Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 11:53 PM UTC

PDB ID	:	7OTP / pdb_00007otp
EMDB ID	:	EMD-13064
Title	:	DNA-PKcs in complex with ATPgammaS-Mg
Authors	:	Liang, S.; Thomas, S.E.; Blundell, T.L.
Deposited on	:	2021-06-10
Resolution	:	3.40 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:

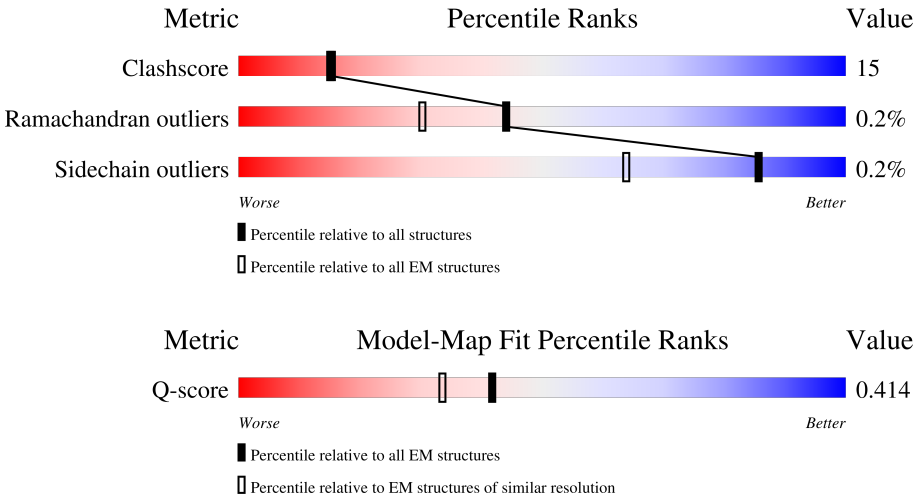
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	4148	5%, 61%, 27%, 12%

2 Entry composition (i)

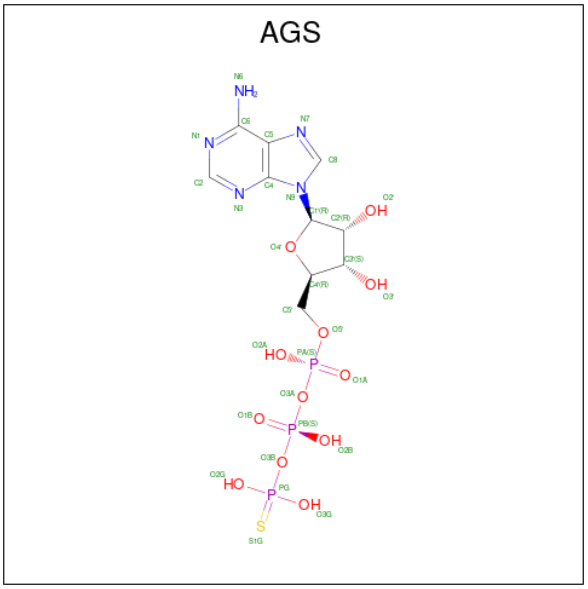
There are 3 unique types of molecules in this entry. The entry contains 29039 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	3656	29006	18606	4902	5307	191	0	0

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
2	A	1	31	10	5	12	3	1	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

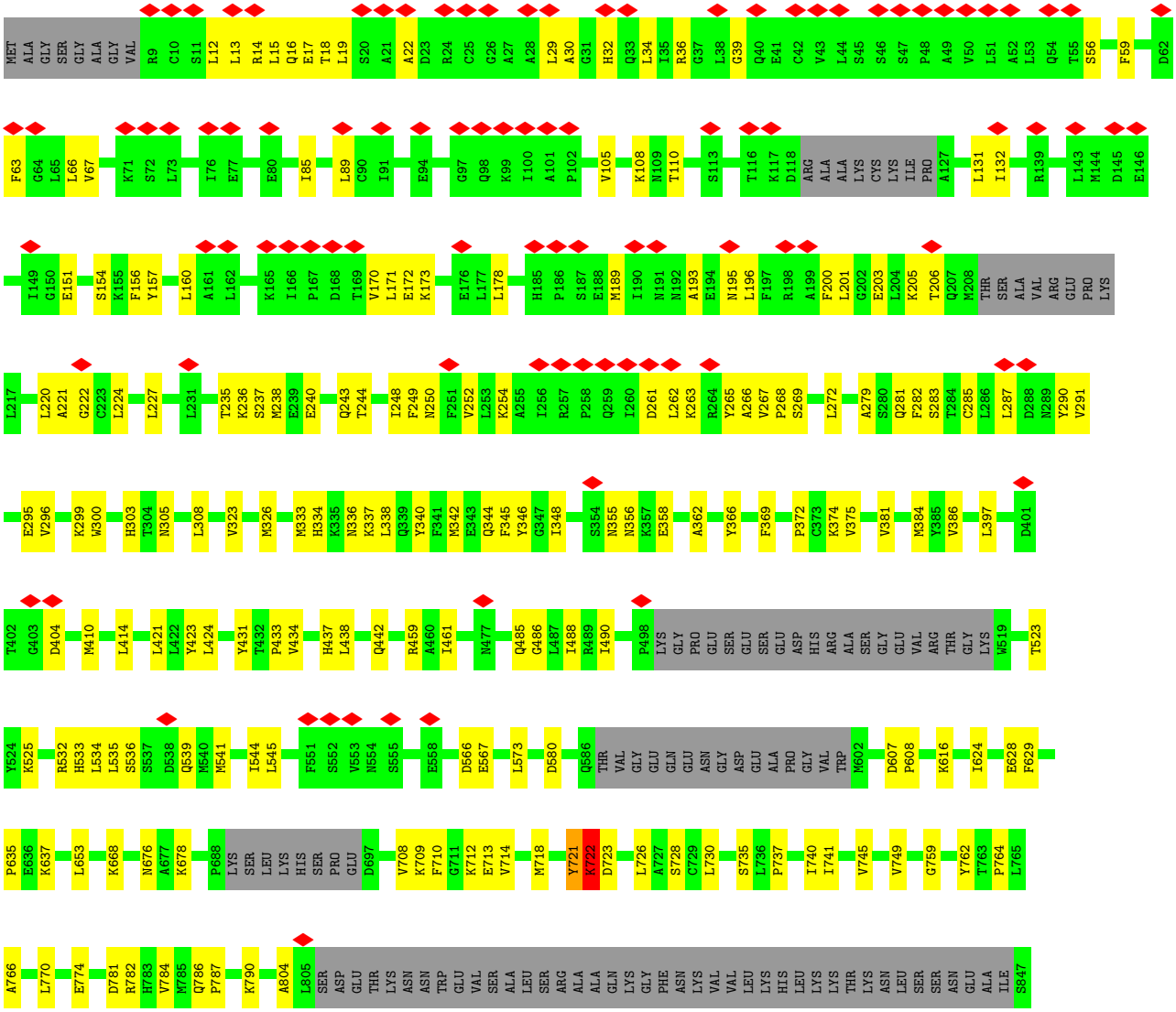
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
3	A	2	2	2	0

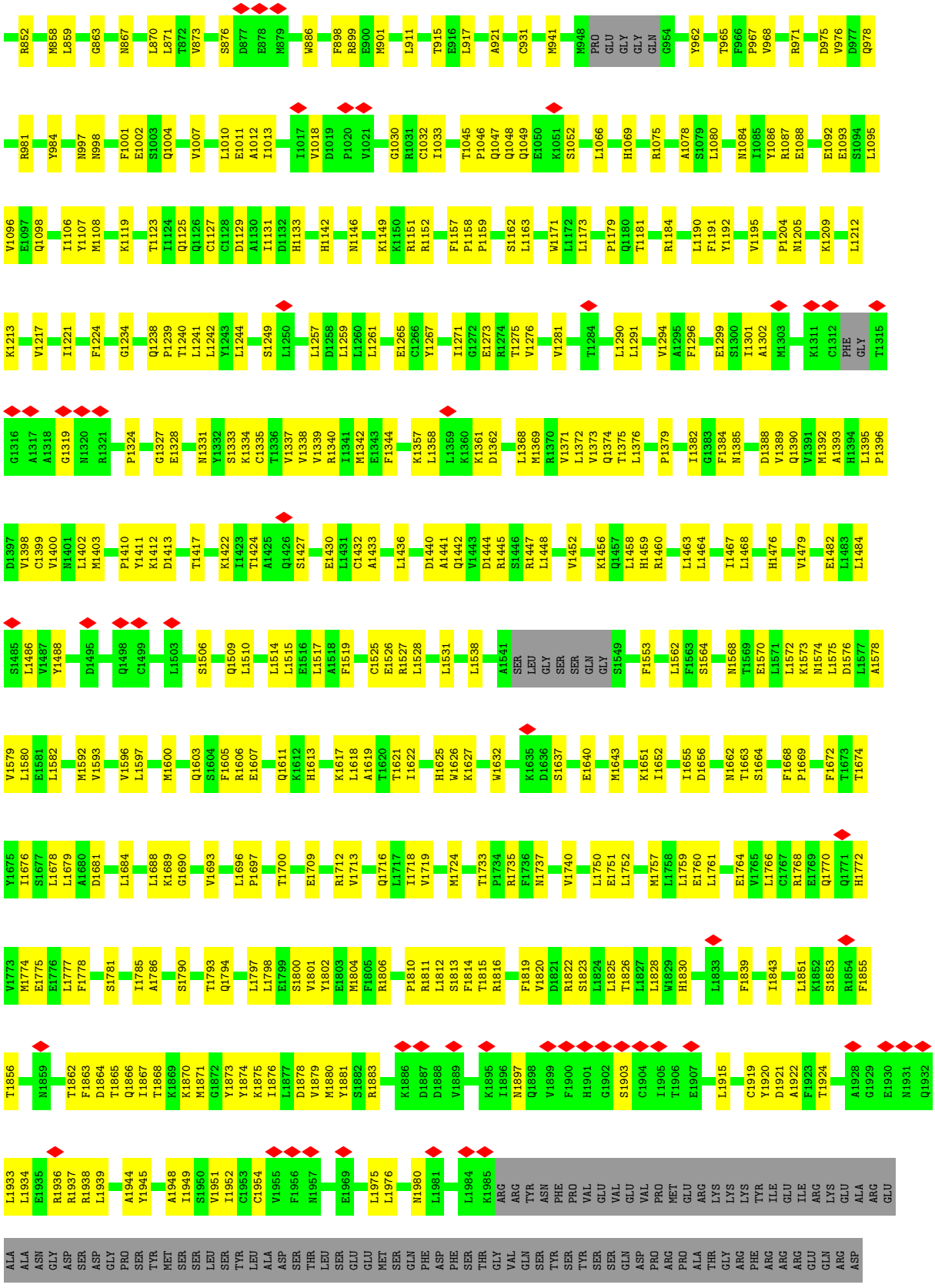
3 Residue-property plots (i)

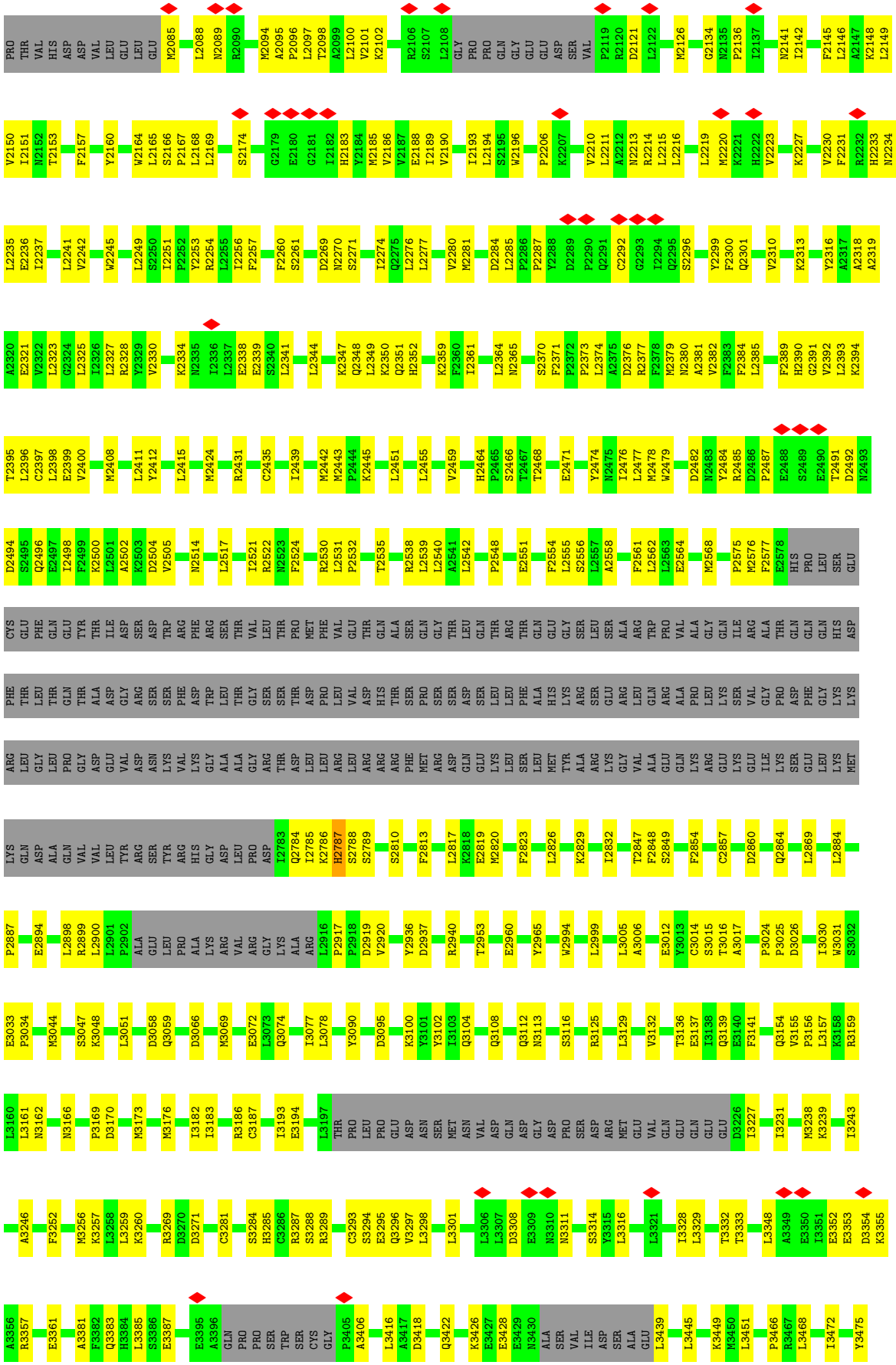
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

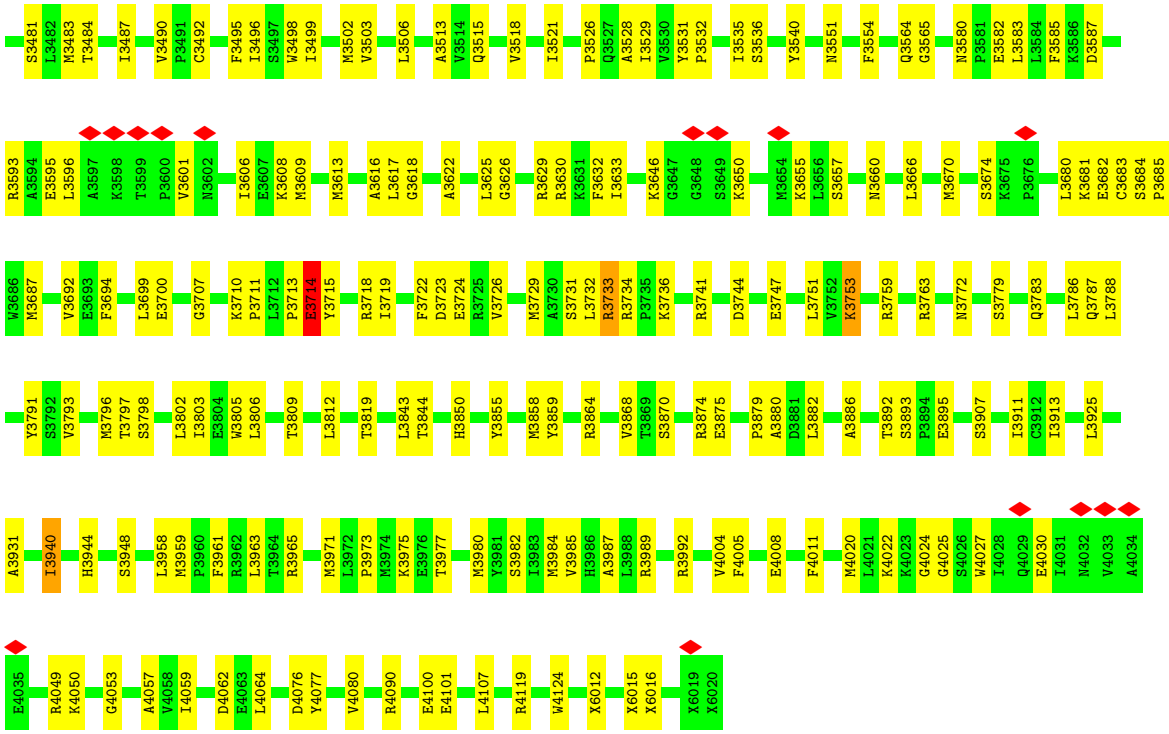
- Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-PKcs

Chain A: 




R852 M858 L859 G863 N867 L870 L871 T872 V873 S876 D877 E878 M879 W886 F898 R899 E900 M901 L911 T915 E916 L917 A921 C931 M941 M948 PRO GLU GLY GLY GLN G954 Y962 T965 F966 P967 V968 R971 D975 V976 D977 Q978
R981 Y984 N997 N998 F1001 E1002 S1003 Q1004 V1007 L1010 E1011 A1012 I1013 I1017 V1018 D1019 P1020 V1021 G1030 R1031 C1032 I1033 T1045 P1046 Q1047 Q1048 Q1049 E1050 K1051 S1052 L1066 H1069 R1075 A1078 S1079 L1080 N1084 I1085 Y1086 R1087 E1088 E1092 E1093 S1094 L1095
V1096 E1097 Q1098 I1106 Y1107 M1108 K1119 T1123 I1124 Q1125 Q1126 C1127 C1128 D1129 A1130 I1131 D1132 H1133 H1142 N1146 K1149 K1150 R1151 R1152 F1157 P1158 P1159 S1162 L1163 W1171 L1172 L1173 P1179 Q1180 T1181 R1184 L1190 F1191 Y1192 V1195 P1204 N1205 K1209 L1212
K1213 V1217 I1221 F1224 G1234 Q1238 P1239 T1240 L1241 L1242 Y1243 L1244 S1249 L1250 L1257 D1258 L1259 L1260 L1261 E1265 C1266 Y1267 I1271 G1272 E1273 R1274 T1275 V1276 V1281 T1284 L1290 L1291 V1294 A1295 F1296 E1299 S1300 I1301 A1302 M1303 K1311 C1312 PHE GLY T1315
G1316 A1317 A1318 G1319 N1320 R1321 P1324 G1327 E1328 N1331 Y1332 S1333 K1334 C1335 T1336 V1337 V1338 V1339 R1340 I1341 M1342 E1343 F1344 K1357 L1358 L1359 K1360 K1361 D1362 L1368 M1369 R1370 V1371 L1372 V1373 Q1374 T1375 L1376 P1379 I1382 G1383 F1384 N1385 D1388 V1389 Q1390 V1391 M1392 A1393 H1394 L1395 P1396
D1397 V1398 C1399 V1400 N1401 L1402 M1403 P1410 Y1411 K1412 D1413 T1417 K1422 I1423 T1424 A1425 Q1426 S1427 E1430 L1431 C1432 A1433 L1436 D1440 A1441 Q1442 V1443 D1444 R1445 S1446 R1447 L1448 V1452 K1456 Q1457 L1458 H1459 R1460 L1463 L1464 I1467 L1468 H1476 V1479 E1482 L1483 L1484
S1485 L1486 V1487 Y1488 D1495 Q1498 C1499 L1503 S1506 Q1509 L1510 L1514 L1515 E1516 L1517 A1518 F1519 C1525 E1526 R1527 L1528 L1531 L1538 A1541 SER LEU GLY SER SER GLN GLY S1549 F1553 L1562 F1563 S1564 N1568 T1569 E1570 L1571 L1572 K1573 N1574 L1575 D1576 L1577 A1578
V1579 L1580 E1581 L1582 M1592 V1593 V1596 L1597 M1600 Q1603 S1604 F1605 R1606 E1607 Q1611 K1612 H1613 K1617 L1618 A1619 T1620 T1621 I1622 H1625 W1626 K1627 W1632 K1635 D1636 S1637 E1640 M1643 K1651 I1652 I1655 D1656 N1662 T1663 S1664 F1668 P1669 F1672 T1673 T1674
Y1675 I1676 S1677 L1678 L1679 A1680 D1681 L1684 L1688 K1689 G1690 V1693 L1696 P1697 T1700 E1709 R1712 V1713 Q1716 L1717 I1718 V1719 M1724 T1733 P1734 R1735 F1736 N1737 V1740 L1750 E1751 L1752 M1757 L1758 L1759 E1760 L1761 E1764 V1765 L1766 C1767 R1768 E1769 Q1770 Q1771 H1772
V1773 M1774 E1775 E1776 L1777 F1778 S1781 I1785 A1786 S1790 T1793 Q1794 L1797 L1798 E1799 S1800 V1801 Y1802 E1803 M1804 F1805 R1806 P1810 R1811 L1812 S1813 F1814 T1815 R1816 F1819 V1820 D1821 R1822 S1823 L1824 L1825 T1826 L1827 L1828 W1829 H1830 L1833 F1839 I1843 L1851 K1852 S1853 R1854 F1855
T1856 N1859 T1862 F1863 D1864 T1865 Q1866 I1867 T1868 K1869 K1870 M1871 G1872 Y1873 Y1874 K1875 I1876 L1877 D1878 V1879 M1880 Y1881 S1882 R1883 K1886 D1887 D1888 V1889 K1895 I1896 N1897 Q1898 V1899 F1900 H1901 G1902 S1903 C1904 I1905 T1906 E1907 L1915 C1919 Y1920 D1921 A1922 F1923 T1924 A1928 G1929 E1930 N1931 Q1932
L1933 L1934 E1935 R1936 R1937 R1938 L1939 A1944 Y1945 A1948 I1949 S1950 V1951 I1952 C1953 C1954 V1955 F1956 N1957 E1969 L1975 L1976 N1980 L1981 L1984 K1985 ARG ARG TYR ASN PHE PRO VAL GLU VAL GLU VAL PRO MET GLU ARG LYS LYS LYS TYR ILE GLU ILE ARG LYS GLU 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 M2094 A2095 P2096 L2097 T2098 A2099 L2100 V2101 K2102 R2106 S2107 L2108 GLY PRO PRO GLN GLY GLU GLU ASP SER VAL P2119 R2120 D2121 L2122 M2126 G2134 N2135 P2136 I2137 N2141 I2142 F2145 L2146 A2147 K2148 L2149
V2150 I2151 N2152 T2153 F2157 Y2160 W2164 L2165 S2166 P2167 L2168 L2169 S2174 G2179 E2180 G2181 I2182 H2183 Y2184 M2185 V2186 V2187 E2188 I2189 V2190 I2193 L2194 S2195 W2196 P2206 K2207 V2210 L2211 A2212 N2213 R2214 L2215 L2216 L2219 M2220 K2221 H2222 V2223 K2227 V2230 F2231 R2232 H2233 N2234
L2235 E2236 I2237 L2241 V2242 W2245 L2249 S2250 I2251 P2252 Y2253 R2254 L2255 I2256 F2257 F2260 S2261 D2269 N2270 S2271 I2274 Q2275 L2276 L2277 V2280 M2281 D2284 L2285 P2286 P2287 Y2288 D2289 P2290 Q2291 C2292 G2293 I2294 Q2295 S2296 Y2299 F2300 Q2301 V2310 K2313 Y2316 A2317 A2318 A2319
A2320 E2321 V2322 L2323 G2324 L2325 I2326 L2327 R2328 Y2329 V2330 K2334 N2335 I2336 L2337 E2338 E2339 S2340 L2341 L2344 K2347 Q2348 L2349 K2350 Q2351 H2352 K2359 F2360 I2361 L2364 N2365 S2370 F2371 P2372 P2373 L2374 A2375 D2376 R2377 F2378 M2379 N2380 A2381 V2382 F2383 F2384 L2385 F2389 H2390 G2391 V2392 L2393 K2394
T2395 L2396 C2397 L2398 E2399 V2400 M2408 L2411 Y2412 L2415 M2424 R2431 C2435 I2439 M2442 M2443 P2444 K2445 L2451 L2455 V2459 H2464 P2465 S2466 T2467 T2468 E2471 Y2474 N2475 I2476 L2477 M2478 W2479 D2482 N2483 Y2484 R2485 D2486 P2487 E2488 S2489 E2490 T2491 D2492 N2493
D2494 S2495 Q2496 E2497 I2498 F2499 K2500 L2501 A2502 K2503 D2504 V2505 N2514 L2517 I2521 R2522 N2523 F2524 R2530 L2531 P2532 T2535 R2538 L2539 L2540 A2541 L2542 P2548 E2551 F2554 L2555 S2556 L2557 A2558 F2561 L2562 L2563 E2564 M2568 P2575 M2576 F2577 E2578 HIS PRO LEU SER GLU
CYS GLU PHE GLN GLU TYR THR ILE ASP SER ASP 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 ALA ARG TRP PRO VAL ALA GLY GLN ILE ARG ALA THR GLN 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 LYS SER VAL GLY PRO ASP PHE GLY LYS LYS
ARG 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 GLN LYS ARG GLU LYS SER GLU LEU LYS MET
LYS GLN ASP ALA GLN VAL VAL LEU TYR ARG SER TYR ARG HIS GLY ASP LEU PRO ASP I2783 Q2784 I2785 K2786 H2787 S2788 S2789 S2810 F2813 L2817 K2818 E2819 M2820 F2823 L2826 K2829 I2832 T2847 F2848 S2849 F2854 C2857 D2860 Q2864 L2869 L2884
P2887 E2894 L2898 R2899 L2900 L2901 P2902 ALA GLU LEU PRO ALA LYS ARG VAL ARG GLY LYS ALA ARG L2916 P2917 P2918 D2919 V2920 Y2936 D2937 R2940 T2953 E2960 Y2965 W2994 L2999 L3005 A3006 E3012 Y3013 C3014 S3015 T3016 A3017 P3024 P3025 D3026 I3030 W3031 S3032
E3033 P3034 M3044 S3047 K3048 L3051 D3058 Q3059 D3066 M3069 E3072 L3073 Q3074 I3077 L3078 Y3090 D3095 K3100 Y3101 Y3102 I3103 Q3104 Q3108 Q3112 N3113 S3116 R3125 L3129 V3132 T3136 E3137 I3138 Q3139 E3140 F3141 Q3154 V3155 P3156 L3157 K3158 R3159
L3160 L3161 N3162 N3166 P3169 D3170 M3173 M3176 I3182 I3183 R3186 C3187 I3193 E3194 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 D3226 I3227 I3231 M3238 K3239 I3243
A3246 F3252 M3256 K3257 L3258 L3259 K3260 R3269 D3270 D3271 C3281 S3284 H3285 C3286 R3287 S3288 R3289 C3293 S3294 E3295 Q3296 V3297 L3298 L3301 L3306 L3307 D3308 E3309 N3310 N3311 S3314 Y3315 L3316 L3321 I3328 L3329 T3332 T3333 L3348 A3349 E3350 I3351 E3352 E3353 D3354 K3355
A3356 R3357 E3361 A3381 F3382 Q3383 H3384 L3385 S3386 E3387 E3395 A3396 GLN PRO PRO SER TRP SER CYS GLY P3405 A3406 L3416 A3417 D3418 Q3422 K3426 E3427 E3428 E3429 N3430 ALA SER VAL ILE ASP SER ALA GLU L3439 L3445 K3449 M3450 L3451 P3466 R3467 L3468 I3472 Y3475


S3481 L3482 M3483 T3484 I3487 V3490 P3491 C3492 F3495 I3496 S3497 W3498 I3499 M3502 V3503 L3506 A3513 V3514 Q3515 V3518 I3521 P3526 Q3527 A3528 I3529 V3530 Y3531 P3532 I3535 S3536 Y3540 N3551 F3554 Q3564 G3565 N3580 P3581 E3582 L3583 L3584 F3585 K3586 D3587
R3593 A3594 E3595 L3596 A3597 K3598 T3599 P3600 V3601 N3602 I3606 E3607 K3608 M3609 M3613 A3616 L3617 G3618 A3622 L3625 G3626 R3629 R3630 K3631 F3632 I3633 K3646 G3647 G3648 S3649 K3650 M3654 K3655 L3656 S3657 N3660 L3666 M3670 S3674 K3675 P3676 L3680 K3681 E3682 C3683 S3684 P3685
W3686 M3687 V3692 E3693 F3694 L3699 E3700 G3707 K3710 P3711 L3712 P3713 E3714 Y3715 R3718 I3719 F3722 D3723 E3724 R3725 V3726 M3729 A3730 S3731 L3732 R3733 R3734 P3735 K3736 R3741 D3744 E3747 L3751 V3752 K3753 R3759 R3763 N3772 S3779 Q3783 L3786 Q3787 L3788
Y3791 S3792 V3793 M3796 T3797 S3798 L3802 I3803 E3804 W3805 L3806 T3809 L3812 T3819 L3843 T3844 H3850 Y3855 M3858 Y3859 R3864 V3868 T3869 S3870 R3874 E3875 P3879 A3880 D3881 L3882 A3886 T3892 S3893 P3894 E3895 S3907 I3911 C3912 I3913 L3925
A3931 I3940 H3944 S3948 L3958 M3959 P3960 F3961 R3962 L3963 T3964 R3965 M3971 L3972 P3973 M3974 K3975 E3976 T3977 M3980 Y3981 S3982 I3983 M3984 V3985 H3986 A3987 L3988 R3989 R3992 V4004 F4005 E4008 F4011 M4020 L4021 K4022 K4023 G4024 G4025 S4026 W4027 I4028 Q4029 E4030 I4031 N4032 V4033 A4034
E4035 R4049 K4050 G4053 A4057 V4058 I4059 D4062 E4063 L4064 D4076 Y4077 V4080 R4090 E4100 E4101 L4107 R4119 W4124 X6012 X6015 X6016 X6019 X6020

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63313	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 ($e^-/Å^2$)	46.8	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	2.339	Depositor
Minimum map value	-1.286	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.23	Depositor
Map size (Å)	339.04, 339.04, 339.04	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.30	0/29498	0.49	4/39889 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3715	TYR	N-CA-C	-9.09	101.15	112.88
1	A	722	LYS	N-CA-C	7.54	117.91	108.19
1	A	1239	PRO	CA-N-CD	-5.26	104.64	112.00
1	A	721	TYR	O-C-N	5.25	129.14	123.10

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	29006	0	29184	810	0
2	A	31	0	11	3	0
3	A	2	0	0	0	0
All	All	29039	0	29195	813	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 15.

All (813) 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)
2:A:6101:AGS:C4'	2:A:6101:AGS:O4'	1.63	1.23
1:A:774:GLU:HG2	1:A:858:MET:HE3	1.53	0.90
1:A:189:MET:HG3	1:A:193:ALA:HB2	1.53	0.90
1:A:3618:GLY:H	1:A:3633:ILE:HD12	1.41	0.85
1:A:3670:MET:O	1:A:3674:SER:HB3	1.76	0.84
1:A:1482:GLU:O	1:A:1486:LEU:HB2	1.77	0.83
1:A:3288:SER:O	1:A:3289:ARG:NH1	2.12	0.83
1:A:1358:LEU:HD21	1:A:1410:PRO:HD2	1.61	0.82
1:A:348:ILE:HD11	1:A:358:GLU:HB2	1.64	0.80
1:A:3162:ASN:ND2	1:A:3166:ASN:OD1	2.15	0.79
1:A:2887:PRO:HG2	1:A:3895:GLU:HG3	1.65	0.79
1:A:1570:GLU:OE2	1:A:1574:ASN:ND2	2.16	0.78
1:A:917:LEU:O	1:A:921:ALA:HB2	1.83	0.78
1:A:1619:ALA:HA	1:A:1652:ILE:HD11	1.65	0.77
1:A:3622:ALA:HB3	1:A:3625:LEU:HB2	1.67	0.77
1:A:1801:VAL:HA	1:A:1804:MET:SD	2.25	0.77
1:A:3700:GLU:HA	1:A:3718:ARG:HA	1.66	0.75
1:A:1828:LEU:O	1:A:1883:ARG:NH2	2.19	0.75
1:A:1871:MET:HE3	1:A:1939:LEU:HD13	1.68	0.75
1:A:240:GLU:HB2	1:A:243:GLN:HE22	1.51	0.74
1:A:1775:GLU:OE1	1:A:1822:ARG:NH1	2.21	0.74
1:A:3243:ILE:HG21	1:A:3259:LEU:HD13	1.69	0.74
1:A:3187:CYS:SG	1:A:3239:LYS:NZ	2.61	0.73
1:A:3483:MET:HE3	1:A:3487:ILE:HD11	1.69	0.73
1:A:2300:PHE:HD2	1:A:2341:LEU:HD13	1.53	0.73
1:A:1632:TRP:O	1:A:1637:SER:OG	2.07	0.72
1:A:3684:SER:HB2	1:A:3685:PRO:HD3	1.72	0.72
1:A:2281:MET:HE1	1:A:2287:PRO:HG3	1.72	0.72
1:A:1881:TYR:HE1	1:A:1954:CYS:HB3	1.54	0.72
1:A:1718:ILE:HD13	1:A:1761:LEU:HD21	1.72	0.72
1:A:13:LEU:HD23	1:A:14:ARG:HE	1.54	0.71
1:A:2347:LYS:HA	1:A:2350:LYS:HD3	1.71	0.71
1:A:2424:MET:HE1	1:A:2439:ILE:HD11	1.71	0.71
1:A:356:ASN:ND2	1:A:404:ASP:O	2.24	0.71
1:A:2786:LYS:NZ	1:A:2788:SER:OG	2.20	0.71
1:A:2194:LEU:HD11	1:A:2241:LEU:HA	1.73	0.70
1:A:3587:ASP:OD2	1:A:3733:ARG:NH2	2.24	0.70
1:A:3985:VAL:HG21	1:A:4101:GLU:HG3	1.72	0.70
1:A:1933:LEU:HD13	1:A:1936:ARG:HB2	1.72	0.69
1:A:3805:TRP:O	1:A:3805:TRP:CD1	2.46	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3855:TYR:HA	1:A:3858:MET:HG3	1.73	0.69
1:A:3606:ILE:HG13	1:A:3609:MET:HE1	1.73	0.69
1:A:254:LYS:NZ	1:A:268:PRO:O	2.26	0.69
1:A:3685:PRO:HB2	1:A:3687:MET:HG3	1.75	0.69
1:A:871:LEU:HD23	1:A:3129:LEU:HD22	1.74	0.69
1:A:1684:LEU:HD23	1:A:1688:LEU:HG	1.74	0.69
1:A:397:LEU:HD11	1:A:437:HIS:HB3	1.74	0.69
1:A:1448:LEU:HD21	1:A:1514:LEU:HD11	1.73	0.68
1:A:3687:MET:HB3	1:A:3722:PHE:CD2	2.29	0.68
1:A:1400:VAL:HG11	1:A:1460:ARG:HG2	1.76	0.68
1:A:863:GLY:O	1:A:867:ASN:ND2	2.27	0.68
1:A:2860:ASP:O	1:A:2864:GLN:NE2	2.27	0.67
1:A:2919:ASP:OD1	1:A:2920:VAL:N	2.28	0.67
1:A:3729:MET:HE2	1:A:3805:TRP:HH2	1.59	0.67
1:A:3616:ALA:O	1:A:3629:ARG:NH2	2.28	0.67
1:A:2216:LEU:HB3	1:A:2220:MET:HE1	1.77	0.66
1:A:2380:ASN:OD1	1:A:2381:ALA:N	2.28	0.66
1:A:1373:VAL:HG11	1:A:1422:LYS:HD3	1.78	0.66
1:A:3298:LEU:HD12	1:A:3333:THR:HG23	1.76	0.66
1:A:2522:ARG:HH22	1:A:2564:GLU:HG3	1.61	0.66
1:A:3596:LEU:HD12	1:A:3601:VAL:HA	1.76	0.66
1:A:3030:ILE:HG23	1:A:3031:TRP:HD1	1.60	0.66
1:A:3580:ASN:HD21	1:A:3734:ARG:HB2	1.61	0.66
1:A:3012:GLU:OE2	1:A:3048:LYS:NZ	2.29	0.66
1:A:12:LEU:HA	1:A:15:LEU:HB3	1.78	0.66
1:A:1445:ARG:HG3	1:A:1510:LEU:HD22	1.78	0.66
1:A:2364:LEU:HG	1:A:2400:VAL:HG21	1.77	0.65
1:A:2459:VAL:HB	1:A:2505:VAL:HG21	1.77	0.65
1:A:1774:MET:SD	1:A:1777:LEU:HB2	2.36	0.65
1:A:1980:ASN:ND2	1:A:2141:ASN:OD1	2.28	0.65
1:A:3137:GLU:OE1	1:A:3186:ARG:NH2	2.24	0.65
1:A:3680:LEU:HD23	1:A:3682:GLU:H	1.62	0.65
1:A:3958:LEU:HD21	1:A:4064:LEU:HD11	1.76	0.65
1:A:372:PRO:HA	1:A:375:VAL:HG12	1.79	0.65
1:A:235:THR:HA	1:A:281:GLN:HE22	1.62	0.64
1:A:1949:ILE:HG23	1:A:2100:LEU:HD12	1.79	0.64
1:A:2379:MET:HG2	1:A:2408:MET:HE2	1.78	0.64
1:A:580:ASP:HB3	1:A:616:LYS:HD2	1.78	0.64
1:A:2216:LEU:HD21	1:A:2249:LEU:HD22	1.79	0.64
1:A:1379:PRO:HB3	1:A:1384:PHE:HD2	1.62	0.64
1:A:3281:CYS:HB2	1:A:3329:LEU:HD23	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2094:MET:HE3	1:A:2145:PHE:HD1	1.63	0.63
1:A:333:MET:HG2	1:A:334:HIS:ND1	2.13	0.63
1:A:2487:PRO:O	1:A:2496:GLN:NE2	2.30	0.63
1:A:3418:ASP:O	1:A:3422:GLN:HG2	1.97	0.63
1:A:265:TYR:O	1:A:269:SER:OG	2.13	0.63
1:A:2223:VAL:HG21	1:A:2276:LEU:HD11	1.79	0.63
1:A:4049:ARG:NH2	1:A:4062:ASP:OD2	2.31	0.63
1:A:3593:ARG:HH21	1:A:3660:ASN:HA	1.63	0.63
1:A:1092:GLU:OE1	1:A:1095:LEU:N	2.32	0.63
1:A:1432:CYS:SG	1:A:1433:ALA:N	2.71	0.63
1:A:3989:ARG:HA	1:A:4100:GLU:OE2	1.99	0.63
1:A:1856:THR:O	1:A:1866:GLN:NE2	2.33	0.62
1:A:1881:TYR:CE1	1:A:1954:CYS:HB3	2.34	0.62
1:A:1459:HIS:HB2	1:A:1464:LEU:HD22	1.80	0.62
1:A:1048:GLN:HE22	1:A:1052:SER:HB2	1.65	0.62
1:A:2174:SER:OG	1:A:2214:ARG:NH2	2.32	0.62
1:A:1240:THR:HG22	1:A:1242:LEU:H	1.64	0.62
1:A:1399:CYS:O	1:A:1403:MET:HG3	2.00	0.62
1:A:2482:ASP:HA	1:A:2485:ARG:HE	1.64	0.62
1:A:709:LYS:NZ	1:A:713:GLU:OE1	2.33	0.62
1:A:2937:ASP:OD1	1:A:3982:SER:OG	2.17	0.62
1:A:3751:LEU:HD22	1:A:3803:ILE:HD11	1.82	0.62
1:A:3843:LEU:HD11	1:A:3858:MET:HG2	1.82	0.61
1:A:2085:MET:HE1	1:A:2089:ASN:H	1.64	0.61
1:A:2150:VAL:HG13	1:A:2157:PHE:HD2	1.65	0.61
1:A:2478:MET:HG2	1:A:2524:PHE:CE1	2.35	0.61
1:A:1864:ASP:HA	1:A:1867:ILE:HG12	1.82	0.61
1:A:2439:ILE:O	1:A:2443:MET:HG2	1.99	0.61
1:A:3963:LEU:HD21	1:A:3980:MET:HE1	1.82	0.61
1:A:3796:MET:CE	1:A:3802:LEU:HG	2.31	0.61
1:A:195:ASN:OD1	1:A:196:LEU:N	2.34	0.60
1:A:2088:LEU:HA	1:A:2094:MET:SD	2.41	0.60
1:A:2471:GLU:HA	1:A:2517:LEU:HD11	1.82	0.60
1:A:3295:GLU:OE2	1:A:3295:GLU:N	2.27	0.60
1:A:3296:GLN:NE2	1:A:3352:GLU:OE1	2.34	0.60
1:A:3284:SER:HB3	1:A:3301:LEU:HD12	1.84	0.60
1:A:386:VAL:HG22	1:A:431:TYR:HE2	1.67	0.60
1:A:787:PRO:O	1:A:790:LYS:NZ	2.34	0.60
1:A:1338:VAL:HG12	1:A:1342:MET:HE3	1.83	0.60
1:A:1603:GLN:OE1	1:A:1606:ARG:NH1	2.33	0.60
1:A:1819:PHE:O	1:A:1823:SER:OG	2.19	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4050:LYS:HE3	1:A:4059:ILE:HG21	1.82	0.60
1:A:1724:MET:O	1:A:1768:ARG:NH1	2.35	0.60
1:A:1261:LEU:HG	1:A:1337:VAL:HG22	1.83	0.60
1:A:2183:HIS:CE1	1:A:2186:VAL:HG23	2.36	0.60
1:A:56:SER:HA	1:A:59:PHE:HD2	1.66	0.59
1:A:917:LEU:O	1:A:921:ALA:CB	2.49	0.59
1:A:3535:ILE:HG21	1:A:3759:ARG:HD3	1.83	0.59
1:A:374:LYS:HD2	1:A:423:TYR:HB3	1.83	0.59
1:A:2786:LYS:O	1:A:2789:SER:N	2.30	0.59
1:A:737:PRO:HD2	1:A:740:ILE:HD12	1.84	0.59
1:A:2898:LEU:HG	1:A:3973:PRO:HG3	1.83	0.59
1:A:3515:GLN:NE2	1:A:3551:ASN:OD1	2.35	0.59
1:A:3681:LYS:NZ	1:A:3723:ASP:O	2.31	0.59
1:A:741:ILE:HG22	1:A:745:VAL:HG22	1.84	0.59
1:A:1444:ASP:OD1	1:A:1447:ARG:NH1	2.36	0.59
1:A:1476:HIS:HB3	1:A:1479:VAL:HG22	1.85	0.59
1:A:1826:THR:O	1:A:1830:HIS:ND1	2.30	0.59
1:A:1873:TYR:HA	1:A:1876:ILE:HG22	1.83	0.59
1:A:1334:LYS:O	1:A:1338:VAL:HG23	2.02	0.59
1:A:1802:TYR:CE1	1:A:1806:ARG:HD3	2.38	0.59
1:A:2443:MET:HE3	1:A:2476:ILE:HG23	1.84	0.59
1:A:2575:PRO:HB2	1:A:2784:GLN:HB3	1.83	0.59
1:A:3154:GLN:HG3	1:A:3227:ILE:HD11	1.85	0.59
1:A:13:LEU:HG	1:A:59:PHE:HZ	1.68	0.59
1:A:154:SER:HA	1:A:157:TYR:HD2	1.68	0.59
1:A:1093:GLU:HA	1:A:1096:VAL:HG12	1.84	0.59
1:A:1357:LYS:HA	1:A:1361:LYS:HB2	1.84	0.58
1:A:1810:PRO:HA	1:A:1816:ARG:HH22	1.68	0.58
1:A:1640:GLU:HA	1:A:1643:MET:HE3	1.84	0.58
1:A:1876:ILE:HG13	1:A:1880:MET:HE1	1.85	0.58
1:A:3687:MET:HB3	1:A:3722:PHE:HD2	1.65	0.58
1:A:2330:VAL:HG22	1:A:2334:LYS:HA	1.84	0.58
1:A:3428:GLU:OE2	1:A:3475:TYR:OH	2.15	0.58
1:A:1786:ALA:HB3	1:A:1830:HIS:HB2	1.84	0.58
1:A:3100:LYS:O	1:A:3104:GLN:HG2	2.03	0.58
1:A:1484:LEU:HD13	1:A:1527:ARG:HH22	1.69	0.58
1:A:1664:SER:H	1:A:1668:PHE:HB3	1.68	0.58
1:A:1750:LEU:HD11	1:A:1759:LEU:HA	1.86	0.58
1:A:2227:LYS:HB2	1:A:2230:VAL:HG12	1.85	0.58
1:A:2391:GLY:O	1:A:2431:ARG:NH2	2.36	0.58
1:A:366:TYR:HE1	1:A:384:MET:HG2	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1506:SER:O	1:A:1509:GLN:NE2	2.37	0.58
1:A:2412:TYR:HA	1:A:2415:LEU:HB2	1.86	0.58
1:A:1375:THR:O	1:A:1379:PRO:HG3	2.04	0.58
1:A:1751:GLU:HA	1:A:1785:ILE:HD11	1.86	0.57
1:A:3864:ARG:NH1	1:A:3868:VAL:HG21	2.19	0.57
1:A:67:VAL:HG13	1:A:110:THR:HG21	1.86	0.57
1:A:3058:ASP:O	1:A:3059:GLN:NE2	2.36	0.57
1:A:2522:ARG:HG2	1:A:2561:PHE:HE1	1.69	0.57
1:A:745:VAL:O	1:A:749:VAL:HG23	2.04	0.57
1:A:1424:THR:HG23	1:A:1427:SER:H	1.70	0.57
1:A:2185:MET:HA	1:A:2188:GLU:CD	2.29	0.57
1:A:3031:TRP:CZ3	1:A:3044:MET:HG3	2.40	0.57
1:A:523:THR:HG23	1:A:525:LYS:H	1.70	0.57
1:A:243:GLN:N	1:A:243:GLN:OE1	2.38	0.56
1:A:1358:LEU:HD11	1:A:1410:PRO:HB2	1.86	0.56
1:A:1757:MET:O	1:A:1760:GLU:HG3	2.05	0.56
1:A:2193:ILE:HA	1:A:2196:TRP:CE3	2.40	0.56
1:A:2149:LEU:O	1:A:2153:THR:HG22	2.05	0.56
1:A:348:ILE:HG23	1:A:362:ALA:HB2	1.88	0.56
1:A:2190:VAL:HA	1:A:2193:ILE:HG12	1.86	0.56
1:A:3030:ILE:HG23	1:A:3031:TRP:CD1	2.40	0.56
1:A:3108:GLN:O	1:A:3112:GLN:HG2	2.05	0.56
1:A:1697:PRO:HG2	1:A:1752:LEU:HD23	1.88	0.56
1:A:1234:GLY:HA2	1:A:1259:LEU:HD22	1.87	0.56
1:A:2365:ASN:ND2	1:A:2399:GLU:OE2	2.31	0.56
1:A:6012:UNK:O	1:A:6016:UNK:N	2.39	0.56
1:A:1192:TYR:OH	1:A:1273:GLU:OE2	2.23	0.56
1:A:1011:GLU:OE2	1:A:1032:CYS:HB3	2.05	0.56
1:A:2256:ILE:HG22	1:A:2260:PHE:CE1	2.41	0.56
1:A:2491:THR:HA	1:A:2496:GLN:HE22	1.69	0.56
1:A:3723:ASP:OD1	1:A:3724:GLU:N	2.38	0.56
1:A:240:GLU:HB2	1:A:243:GLN:NE2	2.20	0.55
1:A:1572:LEU:HD21	1:A:1600:MET:HB3	1.87	0.55
1:A:1184:ARG:NE	1:A:1265:GLU:OE1	2.32	0.55
1:A:2269:ASP:OD1	1:A:2270:ASN:N	2.39	0.55
1:A:608:PRO:HG2	1:A:721:TYR:HE1	1.71	0.55
1:A:1339:VAL:HG23	1:A:1398:VAL:HG11	1.87	0.55
1:A:2334:LYS:HB2	1:A:2338:GLU:HB2	1.89	0.55
1:A:2785:ILE:O	1:A:2789:SER:HB2	2.07	0.55
1:A:414:LEU:HD22	1:A:442:GLN:HE21	1.72	0.55
1:A:3472:ILE:HD11	1:A:3483:MET:SD	2.47	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LYS:HZ1	1:A:272:LEU:N	2.04	0.55
1:A:345:PHE:HA	1:A:348:ILE:HG22	1.88	0.55
1:A:2371:PHE:CD2	1:A:2374:LEU:HB2	2.42	0.55
1:A:236:LYS:HG2	1:A:243:GLN:NE2	2.22	0.55
1:A:3499:ILE:HG21	1:A:3529:ILE:HG13	1.89	0.55
1:A:3596:LEU:HB2	1:A:3601:VAL:HG22	1.88	0.55
1:A:170:VAL:O	1:A:171:LEU:HD22	2.07	0.55
1:A:566:ASP:OD1	1:A:567:GLU:N	2.40	0.54
1:A:3879:PRO:HB2	1:A:3882:LEU:HG	1.89	0.54
1:A:941:MET:HE1	1:A:965:THR:HG21	1.88	0.54
1:A:978:GLN:OE1	1:A:981:ARG:NH2	2.28	0.54
1:A:3796:MET:HE1	1:A:3802:LEU:HG	1.88	0.54
1:A:459:ARG:HH11	1:A:544:ILE:HG13	1.73	0.54
1:A:1388:ASP:HA	1:A:1392:MET:HE2	1.88	0.54
1:A:2999:LEU:HD21	1:A:3015:SER:O	2.07	0.54
1:A:533:HIS:HB3	1:A:541:MET:HE1	1.90	0.54
1:A:2869:LEU:HB2	1:A:2900:LEU:HD13	1.89	0.54
1:A:2379:MET:HA	1:A:2382:VAL:HG22	1.90	0.54
1:A:3626:GLY:O	1:A:3630:ARG:HB2	2.06	0.54
1:A:1709:GLU:HA	1:A:1712:ARG:HG2	1.90	0.54
1:A:2542:LEU:HD21	1:A:2558:ALA:HA	1.89	0.54
1:A:1820:VAL:O	1:A:1825:LEU:HG	2.07	0.54
1:A:3751:LEU:HD12	1:A:3805:TRP:CE3	2.43	0.54
1:A:1488:TYR:CG	1:A:1531:LEU:HD21	2.43	0.53
1:A:1873:TYR:O	1:A:1876:ILE:HG22	2.08	0.53
1:A:3714:GLU:N	1:A:3714:GLU:OE1	2.41	0.53
1:A:2094:MET:HE3	1:A:2145:PHE:CD1	2.43	0.53
1:A:3875:GLU:CG	1:A:3965:ARG:HD3	2.38	0.53
1:A:2148:LYS:HA	1:A:2151:ILE:HD12	1.89	0.53
1:A:3357:ARG:O	1:A:3361:GLU:HG2	2.08	0.53
1:A:1389:VAL:HG23	1:A:1390:GLN:H	1.72	0.53
1:A:1772:HIS:CE1	1:A:1774:MET:HB3	2.44	0.53
1:A:1240:THR:HG23	1:A:1296:PHE:CG	2.44	0.53
1:A:1376:LEU:HD13	1:A:1403:MET:HE1	1.89	0.53
1:A:2371:PHE:HD2	1:A:2374:LEU:HB2	1.71	0.53
1:A:238:MET:HE3	1:A:285:CYS:H	1.73	0.53
1:A:355:ASN:OD1	1:A:356:ASN:N	2.37	0.53
1:A:1301:ILE:HG22	1:A:1334:LYS:HE2	1.90	0.53
1:A:2349:LEU:HA	1:A:2352:HIS:CE1	2.43	0.53
1:A:2439:ILE:HG22	1:A:2443:MET:HE2	1.89	0.53
1:A:3587:ASP:CG	1:A:3733:ARG:HH22	2.16	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1238:GLN:C	1:A:1240:THR:H	2.17	0.53
1:A:1689:LYS:O	1:A:1693:VAL:HG13	2.09	0.53
1:A:3017:ALA:HA	1:A:3031:TRP:CZ2	2.44	0.53
1:A:131:LEU:HD13	1:A:173:LYS:HD2	1.89	0.53
1:A:237:SER:O	1:A:243:GLN:NE2	2.42	0.53
1:A:3137:GLU:CD	1:A:3186:ARG:HE	2.17	0.53
1:A:3506:LEU:HD11	1:A:3518:VAL:HG11	1.89	0.53
1:A:1868:THR:OG1	1:A:1936:ARG:NH2	2.42	0.52
1:A:303:HIS:CE1	1:A:305:ASN:HB2	2.43	0.52
1:A:334:HIS:HA	1:A:337:LYS:HZ3	1.72	0.52
1:A:338:LEU:O	1:A:342:MET:HG2	2.08	0.52
1:A:3072:GLU:C	1:A:3074:GLN:H	2.17	0.52
1:A:238:MET:HE2	1:A:283:SER:H	1.74	0.52
1:A:1825:LEU:HD22	1:A:1879:VAL:HG21	1.91	0.52
1:A:2339:GLU:OE1	1:A:2339:GLU:N	2.41	0.52
1:A:2551:GLU:OE1	1:A:2847:THR:HG23	2.10	0.52
1:A:105:VAL:HA	1:A:108:LYS:HB3	1.91	0.52
1:A:2443:MET:HB3	1:A:2479:TRP:CH2	2.44	0.52
1:A:3699:LEU:HG	1:A:3719:ILE:HD12	1.92	0.52
1:A:3731:SER:OG	1:A:3732:LEU:N	2.42	0.52
1:A:410:MET:HG2	1:A:442:GLN:NE2	2.24	0.52
1:A:2234:ASN:HA	1:A:2237:ILE:HD12	1.91	0.52
1:A:3944:HIS:HB3	1:A:3948:SER:HB2	1.91	0.52
1:A:291:VAL:HG12	1:A:340:TYR:CE2	2.45	0.52
1:A:3711:PRO:O	1:A:3713:PRO:HD3	2.09	0.52
1:A:1897:ASN:HA	1:A:1903:SER:HB2	1.91	0.52
1:A:2443:MET:HB3	1:A:2479:TRP:CZ3	2.44	0.52
1:A:901:MET:HE2	1:A:2535:THR:OG1	2.09	0.52
1:A:931:CYS:O	1:A:984:TYR:OH	2.26	0.52
1:A:1432:CYS:SG	1:A:1486:LEU:HD11	2.50	0.52
1:A:1751:GLU:HA	1:A:1785:ILE:CD1	2.40	0.52
1:A:2384:PHE:HD2	1:A:2385:LEU:HD22	1.75	0.52
1:A:3353:GLU:O	1:A:3355:LYS:N	2.43	0.52
1:A:3186:ARG:HD3	1:A:3238:MET:HE1	1.92	0.52
1:A:3733:ARG:HH21	1:A:4022:LYS:HD3	1.75	0.52
2:A:6101:AGS:O4'	2:A:6101:AGS:C5'	2.49	0.52
1:A:1812:LEU:O	1:A:1815:THR:N	2.33	0.51
1:A:1358:LEU:HD22	1:A:1411:TYR:HE1	1.75	0.51
1:A:3870:SER:OG	1:A:3874:ARG:NH2	2.43	0.51
1:A:1333:SER:O	1:A:1337:VAL:HG23	2.10	0.51
1:A:3499:ILE:O	1:A:3503:VAL:HG22	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4004:VAL:O	1:A:4008:GLU:HG3	2.11	0.51
1:A:1069:HIS:CD2	1:A:3741:ARG:HH21	2.29	0.51
1:A:1205:ASN:HA	1:A:1275:THR:HG23	1.92	0.51
1:A:3285:HIS:HE1	1:A:3332:THR:HB	1.75	0.51
1:A:873:VAL:HA	1:A:876:SER:HB2	1.91	0.51
1:A:1713:VAL:HA	1:A:1716:GLN:CD	2.36	0.51
1:A:3487:ILE:HA	1:A:3490:VAL:HG23	1.91	0.51
1:A:3666:LEU:O	1:A:3670:MET:HG3	2.10	0.51
1:A:287:LEU:HD21	1:A:326:MET:HE1	1.92	0.51
1:A:975:ASP:OD1	1:A:976:VAL:N	2.44	0.51
1:A:2213:ASN:OD1	1:A:2214:ARG:N	2.44	0.51
1:A:2271:SER:HA	1:A:2274:ILE:HD12	1.93	0.51
1:A:2327:LEU:HA	1:A:2330:VAL:HG12	1.93	0.51
1:A:3626:GLY:HA3	1:A:3684:SER:O	2.10	0.51
1:A:3791:TYR:CZ	1:A:3940:ILE:HG22	2.46	0.51
1:A:3844:THR:HB	1:A:3850:HIS:HB3	1.93	0.51
1:A:1716:GLN:HA	1:A:1719:VAL:HG22	1.92	0.51
1:A:36:ARG:HH21	1:A:39:GLY:HA3	1.76	0.51
1:A:678:LYS:NZ	1:A:735:SER:O	2.28	0.51
1:A:1934:LEU:O	1:A:1938:ARG:HB2	2.10	0.51
1:A:3753:LYS:HE3	1:A:3753:LYS:HA	1.92	0.51
1:A:858:MET:HE2	1:A:858:MET:HA	1.92	0.51
1:A:1125:GLN:NE2	1:A:1129:ASP:OD2	2.44	0.51
1:A:3793:VAL:HG22	1:A:3803:ILE:HG22	1.93	0.51
1:A:1525:CYS:HA	1:A:1528:LEU:HB3	1.91	0.50
1:A:1781:SER:O	1:A:1785:ILE:HG12	2.10	0.50
1:A:1871:MET:HA	1:A:1874:TYR:HD2	1.76	0.50
1:A:2165:LEU:HD12	1:A:2166:SER:N	2.26	0.50
1:A:2310:VAL:HA	1:A:2359:LYS:NZ	2.25	0.50
1:A:3439:LEU:HD12	1:A:3439:LEU:O	2.10	0.50
1:A:1007:VAL:O	1:A:1011:GLU:HG3	2.10	0.50
1:A:1564:SER:O	1:A:1568:ASN:ND2	2.44	0.50
1:A:1815:THR:HG22	1:A:1819:PHE:CE1	2.47	0.50
1:A:2253:TYR:H	1:A:2256:ILE:HD13	1.76	0.50
1:A:2849:SER:O	1:A:2849:SER:OG	2.29	0.50
1:A:1296:PHE:O	1:A:1299:GLU:HG3	2.11	0.50
1:A:1618:LEU:O	1:A:1622:ILE:HG22	2.11	0.50
1:A:3685:PRO:CB	1:A:3687:MET:HG3	2.42	0.50
1:A:3496:ILE:HB	1:A:3707:GLY:HA2	1.93	0.50
1:A:16:GLN:NE2	1:A:17:GLU:OE2	2.44	0.50
1:A:2377:ARG:H	1:A:2377:ARG:HD2	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4057:ALA:HB2	1:A:4090:ARG:HD2	1.94	0.50
1:A:131:LEU:HD12	1:A:132:ILE:N	2.26	0.50
1:A:334:HIS:HB3	1:A:337:LYS:HD2	1.93	0.50
1:A:1375:THR:OG1	1:A:1384:PHE:HE2	1.94	0.50
1:A:1482:GLU:HA	1:A:1486:LEU:HD23	1.94	0.50
1:A:1611:GLN:HA	1:A:1613:HIS:CE1	2.46	0.50
1:A:2146:LEU:O	1:A:2150:VAL:HG23	2.12	0.50
1:A:2150:VAL:HG22	1:A:2157:PHE:HE2	1.77	0.50
1:A:1875:LYS:O	1:A:1878:ASP:HB3	2.12	0.50
1:A:2576:MET:HB3	1:A:2787:HIS:NE2	2.27	0.50
1:A:238:MET:HE2	1:A:282:PHE:HA	1.94	0.50
1:A:410:MET:HG2	1:A:442:GLN:HE22	1.76	0.50
1:A:1369:MET:N	1:A:1369:MET:HE2	2.27	0.50
1:A:1384:PHE:CD2	1:A:1395:LEU:HD21	2.46	0.50
1:A:1575:LEU:HA	1:A:1578:ALA:HB3	1.93	0.50
1:A:1593:VAL:O	1:A:1597:LEU:HD23	2.12	0.50
1:A:2411:LEU:HD23	1:A:2442:MET:HG3	1.93	0.49
1:A:250:ASN:O	1:A:254:LYS:HG2	2.11	0.49
1:A:1086:TYR:C	1:A:1088:GLU:H	2.20	0.49
1:A:1244:LEU:H	1:A:1244:LEU:HD23	1.77	0.49
1:A:1812:LEU:HG	1:A:1814:PHE:HB3	1.94	0.49
1:A:2813:PHE:HE1	1:A:2817:LEU:HD11	1.76	0.49
1:A:2884:LEU:HD12	1:A:3116:SER:HB2	1.94	0.49
1:A:3256:MET:SD	1:A:3260:LYS:HD2	2.53	0.49
1:A:3741:ARG:HG2	1:A:3747:GLU:HG2	1.93	0.49
1:A:762:TYR:CD1	1:A:764:PRO:HD2	2.46	0.49
1:A:1607:GLU:O	1:A:1611:GLN:HB2	2.11	0.49
1:A:718:MET:HE1	1:A:730:LEU:HD21	1.95	0.49
1:A:2166:SER:OG	1:A:2167:PRO:HD3	2.12	0.49
1:A:3585:PHE:CD2	1:A:3670:MET:HE1	2.48	0.49
1:A:2464:HIS:CE1	1:A:2466:SER:HB2	2.48	0.49
1:A:340:TYR:O	1:A:344:GLN:HG2	2.13	0.49
1:A:1664:SER:HA	1:A:1669:PRO:HD3	1.93	0.49
1:A:1948:ALA:O	1:A:1952:ILE:HG12	2.13	0.49
1:A:873:VAL:HG11	1:A:3125:ARG:HH12	1.77	0.49
1:A:898:PHE:HB2	1:A:901:MET:O	2.13	0.49
1:A:1975:LEU:HD12	1:A:1976:LEU:HG	1.94	0.49
1:A:2826:LEU:HA	1:A:2829:LYS:HD3	1.95	0.49
1:A:421:LEU:HD12	1:A:424:LEU:HD12	1.95	0.49
1:A:535:LEU:HD23	1:A:637:LYS:HG3	1.94	0.49
1:A:1108:MET:HE1	1:A:1190:LEU:HD22	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1238:GLN:HG2	1:A:1238:GLN:O	2.11	0.49
1:A:1241:LEU:O	1:A:1244:LEU:HB3	2.13	0.49
1:A:1467:ILE:HG22	1:A:1468:LEU:HD22	1.95	0.49
1:A:203:GLU:O	1:A:206:THR:OG1	2.28	0.49
1:A:915:THR:HB	1:A:968:VAL:HG11	1.94	0.49
1:A:1098:GLN:HG3	1:A:1152:ARG:HG3	1.95	0.49
1:A:1750:LEU:HD23	1:A:1785:ILE:HD11	1.93	0.48
1:A:2530:ARG:NH1	1:A:2530:ARG:HG3	2.28	0.48
1:A:3269:ARG:C	1:A:3271:ASP:H	2.20	0.48
1:A:381:VAL:HA	1:A:384:MET:HE3	1.95	0.48
1:A:3859:TYR:CD2	1:A:4077:TYR:HE1	2.31	0.48
1:A:1328:GLU:HA	1:A:1331:ASN:HB2	1.95	0.48
1:A:2277:LEU:O	1:A:2280:VAL:HG12	2.13	0.48
1:A:222:GLY:HA3	1:A:266:ALA:HB1	1.95	0.48
1:A:244:THR:O	1:A:248:ILE:HG13	2.12	0.48
1:A:1301:ILE:HG13	1:A:1302:ALA:H	1.78	0.48
1:A:1515:LEU:HG	1:A:1519:PHE:CE2	2.49	0.48
1:A:3252:PHE:O	1:A:3287:ARG:NH2	2.43	0.48
1:A:1696:LEU:O	1:A:1700:THR:HG23	2.13	0.48
1:A:2189:ILE:O	1:A:2193:ILE:HG23	2.13	0.48
1:A:2233:HIS:HA	1:A:2236:GLU:CD	2.38	0.48
1:A:1249:SER:HB3	1:A:1319:GLY:HA3	1.95	0.48
1:A:1273:GLU:OE1	1:A:1273:GLU:N	2.40	0.48
1:A:2169:LEU:HB3	1:A:2211:LEU:HD11	1.95	0.48
1:A:3726:VAL:HG13	1:A:3736:LYS:HB3	1.96	0.48
1:A:1212:LEU:HD11	1:A:1217:VAL:HA	1.95	0.48
1:A:2348:GLN:HA	1:A:2351:GLN:OE1	2.14	0.48
1:A:2348:GLN:O	1:A:2348:GLN:NE2	2.44	0.48
1:A:2810:SER:HG	1:A:2857:CYS:HG	1.62	0.48
1:A:3182:ILE:HG13	1:A:3183:ILE:N	2.28	0.48
1:A:3613:MET:SD	1:A:3617:LEU:HB2	2.54	0.48
1:A:1127:CYS:O	1:A:1131:ILE:HG13	2.13	0.48
1:A:1267:TYR:HE1	1:A:1281:VAL:HG11	1.78	0.48
1:A:63:PHE:HA	1:A:66:LEU:HD12	1.95	0.48
1:A:397:LEU:HD21	1:A:438:LEU:HD22	1.95	0.48
1:A:267:VAL:HG23	1:A:268:PRO:HD3	1.96	0.48
1:A:345:PHE:HE2	1:A:369:PHE:CE2	2.32	0.48
1:A:901:MET:SD	1:A:2819:GLU:HG2	2.54	0.48
1:A:2257:PHE:CE1	1:A:2261:SER:HB2	2.49	0.48
1:A:2397:CYS:HA	1:A:2400:VAL:HG12	1.96	0.48
1:A:3155:VAL:HG12	1:A:3159:ARG:HH21	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3710:LYS:HB2	1:A:3711:PRO:HD2	1.95	0.48
1:A:2121:ASP:OD1	1:A:2160:TYR:OH	2.32	0.47
1:A:2474:TYR:HB3	1:A:2521:ILE:HD11	1.95	0.47
1:A:3484:THR:HG22	1:A:3513:ALA:HB2	1.96	0.47
1:A:1766:LEU:HD12	1:A:1778:PHE:CD2	2.49	0.47
1:A:2395:THR:O	1:A:2398:LEU:N	2.45	0.47
1:A:2451:LEU:HD23	1:A:2484:TYR:HE2	1.79	0.47
1:A:2522:ARG:NH2	1:A:2564:GLU:HG3	2.28	0.47
1:A:2965:TYR:HB2	1:A:3005:LEU:HD21	1.96	0.47
1:A:4076:ASP:O	1:A:4080:VAL:HG12	2.13	0.47
1:A:962:TYR:HA	1:A:965:THR:HG22	1.95	0.47
1:A:1335:CYS:HB3	1:A:1384:PHE:HE1	1.79	0.47
1:A:1920:TYR:O	1:A:1924:THR:CB	2.63	0.47
1:A:3731:SER:O	1:A:3734:ARG:NH2	2.47	0.47
1:A:3791:TYR:CE1	1:A:3940:ILE:HG22	2.49	0.47
1:A:1605:PHE:HB2	1:A:1655:ILE:HG22	1.96	0.47
1:A:3383:GLN:O	1:A:3387:GLU:HG3	2.14	0.47
1:A:14:ARG:O	1:A:18:THR:HG23	2.14	0.47
1:A:131:LEU:HB2	1:A:173:LYS:HD2	1.95	0.47
1:A:1158:PRO:CD	1:A:1159:PRO:HD2	2.45	0.47
1:A:1374:GLN:OE1	1:A:1382:ILE:HD13	2.15	0.47
1:A:1713:VAL:HA	1:A:1716:GLN:NE2	2.29	0.47
1:A:2466:SER:C	1:A:2468:THR:H	2.23	0.47
1:A:3913:ILE:HG21	1:A:3987:ALA:HB3	1.96	0.47
1:A:221:ALA:HA	1:A:224:LEU:HG	1.96	0.47
1:A:2318:ALA:O	1:A:2321:GLU:HG2	2.13	0.47
1:A:3629:ARG:O	1:A:3633:ILE:HG12	2.15	0.47
1:A:160:LEU:HD21	1:A:178:LEU:HD13	1.97	0.47
1:A:1119:LYS:HD3	1:A:1119:LYS:N	2.30	0.47
1:A:1209:LYS:O	1:A:1213:LYS:HG3	2.15	0.47
1:A:1267:TYR:CD2	1:A:1290:LEU:HD22	2.49	0.47
1:A:1651:LYS:HA	1:A:1651:LYS:HD3	1.79	0.47
1:A:1851:LEU:HD22	1:A:1870:LYS:HG2	1.97	0.47
1:A:2376:ASP:HA	1:A:2379:MET:SD	2.55	0.47
1:A:2474:TYR:HD2	1:A:2517:LEU:HD12	1.79	0.47
1:A:3468:LEU:O	1:A:3472:ILE:HG12	2.15	0.47
1:A:3495:PHE:CD1	1:A:3502:MET:HE1	2.49	0.47
1:A:3763:ARG:HG3	1:A:4011:PHE:HZ	1.80	0.47
1:A:1458:LEU:HD12	1:A:1463:LEU:HB2	1.96	0.47
1:A:3170:ASP:HB3	1:A:3173:MET:HB3	1.97	0.47
1:A:3285:HIS:CE1	1:A:3332:THR:HB	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:ASP:HB3	1:A:784:VAL:HG12	1.97	0.47
1:A:2398:LEU:HD21	1:A:2435:CYS:SG	2.55	0.47
1:A:461:ILE:HG23	1:A:534:LEU:HD21	1.96	0.47
1:A:1651:LYS:O	1:A:1655:ILE:HG23	2.14	0.47
1:A:1690:GLY:O	1:A:1693:VAL:HG22	2.15	0.47
1:A:3786:LEU:O	1:A:3787:GLN:NE2	2.42	0.47
1:A:1001:PHE:N	1:A:1002:GLU:OE2	2.48	0.46
1:A:1324:PRO:C	1:A:1327:GLY:H	2.22	0.46
1:A:1592:MET:O	1:A:1596:VAL:HG23	2.14	0.46
1:A:2233:HIS:O	1:A:2237:ILE:HG13	2.14	0.46
1:A:3156:PRO:O	1:A:3159:ARG:HG2	2.14	0.46
1:A:3012:GLU:HB2	1:A:3047:SER:HB2	1.97	0.46
1:A:3033:GLU:HG3	1:A:3034:PRO:HD3	1.97	0.46
1:A:782:ARG:O	1:A:786:GLN:HB2	2.15	0.46
1:A:1045:THR:HG21	1:A:1047:GLN:HE21	1.81	0.46
1:A:1142:HIS:O	1:A:1146:ASN:ND2	2.48	0.46
1:A:1271:ILE:HD12	1:A:1344:PHE:HE1	1.79	0.46
1:A:1764:GLU:O	1:A:1768:ARG:HG3	2.15	0.46
1:A:1915:LEU:HD13	1:A:1951:VAL:HG11	1.97	0.46
1:A:3014:CYS:C	1:A:3016:THR:H	2.23	0.46
1:A:3699:LEU:HD12	1:A:3700:GLU:H	1.80	0.46
1:A:4064:LEU:HD13	1:A:4077:TYR:HB3	1.98	0.46
1:A:1390:GLN:HA	1:A:1393:ALA:HB3	1.97	0.46
1:A:2530:ARG:HG3	1:A:2530:ARG:HH11	1.79	0.46
1:A:3308:ASP:HB3	1:A:3311:ASN:O	2.16	0.46
1:A:3616:ALA:HB1	1:A:3629:ARG:HH22	1.81	0.46
1:A:1839:PHE:O	1:A:1843:ILE:HG12	2.16	0.46
1:A:1871:MET:HE3	1:A:1939:LEU:CD1	2.43	0.46
1:A:2313:LYS:HA	1:A:2316:TYR:CE2	2.50	0.46
1:A:3348:LEU:HB2	1:A:3352:GLU:HG2	1.97	0.46
1:A:3971:MET:HE1	1:A:3980:MET:HG3	1.97	0.46
1:A:1078:ALA:O	1:A:1107:TYR:OH	2.27	0.46
1:A:1357:LYS:HA	1:A:1361:LYS:HD3	1.98	0.46
1:A:2328:ARG:HH11	1:A:2370:SER:HB3	1.81	0.46
1:A:3515:GLN:HG2	1:A:3554:PHE:CE2	2.51	0.46
1:A:886:TRP:HH2	1:A:915:THR:HG21	1.79	0.46
1:A:1853:SER:O	1:A:1855:PHE:N	2.43	0.46
1:A:2953:THR:HB	1:A:2994:TRP:HE1	1.81	0.46
1:A:3157:LEU:O	1:A:3161:LEU:HG	2.15	0.46
1:A:305:ASN:HB3	1:A:308:LEU:HB3	1.98	0.46
1:A:323:VAL:HA	1:A:326:MET:HG3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1797:LEU:O	1:A:1800:SER:OG	2.27	0.46
1:A:2281:MET:CE	1:A:2287:PRO:HG3	2.43	0.46
1:A:2820:MET:HE3	1:A:2820:MET:HB2	1.81	0.46
1:A:3733:ARG:NH2	1:A:4022:LYS:HD3	2.31	0.46
1:A:296:VAL:O	1:A:300:TRP:CD1	2.69	0.46
1:A:1075:ARG:HH12	1:A:1123:THR:HG21	1.81	0.46
1:A:1573:LYS:HA	1:A:1573:LYS:HD3	1.75	0.46
1:A:2126:MET:HE3	1:A:2160:TYR:HD2	1.81	0.46
1:A:2514:ASN:HD22	1:A:2517:LEU:HD23	1.81	0.46
1:A:3763:ARG:NH1	1:A:4008:GLU:OE1	2.49	0.46
1:A:3819:THR:HG21	1:A:3886:ALA:HB2	1.96	0.46
1:A:3959:MET:SD	1:A:3959:MET:N	2.76	0.46
1:A:205:LYS:HG2	1:A:249:PHE:CE2	2.50	0.46
1:A:1519:PHE:CE1	1:A:1528:LEU:HD22	2.50	0.46
1:A:1579:VAL:HA	1:A:1582:LEU:HD12	1.97	0.46
1:A:3907:SER:O	1:A:3911:ILE:HG23	2.16	0.46
1:A:342:MET:HB3	1:A:346:TYR:CZ	2.50	0.45
1:A:433:PRO:HB3	1:A:6015:UNK:CB	2.46	0.45
1:A:1108:MET:HE2	1:A:1108:MET:HB2	1.85	0.45
1:A:1334:LYS:NZ	1:A:1382:ILE:HB	2.31	0.45
1:A:2786:LYS:O	1:A:2788:SER:N	2.49	0.45
1:A:3699:LEU:HD12	1:A:3700:GLU:N	2.31	0.45
1:A:3729:MET:HE2	1:A:3805:TRP:CH2	2.45	0.45
1:A:3812:LEU:HD12	1:A:3812:LEU:HA	1.81	0.45
1:A:2206:PRO:O	1:A:2210:VAL:HG23	2.16	0.45
1:A:2397:CYS:O	1:A:2400:VAL:HG12	2.16	0.45
1:A:3692:VAL:HG13	1:A:3692:VAL:O	2.16	0.45
1:A:200:PHE:CE1	1:A:224:LEU:HD22	2.51	0.45
1:A:998:ASN:HA	1:A:1001:PHE:CE1	2.51	0.45
1:A:1652:ILE:HD12	1:A:1655:ILE:HD11	1.98	0.45
1:A:1410:PRO:C	1:A:1412:LYS:H	2.24	0.45
1:A:1456:LYS:HB3	1:A:1456:LYS:HE2	1.65	0.45
1:A:2389:PHE:HB2	1:A:2394:LYS:HG2	1.99	0.45
1:A:3466:PRO:HG2	1:A:4004:VAL:HG11	1.99	0.45
1:A:291:VAL:O	1:A:295:GLU:HG2	2.15	0.45
1:A:295:GLU:O	1:A:299:LYS:HG3	2.17	0.45
1:A:1075:ARG:NH1	1:A:1123:THR:HG21	2.31	0.45
1:A:1813:SER:HA	1:A:1816:ARG:HG3	1.99	0.45
1:A:1919:CYS:SG	1:A:1920:TYR:N	2.89	0.45
1:A:2193:ILE:HA	1:A:2196:TRP:HE3	1.82	0.45
1:A:2310:VAL:HA	1:A:2359:LYS:HZ1	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2554:PHE:C	1:A:2556:SER:H	2.24	0.45
1:A:3751:LEU:HD12	1:A:3805:TRP:HE3	1.81	0.45
1:A:3961:PHE:HE2	1:A:4107:LEU:HD13	1.80	0.45
1:A:1440:ASP:HA	1:A:1442:GLN:HE22	1.82	0.45
1:A:3495:PHE:CG	1:A:3502:MET:HE1	2.52	0.45
1:A:3892:THR:OG1	1:A:3893:SER:N	2.49	0.45
1:A:200:PHE:CE2	1:A:227:LEU:HD23	2.52	0.45
1:A:254:LYS:HA	1:A:254:LYS:HD3	1.66	0.45
1:A:3006:ALA:HB3	1:A:3257:LYS:HZ1	1.80	0.45
1:A:3882:LEU:HD23	1:A:3882:LEU:HA	1.80	0.45
1:A:541:MET:O	1:A:545:LEU:HG	2.16	0.45
1:A:3132:VAL:O	1:A:3136:THR:HG23	2.16	0.45
1:A:3961:PHE:CZ	1:A:3984:MET:HE1	2.51	0.45
1:A:16:GLN:HB2	1:A:66:LEU:HD11	1.98	0.45
1:A:261:ASP:OD1	1:A:262:LEU:N	2.50	0.45
1:A:804:ALA:HA	1:A:852:ARG:NH2	2.32	0.45
1:A:2215:LEU:O	1:A:2219:LEU:HG	2.17	0.45
1:A:2256:ILE:HG22	1:A:2260:PHE:HE1	1.79	0.45
1:A:2577:PHE:HB2	1:A:2784:GLN:HA	1.99	0.45
1:A:3449:LYS:HA	1:A:3449:LYS:HD3	1.65	0.45
1:A:635:PRO:HA	1:A:676:ASN:HD22	1.82	0.44
1:A:710:PHE:O	1:A:714:VAL:HG12	2.17	0.44
1:A:1224:PHE:HD2	1:A:1267:TYR:CE1	2.34	0.44
1:A:1790:SER:O	1:A:1794:GLN:HG3	2.16	0.44
1:A:2098:THR:C	1:A:2102:LYS:HZ2	2.25	0.44
1:A:3793:VAL:HG13	1:A:3803:ILE:HG22	1.99	0.44
1:A:1813:SER:O	1:A:1816:ARG:HB2	2.16	0.44
1:A:2464:HIS:ND1	1:A:2466:SER:HB2	2.31	0.44
1:A:3779:SER:O	1:A:3783:GLN:HG3	2.18	0.44
1:A:279:ALA:HA	1:A:282:PHE:HD2	1.82	0.44
1:A:1080:LEU:O	1:A:1084:ASN:ND2	2.45	0.44
1:A:1372:LEU:HD12	1:A:1402:LEU:HD23	1.99	0.44
1:A:1737:ASN:HA	1:A:1740:VAL:HG12	2.00	0.44
1:A:1863:PHE:HZ	1:A:1937:ARG:HH11	1.65	0.44
1:A:2371:PHE:CE1	1:A:2373:PRO:HD2	2.53	0.44
1:A:3451:LEU:HA	1:A:3451:LEU:HD23	1.67	0.44
1:A:3646:LYS:HB3	1:A:3650:LYS:HB2	1.99	0.44
1:A:333:MET:HG2	1:A:334:HIS:CE1	2.52	0.44
1:A:607:ASP:OD1	1:A:607:ASP:N	2.39	0.44
1:A:1151:ARG:HD2	1:A:1163:LEU:HB3	1.98	0.44
1:A:2150:VAL:HG22	1:A:2157:PHE:CE2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2216:LEU:HA	1:A:2219:LEU:HD12	1.98	0.44
1:A:3227:ILE:HD12	1:A:3227:ILE:H	1.82	0.44
1:A:3564:GLN:HG3	1:A:3565:GLY:N	2.32	0.44
1:A:3681:LYS:O	1:A:3685:PRO:HD2	2.17	0.44
1:A:3763:ARG:HG3	1:A:4011:PHE:CZ	2.53	0.44
1:A:3805:TRP:O	1:A:3806:LEU:C	2.61	0.44
1:A:573:LEU:HD23	1:A:573:LEU:HA	1.77	0.44
1:A:1395:LEU:HB3	1:A:1396:PRO:HD3	2.00	0.44
1:A:1793:THR:O	1:A:1797:LEU:HG	2.18	0.44
1:A:1804:MET:O	1:A:1811:ARG:NH2	2.44	0.44
1:A:2319:ALA:O	1:A:2323:LEU:HG	2.18	0.44
1:A:2496:GLN:O	1:A:2500:LYS:HG2	2.18	0.44
1:A:2531:LEU:HA	1:A:2532:PRO:HD3	1.88	0.44
1:A:3805:TRP:O	1:A:3805:TRP:CG	2.69	0.44
1:A:303:HIS:ND1	1:A:308:LEU:HD23	2.32	0.44
1:A:1815:THR:HG22	1:A:1819:PHE:HE1	1.83	0.44
1:A:3176:MET:HE3	1:A:3246:ALA:CA	2.47	0.44
1:A:108:LYS:HZ3	1:A:151:GLU:HA	1.83	0.44
1:A:1724:MET:HA	1:A:1768:ARG:HH22	1.83	0.44
1:A:3104:GLN:OE1	1:A:3139:GLN:NE2	2.51	0.44
1:A:3646:LYS:N	1:A:3650:LYS:HB3	2.33	0.44
1:A:4005:PHE:CD1	1:A:4005:PHE:C	2.95	0.44
1:A:336:ASN:OD1	1:A:337:LYS:N	2.51	0.44
1:A:1440:ASP:CG	1:A:1441:ALA:H	2.25	0.44
1:A:1662:ASN:OD1	1:A:1663:THR:N	2.46	0.44
1:A:2256:ILE:HD12	1:A:2256:ILE:H	1.83	0.44
1:A:2344:LEU:HA	1:A:2347:LYS:NZ	2.33	0.44
1:A:2917:PRO:HB2	1:A:2919:ASP:OD1	2.18	0.44
1:A:3975:LYS:HA	1:A:3975:LYS:HD3	1.86	0.44
1:A:536:SER:O	1:A:539:GLN:HB2	2.18	0.44
1:A:3595:GLU:CD	1:A:3606:ILE:HG21	2.43	0.44
1:A:303:HIS:HE1	1:A:305:ASN:HB2	1.82	0.43
1:A:3859:TYR:HB3	1:A:4076:ASP:OD1	2.18	0.43
1:A:770:LEU:O	1:A:774:GLU:HG3	2.18	0.43
1:A:1452:VAL:HG23	1:A:1517:LEU:HD22	2.00	0.43
1:A:1580:LEU:HD11	1:A:1625:HIS:NE2	2.34	0.43
1:A:2396:LEU:HA	1:A:2399:GLU:OE2	2.18	0.43
1:A:3293:CYS:O	1:A:3297:VAL:HG23	2.18	0.43
1:A:722:LYS:HA	1:A:726:LEU:CB	2.48	0.43
1:A:1664:SER:N	1:A:1668:PHE:HB3	2.33	0.43
1:A:2284:ASP:O	1:A:2285:LEU:HD23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2389:PHE:O	1:A:2390:HIS:ND1	2.50	0.43
1:A:3498:TRP:O	1:A:3502:MET:HG3	2.18	0.43
1:A:1291:LEU:HA	1:A:1294:VAL:HG22	1.99	0.43
1:A:1605:PHE:HD2	1:A:1651:LYS:HZ2	1.64	0.43
1:A:1921:ASP:OD1	1:A:1922:ALA:N	2.52	0.43
1:A:2183:HIS:CE1	1:A:2185:MET:HB2	2.53	0.43
1:A:2960:GLU:HG3	1:A:2965:TYR:HE1	1.83	0.43
1:A:3156:PRO:HA	1:A:3159:ARG:HE	1.84	0.43
1:A:3466:PRO:HB2	1:A:4004:VAL:HG11	2.00	0.43
1:A:3744:ASP:OD1	1:A:3744:ASP:N	2.51	0.43
1:A:3880:ALA:HA	1:A:3965:ARG:NH2	2.33	0.43
1:A:899:ARG:HH21	1:A:2568:MET:HB3	1.83	0.43
1:A:1413:ASP:O	1:A:1417:THR:HG23	2.17	0.43
1:A:1626:TRP:HZ2	1:A:1674:THR:HG21	1.83	0.43
1:A:1672:PHE:O	1:A:1676:ILE:HG12	2.18	0.43
1:A:2296:SER:HA	1:A:2299:TYR:HD2	1.83	0.43
1:A:2376:ASP:OD1	1:A:2377:ARG:HD2	2.19	0.43
1:A:3481:SER:HA	1:A:3484:THR:OG1	2.19	0.43
1:A:3526:PRO:C	1:A:3528:ALA:H	2.27	0.43
1:A:3685:PRO:HB2	1:A:3687:MET:H	1.83	0.43
1:A:4076:ASP:OD1	1:A:4077:TYR:N	2.51	0.43
1:A:290:TYR:CZ	1:A:337:LYS:HB3	2.53	0.43
1:A:759:GLY:HA3	1:A:766:ALA:HB2	1.99	0.43
1:A:2325:LEU:O	1:A:2328:ARG:HG2	2.19	0.43
1:A:3288:SER:OG	1:A:3294:SER:HB2	2.18	0.43
1:A:3809:THR:HG22	1:A:3931:ALA:HA	1.99	0.43
1:A:997:ASN:OD1	1:A:998:ASN:N	2.47	0.43
1:A:1086:TYR:CD2	1:A:1087:ARG:HG3	2.54	0.43
1:A:1217:VAL:O	1:A:1221:ILE:HD12	2.18	0.43
1:A:1617:LYS:O	1:A:1621:THR:HG22	2.19	0.43
1:A:2936:TYR:O	1:A:2940:ARG:HD3	2.18	0.43
1:A:3066:ASP:HA	1:A:3069:MET:HB2	2.01	0.43
1:A:3416:LEU:HG	1:A:3445:LEU:HD21	1.99	0.43
1:A:3582:GLU:HG2	1:A:3583:LEU:N	2.33	0.43
1:A:967:PRO:O	1:A:971:ARG:HG3	2.18	0.43
1:A:1945:TYR:O	1:A:1949:ILE:HG12	2.18	0.43
1:A:2270:ASN:N	1:A:2270:ASN:HD22	2.16	0.43
1:A:2548:PRO:HB2	1:A:2848:PHE:CE2	2.53	0.43
1:A:3012:GLU:HG3	1:A:3048:LYS:HG3	2.00	0.43
1:A:3090:TYR:HE2	1:A:3102:TYR:HE2	1.67	0.43
1:A:1149:LYS:N	1:A:1162:SER:OG	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3655:LYS:C	1:A:3657:SER:H	2.25	0.43
1:A:1655:ILE:HG13	1:A:1656:ASP:N	2.34	0.43
1:A:2478:MET:HG2	1:A:2524:PHE:CD1	2.54	0.43
1:A:2539:LEU:HD13	1:A:2562:LEU:HD11	2.01	0.43
1:A:156:PHE:O	1:A:160:LEU:HG	2.18	0.42
1:A:2371:PHE:CD1	1:A:2373:PRO:HD2	2.54	0.42
1:A:532:ARG:HD3	1:A:637:LYS:HD3	2.00	0.42
1:A:1257:LEU:HD22	1:A:1337:VAL:HG21	2.01	0.42
1:A:1881:TYR:CD2	1:A:1951:VAL:HG23	2.54	0.42
1:A:2443:MET:C	1:A:2445:LYS:H	2.26	0.42
1:A:2492:ASP:C	1:A:2494:ASP:H	2.27	0.42
1:A:3031:TRP:CD1	1:A:3031:TRP:N	2.87	0.42
1:A:434:VAL:O	1:A:438:LEU:HD23	2.18	0.42
1:A:624:ILE:O	1:A:628:GLU:HG2	2.20	0.42
1:A:911:LEU:O	1:A:915:THR:HG23	2.19	0.42
1:A:1157:PHE:HE1	1:A:1171:TRP:CD1	2.37	0.42
1:A:1538:LEU:HD12	1:A:1553:PHE:CE2	2.54	0.42
1:A:3632:PHE:HD1	1:A:3633:ILE:HD13	1.84	0.42
1:A:29:LEU:HA	1:A:32:HIS:HB2	2.02	0.42
1:A:485:GLN:O	1:A:488:ILE:HG22	2.19	0.42
1:A:1086:TYR:CE1	1:A:1133:HIS:CD2	3.08	0.42
1:A:1718:ILE:HG13	1:A:1719:VAL:N	2.34	0.42
1:A:2097:LEU:HD12	1:A:2145:PHE:HZ	1.84	0.42
1:A:3381:ALA:O	1:A:3385:LEU:HD23	2.20	0.42
1:A:534:LEU:HD23	1:A:534:LEU:HA	1.83	0.42
1:A:1179:PRO:HG3	1:A:3694:PHE:CD2	2.54	0.42
1:A:1275:THR:HG22	1:A:1276:VAL:HG23	2.01	0.42
1:A:1301:ILE:HG22	1:A:1334:LYS:HG3	2.02	0.42
1:A:1525:CYS:HB3	1:A:1574:ASN:HD21	1.83	0.42
1:A:1678:LEU:HD12	1:A:1679:LEU:N	2.34	0.42
1:A:4027:TRP:CD2	1:A:4030:GLU:HB3	2.54	0.42
1:A:1385:ASN:HA	1:A:1392:MET:CE	2.49	0.42
1:A:1627:LYS:HD2	1:A:1627:LYS:HA	1.80	0.42
1:A:2894:GLU:HB3	1:A:3973:PRO:HG2	2.02	0.42
1:A:3492:CYS:SG	1:A:3521:ILE:HD13	2.60	0.42
1:A:3580:ASN:ND2	1:A:3734:ARG:HB2	2.30	0.42
1:A:1562:LEU:HD23	1:A:1562:LEU:HA	1.86	0.42
1:A:1794:GLN:O	1:A:1798:LEU:HG	2.19	0.42
1:A:2531:LEU:HD21	1:A:2538:ARG:HG3	2.02	0.42
1:A:2884:LEU:HD11	1:A:3113:ASN:OD1	2.20	0.42
1:A:3031:TRP:HZ3	1:A:3044:MET:HB2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3606:ILE:C	1:A:3608:LYS:H	2.28	0.42
2:A:6101:AGS:O4'	2:A:6101:AGS:O5'	2.36	0.42
1:A:85:ILE:O	1:A:89:LEU:HG	2.19	0.42
1:A:290:TYR:CE1	1:A:337:LYS:HE3	2.55	0.42
1:A:1368:LEU:HA	1:A:1371:VAL:HG12	2.02	0.42
1:A:1526:GLU:OE1	1:A:1526:GLU:N	2.47	0.42
1:A:2504:ASP:OD1	1:A:2504:ASP:C	2.63	0.42
1:A:3095:ASP:OD1	1:A:3095:ASP:N	2.53	0.42
1:A:3169:PRO:HD3	1:A:3182:ILE:HD11	2.01	0.42
1:A:490:ILE:HD11	1:A:629:PHE:CE2	2.54	0.42
1:A:901:MET:HB3	1:A:2823:PHE:CE2	2.55	0.42
1:A:1436:LEU:HD23	1:A:1436:LEU:H	1.84	0.42
1:A:2455:LEU:HD22	1:A:2498:ILE:HG23	2.02	0.42
1:A:172:GLU:HB3	1:A:220:LEU:HD12	2.01	0.42
1:A:653:LEU:HD23	1:A:653:LEU:HA	1.77	0.42
1:A:1046:PRO:HA	1:A:1049:GLN:HB2	2.01	0.42
1:A:1240:THR:HG23	1:A:1296:PHE:CD2	2.54	0.42
1:A:1265:GLU:HG2	1:A:1340:ARG:HD3	2.02	0.42
1:A:2251:ILE:HB	1:A:2253:TYR:CZ	2.55	0.42
1:A:3077:ILE:HG13	1:A:3078:LEU:N	2.34	0.42
1:A:3944:HIS:NE2	1:A:4020:MET:HE1	2.35	0.42
1:A:19:LEU:HG	1:A:34:LEU:HD23	2.01	0.41
1:A:486:GLY:O	1:A:490:ILE:HG23	2.20	0.41
1:A:1086:TYR:O	1:A:1087:ARG:HB2	2.20	0.41
1:A:1427:SER:O	1:A:1430:GLU:HG3	2.19	0.41
1:A:2899:ARG:HE	1:A:2899:ARG:HB3	1.70	0.41
1:A:3051:LEU:HD23	1:A:3051:LEU:HA	1.89	0.41
1:A:3759:ARG:O	1:A:3763:ARG:HG2	2.20	0.41
1:A:3858:MET:HE1	1:A:4119:ARG:HB3	2.01	0.41
1:A:1195:VAL:HG11	1:A:1204:PRO:HA	2.01	0.41
1:A:1238:GLN:C	1:A:1240:THR:N	2.78	0.41
1:A:2095:ALA:HB3	1:A:2096:PRO:HD3	2.01	0.41
1:A:3913:ILE:HD12	1:A:3913:ILE:HA	1.85	0.41
1:A:3959:MET:HE2	1:A:4124:TRP:CH2	2.55	0.41
1:A:971:ARG:HH22	1:A:1018:VAL:HG11	1.86	0.41
1:A:1265:GLU:CG	1:A:1340:ARG:HD3	2.50	0.41
1:A:1576:ASP:O	1:A:1580:LEU:HD13	2.19	0.41
1:A:2098:THR:HA	1:A:2101:VAL:HG22	2.02	0.41
1:A:2142:ILE:O	1:A:2146:LEU:HG	2.20	0.41
1:A:2164:TRP:O	1:A:2167:PRO:HD2	2.20	0.41
1:A:2548:PRO:HB2	1:A:2848:PHE:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3328:ILE:HG13	1:A:3329:LEU:HD12	2.02	0.41
1:A:3499:ILE:CG2	1:A:3529:ILE:HG13	2.50	0.41
1:A:2477:LEU:HA	1:A:2477:LEU:HD23	1.70	0.41
1:A:2540:LEU:HD21	1:A:2832:ILE:HG23	2.02	0.41
1:A:3026:ASP:O	1:A:3030:ILE:HG22	2.20	0.41
1:A:668:LYS:HE2	1:A:728:SER:OG	2.21	0.41
1:A:1301:ILE:HG13	1:A:1302:ALA:N	2.36	0.41
1:A:1376:LEU:HD22	1:A:1403:MET:HE1	2.01	0.41
1:A:2242:VAL:HA	1:A:2249:LEU:HD21	2.02	0.41
1:A:3531:TYR:HB2	1:A:3532:PRO:HD3	2.02	0.41
1:A:3975:LYS:HB2	1:A:3977:THR:HG22	2.03	0.41
1:A:2186:VAL:HA	1:A:2189:ILE:HG22	2.02	0.41
1:A:2813:PHE:CE1	1:A:2817:LEU:HD11	2.54	0.41
1:A:3033:GLU:OE2	1:A:3034:PRO:HG3	2.20	0.41
1:A:3422:GLN:O	1:A:3426:LYS:HG2	2.21	0.41
1:A:3791:TYR:OH	1:A:3940:ILE:HG22	2.20	0.41
1:A:1324:PRO:O	1:A:1327:GLY:N	2.51	0.41
1:A:1389:VAL:HG23	1:A:1390:GLN:N	2.36	0.41
1:A:1843:ILE:HD11	1:A:1880:MET:HE3	2.02	0.41
1:A:2325:LEU:HA	1:A:2328:ARG:HG2	2.03	0.41
1:A:3314:SER:C	1:A:3316:LEU:H	2.28	0.41
1:A:1733:THR:HG22	1:A:1735:ARG:H	1.85	0.41
1:A:1774:MET:HG3	1:A:1778:PHE:CD1	2.56	0.41
1:A:2231:PHE:O	1:A:2235:LEU:HG	2.21	0.41
1:A:22:ALA:O	1:A:30:ALA:HB1	2.21	0.41
1:A:263:LYS:HA	1:A:263:LYS:HD2	1.91	0.41
1:A:459:ARG:NH1	1:A:545:LEU:HD23	2.35	0.41
1:A:708:VAL:O	1:A:712:LYS:HG2	2.21	0.41
1:A:718:MET:HE1	1:A:730:LEU:CD2	2.51	0.41
1:A:1012:ALA:O	1:A:1013:ILE:HD13	2.20	0.41
1:A:1030:GLY:O	1:A:1033:ILE:HG22	2.21	0.41
1:A:1157:PHE:CE2	1:A:1163:LEU:HD11	2.56	0.41
1:A:1173:LEU:HD12	1:A:1191:PHE:CE1	2.56	0.41
1:A:1335:CYS:HB3	1:A:1384:PHE:CE1	2.55	0.41
1:A:1770:GLN:N	1:A:1770:GLN:OE1	2.54	0.41
1:A:1797:LEU:O	1:A:1801:VAL:HG22	2.20	0.41
1:A:2134:GLY:O	1:A:2136:PRO:HD3	2.21	0.41
1:A:2168:LEU:HD12	1:A:2169:LEU:N	2.35	0.41
1:A:2254:ARG:HH12	1:A:2292:CYS:N	2.19	0.41
1:A:2392:VAL:O	1:A:2396:LEU:HG	2.21	0.41
1:A:2555:LEU:HD11	1:A:2854:PHE:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3024:PRO:HA	1:A:3025:PRO:HD3	1.94	0.41
1:A:3797:THR:HG22	1:A:3798:SER:N	2.35	0.41
1:A:3992:ARG:HH12	1:A:4053:GLY:HA2	1.86	0.41
1:A:249:PHE:O	1:A:252:VAL:HG12	2.20	0.41
1:A:1002:GLU:C	1:A:1004:GLN:N	2.78	0.41
1:A:1385:ASN:HA	1:A:1392:MET:HE1	2.03	0.41
1:A:1862:THR:O	1:A:1865:THR:HG22	2.20	0.41
1:A:2284:ASP:C	1:A:2285:LEU:HD23	2.46	0.41
1:A:2318:ALA:HA	1:A:2321:GLU:HG2	2.03	0.41
1:A:2361:ILE:HD11	1:A:2393:LEU:HD23	2.03	0.41
1:A:201:LEU:O	1:A:205:LYS:HG3	2.21	0.40
1:A:2301:GLN:HA	1:A:2344:LEU:HD21	2.03	0.40
1:A:2477:LEU:HD22	1:A:2502:ALA:HA	2.03	0.40
1:A:3194:GLU:HB2	1:A:3231:ILE:CD1	2.51	0.40
1:A:3925:LEU:HA	1:A:3925:LEU:HD23	1.87	0.40
1:A:967:PRO:HD3	1:A:1010:LEU:HD12	2.03	0.40
1:A:1362:ASP:OD1	1:A:1362:ASP:N	2.52	0.40
1:A:2786:LYS:O	1:A:2787:HIS:C	2.65	0.40
1:A:3141:PHE:HE1	1:A:3193:ILE:HG13	1.87	0.40
1:A:3186:ARG:HB2	1:A:3238:MET:HE1	2.02	0.40
1:A:3772:ASN:OD1	1:A:3788:LEU:HB2	2.21	0.40
1:A:1066:LEU:HB3	1:A:1078:ALA:HB2	2.03	0.40
1:A:1181:THR:HG22	1:A:1184:ARG:HH12	1.86	0.40
1:A:3536:SER:HB3	1:A:3540:TYR:HE2	1.86	0.40
1:A:3617:LEU:HA	1:A:3633:ILE:HD11	2.04	0.40
1:A:637:LYS:HA	1:A:637:LYS:HD2	1.74	0.40
1:A:1681:ASP:HB3	1:A:1684:LEU:HD13	2.03	0.40
1:A:2193:ILE:HD12	1:A:2245:TRP:HH2	1.87	0.40
1:A:2251:ILE:HB	1:A:2253:TYR:CE2	2.56	0.40
1:A:859:LEU:HD21	1:A:870:LEU:HD13	2.02	0.40
1:A:1106:ILE:HD13	1:A:1106:ILE:HA	1.89	0.40
1:A:1874:TYR:CE2	1:A:1944:ALA:HB2	2.57	0.40
1:A:2575:PRO:O	1:A:2576:MET:HG2	2.21	0.40
1:A:3238:MET:HE2	1:A:3238:MET:HB3	1.93	0.40
1:A:3683:CYS:SG	1:A:3684:SER:N	2.95	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	3602/4148 (87%)	3284 (91%)	311 (9%)	7 (0%)	43 71

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3714	GLU
1	A	3354	ASP
1	A	3406	ALA
1	A	723	ASP
1	A	2787	HIS
1	A	4024	GLY
1	A	4025	GLY

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	3195/3671 (87%)	3190 (100%)	5 (0%)	87 85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	722	LYS
1	A	3714	GLU
1	A	3733	ARG
1	A	3753	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3940	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	GLN
1	A	442	GLN
1	A	720	GLN
1	A	1048	GLN
1	A	1083	ASN
1	A	1133	HIS
1	A	1331	ASN
1	A	1401	ASN
1	A	2103	HIS
1	A	2152	ASN
1	A	2353	GLN
1	A	2422	GLN
1	A	2784	GLN
1	A	2859	GLN
1	A	3070	HIS
1	A	3081	HIS
1	A	3162	ASN
1	A	3166	ASN
1	A	3250	ASN
1	A	3384	HIS
1	A	3643	HIS
1	A	3664	ASN
1	A	3748	HIS

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

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AGS	A	6101	3	32,33,33	3.61	11 (34%)	45,52,52	2.02	11 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGS	A	6101	3	-	4/21/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6101	AGS	PG-S1G	10.32	2.13	1.90
2	A	6101	AGS	O4'-C4'	8.52	1.63	1.45
2	A	6101	AGS	C3'-C4'	-7.55	1.33	1.53
2	A	6101	AGS	PB-O3A	5.91	1.65	1.59
2	A	6101	AGS	C6-N6	5.26	1.47	1.34
2	A	6101	AGS	O4'-C1'	-5.22	1.29	1.42
2	A	6101	AGS	PB-O3B	4.12	1.63	1.59
2	A	6101	AGS	O2'-C2'	-3.58	1.34	1.43
2	A	6101	AGS	C8-N9	-3.47	1.31	1.37
2	A	6101	AGS	C5-N7	-3.10	1.33	1.39
2	A	6101	AGS	PA-O3A	2.27	1.61	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6101	AGS	C5-C4-N3	-6.26	118.10	126.72
2	A	6101	AGS	N3-C4-N9	4.86	135.43	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	6101	AGS	N3-C2-N1	-4.51	121.75	128.58
2	A	6101	AGS	C2-N3-C4	3.93	121.44	111.83
2	A	6101	AGS	N9-C8-N7	-3.57	108.88	113.94
2	A	6101	AGS	C4-N9-C8	3.18	109.07	105.74
2	A	6101	AGS	C5-N7-C8	2.98	108.13	103.45
2	A	6101	AGS	PB-O3B-PG	-2.83	122.82	133.17
2	A	6101	AGS	C4-C5-N7	-2.74	107.45	110.58
2	A	6101	AGS	C2'-C3'-C4'	2.60	107.64	102.61
2	A	6101	AGS	C3'-C2'-C1'	2.52	106.24	101.46

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	6101	AGS	O4'-C4'-C5'-O5'
2	A	6101	AGS	C3'-C4'-C5'-O5'
2	A	6101	AGS	PB-O3A-PA-O1A
2	A	6101	AGS	PB-O3A-PA-O2A

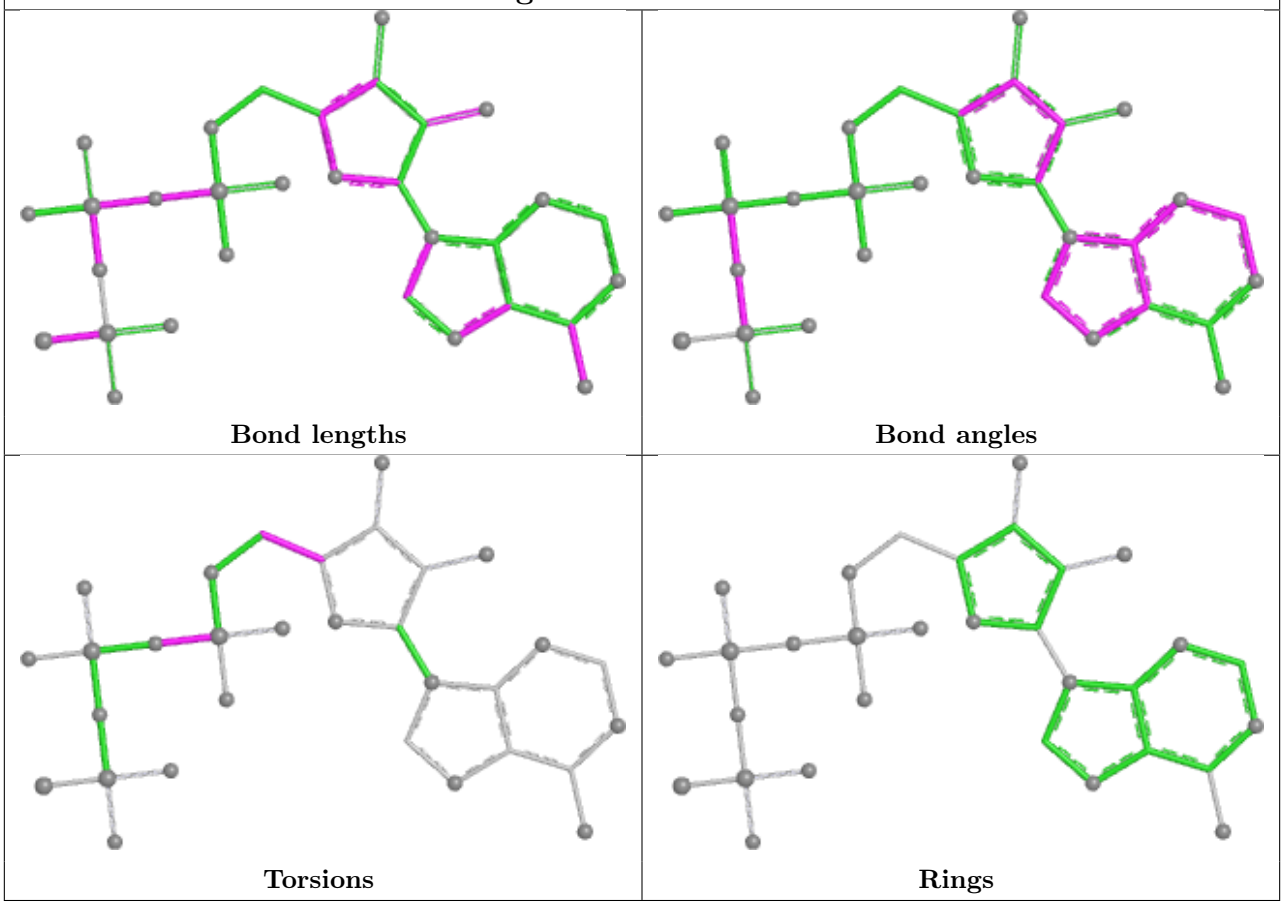
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6101	AGS	3	0

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

Ligand AGS A 6101



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	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4128:MET	C	6001:UNK	N	81.75

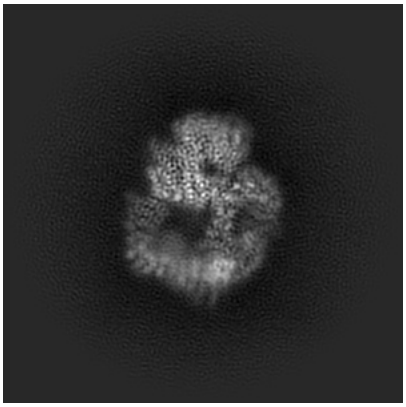
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13064. These allow visual inspection of the internal detail of the map and identification of artifacts.

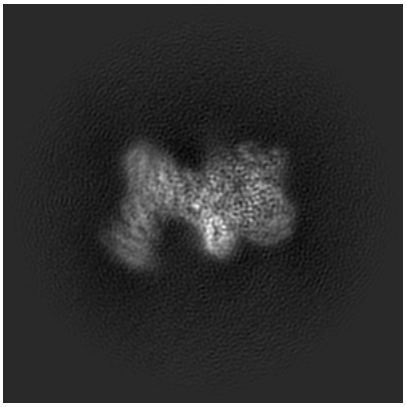
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

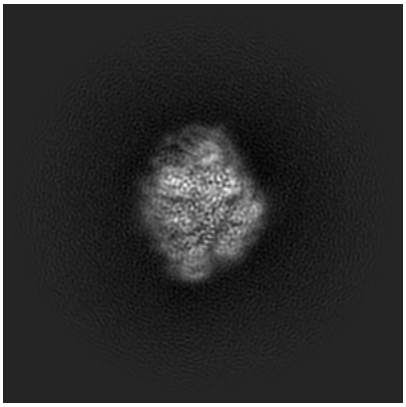
6.1.1 Primary map



X



Y

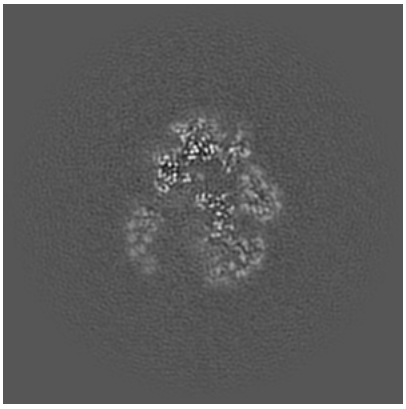


Z

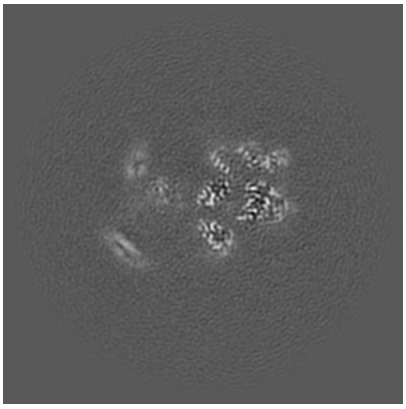
The images above show the map projected in three orthogonal directions.

6.2 Central slices

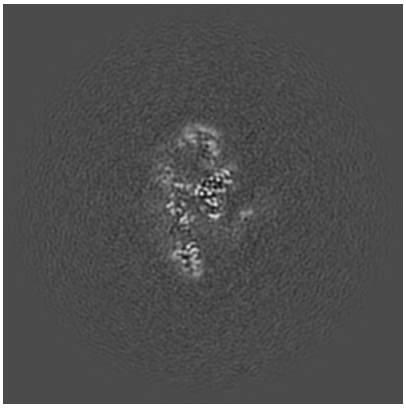
6.2.1 Primary map



X Index: 130



Y Index: 130

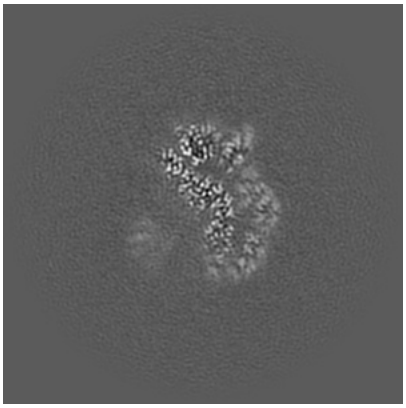


Z Index: 130

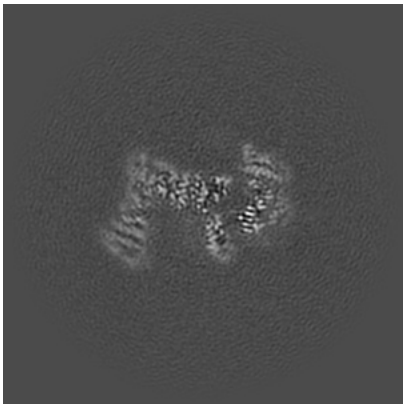
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

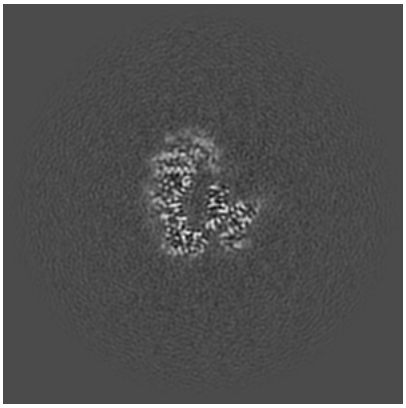
6.3.1 Primary map



X Index: 135



Y Index: 138

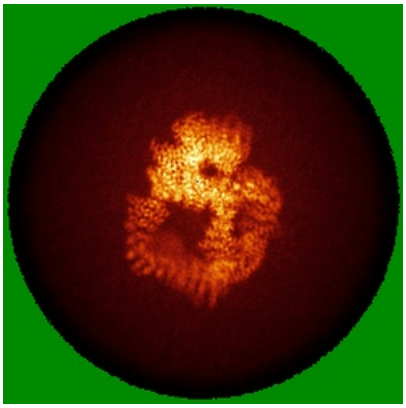


Z Index: 141

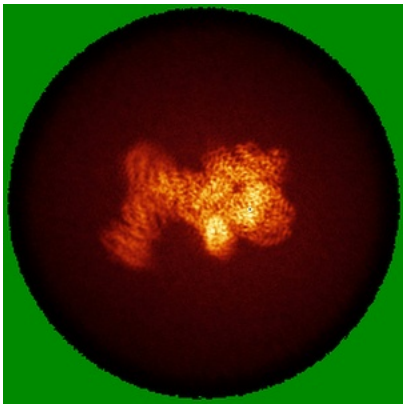
The images above show the largest variance slices of the map in three orthogonal directions.

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

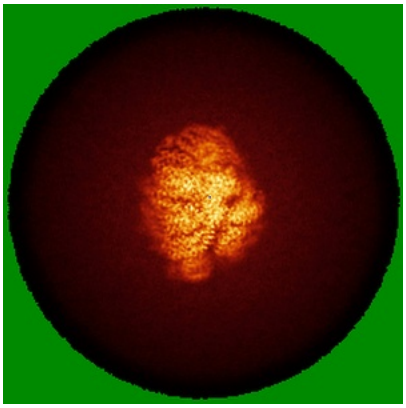
6.4.1 Primary map



X



Y



Z

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

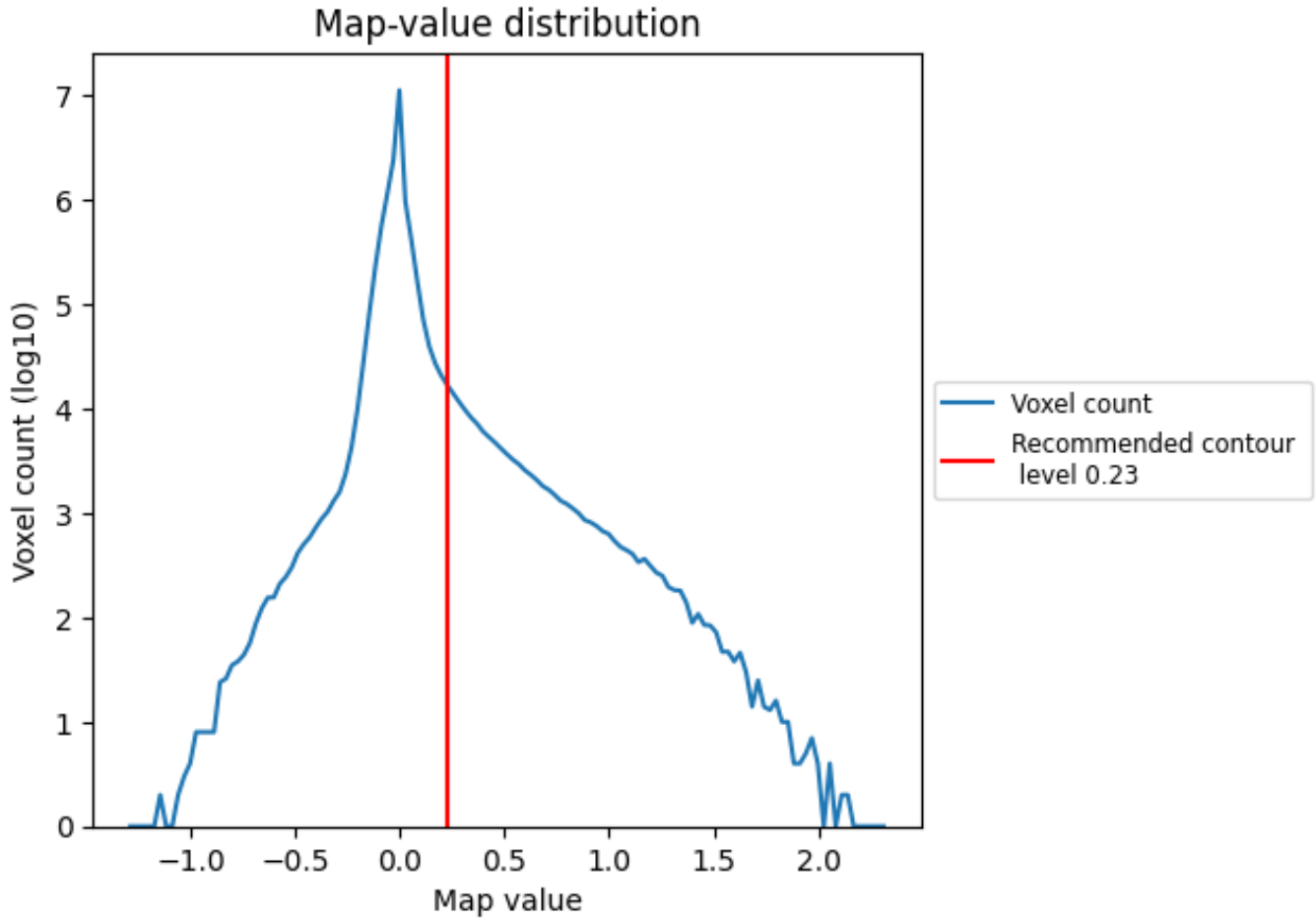
6.6 Mask visualisation (i)

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

7 Map analysis

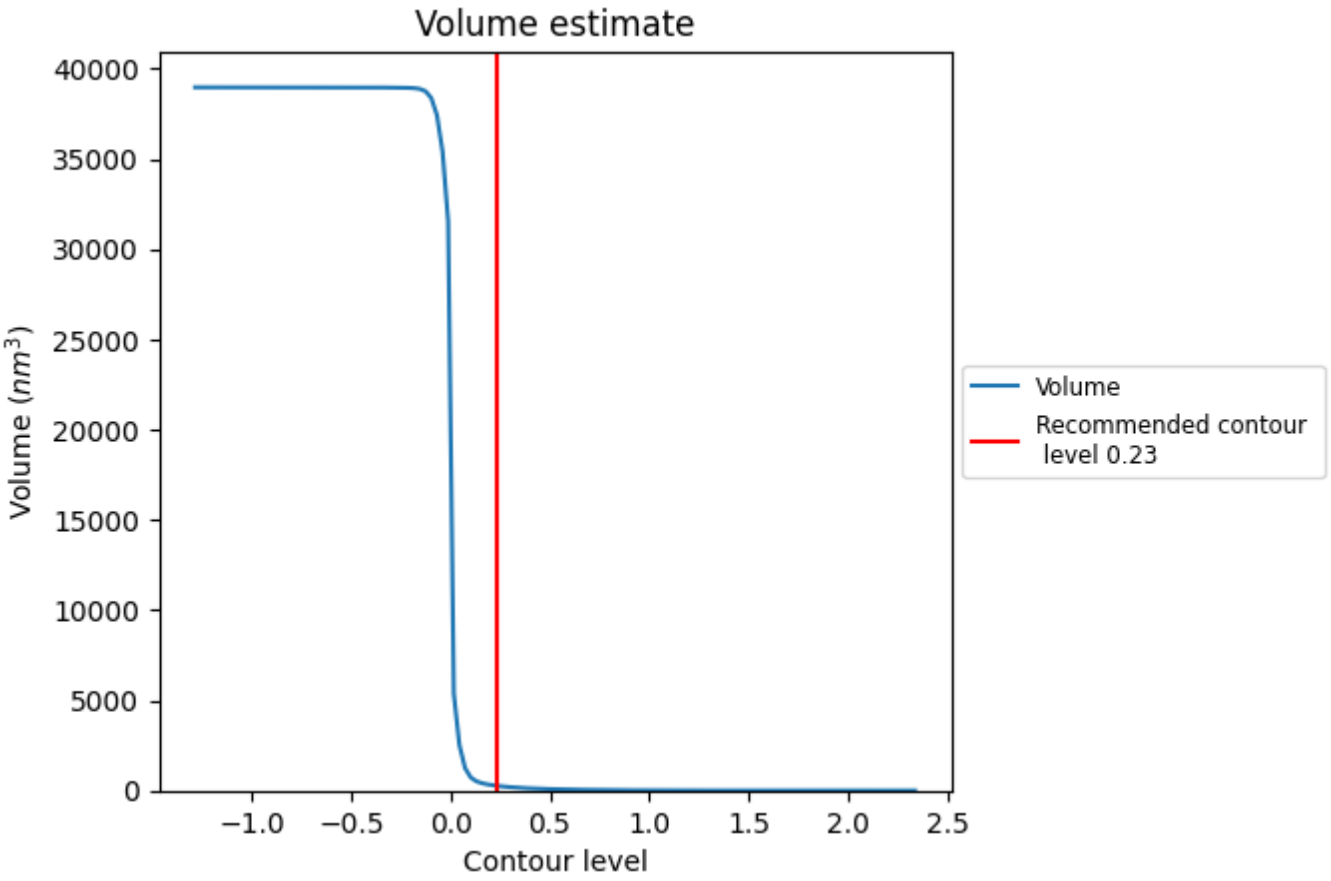
This section contains the results of statistical analysis of the map.

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.

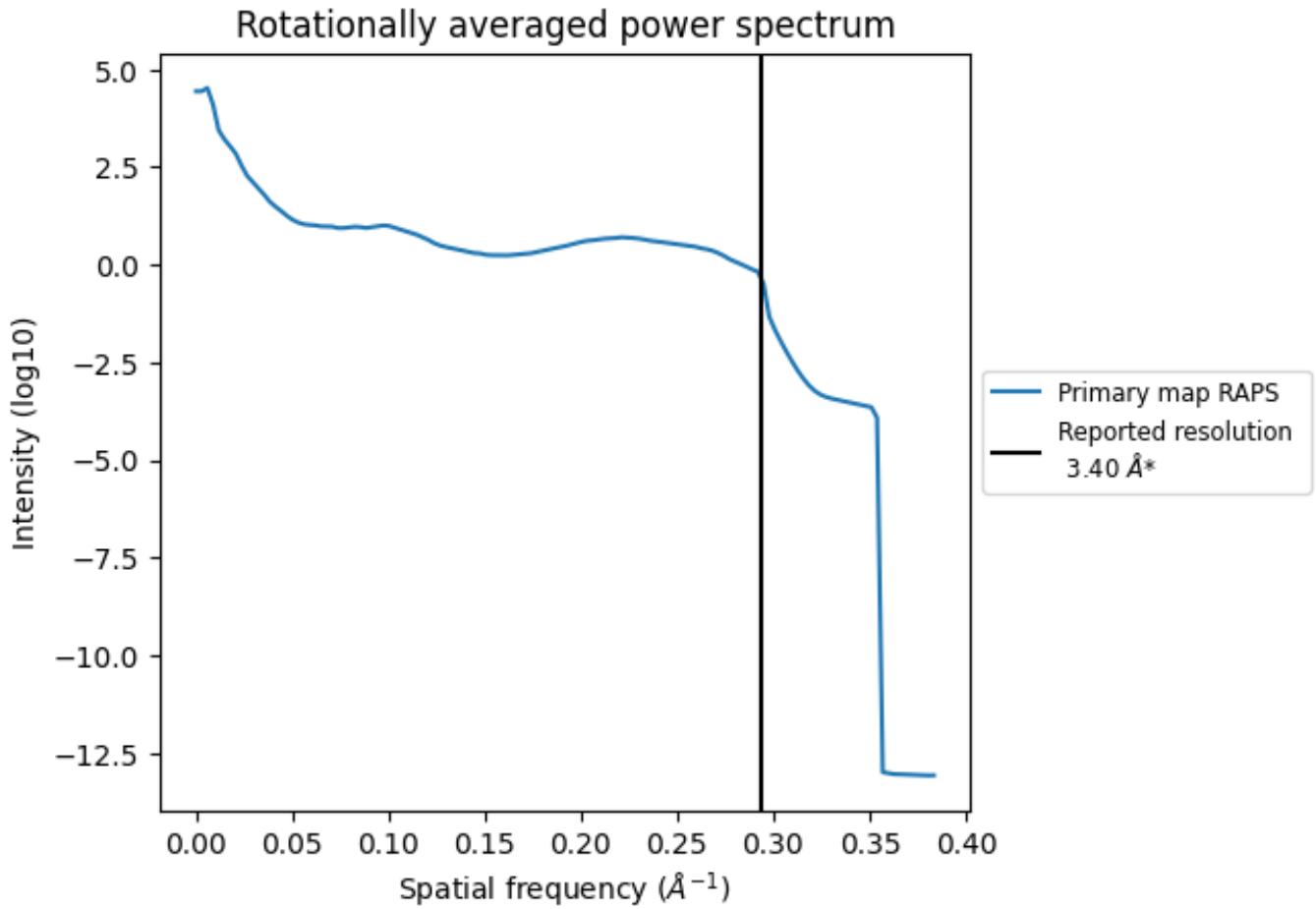
7.2 Volume estimate



The volume at the recommended contour level is 269 nm^3; this corresponds to an approximate mass of 243 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 0.294 $Å^{-1}$

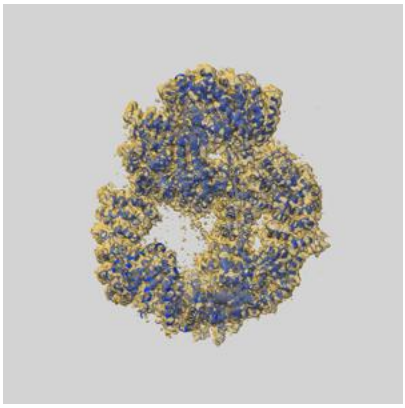
8 Fourier-Shell correlation (i)

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

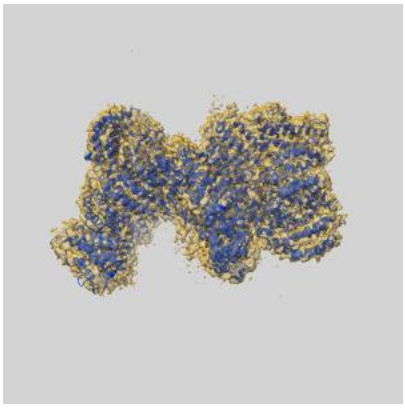
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13064 and PDB model 7OTP. Per-residue inclusion information can be found in section 3 on page 4.

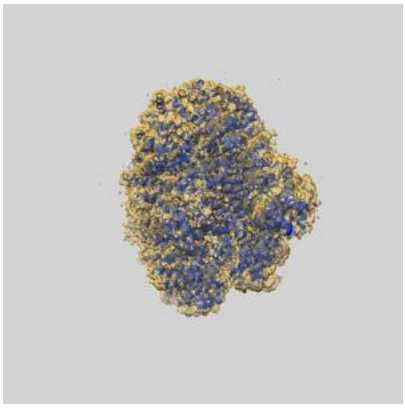
9.1 Map-model overlay



X



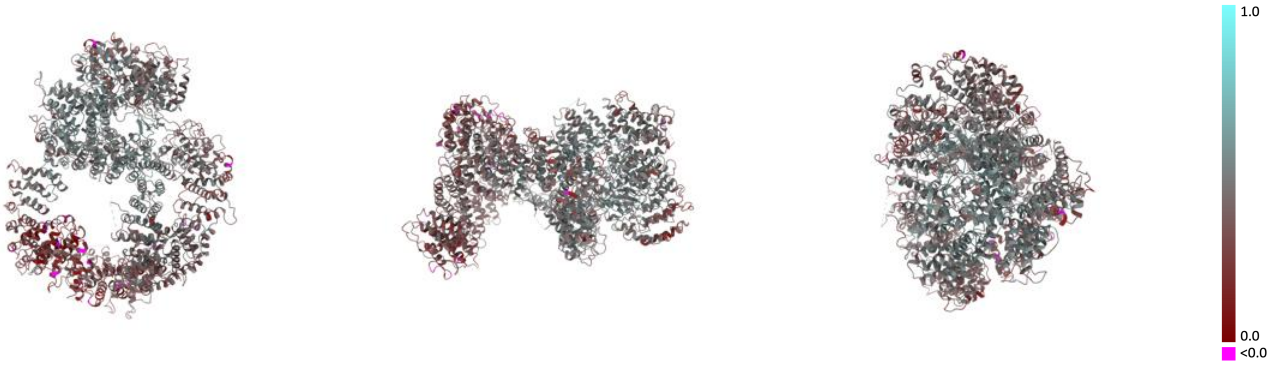
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.23 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.

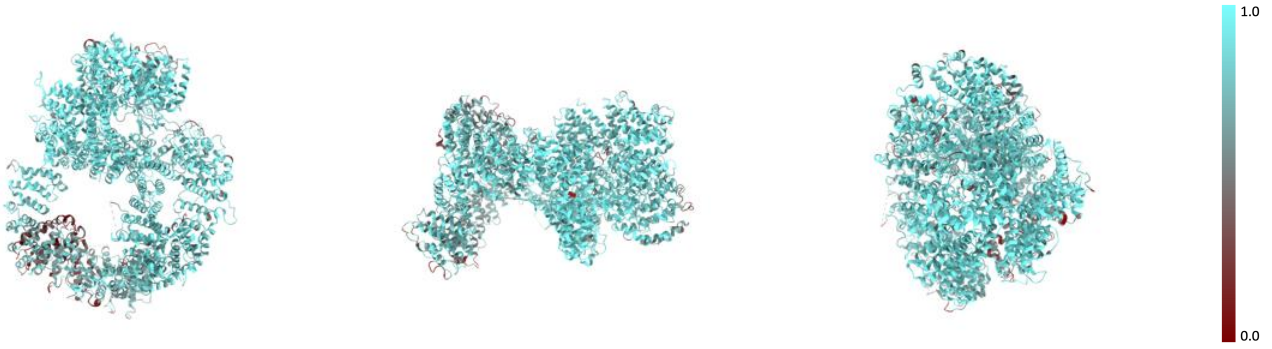
9.2 Q-score mapped to coordinate model (i)



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.

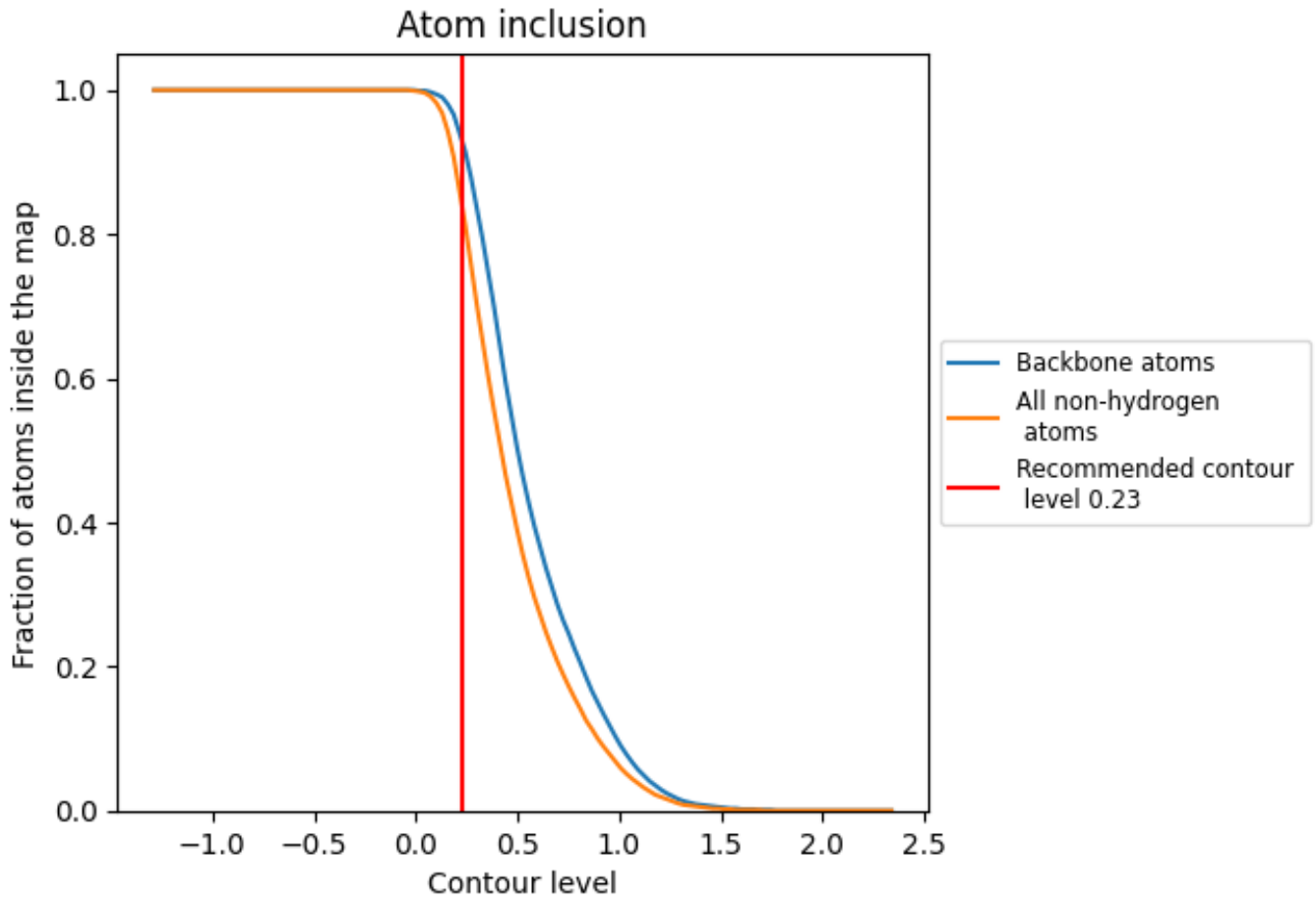
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.23).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.23) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.8360	0.4140
A	0.8360	0.4140