Full wwPDB EM Validation Report

Aug 29, 2024 – 04:39 PM JST

PDB ID	:	8XVG
EMDB ID	:	EMD-38703
Title	:	Structure of human NuA4/TIP60 complex
Authors	:	Chen, K.; Wang, L.; Yu, Z.; Yu, J.; Ren, Y.; Wang, Q.; Xu, Y.
Deposited on	:	2024-01-15
Resolution	:	9.40 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:

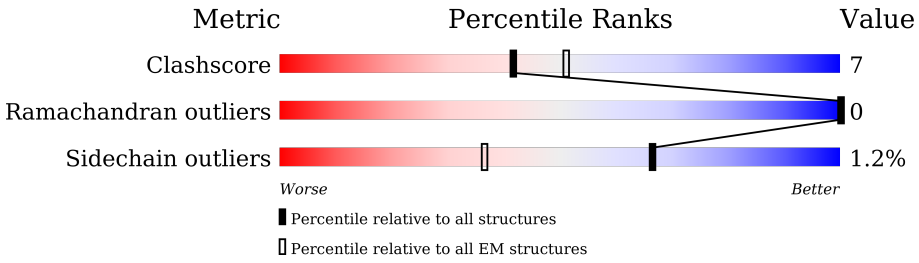
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 9.40 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	L	3830	18% 78% 12% 9%
2	A	456	79% 14% 7%
2	C	456	75% 16% 9%
2	E	456	83% 12% 5%
3	B	463	73% 13% 14%
3	D	463	5% 78% 14% 8%
3	F	463	74% 16% 10%
4	G	467	9% 36% 7% 57%

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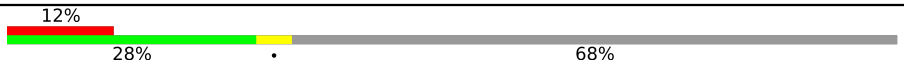
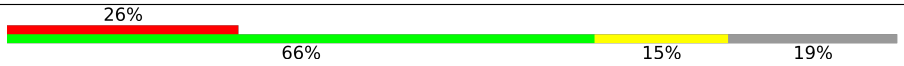
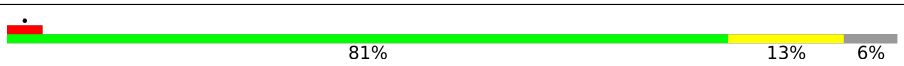
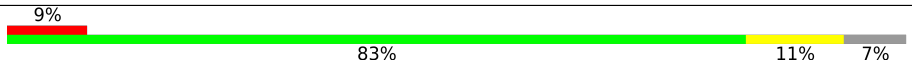
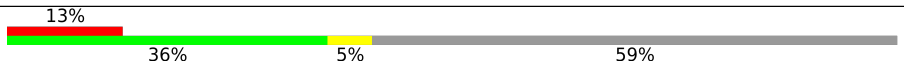
Mol	Chain	Length	Quality of chain
5	H	3123	
6	I	429	
6	J	429	
7	K	375	
8	M	813	
9	N	364	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	ADP	A	501	-	-	X	-
11	ADP	B	501	-	-	X	-
11	ADP	C	501	-	-	X	-
11	ADP	D	501	-	-	X	-
11	ADP	E	501	-	-	X	-
11	ADP	F	501	-	-	X	-
11	ADP	I	501	-	-	X	-
11	ADP	K	401	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 98244 atoms, of which 29886 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Isoform 2 of Transformation/transcription domain-associated protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	L	3485	Total	C	H	N	O	S	2	0
			56537	17940	28534	4845	5023	195		

- Molecule 2 is a protein called RuvB-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	426	Total	C	N	O	S	0	0
			3279	2067	563	633	16		
2	C	416	Total	C	N	O	S	0	0
			3210	2027	552	616	15		
2	E	435	Total	C	N	O	S	0	0
			3344	2106	574	647	17		

- Molecule 3 is a protein called RuvB-like 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	399	Total	C	N	O	S	0	0
			3101	1940	541	605	15		
3	D	427	Total	C	N	O	S	0	0
			3315	2069	584	646	16		
3	F	417	Total	C	N	O	S	0	0
			3242	2025	570	631	16		

- Molecule 4 is a protein called DNA methyltransferase 1-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	201	Total	C	N	O	S	0	0
			1717	1093	316	305	3		

- Molecule 5 is a protein called Isoform 2 of E1A-binding protein p400.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	H	1007	Total	C	H	N	O	S	0	0
			9584	5237	1352	1492	1465	38		

- Molecule 6 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	349	Total	C	N	O	S	0	0
			2715	1716	459	519	21		
6	J	403	Total	C	N	O	S	0	0
			3139	1984	535	597	23		

- Molecule 7 is a protein called ACTB protein (Fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	350	Total	C	N	O	S	0	0
			2733	1736	458	519	20		

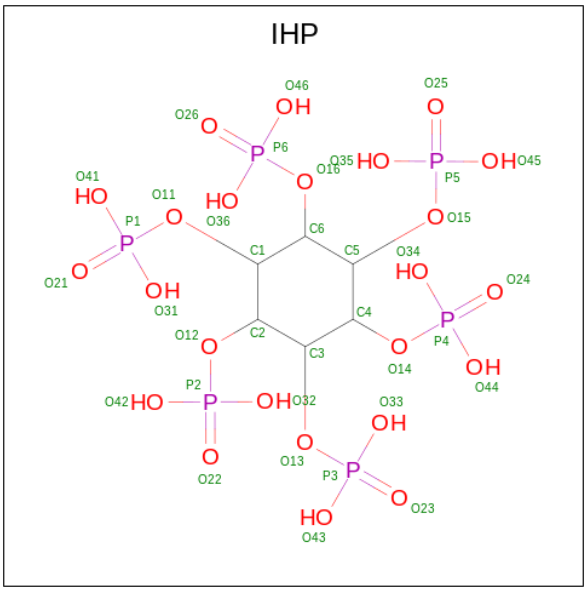
- Molecule 8 is a protein called Isoform 2 of Enhancer of polycomb homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	106	Total	C	N	O	S	0	0
			861	541	166	149	5		

- Molecule 9 is a protein called Vacuolar protein sorting-associated protein 72 homolog.

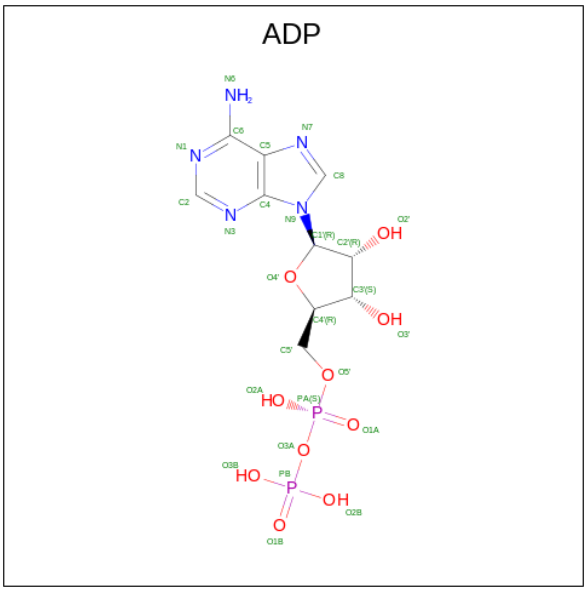
Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	150	Total	C	N	O	S	0	0
			1188	764	213	208	3		

- Molecule 10 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
10	L	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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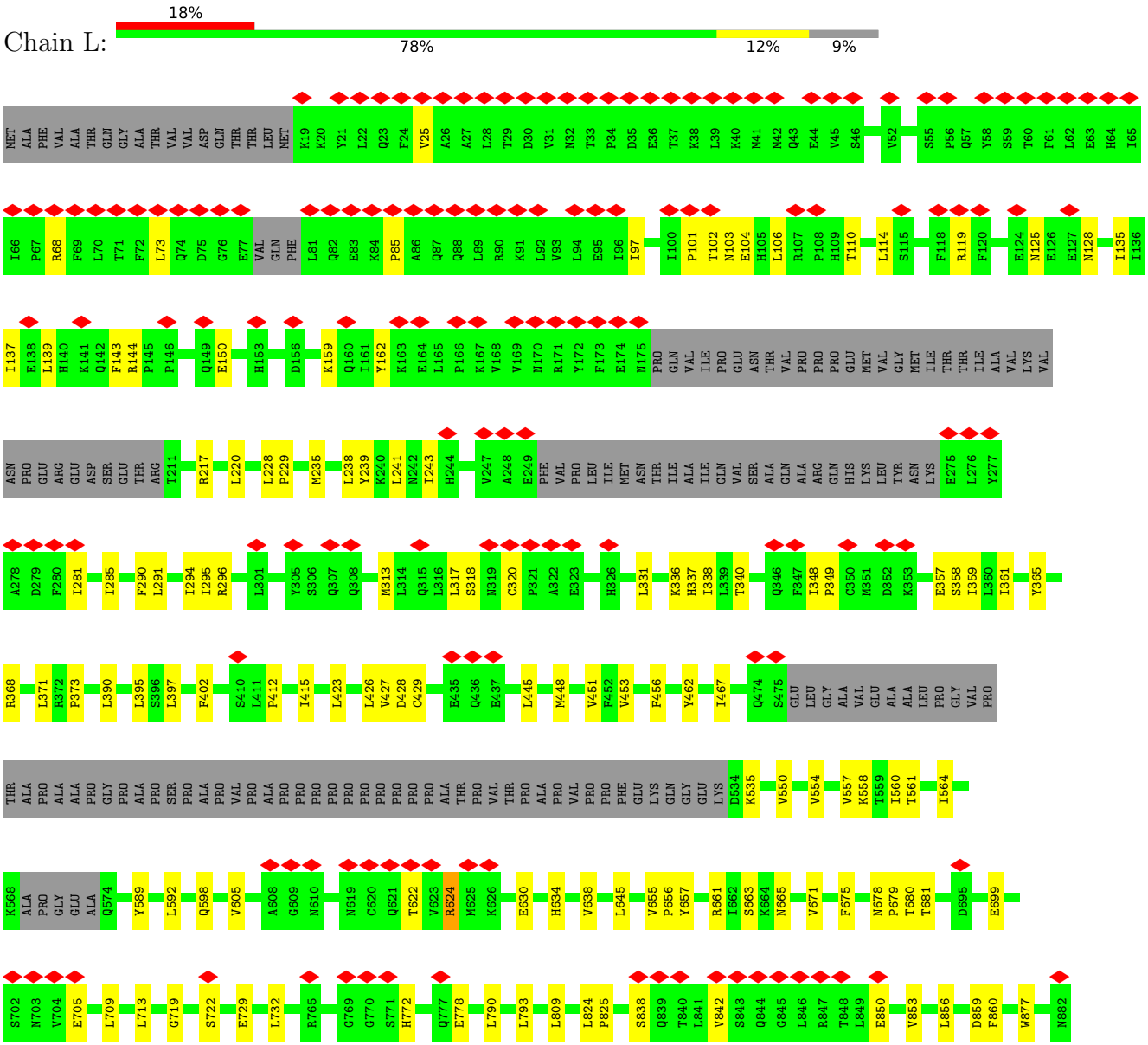
Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	K	1	Total	C	N	O	P	0
			27	10	5	10	2	

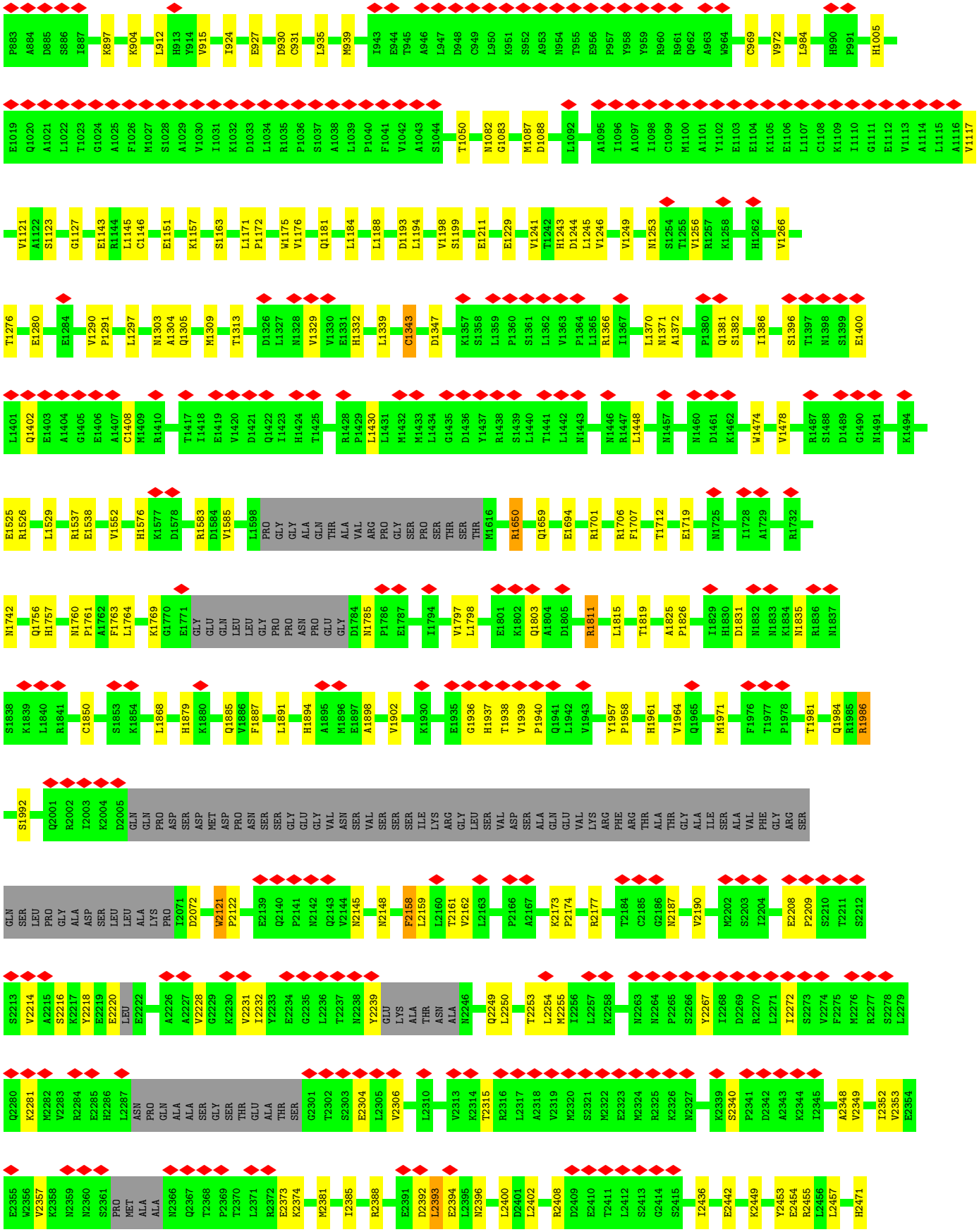
3 Residue-property plots (i)

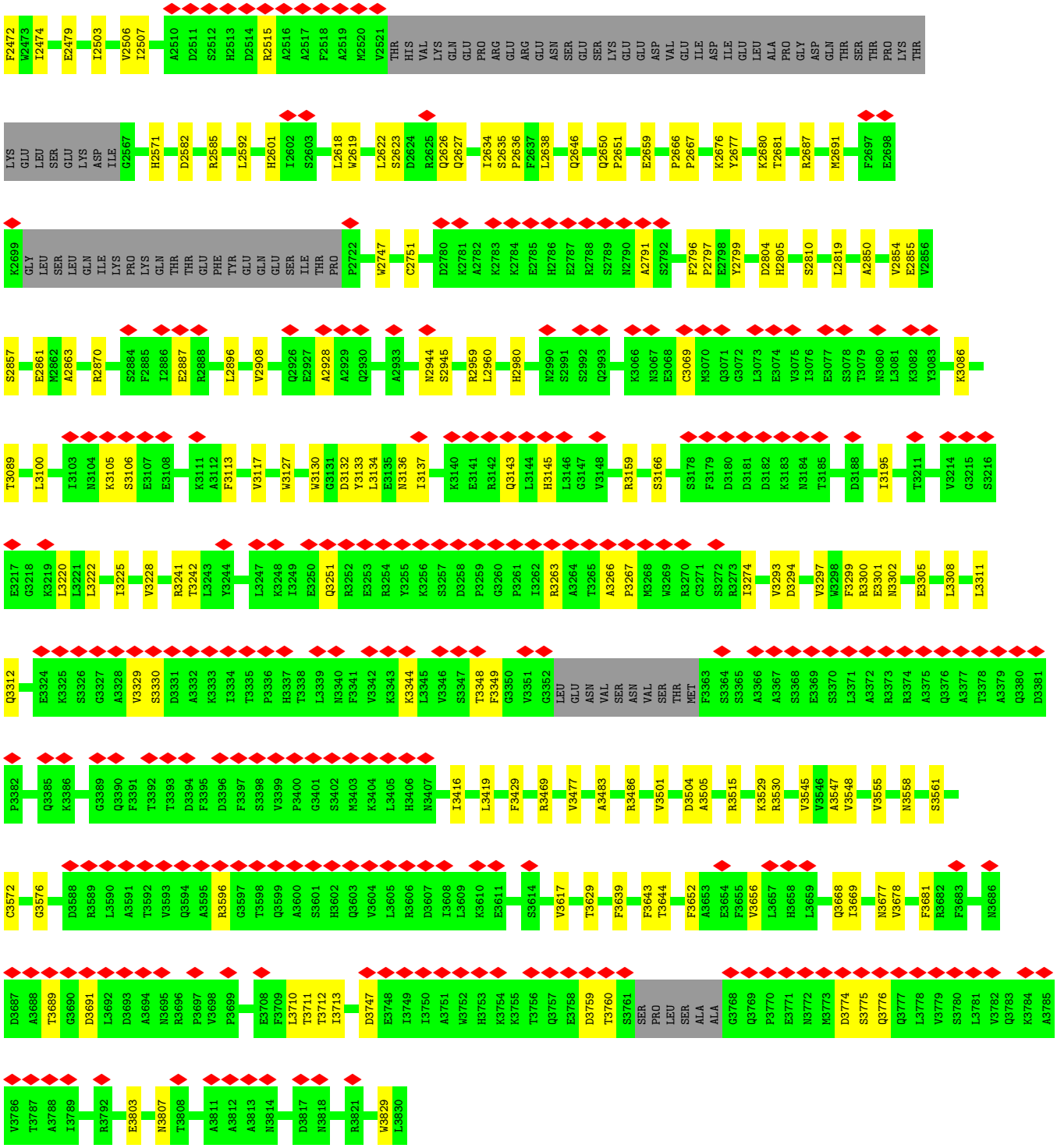
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Isoform 2 of Transformation/transcription domain-associated protein

Chain L:

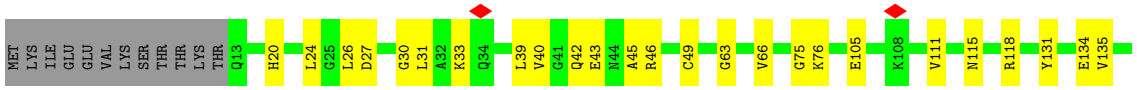


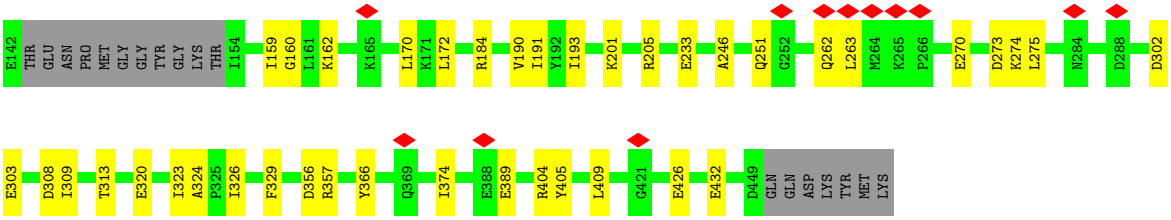

P883 A884 D885 S886 I887 K897 K904 L912 H913 Y914 V915 I924 E927 D930 C931 L935 M939 I943 E944 T945 A946 L947 D948 C949 L950 K951 S952 A953 N954 T955 E956 P957 Y958 Y959 R960 R961 Q962 A963 W964 C969 V972 L984 H990 P991 H1005
E1019 Q1020 A1021 L1022 T1023 G1024 A1025 F1026 M1027 S1028 A1029 V1030 I1031 K1032 D1033 L1034 R1035 P1036 S1037 A1038 L1039 P1040 F1041 V1042 A1043 S1044 T1050 N1082 G1083 M1087 D1088 L1092 A1095 I1096 A1097 I1098 C1099 M1100 A1101 Y1102 E1103 E1104 K1105 E1106 L1107 C1108 K1109 I1110 G1111 E1112 V1113 A1114 L1115 A1116 V1117
V1121 A1122 S1123 G1127 E1143 R1144 L1145 C1146 E1151 K1157 S1163 L1171 P1172 W1175 V1176 Q1181 L1184 L1188 D1193 L1194 V1198 S1199 E1211 E1229 V1241 T1242 H1243 D1244 L1245 V1246 V1249 N1253 S1254 T1255 V1256 R1257 K1258 H1262 V1266
T1276 E1280 E1284 V1290 P1291 L1297 N1303 A1304 Q1305 M1309 T1313 D1326 L1327 N1328 V1329 V1330 E1331 H1332 L1339 C1343 D1347 K1357 S1358 L1359 P1360 S1361 L1362 V1363 P1364 L1365 R1366 I1367 L1370 N1371 A1372 P1380 Q1381 S1382 I1386 S1396 T1397 N1398 S1399 E1400
L1401 Q1402 E1403 A1404 G1405 E1406 A1407 C1408 M1409 R1410 T1417 I1418 E1419 V1420 D1421 Q1422 I1423 H1424 T1425 R1428 P1429 L1430 L1431 M1432 M1433 L1434 G1435 D1436 Y1437 R1438 S1439 L1440 T1441 L1442 N1443 N1446 R1447 L1448 N1457 N1460 D1461 K1462 W1474 V1478 R1487 S1488 D1489 G1490 N1491 K1494
E1525 R1526 L1529 R1537 E1538 V1552 H1576 K1577 D1578 R1583 D1584 V1585 L1598 PRO GLY GLY ALA GLN THR ALA VAL ARG PRO GLY SER PRO SER THR SER THR M1616 R1650 Q1659 E1694 R1701 R1706 F1707 T1712 E1719 N1725 I1728 A1729 R1732
N1742 Q1756 H1757 N1760 P1761 A1762 F1763 L1764 K1769 G1770 E1771 GLY GLU GLN LEU LEU GLY PRO PRO ASN PRO GLU GLY D1784 N1785 P1786 E1787 T1794 V1797 L1798 E1801 K1802 Q1803 A1804 D1805 R1811 L1815 T1819 A1825 P1826 I1829 H1830 D1831 N1832 N1833 K1834 N1835 R1836 N1837
S1838 K1839 L1840 R1841 C1850 S1853 K1854 L1868 H1879 K1880 Q1885 Y1886 F1887 L1891 H1894 A1895 M1896 E1897 A1898 V1902 K1930 E1935 G1936 H1937 T1938 V1939 P1940 Q1941 L1942 V1943 Y1957 P1958 H1961 V1964 Q1965 M1971 F1976 T1977 P1978 T1981 Q1984 R1985 R1986
S1992 Q2001 R2002 I2003 K2004 D2005 GLN GLN PRO ASP SER ASP MET ASP PRO ASN SER SER GLY GLU GLY VAL ASN SER VAL SER SER SER ILE LYS ARG GLY LEU SER VAL ASP SER ALA GLN GLU VAL LYS ARG PHE ARG THR ALA THR GLY ALA ILE SER ALA VAL PHE GLY ARG SER
GLN SER LEU PRO GLY ALA ASP SER LEU LEU ALA LYS PRO I2071 D2072 W2121 P2122 E2139 Q2140 P2141 N2142 Q2143 V2144 N2145 N2148 F2158 L2159 L2160 T2161 V2162 L2163 P2166 A2167 K2173 P2174 R2177 T2184 C2185 G2186 N2187 V2190 M2202 S2203 I2204 E2208 P2209 S2210 T2211 S2212
S2213 V2214 A2215 S2216 K2217 Y2218 E2219 E2220 LEU E2222 A2226 A2227 V2228 G2229 K2230 V2231 I2232 Y2233 E2234 G2235 L2236 T2237 N2238 Y2239 GLU LYS ALA THR ASN ALA N2246 Q2249 L2250 T2253 L2254 M2255 I2256 L2257 K2258 N2263 N2264 P2265 S2266 Y2267 I2268 D2269 R2270 L2271 I2272 S2273 V2274 F2275 M2276 R2277 S2278 L2279
Q2280 K2281 M2282 V2283 R2284 E2285 H2286 L2287 ASN PRO GLN ALA ALA SER GLY SER THR GLU ALA THR SER G2301 T2302 S2303 E2304 L2305 V2306 L2310 V2313 K2314 T2315 R2316 L2317 A2318 V2319 M2320 S2321 M2322 E2323 M2324 R2325 K2326 N2327 K2339 S2340 P2341 D2342 A2343 K2344 I2345 A2348 V2349 I2352 V2353 E2354
E2355 W2356 V2357 K2358 N2359 N2360 S2361 PRO MET ALA ALA N2366 Q2367 T2368 P2369 T2370 L2371 R2372 E2373 K2374 M2381 I2385 R2388 E2391 D2392 L2393 E2394 L2395 N2396 L2400 D2401 L2402 R2408 D2409 E2410 T2411 L2412 S2413 G2414 S2415 I2436 E2442 K2449 Y2453 E2454 R2455 L2456 L2457 H2471



• Molecule 2: RuvB-like 1

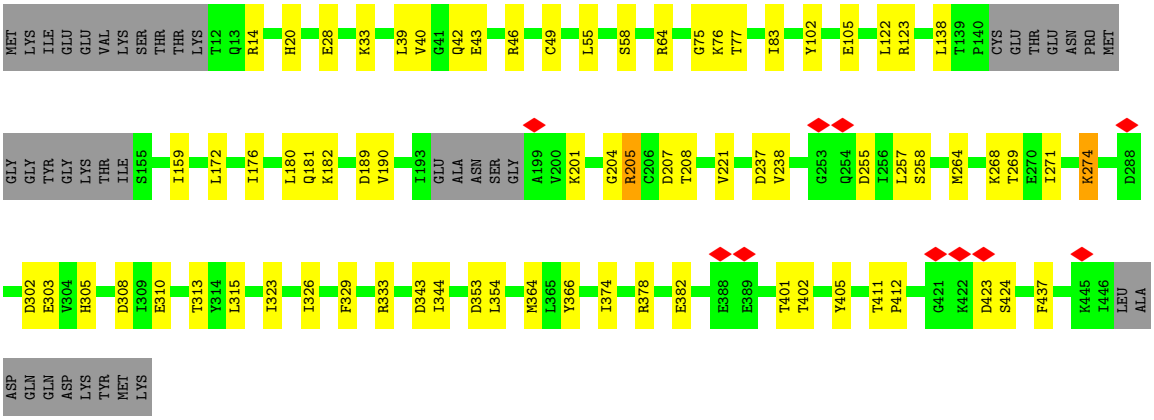
Chain A:





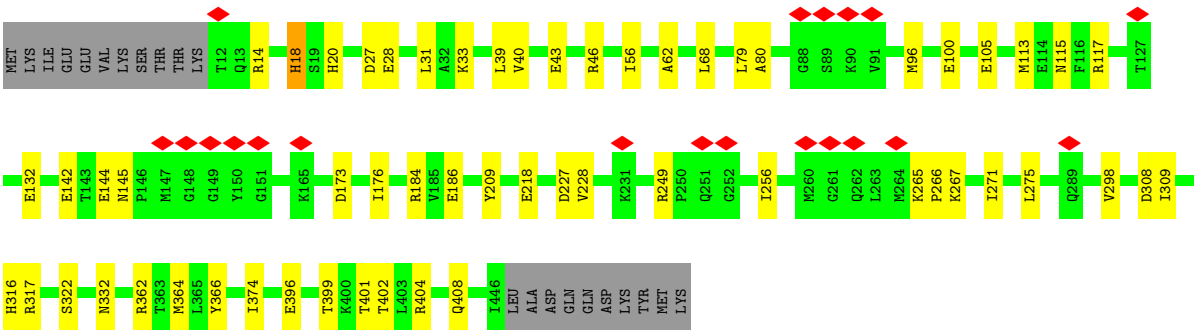
• Molecule 2: RuvB-like 1

Chain C:



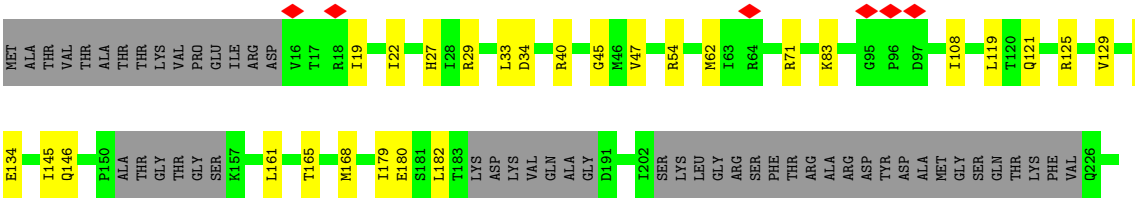
• Molecule 2: RuvB-like 1

Chain E:

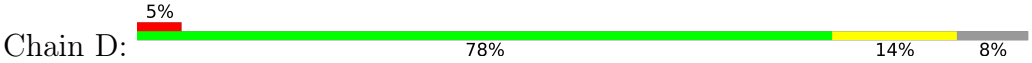


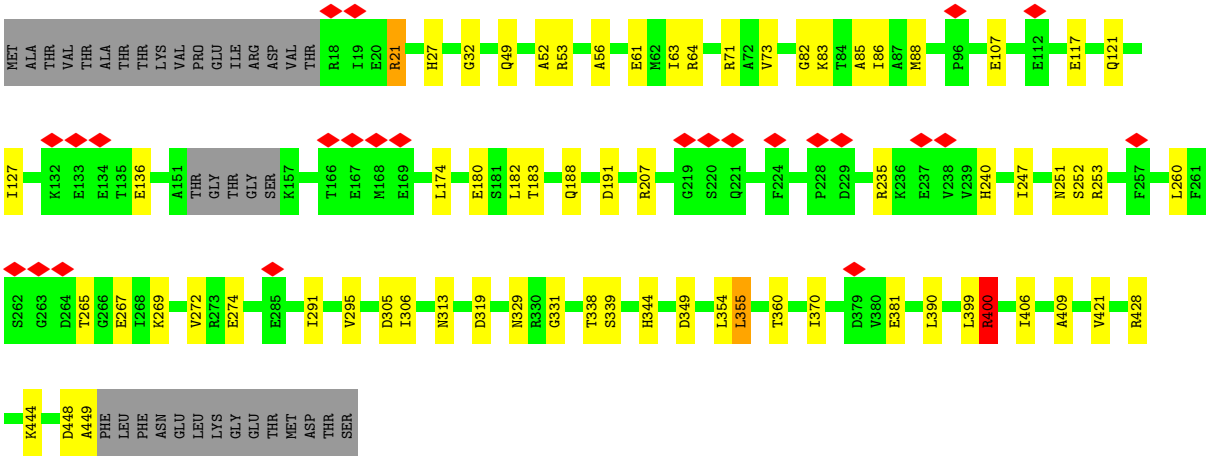
• Molecule 3: RuvB-like 2

Chain B:

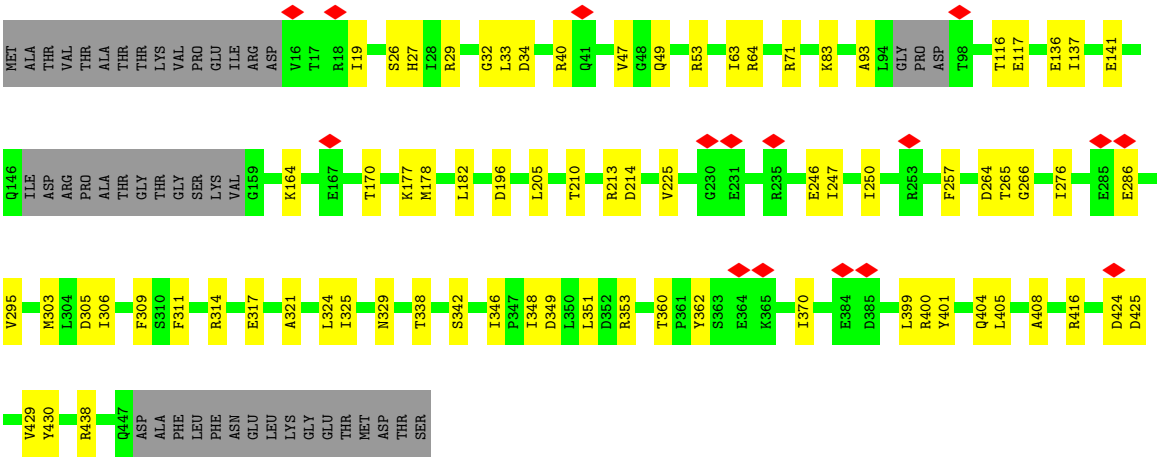


• Molecule 3: RuvB-like 2

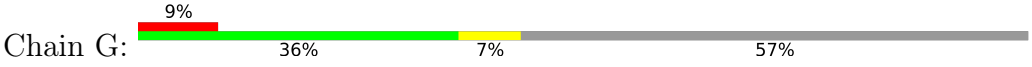


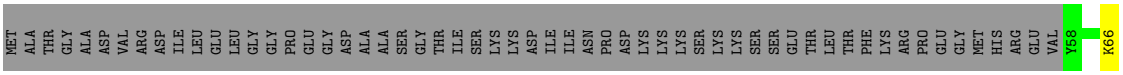


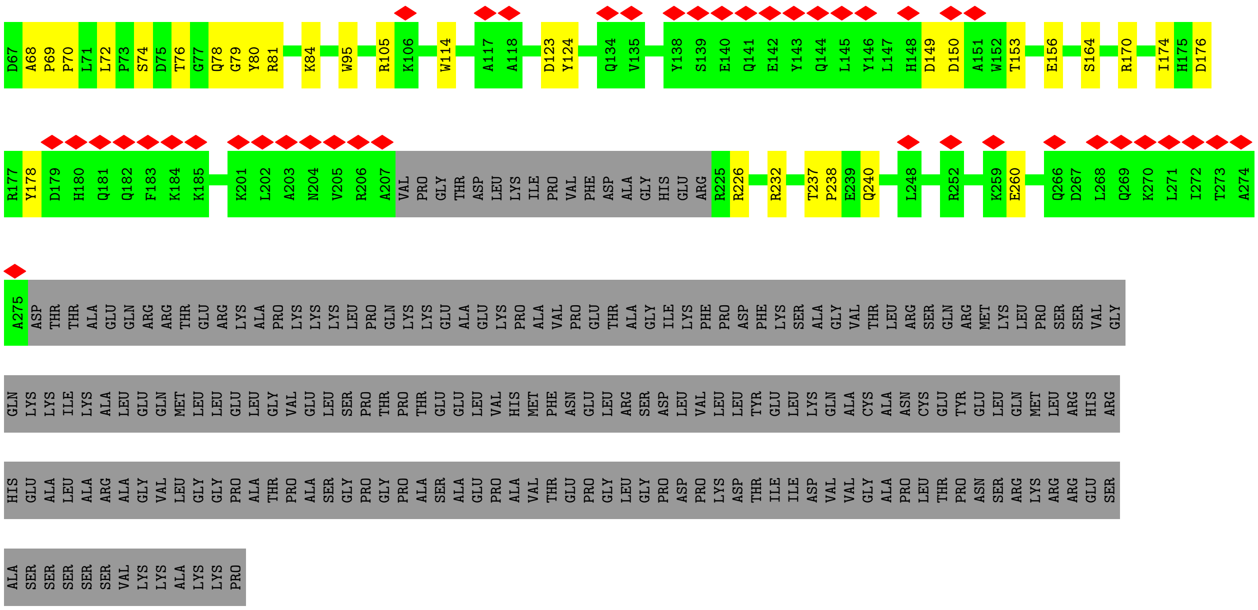
• Molecule 3: RuvB-like 2



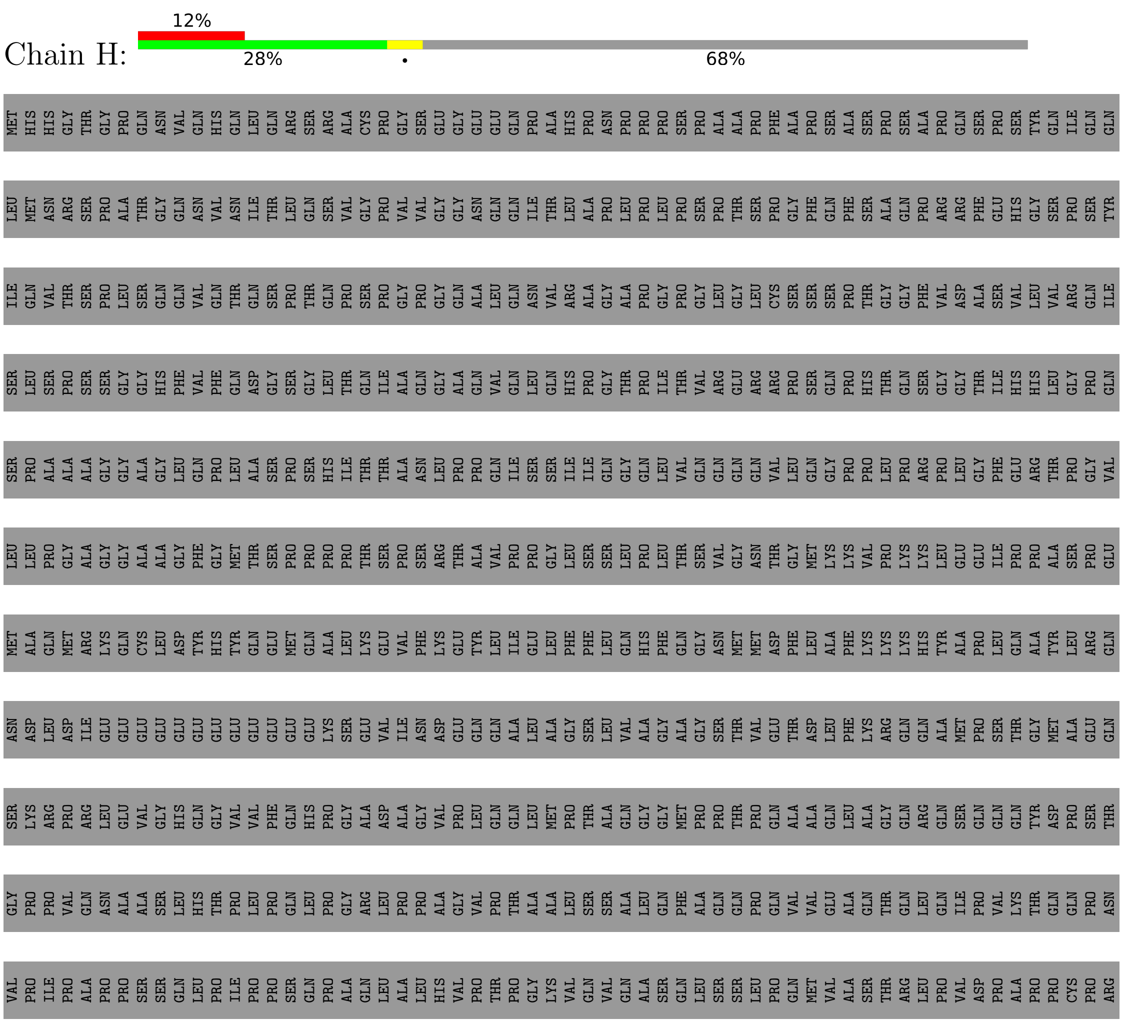
• Molecule 4: DNA methyltransferase 1-associated protein 1

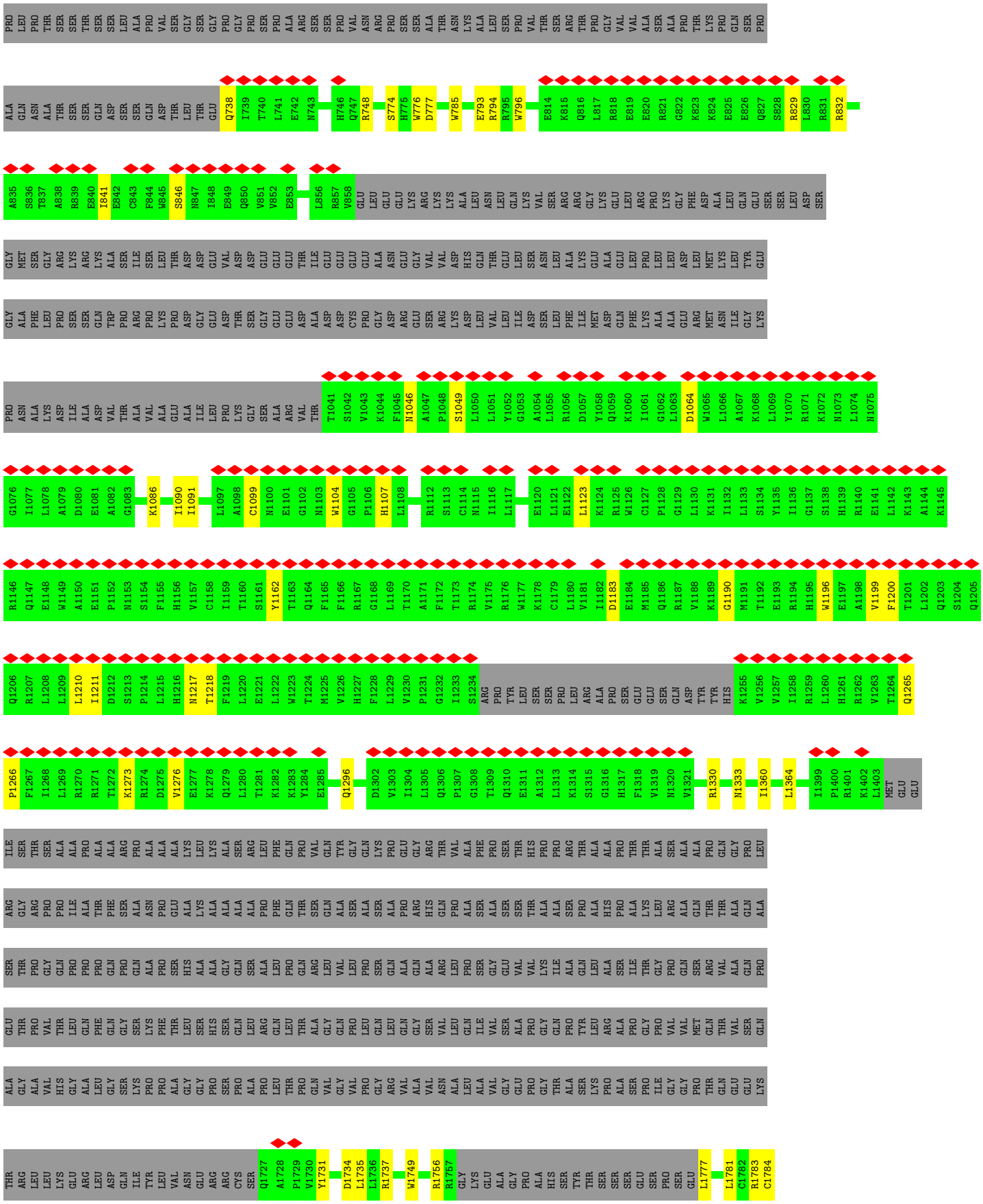


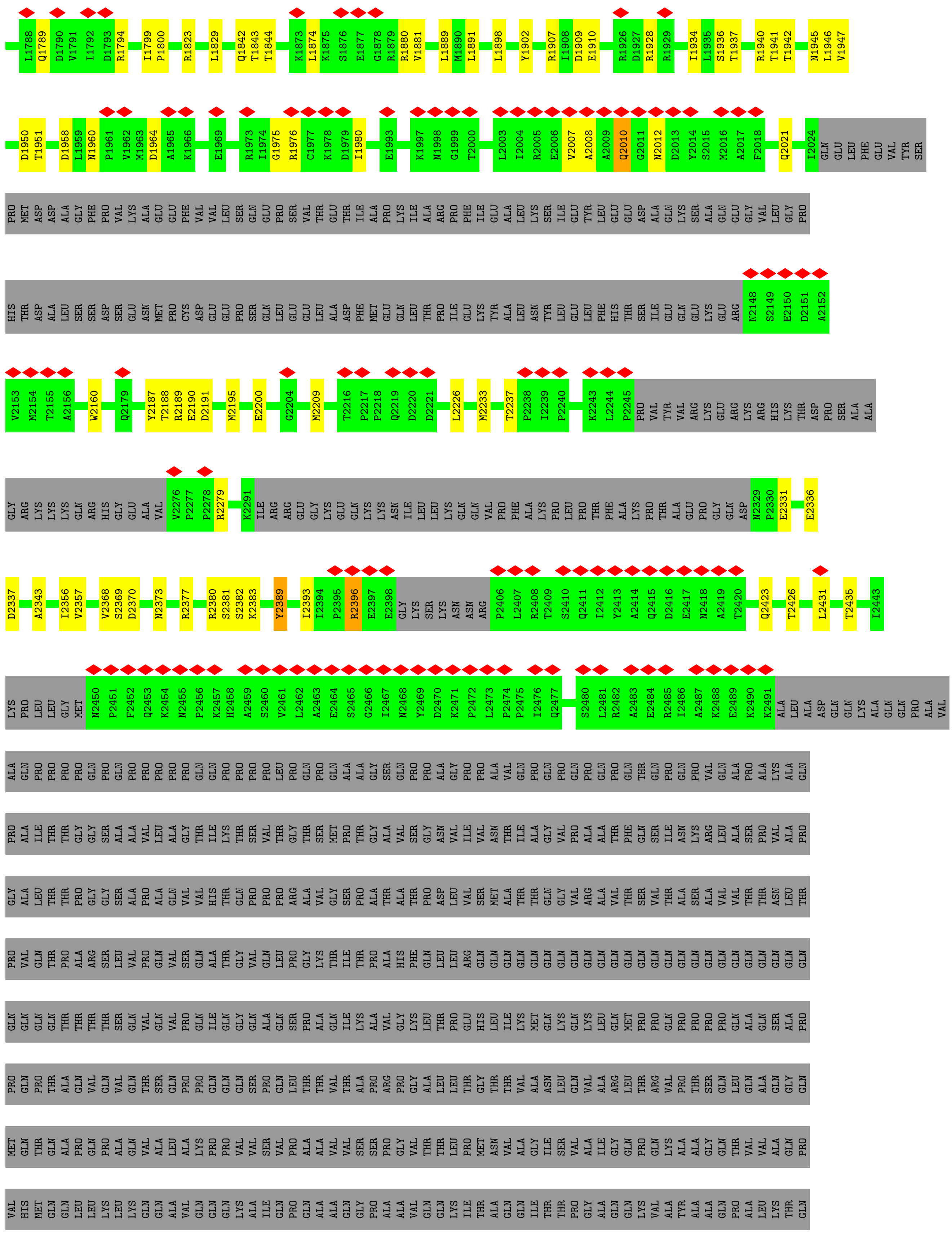


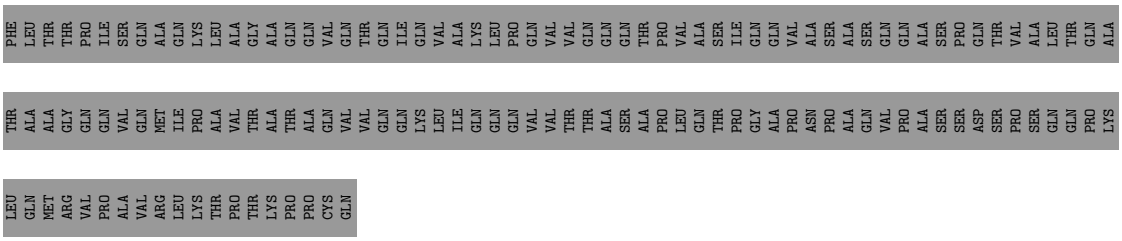


- Molecule 5: Isoform 2 of E1A-binding protein p400



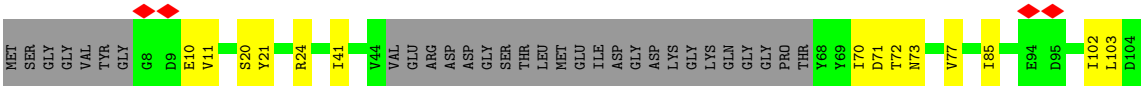

PRO LEU PRO THR SER SER THR SER SER LEU ALA PRO VAL SER GLY SER GLY PRO GLY PRO SER PRO ALA ARG SER SER PRO VAL ASN ARG PRO SER SER ALA THR ASN LYS ALA LEU SER PRO VAL THR SER ARG THR PRO GLY VAL VAL ALA SER ALA PRO THR LYS PRO GLN SER PRO
ALA GLN ASN ALA THR SER SER GLN ASP SER SER GLN ASP THR LEU THR GLU Q738 I739 T740 L741 E742 W743 H746 Q747 R748 S774 H775 W776 D777 W785 E793 R794 R795 W796 E814 K815 Q816 L817 R818 E819 E820 R821 G822 K823 K824 E825 E826 Q827 S828 R829 L830 R831 R832
A835 S836 T837 A838 R839 E840 I841 E842 C843 F844 W845 S846 N847 I848 E849 Q850 V851 V852 E853 L856 R857 V858 GLU LEU GLU GLU LYS ARG LYS LYS ALA LEU ASN LEU GLN LYS VAL SER ARG ARG GLY LYS GLU LEU GLU PHE ASP ALA LEU GLN GLU SER SER LEU ASP SER
GLY MET SER GLY ARG LYS ARG LYS ALA SER ILE SER LEU THR ASP ASP GLU VAL ASP ASP GLU GLU GLU THR ILE GLU GLU GLU ALA ASN GLU GLY VAL VAL ASP HIS GLN THR GLU LEU SER ASN LEU ALA LYS GLU ALA GLU LEU PRO LEU LEU ASP LEU MET LYS LEU TYR GLU
GLY ALA PHE LEU PRO SER SER GLN TRP PRO ARG PRO LYS PRO ASP GLY GLU ASP THR SER GLY GLU GLU ASP ALA ASP ASP CYS PRO GLY ASP ARG GLU SER ARG LYS ASP LEU VAL LEU ILE ASP SER LEU PHE ILE MET ASP GLN PHE LYS ALA ALA GLU ARG MET ASN ILE GLY LYS
PRO ASN ALA LYS ASP ILE ALA ASP VAL THR ALA ALA VAL ALA GLU ALA ILE LEU PRO LYS GLY SER ALA ARG VAL T1041 S1042 V1043 K1044 F1045 N1046 A1047 P1048 S1049 L1050 L1051 Y1052 G1053 A1054 L1055 R1056 D1057 Y1058 Q1059 K1060 I1061 G1062 L1063 D1064 W1065 L1066 A1067 K1068 L1069 Y1070 R1071 K1072 N1073 L1074 N1075
G1076 I1077 L1078 A1079 D1080 E1081 A1082 G1083 K1086 I1090 I1091 L1097 A1098 C1099 N1100 E1101 G1102 N1103 W1104 G1105 P1106 H1107 L1108 R1112 S1113 C1114 N1115 I1116 L1117 E1120 L1121 E1122 L1123 K1124 R1125 W1126 C1127 P1128 G1129 L1130 K1131 I1132 L1133 S1134 Y1135 I1136 G1137 S1138 H1139 R1140 E1141 L1142 K1143 A1144 K1145
R1146 Q1147 E1148 W1149 A1150 E1151 P1152 N1153 S1154 F1155 H1156 V1157 C1158 I1159 T1160 S1161 Y1162 T1163 Q1164 F1165 F1166 R1167 G1168 L1169 T1170 A1171 F1172 T1173 R1174 V1175 R1176 W1177 K1178 C1179 L1180 V1181 I1182 D1183 E1184 M1185 Q1186 R1187 V1188 K1189 G1190 M1191 T1192 E1193 R1194 H1195 W1196 E1197 A1198 V1199 F1200 T1201 L1202 Q1203 S1204 Q1205
Q1206 R1207 L1208 L1209 L1210 I1211 D1212 S1213 P1214 L1215 H1216 N1217 T1218 F1219 L1220 E1221 L1222 W1223 T1224 M1225 V1226 H1227 F1228 L1229 V1230 P1231 G1232 I1233 S1234 ARG PRO TYR LEU SER SER PRO LEU ARG ALA PRO SER GLU GLU SER GLN ASP TYR TYR HIS K1255 V1256 V1257 I1258 R1259 L1260 H1261 R1262 V1263 T1264 Q1265
P1266 F1267 I1268 L1269 R1270 R1271 T1272 K1273 R1274 D1275 V1276 E1277 K1278 Q1279 L1280 T1281 K1282 K1283 Y1284 E1285 Q1296 D1302 V1303 I1304 L1305 Q1306 P1307 G1308 T1309 Q1310 E1311 A1312 L1313 K1314 S1315 G1316 H1317 F1318 V1319 N1320 V1321 R1330 N1333 I1360 L1364 I1399 P1400 R1401 K1402 L1403 MET GLU GLU
ILE SER THR SER ALA ALA PRO ALA ALA ARG PRO ALA ALA ALA LYS LEU LYS ALA SER ARG LEU PHE GLN PRO VAL GLN TYR GLY GLN LYS PRO GLU GLY ARG THR VAL ALA PHE PRO SER THR HIS PRO PRO ARG THR ALA ALA PRO THR THR ALA SER ALA ALA PRO GLN GLY PRO LEU
ARG GLY ARG PRO PRO ILE ALA THR PHE SER ALA ASN PRO GLU ALA LYS ALA ALA ALA PRO PHE GLN THR SER GLN ALA SER ALA SER ALA PRO ARG HIS GLN PRO ALA SER SER THR ALA ALA SER PRO ALA HIS PRO ALA LYS LEU ARG ALA GLN THR THR ALA GLN
SER THR PRO GLY GLN PRO PRO PRO GLN PRO GLN ALA PRO SER HIS ALA ALA ALA GLY GLN SER ALA LEU PRO PRO GLN ARG LEU VAL LEU PRO PRO SER GLN ALA GLN LEU PRO SER GLY GLU VAL VAL LYS ILE ALA GLN LEU GLN LEU ALA SER ILE THR GLY PRO GLN SER ARG VAL ALA GLN PRO
GLU THR PRO VAL THR LEU GLN GLY SER LYS PHE THR LEU SER HIS SER GLN LEU ARG GLN LEU THR ALA GLY GLN LEU GLN GLY SER VAL LEU GLN ILE VAL SER ALA PRO GLY GLN PRO TYR LEU ARG ALA PRO GLY PRO VAL VAL MET GLN THR VAL SER GLN
ALA GLY ALA VAL HIS GLY ALA LEU GLY SER LYS PRO PRO ALA ALA GLY GLY PRO SER PRO ALA ALA PRO LEU THR PRO GLN VAL GLY VAL PRO GLY ARG VAL ALA VAL ASN ALA LEU ALA VAL GLY GLU PRO GLY GLN THR ALA SER LYS PRO ALA SER PRO ILE GLY GLY GLY PRO THR GLN GLU GLU LYS
THR ARG LEU LEU LYS GLU ARG ASP GLN ILE TYR LEU VAL ASN GLU ARG ARG CYS SER Q1727 A1728 P1729 V1730 Y1731 D1734 L1735 L1736 R1737 W1749 R1756 R1757 GLY LYS GLU ALA GLY PRO ALA HIS SER TYR THR SER SER SER GLU SER PRO SER GLU L1777 L1781 C1782 R1783 C1784

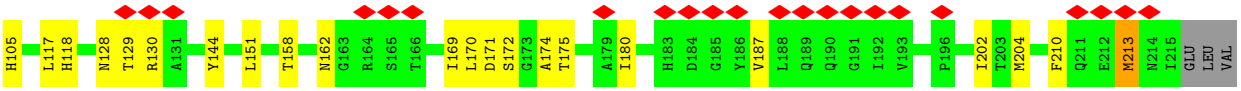

L1788 Q1789 D1790 V1791 I1792 D1793 R1794 I1799 P1800 R1823 L1829 Q1842 T1843 T1844 K1873 L1874 K1875 S1876 E1877 G1878 R1879 R1880 V1881 L1889 M1890 L1891 L1898 Y1902 R1907 I1908 D1909 E1910 R1926 D1927 R1928 R1929 I1934 L1935 S1936 T1937 R1940 T1941 T1942 N1945 L1946 V1947
D1950 T1951 D1958 L1959 N1960 P1961 V1962 M1963 D1964 A1965 K1966 E1969 R1973 I1974 G1975 R1976 C1977 K1978 D1979 I1980 E1993 K1997 N1998 G1999 T2000 L2003 I2004 R2005 E2006 V2007 A2008 A2009 Q2010 G2011 N2012 D2013 Y2014 S2015 M2016 A2017 F2018 Q2021 I2024 GLN GLU LEU PHE GLU VAL TYR SER
PRO MET ASP ASP ALA GLY PHE PRO VAL LYS ALA GLU GLU PHE VAL VAL LEU SER GLN GLU PRO SER VAL THR GLU THR ILE ALA PRO LYS ILE ALA ARG PRO PHE ILE GLU ALA LEU LYS SER ILE GLU TYR LEU GLU GLU ASP ALA GLN LYS SER ALA GLN GLU GLY VAL LEU GLY PRO
HIS THR ASP ALA LEU SER SER ASP SER GLU ASN MET PRO CYS ASP GLU GLU PRO SER GLN LEU GLU GLU LEU ALA ASP PHE MET GLU GLN LEU THR PRO ILE GLU LYS TYR ALA LEU ASN TYR LEU GLU LEU PHE HIS THR SER ILE GLU GLN GLU LYS GLU ARG N2148 S2149 E2150 D2151 A2152
V2153 M2154 T2155 A2156 W2160 Q2179 Y2187 T2188 R2189 E2190 D2191 M2195 E2200 G2204 M2209 T2216 P2217 P2218 Q2219 D2220 D2221 L2226 M2233 T2237 P2238 I2239 P2240 K2243 L2244 P2245 PRO VAL TYR VAL ARG LYS GLU ARG LYS ARG HIS LYS THR ASP PRO SER ALA ALA
GLY ARG LYS LYS GLN ARG HIS GLY GLU ALA VAL V2276 P2277 P2278 R2279 K2291 ILE ARG ARG GLU GLY LYS GLU GLN LYS LYS ASN ILE LEU LEU LYS GLN GLN VAL PRO PHE ALA LYS PRO LEU PRO THR PHE ALA LYS PRO THR ALA GLU PRO GLY GLN ASP N2329 P2330 E2331 E2336
D2337 A2343 I2356 V2357 V2368 S2369 D2370 N2373 R2377 R2380 S2381 S2382 K2383 Y2389 I2393 I2394 P2395 R2396 E2397 E2398 GLY LYS SER LYS ASN ASN ARG P2406 L2407 R2408 T2409 S2410 Q2411 I2412 Y2413 A2414 Q2415 D2416 E2417 N2418 A2419 T2420 Q2423 T2426 L2431 T2435 I2443
LYS PRO LEU LEU GLY MET N2450 P2451 F2452 Q2453 K2454 N2455 P2456 K2457 H2458 A2459 S2460 V2461 L2462 A2463 E2464 S2465 G2466 I2467 N2468 Y2469 D2470 K2471 P2472 L2473 P2474 P2475 I2476 Q2477 S2480 L2481 R2482 A2483 E2484 R2485 I2486 A2487 K2488 E2489 K2490 K2491 ALA LEU ALA ASP GLN GLN LYS ALA GLN GLN PRO ALA VAL
ALA GLN PRO PRO PRO GLN PRO GLN PRO PRO PRO PRO GLN GLN PRO PRO PRO LEU PRO GLN PRO GLN ALA ALA GLY SER GLN PRO PRO ALA GLY PRO PRO ALA VAL GLN PRO GLN PRO GLN PRO GLN PRO GLN THR GLN PRO GLN PRO VAL GLN ALA PRO ALA LYS ALA GLN
PRO ALA ILE THR THR GLY GLY SER ALA ALA VAL LEU ALA GLY THR ILE LYS THR SER VAL THR GLY THR SER MET PRO THR GLY ALA VAL SER GLY ASN VAL ILE VAL ASN THR ILE ALA GLY VAL PRO ALA ALA THR PHE GLN SER ILE ASN LYS ARG LEU ALA SER PRO VAL ALA PRO
GLY ALA LEU THR THR PRO GLY GLY SER ALA PRO ALA GLN VAL VAL HIS THR GLN PRO PRO PRO ARG ALA VAL GLY SER PRO ALA THR ALA THR PRO ASP LEU VAL SER MET ALA THR THR GLN GLY VAL ARG ALA VAL THR SER VAL THR ALA SER ALA VAL VAL THR THR ASN LEU THR
PRO VAL GLN THR PRO ALA ARG SER LEU VAL PRO GLN VAL SER GLN ALA THR GLY VAL GLN LEU PRO GLY LYS THR ILE THR PRO ALA HIS PHE GLN LEU LEU ARG GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN
GLN GLN GLN GLN THR THR THR THR SER GLN VAL GLN VAL PRO GLN ILE GLN GLY GLN ALA GLN SER PRO ALA GLN ILE LYS ALA VAL GLY LYS LEU THR PRO GLU HIS LEU ILE LYS MET GLN LYS GLN LYS LEU GLN MET PRO PRO GLN PRO PRO PRO PRO GLN ALA GLN SER ALA PRO
PRO GLN PRO THR ALA GLN VAL GLN VAL GLN THR SER GLN PRO PRO GLN GLN GLN SER PRO GLN LEU THR THR VAL THR ALA PRO ARG PRO GLY ALA LEU LEU THR GLY THR THR VAL ALA ASN LEU GLN VAL ALA ARG LEU THR ARG VAL PRO THR SER GLN LEU GLN ALA GLN GLY GLN
MET GLN THR GLN ALA PRO GLN PRO ALA GLN VAL ALA LEU ALA LYS PRO PRO VAL VAL SER VAL PRO ALA ALA VAL VAL SER SER PRO GLY VAL THR THR LEU PRO MET ASN VAL ALA GLY ILE SER VAL ALA ILE GLY GLN PRO GLN LYS ALA ALA GLY GLN THR VAL VAL ALA GLN PRO
VAL HIS MET GLN GLN LEU LEU LYS LEU LYS GLN GLN ALA ALA VAL GLN GLN LYS ALA ILE GLN PRO GLN ALA ALA GLN GLY PRO ALA ALA VAL GLN GLN LYS ILE THR ALA GLN GLN ILE THR THR PRO GLY ALA GLN GLN LYS VAL ALA TYR ALA ALA GLN PRO ALA LEU LYS THR GLN

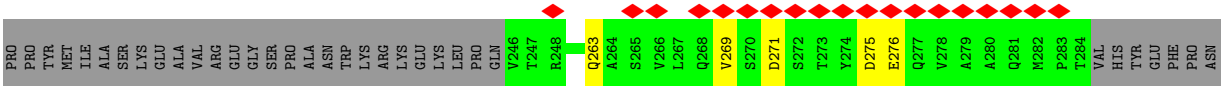


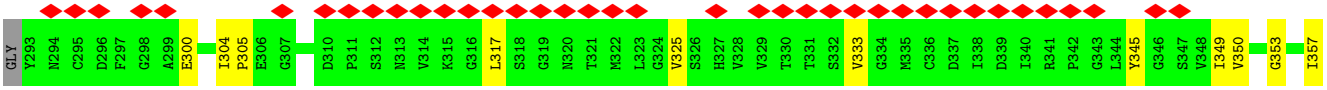
• Molecule 6: Actin-like protein 6A

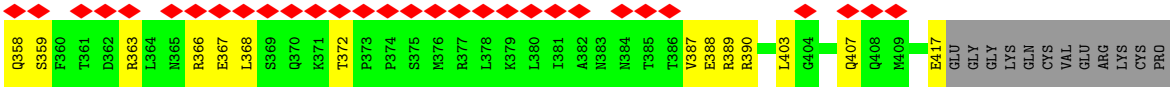
Chain I:





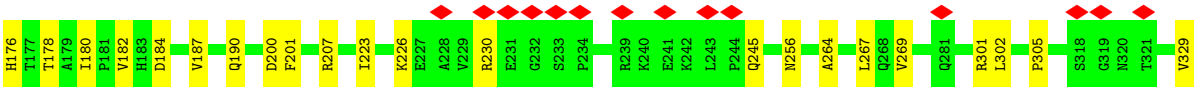






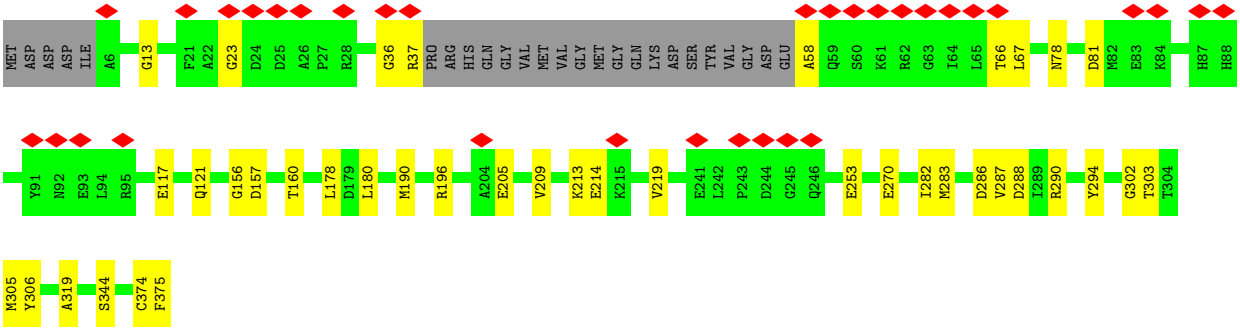
• Molecule 6: Actin-like protein 6A

Chain J:

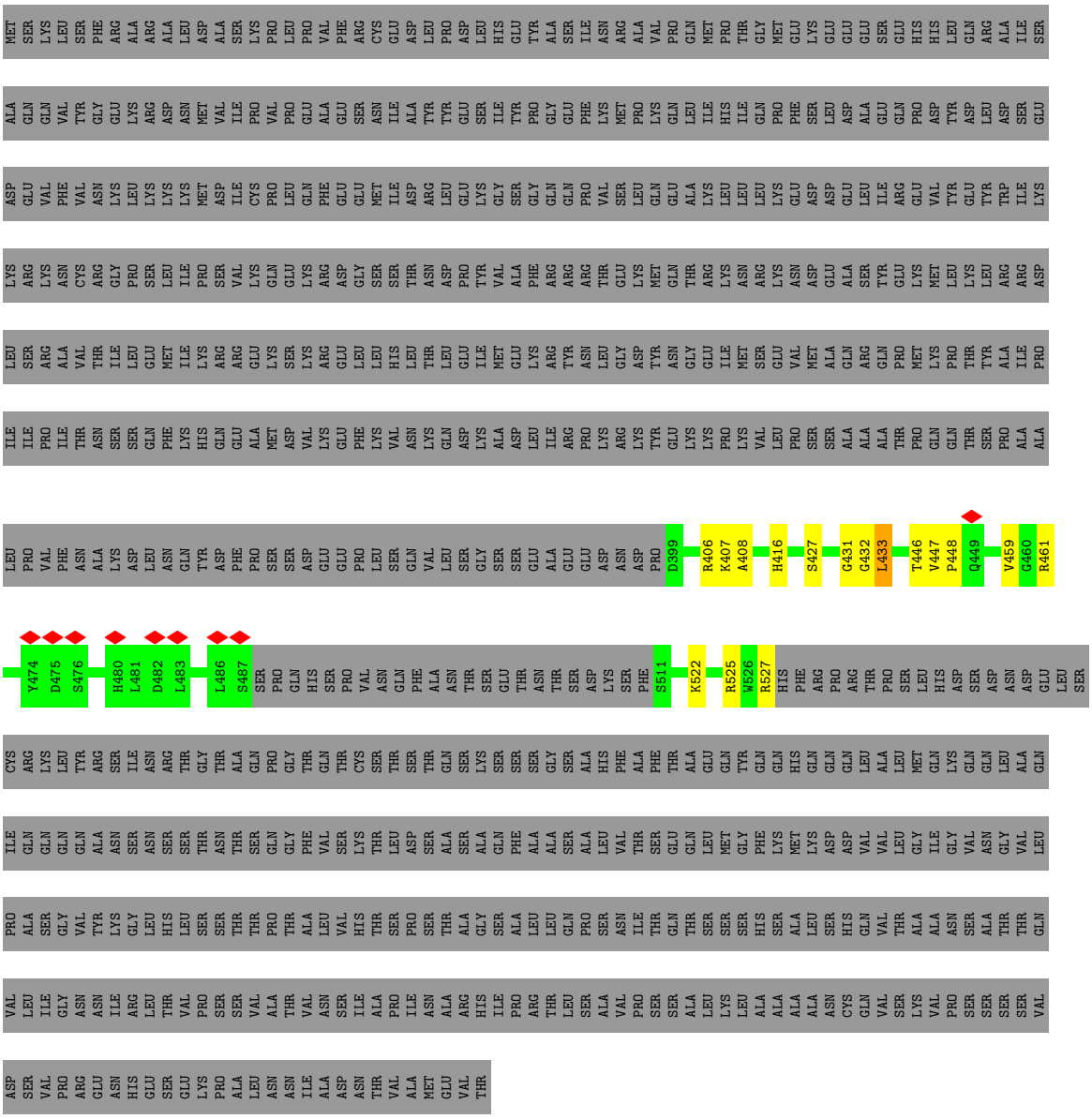


• Molecule 7: ACTB protein (Fragment)

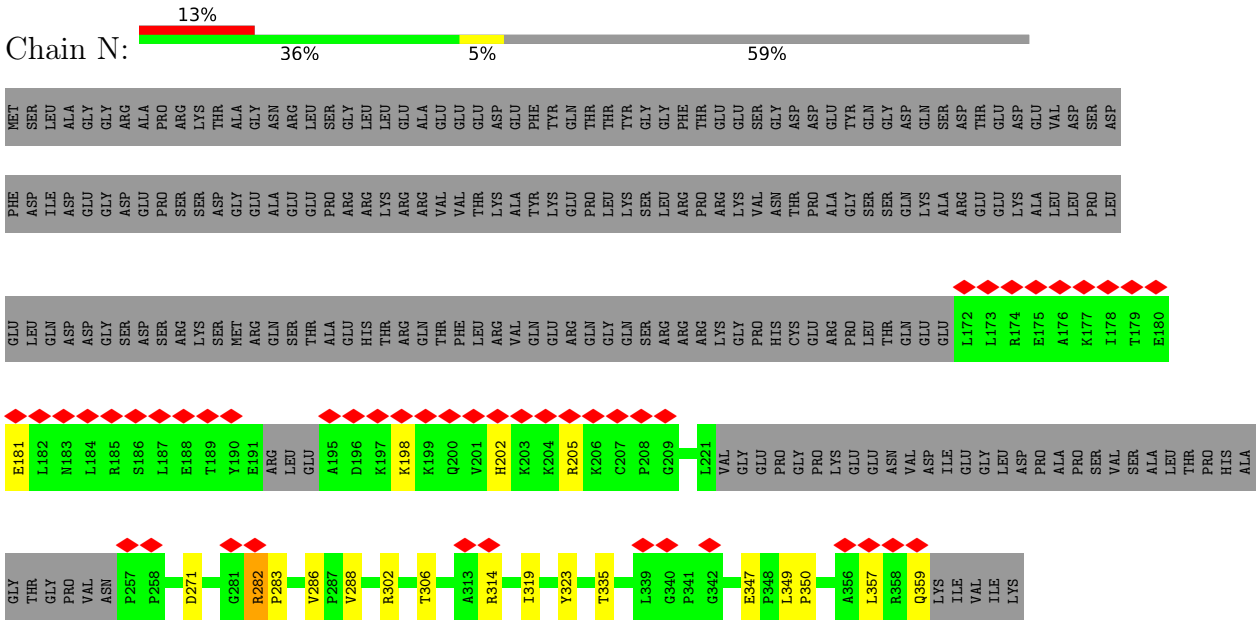
Chain K:



• Molecule 8: Isoform 2 of Enhancer of polycomb homolog 1



• Molecule 9: Vacuolar protein sorting-associated protein 72 homolog


Chain N:
13%
36%
5%
59%
MET SER LEU ALA GLY GLY ARG ALA PRO ARG LYS THR ALA GLY ASN ARG LEU SER GLY LEU LEU GLU ALA GLU GLU GLU ASP GLU PHE TYR GLN THR THR TYR GLY GLY PHE THR GLU GLU SER GLY ASP ASP GLU TYR GLN GLY ASP GLN SER ASP THR GLU ASP GLU VAL ASP SER ASP
PHE ASP ILE ASP GLU GLY ASP GLU PRO SER SER ASP GLY GLU ALA GLU GLU PRO ARG ARG LYS ARG ARG VAL VAL THR LYS ALA TYR LYS GLU PRO LEU LYS SER LEU ARG PRO ARG LYS VAL ASN THR PRO ALA GLY SER SER GLN LYS ALA ARG GLU GLU LYS ALA LEU LEU PRO LEU
GLU LEU GLN ASP ASP GLY SER ASP SER ARG LYS SER MET ARG GLN SER THR ALA GLU HIS THR ARG GLN THR PHE LEU ARG VAL GLN GLU ARG GLN GLY GLN SER ARG ARG ARG LYS GLY PRO HIS CYS GLU ARG PRO LEU THR GLN GLU GLU L172 L173 R174 E175 A176 K177 I178 T179 E180
E181 L182 N183 L184 R185 S186 L187 E188 T189 Y190 E191 ARG LEU GLU A195 D196 K197 K198 K199 Q200 V201 H202 K203 K204 R205 K206 C207 P208 G209 L221 VAL GLY GLU PRO GLY PRO LYS GLU GLU ASN VAL ASP ILE GLU GLY LEU ASP PRO ALA PRO SER VAL SER ALA LEU THR PRO HIS ALA
GLY THR GLY PRO VAL ASN P257 P258 D271 G281 R282 P283 V286 P287 V288 R302 T306 A313 R314 I319 Y323 T335 L339 G340 P341 G342 E347 P348 L349 P350 A356 L357 R358 Q359 LYS ILE VAL ILE LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20275	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.103	Depositor
Minimum map value	-0.056	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	533.6, 533.6, 533.6	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.668, 2.668, 2.668	Depositor

5 Model quality

5.1 Standard geometry

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

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	L	0.24	0/28601	0.38	0/38709
2	A	0.24	0/3321	0.41	0/4476
2	C	0.24	0/3251	0.40	0/4380
2	E	0.24	0/3389	0.40	0/4569
3	B	0.24	0/3134	0.42	0/4219
3	D	0.24	0/3352	0.42	1/4510 (0.0%)
3	F	0.23	0/3276	0.41	0/4405
4	G	0.24	0/1759	0.38	0/2364
5	H	0.23	0/8407	0.38	0/11369
6	I	0.24	0/2771	0.41	0/3756
6	J	0.24	0/3209	0.41	0/4349
7	K	0.24	0/2792	0.39	0/3782
8	M	0.24	0/883	0.42	0/1191
9	N	0.25	0/1225	0.39	0/1669
All	All	0.24	0/69370	0.39	1/93748 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	400	ARG	NE-CZ-NH2	-5.21	117.69	120.30

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	L	28003	28534	28511	302	0
2	A	3279	0	3385	55	0
2	C	3210	0	3324	76	0
2	E	3344	0	3446	60	0
3	B	3101	0	3172	51	0
3	D	3315	0	3391	60	0
3	F	3242	0	3321	70	0
4	G	1717	0	1705	25	0
5	H	8232	1352	8374	94	0
6	I	2715	0	2657	71	0
6	J	3139	0	3077	35	0
7	K	2733	0	2714	42	0
8	M	861	0	841	12	0
9	N	1188	0	1214	16	0
10	L	36	0	6	0	0
11	A	27	0	12	14	0
11	B	27	0	12	9	0
11	C	27	0	12	29	0
11	D	27	0	12	11	0
11	E	27	0	12	20	0
11	F	27	0	11	10	0
11	I	27	0	12	23	0
11	J	27	0	12	6	0
11	K	27	0	11	17	0
All	All	68358	29886	69244	903	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 7.

All (903) 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)
3:F:47:VAL:CG1	3:F:370:ILE:CG2	2.21	1.18
3:F:47:VAL:CG1	3:F:370:ILE:HG22	1.78	1.14
6:I:24:ARG:NH2	11:I:501:ADP:O2'	1.83	1.11
3:F:370:ILE:HD12	3:F:399:LEU:HD21	1.27	1.10
3:F:27:HIS:CE1	11:F:501:ADP:O2'	2.02	1.10
3:F:47:VAL:HG12	3:F:370:ILE:HG22	1.27	1.10
7:K:305:MET:HB2	11:K:401:ADP:C2	1.92	1.04

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:362:TYR:OH	11:B:501:ADP:N7	1.92	1.02
3:F:370:ILE:CD1	3:F:399:LEU:HD21	1.88	1.02
3:D:247:ILE:HG21	3:D:267:GLU:OE2	1.60	0.99
2:C:411:THR:OG1	2:C:412:PRO:HD3	1.63	0.98
2:C:180:LEU:HG	2:C:181:GLN:H	1.29	0.97
1:L:663:SER:HB3	1:L:709:LEU:HD13	1.44	0.97
2:A:366:TYR:OH	11:A:501:ADP:N7	1.98	0.96
2:C:374:ILE:CD1	11:C:501:ADP:N3	2.28	0.96
2:C:374:ILE:CD1	11:C:501:ADP:C4	2.51	0.94
2:C:374:ILE:HD11	11:C:501:ADP:C4	2.02	0.94
3:F:47:VAL:CG1	3:F:370:ILE:HG23	1.96	0.94
3:F:47:VAL:HG11	3:F:370:ILE:HG23	1.49	0.93
2:C:374:ILE:HD11	11:C:501:ADP:N3	1.83	0.92
1:L:3305:GLU:HG2	1:L:3483:ALA:CB	1.99	0.92
6:I:20:SER:HB2	11:I:501:ADP:N7	1.84	0.92
3:F:362:TYR:OH	11:F:501:ADP:N7	2.04	0.91
2:E:404:ARG:NH2	11:E:501:ADP:O3B	2.05	0.89
3:F:400:ARG:NH2	11:F:501:ADP:O2A	2.06	0.89
3:B:362:TYR:CZ	11:B:501:ADP:N7	2.40	0.89
3:F:362:TYR:CZ	11:F:501:ADP:N7	2.40	0.89
1:L:2635:SER:OG	1:L:2636:PRO:HD3	1.73	0.89
7:K:305:MET:HB2	11:K:401:ADP:N1	1.88	0.88
2:E:39:LEU:HD12	11:E:501:ADP:N6	1.89	0.88
3:F:47:VAL:HG11	3:F:370:ILE:CG2	2.00	0.87
1:L:924:ILE:HG13	1:L:2592:LEU:HD21	1.59	0.85
1:L:1719:GLU:HA	1:L:1764:LEU:HD13	1.58	0.85
2:C:374:ILE:HD11	11:C:501:ADP:H1'	1.58	0.84
3:D:247:ILE:CG2	3:D:267:GLU:OE2	2.25	0.84
3:F:27:HIS:HE1	11:F:501:ADP:O2'	1.56	0.83
4:G:76:THR:HG21	5:H:2190:GLU:OE1	1.78	0.83
6:I:70:ILE:CD1	6:I:102:ILE:HA	2.08	0.83
4:G:170:ARG:NH1	6:J:184:ASP:OD2	2.14	0.81
3:B:179:ILE:HD12	3:B:182:LEU:HD11	1.63	0.81
5:H:2209:MET:SD	8:M:525:ARG:NH1	2.54	0.81
2:E:362:ARG:NH1	2:E:364:MET:SD	2.53	0.80
3:F:32:GLY:O	3:F:53:ARG:NH2	2.14	0.80
7:K:160:THR:OG1	7:K:178:LEU:HB3	1.81	0.80
3:B:165:THR:OG1	3:B:168:MET:O	1.99	0.79
3:D:191:ASP:OD1	3:D:207:ARG:NH1	2.16	0.79
2:C:20:HIS:CE1	11:C:501:ADP:O2'	2.35	0.79
5:H:1891:LEU:HD22	5:H:1934:ILE:CG2	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:180:LEU:HG	2:C:181:GLN:N	1.98	0.78
5:H:1880:ARG:O	5:H:1951:THR:OG1	1.99	0.78
2:A:40:VAL:N	11:A:501:ADP:N1	2.31	0.78
1:L:3305:GLU:HG2	1:L:3483:ALA:HB3	1.64	0.78
2:A:320:GLU:OE2	2:A:357:ARG:NH1	2.16	0.78
2:C:366:TYR:OH	11:C:501:ADP:N7	2.16	0.78
2:E:374:ILE:HG12	11:E:501:ADP:C2	2.19	0.78
5:H:829:ARG:NH1	9:N:271:ASP:OD2	2.17	0.78
1:L:924:ILE:HG21	1:L:2592:LEU:HD23	1.64	0.77
7:K:157:ASP:OD1	11:K:401:ADP:O5'	2.00	0.77
2:E:96:MET:SD	2:E:115:ASN:ND2	2.56	0.77
3:F:83:LYS:N	11:F:501:ADP:O1B	2.17	0.77
1:L:103:ASN:O	1:L:144:ARG:NH2	2.18	0.76
2:C:374:ILE:HD12	11:C:501:ADP:C4	2.20	0.76
3:D:247:ILE:CG2	3:D:267:GLU:OE1	2.33	0.76
2:C:75:GLY:HA2	11:C:501:ADP:PA	2.25	0.76
5:H:1330:ARG:NH1	5:H:1958:ASP:OD1	2.19	0.76
3:F:370:ILE:CD1	3:F:399:LEU:CD2	2.63	0.76
1:L:2582:ASP:OD1	1:L:2585:ARG:NH2	2.19	0.76
1:L:3515:ARG:NH2	1:L:3747:ASP:OD2	2.19	0.76
5:H:793:GLU:OE1	8:M:461:ARG:NH1	2.20	0.75
2:C:268:LYS:O	2:C:269:THR:OG1	2.04	0.75
1:L:1831:ASP:OD1	1:L:1835:ASN:ND2	2.19	0.75
3:D:21:ARG:O	2:E:322:SER:OG	2.04	0.75
2:E:218:GLU:OE1	3:F:177:LYS:NZ	2.19	0.75
2:E:18:HIS:HB3	11:E:501:ADP:C3'	2.17	0.75
1:L:3639:PHE:HZ	1:L:3669:ILE:HD11	1.51	0.74
2:E:105:GLU:OE2	3:F:265:THR:OG1	2.02	0.74
6:I:269:VAL:O	6:I:359:SER:OG	2.04	0.74
3:B:83:LYS:HB3	11:B:501:ADP:O1B	1.87	0.74
6:I:21:TYR:CD2	11:I:501:ADP:H3'	2.23	0.73
1:L:663:SER:HB3	1:L:709:LEU:CD1	2.19	0.73
2:A:432:GLU:OE2	3:B:54:ARG:NH1	2.22	0.73
1:L:924:ILE:HG21	1:L:2592:LEU:CD2	2.19	0.72
2:E:332:ASN:ND2	3:F:349:ASP:OD2	2.22	0.72
3:B:407:THR:OG1	2:C:64:ARG:NH2	2.22	0.72
3:F:342:SER:OG	3:F:346:ILE:O	2.07	0.72
2:E:39:LEU:HD12	11:E:501:ADP:C6	2.25	0.72
6:I:70:ILE:HD12	6:I:102:ILE:HD12	1.72	0.71
6:I:70:ILE:HD12	6:I:102:ILE:HA	1.72	0.71
2:C:180:LEU:CG	2:C:181:GLN:H	2.01	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:3305:GLU:HG2	1:L:3483:ALA:HB2	1.73	0.71
9:N:198:LYS:O	9:N:202:HIS:ND1	2.17	0.70
1:L:428:ASP:OD1	1:L:429:CYS:N	2.24	0.70
3:D:247:ILE:CG2	3:D:267:GLU:CD	2.60	0.70
4:G:74:SER:O	5:H:2187:TYR:N	2.25	0.70
6:I:363:ARG:NH1	6:I:367:GLU:OE1	2.25	0.70
3:B:121:GLN:OE1	3:B:125:ARG:NH2	2.25	0.70
2:A:184:ARG:O	2:A:201:LYS:NZ	2.25	0.70
6:I:368:LEU:O	6:I:372:THR:OG1	2.10	0.70
2:E:39:LEU:CD1	11:E:501:ADP:N6	2.55	0.69
4:G:76:THR:HG22	5:H:2189:ARG:HG2	1.73	0.69
6:I:202:ILE:HG22	6:I:304:ILE:HG21	1.72	0.69
3:B:255:GLN:N	3:B:255:GLN:OE1	2.25	0.69
5:H:2331:GLU:O	5:H:2377:ARG:NH1	2.24	0.69
5:H:1049:SER:OG	5:H:1099:CYS:SG	2.51	0.69
6:I:353:GLY:HA3	11:I:501:ADP:H4'	1.74	0.69
6:I:70:ILE:O	6:I:70:ILE:HG13	1.92	0.69
5:H:1907:ARG:NH1	5:H:1909:ASP:OD2	2.26	0.69
5:H:1190:GLY:O	5:H:1196:TRP:NE1	2.26	0.69
2:C:55:LEU:O	2:C:58:SER:OG	2.05	0.68
6:I:117:LEU:O	6:I:118:HIS:ND1	2.27	0.68
2:C:374:ILE:HD12	11:C:501:ADP:N3	2.07	0.68
2:A:263:LEU:HD12	2:A:263:LEU:O	1.93	0.68
5:H:1891:LEU:HD22	5:H:1934:ILE:HG22	1.75	0.68
1:L:2680:LYS:NZ	5:H:2370:ASP:OD1	2.17	0.68
3:F:117:GLU:N	3:F:117:GLU:OE1	2.26	0.68
3:D:448:ASP:OD1	3:D:449:ALA:N	2.26	0.68
4:G:76:THR:CG2	5:H:2190:GLU:OE1	2.42	0.68
1:L:1719:GLU:HA	1:L:1764:LEU:CD1	2.24	0.67
1:L:2408:ARG:NH1	1:L:2442:GLU:OE2	2.26	0.67
2:E:374:ILE:HG12	11:E:501:ADP:N1	2.08	0.67
2:C:49:CYS:SG	2:C:83:ILE:HD11	2.35	0.67
1:L:561:THR:HG21	1:L:638:VAL:HG13	1.76	0.67
7:K:213:LYS:HZ2	11:K:401:ADP:H1'	1.60	0.67
2:A:270:GLU:HB2	2:A:275:LEU:HD23	1.77	0.67
1:L:104:GLU:N	1:L:104:GLU:OE1	2.28	0.67
1:L:1981:THR:O	1:L:1986:ARG:NH2	2.27	0.67
5:H:1734:ASP:OD1	5:H:1737:ARG:NH1	2.28	0.67
1:L:1650:ARG:NH1	1:L:1694:GLU:OE2	2.28	0.66
1:L:2187:ASN:O	1:L:2190:VAL:HG22	1.95	0.66
2:A:63:GLY:N	2:A:324:ALA:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:663:SER:HA	1:L:709:LEU:HD12	1.77	0.66
4:G:68:ALA:HB3	4:G:69:PRO:HD3	1.76	0.66
3:D:390:LEU:HD21	3:D:406:ILE:HG13	1.78	0.66
2:E:27:ASP:OD1	2:E:31:LEU:N	2.28	0.66
6:I:21:TYR:HB3	11:I:501:ADP:H3'	1.78	0.66
1:L:1576:HIS:O	1:L:1583:ARG:NH2	2.28	0.66
2:A:404:ARG:NH2	11:A:501:ADP:H4'	2.10	0.66
6:I:388:GLU:OE1	6:I:388:GLU:N	2.28	0.66
6:J:21:TYR:HD2	11:J:502:ADP:H3'	1.61	0.66
2:E:117:ARG:NE	2:E:275:LEU:HD11	2.11	0.66
6:I:271:ASP:O	6:I:366:ARG:NH1	2.29	0.66
5:H:2337:ASP:OD2	5:H:2396:ARG:NH2	2.28	0.65
6:J:353:GLY:HA3	11:J:502:ADP:H4'	1.78	0.65
2:A:374:ILE:HG12	11:A:501:ADP:C2	2.32	0.65
2:C:14:ARG:NH1	3:D:319:ASP:O	2.28	0.65
1:L:790:LEU:HD22	1:L:809:LEU:HD11	1.78	0.65
3:D:390:LEU:HD21	3:D:406:ILE:CG1	2.27	0.65
3:F:47:VAL:HG13	3:F:370:ILE:CG2	2.26	0.65
7:K:160:THR:HG23	7:K:180:LEU:O	1.95	0.65
6:I:71:ASP:OD1	6:I:72:THR:N	2.28	0.65
1:L:2747:TRP:O	1:L:2751:CYS:N	2.30	0.65
1:L:1211:GLU:OE2	1:L:1266:VAL:HG21	1.96	0.65
1:L:3159:ARG:NH2	1:L:3195:ILE:O	2.30	0.65
2:A:357:ARG:O	3:F:404:GLN:NE2	2.28	0.65
2:C:33:LYS:O	2:C:46:ARG:NH2	2.30	0.65
5:H:1842:GLN:O	5:H:1843:THR:OG1	2.13	0.65
5:H:1936:SER:O	5:H:1937:THR:OG1	2.13	0.65
1:L:2622:LEU:O	1:L:2627:GLN:NE2	2.28	0.65
1:L:2267:TYR:CD1	1:L:2272:ILE:HD11	2.33	0.64
4:G:95:TRP:O	7:K:121:GLN:NE2	2.30	0.64
4:G:176:ASP:O	6:J:190:GLN:NE2	2.30	0.64
5:H:1296:GLN:NE2	5:H:1333:ASN:O	2.30	0.64
1:L:793:LEU:HD11	1:L:1198:VAL:CG2	2.27	0.64
1:L:856:LEU:HD21	1:L:860:PHE:HD2	1.62	0.64
3:F:49:GLN:NE2	3:F:360:THR:O	2.30	0.64
1:L:1898:ALA:O	1:L:1902:VAL:HG22	1.98	0.64
1:L:2249:GLN:O	1:L:2253:THR:HG23	1.98	0.64
2:E:113:MET:CG	2:E:275:LEU:HD21	2.28	0.64
1:L:3105:LYS:O	1:L:3106:SER:OG	2.16	0.63
7:K:283:MET:SD	7:K:290:ARG:NH2	2.72	0.63
1:L:318:SER:O	1:L:365:TYR:OH	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2623:SER:OG	1:L:2626:GLN:OE1	2.15	0.63
6:I:21:TYR:HB3	11:I:501:ADP:H2'	1.81	0.63
2:E:100:GLU:OE2	3:F:314:ARG:NH2	2.32	0.63
5:H:2195:MET:SD	8:M:527:ARG:NE	2.72	0.63
2:E:374:ILE:HG23	11:E:501:ADP:N3	2.14	0.63
6:I:417:GLU:N	6:I:417:GLU:OE1	2.32	0.63
6:J:43:MET:O	6:J:83:GLU:N	2.31	0.62
1:L:3545:VAL:HG22	1:L:3555:VAL:HG23	1.81	0.62
2:A:43:GLU:OE1	2:A:43:GLU:N	2.32	0.62
1:L:2454:GLU:N	1:L:2454:GLU:OE1	2.33	0.62
6:I:170:LEU:HD21	6:I:325:VAL:CG1	2.29	0.62
3:D:247:ILE:HG23	3:D:267:GLU:OE1	1.99	0.62
5:H:2021:GLN:OE1	5:H:2021:GLN:N	2.32	0.62
2:C:374:ILE:HD11	11:C:501:ADP:C1'	2.29	0.62
1:L:622:THR:O	1:L:624:ARG:NH1	2.32	0.62
6:J:264:ALA:HB2	11:J:502:ADP:O2B	1.99	0.62
3:F:264:ASP:OD1	3:F:266:GLY:N	2.33	0.62
5:H:2337:ASP:OD1	5:H:2393:ILE:HD11	2.00	0.62
1:L:1825:ALA:HB3	1:L:1826:PRO:CD	2.29	0.61
6:I:24:ARG:NH2	11:I:501:ADP:HO2'	1.92	0.61
5:H:832:ARG:NH2	9:N:271:ASP:OD1	2.33	0.61
6:I:269:VAL:HG23	6:I:357:ILE:HG21	1.80	0.61
1:L:969:CYS:HB2	1:L:2592:LEU:HD13	1.81	0.61
7:K:13:GLY:HA3	11:K:401:ADP:O2B	1.99	0.61
3:B:62:MET:SD	3:B:71:ARG:NE	2.73	0.61
2:A:162:LYS:O	2:A:205:ARG:NH2	2.34	0.61
1:L:699:GLU:N	1:L:699:GLU:OE1	2.33	0.61
1:L:598:GLN:NE2	1:L:657:TYR:OH	2.33	0.61
1:L:3302:ASN:OD1	1:L:3305:GLU:OE1	2.18	0.61
5:H:738:GLN:N	5:H:738:GLN:OE1	2.34	0.61
1:L:663:SER:CB	1:L:709:LEU:HD13	2.27	0.61
2:A:233:GLU:N	2:A:233:GLU:OE1	2.34	0.61
1:L:295:ILE:HD11	1:L:337:HIS:CB	2.31	0.60
6:I:213:MET:SD	6:I:213:MET:N	2.74	0.60
1:L:2348:ALA:O	1:L:2352:ILE:HG23	2.00	0.60
3:B:249:VAL:O	3:B:255:GLN:NE2	2.32	0.60
3:D:136:GLU:OE1	3:D:235:ARG:NH2	2.34	0.60
2:E:43:GLU:N	2:E:43:GLU:OE1	2.34	0.60
5:H:2010:GLN:O	5:H:2010:GLN:NE2	2.33	0.60
5:H:2343:ALA:HB3	5:H:2368:VAL:HG23	1.82	0.60
3:B:362:TYR:OH	11:B:501:ADP:C5	2.55	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:253:ARG:NH2	5:H:1844:THR:OG1	2.34	0.60
2:E:14:ARG:NH2	3:F:321:ALA:O	2.35	0.60
2:E:209:TYR:CE1	9:N:286:VAL:HG22	2.36	0.60
2:C:411:THR:OG1	2:C:412:PRO:CD	2.45	0.60
6:I:70:ILE:HD12	6:I:102:ILE:CD1	2.31	0.60
1:L:357:GLU:OE2	1:L:397:LEU:HD12	2.02	0.60
2:C:382:GLU:OE2	2:C:411:THR:CG2	2.50	0.59
5:H:1945:ASN:OD1	5:H:1946:LEU:N	2.35	0.59
6:I:21:TYR:CB	11:I:501:ADP:H3'	2.32	0.59
1:L:291:LEU:HD21	1:L:313:MET:SD	2.42	0.59
1:L:3711:THR:O	1:L:3712:THR:OG1	2.17	0.59
3:D:305:ASP:OD1	3:D:306:ILE:N	2.36	0.59
5:H:1784:CYS:SG	5:H:1794:ARG:NH1	2.76	0.59
1:L:2804:ASP:OD1	1:L:2805:HIS:N	2.36	0.59
1:L:3242:THR:OG1	1:L:3547:ALA:O	2.21	0.59
1:L:1894:HIS:O	1:L:1894:HIS:ND1	2.33	0.59
3:F:286:GLU:OE1	3:F:286:GLU:N	2.35	0.59
4:G:72:LEU:H	4:G:72:LEU:HD23	1.67	0.59
7:K:213:LYS:NZ	11:K:401:ADP:H1'	2.18	0.59
2:A:201:LYS:O	5:H:1823:ARG:NH1	2.35	0.59
3:D:240:HIS:ND1	5:H:1789:GLN:OE1	2.35	0.59
7:K:302:GLY:O	11:K:401:ADP:N3	2.35	0.58
9:N:335:THR:OG1	9:N:347:GLU:O	2.11	0.58
1:L:1659:GLN:OE1	1:L:1706:ARG:NH1	2.35	0.58
3:F:416:ARG:NH1	3:F:425:ASP:OD1	2.37	0.58
2:A:75:GLY:HA2	11:A:501:ADP:O2A	2.04	0.58
2:A:111:VAL:O	2:A:115:ASN:ND2	2.36	0.58
2:C:20:HIS:HE1	11:C:501:ADP:O2'	1.86	0.58
3:F:136:GLU:N	3:F:136:GLU:OE1	2.37	0.58
1:L:3711:THR:HG23	1:L:3713:ILE:HG12	1.85	0.58
1:L:2158:PHE:O	1:L:2161:THR:OG1	2.18	0.58
3:F:213:ARG:NH1	3:F:214:ASP:OD1	2.37	0.58
7:K:156:GLY:HA2	11:K:401:ADP:O1B	2.04	0.58
1:L:679:PRO:O	1:L:680:THR:OG1	2.20	0.57
1:L:1050:THR:HG21	1:L:1121:VAL:HG21	1.85	0.57
1:L:1396:SER:N	1:L:1402:GLN:OE1	2.35	0.57
1:L:1961:HIS:O	1:L:1964:VAL:HG22	2.04	0.57
5:H:2431:LEU:O	5:H:2435:THR:HG23	2.04	0.57
6:J:207:ARG:NH2	6:J:256:ASN:OD1	2.37	0.57
1:L:3301:GLU:HG2	1:L:3302:ASN:N	2.19	0.57
2:C:39:LEU:HA	11:C:501:ADP:N1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:305:ASP:OD1	3:F:306:ILE:N	2.37	0.57
7:K:78:ASN:ND2	7:K:81:ASP:OD1	2.37	0.57
3:B:237:GLU:OE1	3:B:237:GLU:N	2.38	0.57
1:L:2626:GLN:OE1	1:L:2626:GLN:N	2.37	0.57
6:I:70:ILE:HD11	6:I:105:HIS:CB	2.34	0.57
1:L:663:SER:CA	1:L:709:LEU:CD1	2.81	0.57
1:L:1381:GLN:OE1	1:L:1381:GLN:N	2.36	0.57
1:L:1981:THR:OG1	1:L:1984:GLN:OE1	2.20	0.57
1:L:2232:ILE:CG2	1:L:2253:THR:HG22	2.35	0.57
1:L:2635:SER:OG	1:L:2636:PRO:CD	2.48	0.57
1:L:1815:LEU:O	1:L:1819:THR:HG23	2.05	0.57
2:C:20:HIS:HE1	11:C:501:ADP:C2'	2.18	0.57
2:A:134:GLU:N	2:A:160:GLY:O	2.34	0.57
9:N:306:THR:HG21	9:N:319:ILE:HG22	1.86	0.57
2:E:308:ASP:OD1	2:E:309:ILE:N	2.38	0.56
1:L:1819:THR:HG22	1:L:1868:LEU:HA	1.86	0.56
1:L:1229:GLU:OE1	1:L:1229:GLU:N	2.37	0.56
2:A:302:ASP:OD1	2:A:303:GLU:N	2.39	0.56
5:H:2369:SER:O	5:H:2373:ASN:ND2	2.39	0.56
2:C:43:GLU:N	2:C:43:GLU:OE1	2.36	0.56
1:L:1474:TRP:O	1:L:1478:VAL:HG23	2.06	0.56
2:A:313:THR:HG21	3:F:303:MET:SD	2.45	0.56
2:C:20:HIS:CE1	11:C:501:ADP:C2'	2.89	0.56
2:C:42:GLN:NE2	2:C:364:MET:O	2.37	0.56
2:E:209:TYR:HE1	9:N:286:VAL:HG22	1.71	0.56
1:L:359:ILE:O	1:L:361:ILE:N	2.39	0.56
3:F:32:GLY:O	3:F:33:LEU:HD12	2.05	0.56
5:H:1940:ARG:HD2	5:H:1942:THR:HG22	1.88	0.56
1:L:1825:ALA:HB3	1:L:1826:PRO:HD3	1.88	0.56
1:L:3106:SER:O	1:L:3133:TYR:OH	2.16	0.56
2:A:308:ASP:OD1	2:A:309:ILE:N	2.37	0.56
2:C:302:ASP:OD1	2:C:303:GLU:N	2.39	0.56
3:D:274:GLU:N	3:D:274:GLU:OE1	2.39	0.56
3:F:400:ARG:HH21	11:F:501:ADP:PA	2.28	0.56
5:H:1086:LYS:NZ	5:H:1211:ILE:O	2.38	0.56
1:L:2453:TYR:CZ	1:L:2457:LEU:HD11	2.40	0.56
1:L:2944:ASN:OD1	1:L:2945:SER:N	2.39	0.56
6:I:21:TYR:CD2	11:I:501:ADP:C3'	2.89	0.56
1:L:1971:MET:SD	1:L:1992:SER:OG	2.64	0.56
2:C:180:LEU:HD23	2:C:182:LYS:HZ2	1.71	0.55
2:C:207:ASP:OD1	2:C:208:THR:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:118:ARG:NE	3:B:270:SER:OG	2.39	0.55
3:F:324:LEU:HD23	3:F:325:ILE:N	2.21	0.55
6:I:300:GLU:OE1	6:I:300:GLU:N	2.37	0.55
7:K:67:LEU:HD12	7:K:67:LEU:O	2.06	0.55
3:B:229:ASP:OD1	3:B:230:GLY:N	2.38	0.55
3:D:188:GLN:N	3:D:191:ASP:OD2	2.39	0.55
1:L:1276:THR:O	1:L:1280:GLU:N	2.40	0.55
6:I:174:ALA:HB3	11:I:501:ADP:C8	2.42	0.55
1:L:2677:TYR:O	1:L:2681:THR:OG1	2.23	0.55
3:F:246:GLU:OE1	5:H:1756:ARG:NH1	2.40	0.55
2:A:20:HIS:NE2	11:A:501:ADP:O2'	2.36	0.55
3:B:435:ASP:OD1	3:B:436:GLU:N	2.40	0.55
2:C:303:GLU:OE1	2:C:305:HIS:NE2	2.39	0.55
3:D:82:GLY:HA2	11:D:501:ADP:O1A	2.06	0.55
6:I:20:SER:HG	11:I:501:ADP:HN61	1.55	0.55
4:G:81:ARG:O	9:N:288:VAL:HG22	2.07	0.55
2:C:401:THR:O	2:C:402:THR:OG1	2.22	0.54
4:G:149:ASP:OD1	4:G:150:ASP:N	2.41	0.54
6:J:81:ASN:O	6:J:245:GLN:NE2	2.39	0.54
1:L:162:TYR:HD2	1:L:241:LEU:HD13	1.72	0.54
1:L:395:LEU:HD22	1:L:426:LEU:HD11	1.89	0.54
2:A:75:GLY:N	11:A:501:ADP:O3B	2.39	0.54
3:B:268:ILE:HG22	3:B:271:GLU:HB2	1.89	0.54
6:I:407:GLN:N	6:I:407:GLN:OE1	2.40	0.54
2:E:20:HIS:NE2	11:E:501:ADP:C2	2.76	0.54
6:I:202:ILE:HD11	6:I:263:GLN:HB2	1.89	0.54
1:L:663:SER:CB	1:L:709:LEU:CD1	2.85	0.54
1:L:2392:ASP:O	1:L:2396:ASN:ND2	2.41	0.54
2:C:102:TYR:OH	2:C:308:ASP:OD1	2.25	0.54
3:F:430:TYR:O	3:F:438:ARG:NH2	2.40	0.54
6:I:70:ILE:HD11	6:I:105:HIS:HB3	1.89	0.54
6:J:38:PRO:O	6:J:70:ILE:HD11	2.07	0.54
1:L:732:LEU:HD13	1:L:732:LEU:O	2.07	0.54
1:L:2267:TYR:CE1	1:L:2272:ILE:HD11	2.43	0.54
2:C:76:LYS:HG2	11:C:501:ADP:O1B	2.06	0.54
2:E:18:HIS:HB3	11:E:501:ADP:H3'	1.88	0.54
2:E:18:HIS:HB3	11:E:501:ADP:O3'	2.08	0.54
2:E:18:HIS:CD2	11:E:501:ADP:H3'	2.43	0.54
2:E:68:LEU:HD13	2:E:79:LEU:HD11	1.89	0.54
3:B:253:ARG:O	3:B:254:THR:OG1	2.22	0.54
1:L:729:GLU:OE2	1:L:772:HIS:ND1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1005:HIS:CE1	1:L:1143:GLU:HG3	2.42	0.54
1:L:2340:SER:OG	1:L:2388:ARG:NH1	2.40	0.54
1:L:2453:TYR:CE2	1:L:2457:LEU:HD11	2.42	0.54
3:D:82:GLY:N	11:D:501:ADP:O3A	2.41	0.54
2:E:33:LYS:O	2:E:46:ARG:NH2	2.41	0.54
1:L:3558:ASN:OD1	1:L:3561:SER:OG	2.08	0.54
2:A:302:ASP:OD2	3:B:314:ARG:NE	2.41	0.54
7:K:196:ARG:NH1	7:K:253:GLU:OE2	2.40	0.54
2:C:374:ILE:CD1	11:C:501:ADP:H1'	2.36	0.53
1:L:3293:VAL:HG22	1:L:3548:VAL:HG21	1.89	0.53
5:H:2190:GLU:OE1	5:H:2190:GLU:N	2.41	0.53
1:L:2304:GLU:N	1:L:2304:GLU:OE1	2.41	0.53
2:C:75:GLY:HA2	11:C:501:ADP:O1A	2.08	0.53
2:E:113:MET:CG	2:E:275:LEU:CD2	2.86	0.53
4:G:240:GLN:NE2	5:H:2233:MET:SD	2.81	0.53
6:I:21:TYR:CG	11:I:501:ADP:H3'	2.44	0.53
1:L:295:ILE:HD11	1:L:337:HIS:HB2	1.91	0.53
1:L:561:THR:HG22	1:L:589:TYR:OH	2.09	0.53
1:L:3311:LEU:HD13	1:L:3416:ILE:HG12	1.90	0.53
5:H:1910:GLU:OE1	5:H:1910:GLU:N	2.42	0.53
3:F:247:ILE:HG22	3:F:276:ILE:HG13	1.90	0.53
3:F:362:TYR:HE2	11:F:501:ADP:HN61	1.57	0.53
3:F:424:ASP:OD1	3:F:425:ASP:N	2.42	0.53
1:L:294:ILE:HG22	1:L:294:ILE:O	2.08	0.53
1:L:663:SER:CA	1:L:709:LEU:HD12	2.39	0.53
1:L:1756:GLN:OE1	1:L:1757:HIS:ND1	2.41	0.53
1:L:3117:VAL:HG21	1:L:3130:TRP:CE3	2.44	0.53
1:L:3308:LEU:HD21	1:L:3419:LEU:HB3	1.91	0.53
1:L:3689:THR:OG1	1:L:3691:ASP:OD1	2.15	0.53
1:L:3803:GLU:OE1	1:L:3807:ASN:ND2	2.42	0.53
3:F:64:ARG:NH2	3:F:93:ALA:O	2.42	0.53
1:L:2471:HIS:O	1:L:2646:GLN:NE2	2.42	0.53
2:A:40:VAL:O	11:A:501:ADP:N6	2.42	0.53
3:B:133:GLU:N	3:B:133:GLU:OE1	2.42	0.53
2:E:28:GLU:OE1	2:E:28:GLU:N	2.40	0.53
3:F:34:ASP:OD1	3:F:40:ARG:NE	2.31	0.53
7:K:213:LYS:NZ	11:K:401:ADP:C1'	2.72	0.53
2:E:227:ASP:OD1	2:E:228:VAL:N	2.42	0.53
1:L:1245:LEU:O	1:L:1249:VAL:HG23	2.10	0.52
3:B:19:ILE:HG22	2:C:323:ILE:HG22	1.91	0.52
2:C:180:LEU:CG	2:C:181:GLN:N	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:1874:LEU:HD13	5:H:1881:VAL:HG22	1.90	0.52
3:F:401:TYR:CE2	3:F:405:LEU:HD11	2.44	0.52
2:A:262:GLN:H	3:B:258:LEU:HD11	1.74	0.52
1:L:1957:TYR:N	1:L:1958:PRO:HD3	2.24	0.52
1:L:2861:GLU:OE1	1:L:2861:GLU:N	2.42	0.52
5:H:2191:ASP:OD1	8:M:446:THR:OG1	2.12	0.52
7:K:302:GLY:HA3	11:K:401:ADP:H5'2	1.90	0.52
1:L:25:VAL:HG22	1:L:68:ARG:NH2	2.25	0.52
1:L:3774:ASP:OD2	1:L:3776:GLN:NE2	2.43	0.52
3:D:82:GLY:CA	11:D:501:ADP:O3A	2.57	0.52
2:E:113:MET:HG2	2:E:275:LEU:CD2	2.39	0.52
5:H:1090:ILE:CD1	5:H:1210:LEU:HD11	2.39	0.52
1:L:1171:LEU:HD12	1:L:1175:TRP:CZ3	2.45	0.52
1:L:3143:GLN:OE1	1:L:3145:HIS:NE2	2.43	0.52
6:J:71:ASP:OD1	6:J:72:THR:N	2.43	0.52
2:C:40:VAL:N	11:C:501:ADP:N1	2.57	0.52
2:A:105:GLU:OE1	2:A:105:GLU:N	2.41	0.52
3:D:27:HIS:NE2	11:D:501:ADP:C2	2.78	0.52
1:L:1538:GLU:OE1	1:L:1538:GLU:N	2.43	0.52
1:L:1936:GLY:O	1:L:1938:THR:HG23	2.09	0.52
3:D:85:ALA:HB2	11:D:501:ADP:O1A	2.09	0.52
7:K:13:GLY:CA	11:K:401:ADP:O2B	2.58	0.52
1:L:114:LEU:HD13	1:L:150:GLU:HB3	1.92	0.51
1:L:1371:ASN:ND2	1:L:1408:CYS:SG	2.83	0.51
2:C:353:ASP:OD1	2:C:354:LEU:N	2.43	0.51
3:D:399:LEU:HD23	11:D:501:ADP:C1'	2.41	0.51
3:D:400:ARG:CZ	11:D:501:ADP:H5'1	2.40	0.51
6:I:390:ARG:HD2	11:I:501:ADP:O3'	2.10	0.51
2:A:356:ASP:OD1	2:A:357:ARG:N	2.43	0.51
3:B:119:LEU:HD21	3:B:312:LEU:HD21	1.92	0.51
1:L:295:ILE:HD11	1:L:337:HIS:HB3	1.91	0.51
1:L:634:HIS:O	1:L:638:VAL:HG23	2.10	0.51
2:A:405:TYR:CE2	2:A:409:LEU:HD11	2.46	0.51
7:K:286:ASP:OD1	7:K:287:VAL:N	2.44	0.51
1:L:661:ARG:O	1:L:665:ASN:N	2.42	0.51
1:L:838:SER:O	1:L:842:VAL:HG13	2.10	0.51
1:L:2145:ASN:O	1:L:2148:ASN:ND2	2.43	0.51
3:D:56:ALA:HB2	3:D:86:ILE:HD11	1.93	0.51
2:E:186:GLU:OE1	2:E:186:GLU:N	2.41	0.51
3:F:370:ILE:HD11	3:F:399:LEU:CD2	2.39	0.51
4:G:260:GLU:OE1	5:H:748:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:217:ARG:HE	1:L:220:LEU:HD21	1.75	0.51
3:B:134:GLU:OE1	3:B:134:GLU:N	2.43	0.51
2:C:423:ASP:OD1	2:C:424:SER:N	2.43	0.51
2:E:132:GLU:N	2:E:132:GLU:OE1	2.44	0.51
3:F:27:HIS:NE2	11:F:501:ADP:N3	2.52	0.51
2:C:405:TYR:OH	2:C:437:PHE:O	2.28	0.51
6:J:343:GLY:O	6:J:347:SER:OG	2.29	0.51
1:L:630:GLU:OE1	1:L:630:GLU:N	2.43	0.51
2:C:40:VAL:HG12	11:C:501:ADP:C2	2.46	0.51
2:C:40:VAL:HG12	11:C:501:ADP:N1	2.26	0.51
2:E:366:TYR:CE2	11:E:501:ADP:N7	2.79	0.51
5:H:1091:ILE:HD11	5:H:1123:LEU:HD22	1.93	0.51
6:I:275:ASP:OD1	6:I:276:GLU:N	2.44	0.51
6:I:390:ARG:NH1	11:I:501:ADP:O3'	2.42	0.50
6:J:99:PHE:CE2	6:J:103:LEU:HD11	2.45	0.50
1:L:2315:THR:HG21	1:L:2352:ILE:HD12	1.92	0.50
1:L:3710:LEU:O	1:L:3711:THR:HG22	2.11	0.50
3:B:250:ILE:HG22	5:H:1364:LEU:HD12	1.93	0.50
3:D:251:ASN:HB3	3:D:267:GLU:OE1	2.11	0.50
6:J:70:ILE:HG23	6:J:70:ILE:O	2.11	0.50
7:K:302:GLY:HA3	11:K:401:ADP:C5'	2.42	0.50
1:L:705:GLU:N	1:L:705:GLU:OE1	2.44	0.50
1:L:1123:SER:O	1:L:1127:GLY:N	2.41	0.50
1:L:2619:TRP:O	1:L:2627:GLN:NE2	2.45	0.50
2:A:66:VAL:O	2:A:329:PHE:N	2.43	0.50
3:D:49:GLN:NE2	3:D:360:THR:O	2.43	0.50
3:F:250:ILE:O	3:F:250:ILE:HG22	2.12	0.50
6:I:333:VAL:HG11	6:I:345:TYR:CZ	2.46	0.50
7:K:36:GLY:O	7:K:58:ALA:N	2.44	0.50
1:L:3100:LEU:O	1:L:3100:LEU:HD23	2.11	0.50
1:L:3294:ASP:O	1:L:3297:VAL:HG12	2.12	0.50
3:B:274:GLU:OE1	3:B:274:GLU:N	2.38	0.50
1:L:915:VAL:HG22	1:L:3629:THR:O	2.12	0.50
1:L:2353:VAL:HG23	1:L:2402:LEU:HD11	1.92	0.50
1:L:2791:ALA:O	5:H:2423:GLN:NE2	2.45	0.50
5:H:1162:TYR:OH	5:H:1183:ASP:O	2.29	0.50
2:A:389:GLU:OE1	2:A:389:GLU:N	2.38	0.50
6:J:329:VAL:O	6:J:333:VAL:HG23	2.11	0.50
1:L:412:PRO:HD2	1:L:415:ILE:HD12	1.94	0.50
1:L:3299:PHE:CE2	1:L:3501:VAL:HG21	2.47	0.50
1:L:3477:VAL:HG21	1:L:3486:ARG:CZ	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:3643:PHE:HE1	1:L:3669:ILE:HD12	1.76	0.50
3:B:145:ILE:HG22	3:B:146:GLN:N	2.26	0.50
3:D:32:GLY:O	3:D:53:ARG:NH2	2.42	0.50
3:F:408:ALA:HB3	3:F:429:VAL:HG11	1.93	0.50
5:H:1975:GLY:O	5:H:1980:ILE:HG21	2.12	0.50
1:L:1400:GLU:OE1	1:L:1400:GLU:N	2.43	0.49
3:B:180:GLU:OE1	3:B:180:GLU:N	2.41	0.49
3:F:170:THR:HG23	9:N:302:ARG:H	1.77	0.49
7:K:302:GLY:O	11:K:401:ADP:C2	2.65	0.49
3:D:21:ARG:HB2	2:E:62:ALA:HB2	1.94	0.49
2:E:117:ARG:HG3	2:E:275:LEU:HD11	1.95	0.49
3:B:45:GLY:O	11:B:501:ADP:C2	2.65	0.49
6:I:21:TYR:HD2	11:I:501:ADP:O3'	1.95	0.49
6:J:169:ILE:N	6:J:169:ILE:HD12	2.27	0.49
1:L:101:PRO:O	1:L:102:THR:HG23	2.12	0.49
1:L:1184:LEU:HD22	1:L:1241:VAL:HG13	1.93	0.49
2:E:142:GLU:OE2	5:H:2160:TRP:NE1	2.45	0.49
4:G:69:PRO:N	4:G:70:PRO:CD	2.76	0.49
1:L:317:LEU:HD22	1:L:331:LEU:HD21	1.93	0.49
3:B:29:ARG:NH2	3:B:377:GLU:OE1	2.44	0.49
5:H:1104:TRP:O	5:H:1107:HIS:NE2	2.44	0.49
5:H:2382:SER:OG	5:H:2383:LYS:N	2.45	0.49
7:K:180:LEU:O	7:K:180:LEU:HD12	2.12	0.49
1:L:97:ILE:HG23	1:L:135:ILE:HD13	1.93	0.49
6:J:182:VAL:HG12	6:J:187:VAL:HG22	1.95	0.49
7:K:178:LEU:HD21	7:K:180:LEU:HD11	1.93	0.49
2:A:404:ARG:NH2	11:A:501:ADP:O3'	2.38	0.49
2:E:79:LEU:HD12	2:E:80:ALA:N	2.27	0.49
5:H:2356:ILE:HG13	5:H:2357:VAL:N	2.28	0.49
7:K:282:ILE:HG21	7:K:294:TYR:CZ	2.48	0.49
1:L:2810:SER:OG	1:L:2819:LEU:HD21	2.13	0.49
3:B:45:GLY:O	11:B:501:ADP:H2	1.96	0.49
3:D:260:LEU:O	2:E:271:ILE:HG22	2.12	0.49
6:I:21:TYR:HD2	11:I:501:ADP:C3'	2.26	0.49
1:L:159:LYS:HG2	1:L:241:LEU:HD11	1.95	0.49
2:E:173:ASP:O	2:E:176:ILE:HG22	2.13	0.49
5:H:841:ILE:HD13	6:I:403:LEU:HD11	1.94	0.49
6:I:174:ALA:HB2	11:I:501:ADP:H5'1	1.94	0.49
9:N:282:ARG:NH1	9:N:283:PRO:O	2.46	0.49
1:L:357:GLU:O	1:L:359:ILE:N	2.46	0.48
1:L:859:ASP:OD1	1:L:860:PHE:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2857:SER:O	1:L:2857:SER:OG	2.32	0.48
5:H:2369:SER:OG	5:H:2381:SER:OG	2.29	0.48
6:I:169:ILE:HD12	6:I:169:ILE:N	2.28	0.48
1:L:2507:ILE:HG22	1:L:2507:ILE:O	2.13	0.48
2:A:131:TYR:N	2:A:193:ILE:O	2.45	0.48
2:C:374:ILE:HD11	11:C:501:ADP:N9	2.26	0.48
2:E:56:ILE:HD13	2:E:298:VAL:HG21	1.94	0.48
2:E:113:MET:SD	2:E:275:LEU:HD21	2.53	0.48
1:L:1347:ASP:OD1	1:L:1366:ARG:NH2	2.46	0.48
3:D:117:GLU:OE1	3:D:121:GLN:NE2	2.47	0.48
3:F:250:ILE:HD11	5:H:1756:ARG:HG3	1.94	0.48
3:B:145:ILE:HG22	3:B:146:GLN:H	1.79	0.48
3:F:178:MET:O	3:F:182:LEU:HD23	2.14	0.48
6:I:350:VAL:O	6:I:389:ARG:NH1	2.45	0.48
1:L:2228:VAL:HA	1:L:2231:VAL:HG12	1.95	0.48
1:L:2634:ILE:O	1:L:2638:LEU:N	2.44	0.48
2:A:426:GLU:N	2:A:426:GLU:OE1	2.47	0.48
2:C:315:LEU:HD21	2:C:329:PHE:CZ	2.48	0.48
1:L:2250:LEU:HD22	1:L:2306:VAL:HG11	1.96	0.48
5:H:1960:ASN:N	5:H:1964:ASP:OD1	2.39	0.48
6:I:170:LEU:HD21	6:I:325:VAL:HG13	1.94	0.48
1:L:1181:GLN:NE2	1:L:1244:ASP:OD2	2.46	0.48
2:A:273:ASP:OD1	2:A:274:LYS:N	2.47	0.48
2:C:105:GLU:N	2:C:105:GLU:OE1	2.47	0.48
1:L:3639:PHE:CZ	1:L:3669:ILE:HD11	2.39	0.48
2:C:176:ILE:O	2:C:176:ILE:HG22	2.14	0.48
1:L:1797:VAL:HG22	1:L:1798:LEU:HD23	1.96	0.47
1:L:3251:GLN:NE2	1:L:3263:ARG:O	2.44	0.47
3:B:129:VAL:HG22	3:B:291:ILE:HG22	1.96	0.47
5:H:1898:LEU:O	5:H:1902:TYR:N	2.47	0.47
6:I:174:ALA:CB	11:I:501:ADP:C8	2.97	0.47
3:B:362:TYR:CE2	11:B:501:ADP:N7	2.82	0.47
3:F:26:SER:O	3:F:29:ARG:NH1	2.47	0.47
5:H:1781:LEU:O	5:H:1783:ARG:NH1	2.45	0.47
2:C:76:LYS:HG2	11:C:501:ADP:PB	2.54	0.47
2:C:255:ASP:OD1	2:C:258:SER:N	2.42	0.47
3:F:264:ASP:OD1	3:F:265:THR:N	2.46	0.47
6:J:354:ASN:O	6:J:357:ILE:HG12	2.15	0.47
1:L:790:LEU:CD2	1:L:809:LEU:HD11	2.44	0.47
1:L:2254:LEU:HD23	1:L:2255:MET:N	2.29	0.47
3:F:317:GLU:OE2	3:F:353:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:445:LEU:HB3	1:L:564:ILE:HG22	1.96	0.47
3:F:309:PHE:CZ	3:F:346:ILE:HG22	2.50	0.47
5:H:2237:THR:HG23	5:H:2237:THR:O	2.15	0.47
5:H:2389:TYR:O	5:H:2393:ILE:HG13	2.13	0.47
7:K:37:ARG:O	7:K:66:THR:OG1	2.30	0.47
1:L:550:VAL:O	1:L:554:VAL:HG23	2.13	0.47
2:C:76:LYS:CG	11:C:501:ADP:O1B	2.63	0.47
3:D:331:GLY:O	3:D:344:HIS:N	2.40	0.47
1:L:235:MET:SD	1:L:296:ARG:NH2	2.81	0.47
1:L:655:VAL:N	1:L:656:PRO:HD2	2.30	0.47
1:L:3617:VAL:HG11	1:L:3829:TRP:CD1	2.49	0.47
3:B:34:ASP:OD1	3:B:40:ARG:NE	2.47	0.47
3:B:161:LEU:HD13	3:B:182:LEU:HD13	1.97	0.47
3:B:424:ASP:OD1	3:B:425:ASP:N	2.48	0.47
6:J:178:THR:HG22	6:J:180:ILE:HG13	1.97	0.47
1:L:1937:HIS:ND1	1:L:1939:VAL:HG13	2.30	0.47
1:L:3299:PHE:CD2	1:L:3501:VAL:HG21	2.50	0.47
1:L:3774:ASP:OD1	1:L:3775:SER:N	2.47	0.47
1:L:1525:GLU:O	1:L:1529:LEU:N	2.48	0.47
1:L:1719:GLU:OE1	1:L:1764:LEU:HD21	2.14	0.47
1:L:2666:PRO:N	1:L:2667:PRO:CD	2.77	0.47
2:C:204:GLY:O	2:C:205:ARG:NE	2.43	0.47
5:H:774:SER:OG	5:H:777:ASP:OD1	2.10	0.47
5:H:1799:ILE:O	5:H:1799:ILE:HG22	2.15	0.47
1:L:3266:ALA:HB3	1:L:3267:PRO:HD3	1.97	0.47
1:L:3311:LEU:HD13	1:L:3416:ILE:CG1	2.44	0.47
2:A:190:VAL:C	2:A:191:ILE:HD12	2.35	0.47
5:H:2336:GLU:OE2	5:H:2380:ARG:NH2	2.48	0.47
1:L:373:PRO:HB3	1:L:415:ILE:HD11	1.96	0.46
2:C:123:ARG:NE	2:C:237:ASP:OD2	2.44	0.46
4:G:123:ASP:OD1	4:G:124:TYR:N	2.46	0.46
6:I:180:ILE:HG23	6:I:187:VAL:HG13	1.98	0.46
7:K:270:GLU:N	7:K:270:GLU:OE1	2.48	0.46
1:L:1938:THR:O	1:L:1939:VAL:C	2.53	0.46
2:E:374:ILE:HG23	11:E:501:ADP:C2	2.49	0.46
6:J:337:ASP:OD1	6:J:338:ILE:N	2.48	0.46
1:L:678:ASN:OD1	1:L:681:THR:OG1	2.26	0.46
1:L:850:GLU:HA	1:L:853:VAL:HG12	1.97	0.46
3:D:370:ILE:HG23	11:D:501:ADP:C2	2.50	0.46
3:D:381:GLU:N	3:D:381:GLU:OE1	2.48	0.46
5:H:1273:LYS:O	5:H:1276:VAL:HG22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:709:LEU:HD23	1:L:713:LEU:CD1	2.46	0.46
1:L:2799:TYR:CD2	5:H:2426:THR:HG21	2.50	0.46
6:I:158:THR:O	6:I:162:ASN:ND2	2.43	0.46
1:L:467:ILE:HD12	1:L:605:VAL:HG11	1.97	0.46
1:L:1313:THR:HG22	1:L:1372:ALA:HA	1.97	0.46
2:E:18:HIS:HD2	11:E:501:ADP:H5'2	1.80	0.46
5:H:1090:ILE:HD12	5:H:1210:LEU:HD11	1.97	0.46
5:H:2200:GLU:O	8:M:522:LYS:NZ	2.49	0.46
6:I:269:VAL:HG23	6:I:357:ILE:CG2	2.44	0.46
1:L:228:LEU:HG	1:L:229:PRO:HD3	1.98	0.46
1:L:3225:ILE:HA	1:L:3228:VAL:HG12	1.98	0.46
5:H:1889:LEU:HD22	5:H:1889:LEU:H	1.81	0.46
1:L:106:LEU:O	1:L:110:THR:OG1	2.32	0.46
2:A:404:ARG:HH21	11:A:501:ADP:H4'	1.79	0.46
2:C:28:GLU:OE1	2:C:28:GLU:N	2.45	0.46
2:C:257:LEU:HD13	5:H:1829:LEU:HD23	1.96	0.46
2:C:271:ILE:HG23	2:C:274:LYS:H	1.80	0.46
3:D:400:ARG:NH2	11:D:501:ADP:H5'1	2.31	0.46
7:K:287:VAL:HG12	7:K:288:ASP:N	2.31	0.46
9:N:349:LEU:N	9:N:350:PRO:HD2	2.30	0.46
1:L:3572:CYS:O	1:L:3576:GLY:N	2.48	0.46
2:A:159:ILE:HB	2:A:170:LEU:HD11	1.97	0.46
5:H:785:TRP:NE1	8:M:459:VAL:O	2.49	0.46
7:K:305:MET:CB	11:K:401:ADP:N1	2.71	0.46
9:N:357:LEU:HD23	9:N:359:GLN:N	2.31	0.46
1:L:930:ASP:OD2	1:L:931:CYS:N	2.49	0.46
1:L:1811:ARG:NH2	1:L:1850:CYS:SG	2.89	0.46
1:L:2850:ALA:O	1:L:2854:VAL:HG23	2.16	0.46
1:L:3222:LEU:HD12	1:L:3274:ILE:HD12	1.97	0.46
3:B:301:VAL:HG21	3:B:326:MET:SD	2.55	0.46
2:E:396:GLU:O	2:E:399:THR:OG1	2.28	0.46
1:L:3311:LEU:HD12	1:L:3312:GLN:N	2.31	0.45
1:L:3668:GLN:N	1:L:3677:ASN:O	2.45	0.45
2:A:246:ALA:O	2:A:251:GLN:NE2	2.49	0.45
4:G:164:SER:HA	4:G:174:ILE:HD11	1.96	0.45
5:H:1217:ASN:O	5:H:1218:THR:OG1	2.30	0.45
2:A:405:TYR:CZ	2:A:409:LEU:HD11	2.51	0.45
4:G:232:ARG:NH2	8:M:406:ARG:O	2.49	0.45
7:K:213:LYS:HZ2	11:K:401:ADP:C1'	2.26	0.45
1:L:448:MET:O	1:L:451:VAL:HG22	2.16	0.45
1:L:2121:TRP:N	1:L:2122:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:119:LEU:HD21	3:B:312:LEU:CD2	2.45	0.45
3:B:370:ILE:HG21	3:B:399:LEU:HD21	1.98	0.45
6:I:170:LEU:N	6:I:349:ILE:O	2.46	0.45
6:J:200:ASP:OD1	6:J:201:PHE:N	2.49	0.45
6:J:387:VAL:HG12	6:J:387:VAL:O	2.16	0.45
7:K:205:GLU:O	7:K:209:VAL:HG23	2.16	0.45
1:L:1253:ASN:HB3	1:L:1256:VAL:HG22	1.98	0.45
1:L:3086:LYS:O	1:L:3089:THR:OG1	2.24	0.45
2:C:122:LEU:N	2:C:238:VAL:O	2.45	0.45
2:C:343:ASP:OD1	2:C:344:ILE:N	2.49	0.45
6:J:176:HIS:HE1	11:J:502:ADP:N6	2.15	0.45
1:L:1193:ASP:O	1:L:3469:ARG:NH1	2.45	0.45
1:L:1760:ASN:HB2	1:L:1761:PRO:HD3	1.99	0.45
1:L:3652:PHE:CE1	1:L:3656:VAL:HG21	2.52	0.45
3:B:108:ILE:HD13	3:B:304:LEU:HD22	1.99	0.45
3:D:251:ASN:OD1	3:D:252:SER:N	2.50	0.45
2:E:39:LEU:CD1	11:E:501:ADP:C6	2.96	0.45
1:L:281:ILE:O	1:L:285:ILE:HG23	2.16	0.45
2:A:39:LEU:HA	11:A:501:ADP:N1	2.32	0.45
5:H:1940:ARG:O	5:H:1941:THR:OG1	2.30	0.45
6:I:358:GLN:O	6:I:359:SER:OG	2.35	0.45
1:L:390:LEU:HD12	1:L:395:LEU:HD21	1.99	0.45
1:L:1343:CYS:HB2	1:L:1370:LEU:HD22	1.99	0.45
3:B:22:ILE:HD12	3:B:22:ILE:N	2.32	0.45
2:E:366:TYR:OH	11:E:501:ADP:N7	2.42	0.45
6:I:353:GLY:HA3	11:I:501:ADP:C4'	2.42	0.45
1:L:2340:SER:O	1:L:2388:ARG:NH1	2.43	0.45
1:L:3348:THR:HG23	1:L:3349:PHE:N	2.31	0.45
3:B:249:VAL:O	3:B:249:VAL:HG12	2.17	0.45
3:D:61:GLU:OE1	3:D:64:ARG:NH2	2.45	0.45
2:E:265:LYS:N	2:E:266:PRO:CD	2.80	0.45
6:I:269:VAL:HG22	6:I:305:PRO:HB3	1.98	0.45
1:L:336:LYS:O	1:L:340:THR:OG1	2.34	0.44
2:C:205:ARG:HB3	2:C:221:VAL:HG22	1.99	0.44
2:E:18:HIS:O	2:E:18:HIS:ND1	2.46	0.44
2:E:401:THR:OG1	2:E:402:THR:N	2.50	0.44
7:K:156:GLY:CA	11:K:401:ADP:O1B	2.65	0.44
1:L:2796:PHE:N	1:L:2797:PRO:HD2	2.31	0.44
1:L:2177:ARG:NH2	1:L:2220:GLU:OE2	2.48	0.44
1:L:2506:VAL:O	1:L:2515:ARG:NH1	2.50	0.44
1:L:2959:ARG:O	1:L:2960:LEU:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:3329:VAL:O	1:L:3330:SER:HB3	2.18	0.44
2:E:408:GLN:O	3:F:71:ARG:NH2	2.50	0.44
9:N:349:LEU:N	9:N:350:PRO:CD	2.80	0.44
1:L:1005:HIS:CD2	1:L:3429:PHE:HZ	2.36	0.44
1:L:2159:LEU:HA	1:L:2162:VAL:HG12	2.00	0.44
1:L:3117:VAL:HG21	1:L:3130:TRP:HE3	1.82	0.44
2:E:18:HIS:HD2	11:E:501:ADP:H3'	1.83	0.44
6:I:21:TYR:HB3	11:I:501:ADP:C3'	2.46	0.44
8:M:407:LYS:NZ	8:M:408:ALA:O	2.51	0.44
8:M:447:VAL:HB	8:M:448:PRO:HD3	1.99	0.44
1:L:1825:ALA:CB	1:L:1826:PRO:CD	2.96	0.44
3:B:250:ILE:HD11	5:H:1360:ILE:O	2.18	0.44
3:D:247:ILE:HG21	3:D:267:GLU:CD	2.27	0.44
6:I:21:TYR:CD2	11:I:501:ADP:O3'	2.68	0.44
5:H:1799:ILE:N	5:H:1800:PRO:HD3	2.33	0.44
5:H:1950:ASP:HB3	5:H:1980:ILE:HG22	2.00	0.44
7:K:374:CYS:SG	7:K:375:PHE:N	2.91	0.44
1:L:671:VAL:HG12	1:L:675:PHE:CE2	2.51	0.44
1:L:2232:ILE:HG21	1:L:2253:THR:HG22	1.98	0.44
1:L:3301:GLU:HG2	1:L:3302:ASN:H	1.83	0.44
3:D:313:ASN:ND2	3:D:349:ASP:OD2	2.51	0.44
3:F:348:ILE:HD13	3:F:351:LEU:HD12	2.00	0.44
5:H:1265:GLN:N	5:H:1266:PRO:HD2	2.33	0.44
6:I:77:VAL:HG23	6:I:77:VAL:O	2.18	0.44
1:L:561:THR:HG22	1:L:589:TYR:CE1	2.53	0.44
2:A:42:GLN:HG3	2:A:45:ALA:HB3	2.00	0.44
3:D:127:ILE:CG2	3:D:291:ILE:HD11	2.48	0.44
3:F:405:LEU:CD2	3:F:429:VAL:HG12	2.48	0.44
5:H:2007:VAL:HG12	5:H:2008:ALA:N	2.32	0.44
8:M:416:HIS:O	8:M:416:HIS:ND1	2.50	0.44
1:L:73:LEU:C	1:L:73:LEU:HD12	2.38	0.44
1:L:295:ILE:HD12	1:L:338:ILE:HG13	1.99	0.44
2:A:24:LEU:HD21	2:A:49:CYS:CB	2.48	0.44
2:A:76:LYS:HG2	11:A:501:ADP:PB	2.58	0.44
3:B:430:TYR:O	3:B:438:ARG:NH1	2.51	0.44
1:L:228:LEU:N	1:L:229:PRO:CD	2.81	0.43
1:L:2887:GLU:OE1	1:L:2887:GLU:N	2.45	0.43
2:C:172:LEU:HD21	2:C:176:ILE:HG21	2.00	0.43
3:F:47:VAL:HG13	3:F:370:ILE:HG23	1.93	0.43
1:L:1172:PRO:O	1:L:1176:VAL:HG13	2.18	0.43
2:A:404:ARG:NH2	11:A:501:ADP:C4'	2.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:1789:GLN:O	5:H:1794:ARG:NH2	2.51	0.43
6:I:151:LEU:N	6:I:151:LEU:HD23	2.33	0.43
1:L:824:LEU:N	1:L:825:PRO:CD	2.81	0.43
1:L:2855:GLU:OE1	1:L:2870:ARG:NH2	2.45	0.43
6:I:175:THR:OG1	11:I:501:ADP:N6	2.52	0.43
6:J:41:ILE:HG22	6:J:70:ILE:HB	1.99	0.43
7:K:282:ILE:HG21	7:K:294:TYR:CE2	2.54	0.43
1:L:969:CYS:HA	1:L:972:VAL:HG22	1.99	0.43
3:B:47:VAL:H	11:B:501:ADP:HN62	1.65	0.43
2:C:77:THR:N	11:C:501:ADP:O1B	2.33	0.43
2:C:138:LEU:HD12	2:C:159:ILE:HG22	2.00	0.43
3:D:355:LEU:HD12	3:D:355:LEU:O	2.18	0.43
5:H:1046:ASN:ND2	5:H:1064:ASP:OD1	2.52	0.43
1:L:561:THR:HG21	1:L:638:VAL:CG1	2.45	0.43
1:L:663:SER:N	1:L:709:LEU:CD1	2.82	0.43
1:L:3132:ASP:O	1:L:3136:ASN:ND2	2.46	0.43
2:A:326:ILE:HD12	2:A:326:ILE:N	2.33	0.43
2:C:75:GLY:HA2	11:C:501:ADP:O3A	2.18	0.43
3:D:83:LYS:H	11:D:501:ADP:PB	2.41	0.43
3:F:205:LEU:HD12	3:F:225:VAL:HB	2.01	0.43
7:K:23:GLY:N	7:K:344:SER:OG	2.50	0.43
8:M:427:SER:O	8:M:431:GLY:N	2.46	0.43
1:L:125:ASN:ND2	1:L:128:ASN:OD1	2.52	0.43
3:B:303:MET:HG3	2:C:313:THR:HG21	2.01	0.43
2:C:326:ILE:HD12	2:C:326:ILE:N	2.34	0.43
2:E:20:HIS:HE1	11:E:501:ADP:O2'	2.01	0.43
4:G:80:TYR:O	4:G:84:LYS:N	2.52	0.43
5:H:1947:VAL:HG11	5:H:1950:ASP:OD1	2.18	0.43
6:I:128:ASN:ND2	6:I:129:THR:O	2.51	0.43
6:J:223:ILE:N	6:J:223:ILE:HD12	2.33	0.43
7:K:303:THR:HG22	7:K:303:THR:O	2.19	0.43
8:M:432:GLY:C	8:M:433:LEU:HD23	2.39	0.43
1:L:558:LYS:HA	1:L:638:VAL:HG22	2.01	0.43
1:L:1087:MET:SD	1:L:1088:ASP:N	2.92	0.43
1:L:3299:PHE:HD2	1:L:3501:VAL:HG11	1.84	0.43
2:A:40:VAL:H	11:A:501:ADP:N6	2.16	0.43
1:L:106:LEU:HD11	1:L:139:LEU:HG	2.00	0.43
1:L:453:VAL:HG23	1:L:592:LEU:HA	2.00	0.43
1:L:3617:VAL:HG11	1:L:3829:TRP:HD1	1.83	0.43
2:C:40:VAL:H	11:C:501:ADP:HN62	1.67	0.43
3:F:137:ILE:HD13	3:F:196:ASP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:1731:TYR:CE2	5:H:1735:LEU:HD11	2.53	0.43
6:I:21:TYR:HB3	11:I:501:ADP:C2'	2.47	0.43
1:L:1290:VAL:HB	1:L:1291:PRO:HD3	2.00	0.43
1:L:3134:LEU:HA	1:L:3137:ILE:HG22	2.01	0.43
2:A:323:ILE:HG22	3:F:19:ILE:HG22	2.01	0.43
3:D:174:LEU:HD13	3:D:182:LEU:HD12	2.01	0.43
7:K:214:GLU:HB2	11:K:401:ADP:N6	2.34	0.43
1:L:1243:HIS:O	1:L:1246:VAL:HG22	2.19	0.43
1:L:1382:SER:O	1:L:1386:ILE:HD13	2.19	0.43
2:A:135:VAL:CG2	2:A:191:ILE:HD13	2.48	0.43
2:C:310:GLU:OE1	2:C:310:GLU:N	2.44	0.43
2:E:144:GLU:OE1	2:E:145:ASN:N	2.52	0.43
5:H:1199:VAL:HG12	5:H:1199:VAL:O	2.19	0.43
6:I:103:LEU:HD23	6:I:144:TYR:CE1	2.54	0.43
9:N:357:LEU:HD23	9:N:359:GLN:H	1.83	0.43
1:L:340:THR:HG22	1:L:340:THR:O	2.19	0.42
1:L:1117:VAL:O	1:L:1121:VAL:HG22	2.18	0.42
2:C:20:HIS:CE1	11:C:501:ADP:H2'	2.53	0.42
5:H:2356:ILE:HG13	5:H:2357:VAL:H	1.85	0.42
1:L:423:LEU:O	1:L:427:VAL:HG23	2.19	0.42
1:L:427:VAL:HG21	1:L:560:ILE:HG12	2.00	0.42
1:L:2349:VAL:O	1:L:2352:ILE:HG12	2.19	0.42
1:L:2863:ALA:HB1	1:L:2896:LEU:HD13	2.01	0.42
1:L:3504:ASP:O	1:L:3505:ALA:HB3	2.18	0.42
3:D:338:THR:OG1	3:D:339:SER:N	2.52	0.42
4:G:78:GLN:OE1	4:G:79:GLY:N	2.52	0.42
1:L:984:LEU:HD13	1:L:2503:ILE:HG21	1.99	0.42
1:L:1329:VAL:HG13	1:L:1332:HIS:H	1.84	0.42
1:L:1430:LEU:HD21	1:L:1448:LEU:HD12	2.01	0.42
3:D:63:ILE:HD13	3:D:295:VAL:HG21	2.00	0.42
3:D:180:GLU:O	3:D:183:THR:OG1	2.32	0.42
3:D:390:LEU:HD21	3:D:406:ILE:HG12	2.02	0.42
4:G:153:THR:HG23	4:G:156:GLU:H	1.84	0.42
6:I:151:LEU:HD23	6:I:151:LEU:H	1.84	0.42
1:L:1082:ASN:OD1	1:L:1083:GLY:N	2.46	0.42
2:C:189:ASP:OD1	2:C:190:VAL:N	2.53	0.42
2:C:315:LEU:HD23	2:C:354:LEU:HD11	2.01	0.42
4:G:174:ILE:O	4:G:178:TYR:N	2.52	0.42
1:L:663:SER:N	1:L:709:LEU:HD11	2.34	0.42
1:L:984:LEU:CD1	1:L:2503:ILE:HG21	2.50	0.42
1:L:2650:GLN:HB3	1:L:2651:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:24:LEU:HD21	2:A:49:CYS:HB2	2.00	0.42
6:I:41:ILE:N	6:I:85:ILE:O	2.45	0.42
6:I:73:ASN:O	6:I:77:VAL:HG22	2.19	0.42
6:J:156:VAL:HG23	6:J:187:VAL:HG23	2.00	0.42
9:N:306:THR:HG22	9:N:323:TYR:HB2	2.01	0.42
1:L:238:LEU:HD13	1:L:241:LEU:HD12	2.01	0.42
1:L:3113:PHE:O	1:L:3117:VAL:HG23	2.20	0.42
6:J:24:ARG:NH1	11:J:502:ADP:O2'	2.53	0.42
3:F:306:ILE:HD13	3:F:338:THR:CG2	2.49	0.42
6:J:334:GLY:O	6:J:341:ARG:NH2	2.52	0.42
1:L:239:TYR:CZ	1:L:243:ILE:HD11	2.54	0.42
1:L:3643:PHE:CE1	1:L:3669:ILE:HD12	2.55	0.42
2:E:256:ILE:O	2:E:256:ILE:HG22	2.19	0.42
2:E:265:LYS:O	2:E:267:LYS:N	2.49	0.42
1:L:348:ILE:N	1:L:349:PRO:HD2	2.33	0.42
1:L:1309:MET:SD	1:L:1339:LEU:HD21	2.60	0.42
1:L:2381:MET:O	1:L:2385:ILE:HG22	2.19	0.42
3:D:247:ILE:HG23	3:D:272:VAL:HG11	2.02	0.42
3:F:210:THR:HG22	3:F:210:THR:O	2.20	0.42
3:D:253:ARG:NH2	5:H:1843:THR:O	2.53	0.42
5:H:2226:LEU:HD13	5:H:2226:LEU:O	2.20	0.42
2:A:26:LEU:HD12	2:A:30:GLY:O	2.18	0.41
3:D:82:GLY:HA2	11:D:501:ADP:PA	2.60	0.41
3:F:141:GLU:N	3:F:164:LYS:O	2.51	0.41
5:H:846:SER:OG	9:N:205:ARG:NH2	2.53	0.41
1:L:1887:PHE:CE2	1:L:1891:LEU:HD11	2.55	0.41
1:L:2072:ASP:N	1:L:2072:ASP:OD1	2.53	0.41
2:A:33:LYS:O	2:A:46:ARG:NH1	2.53	0.41
2:A:170:LEU:C	2:A:170:LEU:HD12	2.39	0.41
2:E:40:VAL:H	11:E:501:ADP:HN62	1.67	0.41
4:G:72:LEU:HD21	5:H:796:TRP:HB2	2.02	0.41
6:I:317:LEU:N	6:I:317:LEU:HD23	2.35	0.41
1:L:1297:LEU:O	1:L:1305:GLN:NE2	2.53	0.41
1:L:3644:THR:HG22	1:L:3710:LEU:HD22	2.01	0.41
1:L:1803:GLN:HA	1:L:1803:GLN:OE1	2.21	0.41
1:L:2216:SER:HG	1:L:2218:TYR:HE1	1.68	0.41
1:L:3678:VAL:HG21	1:L:3681:PHE:CD2	2.56	0.41
3:D:107:GLU:OE2	2:E:317:ARG:NH2	2.49	0.41
6:J:21:TYR:CD2	11:J:502:ADP:H3'	2.48	0.41
1:L:462:TYR:CZ	1:L:1712:THR:HG21	2.55	0.41
1:L:1151:GLU:O	1:L:1157:LYS:NZ	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2214:VAL:HG12	1:L:2214:VAL:O	2.20	0.41
1:L:3344:LYS:O	1:L:3348:THR:HG22	2.20	0.41
5:H:794:ARG:NH1	6:J:31:ASP:OD1	2.53	0.41
5:H:2008:ALA:O	5:H:2012:ASN:OD1	2.38	0.41
6:I:387:VAL:HG22	6:I:387:VAL:O	2.21	0.41
6:J:269:VAL:HG22	6:J:305:PRO:CB	2.51	0.41
1:L:1050:THR:HG21	1:L:1121:VAL:CG2	2.48	0.41
1:L:1552:VAL:HG11	1:L:1585:VAL:CG2	2.50	0.41
1:L:2479:GLU:OE2	1:L:2601:HIS:NE2	2.53	0.41
2:C:76:LYS:N	11:C:501:ADP:O1B	2.54	0.41
4:G:114:TRP:NE1	7:K:117:GLU:OE1	2.48	0.41
5:H:1090:ILE:HD11	5:H:1210:LEU:HD11	2.02	0.41
6:I:171:ASP:OD1	6:I:172:SER:N	2.54	0.41
1:L:1937:HIS:O	1:L:1938:THR:OG1	2.29	0.41
1:L:2239:TYR:O	1:L:2281:LYS:NZ	2.45	0.41
5:H:2187:TYR:O	5:H:2188:THR:OG1	2.29	0.41
6:I:70:ILE:HD11	6:I:105:HIS:HB2	2.02	0.41
6:I:103:LEU:HD23	6:I:144:TYR:CZ	2.56	0.41
6:J:423:CYS:O	6:J:427:LYS:N	2.49	0.41
2:A:27:ASP:OD1	2:A:31:LEU:N	2.54	0.41
2:C:333:ARG:HH22	3:D:306:ILE:HD11	1.86	0.41
2:C:411:THR:HG21	3:D:71:ARG:HH21	1.86	0.41
3:D:247:ILE:HG23	3:D:272:VAL:CG1	2.51	0.41
7:K:178:LEU:CD2	7:K:180:LEU:HD11	2.51	0.41
1:L:557:VAL:O	1:L:561:THR:HG23	2.21	0.41
1:L:1171:LEU:HB3	1:L:1172:PRO:HD2	2.03	0.41
1:L:1957:TYR:N	1:L:1958:PRO:CD	2.84	0.41
1:L:2928:ALA:HB1	1:L:2980:HIS:NE2	2.35	0.41
3:B:33:LEU:O	3:B:40:ARG:NH2	2.53	0.41
3:D:49:GLN:HG3	3:D:52:ALA:HB3	2.02	0.41
3:F:47:VAL:HG12	3:F:370:ILE:CG2	2.04	0.41
3:F:400:ARG:NH2	11:F:501:ADP:PA	2.91	0.41
1:L:877:TRP:CD2	1:L:2908:VAL:HG21	2.56	0.41
1:L:1184:LEU:HG	1:L:1188:LEU:HD23	2.03	0.41
1:L:1366:ARG:O	1:L:1370:LEU:HD23	2.21	0.41
1:L:2400:LEU:HD13	1:L:2436:ILE:HG21	2.02	0.41
3:B:27:HIS:HE1	11:B:501:ADP:O2'	2.04	0.41
3:D:73:VAL:HG22	3:D:355:LEU:HD11	2.03	0.41
3:D:121:GLN:NE2	3:D:265:THR:OG1	2.54	0.41
3:F:116:THR:HG23	3:F:311:PHE:CE1	2.56	0.41
4:G:105:ARG:NH2	6:J:410:TRP:O	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:137:ILE:HD11	1:L:220:LEU:HD12	2.04	0.40
1:L:1194:LEU:HD12	1:L:1199:SER:HB2	2.02	0.40
1:L:2449:LYS:O	1:L:2455:ARG:NE	2.51	0.40
3:B:249:VAL:O	3:B:250:ILE:HD13	2.21	0.40
3:D:329:ASN:O	3:D:329:ASN:ND2	2.54	0.40
3:D:354:LEU:HD12	3:D:354:LEU:C	2.42	0.40
5:H:1777:LEU:N	5:H:1777:LEU:HD22	2.36	0.40
6:I:10:GLU:N	6:I:10:GLU:OE1	2.54	0.40
7:K:219:VAL:HG23	7:K:306:TYR:HB3	2.02	0.40
1:L:1303:ASN:OD1	1:L:1304:ALA:N	2.54	0.40
1:L:1386:ILE:N	1:L:1386:ILE:HD12	2.35	0.40
3:F:63:ILE:HD13	3:F:295:VAL:CG2	2.51	0.40
6:J:267:LEU:HD12	6:J:301:ARG:O	2.22	0.40
1:L:143:PHE:CD1	1:L:228:LEU:HD13	2.57	0.40
1:L:1309:MET:O	1:L:1313:THR:HG23	2.20	0.40
1:L:2208:GLU:N	1:L:2209:PRO:HD2	2.37	0.40
1:L:2357:VAL:HG12	1:L:2374:LYS:HD3	2.04	0.40
1:L:2472:PHE:CE2	1:L:2474:ILE:HD11	2.56	0.40
1:L:2659:GLU:OE2	1:L:2687:ARG:NE	2.46	0.40
6:J:108:LYS:HG2	6:J:109:MET:CE	2.52	0.40
7:K:190:MET:HG3	7:K:209:VAL:HG11	2.03	0.40
1:L:935:LEU:HD11	1:L:2618:LEU:HD23	2.02	0.40
1:L:3241:ARG:NH1	1:L:3548:VAL:O	2.54	0.40
1:L:3759:ASP:OD1	1:L:3760:THR:HG23	2.21	0.40
3:B:336:ARG:NH2	2:C:310:GLU:OE2	2.44	0.40
3:D:409:ALA:HB1	3:D:421:VAL:HG11	2.02	0.40
3:F:83:LYS:NZ	3:F:329:ASN:OD1	2.44	0.40
4:G:237:THR:OG1	4:G:238:PRO:HD3	2.21	0.40
6:I:11:VAL:HG12	6:I:11:VAL:O	2.22	0.40
6:J:226:LYS:NZ	7:K:319:ALA:O	2.49	0.40
1:L:719:GLY:O	1:L:722:SER:OG	2.33	0.40
1:L:1145:LEU:HD13	1:L:1163:SER:HB2	2.03	0.40
1:L:1939:VAL:O	1:L:1940:PRO:C	2.59	0.40
1:L:2173:LYS:N	1:L:2174:PRO:CD	2.84	0.40
1:L:2393:LEU:HD12	1:L:2394:GLU:N	2.36	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	L	3453/3830 (90%)	3332 (96%)	121 (4%)	0	100	100
2	A	422/456 (92%)	410 (97%)	12 (3%)	0	100	100
2	C	410/456 (90%)	394 (96%)	16 (4%)	0	100	100
2	E	433/456 (95%)	419 (97%)	14 (3%)	0	100	100
3	B	391/463 (84%)	374 (96%)	17 (4%)	0	100	100
3	D	423/463 (91%)	406 (96%)	17 (4%)	0	100	100
3	F	411/463 (89%)	397 (97%)	14 (3%)	0	100	100
4	G	197/467 (42%)	187 (95%)	10 (5%)	0	100	100
5	H	987/3123 (32%)	937 (95%)	50 (5%)	0	100	100
6	I	341/429 (80%)	326 (96%)	15 (4%)	0	100	100
6	J	399/429 (93%)	377 (94%)	22 (6%)	0	100	100
7	K	346/375 (92%)	335 (97%)	11 (3%)	0	100	100
8	M	102/813 (12%)	97 (95%)	5 (5%)	0	100	100
9	N	144/364 (40%)	129 (90%)	15 (10%)	0	100	100
All	All	8459/12587 (67%)	8120 (96%)	339 (4%)	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	L	3112/3396 (92%)	3064 (98%)	48 (2%)	60 75
2	A	360/387 (93%)	359 (100%)	1 (0%)	91 92
2	C	353/387 (91%)	348 (99%)	5 (1%)	62 75
2	E	367/387 (95%)	363 (99%)	4 (1%)	70 80
3	B	338/390 (87%)	338 (100%)	0	100 100
3	D	359/390 (92%)	352 (98%)	7 (2%)	52 69
3	F	352/390 (90%)	351 (100%)	1 (0%)	91 92
4	G	179/400 (45%)	177 (99%)	2 (1%)	70 80
5	H	902/2634 (34%)	893 (99%)	9 (1%)	73 82
6	I	299/364 (82%)	295 (99%)	4 (1%)	65 77
6	J	343/364 (94%)	339 (99%)	4 (1%)	67 78
7	K	297/318 (93%)	297 (100%)	0	100 100
8	M	91/718 (13%)	90 (99%)	1 (1%)	70 80
9	N	130/312 (42%)	127 (98%)	3 (2%)	45 64
All	All	7482/10837 (69%)	7393 (99%)	89 (1%)	66 78

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	85	PRO
1	L	119	ARG
1	L	290	PHE
1	L	320	CYS
1	L	358	SER
1	L	368	ARG
1	L	371	LEU
1	L	402	PHE
1	L	456	PHE
1	L	535	LYS
1	L	624	ARG
1	L	645	LEU
1	L	778	GLU
1	L	897	LYS
1	L	904	LYS
1	L	912	LEU
1	L	927	GLU
1	L	939	MET
1	L	1146	CYS

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Mol	Chain	Res	Type
1	L	1343	CYS
1	L	1526	ARG
1	L	1537	ARG
1	L	1650	ARG
1	L	1701	ARG
1	L	1707	PHE
1	L	1742	ASN
1	L	1763	PHE
1	L	1769	LYS
1	L	1785	ASN
1	L	1811	ARG
1	L	1879	HIS
1	L	1885	GLN
1	L	1986	ARG
1	L	2121	TRP
1	L	2158	PHE
1	L	2373	GLU
1	L	2393	LEU
1	L	2571	HIS
1	L	2676	LYS
1	L	2691	MET
1	L	3069	CYS
1	L	3127	TRP
1	L	3166	SER
1	L	3220	LEU
1	L	3300	ARG
1	L	3529	LYS
1	L	3530	ARG
1	L	3596	ARG
2	A	172	LEU
2	C	201	LYS
2	C	205	ARG
2	C	264	MET
2	C	274	LYS
2	C	378	ARG
3	D	21	ARG
3	D	88	MET
3	D	269	LYS
3	D	355	LEU
3	D	400	ARG
3	D	428	ARG
3	D	444	LYS

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Mol	Chain	Res	Type
2	E	18	HIS
2	E	184	ARG
2	E	249	ARG
2	E	316	HIS
3	F	257	PHE
4	G	66	LYS
4	G	226	ARG
5	H	776	TRP
5	H	1200	PHE
5	H	1749	TRP
5	H	1928	ARG
5	H	1976	ARG
5	H	2010	GLN
5	H	2279	ARG
5	H	2389	TYR
5	H	2396	ARG
6	I	130	ARG
6	I	204	MET
6	I	210	PHE
6	I	213	MET
6	J	22	THR
6	J	230	ARG
6	J	302	LEU
6	J	363	ARG
8	M	433	LEU
9	N	181	GLU
9	N	282	ARG
9	N	314	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	51	ASN
1	L	245	ASN
1	L	463	GLN
1	L	598	GLN
1	L	604	GLN
1	L	619	ASN
1	L	621	GLN
1	L	844	GLN
1	L	1056	GLN
1	L	1269	GLN

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Mol	Chain	Res	Type
1	L	1287	GLN
1	L	1371	ASN
1	L	1671	ASN
1	L	2513	HIS
1	L	2627	GLN
1	L	2650	GLN
1	L	2695	GLN
1	L	2828	HIS
1	L	2906	HIS
1	L	3295	GLN
1	L	3406	HIS
1	L	3480	HIS
1	L	3492	HIS
1	L	3827	HIS
2	A	18	HIS
3	B	49	GLN
3	B	302	HIS
2	C	13	GLN
2	C	20	HIS
3	D	121	GLN
3	D	302	HIS
2	E	42	GLN
2	E	115	ASN
2	E	241	HIS
2	E	254	GLN
2	E	373	GLN
3	F	27	HIS
3	F	226	GLN
5	H	792	GLN
5	H	1261	HIS
5	H	1858	GLN
5	H	2010	GLN
5	H	2373	ASN
5	H	2384	GLN
5	H	2387	ASN
5	H	2428	HIS
6	I	128	ASN
6	I	205	GLN
6	I	383	ASN
6	J	190	GLN
6	J	251	HIS
7	K	12	ASN

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Mol	Chain	Res	Type
7	K	88	HIS
7	K	92	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	IHP	L	3901	-	36,36,36	0.74	0	54,60,60	1.41	7 (12%)
11	ADP	B	501	-	24,29,29	1.04	2 (8%)	29,45,45	1.47	3 (10%)
11	ADP	J	502	-	24,29,29	0.96	1 (4%)	29,45,45	1.41	5 (17%)
11	ADP	A	501	-	24,29,29	0.93	1 (4%)	29,45,45	1.59	5 (17%)
11	ADP	I	501	-	24,29,29	1.08	2 (8%)	29,45,45	1.52	4 (13%)
11	ADP	F	501	-	24,29,29	1.07	1 (4%)	29,45,45	1.70	5 (17%)
11	ADP	C	501	-	24,29,29	0.93	1 (4%)	29,45,45	1.61	4 (13%)
11	ADP	K	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.64	5 (17%)
11	ADP	D	501	-	24,29,29	0.98	1 (4%)	29,45,45	1.54	4 (13%)
11	ADP	E	501	-	24,29,29	1.00	1 (4%)	29,45,45	1.56	6 (20%)

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
10	IHP	L	3901	-	-	6/30/54/54	0/1/1/1
11	ADP	B	501	-	-	5/12/32/32	0/3/3/3
11	ADP	J	502	-	-	4/12/32/32	0/3/3/3
11	ADP	A	501	-	-	5/12/32/32	0/3/3/3
11	ADP	I	501	-	-	4/12/32/32	0/3/3/3
11	ADP	F	501	-	-	4/12/32/32	0/3/3/3
11	ADP	C	501	-	-	3/12/32/32	0/3/3/3
11	ADP	K	401	-	-	4/12/32/32	0/3/3/3
11	ADP	D	501	-	-	5/12/32/32	0/3/3/3
11	ADP	E	501	-	-	6/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	501	ADP	C5-C4	3.00	1.48	1.40
11	B	501	ADP	C5-C4	2.75	1.48	1.40
11	I	501	ADP	C5-C4	2.72	1.48	1.40
11	C	501	ADP	C5-C4	2.61	1.47	1.40
11	K	401	ADP	C5-C4	2.49	1.47	1.40
11	A	501	ADP	C5-C4	2.48	1.47	1.40
11	D	501	ADP	C5-C4	2.47	1.47	1.40
11	J	502	ADP	C5-C4	2.45	1.47	1.40
11	E	501	ADP	C5-C4	2.38	1.47	1.40
11	B	501	ADP	O4'-C1'	2.05	1.43	1.41
11	I	501	ADP	C2-N3	2.05	1.35	1.32

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	F	501	ADP	C4-C5-N7	-4.61	104.60	109.40
11	D	501	ADP	PA-O3A-PB	-4.46	117.52	132.83
11	C	501	ADP	PA-O3A-PB	-4.19	118.45	132.83
11	K	401	ADP	PA-O3A-PB	-4.00	119.10	132.83
11	A	501	ADP	PA-O3A-PB	-3.95	119.28	132.83
11	B	501	ADP	C4-C5-N7	-3.94	105.29	109.40
11	E	501	ADP	PA-O3A-PB	-3.92	119.38	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	F	501	ADP	PA-O3A-PB	-3.86	119.57	132.83
11	I	501	ADP	C3'-C2'-C1'	3.53	106.30	100.98
11	B	501	ADP	PA-O3A-PB	-3.50	120.82	132.83
11	K	401	ADP	C4-C5-N7	-3.40	105.85	109.40
11	I	501	ADP	PA-O3A-PB	-3.36	121.30	132.83
11	E	501	ADP	N3-C2-N1	-3.29	123.53	128.68
11	A	501	ADP	N3-C2-N1	-3.17	123.72	128.68
11	A	501	ADP	C3'-C2'-C1'	3.16	105.73	100.98
11	J	502	ADP	N3-C2-N1	-3.12	123.80	128.68
10	L	3901	IHP	O14-C4-C3	3.07	115.93	108.69
11	C	501	ADP	N3-C2-N1	-3.06	123.90	128.68
11	J	502	ADP	PA-O3A-PB	-3.04	122.39	132.83
11	F	501	ADP	C3'-C2'-C1'	3.00	105.50	100.98
11	D	501	ADP	N3-C2-N1	-2.93	124.10	128.68
11	D	501	ADP	C4-C5-N7	-2.91	106.37	109.40
11	I	501	ADP	N3-C2-N1	-2.89	124.16	128.68
11	B	501	ADP	N3-C2-N1	-2.84	124.24	128.68
10	L	3901	IHP	O14-C4-C5	2.80	115.30	108.69
11	K	401	ADP	O3'-C3'-C4'	-2.80	102.94	111.05
10	L	3901	IHP	C6-C5-C4	2.78	116.50	110.41
11	K	401	ADP	N3-C2-N1	-2.73	124.42	128.68
11	C	501	ADP	C3'-C2'-C1'	2.73	105.08	100.98
11	J	502	ADP	C3'-C2'-C1'	2.72	105.08	100.98
11	E	501	ADP	C5'-C4'-C3'	-2.70	105.05	115.18
10	L	3901	IHP	C5-C4-C3	-2.70	104.51	110.41
11	I	501	ADP	C4-C5-N7	-2.63	106.66	109.40
11	D	501	ADP	C3'-C2'-C1'	2.58	104.86	100.98
11	J	502	ADP	C4-C5-N7	-2.56	106.73	109.40
10	L	3901	IHP	C6-C1-C2	2.55	116.00	110.41
11	A	501	ADP	C4-C5-N7	-2.44	106.85	109.40
11	F	501	ADP	N3-C2-N1	-2.44	124.86	128.68
11	J	502	ADP	C2'-C3'-C4'	2.38	107.27	102.64
10	L	3901	IHP	C5-C6-C1	2.35	115.55	110.41
11	C	501	ADP	C4-C5-N7	-2.33	106.97	109.40
11	E	501	ADP	C4-C5-N7	-2.33	106.97	109.40
11	E	501	ADP	C2'-C3'-C4'	2.27	107.06	102.64
10	L	3901	IHP	O15-P5-O25	-2.18	100.96	109.39
11	F	501	ADP	C5-C6-N6	2.17	123.65	120.35
11	E	501	ADP	C3'-C2'-C1'	2.16	104.22	100.98
11	K	401	ADP	O3B-PB-O2B	2.04	115.44	107.64
11	A	501	ADP	C2-N1-C6	2.03	122.22	118.75

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	501	ADP	O4'-C4'-C5'-O5'
11	B	501	ADP	C5'-O5'-PA-O1A
11	B	501	ADP	C5'-O5'-PA-O2A
11	C	501	ADP	C5'-O5'-PA-O1A
11	C	501	ADP	C5'-O5'-PA-O2A
11	D	501	ADP	C5'-O5'-PA-O3A
11	E	501	ADP	C5'-O5'-PA-O1A
11	E	501	ADP	C5'-O5'-PA-O2A
11	E	501	ADP	O4'-C4'-C5'-O5'
11	F	501	ADP	C5'-O5'-PA-O3A
11	I	501	ADP	C5'-O5'-PA-O2A
11	I	501	ADP	C5'-O5'-PA-O3A
11	J	502	ADP	C5'-O5'-PA-O3A
11	K	401	ADP	C5'-O5'-PA-O1A
11	K	401	ADP	C5'-O5'-PA-O2A
11	D	501	ADP	O4'-C4'-C5'-O5'
11	D	501	ADP	C3'-C4'-C5'-O5'
11	E	501	ADP	C3'-C4'-C5'-O5'
11	F	501	ADP	O4'-C4'-C5'-O5'
11	F	501	ADP	C3'-C4'-C5'-O5'
10	L	3901	IHP	C4-C3-O13-P3
11	I	501	ADP	PA-O3A-PB-O3B
11	J	502	ADP	PA-O3A-PB-O3B
10	L	3901	IHP	C1-O11-P1-O41
11	A	501	ADP	C5'-O5'-PA-O3A
11	D	501	ADP	C5'-O5'-PA-O1A
11	F	501	ADP	C5'-O5'-PA-O1A
11	J	502	ADP	C5'-O5'-PA-O2A
11	D	501	ADP	C4'-C5'-O5'-PA
11	B	501	ADP	O4'-C4'-C5'-O5'
11	E	501	ADP	PB-O3A-PA-O2A
10	L	3901	IHP	C4-O14-P4-O24
11	A	501	ADP	C3'-C4'-C5'-O5'
11	K	401	ADP	O4'-C4'-C5'-O5'
11	A	501	ADP	PA-O3A-PB-O2B
11	B	501	ADP	PA-O3A-PB-O2B
10	L	3901	IHP	C1-O11-P1-O31
10	L	3901	IHP	C2-O12-P2-O42
10	L	3901	IHP	C3-O13-P3-O33
11	B	501	ADP	C5'-O5'-PA-O3A
11	C	501	ADP	C5'-O5'-PA-O3A
11	E	501	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
11	K	401	ADP	C5'-O5'-PA-O3A
11	A	501	ADP	C5'-O5'-PA-O1A
11	I	501	ADP	O4'-C4'-C5'-O5'
11	J	502	ADP	O4'-C4'-C5'-O5'

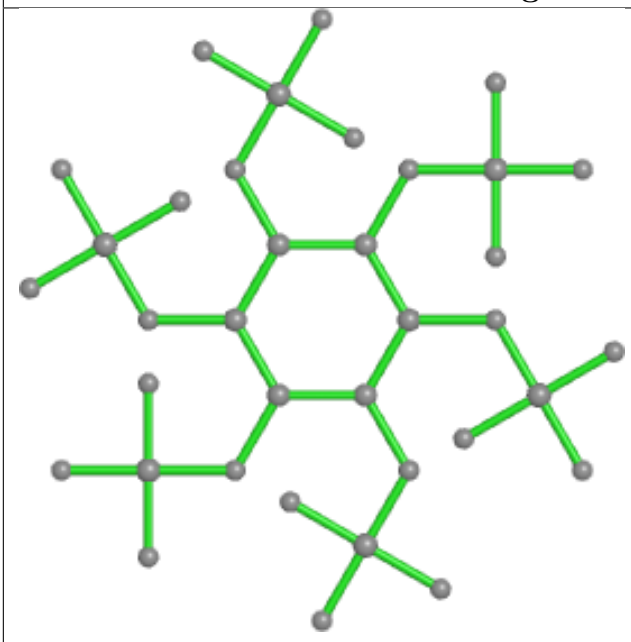
There are no ring outliers.

9 monomers are involved in 139 short contacts:

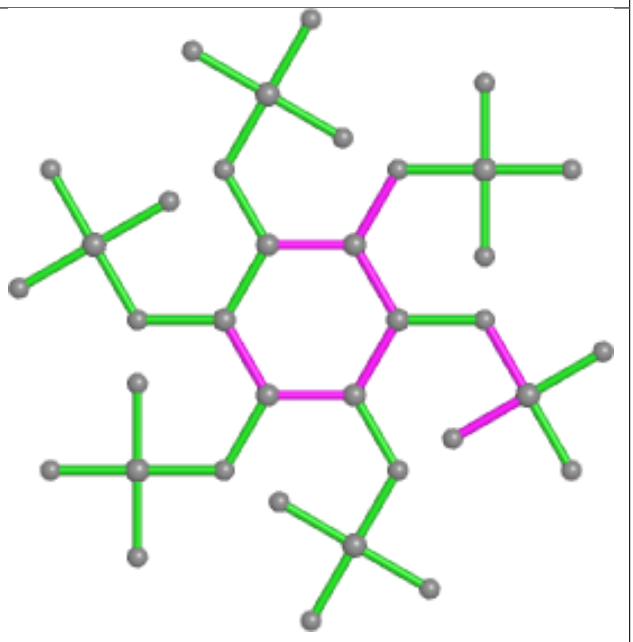
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	501	ADP	9	0
11	J	502	ADP	6	0
11	A	501	ADP	14	0
11	I	501	ADP	23	0
11	F	501	ADP	10	0
11	C	501	ADP	29	0
11	K	401	ADP	17	0
11	D	501	ADP	11	0
11	E	501	ADP	20	0

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.

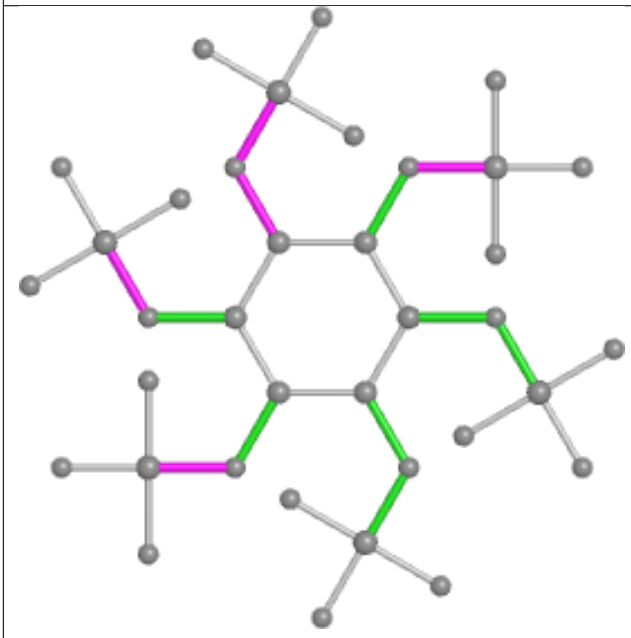
Ligand IHP L 3901



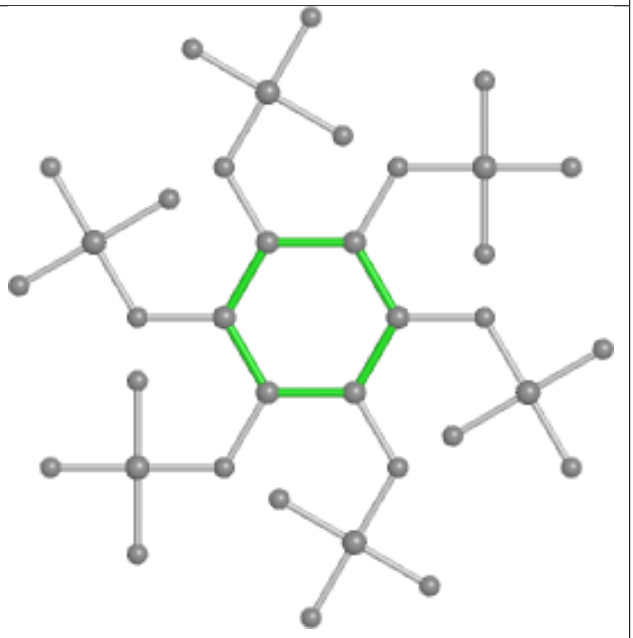
Bond lengths



Bond angles

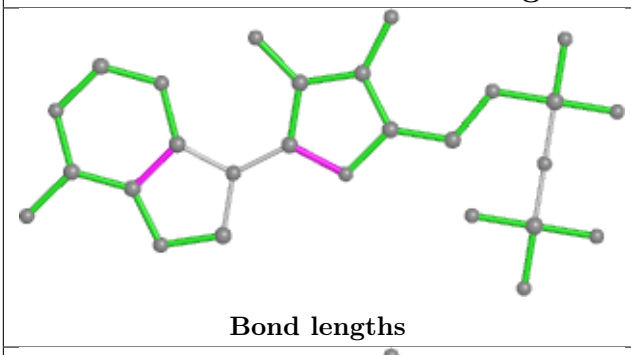


Torsions



Rings

Ligand ADP B 501



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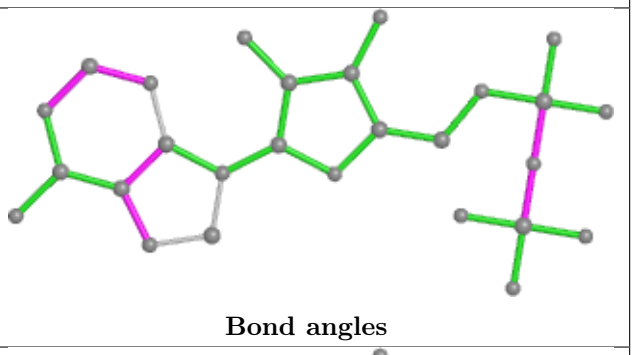
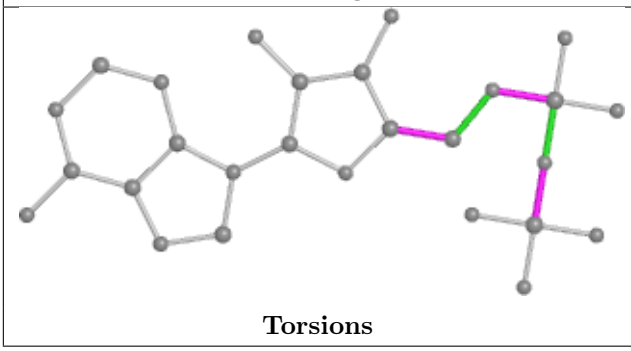


Bond angles



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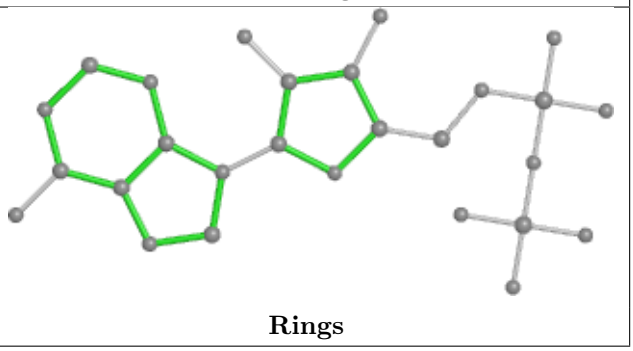
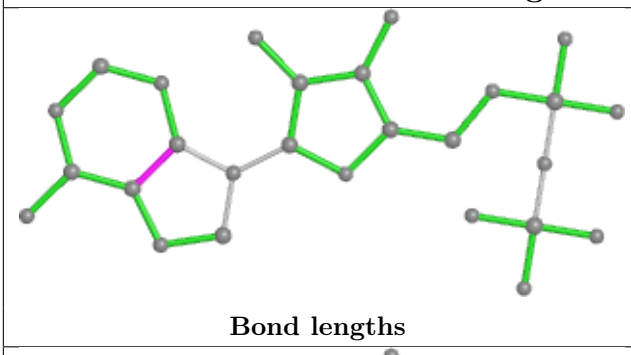


Rings

Ligand ADP J 502



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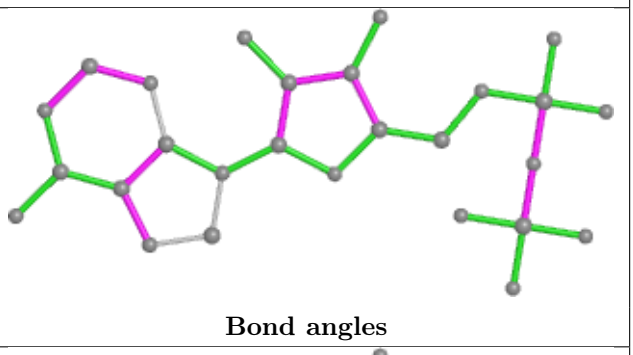

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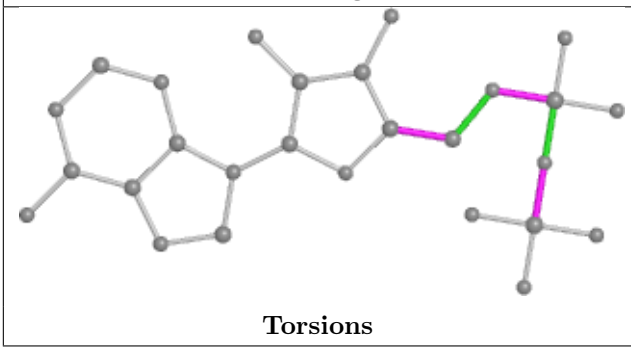

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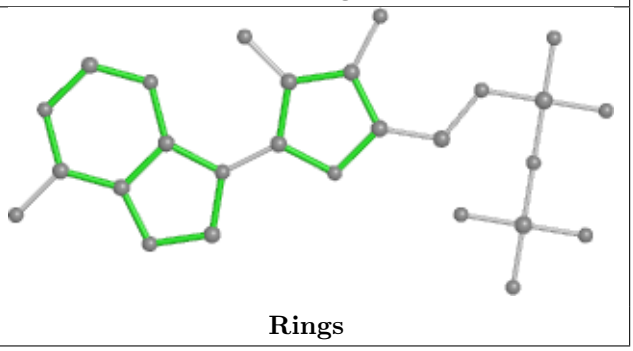
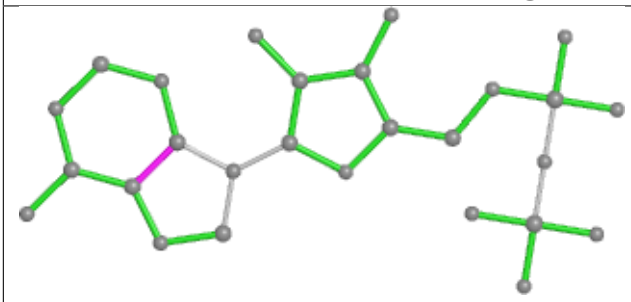
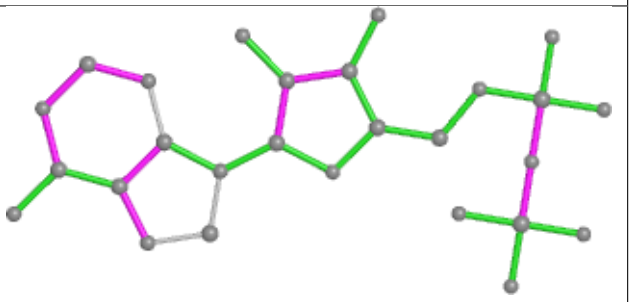
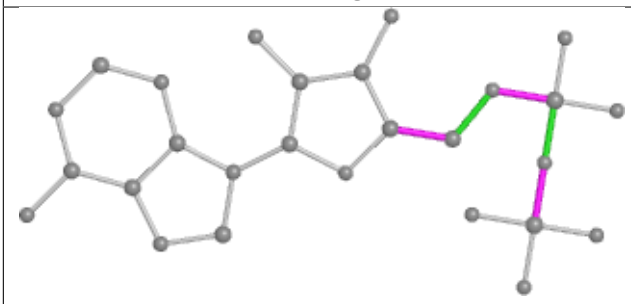
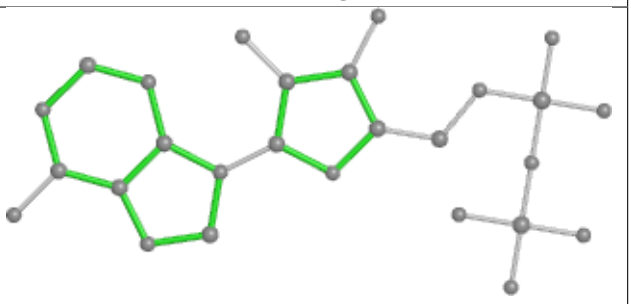
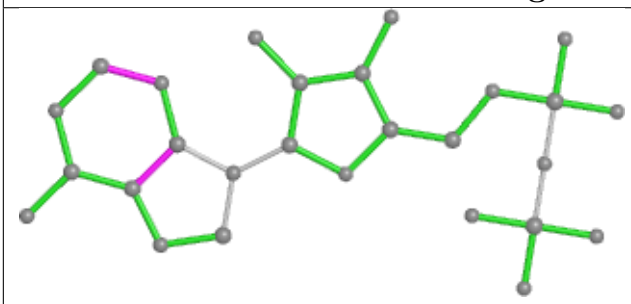
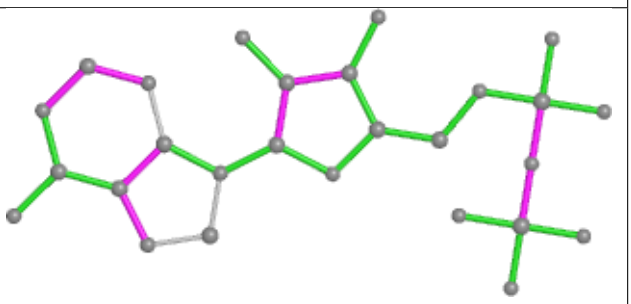
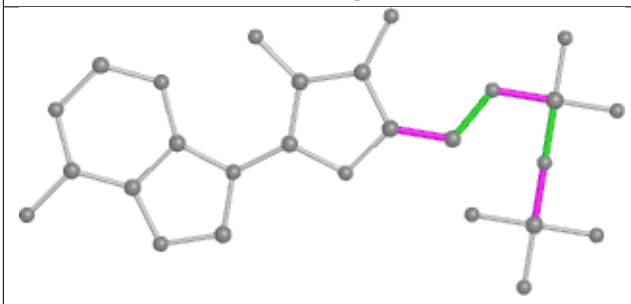
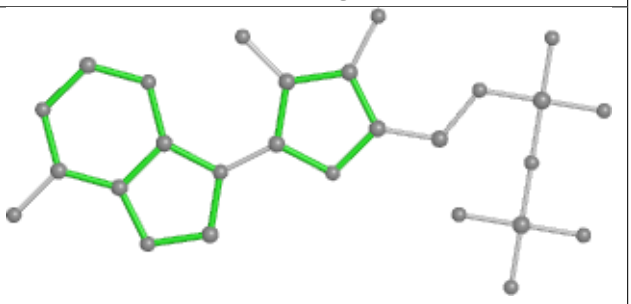
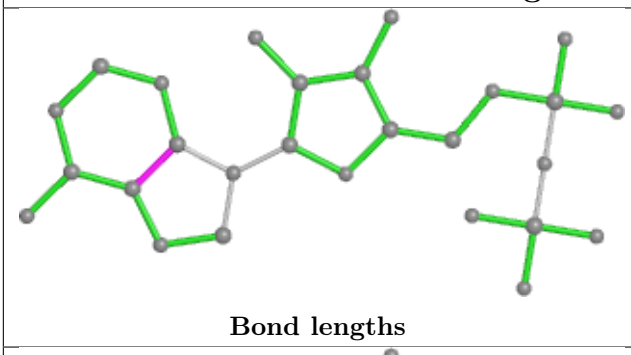


Rings

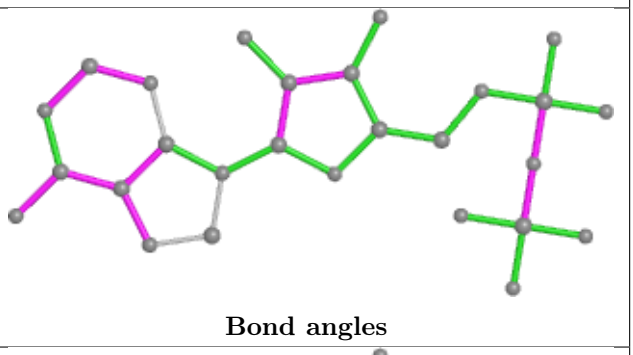
Ligand ADP A 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP I 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

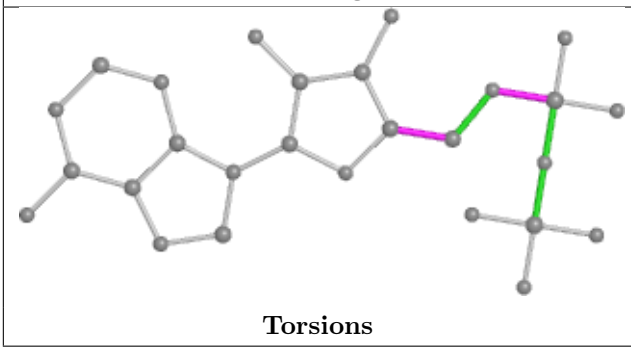
Ligand ADP F 501



Bond lengths



Bond angles



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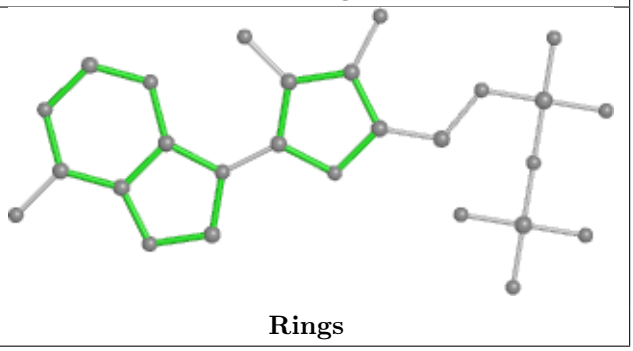
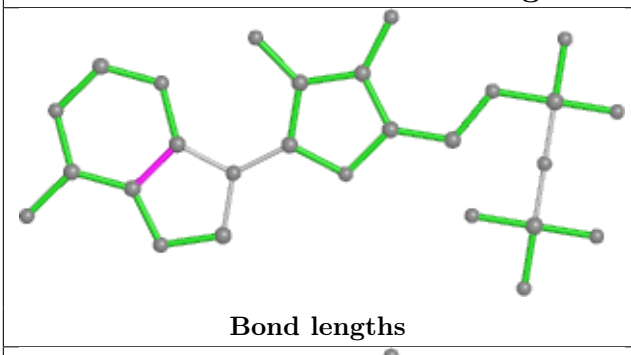
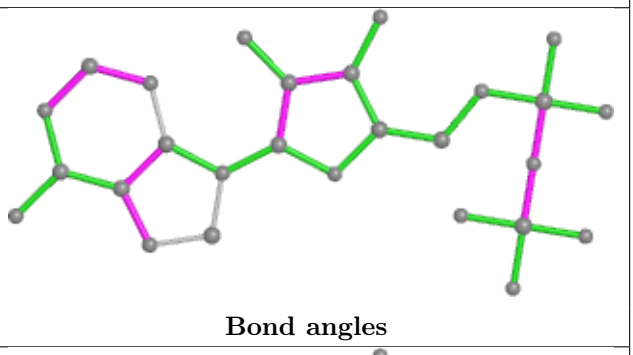


Rings

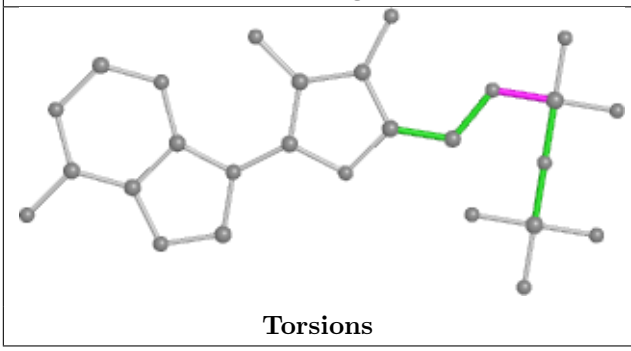
Ligand ADP C 501



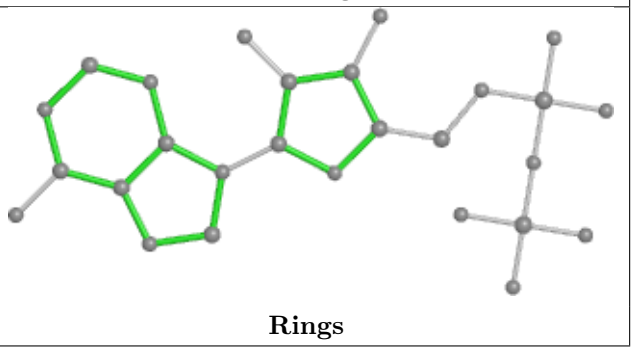
Bond lengths



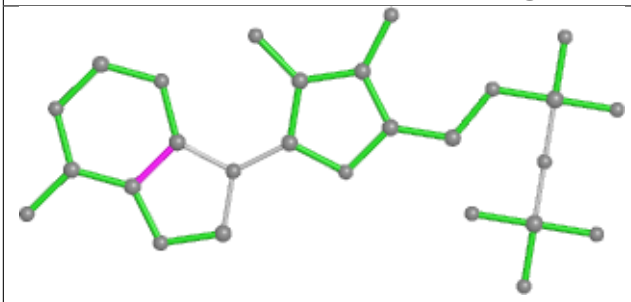
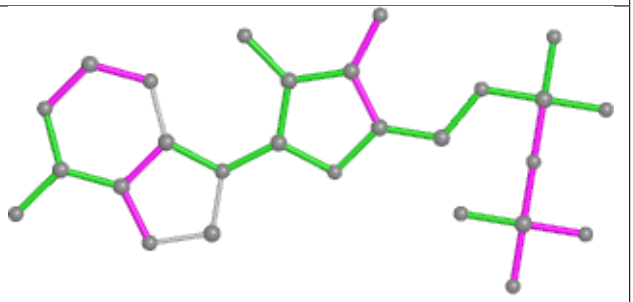
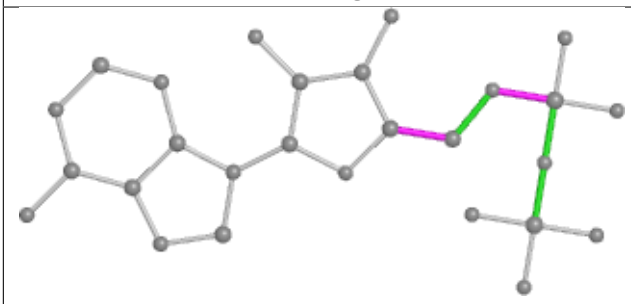
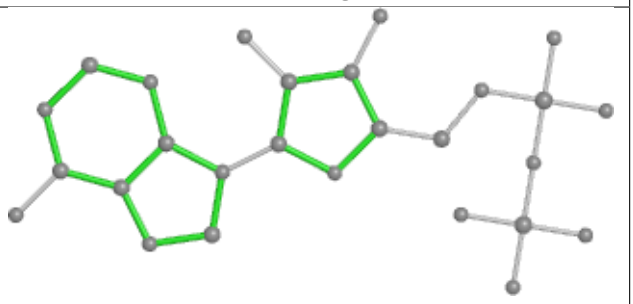
Bond angles

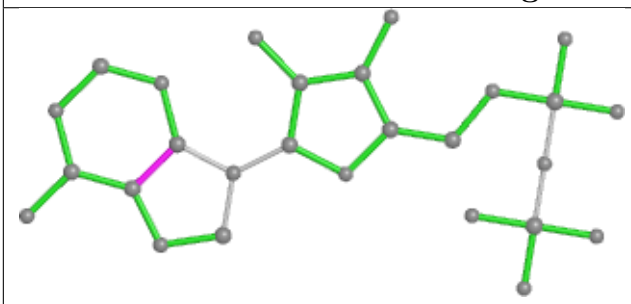
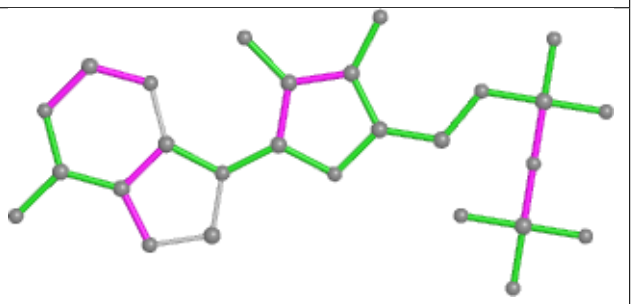
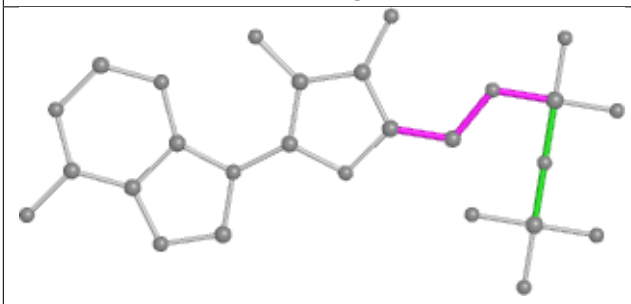
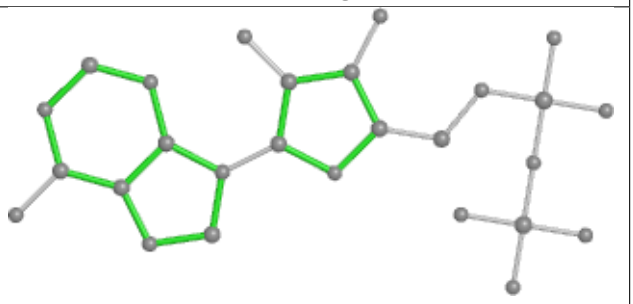


Torsions

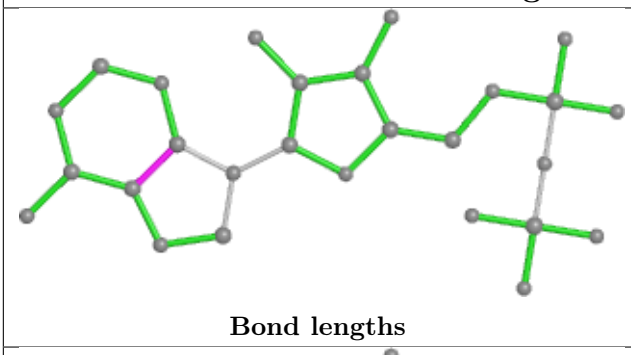


Rings

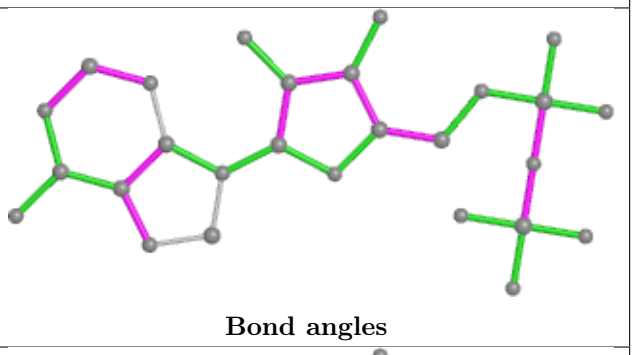
Ligand ADP K 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

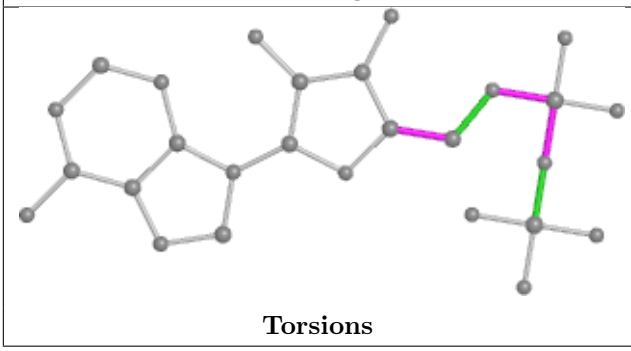
Ligand ADP E 501



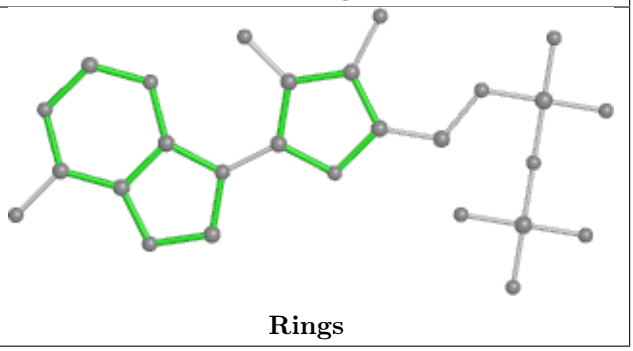
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

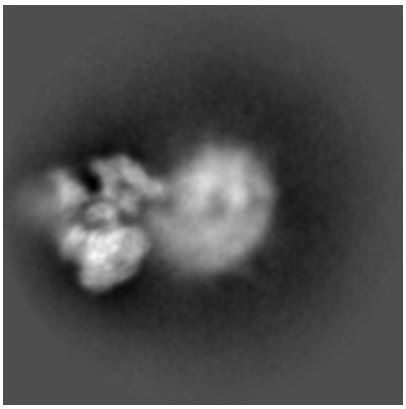
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38703. These allow visual inspection of the internal detail of the map and identification of artifacts.

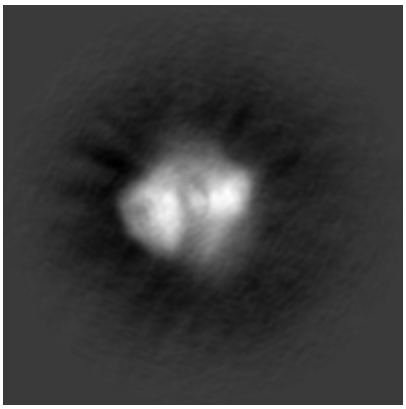
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

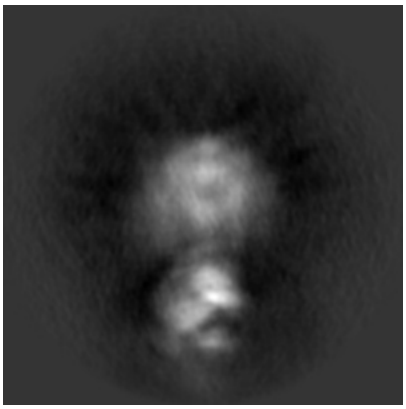
6.1.1 Primary map



X

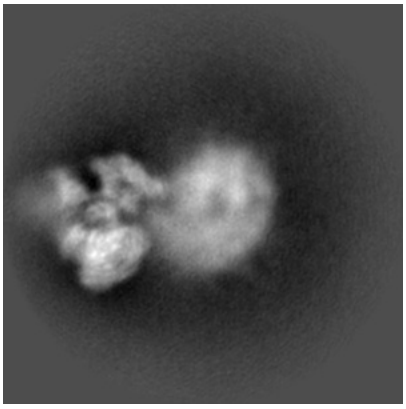


Y

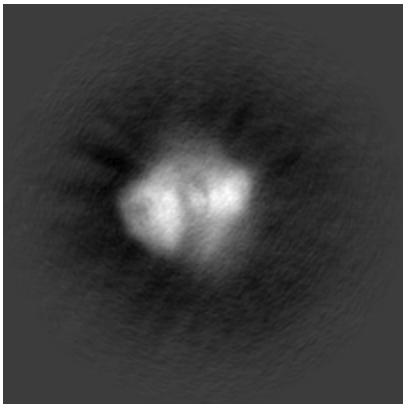


Z

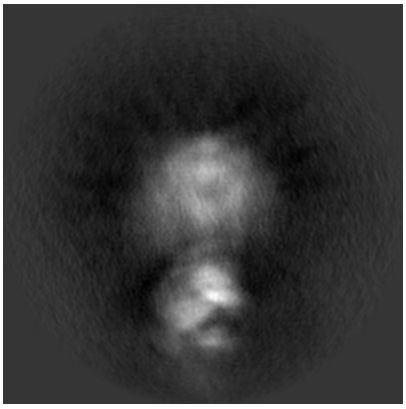
6.1.2 Raw map



X



Y

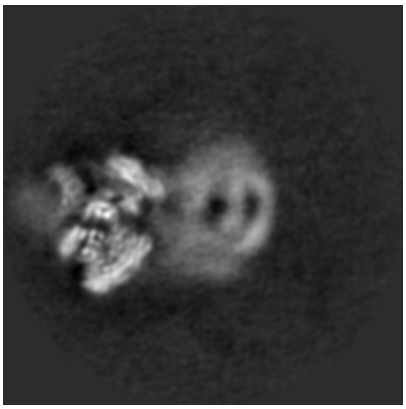


Z

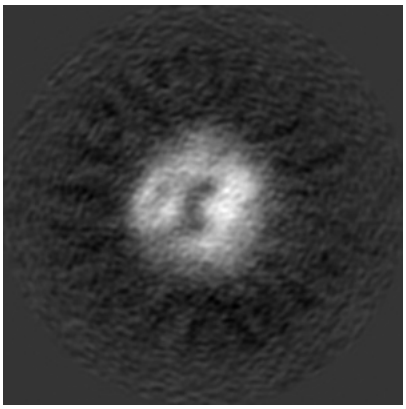
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

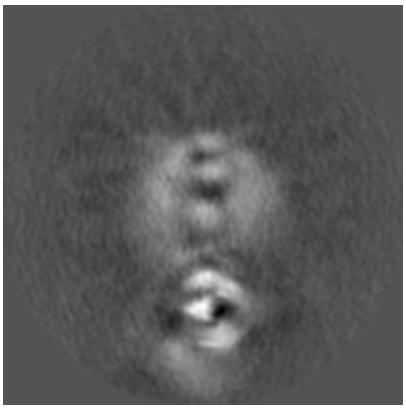
6.2.1 Primary map



X Index: 100

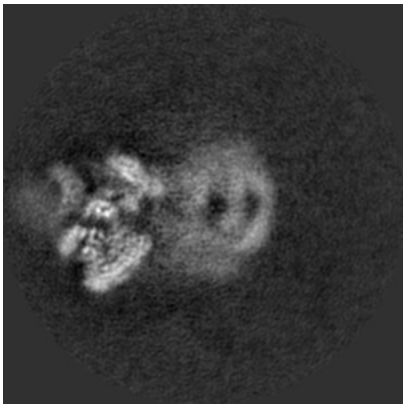


Y Index: 100

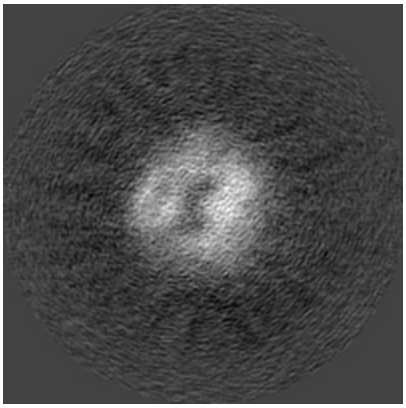


Z Index: 100

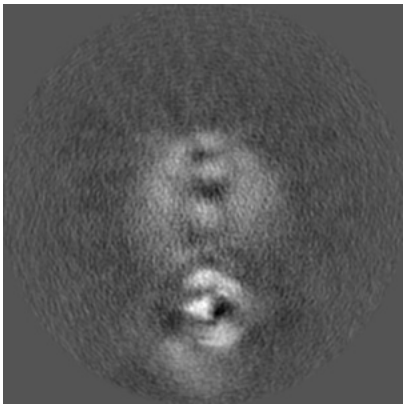
6.2.2 Raw map



X Index: 100



Y Index: 100

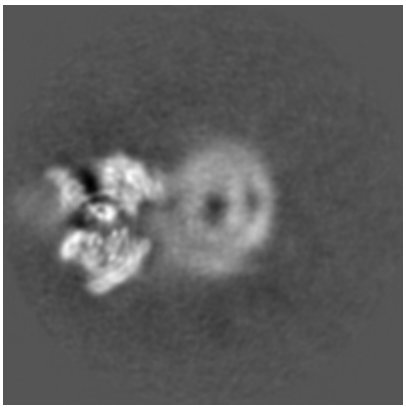


Z Index: 100

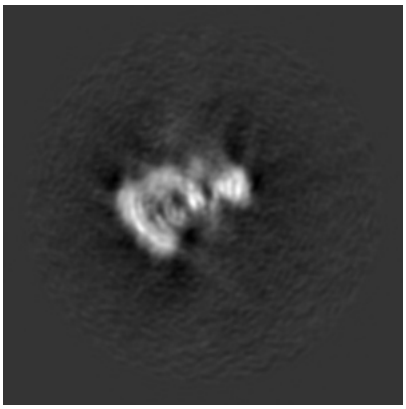
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

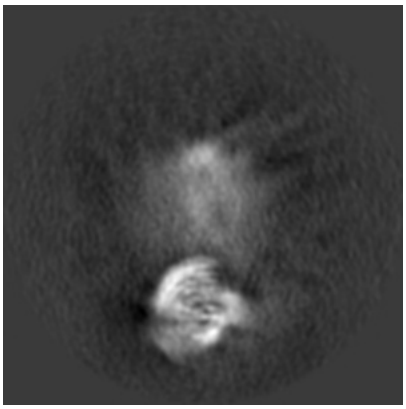
6.3.1 Primary map



X Index: 104

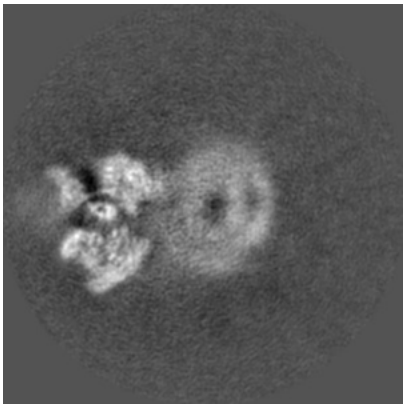


Y Index: 52

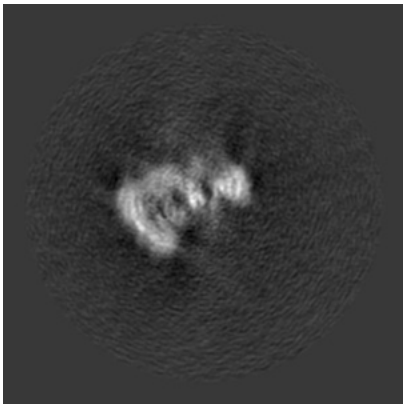


Z Index: 82

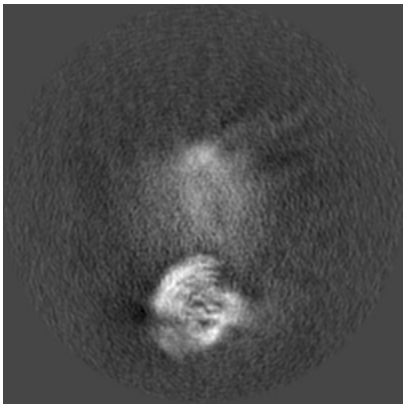
6.3.2 Raw map



X Index: 104



Y Index: 52

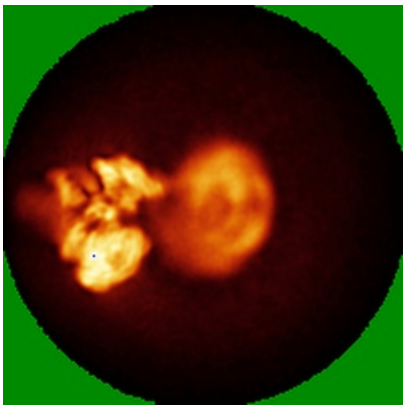


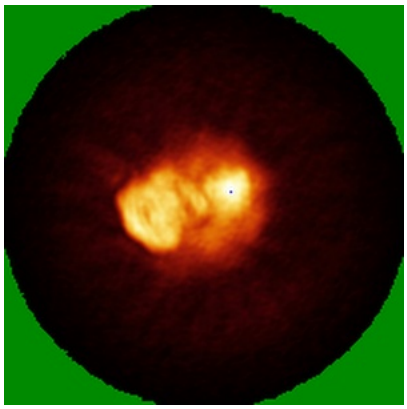
Z Index: 81

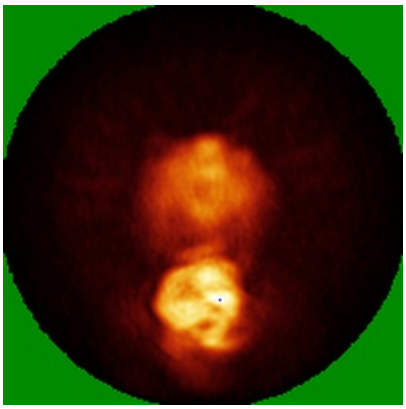
The images above show the largest variance slices of the map in three orthogonal directions.

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

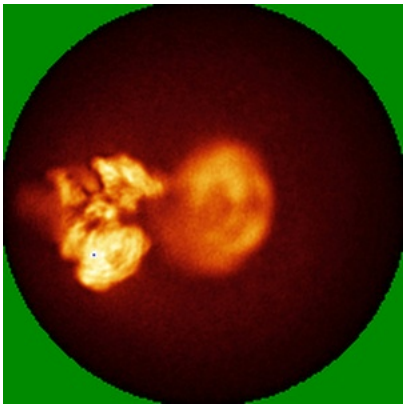
6.4.1 Primary map

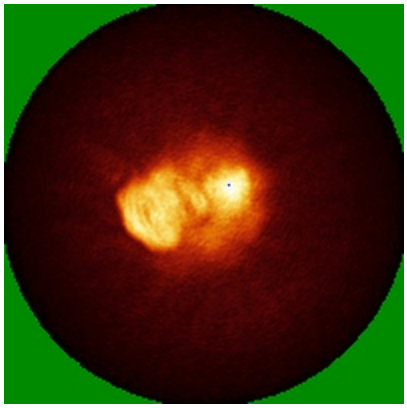

X

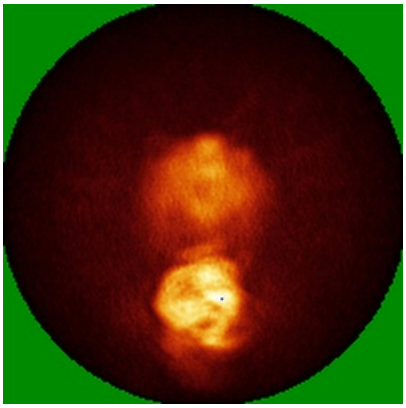

Y


Z

6.4.2 Raw map


X

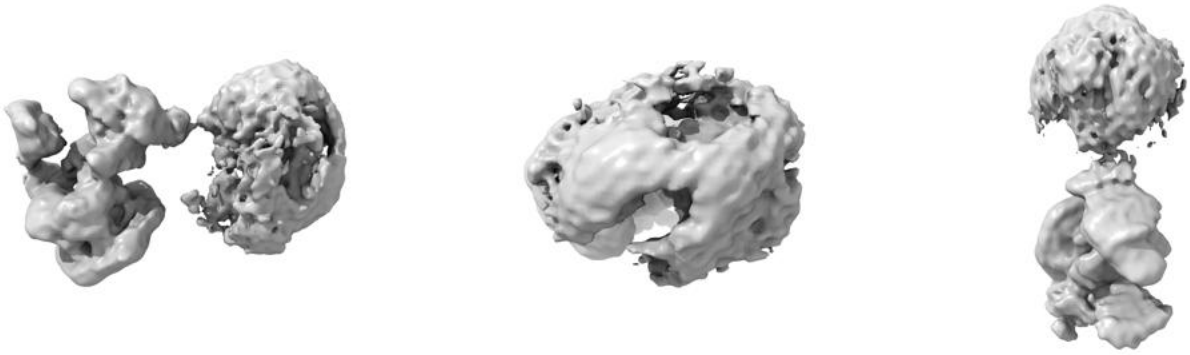

Y


Z

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

6.5 Orthogonal surface views (i)

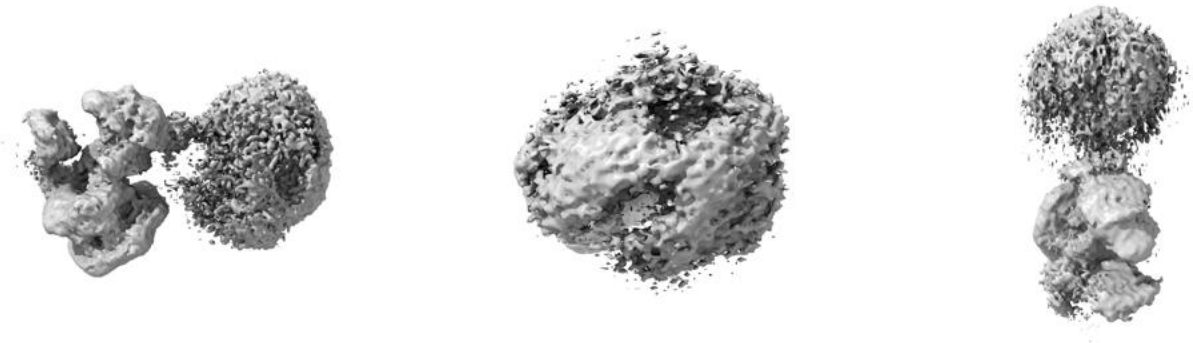
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

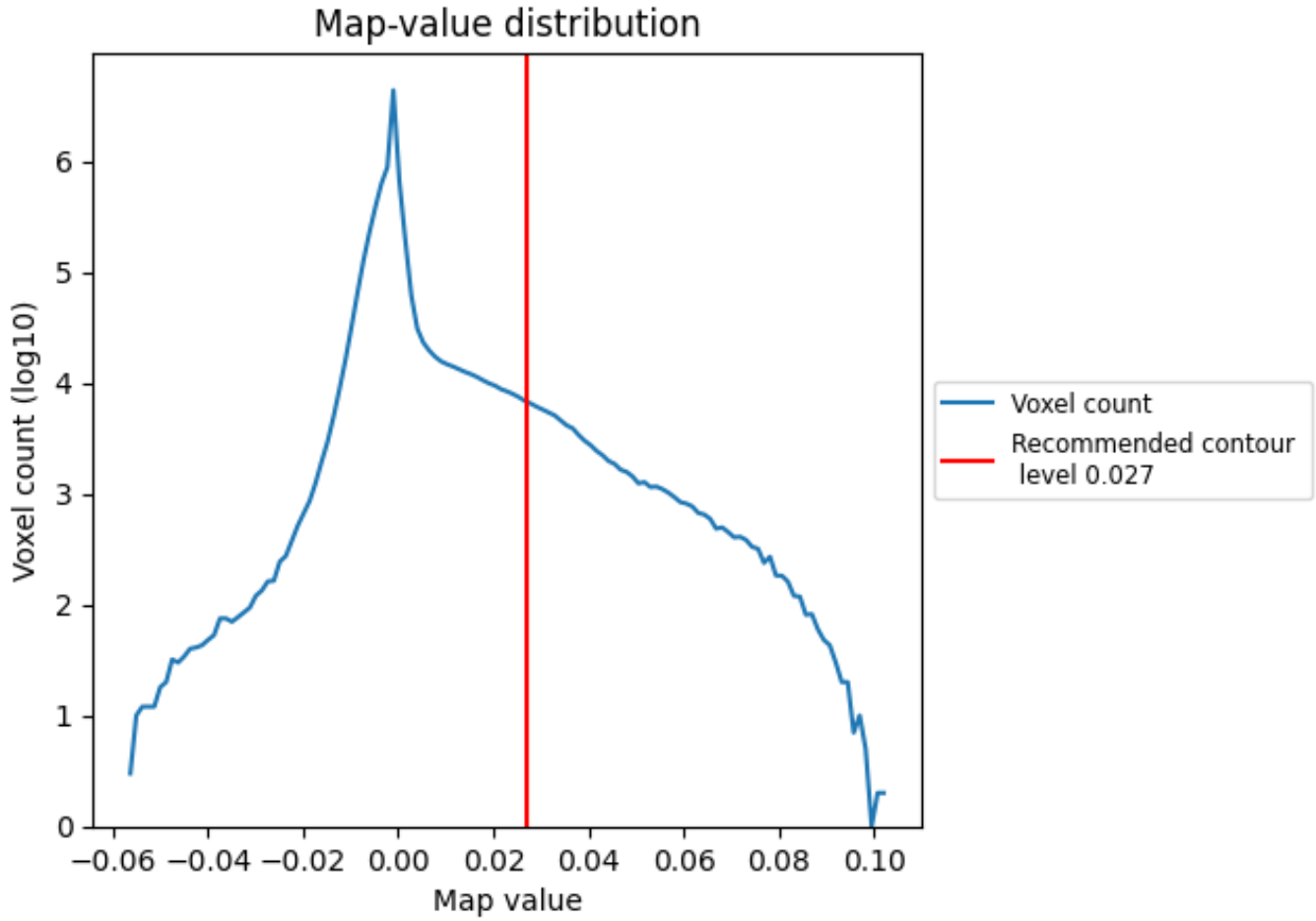
6.6 Mask visualisation (i)

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

7 Map analysis

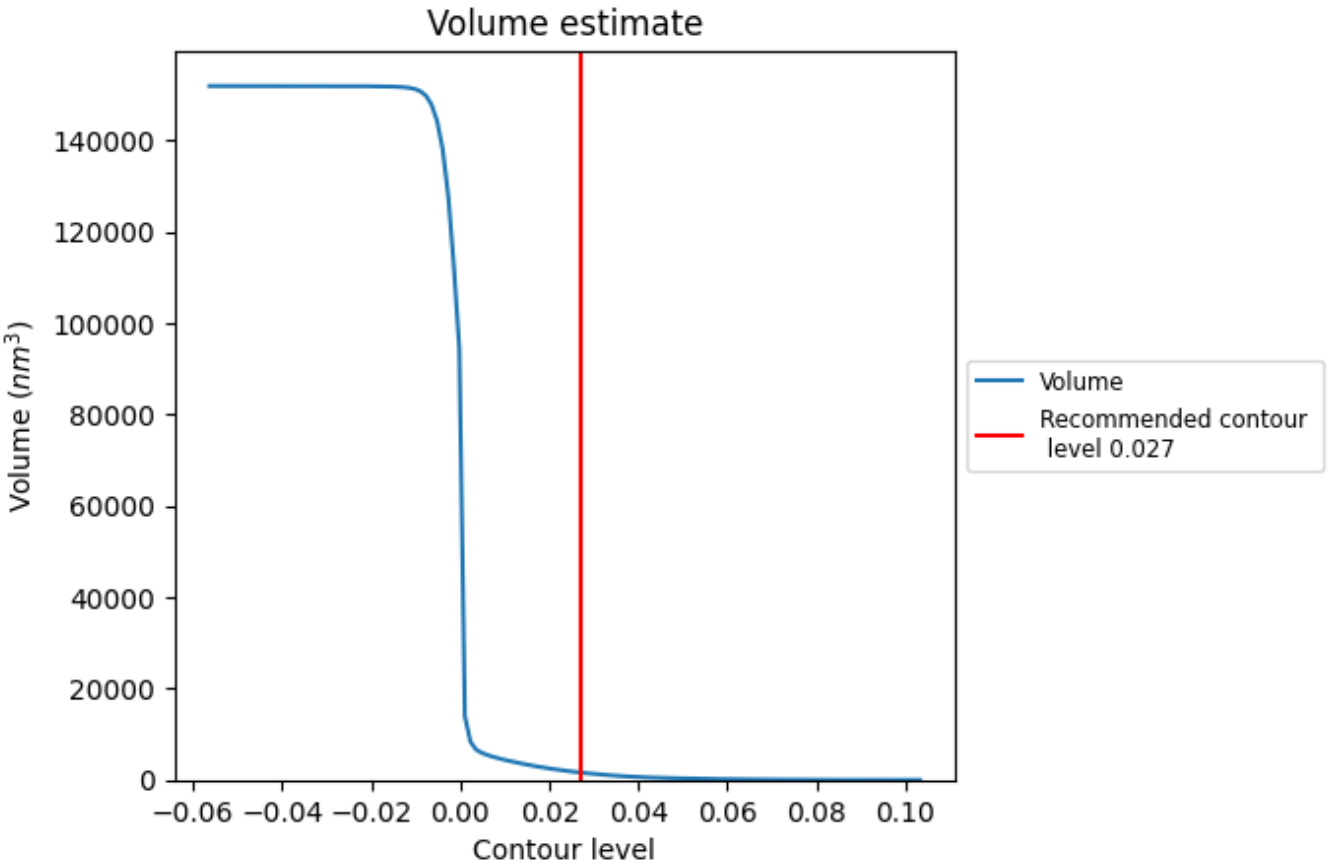
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

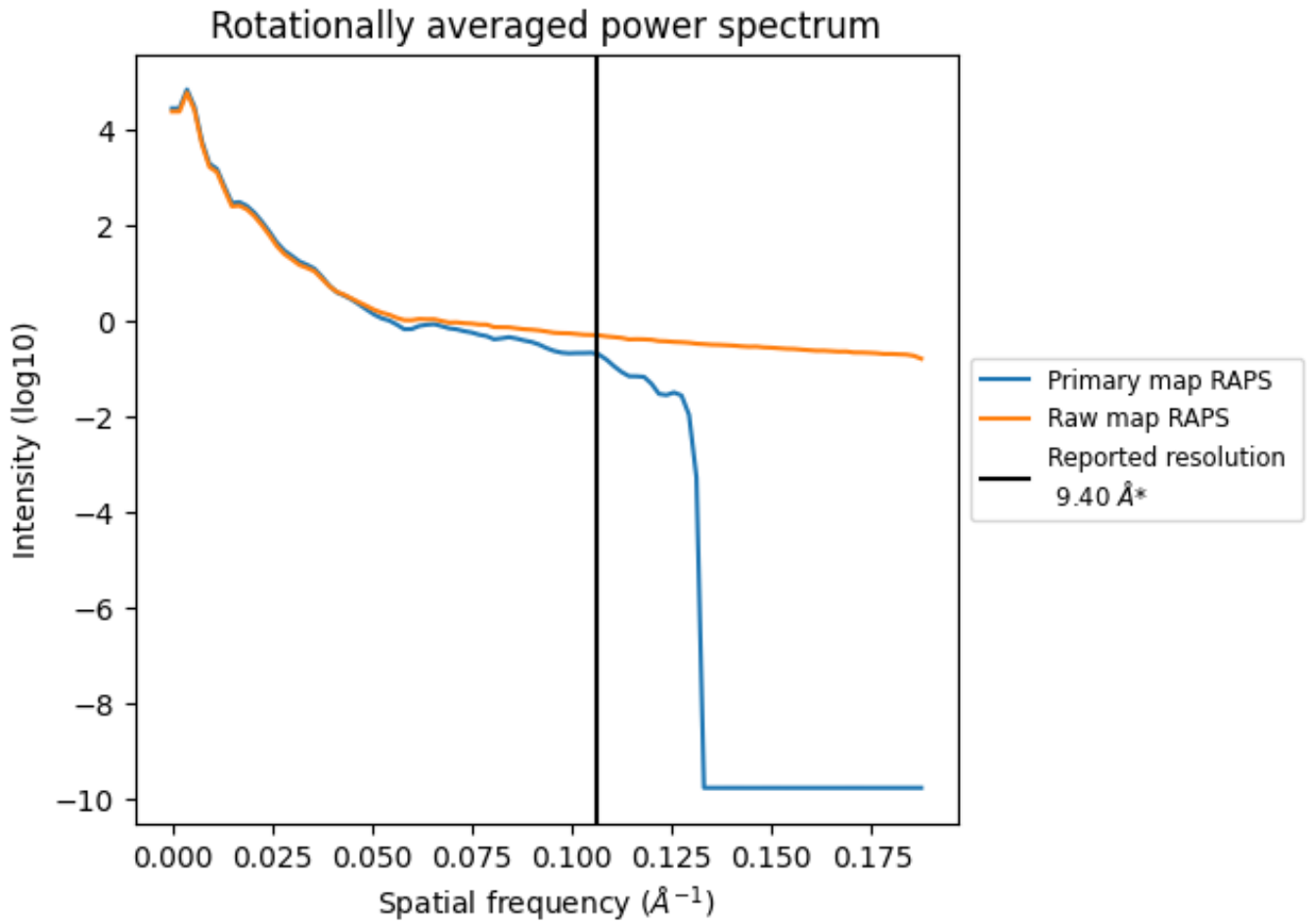
7.2 Volume estimate



The volume at the recommended contour level is 1627 nm^3; this corresponds to an approximate mass of 1470 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)

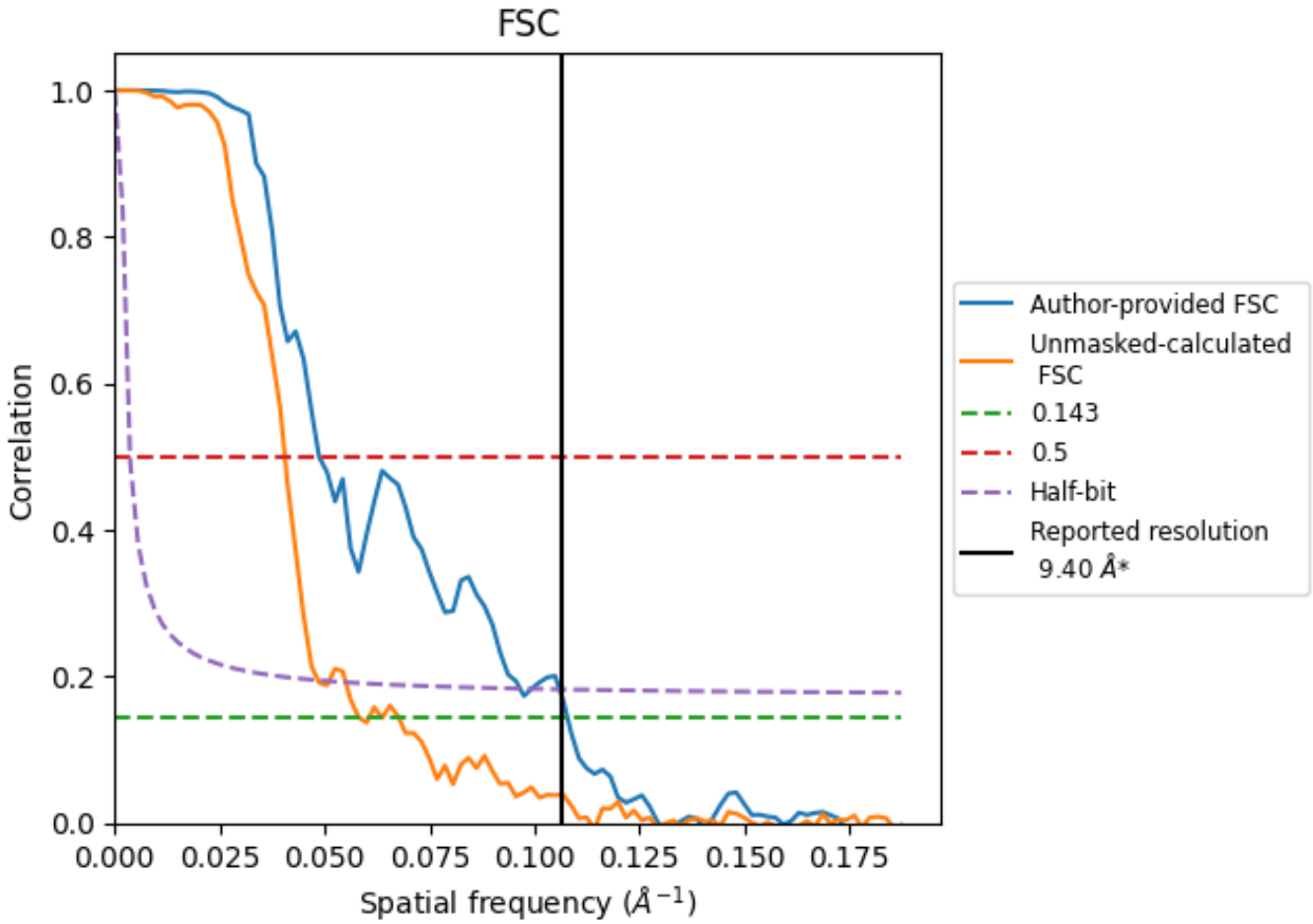


*Reported resolution corresponds to spatial frequency of 0.106 Å^{-1}

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 0.106 Å^{-1}

8.2 Resolution estimates (i)

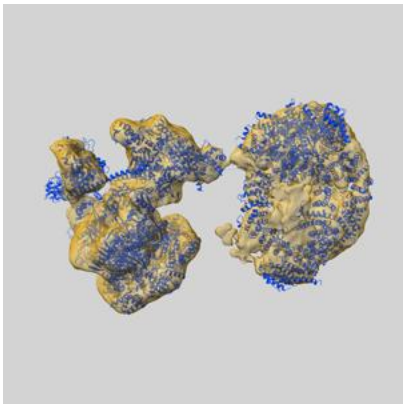
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.40	-	-
Author-provided FSC curve	9.27	20.53	10.36
Unmasked-calculated*	17.15	24.69	20.66

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 17.15 differs from the reported value 9.4 by more than 10 %

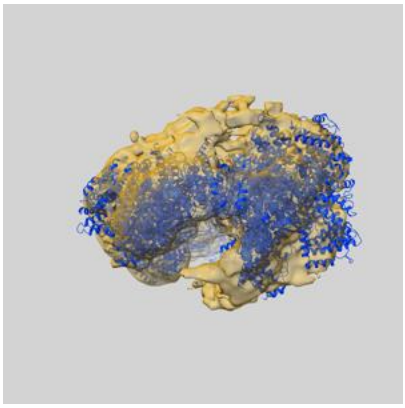
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38703 and PDB model 8XVG. Per-residue inclusion information can be found in section 3 on page 8.

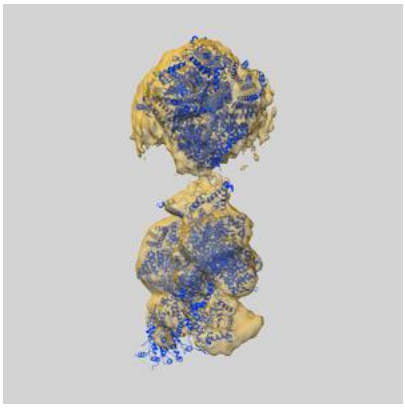
9.1 Map-model overlay



X



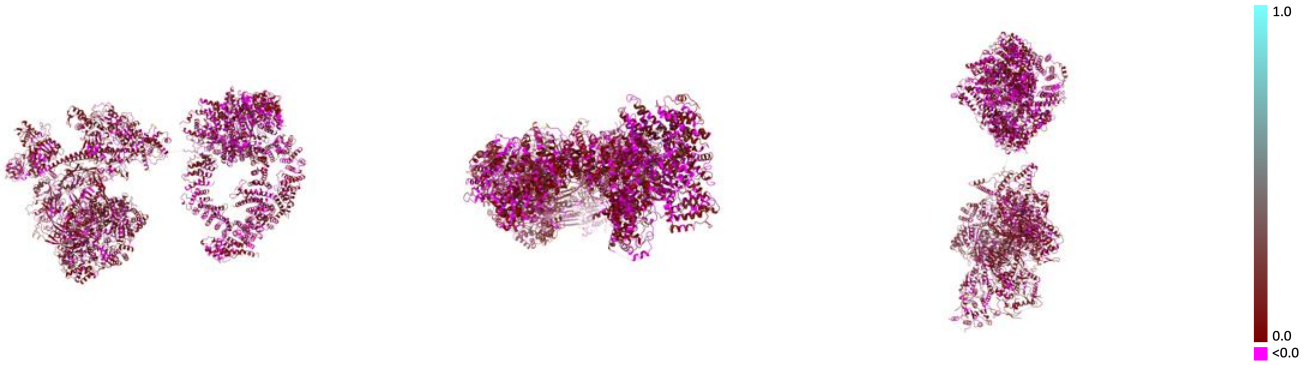
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.027 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.

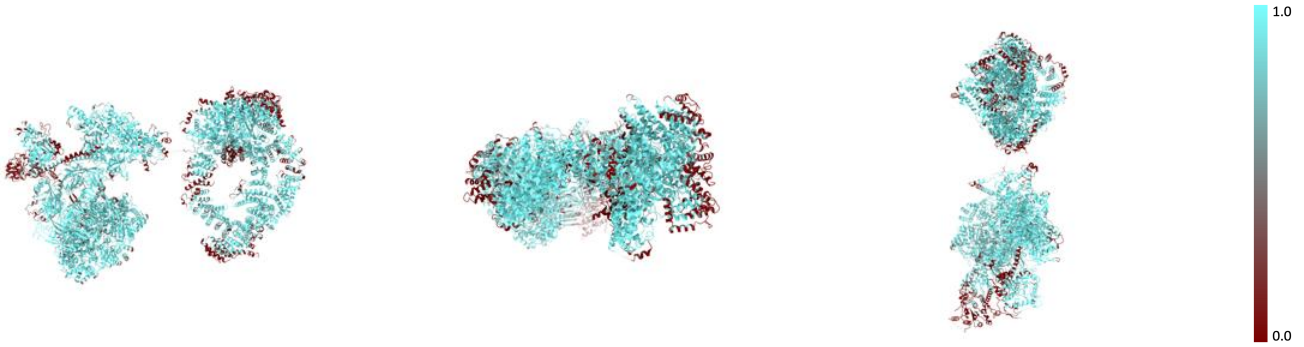
9.2 Q-score mapped to coordinate model (i)



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.

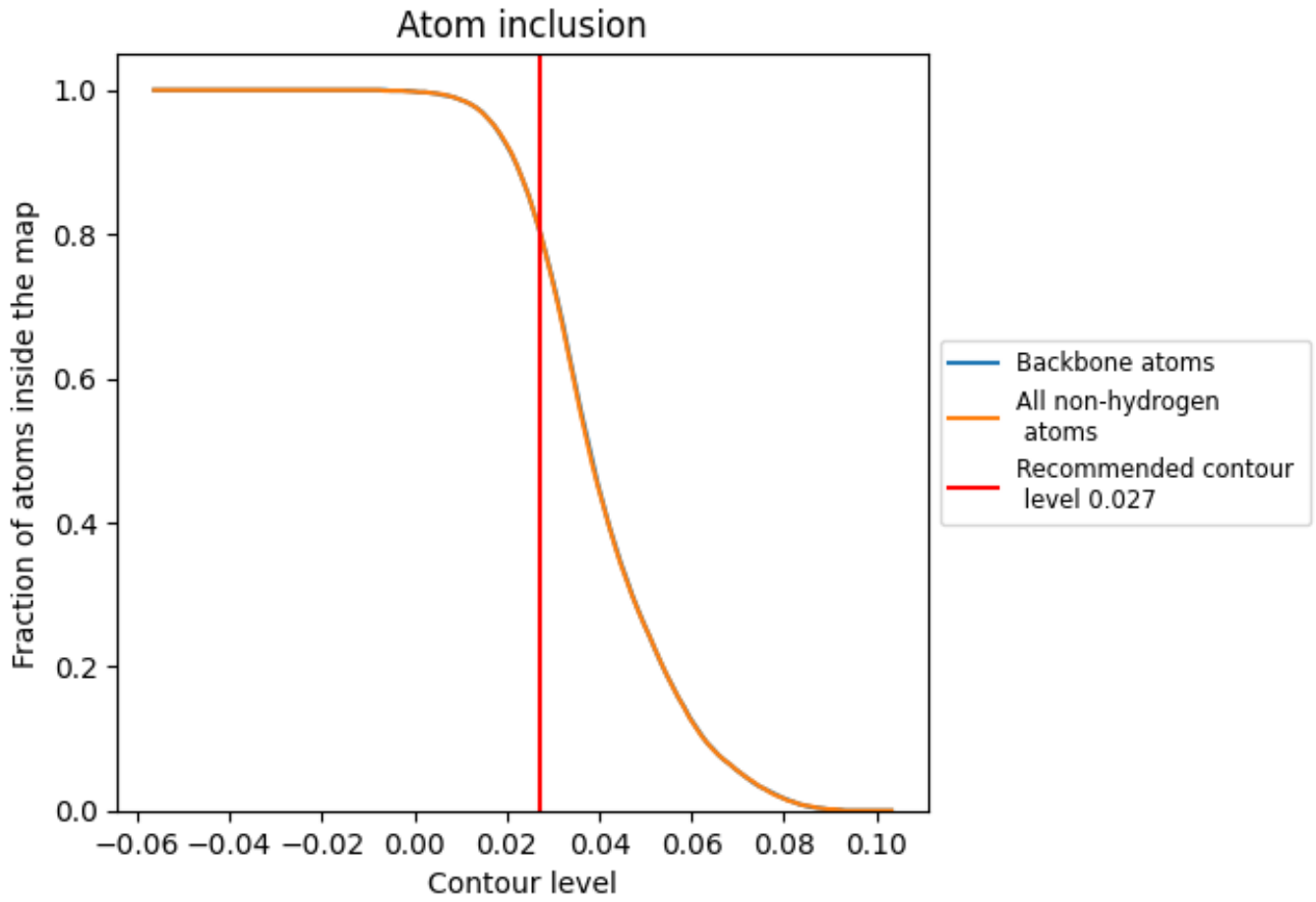
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.027).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8080	0.0570
A	0.9450	0.0660
B	0.9550	0.0760
C	0.9550	0.0880
D	0.9200	0.0760
E	0.9240	0.0890
F	0.9290	0.0720
G	0.7670	0.0670
H	0.6090	0.0650
I	0.6700	0.0730
J	0.9520	0.0760
K	0.8810	0.0750
L	0.7780	0.0340
M	0.8720	0.0700
N	0.6310	0.0620