Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 07:15 PM EST

PDB ID	:	7SIC
EMDB ID	:	EMD-25140
Title	:	Human ATM Dimer
Authors	:	Warren, C.; Pavletich, N.P.
Deposited on	:	2021-10-13
Resolution	:	2.51 Å(reported)

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

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

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

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

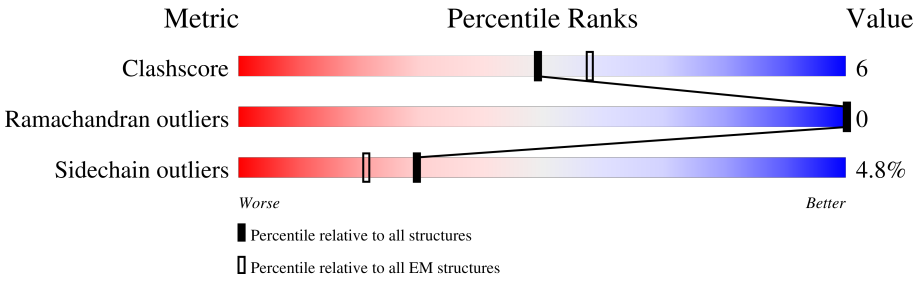
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.51 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	3056	44% 74% 16% • 9%
1	B	3056	44% 74% 16% • 9%

2 Entry composition

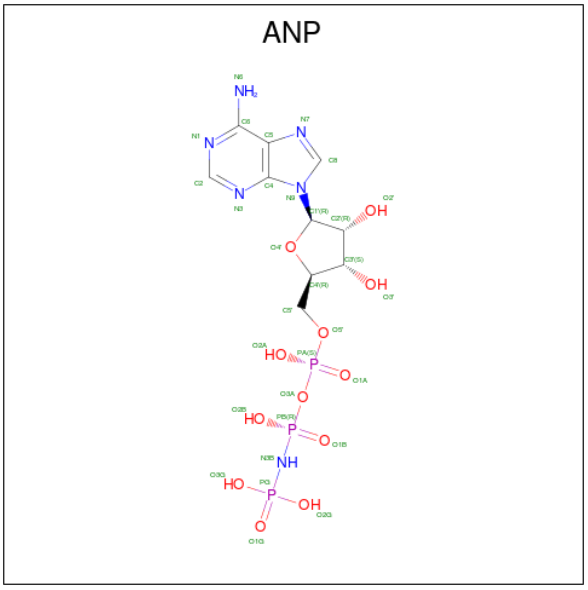
There are 3 unique types of molecules in this entry. The entry contains 44484 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serine-protein kinase ATM.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2773	Total	C	N	O	S	0	0
			22210	14200	3774	4083	153		
1	B	2773	Total	C	N	O	S	0	0
			22210	14200	3774	4083	153		

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	B	1	Total	C	N	O	P	0
			31	10	6	12	3	

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

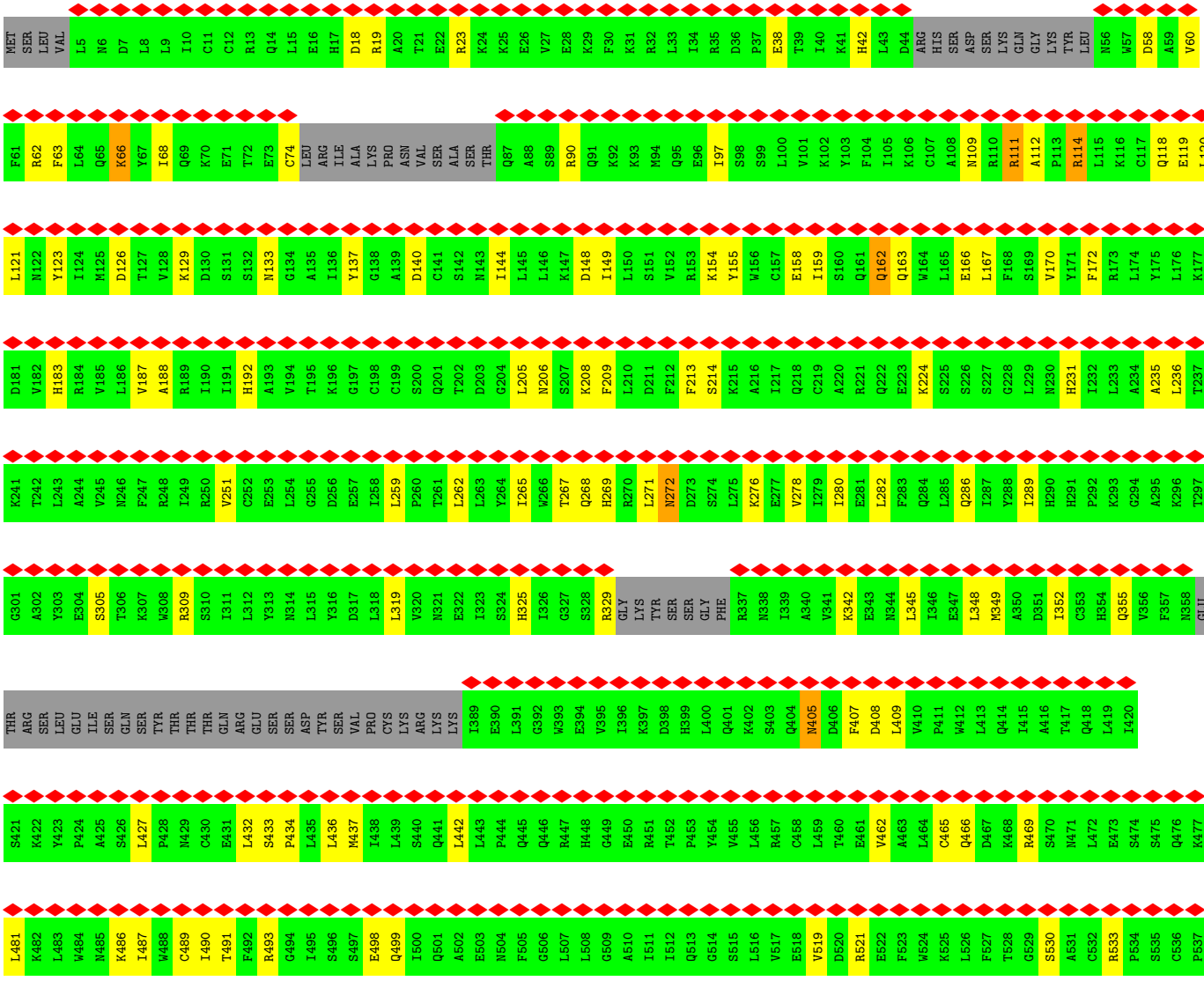
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Mg 1 1	0
3	B	1	Total Mg 1 1	0

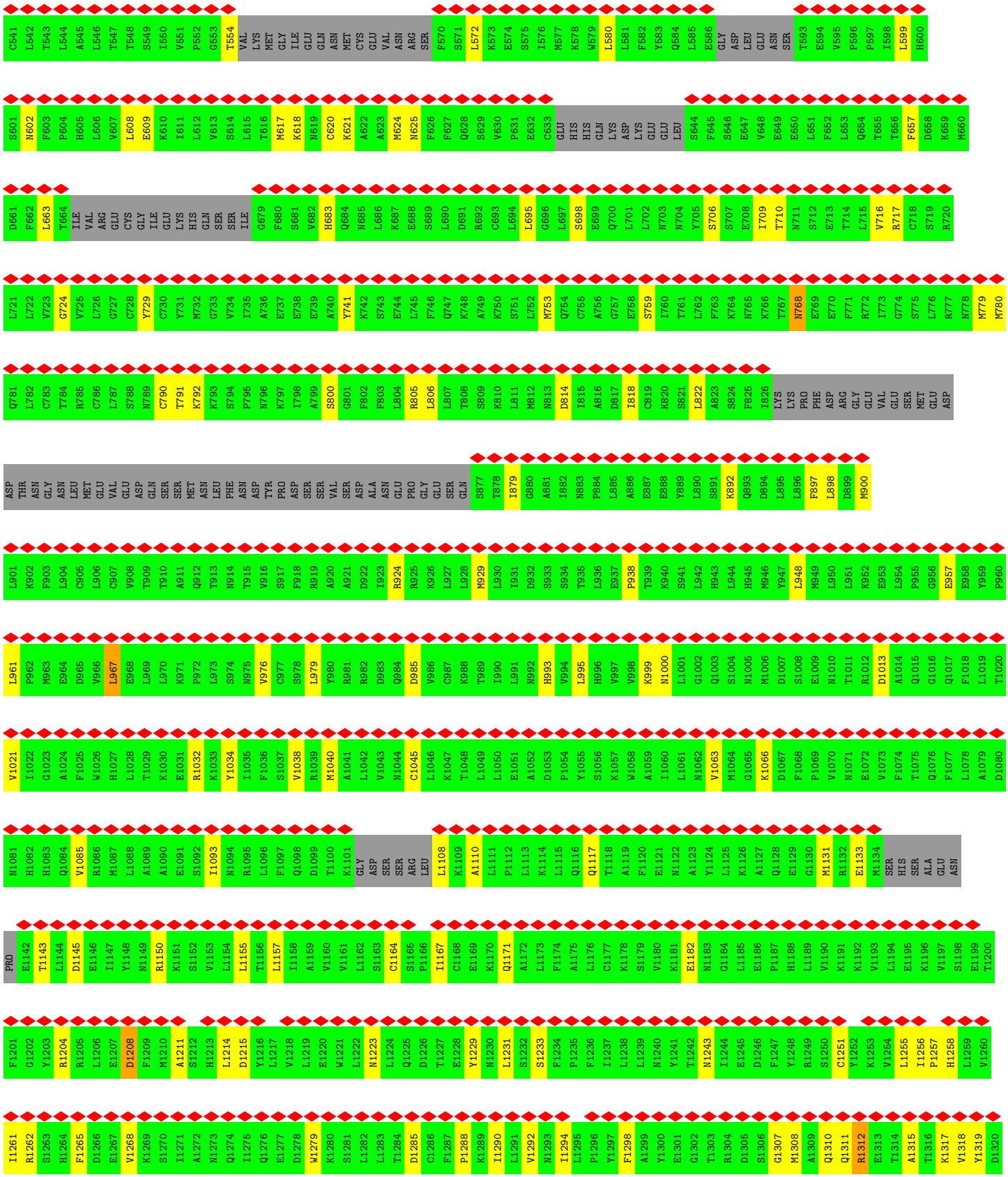
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Serine-protein kinase ATM

Chain A:

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S601 N602 F603 P604 H605 L606 V607 L608 E609 K610 I611 L612 V613 S614 L615 T616 M617 K618 N619 C620 K621 A622 A623 M624 N625 F626 F627 Q628 S629 V630 P631 E632 C633 GLU HIS HIS GLN LYS ASP LYS GLU GLU LEU S644 F645 S646 E647 V648 E649 E650 L651 F652 L653 Q654 T655 T656 F657 D658 K659 M660
D661 F662 L663 T664 ILE VAL ARG GLU CYS GLY ILE GLU LYS HIS GLN SER SER ILE G679 F680 S681 V682 H683 Q684 N685 L686 K687 E688 S689 L690 D691 R692 C693 L694 L695 G696 L697 S698 E699 Q700 L701 L702 N703 N704 Y705 S706 S707 E708 I709 T710 N711 S712 E713 T714 L715 V716 R717 C718 S719 R720
L721 L722 V723 G724 V725 L726 G727 C728 Y729 C730 Y731 M732 G733 V734 I735 A736 E737 E738 E739 A740 Y741 K742 S743 E744 L745 F746 Q747 K748 A749 K750 S751 L752 M753 Q754 C755 A756 G757 E758 S759 I760 T761 L762 F763 K764 N765 K766 T767 N768 E769 E770 F771 R772 I773 G774 S775 L776 R777 N778 M779 M780
Q781 L782 C783 T784 R785 C786 L787 S788 N789 C790 T791 K792 K793 S794 P795 N796 K797 I798 A799 S800 G801 F802 F803 L804 R805 L806 L807 T808 S809 K810 L811 M812 N813 D814 I815 A816 D817 I818 C819 K820 S821 L822 A823 S824 F825 I826 LYS LYS PRO PHE ASP ARG GLY GLU VAL GLU SER MET GLU ASP
ASP THR ASN GLY ASN LEU MET GLU VAL GLU ASP GLN SER SER MET ASN LEU PHE ASN ASP TYR PRO ASP SER SER VAL SER ASP ALA ASN GLU PRO GLY GLU SER GLN S877 T878 I879 G880 A881 I882 N883 P884 L885 A886 E887 E888 Y889 L890 S891 K892 Q893 D894 L895 L896 F897 L898 D899 M900
L901 K902 F903 L904 C905 L906 C907 V908 T909 T910 A911 Q912 T913 N914 T915 V916 S917 F918 R919 A920 A921 D922 I923 R924 R925 K926 L927 L928 M929 L930 I931 D932 S933 S934 T935 L936 E937 P938 T939 K940 S941 L942 H943 L944 H945 M946 Y947 L948 M949 L950 L951 K952 E953 L954 P955 G956 E957 E958 Y959 P960
L961 P962 M963 E964 D965 V966 L967 E968 L969 L970 K971 P972 L973 S974 N975 V976 C977 S978 L979 Y980 R981 R982 D983 Q984 D985 V986 C987 K988 T989 I990 L991 N992 H993 V994 L995 H996 V997 V998 K999 N1000 L1001 G1002 Q1003 S1004 N1005 M1006 D1007 S1008 E1009 N1010 T1011 R1012 D1013 A1014 Q1015 G1016 Q1017 F1018 L1019 T1020
V1021 I1022 G1023 A1024 F1025 W1026 H1027 L1028 T1029 K1030 E1031 R1032 K1033 Y1034 I1035 F1036 S1037 V1038 R1039 M1040 A1041 L1042 V1043 N1044 C1045 L1046 K1047 T1048 L1049 L1050 E1051 A1052 D1053 P1054 Y1055 S1056 K1057 W1058 A1059 I1060 L1061 N1062 V1063 M1064 G1065 K1066 D1067 F1068 P1069 V1070 N1071 E1072 V1073 F1074 T1075 Q1076 F1077 L1078 A1079 D1080
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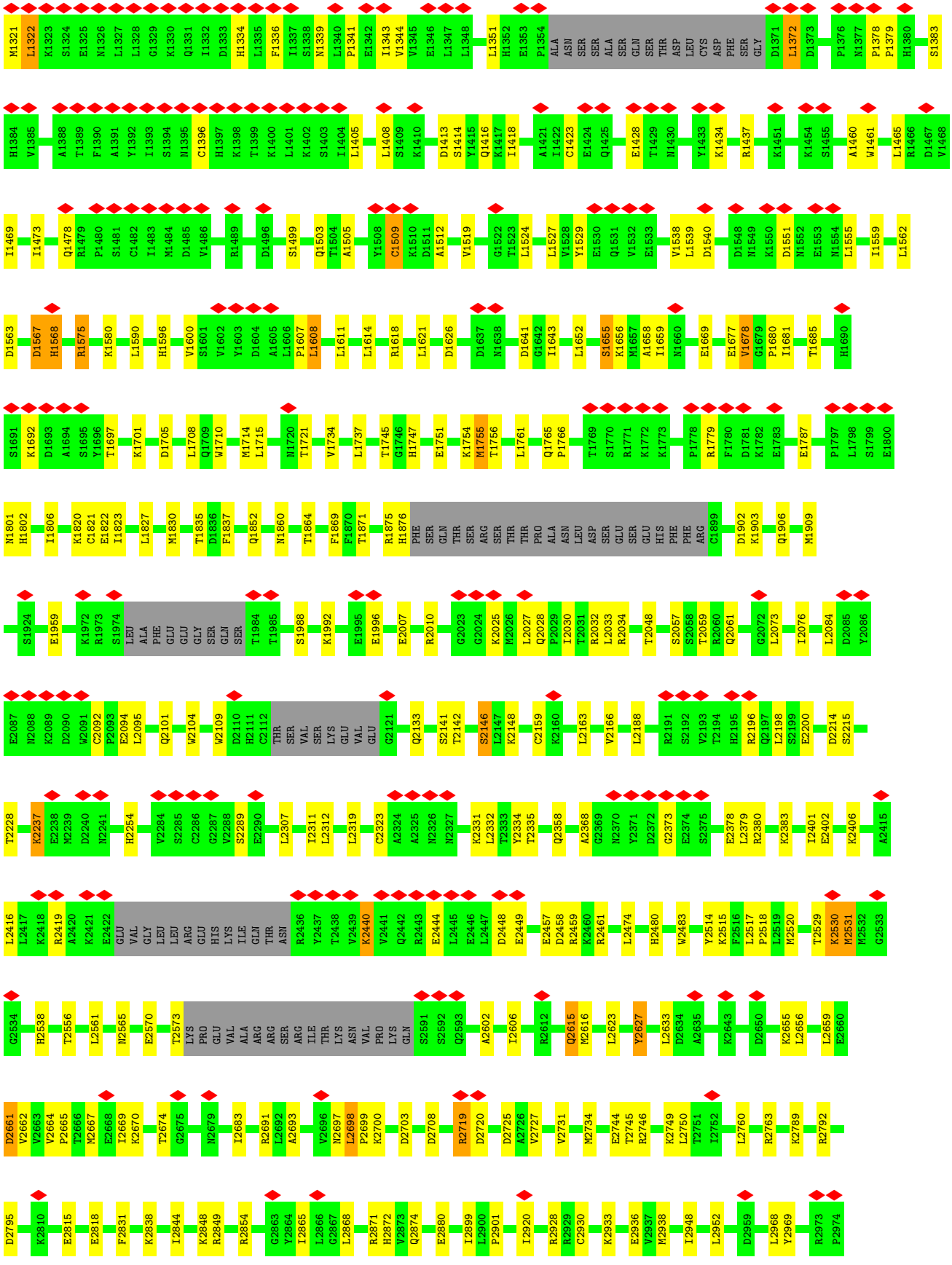
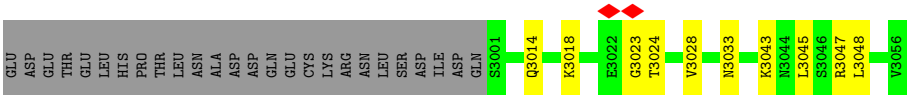
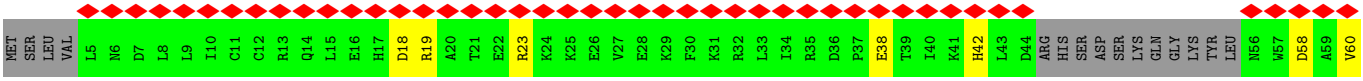
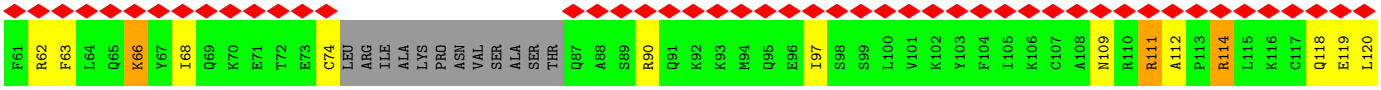
PRO E1142 T1143 L1144 D1145 E1146 I1147 Y1148 N1149 R1150 K1151 S1152 V1153 L1154 L1155 T1156 L1157 I1158 A1159 V1160 V1161 L1162 S1163 C1164 S1165 P1166 I1167 C1168 E1169 K1170 Q1171 A1172 L1173 F1174 A1175 L1176 C1177 K1178 S1179 V1180 K1181 E1182 N1183 G1184 L1185 E1186 P1187 H1188 L1189 V1190 K1191 K1192 V1193 L1194 E1195 K1196 V1197 S1198 E1199 T1200
F1201 G1202 Y1203 R1204 R1205 L1206 E1207 D1208 F1209 M1210 A1211 S1212 H1213 L1214 D1215 Y1216 L1217 V1218 L1219 E1220 W1221 L1222 N1223 L1224 Q1225 D1226 T1227 E1228 Y1229 N1230 L1231 S1232 S1233 F1234 P1235 F1236 I1237 L1238 L1239 N1240 Y1241 T1242 N1243 I1244 E1245 D1246 F1247 Y1248 R1249 S1250 C1251 Y1252 K1253 V1254 L1255 I1256 P1257 H1258 L1259 V1260
I1261 R1262 S1263 H1264 F1265 D1266 E1267 V1268 K1269 S1270 I1271 A1272 N1273 Q1274 I1275 Q1276 E1277 D1278 W1279 K1280 S1281 L1282 L1283 T1284 D1285 C1286 F1287 P1288 K1289 I1290 L1291 V1292 N1293 I1294 L1295 P1296 Y1297 F1298 A1299 Y1300 E1301 G1302 T1303 R1304 D1305 S1306 G1307 M1308 A1309 Q1310 Q1311 R1312 E1313 T1314 A1315 T1316 K1317 V1318 Y1319 D1320

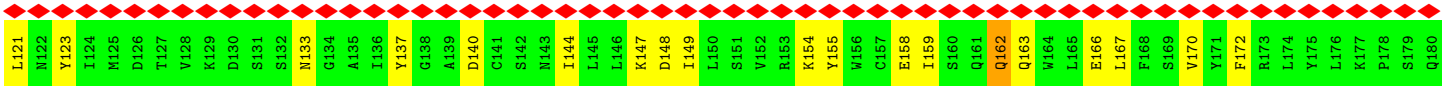


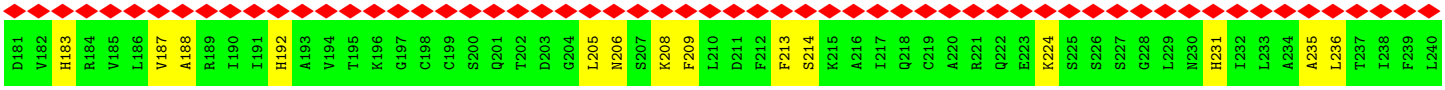


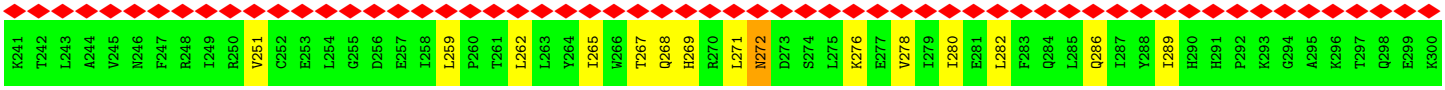
• Molecule 1: Serine-protein kinase ATM

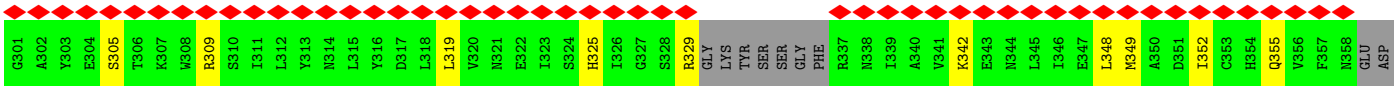


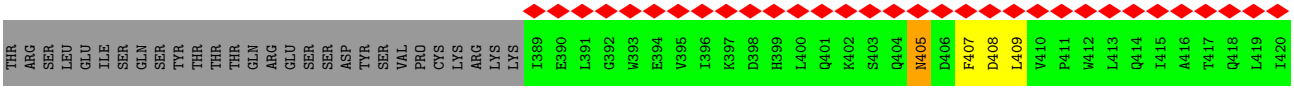


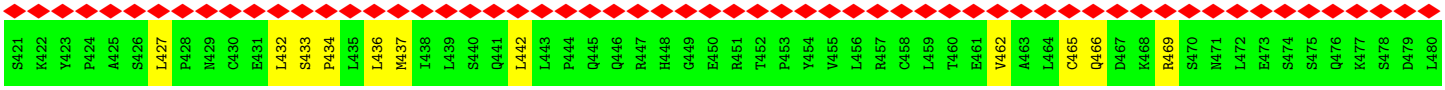


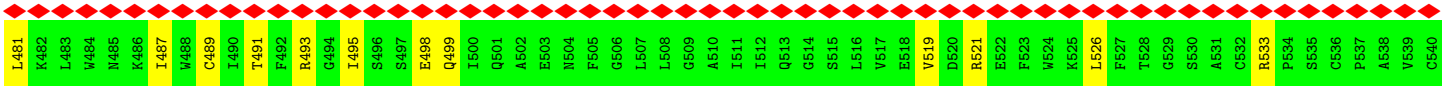


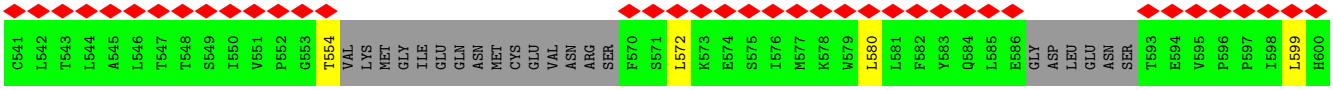


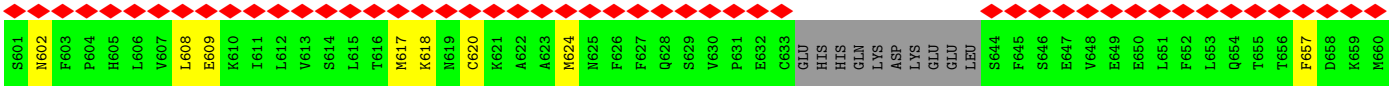


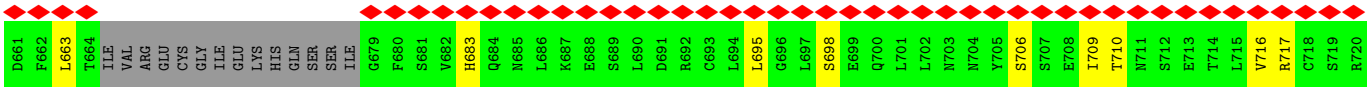


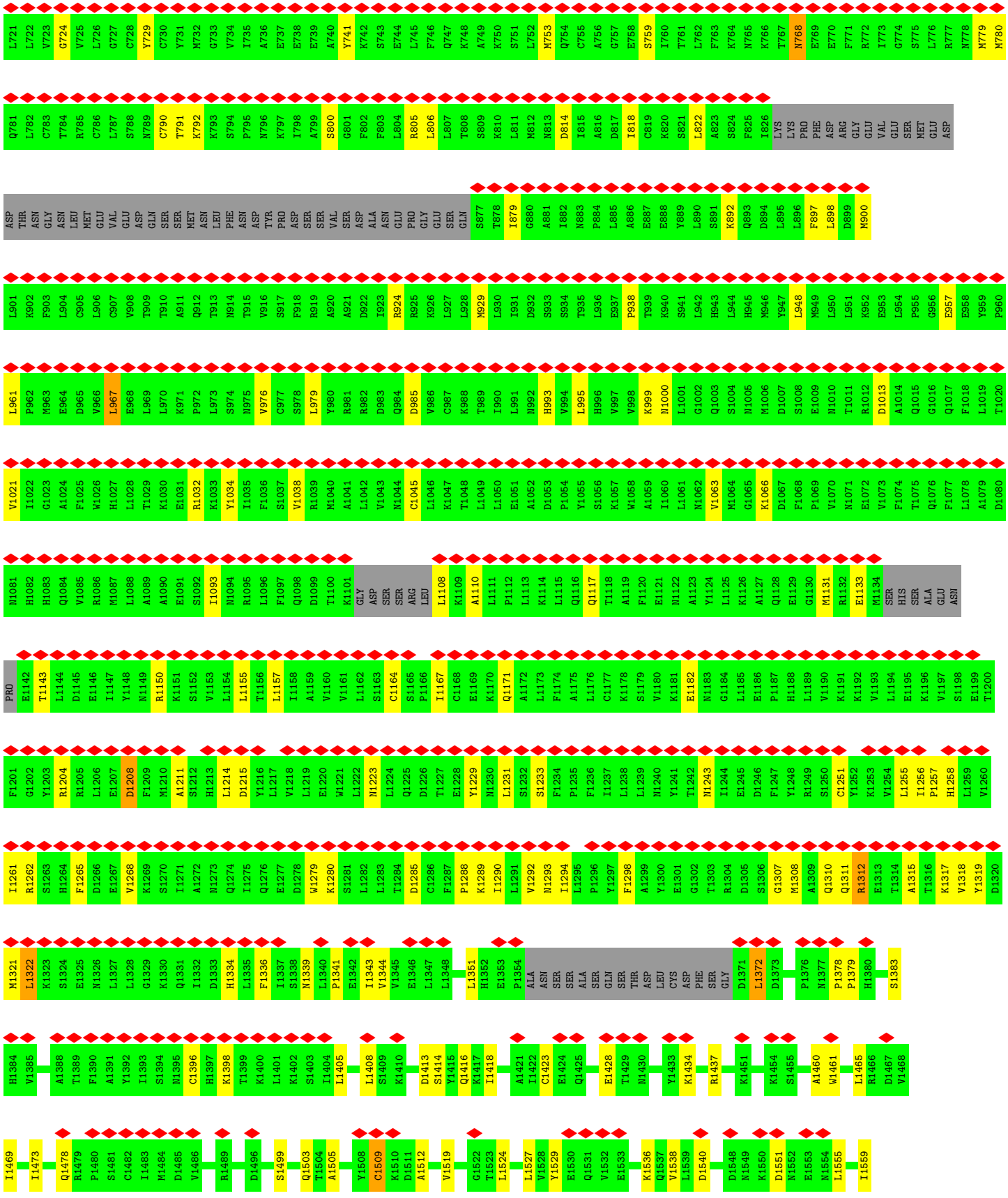








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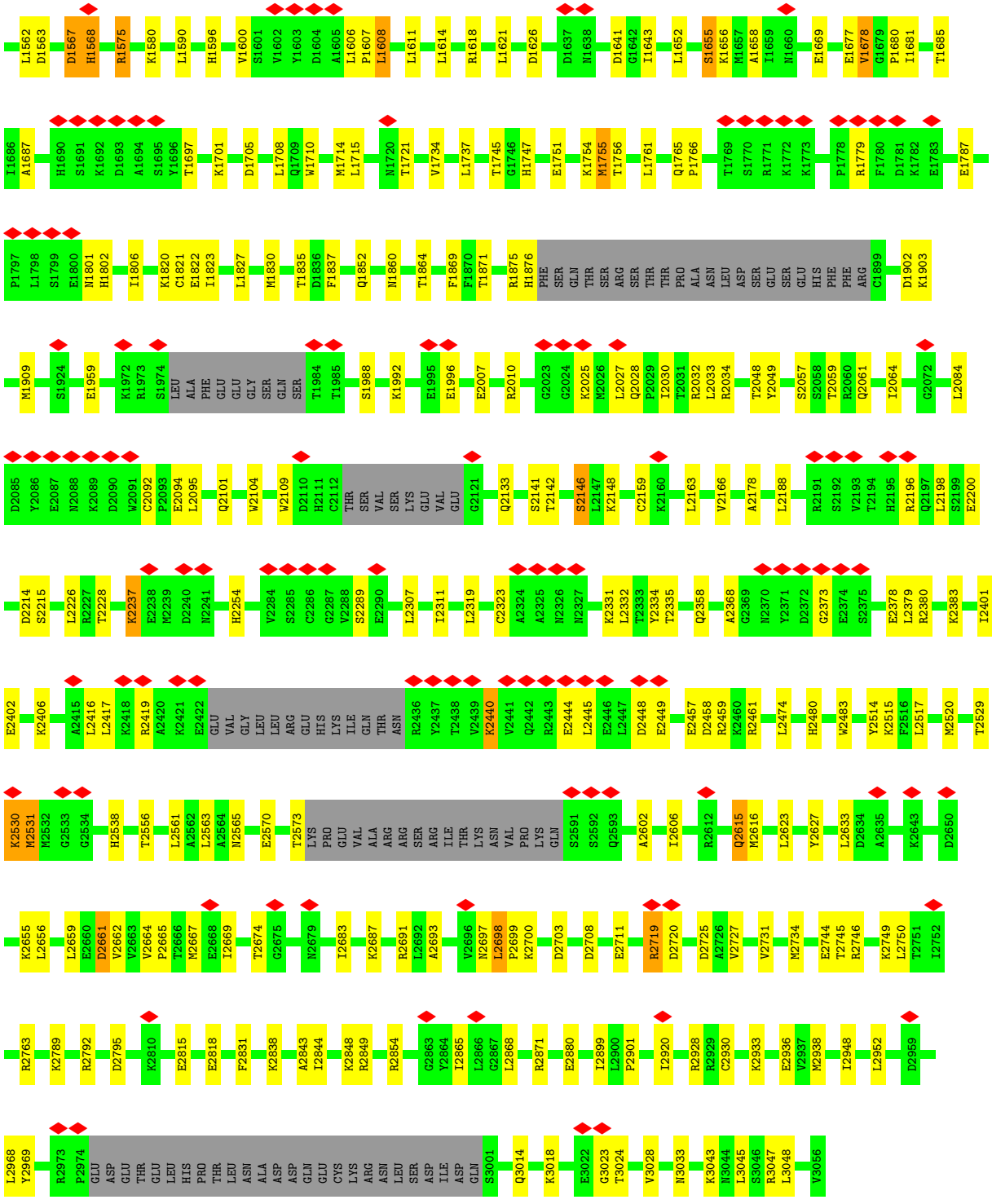
L1562 D1563 D1567 H1568 R1575 K1580 L1590 H1596 V1600 S1601 V1602 Y1603 D1604 A1605 L1606 P1607 L1608 L1611 L1614 R1618 L1621 D1626 D1637 N1638 D1641 G1642 I1643 L1652 S1655 K1656 M1657 A1658 I1659 N1660 E1669 E1677 V1678 G1679 P1680 I1681 T1685
I1686 A1687 H1690 S1691 K1692 D1693 A1694 S1695 Y1696 T1697 K1701 D1705 L1708 Q1709 W1710 M1714 L1715 N1720 T1721 V1734 L1737 T1745 G1746 H1747 E1751 K1754 M1755 T1756 L1761 Q1765 P1766 T1769 S1770 R1771 K1772 K1773 P1778 R1779 F1780 D1781 K1782 E1783 E1787
P1797 L1798 S1799 E1800 N1801 H1802 I1806 K1820 C1821 E1822 I1823 L1827 M1830 T1835 D1836 F1837 Q1852 N1860 T1864 F1869 F1870 T1871 R1875 H1876 PHE SER GLN THR SER ARG SER THR THR PRO ALA ASN LEU ASP SER GLU SER GLU HIS PHE PHE ARG C1899 D1902 K1903
M1909 S1924 E1959 K1972 R1973 S1974 LEU ALA PHE GLU GLU GLY SER GLN SER T1984 T1985 S1988 K1992 E1995 E1996 E2007 R2010 G2023 G2024 K2025 M2026 L2027 Q2028 P2029 I2030 T2031 R2032 L2033 R2034 T2048 Y2049 S2057 S2058 T2059 R2060 Q2061 I2064 G2072 L2084
D2085 Y2086 E2087 N2088 K2089 D2090 W2091 C2092 P2093 E2094 L2095 Q2101 W2104 W2109 D2110 H2111 C2112 THR SER VAL SER LYS GLU VAL GLU G2121 Q2133 S2141 T2142 S2146 L2147 K2148 C2159 K2160 L2163 V2166 A2178 L2188 R2191 S2192 V2193 T2194 H2195 R2196 Q2197 L2198 S2199 E2200
D2214 S2215 L2226 R2227 T2228 K2237 E2238 M2239 D2240 N2241 H2254 V2284 S2285 C2286 G2287 V2288 S2289 E2290 L2307 I2311 L2319 C2323 A2324 A2325 N2326 N2327 K2331 L2332 T2333 Y2334 T2335 Q2358 A2368 G2369 N2370 Y2371 D2372 G2373 E2374 S2375 E2378 L2379 R2380 K2383 I2401
E2402 K2406 A2415 L2416 L2417 K2418 R2419 A2420 K2421 E2422 GLU VAL GLY LEU LEU ARG GLU HIS LYS ILE GLN THR ASN R2436 Y2437 T2438 V2439 K2440 V2441 Q2442 R2443 E2444 L2445 E2446 L2447 D2448 E2449 E2457 D2458 R2459 K2460 R2461 L2474 H2480 W2483 Y2514 K2515 F2516 L2517 M2520 T2529
K2530 M2531 M2532 G2533 G2534 H2538 T2556 L2561 A2562 L2563 A2564 N2565 E2570 T2573 LYS PRO GLU VAL ALA ARG ARG SER ARG ILE THR LYS ASN VAL PRO LYS GLN S2591 S2592 Q2593 A2602 I2606 R2612 Q2615 M2616 L2623 Y2627 L2633 D2634 A2635 K2643 D2650
K2655 L2656 L2659 E2660 D2661 V2662 V2663 V2664 P2665 T2666 M2667 E2668 I2669 T2674 G2675 N2679 I2683 K2687 R2691 L2692 A2693 V2696 M2697 L2698 P2699 K2700 D2703 D2708 E2711 R2719 D2720 D2725 A2726 V2727 V2731 M2734 E2744 T2745 R2746 K2749 L2750 T2751 I2752
R2763 K2789 R2792 D2795 K2810 E2815 E2818 F2831 K2838 A2843 I2844 K2848 R2849 R2854 G2863 Y2864 I2865 L2866 G2867 L2868 R2871 E2880 I2899 L2900 P2901 I2920 R2928 R2929 C2930 K2933 E2936 V2937 M2938 I2948 L2952 D2959
L2968 Y2969 R2973 P2974 GLU ASP GLU THR GLU LEU HIS PRO THR LEU ASN ALA ASP ASP GLN GLU CYS LYS ARG ASN LEU SER ASP ILE ASP GLN S3001 Q3014 K3018 E3022 G3023 T3024 V3028 N3033 K3043 N3044 L3045 S3046 R3047 L3048 V3056

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	303604	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 ($e^-/Å^2$)	53.8	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.222	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	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, ANP

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	0.25	0/22624	0.46	3/30565 (0.0%)
1	B	0.25	0/22624	0.46	3/30565 (0.0%)
All	All	0.25	0/45248	0.46	6/61130 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	663	LEU	CA-CB-CG	5.08	126.97	115.30
1	B	663	LEU	CA-CB-CG	5.08	126.97	115.30
1	A	1372	LEU	CA-CB-CG	5.03	126.87	115.30
1	B	1372	LEU	CA-CB-CG	5.03	126.87	115.30
1	A	1322	LEU	CA-CB-CG	5.01	126.83	115.30
1	B	1322	LEU	CA-CB-CG	5.01	126.83	115.30

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	22210	0	22392	279	0
1	B	22210	0	22392	278	0
2	A	31	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	44484	0	44810	545	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 6.

All (545) 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:B:1312:ARG:HG3	1:B:1312:ARG:HH11	1.31	0.95
1:A:1312:ARG:HG3	1:A:1312:ARG:HH11	1.31	0.93
1:B:2458:ASP:OD1	1:B:2461:ARG:NH2	2.23	0.71
1:B:1509:CYS:HB2	1:B:1512:ALA:HB2	1.73	0.71
1:A:1509:CYS:HB2	1:A:1512:ALA:HB2	1.73	0.71
1:A:272:ASN:OD1	1:A:272:ASN:N	2.19	0.70
1:A:2458:ASP:OD1	1:A:2461:ARG:NH2	2.23	0.70
1:A:1988:SER:OG	1:A:1992:LYS:NZ	2.26	0.69
1:B:1988:SER:OG	1:B:1992:LYS:NZ	2.26	0.69
1:B:272:ASN:OD1	1:B:272:ASN:N	2.19	0.68
1:A:2480:HIS:HB3	1:A:2483:TRP:HD1	1.58	0.68
1:A:2061:GLN:HG2	1:A:2084:LEU:HD21	1.76	0.67
1:A:3043:LYS:HE3	1:A:3047:ARG:NH2	2.10	0.67
1:B:2480:HIS:HB3	1:B:2483:TRP:HD1	1.58	0.67
1:B:1685:THR:HG23	1:B:2166:VAL:HG21	1.76	0.67
1:B:3043:LYS:HE3	1:B:3047:ARG:NH2	2.10	0.67
1:A:1685:THR:HG23	1:A:2166:VAL:HG21	1.76	0.67
1:A:2030:ILE:HD12	1:A:2030:ILE:H	1.60	0.67
1:B:2061:GLN:HG2	1:B:2084:LEU:HD21	1.76	0.67
1:B:2030:ILE:HD12	1:B:2030:ILE:H	1.60	0.66
1:A:319:LEU:HD23	1:A:349:MET:HG2	1.78	0.66
1:A:427:LEU:O	1:A:469:ARG:NH2	2.25	0.66
1:A:1131:MET:HG2	1:A:1150:ARG:HB3	1.76	0.66
1:B:319:LEU:HD23	1:B:349:MET:HG2	1.78	0.66
1:B:1131:MET:HG2	1:B:1150:ARG:HB3	1.76	0.66
1:A:329:ARG:NH2	1:A:407:PHE:O	2.29	0.65
1:B:329:ARG:NH2	1:B:407:PHE:O	2.29	0.65
1:A:1290:ILE:O	1:A:1294:ILE:HD12	1.97	0.65
1:A:1294:ILE:HG23	1:A:1315:ALA:HB1	1.79	0.65
1:A:2969:TYR:OH	2:A:3101:ANP:O2G	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1310:GLN:HE21	1:B:1311:GLN:HE21	1.45	0.64
1:A:1310:GLN:HE21	1:A:1311:GLN:HE21	1.45	0.64
1:B:1290:ILE:O	1:B:1294:ILE:HD12	1.97	0.64
1:B:1223:ASN:OD1	1:B:1262:ARG:NH2	2.32	0.63
1:B:1294:ILE:HG23	1:B:1315:ALA:HB1	1.79	0.63
1:A:1215:ASP:OD2	1:A:1258:HIS:NE2	2.28	0.63
1:B:602:ASN:OD1	1:B:717:ARG:NH1	2.32	0.63
1:B:2368:ALA:HB1	1:B:2383:LYS:HG2	1.80	0.62
1:B:63:PHE:HD1	1:B:66:LYS:HZ1	1.47	0.62
1:B:1747:HIS:O	1:B:1751:GLU:HG2	1.99	0.62
1:B:68:ILE:HD12	1:B:97:ILE:HD12	1.82	0.62
1:B:2744:GLU:HG2	1:B:2933:LYS:HD2	1.81	0.62
1:A:2368:ALA:HB1	1:A:2383:LYS:HG2	1.80	0.62
1:A:2744:GLU:HG2	1:A:2933:LYS:HD2	1.81	0.62
1:A:1223:ASN:OD1	1:A:1262:ARG:NH2	2.32	0.62
1:A:1294:ILE:HG21	1:A:1319:TYR:HB2	1.82	0.62
1:A:1351:LEU:O	1:A:1437:ARG:NH1	2.32	0.62
1:B:1351:LEU:O	1:B:1437:ARG:NH1	2.32	0.62
1:A:1747:HIS:O	1:A:1751:GLU:HG2	1.99	0.61
1:B:2969:TYR:OH	2:B:3101:ANP:O2G	2.15	0.61
1:A:68:ILE:HD12	1:A:97:ILE:HD12	1.82	0.61
1:A:602:ASN:OD1	1:A:717:ARG:NH1	2.32	0.61
1:A:2142:THR:O	1:A:2146:SER:OG	2.19	0.61
1:B:1294:ILE:HG21	1:B:1319:TYR:HB2	1.82	0.60
1:B:2214:ASP:OD1	1:B:2746:ARG:NH1	2.34	0.60
1:A:2664:VAL:HB	1:A:2667:MET:HG3	1.84	0.60
1:A:2697:ASN:HD22	1:A:2719:ARG:HG3	1.66	0.60
1:A:2214:ASP:OD1	1:A:2746:ARG:NH1	2.34	0.60
1:B:2656:LEU:HD13	1:B:2659:LEU:HD11	1.84	0.60
1:B:2142:THR:O	1:B:2146:SER:OG	2.19	0.60
1:B:2378:GLU:OE1	1:B:2378:GLU:N	2.20	0.60
1:B:2697:ASN:HD22	1:B:2719:ARG:HG3	1.66	0.60
1:B:2401:ILE:HG21	1:B:2459:ARG:HB2	1.84	0.60
1:A:1652:LEU:HD13	1:A:2163:LEU:HD21	1.84	0.59
1:B:1652:LEU:HD13	1:B:2163:LEU:HD21	1.84	0.59
1:B:2188:LEU:HD11	1:B:2198:LEU:HD22	1.85	0.59
1:A:3045:LEU:HA	1:A:3048:LEU:HD12	1.85	0.59
1:B:1215:ASP:OD2	1:B:1258:HIS:NE2	2.28	0.59
1:A:2188:LEU:HD11	1:A:2198:LEU:HD22	1.85	0.59
1:A:2401:ILE:HG21	1:A:2459:ARG:HB2	1.84	0.59
1:B:2520:MET:HG2	1:B:2556:THR:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2448:ASP:OD2	1:A:2449:GLU:N	2.36	0.59
1:B:2448:ASP:OD2	1:B:2449:GLU:N	2.36	0.59
1:B:2928:ARG:NH1	1:B:3033:ASN:OD1	2.35	0.59
1:A:1251:CYS:O	1:A:1255:LEU:HG	2.02	0.59
1:A:2520:MET:HG2	1:A:2556:THR:HG22	1.85	0.59
1:A:205:LEU:HD23	1:A:205:LEU:H	1.67	0.59
1:B:3045:LEU:HA	1:B:3048:LEU:HD12	1.85	0.59
1:A:2928:ARG:NH1	1:A:3033:ASN:OD1	2.35	0.58
1:A:1575:ARG:HB3	1:A:1575:ARG:HH11	1.68	0.58
1:B:2664:VAL:HB	1:B:2667:MET:HG3	1.84	0.58
1:A:2633:LEU:HB3	1:A:2700:LYS:HE2	1.85	0.58
1:A:2656:LEU:HD13	1:A:2659:LEU:HD11	1.84	0.58
1:A:618:LYS:HG2	1:A:683:HIS:CD2	2.39	0.58
1:B:1312:ARG:HG3	1:B:1312:ARG:NH1	2.07	0.58
1:B:1575:ARG:HH11	1:B:1575:ARG:HB3	1.68	0.58
1:B:618:LYS:HG2	1:B:683:HIS:CD2	2.39	0.58
1:B:1251:CYS:O	1:B:1255:LEU:HG	2.02	0.58
1:B:205:LEU:HD23	1:B:205:LEU:H	1.67	0.58
1:B:427:LEU:O	1:B:469:ARG:NH2	2.25	0.57
1:A:62:ARG:HB2	1:A:62:ARG:HH11	1.69	0.57
1:B:62:ARG:NH1	1:B:62:ARG:HB2	2.20	0.57
1:A:2719:ARG:HA	1:A:2763:ARG:HG2	1.87	0.56
1:B:2633:LEU:HB3	1:B:2700:LYS:HE2	1.85	0.56
1:A:62:ARG:HB2	1:A:62:ARG:NH1	2.20	0.56
1:A:2101:GLN:HA	1:A:2104:TRP:CD1	2.40	0.56
1:A:111:ARG:HE	1:A:114:ARG:HH22	1.52	0.56
1:B:62:ARG:HB2	1:B:62:ARG:HH11	1.69	0.56
1:B:2101:GLN:HA	1:B:2104:TRP:CD1	2.40	0.56
1:A:19:ARG:O	1:A:23:ARG:N	2.36	0.56
1:B:1208:ASP:N	1:B:1208:ASP:OD1	2.38	0.56
1:A:1745:THR:OG1	1:A:1822:GLU:OE2	2.24	0.56
1:A:1208:ASP:OD1	1:A:1208:ASP:N	2.38	0.55
1:B:2719:ARG:HA	1:B:2763:ARG:HG2	1.87	0.55
1:A:140:ASP:O	1:A:144:ILE:HD12	2.07	0.55
1:B:205:LEU:HD12	1:B:209:PHE:HD1	1.71	0.55
1:A:192:HIS:HA	1:A:235:ALA:HB2	1.88	0.55
1:A:487:ILE:O	1:A:491:THR:HG22	2.06	0.55
1:B:111:ARG:HE	1:B:114:ARG:HH22	1.52	0.55
1:B:192:HIS:HA	1:B:235:ALA:HB2	1.88	0.55
1:A:405:ASN:OD1	1:A:405:ASN:N	2.29	0.54
1:B:487:ILE:O	1:B:491:THR:HG22	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ARG:NH2	1:A:355:GLN:O	2.40	0.54
1:B:162:GLN:O	1:B:162:GLN:NE2	2.34	0.54
1:A:205:LEU:HD12	1:A:209:PHE:HD1	1.71	0.54
1:A:2196:ARG:O	1:A:2200:GLU:HG3	2.08	0.54
1:B:19:ARG:O	1:B:23:ARG:N	2.36	0.54
1:B:140:ASP:O	1:B:144:ILE:HD12	2.07	0.54
1:B:2402:GLU:OE2	1:B:2459:ARG:NE	2.32	0.54
1:A:2901:PRO:HB3	1:B:2444:GLU:OE1	2.08	0.54
1:B:1710:TRP:O	1:B:1714:MET:HG2	2.08	0.54
1:A:2968:LEU:HD11	1:B:2440:LYS:HD3	1.90	0.54
1:B:309:ARG:NH2	1:B:355:GLN:O	2.40	0.54
1:B:1959:GLU:OE2	1:B:2849:ARG:NH1	2.36	0.53
1:B:2196:ARG:O	1:B:2200:GLU:HG3	2.08	0.53
1:A:1182:GLU:OE2	1:A:1229:TYR:OH	2.26	0.53
1:A:2444:GLU:OE1	1:B:2901:PRO:HB3	2.08	0.53
1:B:1182:GLU:OE2	1:B:1229:TYR:OH	2.26	0.53
1:A:2936:GLU:HG3	1:A:3028:VAL:HG21	1.90	0.53
1:B:1318:VAL:O	1:B:1322:LEU:HD12	2.09	0.53
1:A:1567:ASP:O	1:A:1568:HIS:ND1	2.36	0.53
1:B:2936:GLU:HG3	1:B:3028:VAL:HG21	1.90	0.53
1:A:580:LEU:HD22	1:A:608:LEU:HD21	1.91	0.53
1:A:1318:VAL:O	1:A:1322:LEU:HD12	2.09	0.53
1:B:1343:ILE:H	1:B:1343:ILE:HD12	1.74	0.53
1:A:1710:TRP:O	1:A:1714:MET:HG2	2.08	0.52
1:A:2378:GLU:OE1	1:A:2378:GLU:N	2.20	0.52
1:A:1755:MET:SD	1:A:1755:MET:N	2.82	0.52
1:B:580:LEU:HD22	1:B:608:LEU:HD21	1.91	0.52
1:A:2440:LYS:HD3	1:B:2968:LEU:HD11	1.90	0.52
1:A:618:LYS:HG2	1:A:683:HIS:HD2	1.73	0.52
1:A:1312:ARG:HG3	1:A:1312:ARG:NH1	2.07	0.52
1:A:2697:ASN:HB3	1:A:2719:ARG:HD3	1.92	0.52
1:B:618:LYS:HG2	1:B:683:HIS:HD2	1.73	0.52
1:A:1551:ASP:OD1	1:A:1551:ASP:N	2.41	0.52
1:B:1755:MET:SD	1:B:1755:MET:N	2.82	0.52
1:B:2838:LYS:HE2	1:B:2880:GLU:HG2	1.92	0.52
1:A:74:CYS:O	1:A:90:ARG:NH1	2.37	0.52
1:A:162:GLN:O	1:A:162:GLN:NE2	2.34	0.52
1:A:1697:THR:O	1:A:1701:LYS:HG2	2.10	0.52
1:B:1745:THR:OG1	1:B:1822:GLU:OE2	2.24	0.52
1:B:2697:ASN:HB3	1:B:2719:ARG:HD3	1.92	0.52
1:A:1343:ILE:HD12	1:A:1343:ILE:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1211:ALA:HA	1:B:1214:LEU:HB2	1.91	0.51
1:B:405:ASN:OD1	1:B:405:ASN:N	2.29	0.51
1:B:2319:LEU:HD13	1:B:2334:TYR:HA	1.93	0.51
1:A:112:ALA:HB3	1:A:114:ARG:HH11	1.76	0.51
1:B:2745:THR:HG22	1:B:2750:LEU:HD12	1.93	0.51
1:A:2319:LEU:HD13	1:A:2334:TYR:HA	1.93	0.51
1:B:957:GLU:HB2	1:B:999:LYS:HB2	1.93	0.51
1:A:162:GLN:HE21	1:A:162:GLN:C	2.12	0.50
1:A:1211:ALA:HA	1:A:1214:LEU:HB2	1.91	0.50
1:A:1265:PHE:HA	1:A:1268:VAL:HG12	1.93	0.50
1:A:1413:ASP:OD1	1:A:1413:ASP:N	2.45	0.50
1:A:2838:LYS:HE2	1:A:2880:GLU:HG2	1.92	0.50
1:B:1265:PHE:HA	1:B:1268:VAL:HG12	1.93	0.50
1:B:1697:THR:O	1:B:1701:LYS:HG2	2.10	0.50
1:A:2745:THR:HG22	1:A:2750:LEU:HD12	1.93	0.50
1:B:112:ALA:HB3	1:B:114:ARG:HH11	1.76	0.50
1:B:1551:ASP:OD1	1:B:1551:ASP:N	2.41	0.50
1:A:599:LEU:O	1:A:717:ARG:NE	2.44	0.50
1:A:957:GLU:HB2	1:A:999:LYS:HB2	1.93	0.50
1:B:18:ASP:O	1:B:23:ARG:NH1	2.45	0.50
1:B:1992:LYS:O	1:B:1996:GLU:HG3	2.12	0.50
1:A:154:LYS:O	1:A:158:GLU:HG3	2.12	0.50
1:B:706:SER:N	1:B:710:THR:OG1	2.40	0.50
1:B:1655:SER:HB3	1:B:2159:CYS:SG	2.52	0.50
1:A:1655:SER:HB3	1:A:2159:CYS:SG	2.52	0.50
1:A:63:PHE:HD1	1:A:66:LYS:HZ1	1.60	0.50
1:B:521:ARG:HE	1:B:554:THR:HB	1.77	0.49
1:A:18:ASP:O	1:A:23:ARG:NH1	2.45	0.49
1:A:1754:LYS:HG3	1:A:1755:MET:SD	2.52	0.49
1:B:1754:LYS:HG3	1:B:1755:MET:SD	2.52	0.49
1:A:521:ARG:HE	1:A:554:THR:HB	1.77	0.49
1:B:599:LEU:O	1:B:717:ARG:NE	2.44	0.49
1:B:1288:PRO:O	1:B:1292:VAL:HG13	2.13	0.49
1:B:154:LYS:O	1:B:158:GLU:HG3	2.12	0.49
1:A:409:LEU:HD11	1:A:442:LEU:HD11	1.94	0.49
1:B:1875:ARG:O	1:B:1876:HIS:ND1	2.46	0.49
1:A:1473:ILE:HD13	1:A:1519:VAL:HG22	1.95	0.49
1:B:1473:ILE:HD13	1:B:1519:VAL:HG22	1.95	0.49
1:A:938:PRO:HB3	1:A:976:VAL:HG22	1.94	0.49
1:B:938:PRO:HB3	1:B:976:VAL:HG22	1.94	0.49
1:A:2033:LEU:HD21	1:A:2048:THR:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LEU:HD11	1:B:442:LEU:HD11	1.94	0.49
1:A:1656:LYS:HD2	1:A:2163:LEU:HD12	1.95	0.48
1:A:2307:LEU:HD21	1:B:2032:ARG:HD3	1.95	0.48
1:B:162:GLN:HE21	1:B:162:GLN:C	2.13	0.48
1:B:1779:ARG:HH22	1:B:1820:LYS:HD2	1.78	0.48
1:A:1779:ARG:HH22	1:A:1820:LYS:HD2	1.78	0.48
1:A:1875:ARG:O	1:A:1876:HIS:ND1	2.46	0.48
1:B:2033:LEU:HD21	1:B:2048:THR:HB	1.95	0.48
1:A:1288:PRO:O	1:A:1292:VAL:HG13	2.13	0.48
1:A:1344:VAL:HG11	1:A:1418:ILE:HD13	1.94	0.48
1:B:2727:VAL:O	1:B:2731:VAL:HG23	2.14	0.48
1:B:1413:ASP:N	1:B:1413:ASP:OD1	2.45	0.48
1:A:1652:LEU:HB3	1:A:2163:LEU:HD11	1.95	0.48
1:A:1992:LYS:O	1:A:1996:GLU:HG3	2.12	0.48
1:A:2727:VAL:O	1:A:2731:VAL:HG23	2.14	0.48
1:B:251:VAL:HG11	1:B:289:ILE:HD13	1.95	0.48
1:B:657:PHE:CZ	1:B:1155:LEU:HB3	2.49	0.48
1:B:1656:LYS:HD2	1:B:2163:LEU:HD12	1.95	0.48
1:B:74:CYS:O	1:B:90:ARG:NH1	2.37	0.47
1:A:2573:THR:O	1:A:2573:THR:OG1	2.28	0.47
1:A:2865:ILE:HG13	1:A:2938:MET:HG3	1.97	0.47
1:B:1344:VAL:HG11	1:B:1418:ILE:HD13	1.94	0.47
1:B:2228:THR:OG1	1:B:2254:HIS:NE2	2.39	0.47
1:A:2228:THR:OG1	1:A:2254:HIS:NE2	2.39	0.47
1:B:432:LEU:HD21	1:B:466:GLN:HG3	1.97	0.47
1:B:1652:LEU:HB3	1:B:2163:LEU:HD11	1.95	0.47
1:B:1680:PRO:O	1:B:2215:SER:OG	2.26	0.47
1:A:1959:GLU:OE2	1:A:2849:ARG:NH1	2.36	0.47
1:A:1307:GLY:O	1:A:1311:GLN:NE2	2.48	0.47
1:A:2027:LEU:HD13	1:B:2311:ILE:HD11	1.97	0.47
1:A:2311:ILE:HD11	1:B:2027:LEU:HD13	1.97	0.47
1:B:2094:GLU:H	1:B:2094:GLU:CD	2.18	0.47
1:B:2697:ASN:OD1	1:B:2697:ASN:N	2.42	0.47
1:A:119:GLU:OE1	1:A:119:GLU:N	2.46	0.47
1:A:265:ILE:O	1:A:269:HIS:HB2	2.15	0.47
1:A:251:VAL:HG11	1:A:289:ILE:HD13	1.95	0.47
1:A:2032:ARG:HD3	1:B:2307:LEU:HD21	1.95	0.47
1:B:1307:GLY:O	1:B:1311:GLN:NE2	2.48	0.47
1:A:1341:PRO:HG3	1:A:1414:SER:HB2	1.97	0.47
1:A:2406:LYS:HB2	1:A:2406:LYS:HE3	1.73	0.47
1:A:2665:PRO:HD3	1:A:2683:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2865:ILE:HG13	1:B:2938:MET:HG3	1.97	0.47
1:A:657:PHE:CZ	1:A:1155:LEU:HB3	2.49	0.46
1:A:1231:LEU:HD21	1:A:1255:LEU:HB3	1.97	0.46
1:A:2402:GLU:OE2	1:A:2459:ARG:NE	2.32	0.46
1:B:265:ILE:O	1:B:269:HIS:HB2	2.15	0.46
1:B:924:ARG:HD2	1:B:961:LEU:HD21	1.98	0.46
1:A:3014:GLN:HG2	1:A:3018:LYS:NZ	2.30	0.46
1:B:1827:LEU:HD22	1:B:1837:PHE:HZ	1.80	0.46
1:A:342:LYS:HB2	1:A:342:LYS:HE3	1.56	0.46
1:A:2731:VAL:HG21	1:A:2952:LEU:HD21	1.98	0.46
1:B:1231:LEU:HD21	1:B:1255:LEU:HB3	1.97	0.46
1:A:924:ARG:HD2	1:A:961:LEU:HD21	1.98	0.46
1:B:342:LYS:HB2	1:B:342:LYS:HE3	1.56	0.46
1:B:938:PRO:HB2	1:B:979:LEU:HD12	1.97	0.46
1:B:2665:PRO:HD3	1:B:2683:ILE:HD11	1.96	0.46
1:A:1669:GLU:HG3	1:A:2148:LYS:HG3	1.98	0.46
1:B:2025:LYS:HB2	1:B:2025:LYS:HE3	1.79	0.46
1:A:271:LEU:HB3	1:A:276:LYS:HD3	1.98	0.46
1:A:432:LEU:HD21	1:A:466:GLN:HG3	1.97	0.46
1:A:1596:HIS:O	1:A:1600:VAL:HG23	2.16	0.46
1:A:2094:GLU:CD	1:A:2094:GLU:H	2.18	0.46
1:A:938:PRO:HB2	1:A:979:LEU:HD12	1.97	0.46
1:B:716:VAL:HG21	1:B:779:MET:HG3	1.98	0.46
1:B:1341:PRO:HG3	1:B:1414:SER:HB2	1.97	0.46
1:B:1596:HIS:O	1:B:1600:VAL:HG23	2.16	0.46
1:B:533:ARG:HG2	1:B:533:ARG:HH11	1.81	0.46
1:A:1678:VAL:HG23	1:A:1681:ILE:HD12	1.98	0.45
1:B:58:ASP:OD1	1:B:62:ARG:NH2	2.43	0.45
1:B:271:LEU:HB3	1:B:276:LYS:HD3	1.98	0.45
1:A:741:TYR:CE1	1:A:805:ARG:HD3	2.51	0.45
1:A:1680:PRO:O	1:A:2215:SER:OG	2.26	0.45
1:B:753:MET:HG2	1:B:806:LEU:HD13	1.98	0.45
1:B:1527:LEU:HB3	1:B:1538:VAL:HG21	1.99	0.45
1:B:1669:GLU:HG3	1:B:2148:LYS:HG3	1.98	0.45
1:A:533:ARG:HG2	1:A:533:ARG:HH11	1.81	0.45
1:B:206:ASN:HD22	1:B:208:LYS:HG2	1.82	0.45
1:B:2474:LEU:O	1:B:2515:LYS:NZ	2.50	0.45
1:A:120:LEU:HG	1:A:149:ILE:HD11	1.99	0.45
1:A:967:LEU:HD11	1:A:1013:ASP:HB3	1.98	0.45
1:B:1715:LEU:HD22	1:B:1737:LEU:HD23	1.97	0.45
1:B:2237:LYS:HA	1:B:2237:LYS:HD3	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3014:GLN:HG2	1:B:3018:LYS:NZ	2.30	0.45
1:A:109:ASN:ND2	1:A:155:TYR:OH	2.48	0.45
1:A:1527:LEU:HB3	1:A:1538:VAL:HG21	1.99	0.45
1:B:1567:ASP:O	1:B:1568:HIS:ND1	2.36	0.45
1:B:2358:GLN:HA	1:B:2358:GLN:OE1	2.17	0.45
1:A:1465:LEU:HD13	1:A:1469:ILE:HD12	1.99	0.45
1:B:1334:HIS:HD1	1:B:1334:HIS:C	2.19	0.45
1:B:2731:VAL:HG21	1:B:2952:LEU:HD21	1.98	0.45
1:A:60:VAL:HA	1:A:63:PHE:CD2	2.51	0.45
1:A:1034:TYR:HB3	1:A:1038:VAL:HB	1.98	0.45
1:A:2670:LYS:HB2	1:A:2670:LYS:HE2	1.68	0.45
1:B:2570:GLU:CD	1:B:2570:GLU:H	2.20	0.45
1:A:1869:PHE:CE1	1:A:1909:MET:HG3	2.51	0.45
1:A:2763:ARG:NH1	1:A:2763:ARG:HB3	2.32	0.45
1:A:716:VAL:HG21	1:A:779:MET:HG3	1.98	0.45
1:A:1290:ILE:HG22	1:A:1294:ILE:CD1	2.47	0.45
1:A:2693:ALA:HB3	1:A:2699:PRO:HG2	1.99	0.45
1:B:741:TYR:CE1	1:B:805:ARG:HD3	2.51	0.45
1:B:1678:VAL:HG23	1:B:1681:ILE:HD12	1.98	0.45
1:B:2406:LYS:HE3	1:B:2406:LYS:HB2	1.73	0.45
1:A:183:HIS:O	1:A:187:VAL:HG23	2.16	0.45
1:A:753:MET:HG2	1:A:806:LEU:HD13	1.98	0.45
1:A:1257:PRO:O	1:A:1261:ILE:HG22	2.17	0.45
1:A:2474:LEU:O	1:A:2515:LYS:NZ	2.50	0.45
1:B:892:LYS:HD2	1:B:892:LYS:HA	1.74	0.45
1:B:967:LEU:HD11	1:B:1013:ASP:HB3	1.98	0.45
1:B:1257:PRO:O	1:B:1261:ILE:HG22	2.17	0.45
1:B:2025:LYS:HB3	1:B:2028:GLN:HG3	1.99	0.45
1:A:206:ASN:HD22	1:A:208:LYS:HG2	1.82	0.44
1:A:262:LEU:HD11	1:A:282:LEU:HD23	1.99	0.44
1:A:706:SER:N	1:A:710:THR:OG1	2.40	0.44
1:A:1334:HIS:HD1	1:A:1334:HIS:C	2.19	0.44
1:A:1460:ALA:HB2	1:A:1766:PRO:HB3	1.99	0.44
1:A:2358:GLN:OE1	1:A:2358:GLN:HA	2.17	0.44
1:B:120:LEU:HG	1:B:149:ILE:HD11	1.99	0.44
1:B:159:ILE:HG23	1:B:163:GLN:HB2	2.00	0.44
1:B:262:LEU:HD11	1:B:282:LEU:HD23	1.99	0.44
1:B:609:GLU:HG2	1:B:724:GLY:HA3	1.99	0.44
1:B:1643:ILE:HD12	1:B:1643:ILE:HA	1.89	0.44
1:B:2514:TYR:HA	1:B:2517:LEU:HG	2.00	0.44
1:B:2531:MET:H	1:B:2538:HIS:HD2	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:HG23	1:A:163:GLN:HB2	2.00	0.44
1:A:1715:LEU:HD22	1:A:1737:LEU:HD23	1.97	0.44
1:A:1827:LEU:HD22	1:A:1837:PHE:HZ	1.80	0.44
1:B:109:ASN:ND2	1:B:155:TYR:OH	2.48	0.44
1:B:183:HIS:O	1:B:187:VAL:HG23	2.16	0.44
1:B:1802:HIS:HB2	1:B:1902:ASP:OD2	2.17	0.44
1:B:2763:ARG:HB3	1:B:2763:ARG:NH1	2.32	0.44
1:A:121:LEU:HD23	1:A:163:GLN:NE2	2.33	0.44
1:A:948:LEU:HB3	1:A:993:HIS:ND1	2.32	0.44
1:A:1607:PRO:HG2	1:A:1658:ALA:HA	1.99	0.44
1:A:2109:TRP:O	1:A:2133:GLN:NE2	2.51	0.44
1:B:60:VAL:HA	1:B:63:PHE:CD2	2.51	0.44
1:B:1761:LEU:O	1:B:1765:GLN:HG2	2.17	0.44
1:B:1869:PHE:CE1	1:B:1909:MET:HG3	2.51	0.44
1:B:2109:TRP:O	1:B:2133:GLN:NE2	2.51	0.44
1:B:2561:LEU:O	1:B:2565:ASN:N	2.48	0.44
1:A:780:MET:HG3	1:A:900:MET:HG2	1.99	0.44
1:B:224:LYS:HE3	1:B:269:HIS:HA	1.99	0.44
1:B:1378:PRO:HG2	1:B:1379:PRO:HD3	1.98	0.44
1:B:1460:ALA:HB2	1:B:1766:PRO:HB3	1.99	0.44
1:B:2616:MET:HB2	1:B:2661:ASP:HB3	2.00	0.44
1:A:1378:PRO:HG2	1:A:1379:PRO:HD3	1.98	0.44
1:A:1860:ASN:O	1:A:1864:THR:HG22	2.17	0.44
1:A:2025:LYS:HB3	1:A:2028:GLN:HG3	1.99	0.44
1:A:2616:MET:HB2	1:A:2661:ASP:HB3	1.99	0.44
1:B:121:LEU:HD23	1:B:163:GLN:NE2	2.33	0.44
1:B:948:LEU:HB3	1:B:993:HIS:ND1	2.32	0.44
1:B:1465:LEU:HD13	1:B:1469:ILE:HD12	1.99	0.44
1:B:433:SER:O	1:B:437:MET:HG3	2.18	0.44
1:B:780:MET:HG3	1:B:900:MET:HG2	1.99	0.44
1:B:1860:ASN:O	1:B:1864:THR:HG22	2.17	0.44
1:A:433:SER:O	1:A:437:MET:HG3	2.18	0.44
1:A:790:CYS:SG	1:A:792:LYS:HG3	2.58	0.44
1:B:1034:TYR:HB3	1:B:1038:VAL:HB	1.98	0.44
1:B:1280:LYS:HD2	1:B:1280:LYS:HA	1.81	0.44
1:B:3043:LYS:O	1:B:3047:ARG:HG3	2.18	0.44
1:A:706:SER:HB3	1:A:709:ILE:HG13	1.99	0.44
1:A:1117:GLN:NE2	1:A:1171:GLN:OE1	2.48	0.44
1:A:1802:HIS:HB2	1:A:1902:ASP:OD2	2.17	0.44
1:A:2514:TYR:HA	1:A:2517:LEU:HG	2.00	0.44
1:A:2570:GLU:H	1:A:2570:GLU:CD	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1465:LEU:HD21	1:B:1505:ALA:HB2	1.99	0.44
1:B:166:GLU:O	1:B:170:VAL:HG13	2.18	0.44
1:B:706:SER:HB3	1:B:709:ILE:HG13	1.99	0.44
1:A:1465:LEU:HD21	1:A:1505:ALA:HB2	1.99	0.43
1:A:2734:MET:HG2	1:A:2948:ILE:HD13	2.00	0.43
1:B:1607:PRO:HG2	1:B:1658:ALA:HA	1.99	0.43
1:B:2693:ALA:HB3	1:B:2699:PRO:HG2	1.99	0.43
1:A:267:THR:HG22	1:A:268:GLN:OE1	2.18	0.43
1:A:768:ASN:OD1	1:A:768:ASN:N	2.50	0.43
1:A:3043:LYS:O	1:A:3047:ARG:HG3	2.18	0.43
1:A:205:LEU:HD12	1:A:209:PHE:CD1	2.53	0.43
1:A:1066:LYS:HB3	1:A:1066:LYS:HE2	1.55	0.43
1:A:1761:LEU:O	1:A:1765:GLN:HG2	2.17	0.43
1:B:814:ASP:O	1:B:818:ILE:HG13	2.19	0.43
1:B:2749:LYS:HB2	1:B:2749:LYS:HE3	1.62	0.43
1:A:436:LEU:HD12	1:A:436:LEU:HA	1.90	0.43
1:A:554:THR:HG22	1:A:572:LEU:HD22	2.00	0.43
1:A:609:GLU:HG2	1:A:724:GLY:HA3	1.99	0.43
1:B:554:THR:HG22	1:B:572:LEU:HD22	2.00	0.43
1:B:2417:LEU:HD23	1:B:2417:LEU:HA	1.70	0.43
1:A:166:GLU:O	1:A:170:VAL:HG13	2.18	0.43
1:A:2416:LEU:HD22	1:B:2899:ILE:HG22	2.00	0.43
1:A:2899:ILE:HG22	1:B:2416:LEU:HD22	2.00	0.43
1:B:119:GLU:OE1	1:B:119:GLU:N	2.46	0.43
1:A:319:LEU:HD22	1:A:352:ILE:HD12	2.00	0.43
1:A:2332:LEU:HD21	1:A:2379:LEU:HA	2.01	0.43
1:A:2531:MET:H	1:A:2538:HIS:HD2	1.65	0.43
1:A:2570:GLU:OE1	1:A:2570:GLU:N	2.51	0.43
1:A:2691:ARG:HG3	1:A:2691:ARG:HH11	1.84	0.43
1:B:433:SER:HB3	1:B:434:PRO:HD3	2.00	0.43
1:B:1608:LEU:HD23	1:B:1608:LEU:HA	1.83	0.43
1:A:2237:LYS:HA	1:A:2237:LYS:HD3	1.70	0.43
1:A:2335:THR:HG21	1:A:2368:ALA:HB2	2.01	0.43
1:A:2440:LYS:O	1:A:2444:GLU:HG2	2.19	0.43
1:A:2530:LYS:H	1:A:2530:LYS:HD3	1.84	0.43
1:B:133:ASN:HB3	1:B:137:TYR:HD2	1.84	0.43
1:A:63:PHE:HD1	1:A:66:LYS:NZ	2.16	0.43
1:A:2623:LEU:HD22	1:A:2662:VAL:HG11	2.01	0.43
1:B:259:LEU:HD11	1:B:286:GLN:HG3	2.01	0.43
1:B:2440:LYS:O	1:B:2444:GLU:HG2	2.19	0.43
1:B:2734:MET:HG2	1:B:2948:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3043:LYS:HA	1:B:3043:LYS:HD2	1.85	0.43
1:B:319:LEU:HD22	1:B:352:ILE:HD12	2.00	0.43
1:B:790:CYS:SG	1:B:792:LYS:HG3	2.58	0.43
1:B:2570:GLU:OE1	1:B:2570:GLU:N	2.51	0.43
1:A:1294:ILE:HG22	1:A:1298:PHE:CE1	2.54	0.43
1:B:1290:ILE:HG22	1:B:1294:ILE:CD1	2.47	0.43
1:B:2332:LEU:HD21	1:B:2379:LEU:HA	2.01	0.43
1:A:38:GLU:O	1:A:42:HIS:HB2	2.19	0.42
1:A:224:LYS:HE3	1:A:269:HIS:HA	1.99	0.42
1:B:38:GLU:O	1:B:42:HIS:HB2	2.19	0.42
1:B:768:ASN:OD1	1:B:768:ASN:N	2.50	0.42
1:B:1093:ILE:HG21	1:B:1157:LEU:HD12	2.01	0.42
1:B:1294:ILE:HG22	1:B:1298:PHE:CE1	2.54	0.42
1:B:2602:ALA:O	1:B:2606:ILE:HG12	2.19	0.42
1:A:192:HIS:CE1	1:A:879:ILE:HG13	2.54	0.42
1:A:433:SER:HB3	1:A:434:PRO:HD3	2.00	0.42
1:A:1256:ILE:HG12	1:A:1268:VAL:HG23	2.01	0.42
1:A:2010:ARG:CZ	1:A:2034:ARG:HD2	2.49	0.42
1:B:192:HIS:CE1	1:B:879:ILE:HG13	2.55	0.42
1:A:2561:LEU:O	1:A:2565:ASN:N	2.48	0.42
1:B:205:LEU:HD12	1:B:209:PHE:CD1	2.53	0.42
1:B:267:THR:HG22	1:B:268:GLN:OE1	2.18	0.42
1:B:1117:GLN:NE2	1:B:1171:GLN:OE1	2.48	0.42
1:B:1820:LYS:HB2	1:B:1852:GLN:HG3	2.02	0.42
1:B:2691:ARG:NH1	1:B:2691:ARG:HG3	2.34	0.42
1:A:892:LYS:HA	1:A:892:LYS:HD2	1.74	0.42
1:A:1643:ILE:HD12	1:A:1643:ILE:HA	1.89	0.42
1:A:1820:LYS:HB2	1:A:1852:GLN:HG3	2.02	0.42
1:A:2312:LEU:HD12	1:A:2312:LEU:HA	1.88	0.42
1:B:1256:ILE:HG12	1:B:1268:VAL:HG23	2.01	0.42
1:B:2010:ARG:CZ	1:B:2034:ARG:HD2	2.49	0.42
1:B:2563:LEU:HD23	1:B:2563:LEU:HA	1.80	0.42
1:A:1093:ILE:HG21	1:A:1157:LEU:HD12	2.01	0.42
1:B:1536:LYS:HA	1:B:1536:LYS:HD2	1.85	0.42
1:B:1606:LEU:HD12	1:B:1606:LEU:HA	1.80	0.42
1:A:436:LEU:HD13	1:A:462:VAL:HG11	2.02	0.42
1:A:814:ASP:O	1:A:818:ILE:HG13	2.19	0.42
1:A:1705:ASP:HB3	1:A:1708:LEU:HG	2.00	0.42
1:A:2691:ARG:HG3	1:A:2691:ARG:NH1	2.34	0.42
1:B:188:ALA:HB1	1:B:231:HIS:HB2	2.02	0.42
1:A:530:SER:O	1:A:530:SER:OG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1405:LEU:HA	1:A:1408:LEU:HB2	2.02	0.42
1:A:3043:LYS:HD2	1:A:3043:LYS:HA	1.85	0.42
1:B:436:LEU:HD13	1:B:462:VAL:HG11	2.02	0.42
1:B:1499:SER:O	1:B:1503:GLN:HG3	2.20	0.42
1:B:2691:ARG:HG3	1:B:2691:ARG:HH11	1.84	0.42
1:B:2708:ASP:OD1	1:B:2708:ASP:N	2.53	0.42
1:A:259:LEU:HD11	1:A:286:GLN:HG3	2.01	0.42
1:A:822:LEU:HD23	1:A:897:PHE:HB2	2.02	0.42
1:A:2708:ASP:OD1	1:A:2708:ASP:N	2.53	0.42
1:B:822:LEU:HD23	1:B:897:PHE:HB2	2.02	0.42
1:B:1705:ASP:HB3	1:B:1708:LEU:HG	2.00	0.42
1:A:2025:LYS:HB2	1:A:2025:LYS:HE3	1.79	0.42
1:A:2092:CYS:SG	1:A:2095:LEU:HB2	2.60	0.42
1:A:2602:ALA:O	1:A:2606:ILE:HG12	2.19	0.42
1:B:206:ASN:ND2	1:B:208:LYS:HG2	2.35	0.42
1:B:1461:TRP:CH2	1:B:1465:LEU:HD23	2.55	0.42
1:B:1590:LEU:HD11	1:B:1621:LEU:HD23	2.02	0.42
1:B:2792:ARG:NE	1:B:2795:ASP:OD2	2.52	0.42
1:A:133:ASN:HB3	1:A:137:TYR:HD2	1.84	0.42
1:A:1461:TRP:CH2	1:A:1465:LEU:HD23	2.55	0.42
1:A:2698:LEU:HD12	1:A:2698:LEU:H	1.85	0.42
1:A:2792:ARG:NE	1:A:2795:ASP:OD2	2.52	0.42
1:B:2335:THR:HG21	1:B:2368:ALA:HB2	2.01	0.42
1:A:621:LYS:O	1:A:625:ASN:ND2	2.49	0.41
1:A:1499:SER:O	1:A:1503:GLN:HG3	2.20	0.41
1:A:1555:LEU:O	1:A:1559:ILE:HG13	2.20	0.41
1:A:1608:LEU:HA	1:A:1608:LEU:HD23	1.83	0.41
1:B:805:ARG:HE	1:B:805:ARG:HB3	1.79	0.41
1:B:2573:THR:O	1:B:2573:THR:OG1	2.28	0.41
1:B:2623:LEU:HD22	1:B:2662:VAL:HG11	2.01	0.41
1:A:2854:ARG:HG2	1:A:2930:CYS:SG	2.60	0.41
1:B:2530:LYS:H	1:B:2530:LYS:HD3	1.84	0.41
1:A:206:ASN:ND2	1:A:208:LYS:HG2	2.35	0.41
1:B:2844:ILE:O	1:B:2848:LYS:HG2	2.21	0.41
1:A:1590:LEU:HD11	1:A:1621:LEU:HD23	2.02	0.41
1:A:2749:LYS:HE3	1:A:2749:LYS:HB2	1.62	0.41
1:A:3018:LYS:HE2	1:B:3023:GLY:O	2.20	0.41
1:A:1290:ILE:HG22	1:A:1294:ILE:HD11	2.03	0.41
1:A:1659:ILE:HD13	1:A:1659:ILE:HA	1.92	0.41
1:B:2092:CYS:SG	1:B:2095:LEU:HB2	2.60	0.41
1:A:213:PHE:CG	1:A:236:LEU:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3023:GLY:O	1:B:3018:LYS:HE2	2.20	0.41
1:B:1398:LYS:H	1:B:1398:LYS:HG2	1.67	0.41
1:B:1416:GLN:NE2	1:B:1734:VAL:HG21	2.35	0.41
1:B:2331:LYS:HZ2	1:B:2373:GLY:H	1.68	0.41
1:A:1539:LEU:HD13	1:A:1539:LEU:HA	1.91	0.41
1:A:1677:GLU:OE1	1:A:1677:GLU:HA	2.21	0.41
1:A:1903:LYS:HA	1:A:1903:LYS:HD3	1.90	0.41
1:A:2844:ILE:O	1:A:2848:LYS:HG2	2.21	0.41
1:B:2854:ARG:HG2	1:B:2930:CYS:SG	2.60	0.41
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.87	0.41
1:A:486:LYS:O	1:A:490:ILE:HG13	2.21	0.41
1:A:1821:CYS:SG	1:A:1823:ILE:HG13	2.60	0.41
1:A:2815:GLU:O	1:A:2818:GLU:HG3	2.21	0.41
1:A:2868:LEU:HG	1:A:2871:ARG:HD3	2.02	0.41
1:B:213:PHE:CG	1:B:236:LEU:HD13	2.56	0.41
1:B:1066:LYS:HB3	1:B:1066:LYS:HE2	1.55	0.41
1:B:1290:ILE:HG22	1:B:1294:ILE:HD11	2.03	0.41
1:B:1555:LEU:O	1:B:1559:ILE:HG13	2.20	0.41
1:B:1821:CYS:SG	1:B:1823:ILE:HG13	2.60	0.41
1:B:2815:GLU:O	1:B:2818:GLU:HG3	2.21	0.41
1:A:126:ASP:HA	1:A:129:LYS:HB2	2.03	0.41
1:A:657:PHE:HZ	1:A:1155:LEU:HB3	1.85	0.41
1:A:1110:ALA:HB3	1:A:1372:LEU:HD21	2.03	0.41
1:A:1524:LEU:O	1:A:1527:LEU:HB2	2.21	0.41
1:B:147:LYS:HA	1:B:147:LYS:HD3	1.94	0.41
1:B:495:ILE:HG21	1:B:526:LEU:HD21	2.03	0.41
1:B:657:PHE:HZ	1:B:1155:LEU:HB3	1.85	0.41
1:B:1339:ASN:OD1	1:B:1339:ASN:N	2.54	0.41
1:B:1405:LEU:HA	1:B:1408:LEU:HB2	2.02	0.41
1:B:2163:LEU:HD23	1:B:2163:LEU:HA	1.89	0.41
1:B:2417:LEU:HD13	1:B:2445:LEU:HD22	2.03	0.41
1:B:2687:LYS:HZ2	1:B:2711:GLU:HG2	1.85	0.41
1:B:2868:LEU:HG	1:B:2871:ARG:HD3	2.02	0.41
1:B:2178:ALA:HB1	1:B:2226:LEU:HD23	2.03	0.41
1:B:2669:ILE:HD12	1:B:2669:ILE:N	2.36	0.41
1:A:188:ALA:HB1	1:A:231:HIS:HB2	2.02	0.40
1:A:280:ILE:HG23	1:A:348:LEU:HD22	2.03	0.40
1:A:2517:LEU:N	1:A:2518:PRO:HD2	2.36	0.40
1:A:2627:TYR:HB3	1:A:2760:LEU:HD13	2.03	0.40
1:B:1611:LEU:O	1:B:1614:LEU:HB2	2.21	0.40
1:B:2049:TYR:HB3	1:B:2064:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1416:GLN:NE2	1:A:1734:VAL:HG21	2.35	0.40
1:B:1677:GLU:HA	1:B:1677:GLU:OE1	2.21	0.40
1:B:1903:LYS:HD3	1:B:1903:LYS:HA	1.90	0.40
1:A:58:ASP:OD1	1:A:62:ARG:NH2	2.43	0.40
1:A:1040:MET:HG3	1:A:1085:VAL:HG22	2.04	0.40
1:A:1611:LEU:O	1:A:1614:LEU:HB2	2.21	0.40
1:A:1692:LYS:HE3	1:A:1692:LYS:HB3	1.87	0.40
1:A:2331:LYS:HZ2	1:A:2373:GLY:H	1.70	0.40
1:A:2615:GLN:NE2	1:A:2615:GLN:O	2.53	0.40
1:B:280:ILE:HG23	1:B:348:LEU:HD22	2.03	0.40
1:B:1289:LYS:O	1:B:1293:ASN:ND2	2.53	0.40
1:B:1524:LEU:O	1:B:1527:LEU:HB2	2.21	0.40
1:B:2615:GLN:NE2	1:B:2615:GLN:O	2.53	0.40
1:A:2669:ILE:HD12	1:A:2669:ILE:N	2.36	0.40
1:A:2872:HIS:CE1	1:A:2874:GLN:HB2	2.57	0.40
1:B:2698:LEU:HD12	1:B:2698:LEU:H	1.85	0.40
1:A:1310:GLN:NE2	1:A:1311:GLN:HE21	2.15	0.40
1:A:1339:ASN:OD1	1:A:1339:ASN:N	2.54	0.40
1:A:1902:ASP:O	1:A:1906:GLN:HG3	2.21	0.40
1:A:2073:LEU:HD22	1:A:2076:ILE:HD12	2.03	0.40
1:B:63:PHE:HD1	1:B:66:LYS:NZ	2.16	0.40
1:B:1110:ALA:HB3	1:B:1372:LEU:HD21	2.03	0.40
1:B:1687:ALA:HB1	1:B:2843:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2735/3056 (90%)	2687 (98%)	48 (2%)	0	100	100
1	B	2735/3056 (90%)	2687 (98%)	48 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5470/6112 (90%)	5374 (98%)	96 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2469/2780 (89%)	2350 (95%)	119 (5%)	25 48
1	B	2469/2780 (89%)	2351 (95%)	118 (5%)	25 48
All	All	4938/5560 (89%)	4701 (95%)	237 (5%)	29 48

All (237) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LYS
1	A	111	ARG
1	A	114	ARG
1	A	118	GLN
1	A	123	TYR
1	A	148	ASP
1	A	162	GLN
1	A	167	LEU
1	A	172	PHE
1	A	214	SER
1	A	272	ASN
1	A	278	VAL
1	A	305	SER
1	A	325	HIS
1	A	405	ASN
1	A	408	ASP
1	A	465	CYS
1	A	481	LEU
1	A	489	CYS
1	A	493	ARG

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Mol	Chain	Res	Type
1	A	498	GLU
1	A	499	GLN
1	A	519	VAL
1	A	617	MET
1	A	620	CYS
1	A	624	MET
1	A	695	LEU
1	A	698	SER
1	A	729	TYR
1	A	759	SER
1	A	768	ASN
1	A	791	THR
1	A	800	SER
1	A	898	LEU
1	A	929	MET
1	A	967	LEU
1	A	985	ASP
1	A	995	LEU
1	A	1000	ASN
1	A	1021	VAL
1	A	1032	ARG
1	A	1045	CYS
1	A	1063	VAL
1	A	1108	LEU
1	A	1133	GLU
1	A	1143	THR
1	A	1145	ASP
1	A	1164	CYS
1	A	1167	ILE
1	A	1204	ARG
1	A	1208	ASP
1	A	1233	SER
1	A	1243	ASN
1	A	1279	TRP
1	A	1285	ASP
1	A	1308	MET
1	A	1312	ARG
1	A	1317	LYS
1	A	1321	MET
1	A	1336	PHE
1	A	1383	SER
1	A	1396	CYS

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Mol	Chain	Res	Type
1	A	1423	CYS
1	A	1428	GLU
1	A	1434	LYS
1	A	1478	GLN
1	A	1509	CYS
1	A	1529	TYR
1	A	1540	ASP
1	A	1562	LEU
1	A	1563	ASP
1	A	1567	ASP
1	A	1568	HIS
1	A	1575	ARG
1	A	1580	LYS
1	A	1608	LEU
1	A	1618	ARG
1	A	1626	ASP
1	A	1641	ASP
1	A	1655	SER
1	A	1678	VAL
1	A	1721	THR
1	A	1755	MET
1	A	1756	THR
1	A	1787	GLU
1	A	1801	ASN
1	A	1806	ILE
1	A	1830	MET
1	A	1835	THR
1	A	1871	THR
1	A	2007	GLU
1	A	2057	SER
1	A	2059	THR
1	A	2141	SER
1	A	2146	SER
1	A	2237	LYS
1	A	2289	SER
1	A	2323	CYS
1	A	2380	ARG
1	A	2419	ARG
1	A	2440	LYS
1	A	2457	GLU
1	A	2529	THR
1	A	2530	LYS

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Mol	Chain	Res	Type
1	A	2531	MET
1	A	2615	GLN
1	A	2627	TYR
1	A	2655	LYS
1	A	2661	ASP
1	A	2674	THR
1	A	2698	LEU
1	A	2703	ASP
1	A	2719	ARG
1	A	2720	ASP
1	A	2725	ASP
1	A	2789	LYS
1	A	2831	PHE
1	A	2920	ILE
1	A	3024	THR
1	B	66	LYS
1	B	111	ARG
1	B	114	ARG
1	B	118	GLN
1	B	123	TYR
1	B	148	ASP
1	B	162	GLN
1	B	167	LEU
1	B	172	PHE
1	B	214	SER
1	B	272	ASN
1	B	278	VAL
1	B	305	SER
1	B	325	HIS
1	B	405	ASN
1	B	408	ASP
1	B	465	CYS
1	B	481	LEU
1	B	489	CYS
1	B	493	ARG
1	B	498	GLU
1	B	499	GLN
1	B	519	VAL
1	B	617	MET
1	B	620	CYS
1	B	624	MET
1	B	695	LEU

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Mol	Chain	Res	Type
1	B	698	SER
1	B	729	TYR
1	B	759	SER
1	B	768	ASN
1	B	791	THR
1	B	800	SER
1	B	898	LEU
1	B	929	MET
1	B	967	LEU
1	B	985	ASP
1	B	995	LEU
1	B	1000	ASN
1	B	1021	VAL
1	B	1032	ARG
1	B	1045	CYS
1	B	1063	VAL
1	B	1108	LEU
1	B	1133	GLU
1	B	1143	THR
1	B	1164	CYS
1	B	1167	ILE
1	B	1204	ARG
1	B	1208	ASP
1	B	1233	SER
1	B	1243	ASN
1	B	1279	TRP
1	B	1285	ASP
1	B	1308	MET
1	B	1312	ARG
1	B	1317	LYS
1	B	1321	MET
1	B	1336	PHE
1	B	1383	SER
1	B	1396	CYS
1	B	1423	CYS
1	B	1428	GLU
1	B	1434	LYS
1	B	1478	GLN
1	B	1509	CYS
1	B	1529	TYR
1	B	1540	ASP
1	B	1562	LEU

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Mol	Chain	Res	Type
1	B	1563	ASP
1	B	1567	ASP
1	B	1568	HIS
1	B	1575	ARG
1	B	1580	LYS
1	B	1608	LEU
1	B	1618	ARG
1	B	1626	ASP
1	B	1641	ASP
1	B	1655	SER
1	B	1678	VAL
1	B	1721	THR
1	B	1755	MET
1	B	1756	THR
1	B	1787	GLU
1	B	1801	ASN
1	B	1806	ILE
1	B	1830	MET
1	B	1835	THR
1	B	1871	THR
1	B	2007	GLU
1	B	2057	SER
1	B	2059	THR
1	B	2141	SER
1	B	2146	SER
1	B	2237	LYS
1	B	2289	SER
1	B	2323	CYS
1	B	2380	ARG
1	B	2419	ARG
1	B	2440	LYS
1	B	2457	GLU
1	B	2529	THR
1	B	2530	LYS
1	B	2531	MET
1	B	2615	GLN
1	B	2627	TYR
1	B	2655	LYS
1	B	2661	ASP
1	B	2674	THR
1	B	2698	LEU
1	B	2703	ASP

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Mol	Chain	Res	Type
1	B	2719	ARG
1	B	2720	ASP
1	B	2725	ASP
1	B	2789	LYS
1	B	2831	PHE
1	B	2920	ILE
1	B	3024	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	163	GLN
1	A	1311	GLN
1	B	118	GLN
1	B	163	GLN
1	B	1311	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ANP	B	3101	3	29,33,33	1.08	4 (13%)	31,52,52	1.09	2 (6%)
2	ANP	A	3101	3	29,33,33	1.08	4 (13%)	31,52,52	1.09	2 (6%)

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	ANP	B	3101	3	-	4/14/38/38	0/3/3/3
2	ANP	A	3101	3	-	4/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3101	ANP	PG-O1G	2.43	1.50	1.46
2	B	3101	ANP	PG-O1G	2.43	1.50	1.46
2	A	3101	ANP	PG-N3B	2.39	1.69	1.63
2	B	3101	ANP	PG-N3B	2.39	1.69	1.63
2	A	3101	ANP	PB-O3A	-2.39	1.56	1.59
2	B	3101	ANP	PB-O3A	-2.39	1.56	1.59
2	A	3101	ANP	PB-O1B	2.28	1.49	1.46
2	B	3101	ANP	PB-O1B	2.28	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3101	ANP	PB-O3A-PA	-4.02	118.45	132.62
2	B	3101	ANP	PB-O3A-PA	-4.02	118.45	132.62
2	A	3101	ANP	C5-C6-N6	2.25	123.78	120.35
2	B	3101	ANP	C5-C6-N6	2.25	123.78	120.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3101	ANP	PB-N3B-PG-O1G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	3101	ANP	PG-N3B-PB-O1B
2	B	3101	ANP	PB-N3B-PG-O1G
2	B	3101	ANP	PG-N3B-PB-O1B
2	A	3101	ANP	O4'-C4'-C5'-O5'
2	B	3101	ANP	O4'-C4'-C5'-O5'
2	A	3101	ANP	C3'-C4'-C5'-O5'
2	B	3101	ANP	C3'-C4'-C5'-O5'

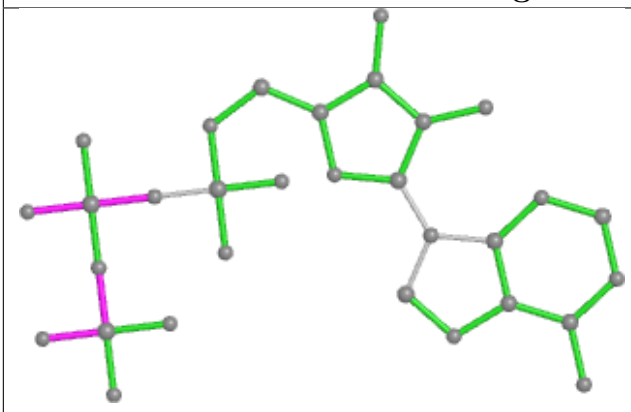
There are no ring outliers.

2 monomers are involved in 2 short contacts:

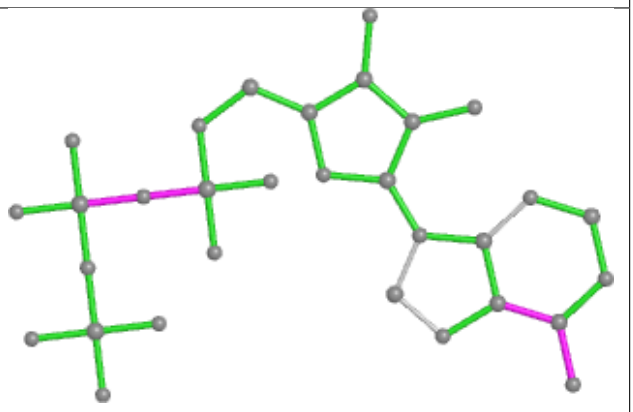
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3101	ANP	1	0
2	A	3101	ANP	1	0

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.

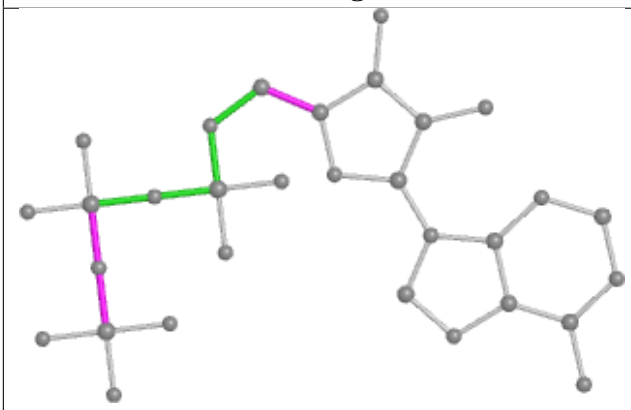
Ligand ANP B 3101



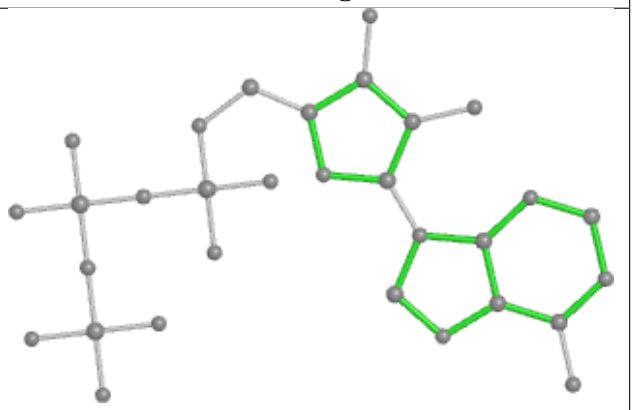
Bond lengths



Bond angles

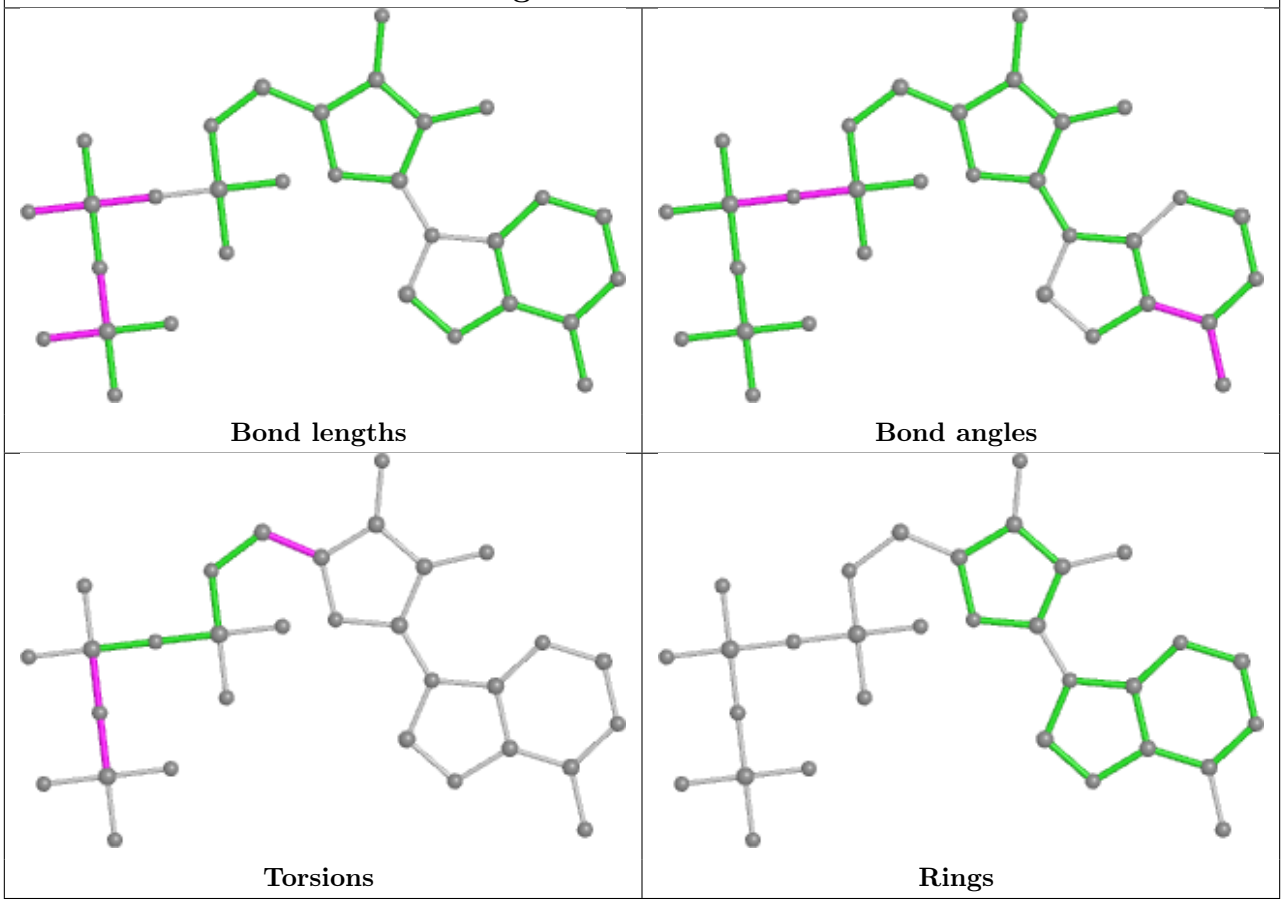


Torsions



Rings

Ligand ANP A 3101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

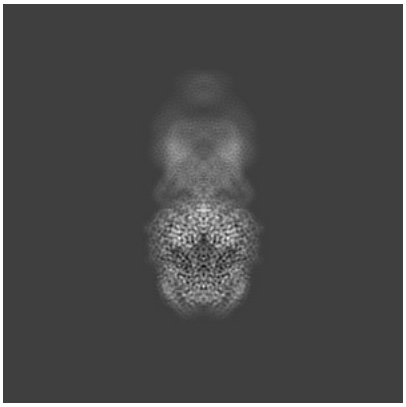
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25140. These allow visual inspection of the internal detail of the map and identification of artifacts.

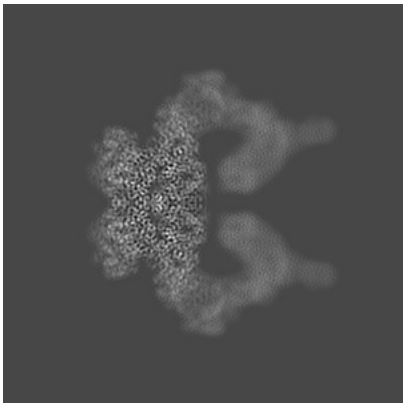
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

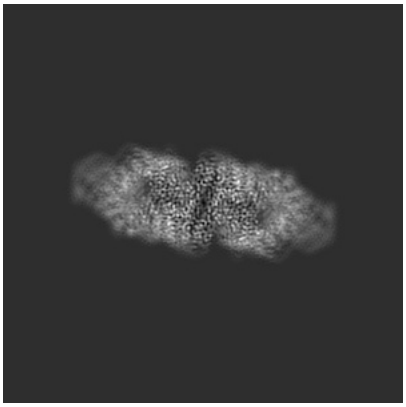
6.1.1 Primary map



X



Y



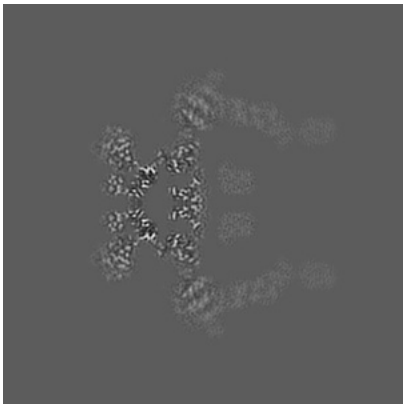
Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 150



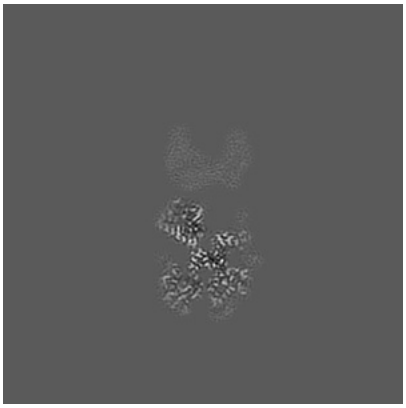
Y Index: 150

Z Index: 150

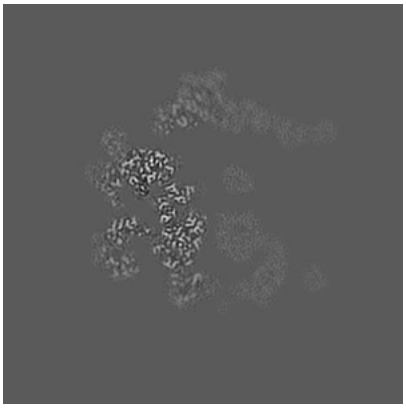
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

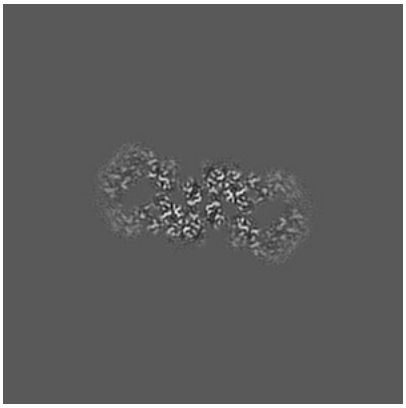
6.3.1 Primary map



X Index: 127



Y Index: 140



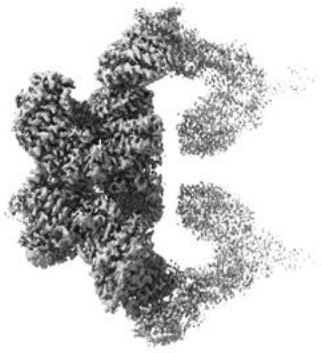
Z Index: 128

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

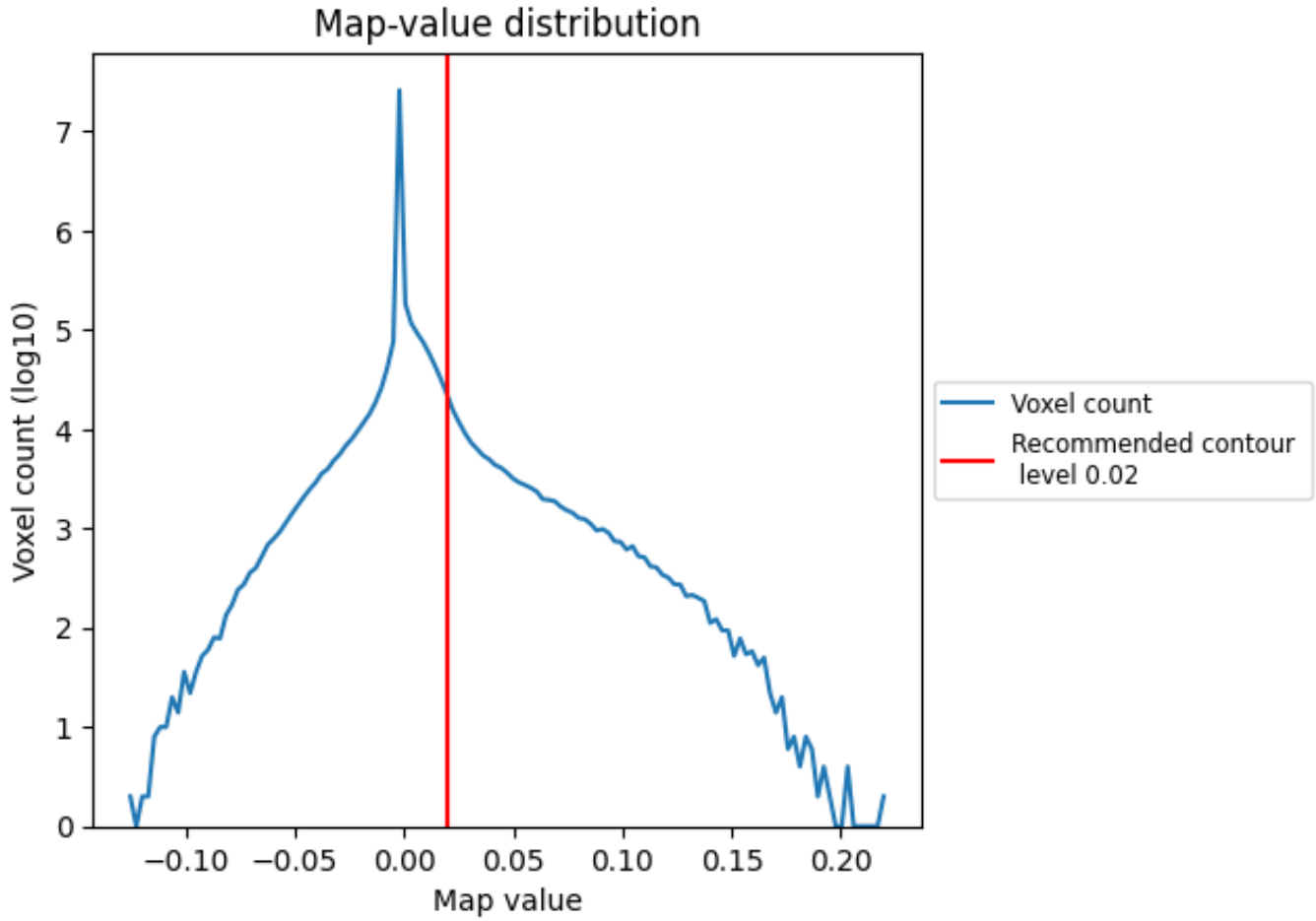
6.5 Mask visualisation (i)

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

7 Map analysis

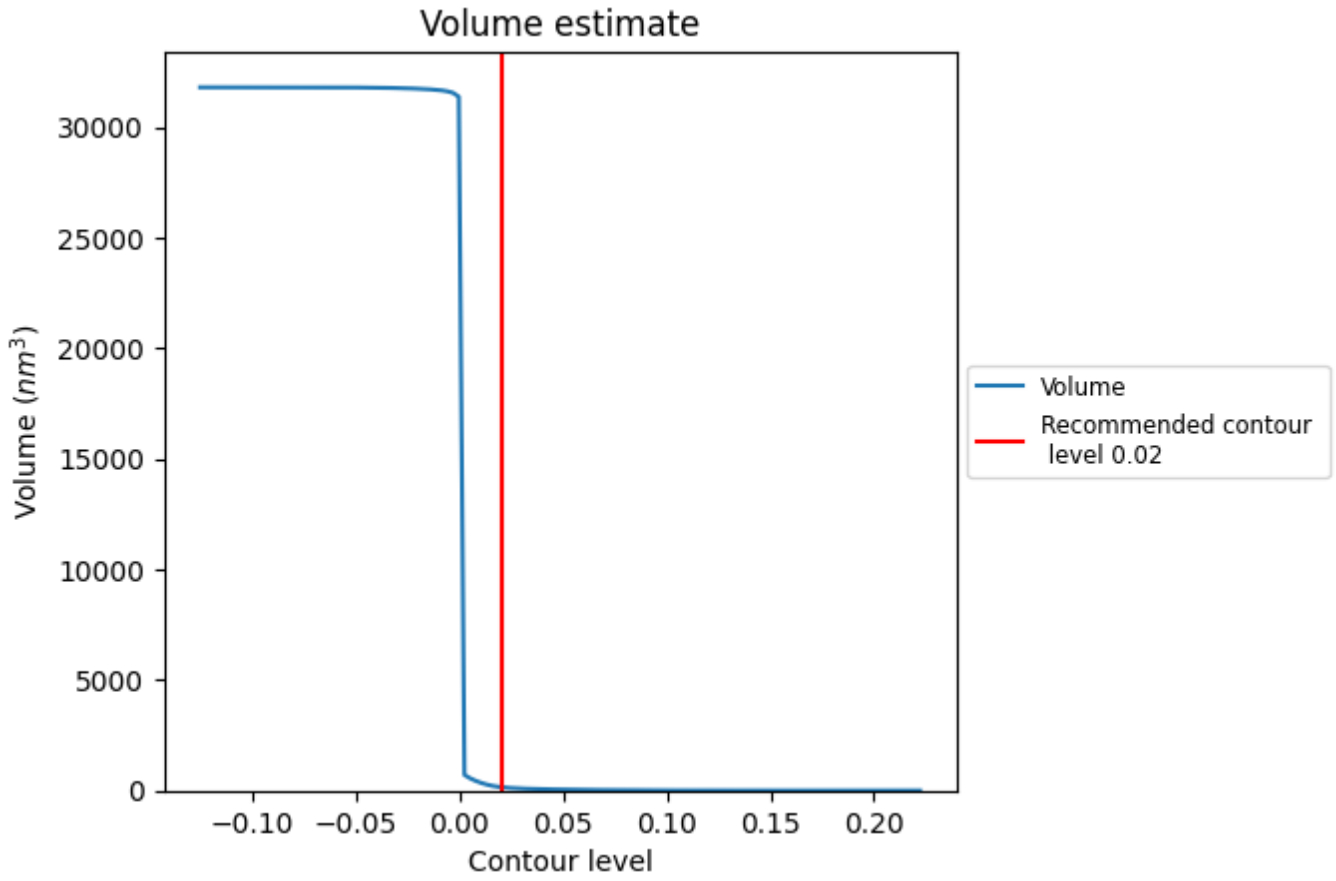
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

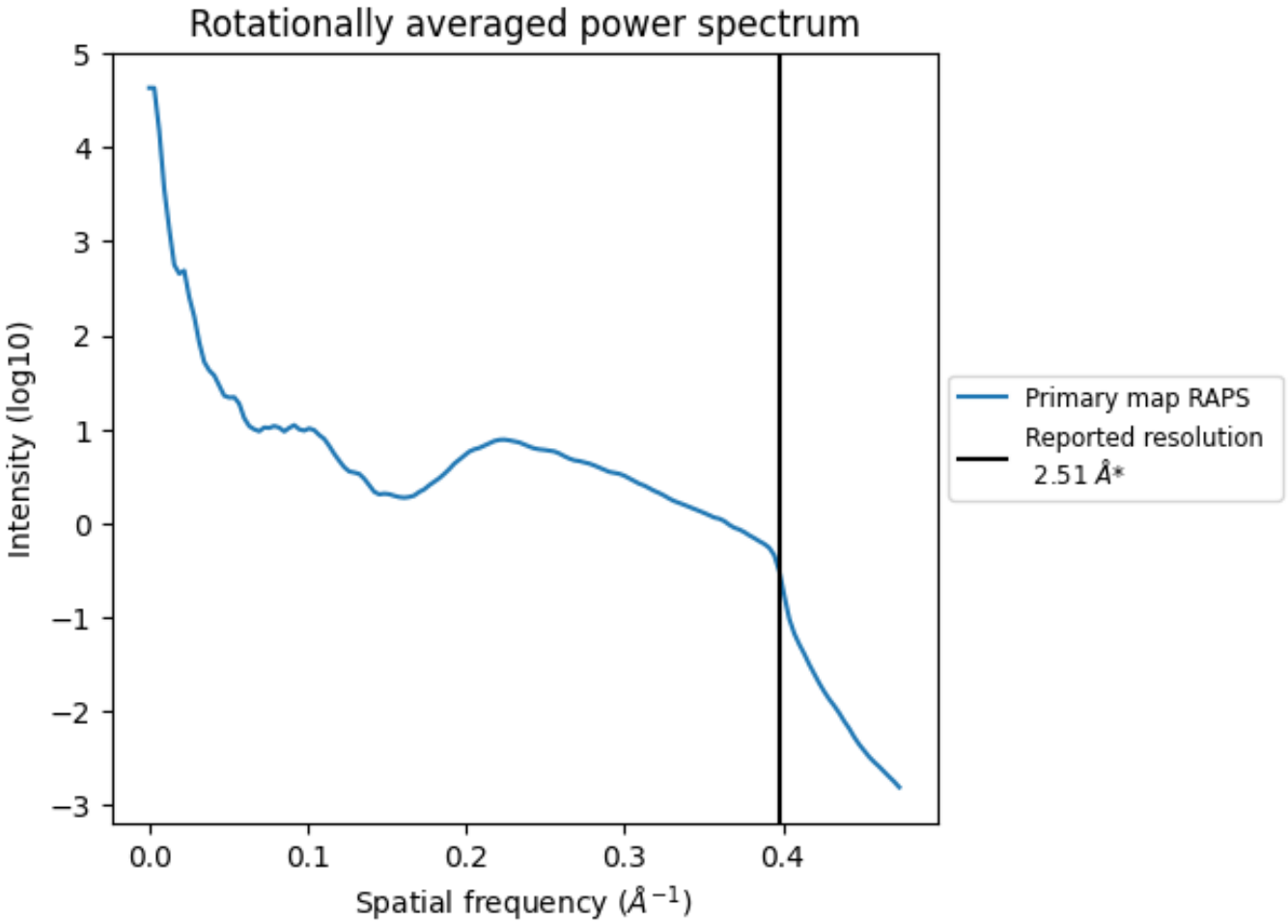
7.2 Volume estimate



The volume at the recommended contour level is 154 nm^3; this corresponds to an approximate mass of 139 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)

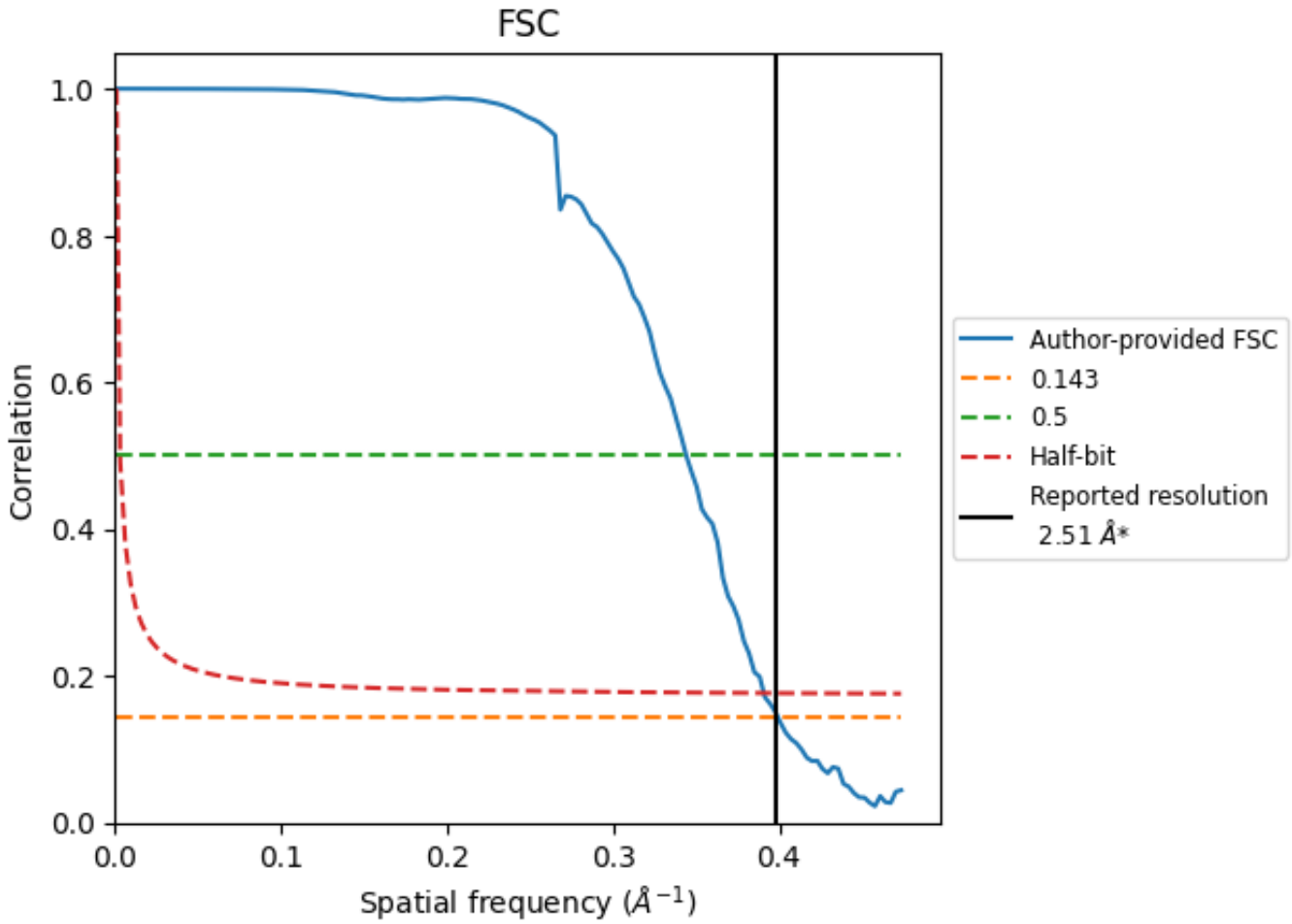


*Reported resolution corresponds to spatial frequency of 0.398 Å^{-1}

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 0.398 Å^{-1}

8.2 Resolution estimates (i)

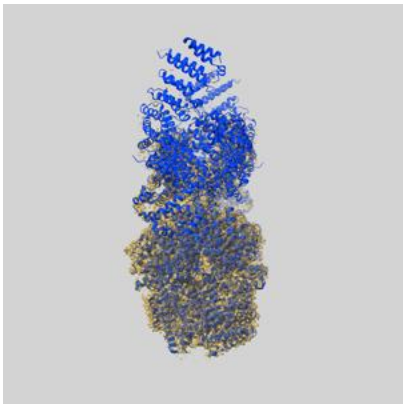
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.51	-	-
Author-provided FSC curve	2.50	2.91	2.56
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

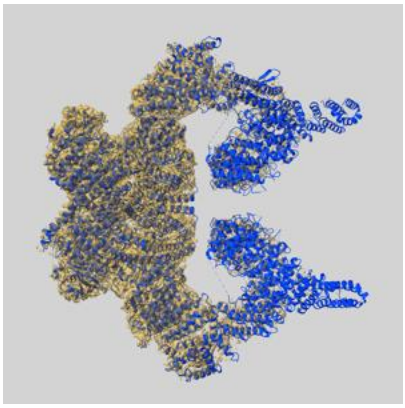
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25140 and PDB model 7SIC. Per-residue inclusion information can be found in section 3 on page 5.

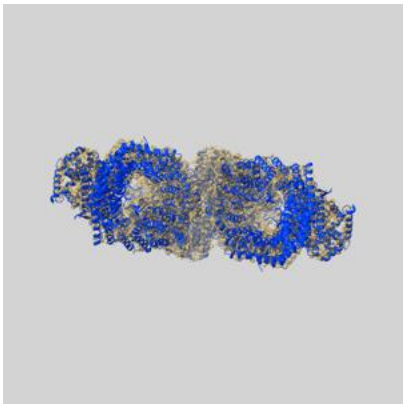
9.1 Map-model overlay



X



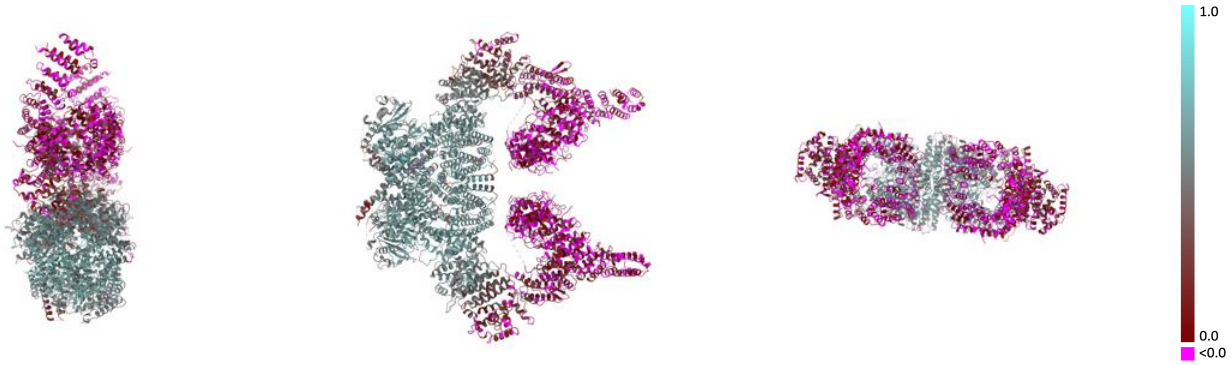
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

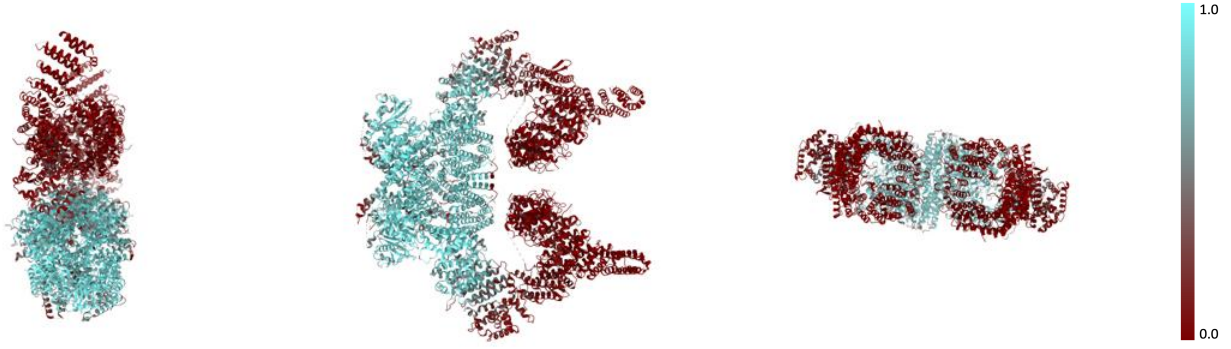
9.2 Q-score mapped to coordinate model



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.

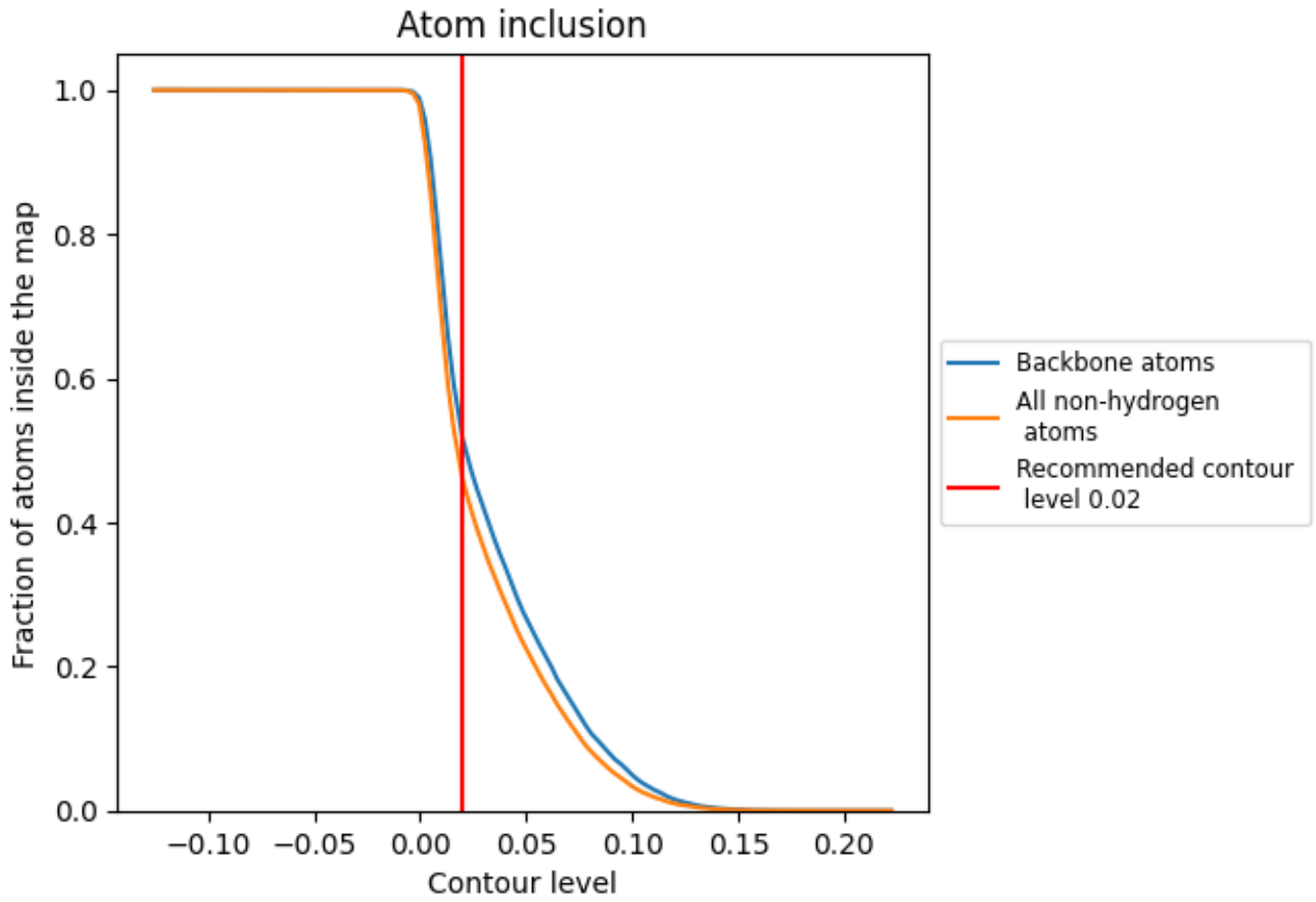
9.3 Atom inclusion mapped to coordinate model



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 52% of all backbone atoms, 46% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4604	0.3400
A	0.4604	0.3400
B	0.4604	0.3400