165

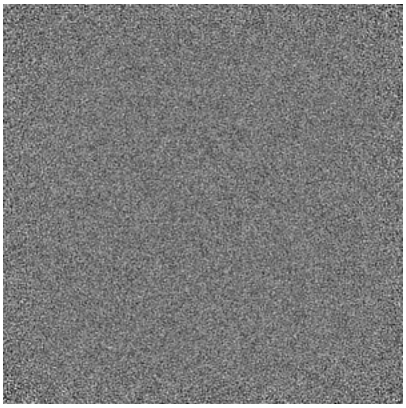


Y Index: 176

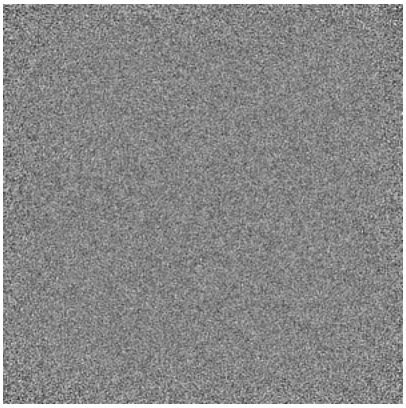


Z Index: 169

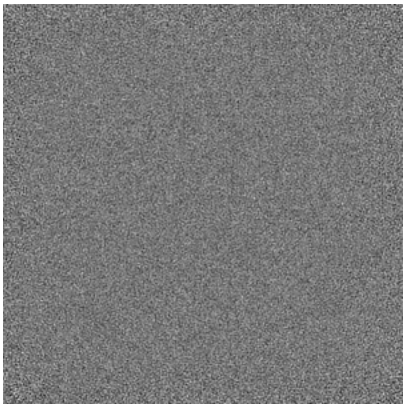
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

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

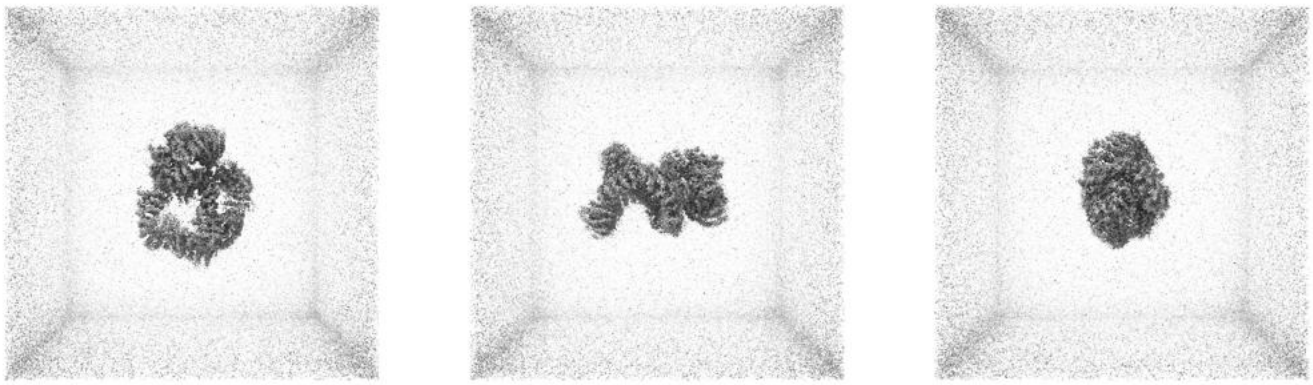
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.125. 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.

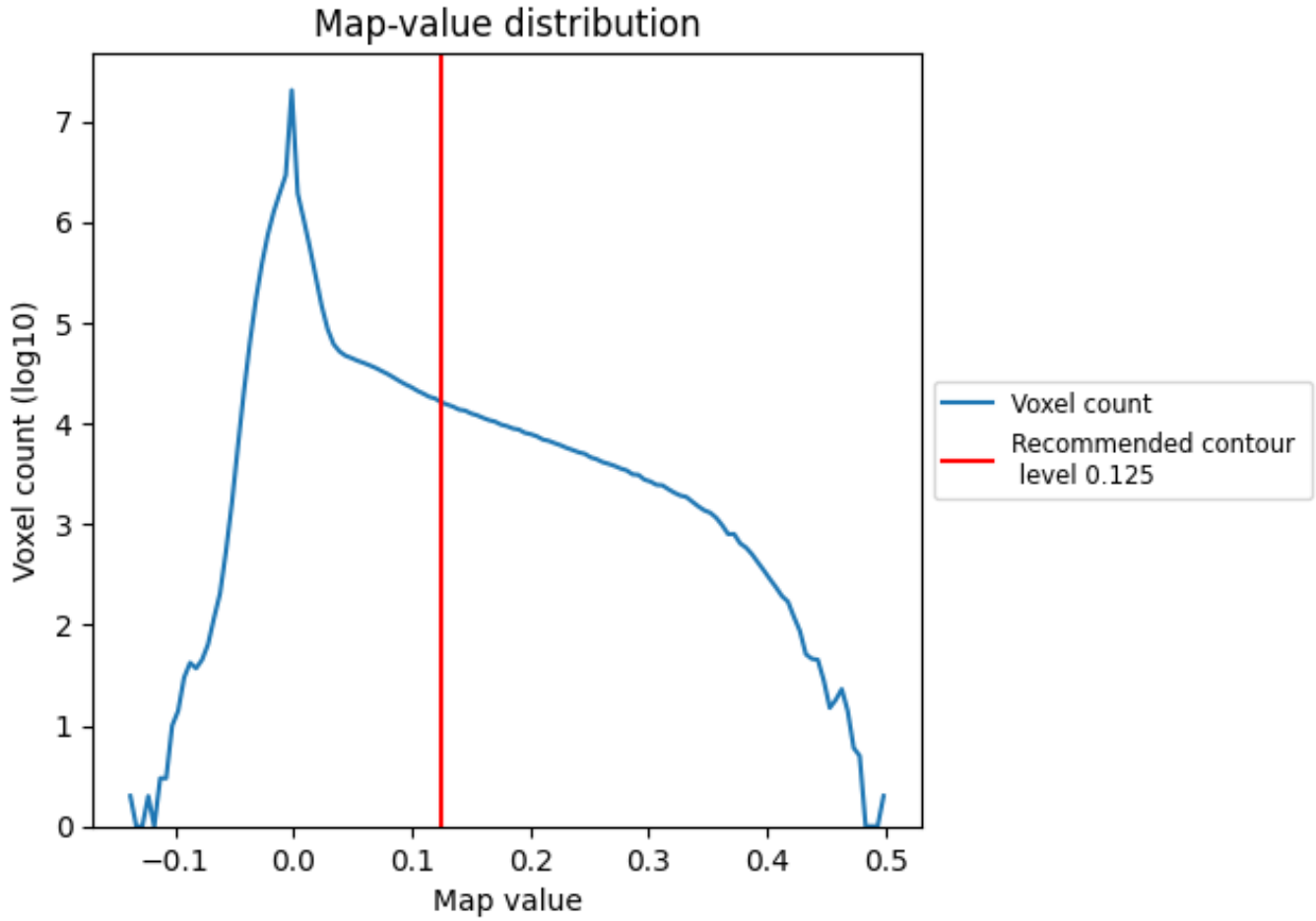
6.5 Mask visualisation (i)

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

7 Map analysis

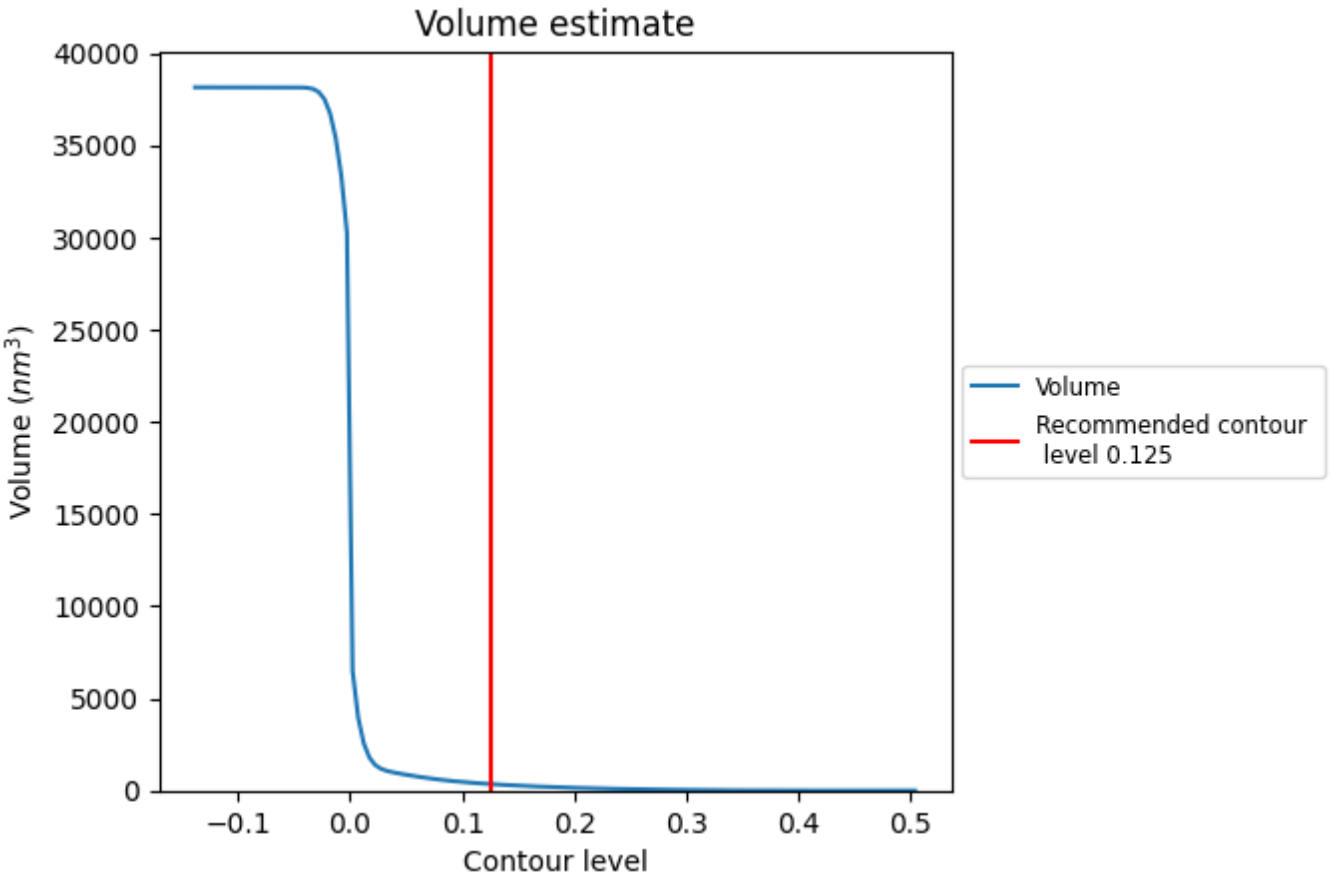
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

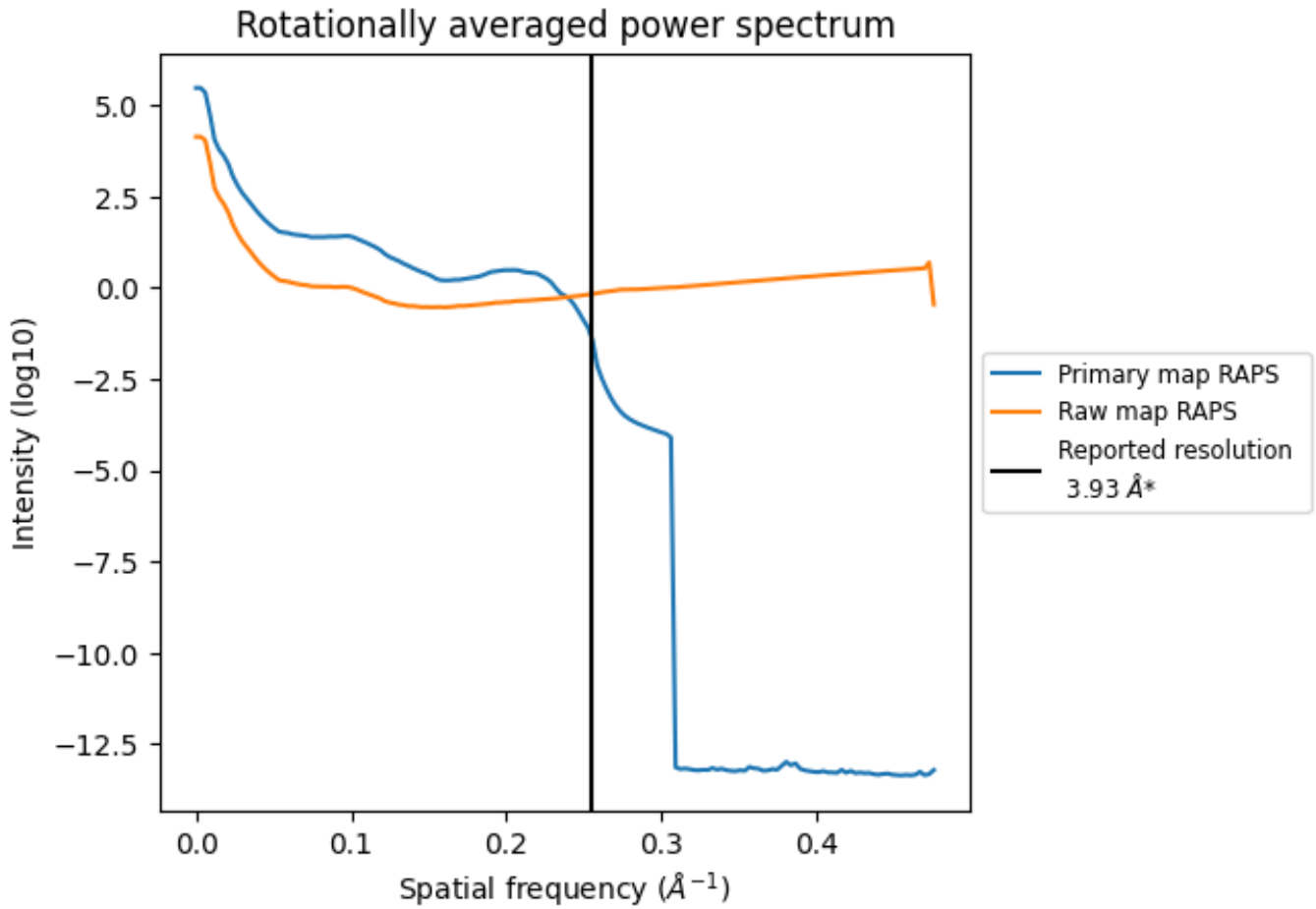
7.2 Volume estimate (i)



The volume at the recommended contour level is 352 nm^3; this corresponds to an approximate mass of 318 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)

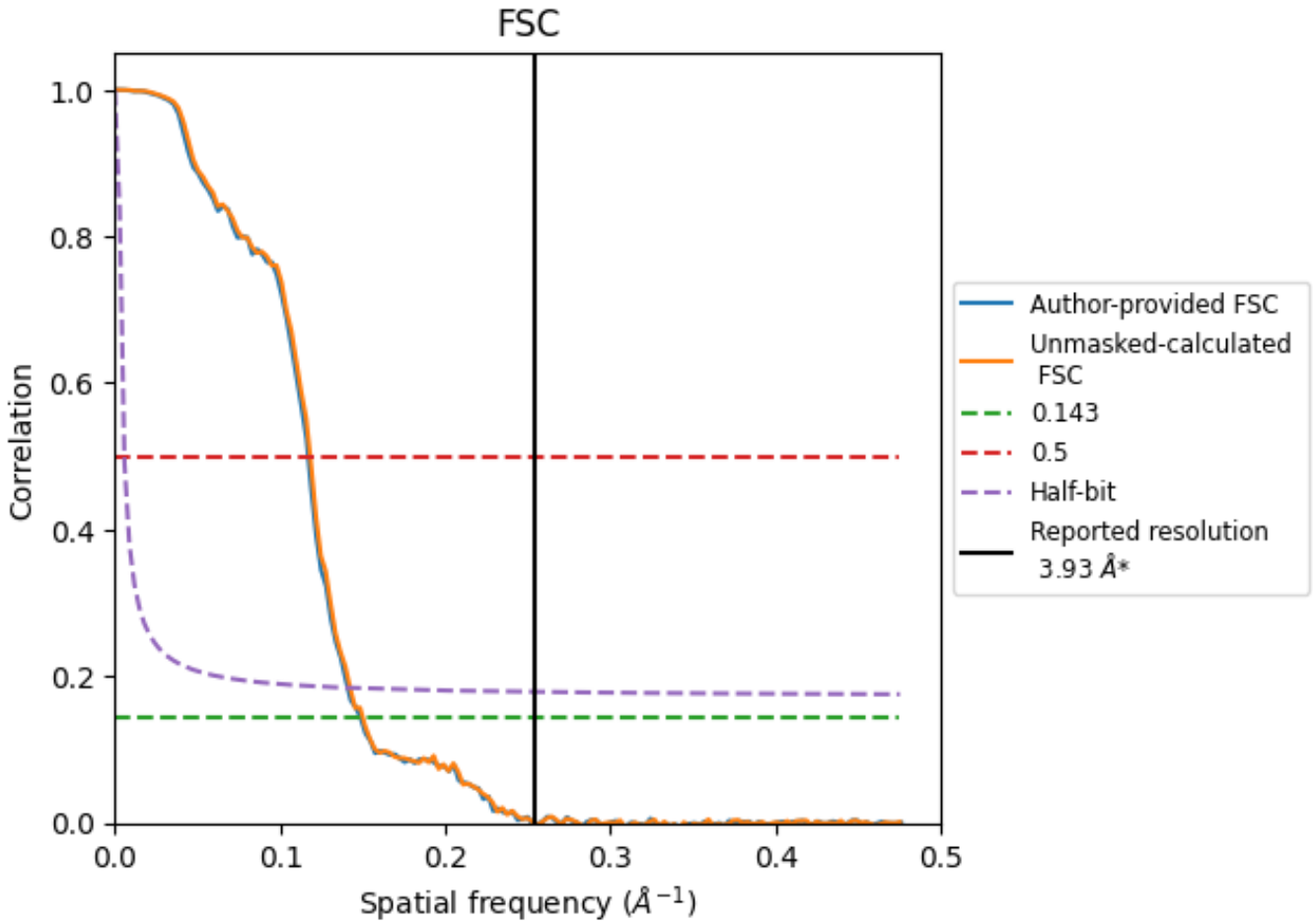


*Reported resolution corresponds to spatial frequency of 0.254 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.254 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.93	-	-
Author-provided FSC curve	6.72	8.54	7.09
Unmasked-calculated*	6.66	8.45	7.02

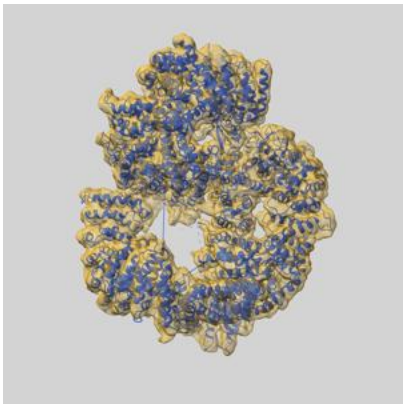
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.72 differs from the reported value 3.93 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.66 differs from the reported value 3.93 by more than 10 %

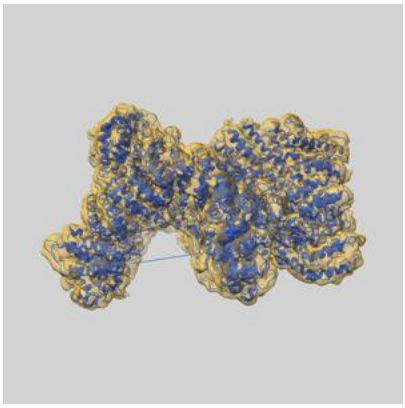
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11215 and PDB model 6ZH6. Per-residue inclusion information can be found in section 3 on page 4.

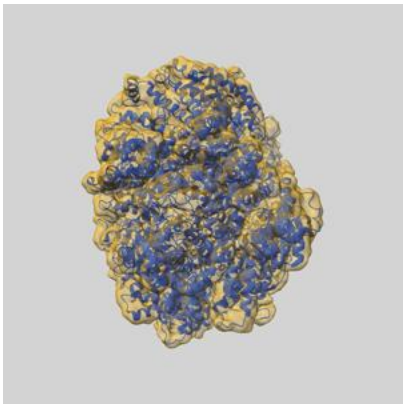
9.1 Map-model overlay



X



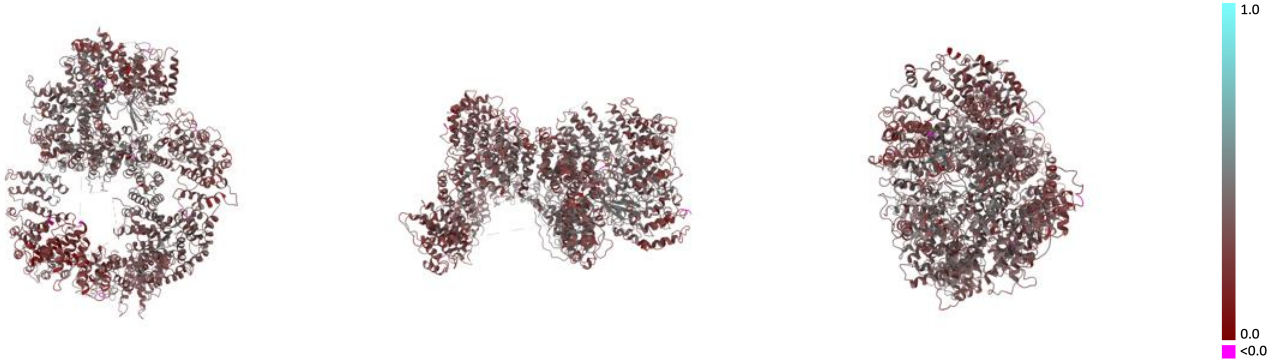
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

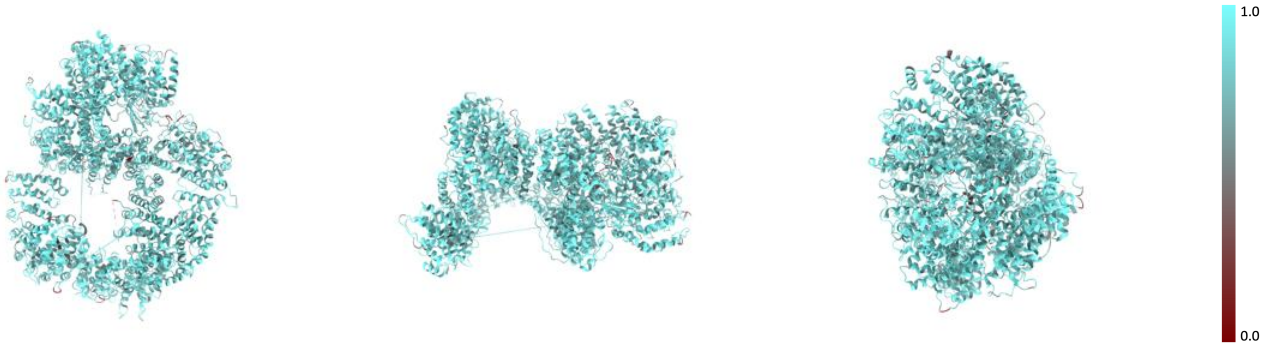
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

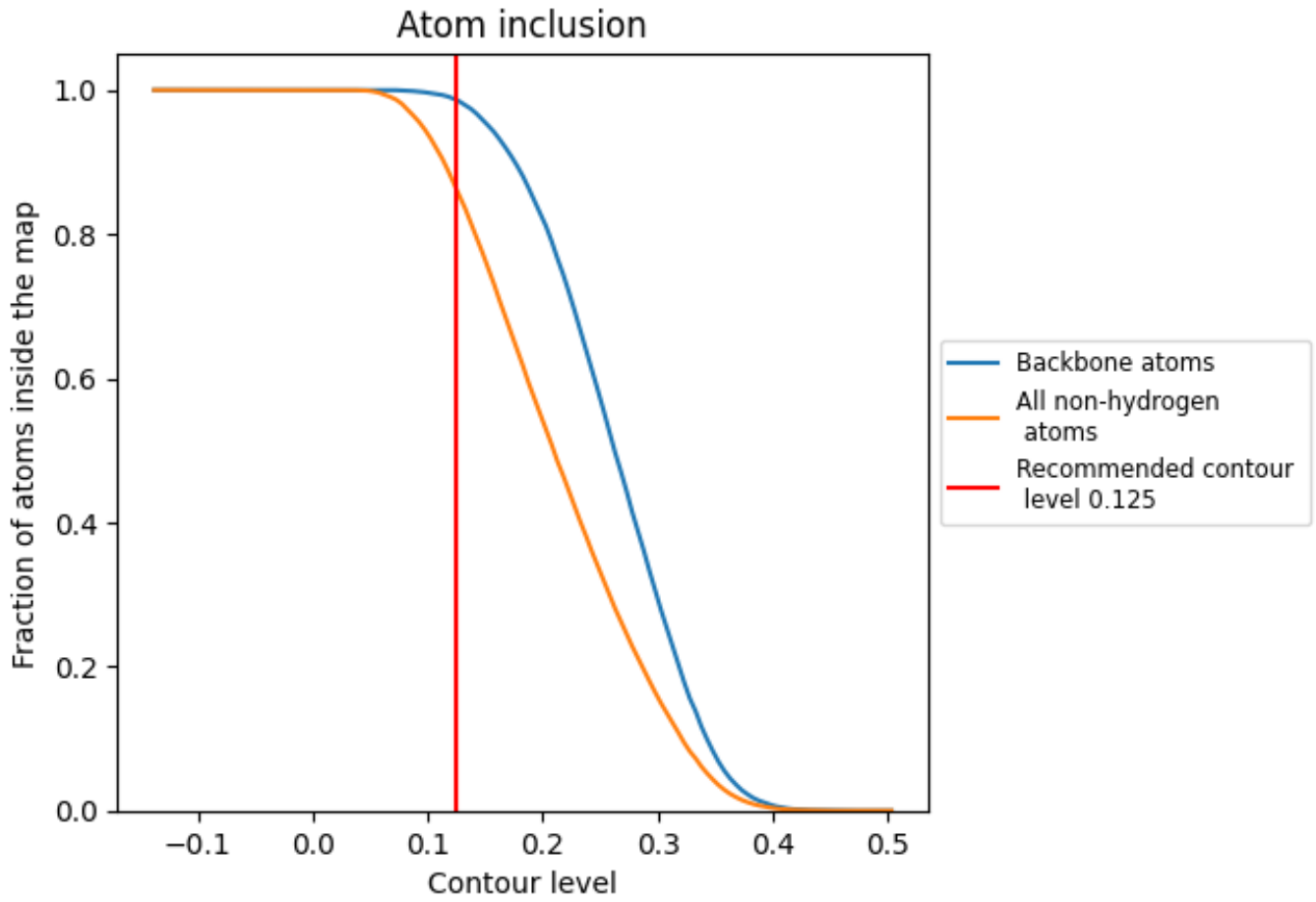
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.125).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8622	0.3350
A	0.8620	0.3350
B	0.9206	0.3380