Full wwPDB EM Validation Report ⓘ

Apr 23, 2024 – 06:59 am BST

PDB ID	:	6ZFP
EMDB ID	:	EMD-11185
Title	:	Cryo-EM structure of DNA-PKcs (State 2)
Authors	:	Chaplin, A.K.; Hardwick, S.W.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on	:	2020-06-17
Resolution	:	3.24 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:

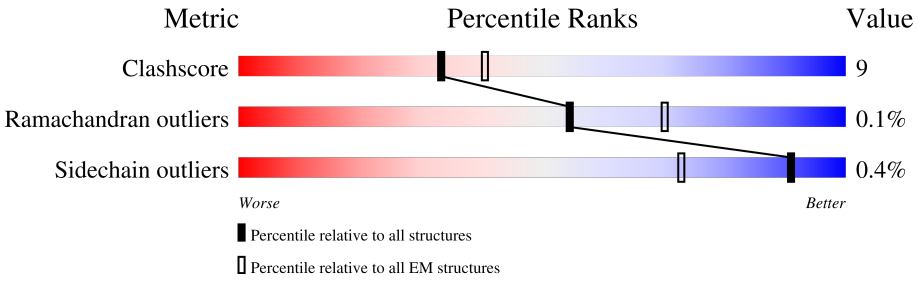
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.24 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	71% 18% 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 29385 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, DNA-PKcs.

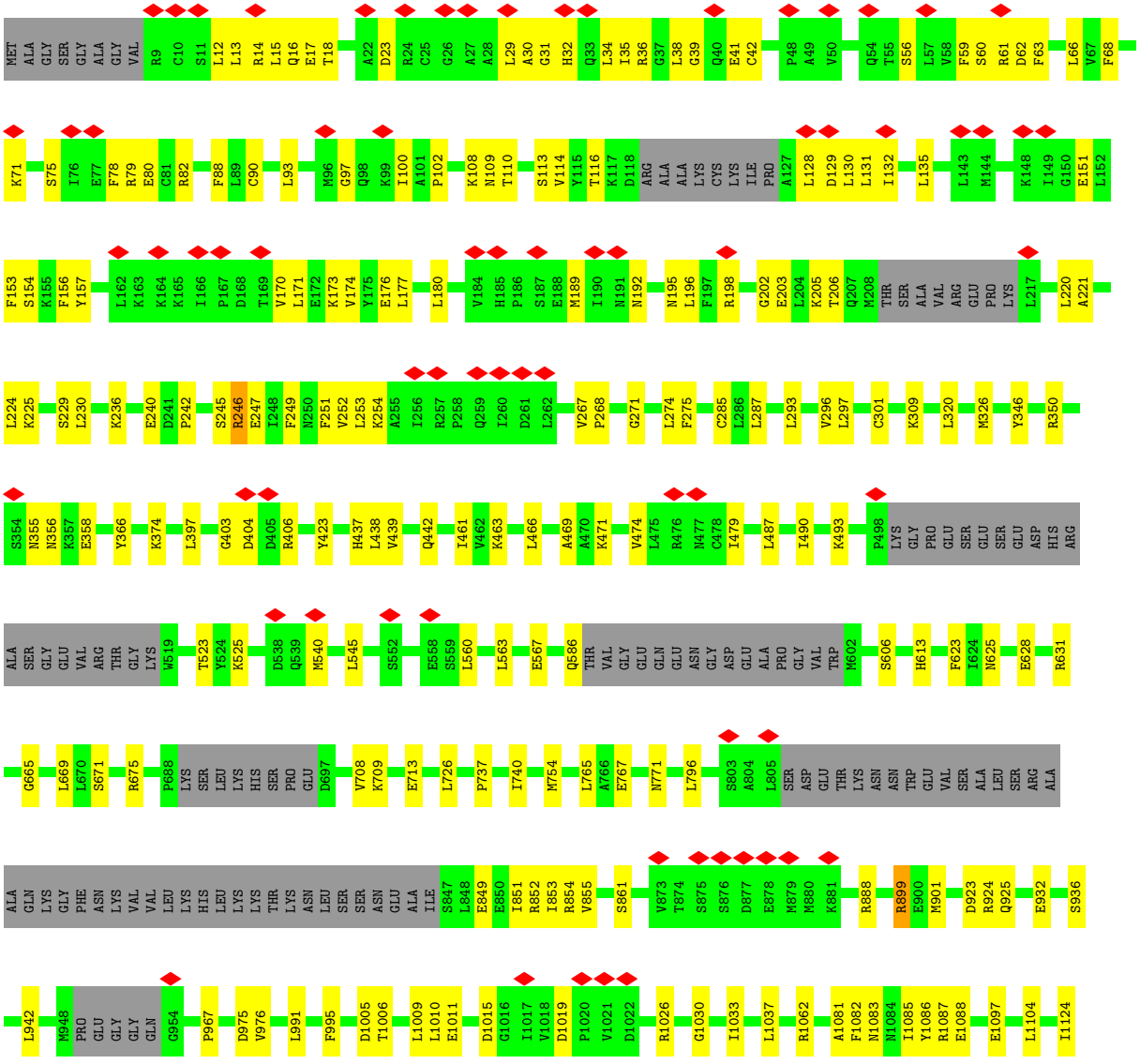
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3704	29385	18849	4964	5379	193	0	0

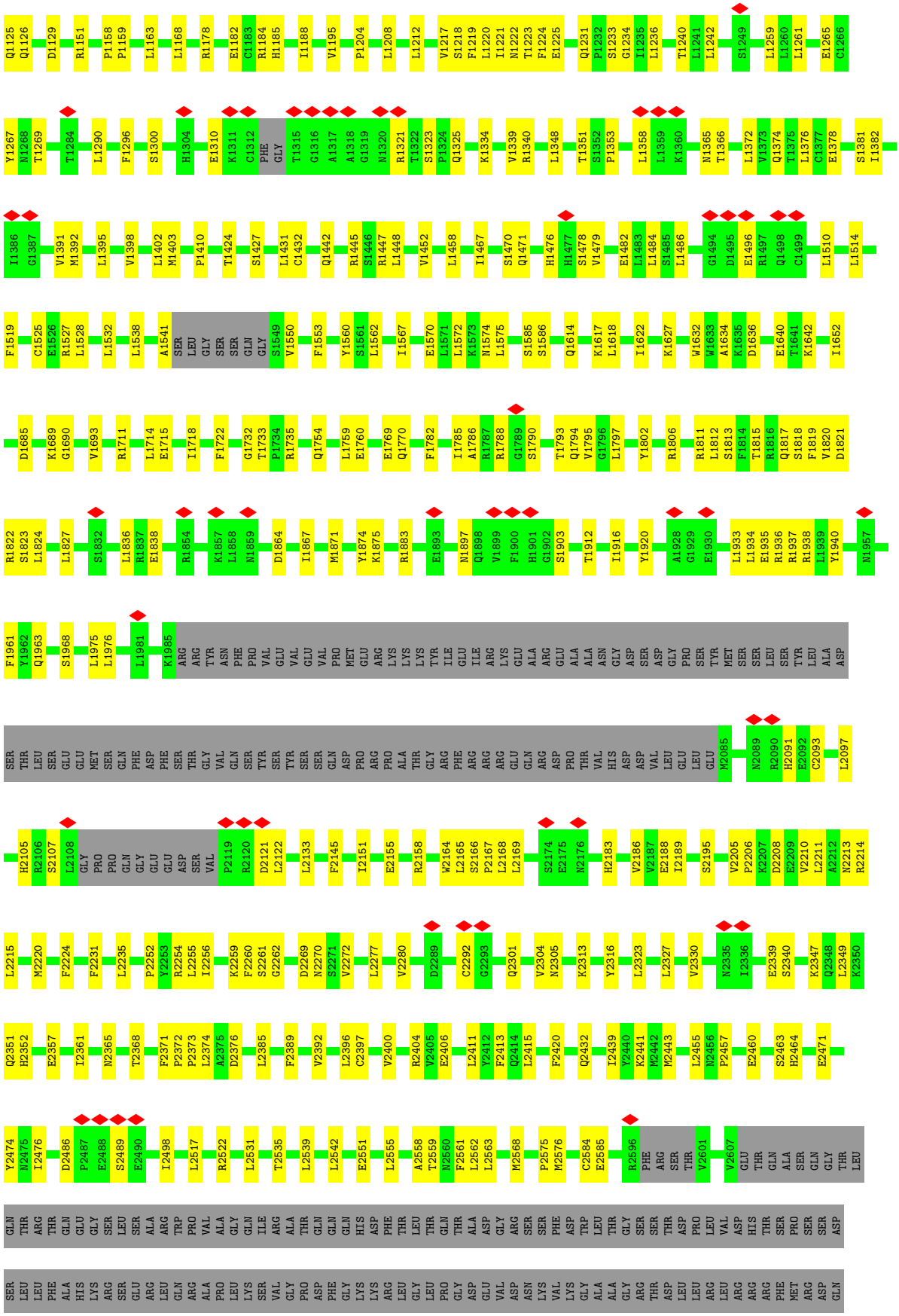
3 Residue-property plots (i)

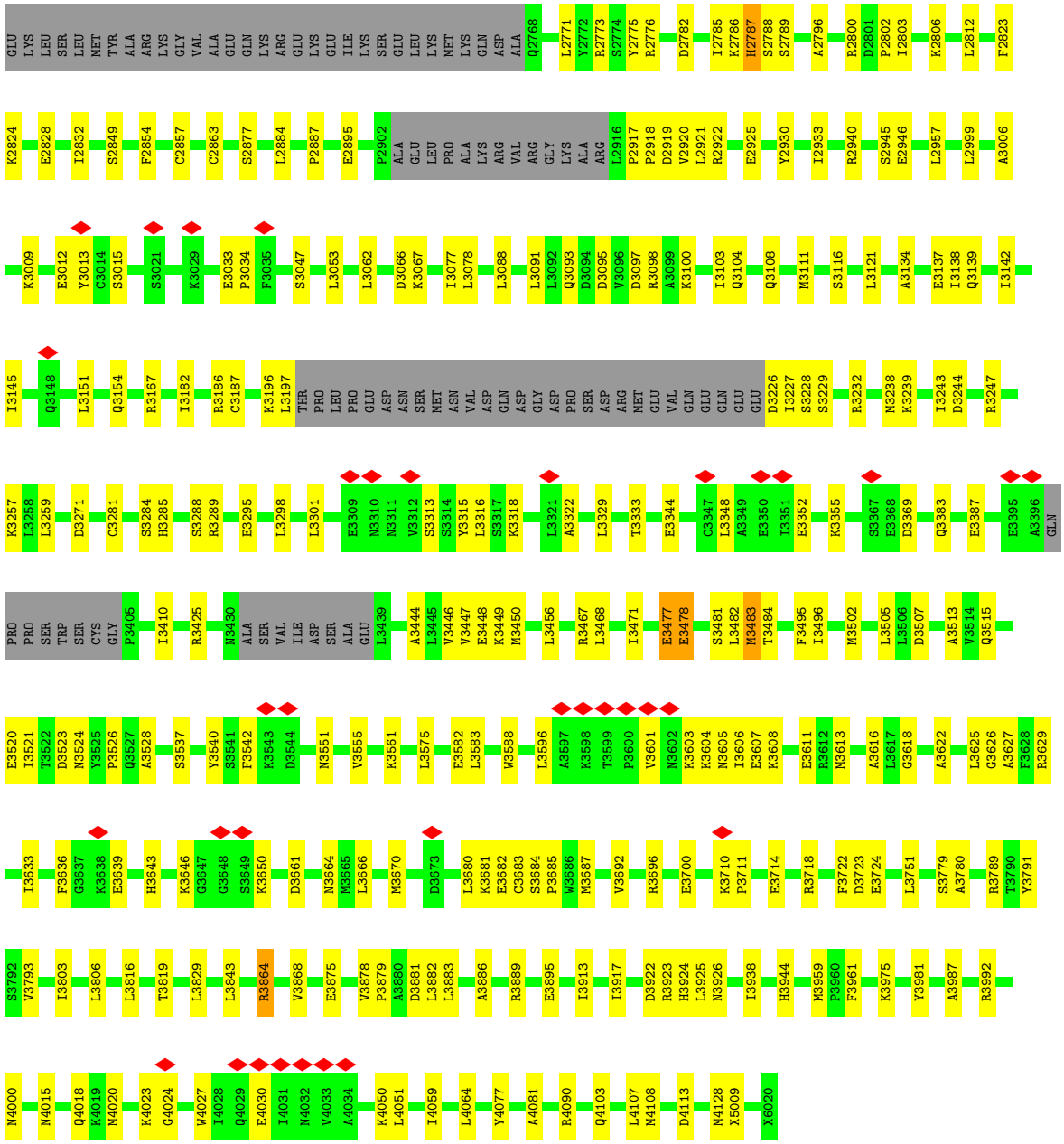
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:




Q1125 Q1126 D1129 R1151 P1158 P1159 L1163 L1168 R1178 E1182 C1183 R1184 H1185 I1188 V1195 P1204 L1208 L1212 V1217 S1218 F1219 L1220 I1221 N1222 T1223 F1224 E1225 Q1231 P1232 S1233 G1234 I1235 L1236 T1240 L1241 L1242 S1249 L1259 L1260 L1261 E1265 C1266
Y1267 N1268 T1269 T1284 L1290 F1296 S1300 H1304 E1310 K1311 C1312 PHE GLY T1315 G1316 A1317 A1318 G1319 N1320 R1321 T1322 S1323 P1324 Q1325 K1334 V1339 R1340 L1348 T1351 S1352 P1353 L1358 L1359 K1360 N1366 T1366 L1372 V1373 Q1374 T1375 L1376 C1377 E1378 S1381 I1382
I1386 G1387 V1391 M1392 L1395 V1398 L1402 M1403 P1410 T1424 S1427 L1431 C1432 Q1442 R1445 S1446 R1447 L1448 V1452 L1458 I1467 S1470 Q1471 H1476 H1477 S1478 V1479 E1482 L1483 L1484 S1485 L1486 G1494 D1495 E1496 R1497 Q1498 C1499 L1510 L1514
F1519 C1525 E1526 R1527 L1528 L1532 L1538 A1541 SER LEU GLY SER SER GLN GLY S1549 V1550 F1553 Y1560 S1561 L1562 I1567 E1570 L1571 L1572 K1573 N1574 L1575 S1585 S1586 Q1614 K1617 L1618 I1622 K1627 W1632 W1633 A1634 K1635 D1636 E1640 T1641 K1642 I1652
D1685 K1689 G1690 V1693 R1711 L1714 E1715 I1718 F1722 G1732 T1733 P1734 R1735 Q1754 L1759 E1760 E1769 Q1770 F1782 I1785 A1786 R1787 R1788 G1789 S1790 T1793 Q1794 V1795 G1796 L1797 Y1802 R1806 R1811 L1812 S1813 F1814 T1815 R1816 Q1817 S1818 F1819 V1820 D1821
R1822 S1823 L1824 L1827 S1832 L1836 R1837 E1838 R1854 K1857 L1858 N1859 D1864 I1867 M1871 Y1874 K1875 R1883 E1893 N1897 Q1898 V1899 F1900 H1901 G1902 S1903 T1912 I1916 Y1920 A1928 G1929 E1930 L1933 L1934 E1935 R1936 R1937 R1938 L1939 Y1940 N1957
F1961 Y1962 Q1963 S1968 L1975 L1976 L1981 K1985 ARG ARG TYR ASN PHE PRO VAL GLU VAL GLU VAL PRO MET GLU ARG 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 GLU GLN ARG ASP PRO THR VAL HIS ASP ASP VAL LEU GLU LEU GLU M2085 N2089 R2090 H2091 E2092 C2093 L2097
H2105 R2106 S2107 L2108 GLY PRO PRO GLN GLY GLU GLU ASP SER VAL P2119 R2120 D2121 L2122 L2133 F2145 I2151 E2155 R2158 W2164 L2165 S2166 P2167 L2168 L2169 S2174 E2175 N2176 H2183 V2186 V2187 E2188 I2189 S2195 V2205 P2206 K2207 D2208 E2209 V2210 L2211 A2212 N2213 R2214
L2215 M2220 F2224 F2231 L2235 P2252 Y2253 R2254 L2255 I2256 K2259 F2260 S2261 G2262 D2269 N2270 S2271 V2272 L2277 V2280 D2289 C2292 G2293 Q2301 V2304 N2305 K2313 Y2316 L2323 L2327 V2330 N2335 I2336 E2339 S2340 K2347 Q2348 L2349 K2350
Q2351 H2352 E2357 I2361 N2365 T2368 F2371 P2372 P2373 L2374 A2375 D2376 L2385 F2389 V2392 L2396 C2397 V2400 R2404 V2405 E2406 L2411 Y2412 F2413 Q2414 L2415 F2420 Q2432 I2439 Y2440 K2441 M2442 M2443 L2455 N2456 P2457 E2460 S2463 H2464 E2471
Y2474 N2475 I2476 D2486 P2487 E2488 S2489 E2490 I2498 L2517 R2522 L2531 T2535 L2539 L2542 E2551 L2555 A2558 T2559 N2560 F2561 L2562 L2563 M2568 P2575 M2576 C2584 E2585 R2596 PHE ARG SER THR V2601 V2607 GLU THR GLN ALA SER GLN GLY THR LEU
GLN THR ARG THR GLN GLU GLY SER LEU SER ALA ARG TRP PRO VAL ALA GLY GLN ILE ARG ALA THR GLN GLN GLN HIS ASP PHE THR LEU GLY LEU PRO GLY ASP GLU VAL ASP ASN LYS VAL LYS GLY ALA ALA 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 LYS SER VAL GLY PRO ASP PHE GLY LYS LYS ARG LEU LEU GLY LEU PRO GLY ASP GLU VAL ASP ASN LYS VAL LYS GLY ALA ALA GLY ARG THR ASP LEU LEU ARG LEU ARG ARG ARG PHE MET ARG ASP GLN


GLU LYS LEU SER LEU MET TYR ALA ARG LYS GLY VAL ALA GLU GLN LYS ARG GLU LYS GLU ILE LYS SER GLU LEU LYS MET LYS GLN ASP ALA Q2768 L2771 Y2772 R2773 S2774 Y2775 R2776 D2782 I2785 K2786 H2787 S2788 S2789 A2796 R2800 D2801 P2802 I2803 K2806 L2812 F2823
K2824 E2828 I2832 S2849 F2854 C2857 C2863 S2877 L2884 P2887 E2895 P2902 ALA GLU LEU PRO ALA LYS ARG VAL ARG GLY LYS ALA ARG L2916 P2917 P2918 D2919 V2920 L2921 R2922 E2925 Y2930 I2933 R2940 S2945 E2946 L2957 L2999 A3006
K3009 E3012 Y3013 C3014 S3015 S3021 K3029 E3033 P3034 F3035 S3047 L3053 L3062 D3066 K3067 I3077 L3078 L3088 L3091 L3092 Q3093 D3094 D3095 V3096 D3097 R3098 A3099 K3100 I3103 Q3104 Q3108 M3111 S3116 L3121 A3134 E3137 I3138 Q3139 I3142
I3145 Q3148 L3151 Q3154 R3167 I3182 R3186 C3187 K3196 L3197 THR PRO LEU PRO GLU ASP ASN SER MET ASN VAL ASP GLN ASP GLY ASP PRO SER ASP ARG MET GLU VAL GLN GLU GLN GLU GLU D3226 I3227 S3228 S3229 R3232 M3238 K3239 I3243 D3244 R3247
K3257 L3258 L3259 D3271 C3281 S3284 H3285 S3288 R3289 E3295 L3298 L3301 E3309 N3310 N3311 Y3312 S3313 S3314 Y3315 L3316 S3317 K3318 L3321 A3322 L3329 T3333 E3344 C3347 L3348 A3349 E3350 I3351 E3352 K3355 S3367 E3368 D3369 Q3383 E3387 E3395 A3396 GLN
PRO PRO SER TRP SER CYS GLY P3405 I3410 R3425 N3430 ALA SER VAL ILE ASP SER ALA GLU L3439 A3444 L3445 V3446 V3447 E3448 K3449 M3450 L3456 R3467 L3468 I3471 E3477 E3478 S3481 L3482 M3483 T3484 F3495 I3496 M3502 L3505 L3506 D3507 A3513 V3514 Q3515
E3520 I3521 T3522 D3523 N3524 Y3525 P3526 Q3527 A3528 S3537 Y3540 S3541 F3542 K3543 D3544 N3551 V3555 K3561 L3575 E3582 L3583 W3588 L3596 A3597 K3598 T3599 P3600 V3601 N3602 K3603 K3604 N3605 I3606 E3607 K3608 E3611 R3612 M3613 A3616 L3617 G3618 A3622 L3625 G3626 A3627 F3628 R3629
I3633 F3636 G3637 K3638 E3639 H3643 K3646 G3647 G3648 S3649 K3650 D3661 N3664 M3665 L3666 M3670 D3673 L3680 K3681 E3682 C3683 S3684 P3685 W3686 M3687 V3692 R3696 E3700 K3710 P3711 E3714 R3718 F3722 D3723 E3724 L3751 S3779 A3780 R3789 T3790 Y3791
S3792 V3793 I3803 L3806 L3816 T3819 L3829 L3843 R3864 V3868 E3875 V3878 P3879 A3880 D3881 L3882 L3883 A3886 R3889 E3895 I3913 I3917 D3922 R3923 H3924 L3925 N3926 I3938 H3944 M3959 P3960 F3961 K3975 Y3981 A3987 R3992
N4000 N4015 Q4018 K4019 M4020 K4023 G4024 W4027 I4028 Q4029 E4030 I4031 N4032 V4033 A4034 K4050 L4051 I4059 L4064 Y4077 A4081 R4090 Q4103 L4107 M4108 D4113 M4128 X5009 X6020

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80688	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 ($e^-/Å^2$)	53.95	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.352	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	280.36002, 280.36002, 280.36002	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.652, 0.652, 0.652	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	0.33	0/29848	0.46	0/40366

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	29385	0	29509	506	0
All	All	29385	0	29509	506	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 9.

All (506) 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:3444:ALA:HA	1:A:3482:LEU:CD2	1.99	0.93
1:A:3618:GLY:H	1:A:3633:ILE:HD12	1.46	0.80
1:A:3444:ALA:O	1:A:3482:LEU:HD21	1.83	0.79
1:A:899:ARG:HE	1:A:2568:MET:HB2	1.48	0.78
1:A:403:GLY:H	1:A:406:ARG:HH12	1.29	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1212:LEU:HD11	1:A:1217:VAL:HA	1.69	0.75
1:A:3186:ARG:HD3	1:A:3238:MET:HE3	1.69	0.75
1:A:4050:LYS:HE3	1:A:4059:ILE:HG21	1.71	0.73
1:A:2796:ALA:O	1:A:2800:ARG:NH1	2.21	0.73
1:A:3298:LEU:HD12	1:A:3333:THR:HG23	1.69	0.73
1:A:3444:ALA:CA	1:A:3482:LEU:CD2	2.66	0.72
1:A:1933:LEU:HD13	1:A:1936:ARG:HB3	1.71	0.72
1:A:3288:SER:O	1:A:3289:ARG:NH1	2.20	0.71
1:A:3444:ALA:HB1	1:A:3482:LEU:HD22	1.72	0.71
1:A:356:ASN:ND2	1:A:404:ASP:O	2.24	0.71
1:A:3444:ALA:CB	1:A:3482:LEU:HD22	2.21	0.71
1:A:2151:ILE:HG21	1:A:2188:GLU:HG2	1.73	0.71
1:A:3520:GLU:OE2	1:A:3524:ASN:ND2	2.25	0.70
1:A:3187:CYS:SG	1:A:3239:LYS:NZ	2.62	0.70
1:A:1240:THR:HG22	1:A:1242:LEU:H	1.56	0.69
1:A:767:GLU:HG2	1:A:851:ILE:HD11	1.75	0.69
1:A:1097:GLU:OE2	1:A:1151:ARG:NH2	2.25	0.69
1:A:899:ARG:NH2	1:A:2568:MET:SD	2.65	0.69
1:A:1083:ASN:ND2	1:A:1126:GLN:OE1	2.26	0.68
1:A:3281:CYS:HB2	1:A:3329:LEU:HD23	1.75	0.68
1:A:936:SER:OG	1:A:2773:ARG:NH1	2.27	0.68
1:A:1484:LEU:HD11	1:A:1527:ARG:HH12	1.57	0.68
1:A:3145:ILE:HD11	1:A:3196:LYS:HD2	1.74	0.68
1:A:1225:GLU:HB3	1:A:1236:LEU:HB2	1.75	0.68
1:A:709:LYS:NZ	1:A:713:GLU:OE2	2.27	0.67
1:A:16:GLN:NE2	1:A:17:GLU:OE2	2.27	0.66
1:A:75:SER:H	1:A:78:PHE:HB3	1.59	0.66
1:A:1185:HIS:NE2	1:A:1265:GLU:OE2	2.26	0.66
1:A:1334:LYS:NZ	1:A:1382:ILE:O	2.29	0.66
1:A:38:LEU:O	1:A:41:GLU:HB3	1.95	0.66
1:A:4064:LEU:HD13	1:A:4077:TYR:HB3	1.78	0.66
1:A:247:GLU:HG2	1:A:285:CYS:HB3	1.76	0.65
1:A:1432:CYS:HB3	1:A:1486:LEU:HD11	1.79	0.65
1:A:90:CYS:O	1:A:93:LEU:HB3	1.98	0.64
1:A:93:LEU:O	1:A:97:GLY:N	2.25	0.64
1:A:2365:ASN:HD22	1:A:2396:LEU:HD13	1.63	0.64
1:A:1151:ARG:NH1	1:A:1163:LEU:O	2.31	0.64
1:A:2563:LEU:HD13	1:A:2812:LEU:HD11	1.79	0.63
1:A:1897:ASN:HB3	1:A:1903:SER:HB2	1.81	0.63
1:A:3924:HIS:ND1	1:A:3926:ASN:OD1	2.29	0.63
1:A:3009:LYS:O	1:A:3013:TYR:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LYS:HA	1:A:176:GLU:HG3	1.81	0.63
1:A:374:LYS:HD2	1:A:423:TYR:HB3	1.82	0.62
1:A:1754:GLN:HA	1:A:1785:ILE:HD11	1.82	0.62
1:A:3444:ALA:HA	1:A:3482:LEU:HD21	1.82	0.62
1:A:463:LYS:HD3	1:A:545:LEU:HD22	1.80	0.61
1:A:2169:LEU:HD11	1:A:2215:LEU:HD22	1.80	0.61
1:A:2439:ILE:O	1:A:2443:MET:HG3	2.00	0.61
1:A:3515:GLN:NE2	1:A:3551:ASN:OD1	2.34	0.61
1:A:3448:GLU:HB3	1:A:3482:LEU:HD11	1.81	0.61
1:A:3495:PHE:HB3	1:A:3502:MET:HE3	1.82	0.61
1:A:3992:ARG:NH1	1:A:4103:GLN:OE1	2.33	0.61
1:A:2155:GLU:OE2	1:A:2158:ARG:NH2	2.34	0.60
1:A:3723:ASP:OD1	1:A:3724:GLU:N	2.35	0.60
1:A:2195:SER:O	1:A:5009:UNK:N	2.34	0.60
1:A:3864:ARG:NH1	1:A:3868:VAL:HG21	2.17	0.60
1:A:1733:THR:HG22	1:A:1735:ARG:H	1.67	0.60
1:A:3666:LEU:O	1:A:3670:MET:HG3	2.01	0.60
1:A:3477:GLU:HA	1:A:3477:GLU:OE1	2.01	0.60
1:A:3425:ARG:NH1	1:A:4000:ASN:OD1	2.35	0.60
1:A:2406:GLU:OE1	1:A:2441:LYS:NZ	2.34	0.59
1:A:4023:LYS:HG2	1:A:4024:GLY:H	1.67	0.59
1:A:1358:LEU:HD11	1:A:1410:PRO:HG2	1.84	0.59
1:A:3639:GLU:O	1:A:3643:HIS:N	2.28	0.59
1:A:3137:GLU:OE1	1:A:3186:ARG:NH2	2.35	0.59
1:A:3444:ALA:CA	1:A:3482:LEU:HD21	2.33	0.59
1:A:3646:LYS:H	1:A:3650:LYS:HB3	1.68	0.59
1:A:131:LEU:HD22	1:A:173:LYS:HD2	1.85	0.59
1:A:1871:MET:HG2	1:A:1940:TYR:HA	1.85	0.58
1:A:3444:ALA:HB2	1:A:3478:GLU:HG2	1.85	0.58
1:A:3154:GLN:OE1	1:A:3226:ASP:N	2.37	0.58
1:A:1125:GLN:NE2	1:A:1129:ASP:OD2	2.37	0.58
1:A:3684:SER:HB2	1:A:3685:PRO:HD3	1.85	0.58
1:A:2091:HIS:CE1	1:A:2093:CYS:SG	2.96	0.58
1:A:2357:GLU:HB3	1:A:2385:LEU:HD21	1.85	0.58
1:A:3284:SER:HB3	1:A:3301:LEU:HD12	1.84	0.58
1:A:1975:LEU:HD12	1:A:1976:LEU:HD12	1.86	0.58
1:A:4081:ALA:O	1:A:4090:ARG:NH1	2.36	0.58
1:A:4090:ARG:NH2	1:A:4113:ASP:OD2	2.37	0.57
1:A:1267:TYR:CD2	1:A:1290:LEU:HD22	2.39	0.57
1:A:205:LYS:HG2	1:A:249:PHE:HZ	1.70	0.57
1:A:628:GLU:OE2	1:A:631:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:LEU:HD23	1:A:1168:LEU:HD21	1.86	0.57
1:A:2361:ILE:HD12	1:A:2389:PHE:HE2	1.67	0.57
1:A:606:SER:OG	1:A:1026:ARG:NH2	2.37	0.56
1:A:108:LYS:HZ2	1:A:156:PHE:HZ	1.52	0.56
1:A:229:SER:HA	1:A:274:LEU:HD13	1.88	0.56
1:A:2919:ASP:OD1	1:A:2920:VAL:N	2.38	0.56
1:A:3961:PHE:HE2	1:A:4107:LEU:HD13	1.70	0.56
1:A:2260:PHE:O	1:A:2270:ASN:ND2	2.38	0.56
1:A:2347:LYS:O	1:A:2351:GLN:NE2	2.37	0.56
1:A:3244:ASP:OD1	1:A:3247:ARG:NH1	2.37	0.56
1:A:13:LEU:HD23	1:A:14:ARG:HE	1.70	0.56
1:A:1011:GLU:O	1:A:1015:ASP:N	2.38	0.56
1:A:1769:GLU:O	1:A:1822:ARG:NH2	2.24	0.56
1:A:3596:LEU:HD12	1:A:3601:VAL:HA	1.88	0.56
1:A:205:LYS:HG2	1:A:249:PHE:CZ	2.41	0.56
1:A:901:MET:SD	1:A:2535:THR:OG1	2.64	0.56
1:A:1525:CYS:SG	1:A:1574:ASN:ND2	2.78	0.56
1:A:3751:LEU:HD22	1:A:3803:ILE:HD11	1.87	0.56
1:A:203:GLU:O	1:A:206:THR:OG1	2.20	0.56
1:A:1754:GLN:HG3	1:A:1785:ILE:HG13	1.88	0.56
1:A:1541:ALA:HB2	1:A:1550:VAL:HG12	1.87	0.56
1:A:1961:PHE:O	1:A:1961:PHE:CD1	2.59	0.56
1:A:2224:PHE:HB2	1:A:2272:VAL:HG11	1.87	0.56
1:A:3295:GLU:OE2	1:A:3295:GLU:N	2.33	0.56
1:A:1819:PHE:O	1:A:1823:SER:OG	2.22	0.55
1:A:1867:ILE:O	1:A:1871:MET:HG3	2.06	0.55
1:A:1874:TYR:HE2	1:A:1940:TYR:HE1	1.54	0.55
1:A:771:ASN:OD1	1:A:854:ARG:NH2	2.40	0.55
1:A:1224:PHE:HD2	1:A:1267:TYR:HE1	1.55	0.55
1:A:3661:ASP:HA	1:A:3664:ASN:HD21	1.71	0.55
1:A:1442:GLN:HG3	1:A:1445:ARG:HH12	1.71	0.55
1:A:2254:ARG:NH1	1:A:2292:CYS:O	2.39	0.55
1:A:2443:MET:SD	1:A:2476:ILE:HG23	2.46	0.55
1:A:56:SER:HA	1:A:59:PHE:CD2	2.42	0.55
1:A:1484:LEU:HD11	1:A:1527:ARG:NH1	2.22	0.55
1:A:1759:LEU:HD12	1:A:1785:ILE:HD13	1.88	0.55
1:A:2168:LEU:HD22	1:A:2189:ILE:HD11	1.89	0.55
1:A:3608:LYS:O	1:A:3611:GLU:HG3	2.07	0.55
1:A:849:GLU:OE1	1:A:3108:GLN:NE2	2.38	0.54
1:A:3605:ASN:OD1	1:A:3606:ILE:N	2.40	0.54
1:A:4027:TRP:HE3	1:A:4030:GLU:HB3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ASP:OD1	1:A:129:ASP:N	2.40	0.54
1:A:1267:TYR:HD2	1:A:1290:LEU:HD22	1.72	0.54
1:A:2411:LEU:HD11	1:A:2415:LEU:HD23	1.90	0.54
1:A:932:GLU:OE2	1:A:2771:LEU:HD13	2.08	0.54
1:A:3680:LEU:HD23	1:A:3682:GLU:H	1.72	0.54
1:A:131:LEU:O	1:A:135:LEU:HG	2.08	0.54
1:A:1920:TYR:HE1	1:A:1963:GLN:CB	2.20	0.54
1:A:355:ASN:HB3	1:A:358:GLU:HG2	1.90	0.54
1:A:3710:LYS:HB2	1:A:3711:PRO:HD2	1.88	0.54
1:A:1920:TYR:CE1	1:A:1963:GLN:CB	2.91	0.54
1:A:267:VAL:HG23	1:A:268:PRO:HD3	1.90	0.54
1:A:79:ARG:HA	1:A:82:ARG:HB2	1.90	0.53
1:A:796:LEU:HD23	1:A:855:VAL:HG13	1.91	0.53
1:A:2474:TYR:HD2	1:A:2517:LEU:HD12	1.74	0.53
1:A:3627:ALA:HB3	1:A:3683:CYS:HB2	1.90	0.53
1:A:56:SER:HA	1:A:59:PHE:HD2	1.73	0.53
1:A:1351:THR:HG22	1:A:1353:PRO:HD2	1.90	0.53
1:A:1528:LEU:HD21	1:A:1567:ILE:HG23	1.90	0.53
1:A:1812:LEU:O	1:A:1815:THR:N	2.36	0.53
1:A:2918:PRO:HB2	1:A:2922:ARG:HH22	1.73	0.53
1:A:59:PHE:HA	1:A:62:ASP:HB2	1.91	0.53
1:A:2091:HIS:HE1	1:A:2093:CYS:SG	2.32	0.53
1:A:3495:PHE:HB3	1:A:3502:MET:CE	2.38	0.53
1:A:2999:LEU:HD21	1:A:3015:SER:O	2.09	0.53
1:A:3033:GLU:HG3	1:A:3034:PRO:HD3	1.91	0.53
1:A:1585:SER:O	1:A:1585:SER:OG	2.27	0.52
1:A:3661:ASP:HA	1:A:3664:ASN:ND2	2.24	0.52
1:A:2933:ILE:HD11	1:A:3121:LEU:HD22	1.91	0.52
1:A:2555:LEU:HD11	1:A:2854:PHE:HA	1.91	0.52
1:A:3348:LEU:O	1:A:3352:GLU:HG2	2.09	0.52
1:A:3622:ALA:HB3	1:A:3625:LEU:HB2	1.91	0.52
1:A:3097:ASP:OD1	1:A:3098:ARG:N	2.37	0.52
1:A:1519:PHE:CG	1:A:1570:GLU:HG3	2.45	0.52
1:A:3496:ILE:HD11	1:A:3521:ILE:HD11	1.92	0.52
1:A:170:VAL:O	1:A:171:LEU:HD22	2.10	0.52
1:A:1634:ALA:O	1:A:1642:LYS:NZ	2.29	0.52
1:A:2205:VAL:HB	1:A:2208:ASP:HB2	1.92	0.52
1:A:2121:ASP:OD1	1:A:2121:ASP:N	2.43	0.52
1:A:2457:PRO:O	1:A:2460:GLU:HG2	2.10	0.52
1:A:3053:LEU:HD11	1:A:3088:LEU:HD13	1.92	0.52
1:A:3507:ASP:HB3	1:A:3540:TYR:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ASP:HA	1:A:30:ALA:HB1	1.93	0.51
1:A:3243:ILE:HD13	1:A:3259:LEU:HD13	1.92	0.51
1:A:1086:TYR:O	1:A:1087:ARG:HB2	2.11	0.51
1:A:13:LEU:O	1:A:14:ARG:NE	2.43	0.51
1:A:1378:GLU:HG2	1:A:1378:GLU:O	2.10	0.51
1:A:1586:SER:O	1:A:1632:TRP:NE1	2.43	0.51
1:A:708:VAL:HG22	1:A:740:ILE:HG23	1.92	0.51
1:A:1224:PHE:HD2	1:A:1267:TYR:CE1	2.28	0.51
1:A:1575:LEU:H	1:A:1575:LEU:HD23	1.76	0.51
1:A:967:PRO:HD3	1:A:1010:LEU:HD12	1.93	0.51
1:A:2256:ILE:HG22	1:A:2260:PHE:HE2	1.76	0.51
1:A:3629:ARG:O	1:A:3633:ILE:HG12	2.11	0.51
1:A:1037:LEU:HD23	1:A:1085:ILE:HB	1.93	0.50
1:A:1934:LEU:O	1:A:1938:ARG:N	2.43	0.50
1:A:3646:LYS:N	1:A:3650:LYS:HB3	2.25	0.50
1:A:1818:SER:HA	1:A:1821:ASP:HB3	1.94	0.50
1:A:2259:LYS:HB3	1:A:2272:VAL:HG23	1.94	0.50
1:A:242:PRO:O	1:A:245:SER:OG	2.24	0.50
1:A:1532:LEU:HD11	1:A:1560:TYR:HB2	1.94	0.50
1:A:2828:GLU:O	1:A:2832:ILE:HG12	2.12	0.50
1:A:1234:GLY:HA2	1:A:1259:LEU:HD22	1.93	0.50
1:A:2368:THR:HG23	1:A:2372:PRO:HA	1.93	0.50
1:A:2522:ARG:HG2	1:A:2561:PHE:HE1	1.76	0.50
1:A:3944:HIS:NE2	1:A:4020:MET:SD	2.85	0.50
1:A:59:PHE:HB3	1:A:63:PHE:CE1	2.47	0.50
1:A:1374:GLN:HE22	1:A:1381:SER:HB3	1.76	0.50
1:A:3444:ALA:CA	1:A:3482:LEU:HD22	2.42	0.49
1:A:1817:GLN:OE1	1:A:1936:ARG:NH2	2.41	0.49
1:A:2584:CYS:SG	1:A:2585:GLU:N	2.85	0.49
1:A:2806:LYS:HG3	1:A:2857:CYS:HB2	1.93	0.49
1:A:403:GLY:O	1:A:406:ARG:NH1	2.46	0.49
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	1.94	0.49
1:A:1470:SER:HB3	1:A:1476:HIS:CD2	2.48	0.49
1:A:3596:LEU:HB2	1:A:3601:VAL:HG22	1.94	0.49
1:A:1006:THR:HG22	1:A:1009:LEU:HB2	1.94	0.49
1:A:1208:LEU:HD21	1:A:1220:LEU:HD11	1.94	0.49
1:A:1871:MET:HE1	1:A:1936:ARG:HH21	1.77	0.49
1:A:3062:LEU:HD13	1:A:3093:GLN:NE2	2.28	0.49
1:A:2542:LEU:HD21	1:A:2558:ALA:HA	1.95	0.49
1:A:36:ARG:HH21	1:A:39:GLY:HA3	1.76	0.49
1:A:251:PHE:HA	1:A:254:LYS:HZ2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2463:SER:O	1:A:2463:SER:OG	2.31	0.49
1:A:3446:VAL:O	1:A:3450:MET:HG2	2.13	0.49
1:A:2261:SER:OG	1:A:2262:GLY:N	2.46	0.48
1:A:2877:SER:OG	1:A:2925:GLU:HB3	2.13	0.48
1:A:397:LEU:HD21	1:A:438:LEU:HD22	1.95	0.48
1:A:2415:LEU:HD12	1:A:2420:PHE:CD1	2.48	0.48
1:A:1685:ASP:OD1	1:A:1685:ASP:N	2.42	0.48
1:A:3227:ILE:HD12	1:A:3227:ILE:H	1.78	0.48
1:A:3444:ALA:HA	1:A:3482:LEU:HD23	1.92	0.48
1:A:1782:PHE:HA	1:A:1785:ILE:HG22	1.94	0.48
1:A:3104:GLN:OE1	1:A:3139:GLN:NE2	2.46	0.48
1:A:3151:LEU:HD21	1:A:3197:LEU:HA	1.95	0.48
1:A:3616:ALA:O	1:A:3629:ARG:NH2	2.47	0.48
1:A:975:ASP:OD1	1:A:976:VAL:N	2.45	0.48
1:A:1864:ASP:HA	1:A:1867:ILE:HG12	1.95	0.48
1:A:2301:GLN:OE1	1:A:2305:ASN:ND2	2.46	0.48
1:A:2313:LYS:HA	1:A:2316:TYR:CE2	2.48	0.48
1:A:2786:LYS:O	1:A:2788:SER:N	2.47	0.48
1:A:3313:SER:HA	1:A:3316:LEU:HB2	1.96	0.48
1:A:253:LEU:HD11	1:A:271:GLY:HA3	1.94	0.48
1:A:1339:VAL:HG23	1:A:1398:VAL:HG21	1.95	0.48
1:A:12:LEU:O	1:A:16:GLN:HG2	2.14	0.47
1:A:301:CYS:O	1:A:309:LYS:NZ	2.38	0.47
1:A:1912:THR:O	1:A:1916:ILE:HG12	2.14	0.47
1:A:1471:GLN:N	1:A:1471:GLN:OE1	2.48	0.47
1:A:2097:LEU:HD12	1:A:2145:PHE:HZ	1.78	0.47
1:A:2304:VAL:HG12	1:A:2323:LEU:HD11	1.96	0.47
1:A:3444:ALA:C	1:A:3482:LEU:HD21	2.33	0.47
1:A:346:TYR:HB3	1:A:350:ARG:HH12	1.78	0.47
1:A:1323:SER:O	1:A:1325:GLN:N	2.48	0.47
1:A:2884:LEU:HD12	1:A:3116:SER:HB2	1.96	0.47
1:A:2432:GLN:OE1	1:A:2464:HIS:NE2	2.45	0.47
1:A:63:PHE:O	1:A:66:LEU:HB2	2.15	0.47
1:A:439:VAL:O	1:A:442:GLN:HB3	2.15	0.47
1:A:1009:LEU:HD21	1:A:1062:ARG:NH1	2.29	0.47
1:A:1933:LEU:HD12	1:A:1937:ARG:HG3	1.96	0.47
1:A:2091:HIS:CE1	1:A:2093:CYS:HG	2.32	0.47
1:A:1231:GLN:O	1:A:1233:SER:N	2.47	0.47
1:A:1793:THR:O	1:A:1797:LEU:HG	2.15	0.47
1:A:2206:PRO:O	1:A:2210:VAL:HG23	2.14	0.47
1:A:2213:ASN:OD1	1:A:2214:ARG:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2269:ASP:OD1	1:A:2269:ASP:N	2.46	0.47
1:A:942:LEU:HD11	1:A:991:LEU:HD21	1.97	0.47
1:A:14:ARG:O	1:A:18:THR:HG23	2.15	0.47
1:A:540:MET:SD	1:A:540:MET:N	2.88	0.47
1:A:1689:LYS:O	1:A:1693:VAL:HG13	2.15	0.46
1:A:2107:SER:O	1:A:2107:SER:OG	2.32	0.46
1:A:1711:ARG:NH2	1:A:1760:GLU:OE1	2.48	0.46
1:A:2376:ASP:OD1	1:A:2404:ARG:NE	2.41	0.46
1:A:1484:LEU:HD21	1:A:1527:ARG:HH22	1.80	0.46
1:A:2940:ARG:HG2	1:A:2957:LEU:HD22	1.95	0.46
1:A:3066:ASP:OD1	1:A:3067:LYS:N	2.48	0.46
1:A:195:ASN:O	1:A:198:ARG:HG3	2.15	0.46
1:A:1572:LEU:HD21	1:A:1618:LEU:HD22	1.96	0.46
1:A:3344:GLU:OE2	1:A:3348:LEU:HD23	2.15	0.46
1:A:3444:ALA:HB2	1:A:3478:GLU:CG	2.44	0.46
1:A:3449:LYS:HD3	1:A:3449:LYS:HA	1.72	0.46
1:A:726:LEU:HD21	1:A:754:MET:SD	2.55	0.46
1:A:3137:GLU:CD	1:A:3186:ARG:HE	2.19	0.46
1:A:861:SER:O	1:A:3167:ARG:NH1	2.46	0.46
1:A:2785:ILE:O	1:A:2789:SER:HB2	2.16	0.46
1:A:3100:LYS:HB3	1:A:3100:LYS:HE3	1.77	0.46
1:A:100:ILE:HB	1:A:102:PRO:HD3	1.98	0.46
1:A:1158:PRO:N	1:A:1159:PRO:HD2	2.31	0.46
1:A:2559:THR:O	1:A:2563:LEU:HB2	2.16	0.46
1:A:2361:ILE:HD12	1:A:2389:PHE:CE2	2.50	0.46
1:A:3447:VAL:HG22	1:A:3468:LEU:HD22	1.98	0.46
1:A:586:GLN:HB2	1:A:613:HIS:CD2	2.51	0.45
1:A:189:MET:SD	1:A:189:MET:N	2.90	0.45
1:A:2365:ASN:ND2	1:A:2396:LEU:HD13	2.27	0.45
1:A:3779:SER:OG	1:A:3780:ALA:N	2.50	0.45
1:A:1786:ALA:HB2	1:A:1827:LEU:HD23	1.99	0.45
1:A:180:LEU:HA	1:A:230:LEU:HD21	1.97	0.45
1:A:242:PRO:C	1:A:246:ARG:HE	2.20	0.45
1:A:404:ASP:HB2	1:A:1732:GLY:O	2.17	0.45
1:A:487:LEU:HD12	1:A:490:ILE:HD11	1.99	0.45
1:A:1188:ILE:HD13	1:A:1269:THR:HG21	1.98	0.45
1:A:1372:LEU:HD13	1:A:1402:LEU:HD23	1.98	0.45
1:A:2576:MET:HB3	1:A:2787:HIS:CD2	2.52	0.45
1:A:3369:ASP:OD1	1:A:3369:ASP:N	2.49	0.45
1:A:2877:SER:HG	1:A:2925:GLU:HB3	1.82	0.45
1:A:114:VAL:HG12	1:A:130:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1221:ILE:HD12	1:A:1221:ILE:H	1.82	0.45
1:A:2372:PRO:O	1:A:2374:LEU:N	2.50	0.45
1:A:3444:ALA:CB	1:A:3482:LEU:CD2	2.93	0.45
1:A:1572:LEU:HB3	1:A:1614:GLN:HE21	1.81	0.45
1:A:2539:LEU:HD13	1:A:2562:LEU:HD11	1.97	0.45
1:A:2930:TYR:HA	1:A:2933:ILE:HG22	1.98	0.45
1:A:3410:ILE:HD11	1:A:3456:LEU:HB3	1.98	0.45
1:A:3922:ASP:O	1:A:3923:ARG:NE	2.49	0.45
1:A:2551:GLU:OE2	1:A:2849:SER:OG	2.28	0.45
1:A:3484:THR:HG23	1:A:3513:ALA:HA	1.97	0.45
1:A:1124:ILE:HG23	1:A:1182:GLU:HG2	1.99	0.44
1:A:3793:VAL:HG13	1:A:3803:ILE:HG22	1.99	0.44
1:A:1478:SER:O	1:A:1482:GLU:HG3	2.17	0.44
1:A:3636:PHE:CE2	1:A:3670:MET:HG2	2.52	0.44
1:A:1019:ASP:HA	1:A:1026:ARG:HH11	1.83	0.44
1:A:1458:LEU:HD13	1:A:1467:ILE:HD11	2.00	0.44
1:A:3467:ARG:O	1:A:3471:ILE:HG12	2.17	0.44
1:A:3925:LEU:HD23	1:A:3925:LEU:HA	1.75	0.44
1:A:154:SER:HA	1:A:157:TYR:HD2	1.82	0.44
1:A:225:LYS:HZ3	1:A:253:LEU:HD13	1.82	0.44
1:A:275:PHE:CZ	1:A:293:LEU:HD21	2.53	0.44
1:A:1538:LEU:HD12	1:A:1553:PHE:CE1	2.52	0.44
1:A:1815:THR:O	1:A:1818:SER:OG	2.25	0.44
1:A:1864:ASP:N	1:A:1864:ASP:OD1	2.50	0.44
1:A:2327:LEU:HA	1:A:2330:VAL:HG12	1.99	0.44
1:A:2945:SER:HB2	1:A:2946:GLU:OE1	2.17	0.44
1:A:849:GLU:OE2	1:A:852:ARG:NH1	2.50	0.44
1:A:1640:GLU:OE1	1:A:1640:GLU:N	2.50	0.44
1:A:2183:HIS:CE1	1:A:2186:VAL:HG23	2.52	0.44
1:A:2471:GLU:HA	1:A:2517:LEU:HD11	1.98	0.44
1:A:2575:PRO:HA	1:A:2786:LYS:H	1.83	0.44
1:A:2849:SER:OG	1:A:2849:SER:O	2.36	0.44
1:A:3575:LEU:HD23	1:A:3575:LEU:HA	1.81	0.44
1:A:3881:ASP:OD1	1:A:3881:ASP:N	2.50	0.44
1:A:1300:SER:O	1:A:1300:SER:OG	2.32	0.44
1:A:3088:LEU:HD23	1:A:3088:LEU:HA	1.74	0.44
1:A:3700:GLU:HA	1:A:3718:ARG:HA	1.99	0.44
1:A:131:LEU:HD12	1:A:132:ILE:N	2.33	0.44
1:A:151:GLU:HB3	1:A:153:PHE:CE1	2.53	0.44
1:A:923:ASP:C	1:A:925:GLN:H	2.21	0.44
1:A:2863:CYS:SG	1:A:2895:GLU:HG3	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3878:VAL:HG21	1:A:4128:MET:HB3	1.98	0.44
1:A:3981:TYR:HD1	1:A:4108:MET:HE2	1.82	0.44
1:A:1448:LEU:HD21	1:A:1514:LEU:HD11	1.99	0.44
1:A:1636:ASP:N	1:A:1636:ASP:OD1	2.50	0.44
1:A:1715:GLU:HA	1:A:1718:ILE:HG12	1.98	0.44
1:A:2097:LEU:HD23	1:A:2097:LEU:HA	1.81	0.44
1:A:3285:HIS:HD2	1:A:3298:LEU:HD11	1.83	0.44
1:A:3819:THR:HG21	1:A:3886:ALA:HB2	2.00	0.44
1:A:1178:ARG:O	1:A:1184:ARG:NH2	2.51	0.43
1:A:2887:PRO:HB2	1:A:3895:GLU:HG3	2.00	0.43
1:A:3626:GLY:HA3	1:A:3684:SER:O	2.18	0.43
1:A:4107:LEU:HD23	1:A:4107:LEU:HA	1.79	0.43
1:A:1427:SER:O	1:A:1431:LEU:HD23	2.18	0.43
1:A:1820:VAL:HG12	1:A:1824:LEU:HD23	2.00	0.43
1:A:225:LYS:HZ3	1:A:253:LEU:HD22	1.82	0.43
1:A:493:LYS:O	1:A:625:ASN:ND2	2.51	0.43
1:A:671:SER:O	1:A:675:ARG:HG3	2.18	0.43
1:A:3603:LYS:HB3	1:A:3606:ILE:HG22	1.98	0.43
1:A:59:PHE:O	1:A:63:PHE:N	2.52	0.43
1:A:1770:GLN:N	1:A:1770:GLN:OE1	2.51	0.43
1:A:2522:ARG:HG2	1:A:2561:PHE:CE1	2.52	0.43
1:A:3383:GLN:O	1:A:3387:GLU:HG3	2.17	0.43
1:A:1690:GLY:HA2	1:A:1693:VAL:HG22	2.00	0.43
1:A:1802:TYR:O	1:A:1806:ARG:HG2	2.19	0.43
1:A:3186:ARG:HD3	1:A:3238:MET:CE	2.44	0.43
1:A:3523:ASP:OD1	1:A:3561:LYS:NZ	2.31	0.43
1:A:3588:TRP:CD1	1:A:3613:MET:HB2	2.52	0.43
1:A:1586:SER:O	1:A:1586:SER:OG	2.34	0.43
1:A:1627:LYS:HD2	1:A:1627:LYS:HA	1.83	0.43
1:A:3604:LYS:HA	1:A:3607:GLU:HG2	2.00	0.43
1:A:3714:GLU:N	1:A:3714:GLU:OE1	2.51	0.43
1:A:79:ARG:O	1:A:82:ARG:HB2	2.19	0.43
1:A:1365:ASN:OD1	1:A:1366:THR:N	2.51	0.43
1:A:174:VAL:O	1:A:177:LEU:HG	2.18	0.43
1:A:253:LEU:HD12	1:A:254:LYS:N	2.34	0.43
1:A:346:TYR:HD1	1:A:366:TYR:HH	1.66	0.43
1:A:221:ALA:O	1:A:225:LYS:HE3	2.18	0.43
1:A:2220:MET:HB3	1:A:2255:LEU:HD22	2.01	0.43
1:A:320:LEU:HD23	1:A:320:LEU:HA	1.80	0.43
1:A:563:LEU:O	1:A:567:GLU:HG2	2.19	0.43
1:A:1391:VAL:HG13	1:A:1392:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1622:ILE:HG21	1:A:1652:ILE:HD11	2.00	0.43
1:A:287:LEU:HG	1:A:326:MET:SD	2.59	0.42
1:A:1476:HIS:HB3	1:A:1479:VAL:HG22	2.01	0.42
1:A:1935:GLU:OE2	1:A:1938:ARG:NE	2.34	0.42
1:A:2415:LEU:HD12	1:A:2420:PHE:CG	2.53	0.42
1:A:2531:LEU:HD12	1:A:2531:LEU:HA	1.88	0.42
1:A:3227:ILE:O	1:A:3228:SER:HB3	2.19	0.42
1:A:466:LEU:HB3	1:A:560:LEU:HD22	2.01	0.42
1:A:1218:SER:O	1:A:1222:ASN:ND2	2.52	0.42
1:A:3542:PHE:HZ	1:A:3555:VAL:HG11	1.84	0.42
1:A:3975:LYS:HA	1:A:3975:LYS:HD3	1.93	0.42
1:A:192:ASN:N	1:A:192:ASN:OD1	2.52	0.42
1:A:765:LEU:HD23	1:A:765:LEU:HA	1.72	0.42
1:A:853:ILE:HA	1:A:3111:MET:HE1	2.00	0.42
1:A:1714:LEU:HD23	1:A:1714:LEU:HA	1.86	0.42
1:A:3095:ASP:N	1:A:3095:ASP:OD1	2.52	0.42
1:A:240:GLU:HB3	1:A:242:PRO:HD2	2.01	0.42
1:A:469:ALA:HB2	1:A:479:ILE:HD11	2.02	0.42
1:A:737:PRO:HD2	1:A:740:ILE:HD12	2.01	0.42
1:A:1358:LEU:HD21	1:A:1410:PRO:HB2	2.01	0.42
1:A:1496:GLU:OE1	1:A:1496:GLU:N	2.42	0.42
1:A:2486:ASP:HB3	1:A:2489:SER:HB2	2.01	0.42
1:A:3789:ARG:HG2	1:A:3938:ILE:HG12	2.01	0.42
1:A:1395:LEU:O	1:A:1398:VAL:HG22	2.20	0.42
1:A:2166:SER:OG	1:A:2167:PRO:HD3	2.20	0.42
1:A:2455:LEU:HD22	1:A:2498:ILE:HG23	2.01	0.42
1:A:2576:MET:HB3	1:A:2787:HIS:NE2	2.34	0.42
1:A:3582:GLU:HG2	1:A:3583:LEU:N	2.35	0.42
1:A:3681:LYS:O	1:A:3685:PRO:HD2	2.19	0.42
1:A:3879:PRO:HB2	1:A:3882:LEU:HG	2.01	0.42
1:A:128:LEU:HD13	1:A:131:LEU:HD21	2.02	0.42
1:A:355:ASN:OD1	1:A:356:ASN:N	2.52	0.42
1:A:623:PHE:CE2	1:A:665:GLY:HA3	2.54	0.42
1:A:3077:ILE:HG13	1:A:3078:LEU:N	2.34	0.42
1:A:113:SER:O	1:A:116:THR:OG1	2.31	0.42
1:A:236:LYS:HD3	1:A:246:ARG:HH12	1.84	0.42
1:A:523:THR:HG23	1:A:525:LYS:H	1.85	0.42
1:A:1242:LEU:HA	1:A:1310:GLU:HB2	2.01	0.42
1:A:1376:LEU:HD13	1:A:1403:MET:HE1	2.01	0.42
1:A:1448:LEU:O	1:A:1452:VAL:HG13	2.20	0.42
1:A:3229:SER:OG	1:A:3232:ARG:NH1	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3318:LYS:O	1:A:3322:ALA:HB3	2.19	0.42
1:A:3526:PRO:C	1:A:3528:ALA:H	2.23	0.42
1:A:3829:LEU:HD23	1:A:3829:LEU:HA	1.92	0.42
1:A:3875:GLU:O	1:A:3878:VAL:HG12	2.19	0.42
1:A:3917:ILE:HD13	1:A:4051:LEU:HD21	2.00	0.42
1:A:109:ASN:OD1	1:A:110:THR:N	2.53	0.42
1:A:3006:ALA:HB3	1:A:3257:LYS:HE2	2.01	0.42
1:A:3138:ILE:O	1:A:3142:ILE:HG12	2.20	0.42
1:A:3271:ASP:HB2	1:A:3315:TYR:CE2	2.55	0.42
1:A:42:CYS:HA	1:A:88:PHE:CE1	2.55	0.42
1:A:195:ASN:OD1	1:A:196:LEU:N	2.52	0.42
1:A:1195:VAL:HG11	1:A:1204:PRO:HA	2.01	0.42
1:A:4015:ASN:O	1:A:4018:GLN:HG3	2.20	0.42
1:A:12:LEU:HA	1:A:15:LEU:HB3	2.00	0.42
1:A:60:SER:OG	1:A:61:ARG:N	2.53	0.42
1:A:251:PHE:HA	1:A:254:LYS:NZ	2.35	0.41
1:A:1431:LEU:HD11	1:A:1447:ARG:NH2	2.35	0.41
1:A:31:GLY:HA2	1:A:34:LEU:HB2	2.03	0.41
1:A:669:LEU:HD12	1:A:669:LEU:HA	1.90	0.41
1:A:1424:THR:HG23	1:A:1427:SER:H	1.85	0.41
1:A:1871:MET:O	1:A:1875:LYS:HG3	2.20	0.41
1:A:2802:PRO:HG2	1:A:2803:ILE:HD12	2.02	0.41
1:A:2921:LEU:O	1:A:2925:GLU:HG2	2.19	0.41
1:A:29:LEU:HD13	1:A:32:HIS:HB3	2.02	0.41
1:A:442:GLN:HG3	1:A:461:ILE:HD11	2.02	0.41
1:A:888:ARG:HB3	1:A:3889:ARG:HH21	1.85	0.41
1:A:995:PHE:HB3	1:A:1005:ASP:OD1	2.19	0.41
1:A:1374:GLN:HE22	1:A:1381:SER:CB	2.33	0.41
1:A:2252:PRO:C	1:A:2254:ARG:H	2.24	0.41
1:A:2397:CYS:O	1:A:2400:VAL:HG12	2.20	0.41
1:A:2771:LEU:HD12	1:A:2775:TYR:HE2	1.85	0.41
1:A:220:LEU:O	1:A:224:LEU:HG	2.21	0.41
1:A:3537:SER:HA	1:A:3540:TYR:CE2	2.55	0.41
1:A:202:GLY:HA2	1:A:205:LYS:HE2	2.02	0.41
1:A:1538:LEU:HD12	1:A:1553:PHE:HE1	1.86	0.41
1:A:1575:LEU:HD11	1:A:1617:LYS:HG3	2.03	0.41
1:A:3791:TYR:HB3	1:A:3806:LEU:HD21	2.02	0.41
1:A:3913:ILE:HG21	1:A:3987:ALA:HB3	2.02	0.41
1:A:36:ARG:NE	1:A:36:ARG:HA	2.36	0.41
1:A:2211:LEU:HA	1:A:2214:ARG:HG2	2.02	0.41
1:A:2277:LEU:O	1:A:2280:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3816:LEU:HD21	1:A:3883:LEU:HD13	2.01	0.41
1:A:275:PHE:HZ	1:A:293:LEU:HD21	1.84	0.41
1:A:1081:ALA:O	1:A:1085:ILE:HG23	2.21	0.41
1:A:1261:LEU:CD1	1:A:1340:ARG:HG3	2.51	0.41
1:A:1795:VAL:HG21	1:A:1838:GLU:HG3	2.03	0.41
1:A:2349:LEU:HA	1:A:2352:HIS:CE1	2.56	0.41
1:A:3687:MET:HB3	1:A:3722:PHE:CD1	2.56	0.41
1:A:68:PHE:O	1:A:71:LYS:HB2	2.21	0.41
1:A:991:LEU:HD23	1:A:991:LEU:HA	1.85	0.41
1:A:1086:TYR:C	1:A:1088:GLU:H	2.22	0.41
1:A:1219:PHE:O	1:A:1223:THR:HG23	2.21	0.41
1:A:35:ILE:HG21	1:A:80:GLU:HB3	2.02	0.41
1:A:296:VAL:HG23	1:A:297:LEU:HD12	2.03	0.41
1:A:1240:THR:HG23	1:A:1296:PHE:CG	2.56	0.41
1:A:1718:ILE:O	1:A:1722:PHE:HB2	2.20	0.41
1:A:1836:LEU:HD21	1:A:1883:ARG:HH21	1.85	0.41
1:A:2339:GLU:HG2	1:A:2340:SER:N	2.36	0.41
1:A:2392:VAL:O	1:A:2396:LEU:HD23	2.21	0.41
1:A:3012:GLU:HB2	1:A:3047:SER:HB2	2.02	0.41
1:A:3134:ALA:HB2	1:A:3182:ILE:HG22	2.03	0.41
1:A:3227:ILE:HG22	1:A:3228:SER:N	2.36	0.41
1:A:3692:VAL:HG13	1:A:3692:VAL:O	2.21	0.41
1:A:3843:LEU:HD23	1:A:3843:LEU:HA	1.87	0.41
1:A:397:LEU:HD22	1:A:437:HIS:HB3	2.03	0.41
1:A:1348:LEU:HD23	1:A:1348:LEU:HA	1.84	0.41
1:A:2231:PHE:O	1:A:2235:LEU:HD23	2.21	0.41
1:A:2371:PHE:CD1	1:A:2373:PRO:HD2	2.56	0.41
1:A:2392:VAL:HG12	1:A:2396:LEU:HD23	2.03	0.41
1:A:3959:MET:HE3	1:A:3959:MET:H	1.86	0.41
1:A:2164:TRP:C	1:A:2167:PRO:HD2	2.42	0.40
1:A:2917:PRO:HB2	1:A:2919:ASP:OD1	2.20	0.40
1:A:3483:MET:O	1:A:3483:MET:HG3	2.16	0.40
1:A:3685:PRO:HB2	1:A:3687:MET:H	1.86	0.40
1:A:1445:ARG:HG3	1:A:1510:LEU:HD13	2.03	0.40
1:A:2411:LEU:C	1:A:2413:PHE:H	2.24	0.40
1:A:3091:LEU:HD23	1:A:3091:LEU:HA	1.88	0.40
1:A:3505:LEU:HD23	1:A:3505:LEU:H	1.86	0.40
1:A:1754:GLN:HE22	1:A:1788:ARG:HD2	1.86	0.40
1:A:2133:LEU:HD23	1:A:2164:TRP:CZ3	2.56	0.40
1:A:2776:ARG:NE	1:A:2782:ASP:OD1	2.54	0.40
1:A:471:LYS:HB2	1:A:474:VAL:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1030:GLY:O	1:A:1033:ILE:HG22	2.21	0.40
1:A:1562:LEU:HD23	1:A:1562:LEU:HA	1.85	0.40
1:A:2122:LEU:HD12	1:A:2122:LEU:HA	1.93	0.40
1:A:3100:LYS:O	1:A:3103:ILE:HG22	2.21	0.40
1:A:249:PHE:O	1:A:252:VAL:HG12	2.21	0.40
1:A:1790:SER:O	1:A:1794:GLN:HG3	2.21	0.40
1:A:2165:LEU:HA	1:A:2165:LEU:HD12	1.81	0.40
1:A:2823:PHE:CD2	1:A:2824:LYS:HG3	2.57	0.40
1:A:3478:GLU:N	1:A:3478:GLU:CD	2.75	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	3640/4156 (88%)	3332 (92%)	304 (8%)	4 (0%)	51 83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3481	SER
1	A	2787	HIS
1	A	1968	SER
1	A	1813	SER

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	3234/3671 (88%)	3222 (100%)	12 (0%)	91 95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	ARG
1	A	899	ARG
1	A	924	ARG
1	A	1321	ARG
1	A	1811	ARG
1	A	2105	HIS
1	A	3355	LYS
1	A	3477	GLU
1	A	3478	GLU
1	A	3483	MET
1	A	3696	ARG
1	A	3864	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1083	ASN
1	A	1374	GLN
1	A	1574	ASN
1	A	2091	HIS
1	A	2305	ASN
1	A	2351	GLN
1	A	2365	ASN
1	A	3139	GLN
1	A	3515	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	95.34
1	A	5016:UNK	C	6001:UNK	N	49.10

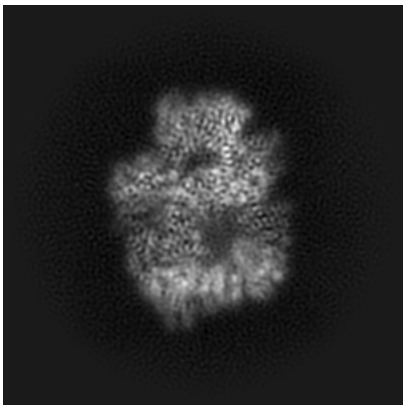
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11185. These allow visual inspection of the internal detail of the map and identification of artifacts.

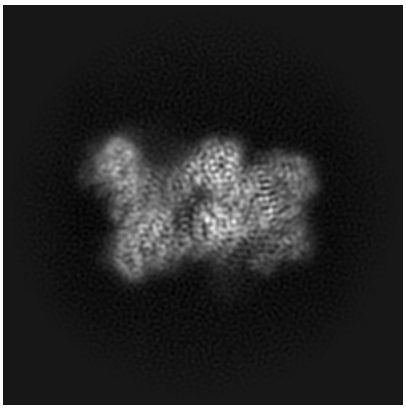
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

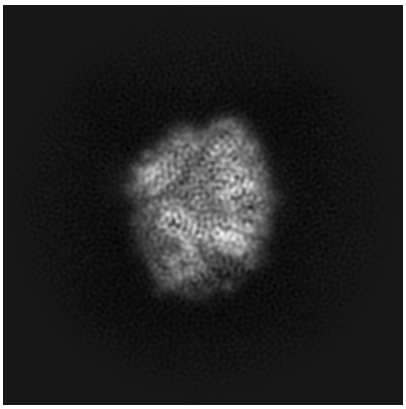
6.1.1 Primary map



X

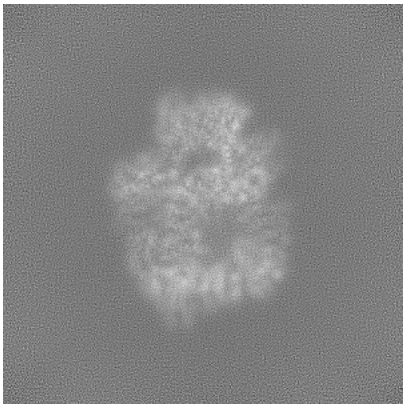


Y

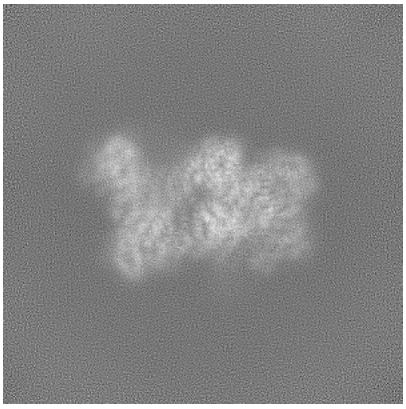


Z

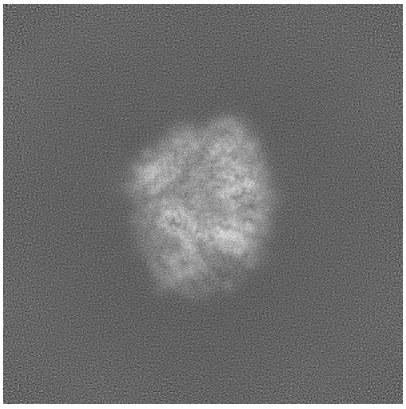
6.1.2 Raw map



X



Y

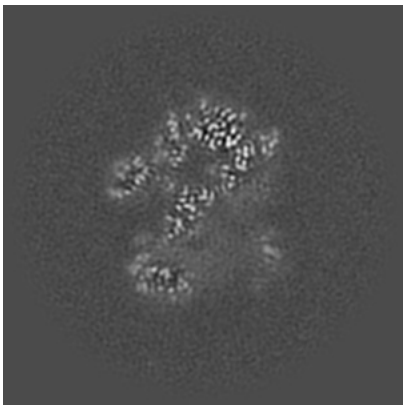


Z

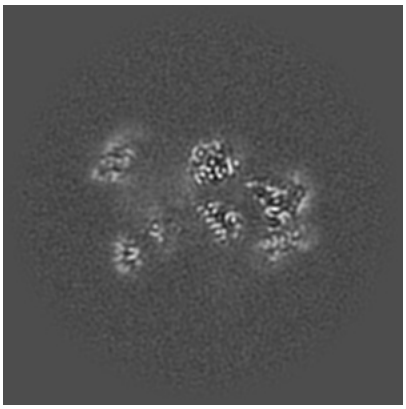
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

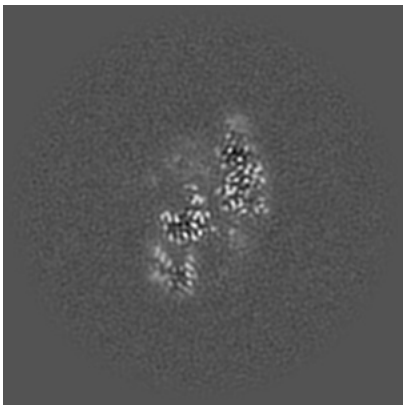
6.2.1 Primary map



X Index: 215

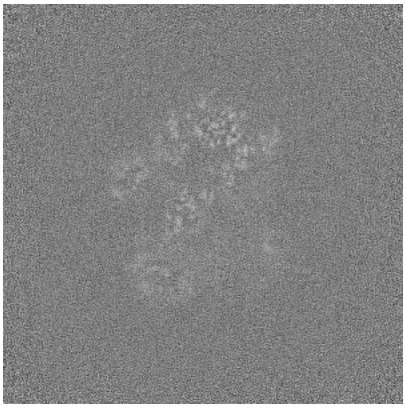


Y Index: 215

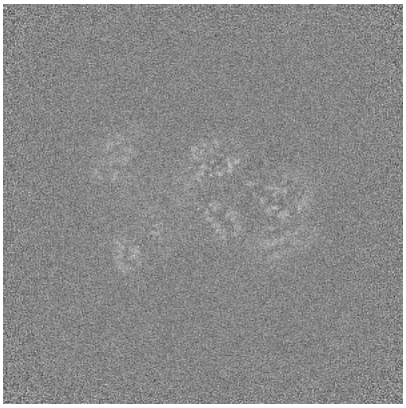


Z Index: 215

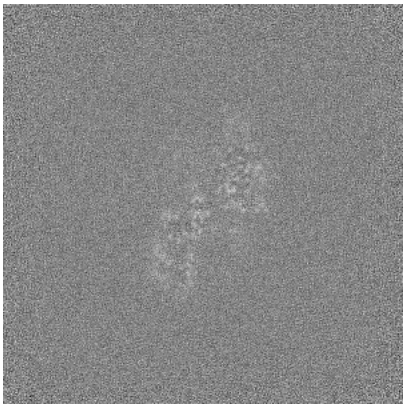
6.2.2 Raw map



X Index: 215



Y Index: 215

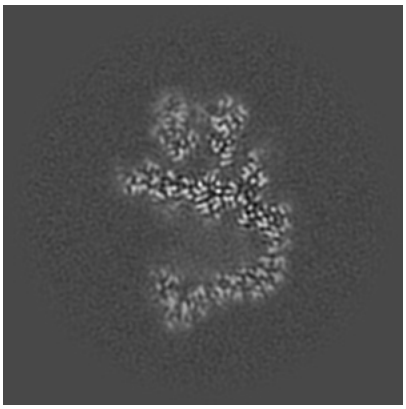


Z Index: 215

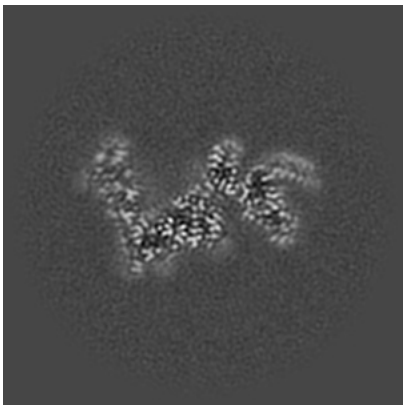
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

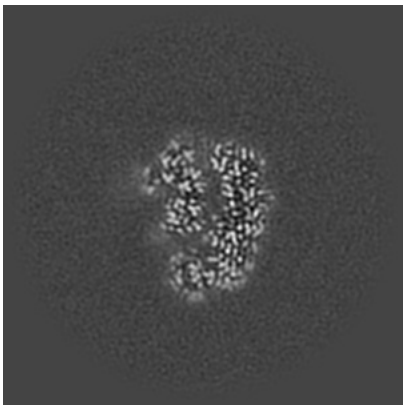
6.3.1 Primary map



X Index: 247

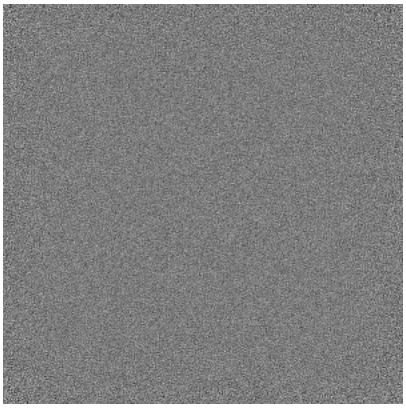


Y Index: 187

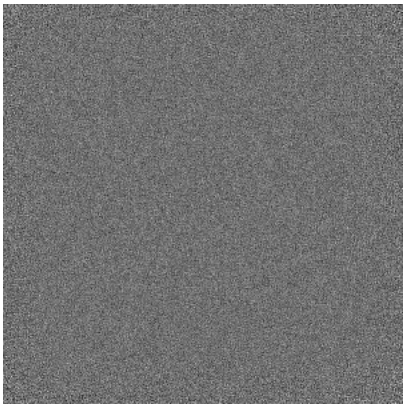


Z Index: 232

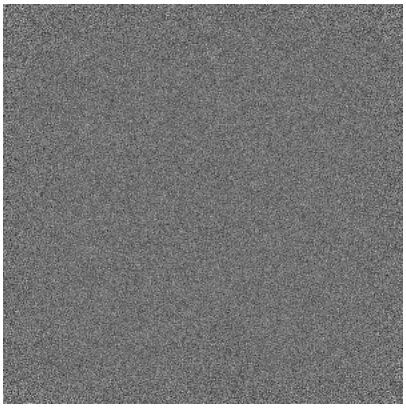
6.3.2 Raw map



X Index: 0



Y Index: 0

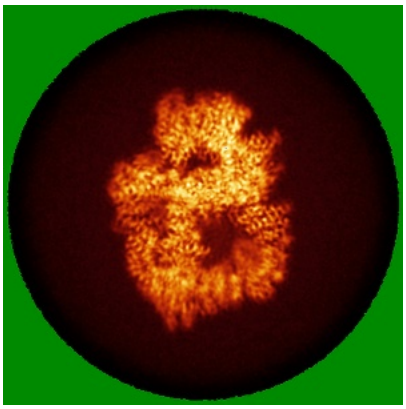


Z Index: 0

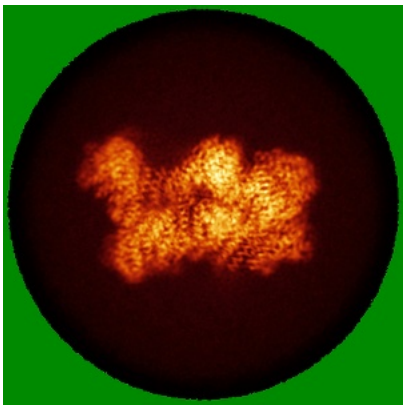
The images above show the largest variance slices of the map in three orthogonal directions.

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

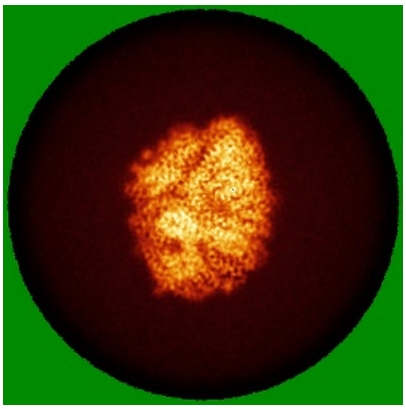
6.4.1 Primary map



X

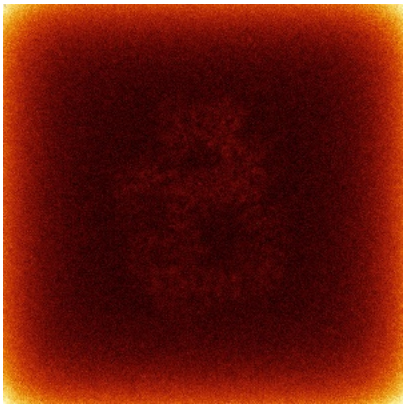


Y

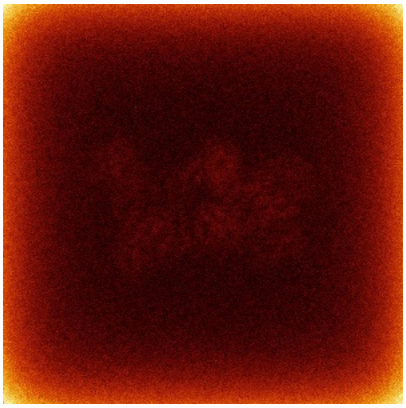


Z

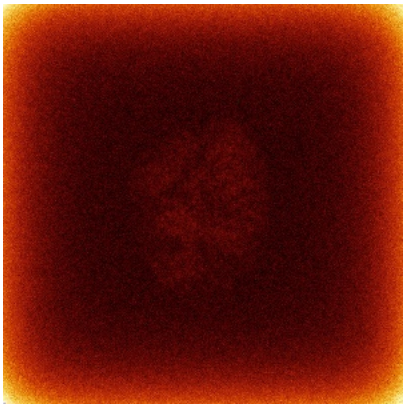
6.4.2 Raw map



X



Y

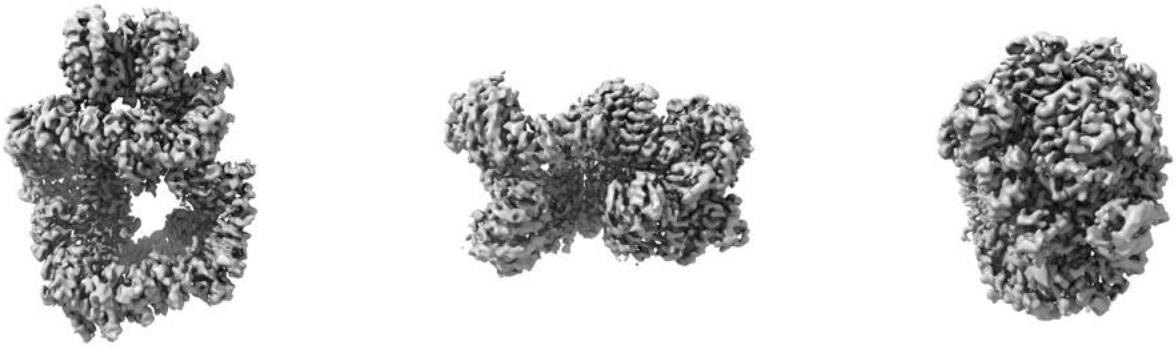


Z

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

6.5 Orthogonal surface views (i)

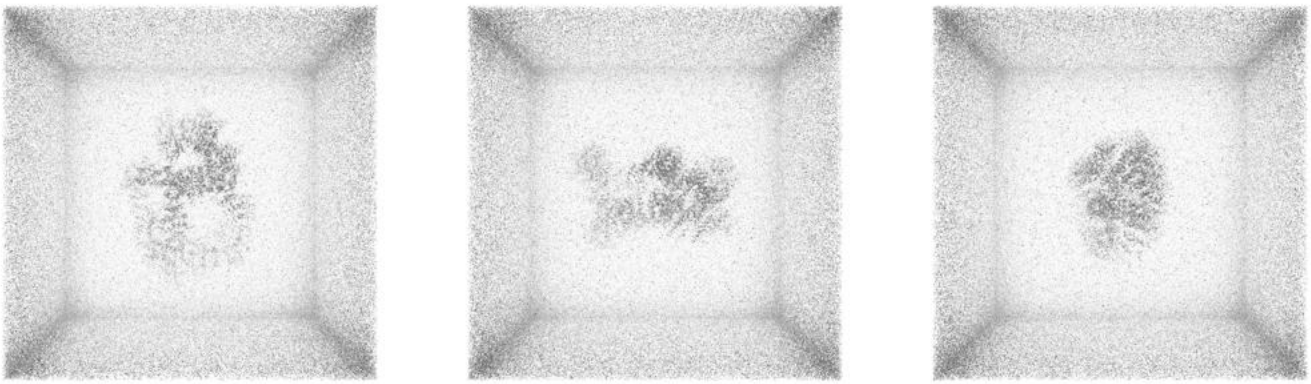
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

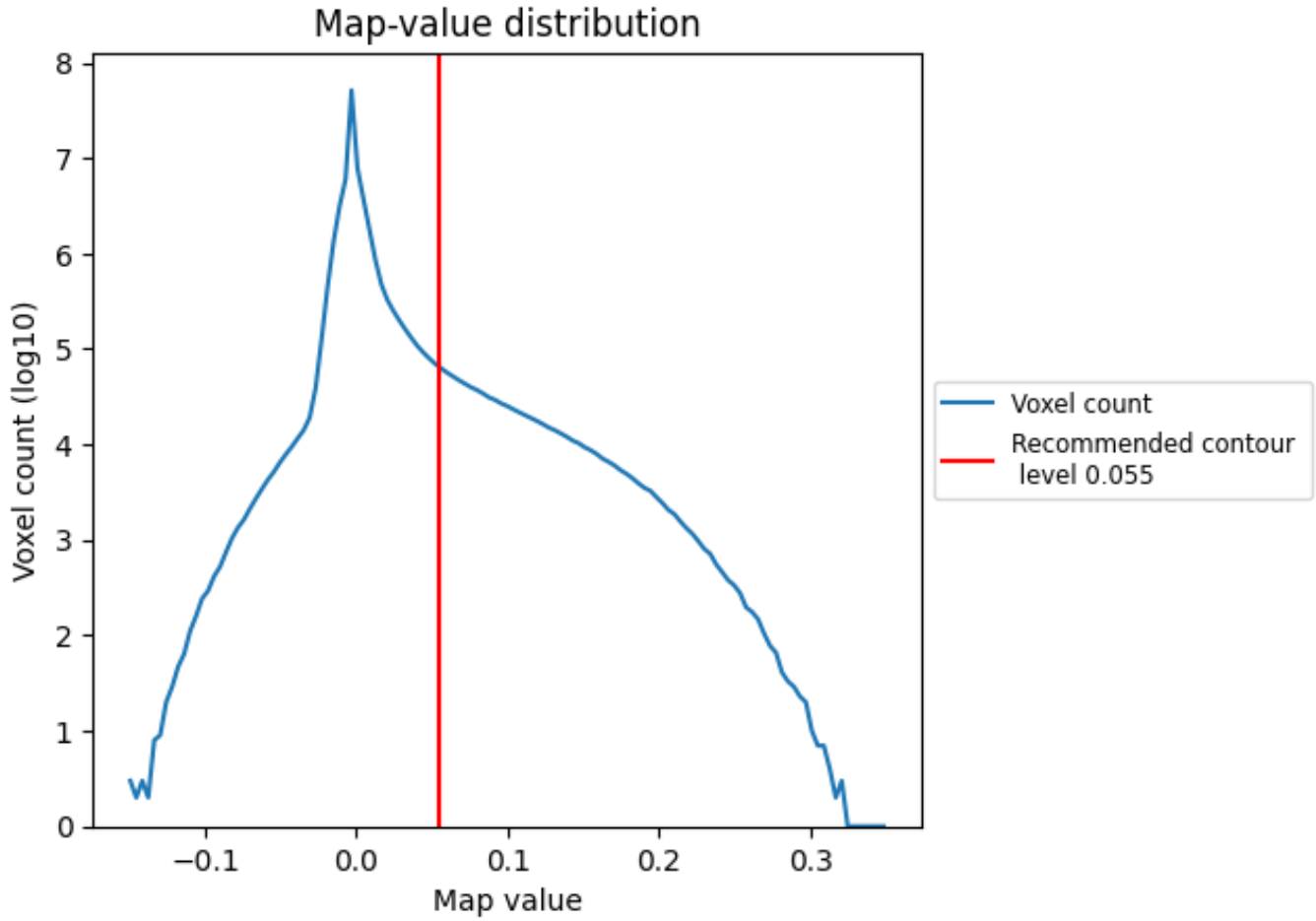
6.6 Mask visualisation (i)

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

7 Map analysis

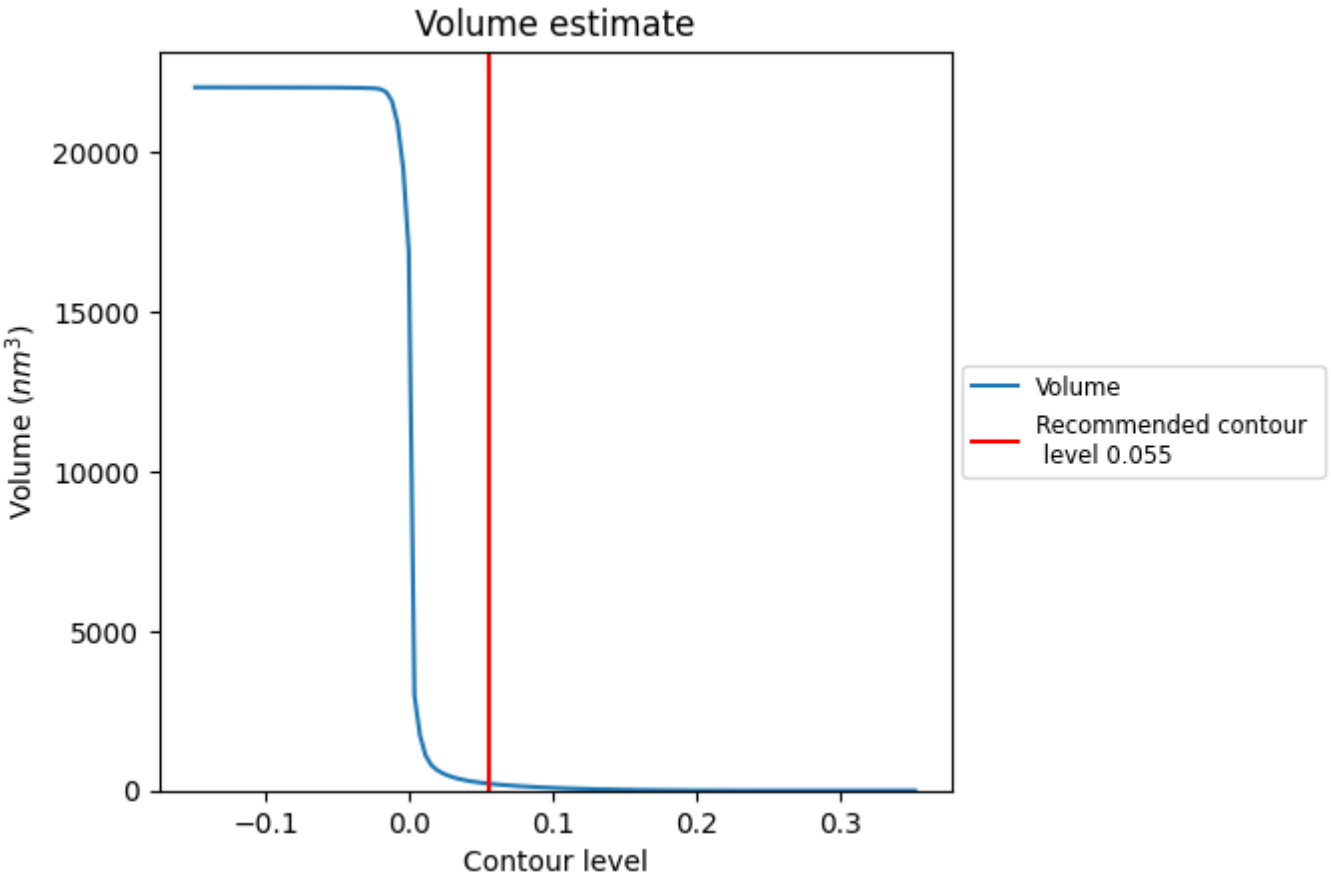
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

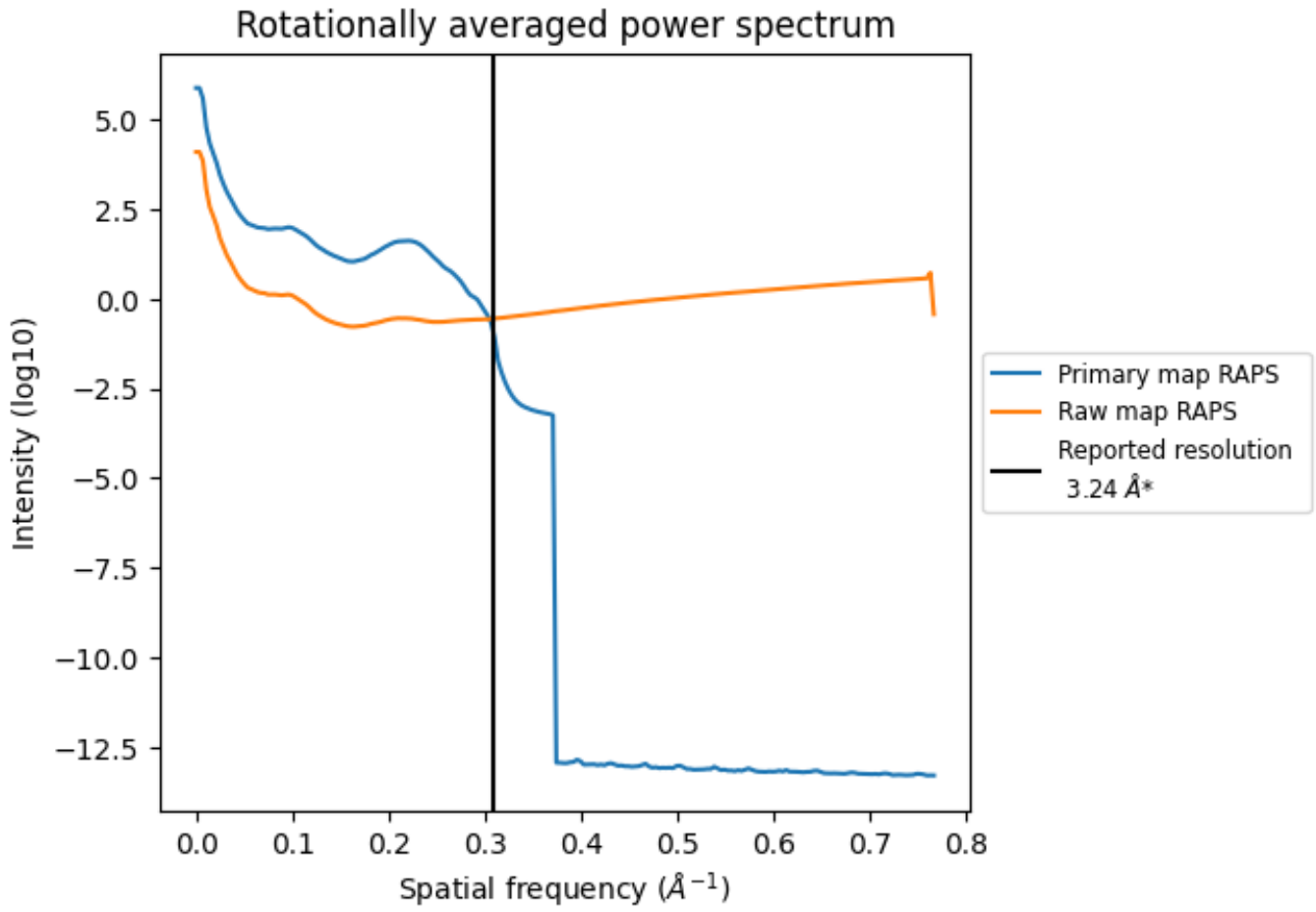
7.2 Volume estimate



The volume at the recommended contour level is 218 nm^3; this corresponds to an approximate mass of 197 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)

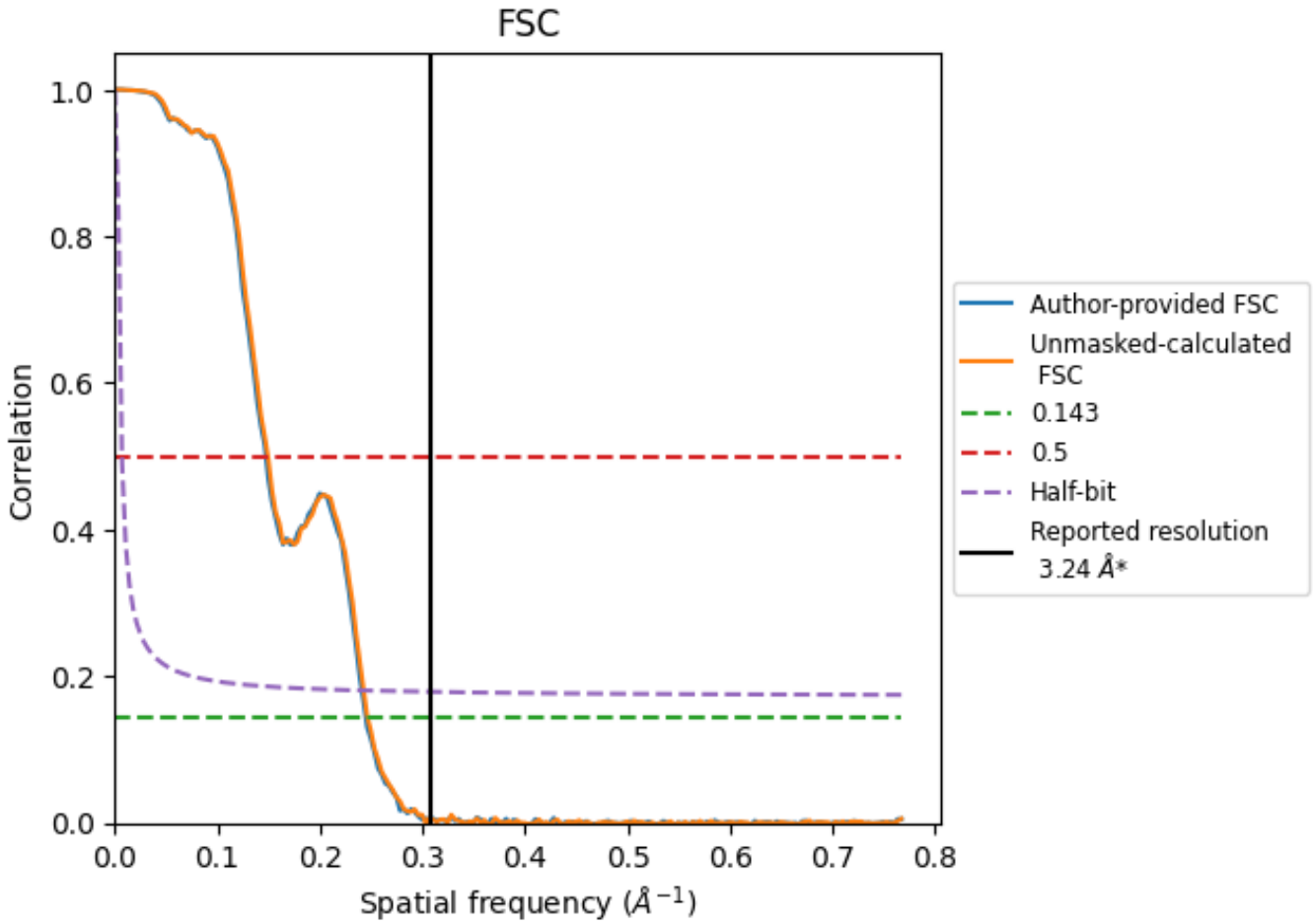


*Reported resolution corresponds to spatial frequency of 0.309 Å^{-1}

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 0.309 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	4.08	6.78	4.15
Unmasked-calculated*	4.06	6.70	4.12

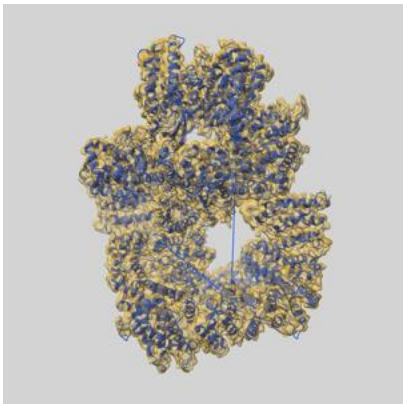
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.08 differs from the reported value 3.24 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.06 differs from the reported value 3.24 by more than 10 %

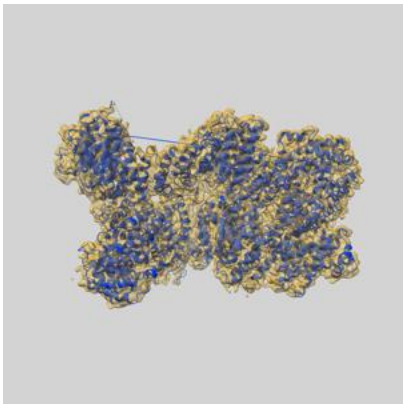
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11185 and PDB model 6ZFP. Per-residue inclusion information can be found in section 3 on page 4.

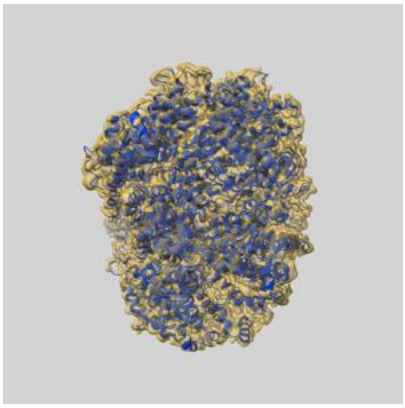
9.1 Map-model overlay



X



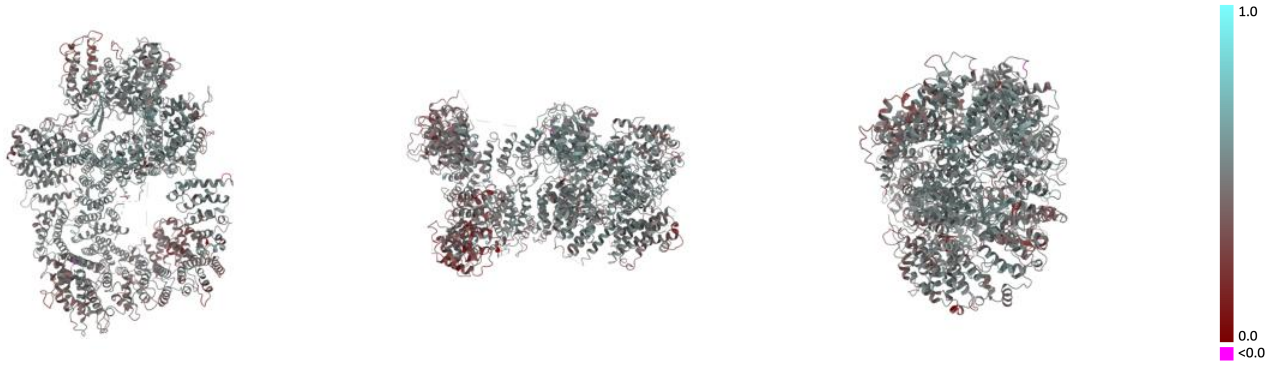
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.055 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.

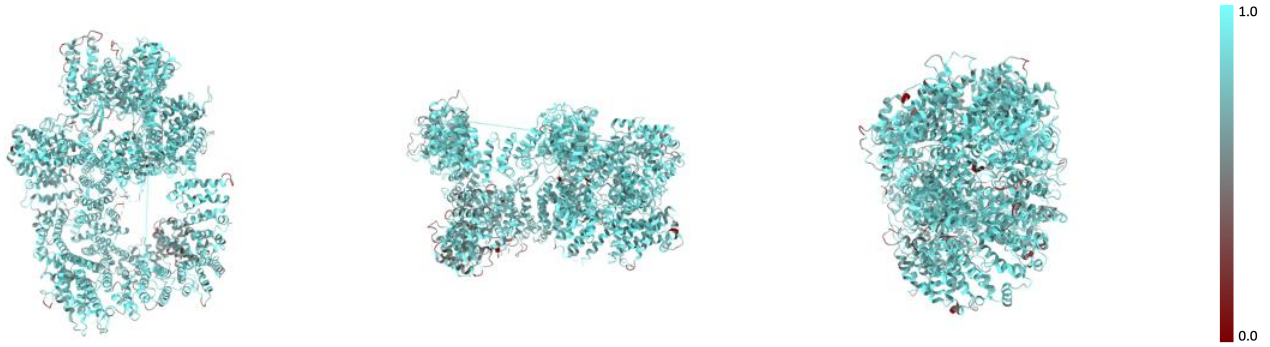
9.2 Q-score mapped to coordinate model (i)



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.

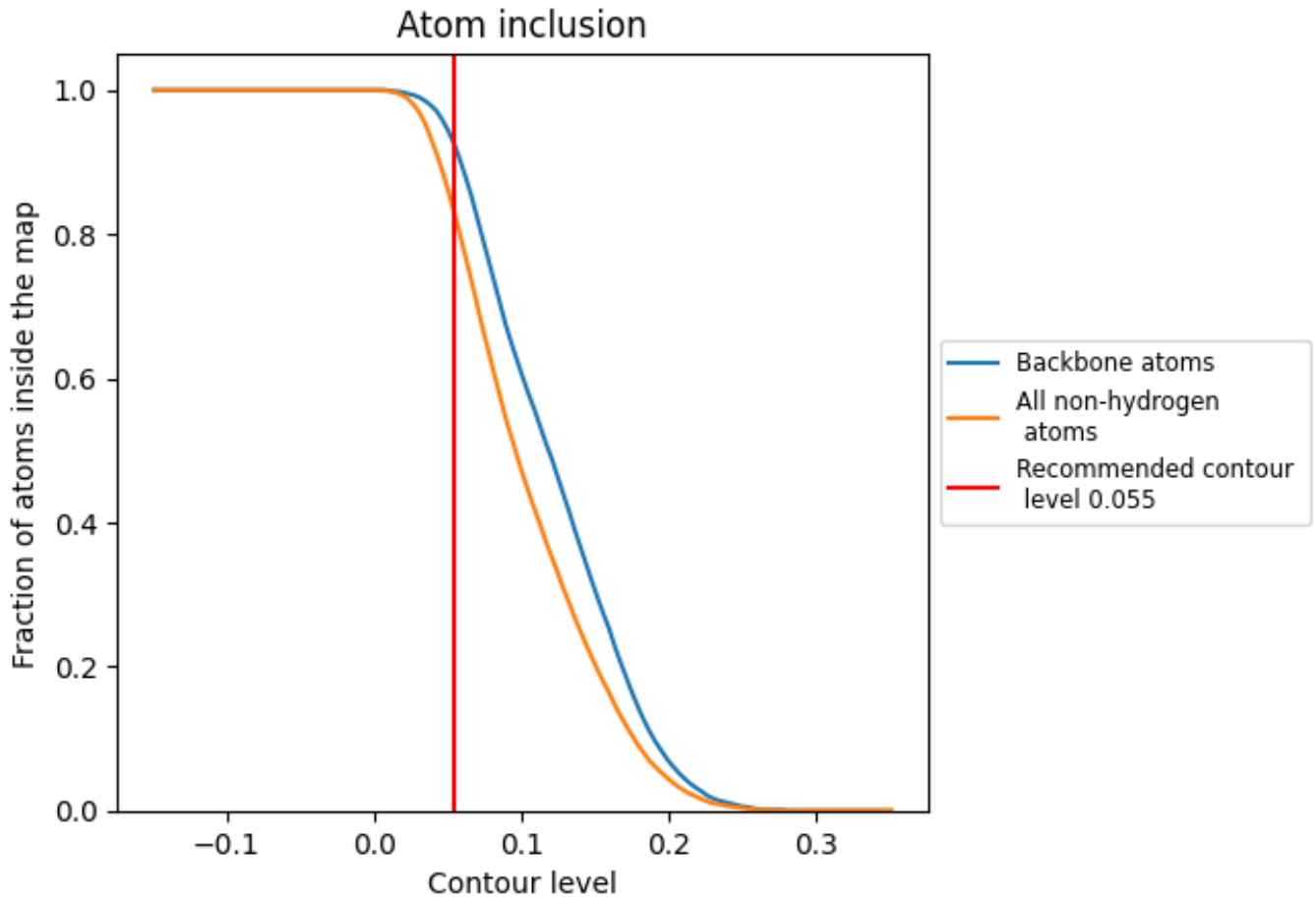
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.055).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 83% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8280	0.4720
A	0.8280	0.4720