



# Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 10:26 am BST

PDB ID : 8RC0  
EMDB ID : EMD-19041  
Title : Structure of the human 20S U5 snRNP  
Authors : Schneider, S.; Galej, W.P.  
Deposited on : 2023-12-05  
Resolution : 3.20 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](mailto: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>.

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

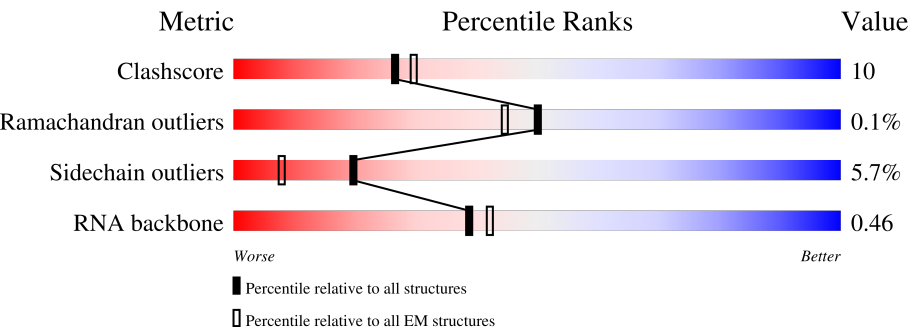
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 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.



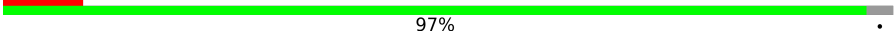
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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  $\leq 5\%$ . 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	F	341	<div><div></div><div>28%11%59%</div></div>
2	A	2335	<div><div>23%</div><div>65%25%8%</div></div>
3	5	117	<div><div></div><div>30%46%9%11%</div></div>
4	E	941	<div><div>5%</div><div>94%</div></div>
5	D	820	<div><div>28%</div><div>65%5%29%</div></div>
6	G	357	<div><div>75%</div><div>81%14%</div></div>
7	B	2136	<div><div>81%</div><div>18%</div></div>

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Mol	Chain	Length	Quality of chain
8	i	119	 68%32%
9	k	126	 67%33%
10	l	92	 84%16%
11	m	86	 85%15%
12	n	76	 9%97%
13	j	118	 9%83%17%
14	h	240	 30%70%
15	C	972	 66%20%13%

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 40648 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CD2 antigen cytoplasmic tail-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	140	Total	C	N	O	S	0	0
			889	554	165	169	1		

- Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	2153	Total	C	N	O	S	0	0
			16709	10694	2952	2994	69		

- Molecule 3 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	104	Total	C	N	O	P	0	0
			2192	983	372	734	103		

- Molecule 4 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	60	Total	C	N	O	S	0	0
			516	314	93	108	1		

- Molecule 5 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	580	Total	C	N	O	S	7	0
			2941	1609	666	664	2		

- Molecule 6 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	306	Total	C	N	O		0	0
			1507	894	306	307			

- Molecule 7 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	B	1748	Total	C	N	O	0	0
			6992	3496	1748	1748		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	i	81	Total	C	N	O	0	0
			324	162	81	81		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	k	84	Total	C	N	O	0	0
			336	168	84	84		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	l	77	Total	C	N	O	0	0
			308	154	77	77		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	m	73	Total	C	N	O	0	0
			292	146	73	73		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	n	74	Total	C	N	O	0	0
			297	148	74	75		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	j	98	Total	C	N	O	0	0
			392	196	98	98		

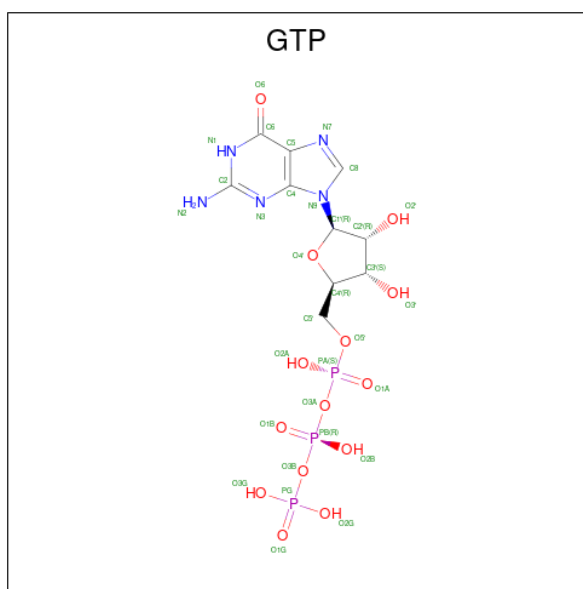
- Molecule 14 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	h	73	Total	C	N	O	0	0
			292	146	73	73		

- Molecule 15 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	847	Total	C	N	O	S	0	0
			6629	4238	1108	1250	33		

- Molecule 16 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	C	1	Total	C	N	O	P	0
			32	10	5	14	3	







K2293	G2294	Y2295	L2296	Q2297	L2298	A2299	N2300	P2301	K2302	E2303	F2304	V2305	H2306	E2307	V2308	H2309	R2310	P2311	S2312	H2313	P2314	L2315	N2316	F2317	A2318	L2319	L2320	Q2321	E2322	G2323	E2324	V2325	S2326	S2327	A2328	D2329	R2330	E2331	D2332	L2333	Y2334	A2335																		
S2233	G2234	Y2235	E2236	W2237	G2238	R2239	Q2240	N2241	T2242	D2243	K2244	G2245	N2246	N2247	P2248	K2249	G2250	Y2251	L2252	P2253	S2254	H2255	Y2256	E2257	R2258	V2259	Q2260	M2261	L2262	L2263	S2264	D2265	R2266	F2267	L2268	G2269	F2270	F2271	M2272	V2273	P2274	A2275	Q2276	S2277	S2278	W2279	N2280	Y2281	N2282	F2283	M2284	G2285	V2286	R2287	H2288	D2289	P2290	N2291	M2292	
E2173	P2174	L2175	G2176	W2177	L2178	H2179	T2180	Q2181	P2182	N2183	E2184	S2185	P2186	Q2187	L2188	S2189	P2190	Q2191	D2192	V2193	T2194	T2195	H2196	A2197	K2198	L2199	W2200	A2201	D2202	N2203	P2204	S2205	W2206	D2207	G2208	E2209	K2210	T2211	L2212	L2213	L2214	T2215	C2216	S2217	F2218	T2219	P2220	G2221	S2222	C2223	T2224	L2225	T2226	A2227	Y2228	K2229	L2230	T2231	P2232	
K2113	F2114	I2115	C2116	L2117	S2118	D2119	L2120	R2121	A2122	Q2123	I2124	A2125	G2126	Y2127	L2128	Y2129	G2130	V2131	S2132	P2133	P2134	D2135	N2136	T2137	Q2138	V2139	K2140	E2141	L2142	R2143	C2144	I2145	V2146	M2147	V2148	P2149	Q2150	W2151	G2152	T2153	H2154	Q2155	T2156	V2157	H2158	L2159	P2160	G2161	Q2162	L2163	P2164	Q2165	H2166	E2167	Y2168	L2169	K2170	E2171	M2172	
GLU	ILE	THR	SER	THR	THR	SER	ASN	TYR	GLU	THR	GLN	THR	F2067	S2068	S2069	T2070	T2071	E2072	W2073	R2074	V2075	R2076	A2077	T2078	S2079	A2080	A2081	N2082	L2083	H2084	L2085	R2086	T2087	N2088	H2089	T2090	Y2091	V2092	S2093	S2094	D2095	D2096	L2097	K2098	E2099	T2100	G2101	Y2102	T2103	Y2104	L2105	L2106	P2107	K2108	N2109	V2110	L2111	K2112		
K1993	K1994	N1995	M1996	V1997	N1998	V1999	A2000	S2001	L2002	T2003	Q2004	S2005	E2006	T2007	R2008	D2009	I2010	I2011	L2012	G2013	M2014	E2015	S2016	SER	ALA	PRO	SER	GLN	GLN	ARG	GLN	ILE	ALA	GLU	ILE	GLU	LYS	GLN	THR	LYS	GLU	GLN	SER	GLN	LEU	THR	ALA	THR	GLN	THR	ARG	THR	VAL	ASN	LYS	HIS	GLY	ASP		
F1933	S1934	R1935	L1936	L1937	L1938	L1939	L1940	R1941	A1942	L1943	H1944	V1945	N1946	T1947	D1948	R1949	A1950	K1951	V1952	L1953	L1954	K1955	P1956	D1957	ALA	K1958	T1959	T1960	L1961	T1962	E1963	P1964	H1965	H1966	T1967	N1968	P1969	T1970	L1971	T1972	D1973	E1974	E1975	W1976	L1977	K1978	V1979	E1980	V1981	Q1982	L1983	K1984	D1985	L1986	I1987	L1988	A1989	D1990	Y1991	G1992
E1873	V1874	H1875	L1876	L1877	D1878	F1879	P1880	M1881	I1882	L1883	I1884	K1885	G1886	S1887	E1888	L1889	Q1890	L1891	P1892	F1893	Q1894	A1895	C1896	D1897	K1898	V1899	E1900	K1901	F1902	G1903	D1904	L1905	I1906	L1907	K1908	A1909	T1910	E1911	P1912	Q1913	M1914	V1915	L1916	F1917	M1918	L1919	Y1920	D1921	D1922	W1923	L1924	K1925	T1926	I1927	S1928	Y1930	T1931	A1932		

• Molecule 3: U5 snRNA

Chain 5: 30% 46% 9% 11%

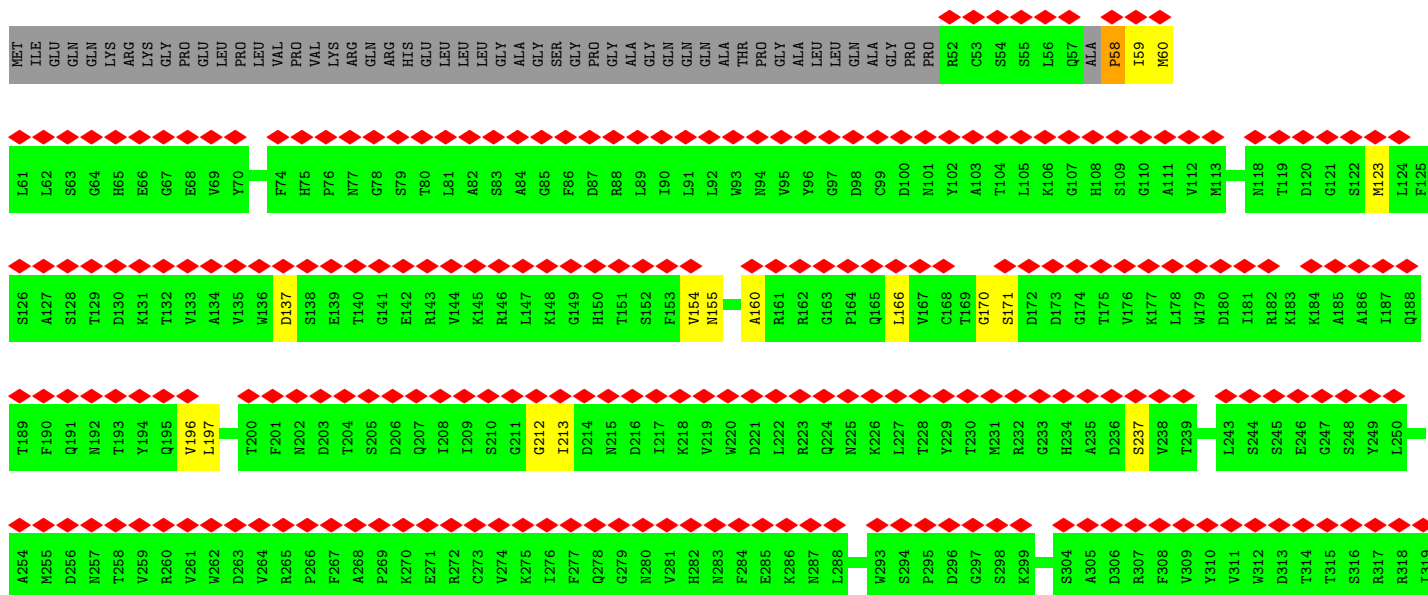
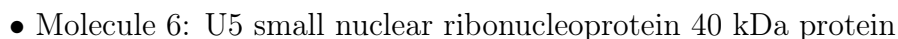
A	U	A3	C4	U5	C6	U7	G8	G9	U12	C13	U14	C15	U16	U17	C18	A19	G20	A21	U22	C23	G24	C25	A26	U27	A28	A29	A30	U34	U35	C36	G37	C38	C	U	U	U	U	A44	A47	A48	A49	G50	A51	U52	C55	C56	G57	U58	G59	G60	A61	G62	A63	G64	G65
A66	A67	C68	A69	A70	C71	G75	A76	G77	U78	C	U	U	A	A	A	C	C85	C86	U94	G95	A96	G97	G98	U105	U106	U107	U108	G109	C110	A111	A112	G113	G114	A117																					

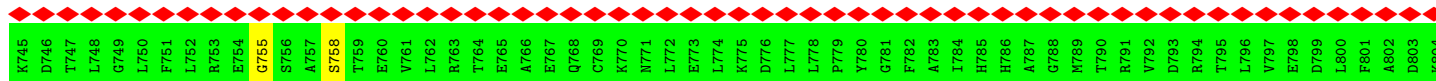
• Molecule 4: Pre-mRNA-processing factor 6

Chain E: 5% 94%

MET	ASN	LYS	LYS	LYS	PRO	PHE	LEU	GLY	MET	PRO	ALA	PRO	LEU	GLY	TYR	VAL	PRO	GLY	LEU	GLY	ARG	GLY	ALA	THR	PHE	THR	THR	ARG	SER	ASP	ILE	GLY	PRO	ALA	ARG	ASP	ALA	ASN	ASP	PRO	VAL	ASP	ASP	ARG	HIS	ALA	PRO	PRO	GLY	LYS	ARG	THR	VAL	GLY	ASP	GLN	MET
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L1525	P1465	V1405	N1345	S1285	V1225	I1165	A1105	P1045	G985	L925	G865	H805
H1526	V1466	V1406	V1346	F1286	E1226	R1166	Q1106	I1046	R986	Y926	E866	I806
I1527	L1467	L1407	F1347	A1287	D1227	M1167	L1107	P1047	T987	I927	G867	Q807
Q1528	E1468	L1408	V1348	H1288	V1228	P1168	T1108	V1048	A988	R928	I868	V808
G1529	V1469	T1409	G1349	L1289	D1229	K1169	K1109	K1049	S989	M929	L869	L809
F1530	G1470	G1410	A1350	I1290	S1230	M1170	K1110	E1050	H990	L930	I870	V810
M1531	C1471	E1411	P1351	L1291	E1231	G1171	T1111	S1051	Y991	R931	T871	S811
I1532	S1472	T1412	T1352	P1292	V1232	K1172	L1112	I1052	Y992	S932	S872	T812
S1533	S1473	G1413	G1353	E1293	I1233	T1173	M1113	E1053	P993	P933	H873	A813
H1534	M1474	T1414	S1354	K1294	L1234	T1174	L1114	E1054	T994	T934	G874	T814
T1535	R1475	D1415	G1355	Y1295	H1235	H1175	C1115	P1055	N995	L935	E875	L815
Q1536	Y1476	L1416	K1356	P1296	H1236	K1176	K1116	S1056	D996	Y936	L876	A816
T1537	I1477	K1417	T1357	P1297	E1237	V1177	M1117	A1057	T997	G937	G877	W817
R1538	S1478	L1418	I1358	P1298	V1238	Y1178	I1118	K1058	V998	I938	Y878	G818
L1539	S1479	L1419	C1359	T1299	F1239	H1179	D1119	I1059	Q999	S939	Y879	V819
L1540	Q1480	G1420	A1360	E1300	L1240	L1180	K1120	N1060	T1000	H940	L880	N820
S1541	I1481	K1421	E1361	L1301	L1241	F1181	R1121	V1061	Y1001	D941	S881	L821
M1542	E1482	G1422	F1362	L1302	K1242	P1182	M1122	L1062	M1002	D942	L882	P822
A1543	R1483	N1423	A1363	D1303	A1243	K1183	W1123	L1063	Q1003	L943	L883	A823
K1544	P1484	I1424	I1364	L1304	K1244	L1184	Q1124	Q1064	L1004	K944	N884	H824
P1545	I1485	I1425	L1365	Q1305	Y1245	L1185	M1125	A1065	L1005	G945	Q885	T825
V1546	R1486	I1426	R1366	P1306	A1246	L1186	M1126	F1066	K1006	D946	Q886	V826
Y1547	I1487	S1427	M1367	L1307	Q1247	S1187	C1127	I1067	P1007	P947	L887	I827
H1548	V1488	T1428	L1368	P1308	D1248	V1188	P1128	Q1068	T1008	L948	P888	I828
A1549	P1489	P1429	L1369	V1309	E1249	H1189	L1129	Q1069	L1009	L949	I889	K829
I1550	L1490	E1430	Q1370	S1310	H1250	L1190	R1130	L1070	S1010	D950	E890	G830
T1551	S1491	K1431	S1371	A1311	L1251	Q1191	Q1131	K1071	E1011	Q951	S891	T831
K1552	S1492	W1432	S1372	L1312	I1252	P1192	F1132	L1072	I1012	R952	Q892	Q832
H1553	S1493	D1433	E1373	L1313	T1253	L1193	R1133	E1073	R953	L953	M893	V833
S1554	L1494	I1434	G1374	M1314	F1254	T1194	K1134	G1074	L1014	L954	Y894	Y834
P1555	S1495	L1435	R1375	S1315	F1255	R1195	L1135	F1075	F1015	D955	S895	S835
K1556	N1496	S1436	C1376	A1316	V1256	S1196	P1136	A1076	R1016	V956	K896	P836
P1557	K1497	R1437	Y1377	F1317	P1257	L1197	E1137	L1077	V1017	R957	L897	E837
V1558	A1498	L1438	V1378	E1318	V1258	L1198	E1138	M1078	F1018	H958	P898	K838
I1559	D1499	W1439	I1379	S1319	F1259	K1199	V1139	A1079	S1019	T959	D899	G839
I1560	V1500	K1440	T1380	L1320	E1260	V1200	V1140	D1080	L1020	A960	M900	R840
V1561	A1501	Q1441	P1381	Y1321	P1261	E1201	K1141	M1081	S1021	A961	L901	W841
F1562	H1502	L1442	M1382	Q1322	L1262	L1202	K1142	V1082	S1022	L962	N902	T842
V1563	V1503	K1443	E1383	D1323	P1263	T1203	I1143	Y1083	E1023	M963	A903	E843
P1564	L1504	M1444	A1384	K1324	P1264	L1204	E1144	V1084	F1024	L964	E904	L844
S1565	G1505	V1445	L1385	F1325	Q1265	T1205	K1145	T1085	K1025	D965	I905	G845
R1566	C1506	Q1446	A1386	P1326	V1266	P1206	K1146	Q1086	M1026	K966	V906	A846
K1567	S1507	N1447	E1387	F1327	F1267	D1207	M1147	S1087	I1027	N967	L907	L847
Q1568	A1508	I1448	Q1388	F1328	I1268	F1208	F1148	A1088	T1028	N968	G908	D848
T1569	T1509	M1449	V1389	M1329	Q1269	Q1209	P1149	G1089	V1029	L969	N909	I849
R1570	S1510	L1450	Y1390	P1330	V1270	W1210	F1150	R1090	R1030	V970	V910	L850
L1571	T1511	F1451	M1391	I1331	V1271	D1211	E1151	L1091	E1031	K971	Q911	Q851
T1572	F1512	Y1452	D1392	Q1332	S1272	E1212	R1152	M1092	E1032	Y972	N912	M852
A1573	N1513	V1453	W1393	T1333	D1273	K1213	L1153	R1093	E1033	D973	A913	L853
I1574	F1514	D1454	Y1394	Q1334	R1274	V1214	Y1154	A1094	K1034	K974	K914	G854
D1575	H1515	E1455	E1395	V1335	W1275	H1215	D1155	I1095	L1035	K975	D915	R855
I1576	P1516	V1456	K1396	F1336	L1276	G1216	L1156	F1096	E1036	T976	A916	A856
L1577	N1517	H1457	F1397	T1337	S1277	S1217	M1157	E1097	V1037	G977	V917	G857
T1578	V1518	L1458	Q1398	M1338	C1278	S1218	H1158	I1098	Q1038	N978	N918	R858
I1579	R1519	I1459	D1399	V1339	E1279	E1219	M1159	V1099	K1039	F979	W919	P859
C1580	P1520	G1460	R1400	V1340	T1280	A1220	E1160	L1100	L1040	Q980	L920	Q860
A1581	V1521	G1461	L1401	M1341	Q1281	F1221	I1161	L1101	L1041	V981	G921	Y861
I1582	P1522	I1462	N1402	S1342	L1282	W1222	I1162	R1102	E1042	T982	Y922	T862
D1583	L1523	N1463	K1403	D1343	P1283	L1223	E1163	G1103	R1043	E983	A923	T863
I1584	E1524	G1464	K1404	D1344	V1284	L1224	L1164	W1104	V1044	L984	Y924	K864





L887	R888	T889	H890	T891	S897	L898	V907	K914	S915	I916	V917	I918	P925	H928	R931	I935	R938	K941	S944	E945	D946	V947	K951	PHE	PHE	ASP	ASP	PRO	MET	LEU	LEU	GLU	LEU	ALA	LYS	GLN	ASP	GLN	ASP	VAL	ASP	ASN	TYR	PRO	MET			
I732	F735	G736	P737	P742	N743	I744	D747	D748	T749	K756	D764	F770	R775	L779	C780	K788	I808	S818	M822	A823	T824	E829	P830	V834	E835	V836	A845	V846	V849	R854	G855	H856	D860	A877	I878	D879	S880	F881	G882	F883								
I559	T562	A563	E573	M603	Y614	S616	L617	S624	L635	D638	R645	I651	V659	V660	E668	T669	S670	K673	C674	E677	I685	L692	E693	K694	G695	L696	A697	E698	E701	N702	Q719	T720	K721	Y722	D723	H724	L727	S731										
L418	K421	K422	F430	M433	Q436	H437	P441	A445	K446	P447	K448	I449	G455	S459	M465	P473	T478	T479	S483	F490	G494	S498	E512	E517	E520	C525	R529	L530	H531	S532	S533	V534	A535	R536	V537	H538	I539	R543										
H140	T143	C144	F145	V146	D147	C148	L149	I150	H154	F155	E156	K159	D164	L165	C166	Y167	T168	T173	R177	V186	D192	T193	T205	F211	S212	D213	E214	V215	T216	L219	F228	I229	D230	E233	M236	L237	N238	T239	E240	R241	L242	I243	V247					
GLU	ASP	LYS	LYS	TYR	PRO	THR	ALA	GLU	ASN	TYR	ILE	GLY	PRO	GLU	LEU	ASP	THR	ILE	GLN	LEU	THR	GLU	PRO	ILE	ILE	LYS	PRO	VAL	LYS	THR	LYS	PHE	THR	LEU	M105	L109	P110	V111	T112	L119	M123	M131	V132	T133	H137			



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	237698	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 ( $e^-/\text{\AA}^2$ )	40.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.462	Depositor
Minimum map value	-1.224	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	526.68, 526.68, 526.68	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	F	0.28	0/898	0.61	1/1227 (0.1%)
2	A	0.33	0/17137	0.55	8/23327 (0.0%)
3	5	0.34	0/2444	0.93	9/3798 (0.2%)
4	E	0.24	0/519	0.54	0/688
5	D	0.26	0/2955	0.55	0/3773
6	G	0.24	0/1506	0.49	0/2091
7	B	0.23	0/6990	0.45	0/8734
8	i	0.22	0/323	0.49	0/402
9	k	0.23	0/335	0.50	0/417
10	l	0.22	0/307	0.49	0/382
11	m	0.24	0/291	0.49	0/362
12	n	0.23	0/296	0.50	0/367
13	j	0.23	0/390	0.48	0/484
14	h	0.24	0/290	0.50	0/359
15	C	0.40	0/6777	0.57	2/9214 (0.0%)
All	All	0.31	0/41458	0.57	20/55625 (0.0%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	784	LEU	CA-CB-CG	9.26	136.59	115.30
3	5	23	C	N1-C2-O2	8.27	123.86	118.90
3	5	57	G	O4'-C1'-N9	7.79	114.43	108.20
3	5	58	U	O5'-P-OP2	-7.53	98.92	105.70
3	5	23	C	C2-N1-C1'	7.30	126.84	118.80
3	5	23	C	N3-C2-O2	-7.06	116.96	121.90
2	A	1119	ASP	CB-CG-OD1	6.68	124.31	118.30
1	F	209	MET	CA-CB-CG	5.51	122.66	113.30
3	5	22	U	N1-C2-O2	5.48	126.63	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	71	C	N1-C2-O2	5.40	122.14	118.90
15	C	144	CYS	N-CA-CB	5.29	120.12	110.60
2	A	839	LEU	CA-CB-CG	5.26	127.41	115.30
3	5	23	C	C6-N1-C1'	-5.23	114.53	120.80
2	A	997	LEU	CA-CB-CG	5.23	127.32	115.30
2	A	856	LEU	CA-CB-CG	5.21	127.29	115.30
3	5	71	C	C2-N1-C1'	5.21	124.53	118.80
15	C	860	ASP	CB-CG-OD1	5.07	122.87	118.30
2	A	1426	ASP	CB-CG-OD1	5.05	122.84	118.30
2	A	821	ARG	CA-CB-CG	5.02	124.45	113.40
2	A	1307	MET	CA-CB-CG	5.01	121.82	113.30

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	F	889	0	721	36	0
2	A	16709	0	15543	439	0
3	5	2192	0	1111	42	0
4	E	516	0	501	10	0
5	D	2941	0	1555	41	0
6	G	1507	0	682	8	0
7	B	6992	0	1835	13	0
8	i	324	0	85	0	0
9	k	336	0	95	0	0
10	l	308	0	83	0	0
11	m	292	0	86	0	0
12	n	297	0	84	0	0
13	j	392	0	98	0	0
14	h	292	0	78	0	0
15	C	6629	0	6607	134	0
16	C	32	0	12	1	0
All	All	40648	0	29176	679	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 10.

All (679) 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)
15:C:173:THR:O	15:C:177:ARG:HB2	1.68	0.94
2:A:200:ASP:OD1	2:A:240:ARG:NH2	2.09	0.86
2:A:370:PRO:HG2	15:C:304:LEU:HD21	1.59	0.82
2:A:1013:ASN:HA	2:A:1031:ILE:HD13	1.62	0.81
2:A:143:GLN:NE2	2:A:207:PHE:O	2.14	0.81
2:A:886:LEU:HD12	2:A:887:THR:HG23	1.64	0.79
5:D:351:ARG:HH22	5:D:355:ARG:HA	1.49	0.77
2:A:821:ARG:HH12	2:A:823:SER:HB3	1.52	0.75
1:F:168:ARG:H	1:F:222:ARG:HD2	1.52	0.74
1:F:166:LEU:O	1:F:222:ARG:NH1	2.21	0.74
2:A:147:MET:O	2:A:151:MET:HG3	1.89	0.73
2:A:469:LYS:NZ	3:5:59:G:N7	2.36	0.73
15:C:829:GLU:HG3	15:C:907:VAL:HG22	1.70	0.73
2:A:585:VAL:HG11	2:A:637:TRP:CZ2	2.24	0.72
2:A:1016:VAL:HA	2:A:1025:THR:HA	1.69	0.72
2:A:1536:LEU:O	2:A:1539:SER:OG	2.08	0.72
2:A:904:HIS:HE1	2:A:1239:ARG:HH12	1.37	0.71
2:A:781:ARG:NH2	2:A:1022:MET:HB3	2.04	0.71
2:A:1628:ASP:H	2:A:1661:TRP:HE1	1.38	0.71
15:C:140:HIS:NE2	15:C:233:GLU:OE1	2.24	0.71
2:A:461:HIS:HD2	3:5:27:U:H3	1.39	0.70
15:C:156:GLU:OE2	15:C:156:GLU:N	2.18	0.70
2:A:817:LEU:HD13	2:A:999:LEU:HD22	1.72	0.70
2:A:885:LEU:HD23	2:A:1008:TYR:HD2	1.56	0.69
2:A:1303:LEU:HD11	2:A:1542:ILE:HD13	1.73	0.69
2:A:1094:ARG:HH22	2:A:1190:CYS:H	1.37	0.69
6:G:160:ALA:HB3	6:G:166:LEU:H	1.58	0.69
2:A:549:GLU:HB3	2:A:591:MET:HG2	1.76	0.68
2:A:1701:VAL:HA	2:A:1716:GLY:HA3	1.75	0.68
5:D:351:ARG:HH12	5:D:355:ARG:HG2	1.57	0.68
15:C:685:ILE:HD11	15:C:808:ILE:HD11	1.74	0.67
2:A:1660:TYR:OH	2:A:1717:ASN:O	2.12	0.67
2:A:1577:PHE:HA	2:A:1581:LEU:HD13	1.75	0.67
15:C:573:GLU:OE1	15:C:573:GLU:N	2.28	0.67
2:A:1425:LYS:HE2	2:A:1425:LYS:H	1.58	0.67
2:A:318:TYR:O	15:C:645:ARG:NH1	2.27	0.67
2:A:1444:GLN:HG3	2:A:1445:TYR:HD1	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1626:CYS:SG	2:A:1627:ALA:N	2.67	0.67
2:A:474:ARG:NH2	3:5:14:U:OP2	2.28	0.67
2:A:1005:ILE:O	2:A:1009:MET:HG2	1.95	0.66
2:A:1581:LEU:HD12	2:A:1746:ARG:HH11	1.60	0.66
2:A:1607:GLU:N	2:A:1632:PHE:O	2.27	0.66
2:A:444:ARG:NH2	5:D:281:ASP:OD2	2.28	0.66
2:A:1316:PHE:HB3	2:A:1327:MET:HG3	1.76	0.66
2:A:1622:MET:O	2:A:1687:TYR:OH	2.13	0.66
2:A:1499:GLU:N	2:A:1499:GLU:OE1	2.27	0.66
2:A:150:MET:HE2	2:A:193:LEU:HD12	1.77	0.66
2:A:292:ASP:OD2	2:A:1130:ASN:ND2	2.27	0.66
15:C:887:LEU:O	15:C:891:THR:OG1	2.12	0.66
2:A:1123:GLU:N	2:A:1123:GLU:OE2	2.29	0.66
2:A:170:ASP:OD1	2:A:171:ASP:N	2.29	0.66
2:A:341:LYS:O	5:D:301:ARG:NH1	2.28	0.66
2:A:879:SER:HB2	2:A:883:ARG:HH21	1.61	0.66
15:C:215:VAL:HG11	15:C:242:LEU:HD22	1.78	0.66
2:A:1730:MET:SD	2:A:1730:MET:N	2.69	0.65
2:A:158:ARG:HG2	5:D:372:ILE:HG12	1.77	0.65
1:F:165:LEU:HG	1:F:222:ARG:HH12	1.61	0.65
2:A:1544:ARG:HG2	2:A:1546:ASN:H	1.62	0.65
2:A:820:ARG:NH1	2:A:1063:GLY:O	2.23	0.65
15:C:674:CYS:SG	15:C:818:SER:OG	2.53	0.65
15:C:146:VAL:HG11	15:C:186:VAL:HG21	1.79	0.65
1:F:206:ALA:O	1:F:210:VAL:HG23	1.97	0.64
2:A:530:LEU:HD22	2:A:534:GLU:HB3	1.79	0.64
2:A:950:LEU:HD12	2:A:1379:PHE:CD1	2.33	0.64
2:A:1179:SER:O	2:A:1201:ARG:NH2	2.19	0.64
15:C:335:ASN:ND2	15:C:338:GLU:OE1	2.30	0.64
15:C:517:GLU:N	15:C:517:GLU:OE2	2.31	0.64
2:A:156:ARG:NH1	2:A:157:ASP:OD1	2.31	0.64
2:A:1589:ILE:HA	2:A:1733:ILE:HD11	1.80	0.64
2:A:1425:LYS:HE2	2:A:1425:LYS:N	2.13	0.64
2:A:2103:THR:HB	2:A:2139:VAL:HG23	1.80	0.63
15:C:359:LYS:HE3	15:C:359:LYS:HA	1.80	0.63
15:C:692:LEU:HD12	15:C:788:LYS:HB2	1.80	0.63
2:A:97:HIS:ND1	2:A:649:GLU:OE2	2.22	0.63
15:C:366:GLN:NE2	15:C:375:GLU:OE2	2.31	0.63
2:A:825:ILE:HB	2:A:1001:VAL:HA	1.81	0.63
2:A:974:ASN:OD1	2:A:1100:ARG:NH1	2.32	0.63
2:A:1094:ARG:NH2	2:A:1190:CYS:H	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2196:HIS:HD2	2:A:2230:LEU:HD22	1.63	0.63
2:A:171:ASP:OD2	2:A:523:ASN:ND2	2.31	0.63
2:A:832:TYR:HB3	2:A:835:ASP:HB3	1.81	0.63
2:A:485:THR:OG1	2:A:486:LYS:N	2.31	0.62
2:A:2207:ASP:HB3	2:A:2210:LYS:HG2	1.80	0.62
15:C:603:MET:HB2	15:C:651:ILE:HD11	1.81	0.62
1:F:165:LEU:HG	1:F:222:ARG:NH1	2.13	0.62
2:A:857:ASN:H	2:A:860:GLN:HB2	1.63	0.62
2:A:1579:ALA:O	2:A:1584:LYS:NZ	2.29	0.62
1:F:164:LEU:O	1:F:198:ARG:NH2	2.32	0.62
2:A:2086:ARG:NH1	2:A:2219:THR:O	2.32	0.62
2:A:923:ASP:OD2	2:A:1439:ARG:NH1	2.27	0.62
15:C:512:GLU:OE1	15:C:562:THR:OG1	2.18	0.62
2:A:1687:TYR:O	2:A:1693:SER:OG	2.16	0.62
2:A:608:LEU:HD13	2:A:632:ALA:HB1	1.81	0.62
3:5:17:U:H3	3:5:60:G:H1	1.48	0.62
5:D:361:LYS:HD3	5:D:362:LEU:HD22	1.82	0.62
2:A:1141:ARG:H	2:A:1182:ASN:ND2	1.97	0.62
15:C:473:PRO:O	15:C:498:SER:OG	2.13	0.62
2:A:1002:ASP:OD2	2:A:1004:ASN:ND2	2.33	0.62
2:A:157:ASP:OD2	5:D:368:ARG:NH2	2.22	0.61
15:C:780:CYS:O	15:C:941:LYS:NZ	2.33	0.61
2:A:885:LEU:HD22	2:A:1005:ILE:HD12	1.82	0.61
2:A:2278:SER:OG	2:A:2309:HIS:NE2	2.25	0.61
15:C:133:THR:HG21	15:C:219:LEU:HD23	1.80	0.61
4:E:113:ASP:OD1	4:E:113:ASP:N	2.33	0.61
2:A:784:LEU:HB2	2:A:1024:HIS:NE2	2.16	0.61
2:A:1612:GLU:HG2	2:A:1627:ALA:HB3	1.81	0.61
2:A:946:GLU:HB2	2:A:950:LEU:HD22	1.83	0.61
2:A:1576:ILE:HG23	2:A:1577:PHE:HD1	1.65	0.61
5:D:370:TRP:HB3	5:D:374:ARG:HH12	1.66	0.61
2:A:2105:ILE:HG12	2:A:2262:LEU:HD21	1.82	0.61
2:A:2197:ALA:HA	2:A:2200:MET:HG2	1.83	0.61
2:A:1482:GLU:OE1	2:A:1483:GLY:N	2.35	0.60
2:A:343:GLU:N	2:A:343:GLU:OE1	2.33	0.60
2:A:837:LYS:HA	2:A:840:ILE:HD12	1.83	0.60
5:D:370:TRP:O	5:D:374:ARG:HG2	2.02	0.60
15:C:834:VAL:HG11	15:C:883:PHE:HE2	1.67	0.60
15:C:144:CYS:SG	15:C:147:ASP:HB2	2.41	0.60
2:A:1426:ASP:O	2:A:1429:THR:N	2.34	0.60
3:5:47:A:O2'	3:5:48:A:O5'	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:56:C:H2'	3:5:57:G:H5'	1.84	0.60
2:A:1365:ILE:HG12	2:A:1366:PRO:HD2	1.83	0.59
5:D:361:LYS:HD3	5:D:362:LEU:H	1.66	0.59
2:A:2188:LEU:O	2:A:2251:TYR:OH	2.18	0.59
4:E:154:GLU:HA	4:E:157:TRP:HD1	1.67	0.59
2:A:112:GLN:HE21	2:A:189:GLU:HA	1.67	0.59
5:D:341:ARG:HH22	5:D:342:LYS:HE2	1.68	0.59
2:A:790:ARG:HH22	2:A:1028:TYR:HB3	1.67	0.59
2:A:1384:ARG:HH11	2:A:2220:PRO:HB2	1.68	0.59
2:A:1676:ILE:HD13	2:A:1706:ASP:HB2	1.84	0.59
2:A:470:ARG:HB2	4:E:115:ARG:HG3	1.84	0.58
2:A:2214:ILE:HG12	2:A:2227:ALA:HB2	1.85	0.58
2:A:494:LEU:HD21	2:A:562:VAL:HG21	1.86	0.58
2:A:1576:ILE:HG23	2:A:1577:PHE:CD1	2.38	0.58
5:D:352:TRP:O	5:D:355:ARG:NE	2.33	0.58
2:A:381:PRO:HD2	15:C:334:ILE:HG22	1.85	0.58
2:A:436:PRO:HG2	2:A:439:GLN:HG3	1.84	0.58
2:A:888:GLN:OE1	2:A:889:ARG:N	2.35	0.58
2:A:164:MET:HG2	2:A:569:VAL:HG11	1.85	0.58
2:A:2278:SER:HG	2:A:2309:HIS:CD2	2.18	0.58
3:5:17:U:H2'	3:5:18:C:C6	2.38	0.58
2:A:1300:LYS:HG2	2:A:1311:PHE:CD2	2.38	0.58
2:A:1570:LYS:O	2:A:1574:ILE:HG22	2.03	0.58
2:A:1497:THR:OG1	2:A:1499:GLU:OE1	2.16	0.58
15:C:144:CYS:O	15:C:148:CYS:SG	2.62	0.58
2:A:780:THR:O	2:A:784:LEU:HD23	2.04	0.58
2:A:805:GLU:O	2:A:809:VAL:HG12	2.04	0.58
2:A:835:ASP:O	2:A:839:LEU:HD12	2.03	0.58
15:C:165:LEU:HD12	15:C:167:TYR:HB2	1.86	0.57
2:A:2193:VAL:HG23	2:A:2230:LEU:HD11	1.86	0.57
15:C:166:CYS:O	15:C:168:THR:N	2.37	0.57
2:A:2149:PRO:HB3	2:A:2281:TYR:CE1	2.38	0.57
15:C:145:PHE:HE2	15:C:430:PHE:CD1	2.22	0.57
2:A:1434:LYS:O	2:A:1439:ARG:NH2	2.35	0.57
2:A:1637:TRP:N	2:A:1657:THR:O	2.38	0.57
15:C:436:GLN:OE1	15:C:437:HIS:NE2	2.38	0.57
1:F:169:GLU:OE2	1:F:174:ALA:N	2.38	0.57
2:A:776:LEU:O	2:A:780:THR:HG23	2.03	0.57
2:A:946:GLU:CB	2:A:950:LEU:HD22	2.35	0.57
2:A:1304:ASN:OD1	2:A:1305:SER:N	2.38	0.57
15:C:159:LYS:HA	15:C:165:LEU:HD23	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:488:ASP:OD1	2:A:489:TRP:N	2.38	0.56
15:C:258:ASN:OD1	15:C:259:LYS:N	2.39	0.56
2:A:252:ASP:OD1	2:A:252:ASP:N	2.37	0.56
2:A:511:LYS:HB2	2:A:513:LEU:HG	1.86	0.56
1:F:161:LEU:HD11	1:F:225:LEU:HD22	1.86	0.56
2:A:850:TYR:HE1	2:A:860:GLN:HG2	1.71	0.56
2:A:1403:LEU:HD13	2:A:1408:LEU:HD11	1.87	0.56
15:C:110:PRO:HD2	15:C:537:TYR:CE2	2.41	0.56
15:C:213:ASP:OD2	15:C:616:SER:OG	2.17	0.56
6:G:197:LEU:H	6:G:212:GLY:HA2	1.69	0.56
2:A:1587:GLU:O	2:A:1591:MET:HG3	2.06	0.56
2:A:839:LEU:O	2:A:843:LEU:HD12	2.06	0.55
2:A:903:SER:OG	2:A:904:HIS:ND1	2.40	0.55
2:A:1283:GLU:N	2:A:1283:GLU:OE1	2.36	0.55
2:A:1342:TRP:NE1	2:A:1353:PHE:HB2	2.21	0.55
3:5:66:A:HO2'	3:5:67:A:H8	1.55	0.55
2:A:1193:GLU:HB3	2:A:1231:ARG:HB2	1.89	0.55
2:A:1251:SER:O	2:A:1254:THR:HG23	2.05	0.55
2:A:1264:ASN:ND2	2:A:1326:GLY:O	2.33	0.55
5:D:316:GLN:HE22	5:D:318:ARG:HA	1.70	0.55
15:C:559:ILE:HG21	15:C:563:ALA:HB2	1.87	0.55
15:C:677:GLU:N	15:C:677:GLU:OE1	2.40	0.55
1:F:210:VAL:HG13	1:F:215:LEU:HA	1.87	0.55
2:A:357:ASN:OD1	5:D:327:ARG:NH2	2.39	0.55
2:A:1094:ARG:HH22	2:A:1190:CYS:N	2.03	0.55
2:A:1602:ASP:OD1	2:A:1602:ASP:N	2.35	0.55
2:A:876:GLU:OE1	2:A:880:ARG:NH1	2.31	0.55
3:5:109:G:H2'	3:5:110:C:C6	2.42	0.55
2:A:1047:VAL:HG12	2:A:1048:MET:HE3	1.89	0.55
1:F:123:ILE:O	1:F:127:LYS:N	2.37	0.54
1:F:71:VAL:HG21	2:A:1574:ILE:HG23	1.88	0.54
2:A:1276:GLU:OE1	2:A:1375:TRP:N	2.40	0.54
15:C:737:PRO:O	15:C:775:ARG:NH2	2.40	0.54
15:C:846:VAL:HG22	15:C:887:LEU:HD11	1.88	0.54
15:C:946:ASP:OD1	15:C:947:VAL:N	2.38	0.54
1:F:71:VAL:HG23	2:A:1575:GLN:HB2	1.89	0.54
2:A:1384:ARG:HD2	2:A:1384:ARG:C	2.27	0.54
15:C:186:VAL:HG22	15:C:535:ALA:HB2	1.89	0.54
1:F:66:LEU:HD21	1:F:101:PHE:HD2	1.72	0.54
1:F:95:GLU:N	1:F:95:GLU:OE1	2.40	0.54
2:A:904:HIS:CE1	2:A:1239:ARG:HH12	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:19:A:N3	3:5:21:A:N6	2.56	0.54
2:A:1730:MET:HA	2:A:1733:ILE:HG22	1.90	0.54
2:A:1560:ILE:HD11	2:A:1668:TRP:CD1	2.43	0.54
2:A:2146:VAL:HG11	2:A:2164:PRO:HB3	1.89	0.54
2:A:881:ILE:HG12	2:A:918:THR:HA	1.89	0.53
2:A:1573:LEU:HA	2:A:1576:ILE:HG22	1.90	0.53
15:C:357:THR:OG1	15:C:359:LYS:O	2.26	0.53
1:F:165:LEU:O	1:F:222:ARG:NH2	2.39	0.53
1:F:105:GLY:HA3	2:A:1532:ARG:HD2	1.88	0.53
2:A:1404:THR:OG1	2:A:1407:ASP:OD2	2.24	0.53
2:A:2181:GLN:HB2	2:A:2217:SER:HA	1.91	0.53
2:A:939:TRP:NE1	2:A:1049:ASP:OD2	2.39	0.53
4:E:116:ARG:HE	4:E:119:ARG:HD2	1.73	0.53
1:F:168:ARG:N	1:F:222:ARG:HD2	2.22	0.53
2:A:835:ASP:OD1	2:A:836:THR:N	2.42	0.53
2:A:1537:TRP:HB2	2:A:1751:LEU:HD22	1.91	0.53
3:5:111:A:H2'	3:5:112:A:C8	2.43	0.53
1:F:102:ASP:OD1	1:F:106:ASN:N	2.29	0.53
2:A:429:ASN:OD1	2:A:432:ARG:NH1	2.41	0.53
5:D:320:TYR:O	5:D:324:MET:HG2	2.09	0.53
2:A:178:TYR:HB2	2:A:494:LEU:HD12	1.90	0.53
2:A:648:LEU:O	2:A:652:LEU:HD13	2.08	0.53
2:A:881:ILE:HG23	2:A:918:THR:HG23	1.89	0.53
2:A:885:LEU:HD23	2:A:1008:TYR:CD2	2.41	0.53
2:A:1032:ARG:HD3	2:A:1445:TYR:CE2	2.43	0.53
2:A:1342:TRP:HB2	2:A:1486:GLU:HB2	1.91	0.53
15:C:144:CYS:SG	15:C:144:CYS:O	2.67	0.53
15:C:145:PHE:CG	15:C:228:PHE:HZ	2.27	0.53
15:C:614:TYR:HB2	15:C:617:LEU:HB2	1.90	0.53
3:5:7:U:H3'	3:5:8:G:H8	1.74	0.53
15:C:749:THR:O	15:C:756:LYS:NZ	2.36	0.53
3:5:12:U:H3	3:5:65:G:H1	1.58	0.52
3:5:69:A:H2'	3:5:70:A:O4'	2.09	0.52
3:5:67:A:H2'	3:5:68:C:C6	2.44	0.52
15:C:150:ILE:O	15:C:154:HIS:HB2	2.09	0.52
15:C:724:TRP:HZ3	15:C:732:ILE:HD11	1.74	0.52
2:A:651:TRP:CE3	2:A:652:LEU:HD12	2.44	0.52
5:D:370:TRP:HB3	5:D:374:ARG:NH1	2.25	0.52
15:C:243:ILE:O	15:C:247:VAL:HG13	2.08	0.52
2:A:837:LYS:HD2	2:A:1429:THR:HG23	1.90	0.52
15:C:829:GLU:OE2	15:C:854:ARG:NH1	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:63:A:H2'	3:5:64:G:H8	1.73	0.52
2:A:1410:ASP:OD1	2:A:1410:ASP:N	2.41	0.52
3:5:63:A:H2'	3:5:64:G:C8	2.45	0.52
2:A:1031:ILE:HG22	2:A:1033:GLY:H	1.74	0.52
3:5:110:C:H2'	3:5:111:A:H8	1.75	0.52
15:C:836:VAL:HG22	15:C:897:SER:HB3	1.91	0.52
5:D:344:ARG:O	5:D:344:ARG:HD3	2.09	0.51
7:B:526:ASN:O	7:B:529:GLY:N	2.44	0.51
15:C:144:CYS:HA	15:C:147:ASP:CG	2.31	0.51
2:A:992:LEU:O	2:A:996:LEU:HD23	2.10	0.51
2:A:1107:ARG:O	2:A:1111:GLN:NE2	2.36	0.51
2:A:2103:THR:O	2:A:2140:LYS:N	2.33	0.51
2:A:2125:ALA:HB3	2:A:2159:LEU:HD21	1.93	0.51
7:B:1225:VAL:O	7:B:1234:LEU:N	2.41	0.51
2:A:888:GLN:OE1	2:A:890:ALA:N	2.43	0.51
2:A:1447:VAL:HG12	2:A:1449:LYS:H	1.76	0.51
2:A:1582:TRP:CZ2	2:A:1666:LEU:HB2	2.45	0.51
15:C:779:LEU:O	15:C:938:ARG:NH1	2.43	0.51
2:A:1458:GLN:HE22	2:A:1463:LYS:HE2	1.75	0.51
15:C:731:SER:HB3	15:C:747:ASP:OD1	2.11	0.51
15:C:166:CYS:C	15:C:168:THR:H	2.13	0.51
2:A:979:SER:OG	2:A:980:ARG:N	2.43	0.51
2:A:1000:ILE:HD13	2:A:1001:VAL:HG13	1.93	0.51
2:A:1311:PHE:HE1	2:A:1315:VAL:HG21	1.76	0.51
15:C:212:SER:O	15:C:216:THR:HG23	2.11	0.51
2:A:214:ARG:HG3	2:A:225:TYR:CD1	2.45	0.51
2:A:1119:ASP:OD1	2:A:1119:ASP:O	2.29	0.51
2:A:1544:ARG:HD2	2:A:1546:ASN:HB2	1.92	0.51
4:E:114:GLU:HA	4:E:117:LYS:HB2	1.92	0.51
5:D:341:ARG:NH1	5:D:342:LYS:HA	2.25	0.51
15:C:478:THR:HA	15:C:494:GLY:HA3	1.93	0.51
2:A:982:GLU:OE2	2:A:1172:ASN:ND2	2.44	0.51
2:A:880:ARG:O	2:A:883:ARG:HG2	2.12	0.50
1:F:95:GLU:OE2	2:A:1570:LYS:NZ	2.39	0.50
2:A:897:GLU:O	2:A:908:VAL:N	2.41	0.50
15:C:305:GLY:O	15:C:433:MET:HG3	2.11	0.50
2:A:395:THR:HG22	2:A:396:ASP:H	1.75	0.50
2:A:595:LYS:NZ	3:5:30:A:OP1	2.44	0.50
15:C:944:SER:OG	15:C:945:GLU:N	2.44	0.50
2:A:441:VAL:O	2:A:445:VAL:HG23	2.12	0.50
2:A:1056:HIS:O	2:A:1060:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1384:ARG:HE	2:A:1385:VAL:HG23	1.77	0.50
2:A:321:ASN:O	15:C:645:ARG:NH2	2.45	0.50
2:A:1659:LYS:HZ3	2:A:1661:TRP:HB2	1.75	0.50
3:5:57:G:O2'	3:5:58:U:O5'	2.19	0.50
15:C:727:LEU:O	15:C:731:SER:OG	2.17	0.50
15:C:918:ILE:O	15:C:918:ILE:HD12	2.12	0.50
2:A:1006:ALA:O	2:A:1010:THR:OG1	2.21	0.50
3:5:51:A:H2'	3:5:52:U:C6	2.46	0.50
2:A:631:ALA:O	2:A:635:ARG:HG3	2.11	0.50
2:A:1606:ILE:HG12	2:A:1637:TRP:HZ2	1.76	0.50
2:A:1433:ASP:HB3	2:A:1460:HIS:HE1	1.77	0.50
15:C:111:VAL:N	15:C:156:GLU:OE1	2.45	0.50
15:C:483:SER:HB2	15:C:490:PHE:CE2	2.47	0.50
2:A:162:LYS:N	5:D:375:GLU:OE1	2.35	0.49
2:A:224:THR:OG1	3:5:12:U:OP1	2.16	0.49
2:A:534:GLU:N	2:A:534:GLU:OE1	2.46	0.49
2:A:1021:ASP:OD1	2:A:1022:MET:N	2.45	0.49
3:5:60:G:H2'	3:5:61:A:C8	2.46	0.49
2:A:809:VAL:O	2:A:812:THR:HG22	2.12	0.49
2:A:1503:TRP:HE1	2:A:1533:ARG:HD2	1.77	0.49
3:5:12:U:H2'	3:5:13:C:C6	2.48	0.49
5:D:341:ARG:HH12	5:D:342:LYS:HE2	1.77	0.49
15:C:455:GLY:O	15:C:459:SER:OG	2.27	0.49
15:C:701:GLU:HG3	15:C:742:PRO:HG3	1.93	0.49
2:A:825:ILE:HD12	2:A:929:GLU:HB3	1.94	0.49
3:5:34:U:H2'	3:5:35:U:C6	2.47	0.49
15:C:299:ILE:O	15:C:306:ASN:ND2	2.45	0.49
2:A:1093:ASP:N	2:A:1093:ASP:OD1	2.45	0.49
3:5:26:A:H2'	3:5:27:U:O4'	2.12	0.49
2:A:420:ARG:NH1	3:5:57:G:H5''	2.28	0.49
2:A:469:LYS:HB3	2:A:471:TYR:CE1	2.47	0.49
15:C:304:LEU:O	15:C:437:HIS:NE2	2.45	0.49
2:A:469:LYS:HB3	2:A:471:TYR:HE1	1.78	0.49
2:A:981:PHE:HB2	2:A:1093:ASP:O	2.12	0.49
2:A:293:TRP:HB2	2:A:1141:ARG:HB3	1.94	0.49
5:D:328:ARG:HG2	5:D:332:GLU:HB2	1.94	0.49
5:D:359:GLN:OE1	5:D:359:GLN:N	2.46	0.49
15:C:925:PRO:HD2	15:C:928:HIS:NE2	2.27	0.49
2:A:261:LYS:HD2	2:A:328:HIS:HB3	1.93	0.49
2:A:1645:LEU:HB2	2:A:1714:ALA:H	1.78	0.49
2:A:2124:ILE:HD12	2:A:2147:MET:HE1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:893:GLU:OE1	2:A:893:GLU:N	2.45	0.49
2:A:1382:SER:HA	2:A:1415:GLY:HA2	1.94	0.49
15:C:320:LEU:HD21	15:C:344:TRP:HB2	1.95	0.48
2:A:613:TYR:HD2	2:A:617:ASN:HD21	1.61	0.48
2:A:1342:TRP:CD1	2:A:1353:PHE:HB2	2.48	0.48
2:A:1693:SER:HB2	2:A:1695:TYR:CZ	2.48	0.48
5:D:371:ARG:HG2	5:D:374:ARG:HH21	1.77	0.48
1:F:214:ASN:OD1	1:F:216:GLY:N	2.38	0.48
2:A:2227:ALA:HB3	2:A:2261:MET:SD	2.54	0.48
7:B:537:LYS:N	7:B:608:LEU:O	2.45	0.48
7:B:1663:ILE:O	7:B:1705:MET:N	2.45	0.48
2:A:196:ASP:N	2:A:200:ASP:OD2	2.46	0.48
2:A:794:TYR:HA	2:A:800:TYR:CE1	2.48	0.48
2:A:1308:PRO:HB3	2:A:1548:TYR:CE1	2.48	0.48
2:A:1385:VAL:HG21	2:A:1414:ARG:HB3	1.95	0.48
15:C:659:VAL:HG22	15:C:660:VAL:H	1.77	0.48
2:A:530:LEU:HD22	2:A:534:GLU:CB	2.42	0.48
2:A:651:TRP:CZ3	2:A:652:LEU:HD12	2.49	0.48
2:A:1581:LEU:HD12	2:A:1746:ARG:NH1	2.26	0.48
3:5:16:U:H2'	3:5:17:U:C6	2.48	0.48
2:A:336:ASN:O	15:C:262:ARG:NH2	2.46	0.48
2:A:395:THR:HG22	2:A:396:ASP:N	2.28	0.48
15:C:697:ALA:HB1	15:C:742:PRO:HB3	1.95	0.48
2:A:181:ASN:OD1	2:A:181:ASN:N	2.47	0.48
15:C:624:SER:O	15:C:624:SER:OG	2.30	0.48
2:A:815:HIS:HA	2:A:818:GLU:OE1	2.13	0.48
2:A:1030:ILE:HG22	2:A:1032:ARG:H	1.79	0.48
15:C:144:CYS:HA	15:C:147:ASP:HB2	1.95	0.48
2:A:845:ARG:HH12	2:A:1457:HIS:CD2	2.31	0.48
2:A:1127:GLY:O	2:A:1170:TRP:NE1	2.33	0.48
2:A:1659:LYS:HE2	2:A:1696:PRO:HB2	1.96	0.48
4:E:112:MET:HA	4:E:112:MET:HE2	1.96	0.48
15:C:724:TRP:CZ3	15:C:732:ILE:HD11	2.49	0.48
1:F:175:LEU:HD13	2:A:61:MET:HE1	1.96	0.47
2:A:1399:GLN:HA	7:B:1051:SER:N	2.29	0.47
2:A:1581:LEU:O	2:A:1585:ILE:HG12	2.14	0.47
2:A:112:GLN:NE2	2:A:189:GLU:HA	2.28	0.47
2:A:1657:THR:HG21	2:A:1699:THR:HG21	1.97	0.47
2:A:152:ARG:HH22	5:D:308:ASP:HB2	1.79	0.47
2:A:804:GLU:HA	2:A:807:VAL:HG22	1.96	0.47
2:A:1582:TRP:NE1	2:A:1619:SER:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:320:TYR:OH	15:C:881:PHE:HB3	2.12	0.47
5:D:357:TRP:HB3	5:D:369:ASP:OD1	2.14	0.47
2:A:67:ARG:HD3	2:A:179:ALA:HB2	1.97	0.47
2:A:1744:ARG:O	2:A:1747:ILE:HG22	2.15	0.47
2:A:2108:LYS:HD3	2:A:2263:LEU:HD23	1.97	0.47
2:A:2280:ASN:HB3	2:A:2309:HIS:CG	2.50	0.47
7:B:1620:LEU:N	7:B:1645:VAL:O	2.46	0.47
7:B:1196:SER:O	7:B:1258:VAL:N	2.41	0.47
7:B:1347:PHE:O	7:B:1512:PHE:N	2.43	0.47
15:C:144:CYS:HA	15:C:147:ASP:CB	2.45	0.47
2:A:422:LEU:H	2:A:422:LEU:HD23	1.79	0.47
2:A:787:GLU:OE2	2:A:790:ARG:NE	2.42	0.47
2:A:795:LEU:HD12	2:A:796:LYS:HD3	1.98	0.47
2:A:1314:VAL:HG13	2:A:1478:LEU:HD13	1.96	0.47
15:C:736:GLY:N	15:C:743:ASN:O	2.48	0.47
2:A:1644:LEU:N	2:A:1647:ASP:OD2	2.41	0.46
2:A:2131:VAL:HG13	2:A:2172:MET:HG2	1.97	0.46
6:G:154:VAL:HA	6:G:171:SER:HA	1.97	0.46
15:C:720:THR:HG23	15:C:721:LYS:HD3	1.97	0.46
2:A:343:GLU:HG2	2:A:344:ASP:OD1	2.15	0.46
2:A:776:LEU:HA	2:A:779:LEU:HD12	1.98	0.46
2:A:2190:PRO:HA	2:A:2193:VAL:HG12	1.98	0.46
2:A:2281:TYR:HA	2:A:2284:MET:HE3	1.98	0.46
2:A:1991:TYR:O	2:A:1995:ASN:N	2.47	0.46
5:D:322:ASP:OD1	5:D:322:ASP:N	2.49	0.46
15:C:230:ASP:OD2	15:C:262:ARG:NH1	2.49	0.46
15:C:445:ALA:O	15:C:449:ILE:HG12	2.15	0.46
2:A:834:HIS:O	2:A:838:LEU:HD13	2.16	0.46
2:A:1391:LEU:O	2:A:1394:GLN:HG3	2.14	0.46
5:D:351:ARG:HG3	5:D:351:ARG:HH11	1.80	0.46
2:A:843:LEU:HD21	2:A:870:ALA:HB3	1.97	0.46
2:A:980:ARG:NH2	2:A:1094:ARG:HD2	2.30	0.46
3:5:60:G:H2'	3:5:61:A:H8	1.79	0.46
1:F:173:GLY:HA2	1:F:176:ARG:HB2	1.98	0.46
2:A:1487:HIS:HB3	2:A:1541:THR:HB	1.98	0.46
15:C:421:LYS:HE3	15:C:421:LYS:HB2	1.58	0.46
15:C:347:ILE:HG13	15:C:357:THR:O	2.16	0.46
2:A:817:LEU:HD13	2:A:999:LEU:CD2	2.44	0.46
2:A:887:THR:O	2:A:889:ARG:HG2	2.16	0.46
2:A:1271:MET:O	2:A:1271:MET:HG3	2.15	0.46
15:C:696:LEU:HD13	15:C:722:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:GLY:HA3	1:F:109:LEU:HD22	1.97	0.46
2:A:361:HIS:CE1	2:A:362:ARG:HG2	2.50	0.46
4:E:112:MET:HA	4:E:112:MET:CE	2.46	0.46
1:F:200:ASP:O	2:A:68:LYS:HE2	2.15	0.45
2:A:313:LYS:HZ1	5:D:253:ARG:HH22	1.64	0.45
7:B:1455:GLU:N	7:B:1490:LEU:O	2.48	0.45
15:C:520:GLU:OE2	15:C:520:GLU:N	2.45	0.45
15:C:531:TRP:HB3	15:C:538:HIS:HB3	1.98	0.45
2:A:530:LEU:HD23	2:A:530:LEU:HA	1.83	0.45
2:A:1391:LEU:HD23	2:A:1391:LEU:HA	1.85	0.45
3:5:65:G:O6	3:5:66:A:N6	2.49	0.45
5:D:361:LYS:HG3	5:D:363:ASP:OD1	2.16	0.45
2:A:899:MET:O	2:A:905:LEU:HD13	2.16	0.45
2:A:1274:PHE:O	2:A:1278:VAL:HG23	2.16	0.45
2:A:794:TYR:HA	2:A:800:TYR:HE1	1.82	0.45
2:A:899:MET:HE2	2:A:908:VAL:HG21	1.99	0.45
15:C:479:THR:HA	15:C:562:THR:HG22	1.99	0.45
2:A:719:CYS:O	2:A:723:ASN:N	2.50	0.45
2:A:922:LEU:HD12	2:A:1036:PHE:CD2	2.52	0.45
2:A:2107:PRO:HG2	2:A:2110:VAL:HG22	1.98	0.45
2:A:2164:PRO:HB3	2:A:2296:LEU:HD11	1.98	0.45
2:A:2303:GLU:O	2:A:2309:HIS:ND1	2.48	0.45
15:C:668:GLU:OE1	15:C:824:THR:OG1	2.28	0.45
2:A:120:TYR:HE2	2:A:485:THR:HG22	1.82	0.45
15:C:192:ASP:OD1	15:C:193:THR:N	2.47	0.45
2:A:374:ASP:N	2:A:374:ASP:OD1	2.48	0.45
2:A:788:GLN:OE1	2:A:1024:HIS:HB3	2.16	0.45
2:A:823:SER:OG	2:A:933:ARG:NH1	2.48	0.45
2:A:896:ILE:HA	2:A:908:VAL:O	2.17	0.45
2:A:1422:LEU:HD12	2:A:1427:ARG:HH21	1.82	0.45
2:A:1533:ARG:HD3	2:A:1752:GLN:OE1	2.15	0.45
15:C:670:SER:HB2	15:C:822:MET:HB2	1.97	0.45
15:C:674:CYS:SG	15:C:822:MET:HG3	2.57	0.45
15:C:830:PRO:HG2	15:C:877:ALA:HB3	1.99	0.45
2:A:2187:GLN:HB2	2:A:2256:TYR:OH	2.17	0.45
6:G:213:ILE:HA	6:G:237:SER:HA	1.98	0.45
2:A:1659:LYS:HD2	2:A:1660:TYR:N	2.31	0.45
1:F:210:VAL:HA	1:F:214:ASN:O	2.17	0.44
15:C:137:HIS:HA	15:C:238:ASN:HB3	2.00	0.44
2:A:308:ILE:HD12	2:A:320:TYR:HE1	1.81	0.44
2:A:1426:ASP:OD1	2:A:1429:THR:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2106:LEU:HD12	2:A:2107:PRO:HD2	2.00	0.44
2:A:1146:ASP:OD2	2:A:1181:ASP:HB2	2.16	0.44
2:A:1341:ARG:HG2	2:A:1354:ARG:HG3	1.98	0.44
15:C:143:THR:HG22	15:C:147:ASP:OD2	2.18	0.44
1:F:200:ASP:N	1:F:200:ASP:OD1	2.43	0.44
2:A:409:ARG:HG3	2:A:410:PRO:HA	2.00	0.44
3:5:17:U:H2'	3:5:18:C:H6	1.82	0.44
7:B:755:GLY:O	7:B:758:SER:N	2.50	0.44
1:F:90:PHE:O	2:A:1574:ILE:HD12	2.18	0.44
2:A:997:LEU:HG	2:A:1000:ILE:HD11	2.00	0.44
2:A:1051:LEU:HD12	2:A:1162:PRO:HD3	2.00	0.44
2:A:1251:SER:HB2	2:A:1259:ILE:HD11	1.99	0.44
2:A:464:PRO:HG2	3:5:23:C:C6	2.52	0.44
2:A:895:GLY:HA2	2:A:1018:ASN:O	2.16	0.44
2:A:913:PRO:HA	2:A:916:LYS:HB2	1.99	0.44
2:A:988:ILE:HG12	2:A:1044:TYR:CE2	2.52	0.44
2:A:2207:ASP:H	2:A:2210:LYS:HZ2	1.66	0.44
2:A:912:GLU:OE1	2:A:914:LEU:HB2	2.17	0.44
2:A:1577:PHE:HE2	2:A:1582:TRP:CE3	2.36	0.44
2:A:2280:ASN:ND2	2:A:2304:PHE:O	2.49	0.44
3:5:76:A:H2'	3:5:77:G:C8	2.53	0.44
2:A:1018:ASN:HB2	2:A:1023:ASN:HB3	2.00	0.44
3:5:48:A:H2'	3:5:49:A:H8	1.83	0.44
5:D:341:ARG:HH11	5:D:345:LYS:HE3	1.82	0.44
1:F:120:LEU:HD22	2:A:539:ARG:HD2	2.00	0.44
2:A:613:TYR:HD2	2:A:617:ASN:ND2	2.15	0.44
2:A:986:GLU:OE1	2:A:986:GLU:N	2.44	0.44
2:A:1416:ILE:HD13	2:A:1416:ILE:HA	1.87	0.44
2:A:1661:TRP:CD1	2:A:1662:ILE:N	2.86	0.44
15:C:236:MET:O	15:C:240:GLU:HG3	2.18	0.44
15:C:534:VAL:HG12	15:C:535:ALA:H	1.82	0.44
2:A:950:LEU:HD12	2:A:1379:PHE:CE1	2.53	0.43
2:A:1088:PHE:CD1	2:A:1097:ILE:HG12	2.53	0.43
2:A:2149:PRO:HB2	2:A:2292:MET:HE3	2.00	0.43
2:A:491:GLU:O	2:A:495:GLN:HG3	2.18	0.43
2:A:944:ASP:N	2:A:944:ASP:OD1	2.51	0.43
2:A:1116:GLU:HG2	2:A:1117:HIS:CD2	2.53	0.43
2:A:1621:LYS:N	2:A:1622:MET:HE3	2.33	0.43
2:A:1779:PHE:O	2:A:1809:ILE:HA	2.17	0.43
2:A:445:VAL:HG22	5:D:281:ASP:HB2	2.00	0.43
2:A:899:MET:HE1	2:A:1448:LEU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1342:TRP:CH2	2:A:1344:LYS:HB2	2.53	0.43
4:E:113:ASP:HB2	4:E:120:ARG:NH2	2.33	0.43
5:D:366:THR:OG1	5:D:367:ASP:N	2.51	0.43
2:A:188:LEU:HD11	2:A:567:GLY:HA2	2.01	0.43
2:A:960:ASN:OD1	2:A:1225:THR:OG1	2.34	0.43
2:A:1342:TRP:CZ3	2:A:1344:LYS:HB2	2.53	0.43
15:C:446:LYS:HB3	15:C:447:PRO:HD3	2.00	0.43
2:A:839:LEU:HD11	2:A:878:LEU:HG	2.00	0.43
2:A:1396:ALA:HA	2:A:1399:GLN:HB2	2.01	0.43
2:A:1606:ILE:HG12	2:A:1637:TRP:CZ2	2.54	0.43
2:A:2133:PRO:HD2	2:A:2139:VAL:HG13	2.00	0.43
3:5:8:G:C2'	3:5:9:G:H5'	2.49	0.43
15:C:205:THR:HB	15:C:215:VAL:HG22	1.99	0.43
15:C:537:TYR:HD1	15:C:537:TYR:H	1.67	0.43
15:C:698:GLU:O	15:C:702:ASN:HB2	2.19	0.43
2:A:2086:ARG:NH1	2:A:2222:SER:O	2.47	0.43
15:C:370:VAL:HA	15:C:374:LEU:HB2	2.00	0.43
2:A:176:LEU:HD23	2:A:181:ASN:ND2	2.34	0.43
2:A:1318:THR:HB	2:A:1324:GLY:HA3	2.00	0.43
15:C:137:HIS:CE1	15:C:898:LEU:HD12	2.54	0.43
2:A:275:GLY:H	5:D:282:THR:HB	1.84	0.43
2:A:449:LYS:HD3	2:A:449:LYS:HA	1.84	0.43
2:A:919:ASP:N	2:A:919:ASP:OD1	2.52	0.43
2:A:1223:GLU:HA	2:A:1224:ARG:NH2	2.33	0.43
2:A:106:MET:HE2	2:A:578:LEU:HD13	2.01	0.43
2:A:430:TRP:HB3	2:A:611:LEU:HD11	2.00	0.43
2:A:950:LEU:HD21	2:A:954:LYS:HE3	2.01	0.43
2:A:1103:ALA:O	2:A:1107:ARG:HG3	2.19	0.43
2:A:1222:LYS:NZ	2:A:2088:ASN:O	2.39	0.43
2:A:1459:ARG:HG3	2:A:1459:ARG:HH11	1.83	0.43
2:A:2115:ILE:O	2:A:2118:SER:OG	2.36	0.43
5:D:324:MET:O	5:D:328:ARG:HB2	2.19	0.43
7:B:1299:THR:N	7:B:1513:ASN:O	2.46	0.43
2:A:833:LYS:HE3	2:A:834:HIS:HE1	1.84	0.43
2:A:1320:LYS:HA	2:A:1324:GLY:O	2.19	0.43
2:A:1607:GLU:HB2	2:A:1634:SER:N	2.34	0.43
2:A:1728:GLN:O	2:A:1732:LYS:HG2	2.18	0.43
15:C:164:ASP:OD1	15:C:164:ASP:N	2.46	0.43
2:A:318:TYR:HB2	15:C:638:ASP:OD1	2.19	0.42
2:A:722:ALA:HA	2:A:1022:MET:HB2	2.00	0.42
2:A:841:LEU:HD21	2:A:1429:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2188:LEU:HD13	2:A:2228:TYR:CD1	2.54	0.42
3:5:22:U:O2	3:5:22:U:H2'	2.19	0.42
15:C:374:LEU:HA	15:C:374:LEU:HD23	1.82	0.42
1:F:205:LEU:HA	1:F:208:GLN:OE1	2.19	0.42
2:A:513:LEU:HD13	2:A:516:LEU:HD12	2.00	0.42
2:A:1600:GLU:HG2	2:A:1725:LEU:HD13	2.01	0.42
2:A:1623:ASN:OD1	2:A:1624:SER:N	2.52	0.42
5:D:287:ASN:O	5:D:291:LYS:HG3	2.19	0.42
2:A:89:LEU:HD21	2:A:506:LEU:HD11	2.01	0.42
2:A:251:ASP:HB3	2:A:253:ASN:H	1.84	0.42
2:A:279:PHE:HE2	2:A:456:LEU:HG	1.84	0.42
2:A:462:ARG:HG3	2:A:463:PRO:HD2	2.02	0.42
2:A:809:VAL:HG22	2:A:996:LEU:HD11	2.01	0.42
2:A:901:LEU:HD22	2:A:901:LEU:H	1.84	0.42
2:A:1275:ARG:HH22	2:A:1464:LEU:HB3	1.85	0.42
2:A:1311:PHE:CD1	2:A:1312:PRO:HD2	2.54	0.42
2:A:2273:VAL:HG22	2:A:2274:PRO:HD2	2.02	0.42
5:D:328:ARG:HB3	5:D:333:LYS:HG3	2.01	0.42
6:G:196:VAL:HA	6:G:212:GLY:HA3	2.00	0.42
2:A:685:LEU:HA	4:E:138:ILE:HD13	2.01	0.42
2:A:785:LYS:O	2:A:789:GLU:HG2	2.19	0.42
2:A:911:VAL:HG12	2:A:916:LYS:HG3	2.01	0.42
2:A:1188:ASN:C	2:A:1188:ASN:HD22	2.21	0.42
2:A:1384:ARG:NE	2:A:1385:VAL:HG23	2.33	0.42
6:G:123:MET:HA	6:G:137:ASP:HA	2.00	0.42
15:C:133:THR:HG21	15:C:219:LEU:CD2	2.48	0.42
1:F:209:MET:HG3	1:F:217:VAL:CG2	2.50	0.42
2:A:93:LYS:HB3	2:A:93:LYS:HE3	1.86	0.42
2:A:406:TRP:CZ2	15:C:266:GLU:HG2	2.55	0.42
2:A:425:PRO:HB2	2:A:428:LYS:HB2	2.01	0.42
2:A:563:GLN:NE2	2:A:568:ASN:OD1	2.51	0.42
2:A:1426:ASP:HB3	2:A:1459:ARG:NH2	2.34	0.42
2:A:1663:ASP:HB3	2:A:1702:LEU:HA	2.01	0.42
2:A:1806:ALA:HA	2:A:1820:LYS:O	2.19	0.42
3:5:113:G:H2'	3:5:114:G:H8	1.84	0.42
7:B:1377:VAL:O	7:B:1452:VAL:N	2.46	0.42
15:C:328:ALA:O	15:C:332:GLY:HA2	2.19	0.42
15:C:412:ILE:HD13	15:C:412:ILE:HA	1.88	0.42
2:A:1414:ARG:NH1	2:A:1414:ARG:HG3	2.33	0.42
15:C:735:PHE:HD1	15:C:735:PHE:HA	1.69	0.42
15:C:845:ALA:O	15:C:849:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:ASP:OD1	1:F:105:GLY:N	2.52	0.42
1:F:165:LEU:HD11	1:F:170:THR:O	2.20	0.42
2:A:134:TRP:HZ2	3:5:58:U:OP2	2.02	0.42
2:A:380:LEU:HA	2:A:380:LEU:HD12	1.82	0.42
2:A:888:GLN:HG3	2:A:891:PHE:CE1	2.54	0.42
2:A:1077:ILE:HD12	2:A:1078:ALA:N	2.34	0.42
2:A:1109:LEU:HG	2:A:1152:ALA:HB1	2.01	0.42
5:D:366:THR:HG23	5:D:369:ASP:H	1.84	0.42
2:A:544:PHE:HA	2:A:651:TRP:CH2	2.55	0.42
2:A:1504:GLU:N	2:A:1504:GLU:OE1	2.53	0.42
2:A:2196:HIS:CG	2:A:2213:ILE:HD11	2.55	0.42
15:C:211:PHE:HE2	15:C:635:LEU:HD23	1.85	0.42
15:C:719:GLN:HG2	15:C:724:TRP:O	2.20	0.42
2:A:902:TYR:HB2	2:A:1242:ASN:CG	2.40	0.42
2:A:1090:ARG:HG2	2:A:1091:TYR:O	2.19	0.42
2:A:1344:LYS:HA	2:A:1491:LYS:NZ	2.35	0.42
2:A:1565:LYS:HB3	2:A:1565:LYS:HE2	1.73	0.42
7:B:1404:LYS:O	7:B:1423:ASN:N	2.47	0.42
15:C:532:ILE:HD13	15:C:532:ILE:HA	1.88	0.42
2:A:950:LEU:CD2	2:A:954:LYS:HE3	2.50	0.42
2:A:1241:HIS:HE1	2:A:1290:LYS:HE2	1.84	0.42
2:A:1343:SER:OG	2:A:1352:HIS:ND1	2.48	0.42
15:C:313:GLN:HB2	16:C:1001:GTP:C6	2.55	0.42
2:A:152:ARG:NH2	5:D:308:ASP:HB2	2.35	0.41
2:A:944:ASP:HB3	2:A:1436:TRP:NE1	2.35	0.41
2:A:1218:ASN:OD1	2:A:1220:VAL:HG22	2.20	0.41
2:A:1341:ARG:HD3	2:A:1352:HIS:HB3	2.01	0.41
3:5:37:G:N2	3:5:44:A:N3	2.68	0.41
3:5:112:A:H2'	3:5:113:G:C8	2.55	0.41
2:A:2127:TYR:HE2	2:A:2148:VAL:HG21	1.85	0.41
2:A:1612:GLU:HB2	2:A:1630:LEU:HD21	2.02	0.41
15:C:388:VAL:HG11	15:C:412:ILE:HD11	2.01	0.41
2:A:1194:CYS:HB3	2:A:1228:CYS:SG	2.60	0.41
2:A:1458:GLN:NE2	2:A:1463:LYS:HE2	2.35	0.41
5:D:378:SER:OG	5:D:630:GLY:O	2.37	0.41
15:C:537:TYR:CE2	15:C:539:ILE:HD11	2.56	0.41
15:C:692:LEU:HD11	15:C:744:ILE:HG13	2.03	0.41
2:A:902:TYR:HB2	2:A:1242:ASN:ND2	2.36	0.41
2:A:1392:LYS:O	2:A:1395:GLU:HG3	2.20	0.41
2:A:1548:TYR:HB3	2:A:1551:PHE:CE2	2.55	0.41
2:A:1576:ILE:HD11	2:A:1746:ARG:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2093:SER:HB3	2:A:2258:ARG:NH2	2.36	0.41
6:G:58:PRO:O	6:G:60:MET:N	2.53	0.41
2:A:310:THR:O	2:A:314:ILE:HG12	2.20	0.41
2:A:1443:LYS:HA	2:A:1443:LYS:HD3	1.88	0.41
2:A:1482:GLU:H	2:A:1482:GLU:HG3	1.53	0.41
2:A:2149:PRO:HB2	2:A:2292:MET:CE	2.51	0.41
5:D:290:TYR:CE2	15:C:889:THR:HG21	2.54	0.41
15:C:418:LEU:O	15:C:422:LYS:HG2	2.20	0.41
15:C:736:GLY:HA2	15:C:743:ASN:HB2	2.03	0.41
2:A:461:HIS:HD2	3:5:27:U:N3	2.12	0.41
2:A:1384:ARG:NH1	2:A:2220:PRO:HB2	2.34	0.41
2:A:1414:ARG:HG3	2:A:1414:ARG:HH11	1.86	0.41
2:A:2163:LEU:HD21	2:A:2206:TRP:NE1	2.35	0.41
2:A:2183:ASN:OD1	2:A:2183:ASN:N	2.53	0.41
15:C:529:ARG:O	15:C:530:LEU:HD23	2.21	0.41
15:C:916:ILE:HD12	15:C:928:HIS:ND1	2.36	0.41
2:A:344:ASP:OD1	5:D:339:ARG:NE	2.53	0.41
2:A:1321:GLU:HG2	2:A:1322:LEU:HD12	2.02	0.41
2:A:1582:TRP:NE1	2:A:1666:LEU:HD12	2.36	0.41
2:A:1593:LEU:HD12	2:A:1629:ILE:HD12	2.02	0.41
15:C:177:ARG:NH2	15:C:638:ASP:OD2	2.50	0.41
15:C:931:ARG:O	15:C:935:ILE:HG23	2.20	0.41
1:F:73:GLY:HA3	2:A:1578:ARG:HB2	2.02	0.41
2:A:137:GLU:O	2:A:141:ILE:HG13	2.20	0.41
2:A:882:LYS:HA	2:A:885:LEU:HD12	2.03	0.41
2:A:1627:ALA:HA	2:A:1661:TRP:NE1	2.36	0.41
2:A:1638:ASN:O	2:A:1720:PRO:HD3	2.20	0.41
2:A:1670:ASP:O	2:A:1674:HIS:HB3	2.21	0.41
6:G:155:ASN:N	6:G:170:GLY:O	2.44	0.41
15:C:110:PRO:HD2	15:C:537:TYR:CD2	2.55	0.41
15:C:131:ASN:ND2	15:C:441:PRO:HG3	2.35	0.41
15:C:449:ILE:HD12	15:C:465:MET:HE3	2.03	0.41
15:C:854:ARG:NE	15:C:879:ASP:OD2	2.49	0.41
2:A:87:VAL:HG13	4:E:101:ALA:HB2	2.03	0.41
2:A:565:ARG:HD2	2:A:565:ARG:HA	1.95	0.41
2:A:1017:ILE:N	2:A:1024:HIS:O	2.33	0.41
2:A:1057:ARG:HA	2:A:1057:ARG:HD2	1.81	0.41
2:A:1106:ALA:O	2:A:1110:ILE:HG13	2.20	0.41
2:A:1645:LEU:O	2:A:1723:LYS:HE3	2.20	0.41
3:5:37:G:C2	3:5:44:A:C4	3.09	0.41
15:C:119:LEU:O	15:C:123:MET:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:764:ASP:OD1	15:C:764:ASP:C	2.59	0.41
1:F:225:LEU:HD12	1:F:226:ALA:N	2.36	0.40
2:A:387:PHE:CZ	15:C:326:ILE:HG22	2.56	0.40
2:A:507:LEU:HD22	2:A:655:LEU:HD23	2.03	0.40
2:A:531:THR:HB	2:A:534:GLU:OE1	2.21	0.40
2:A:836:THR:O	2:A:840:ILE:HG13	2.20	0.40
2:A:1171:GLU:H	2:A:1171:GLU:HG3	1.63	0.40
2:A:1543:ASN:O	2:A:1563:HIS:ND1	2.51	0.40
2:A:641:MET:HE2	2:A:641:MET:HB3	1.95	0.40
2:A:987:LYS:HA	2:A:1028:TYR:CE2	2.57	0.40
15:C:145:PHE:CE2	15:C:430:PHE:CD1	3.05	0.40
15:C:215:VAL:HG11	15:C:242:LEU:CD2	2.49	0.40
2:A:1214:TRP:CE2	2:A:1230:LEU:HD11	2.56	0.40
2:A:1809:ILE:O	2:A:1818:PHE:N	2.40	0.40
2:A:2076:ARG:HB3	2:A:2305:TYR:OH	2.21	0.40
2:A:2189:SER:OG	2:A:2191:GLN:OE1	2.39	0.40
1:F:108:PHE:CD1	1:F:108:PHE:N	2.89	0.40
2:A:444:ARG:HE	2:A:444:ARG:HB2	1.67	0.40
2:A:1551:PHE:HB3	2:A:1552:GLN:H	1.60	0.40
2:A:2125:ALA:HB3	2:A:2157:VAL:HG11	2.03	0.40
2:A:2284:MET:SD	2:A:2284:MET:O	2.80	0.40
1:F:177:ARG:HD3	1:F:178:LEU:N	2.36	0.40
2:A:72:ASP:N	2:A:72:ASP:OD1	2.55	0.40
2:A:1064:PRO:HA	2:A:1065:PRO:HD3	1.97	0.40
2:A:1211:ASP:OD1	2:A:1211:ASP:N	2.53	0.40
2:A:1639:VAL:HG21	2:A:1699:THR:HG21	2.04	0.40
2:A:2072:GLU:HG3	2:A:2076:ARG:HD3	2.04	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	F	134/341 (39%)	121 (90%)	12 (9%)	1 (1%)	19	54
2	A	2137/2335 (92%)	2045 (96%)	91 (4%)	1 (0%)	100	100
4	E	56/941 (6%)	55 (98%)	1 (2%)	0	100	100
5	D	571/820 (70%)	566 (99%)	5 (1%)	0	100	100
6	G	304/357 (85%)	284 (93%)	18 (6%)	2 (1%)	19	54
7	B	1744/2136 (82%)	1716 (98%)	28 (2%)	0	100	100
8	i	79/119 (66%)	76 (96%)	3 (4%)	0	100	100
9	k	82/126 (65%)	79 (96%)	3 (4%)	0	100	100
10	l	75/92 (82%)	75 (100%)	0	0	100	100
11	m	71/86 (83%)	70 (99%)	1 (1%)	0	100	100
12	n	72/76 (95%)	72 (100%)	0	0	100	100
13	j	94/118 (80%)	92 (98%)	2 (2%)	0	100	100
14	h	69/240 (29%)	68 (99%)	1 (1%)	0	100	100
15	C	845/972 (87%)	802 (95%)	43 (5%)	0	100	100
All	All	6333/8759 (72%)	6121 (97%)	208 (3%)	4 (0%)	50	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1020	LYS
1	F	126	VAL
6	G	59	ILE
6	G	58	PRO

### 5.3.2 Protein sidechains ⓘ

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	F	59/281 (21%)	50 (85%)	9 (15%)	2	11
2	A	1626/2108 (77%)	1536 (94%)	90 (6%)	18	51
4	E	55/792 (7%)	51 (93%)	4 (7%)	11	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	D	115/721 (16%)	102 (89%)	13 (11%)	4	22
15	C	737/866 (85%)	704 (96%)	33 (4%)	23	56
All	All	2592/4768 (54%)	2443 (94%)	149 (6%)	20	50

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	90	PHE
1	F	92	LEU
1	F	122	ASN
1	F	177	ARG
1	F	195	SER
1	F	200	ASP
1	F	208	GLN
1	F	222	ARG
1	F	225	LEU
2	A	60	ASP
2	A	86	ARG
2	A	87	VAL
2	A	97	HIS
2	A	106	MET
2	A	156	ARG
2	A	164	MET
2	A	181	ASN
2	A	210	HIS
2	A	217	ARG
2	A	221	ASN
2	A	227	ARG
2	A	271	MET
2	A	292	ASP
2	A	297	ASN
2	A	310	THR
2	A	346	ASP
2	A	374	ASP
2	A	379	GLU
2	A	390	ASP
2	A	422	LEU
2	A	485	THR
2	A	498	ARG
2	A	506	LEU
2	A	510	ARG

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Mol	Chain	Res	Type
2	A	600	ARG
2	A	611	LEU
2	A	621	VAL
2	A	773	LYS
2	A	781	ARG
2	A	793	ASN
2	A	821	ARG
2	A	871	TYR
2	A	886	LEU
2	A	904	HIS
2	A	934	ARG
2	A	981	PHE
2	A	995	ARG
2	A	1008	TYR
2	A	1019	TYR
2	A	1023	ASN
2	A	1024	HIS
2	A	1026	ASN
2	A	1044	TYR
2	A	1055	LEU
2	A	1061	MET
2	A	1067	MET
2	A	1070	ASP
2	A	1089	CYS
2	A	1111	GLN
2	A	1176	SER
2	A	1180	LYS
2	A	1184	ASN
2	A	1188	ASN
2	A	1193	GLU
2	A	1194	CYS
2	A	1210	LYS
2	A	1211	ASP
2	A	1224	ARG
2	A	1234	ASP
2	A	1244	VAL
2	A	1249	MET
2	A	1255	THR
2	A	1298	ARG
2	A	1301	ILE
2	A	1307	MET
2	A	1311	PHE

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Mol	Chain	Res	Type
2	A	1341	ARG
2	A	1425	LYS
2	A	1428	HIS
2	A	1432	TYR
2	A	1441	ASP
2	A	1482	GLU
2	A	1494	TYR
2	A	1502	PHE
2	A	1537	TRP
2	A	1539	SER
2	A	1591	MET
2	A	1610	GLN
2	A	1615	HIS
2	A	1622	MET
2	A	1652	MET
2	A	1659	LYS
2	A	1667	ARG
2	A	1686	ASP
2	A	1710	ASN
2	A	1728	GLN
2	A	1734	MET
2	A	2249	LYS
2	A	2284	MET
4	E	108	LEU
4	E	110	LYS
4	E	111	ARG
4	E	113	ASP
5	D	243	LYS
5	D	271	LYS
5	D	279	SER
5	D	280	GLU
5	D	282	THR
5	D	311	GLN
5	D	322	ASP
5	D	328	ARG
5	D	330	LEU
5	D	341	ARG
5	D	350	GLN
5	D	351	ARG
5	D	375	GLU
15	C	109	LEU
15	C	112	THR

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Mol	Chain	Res	Type
15	C	261	ASP
15	C	315	SER
15	C	323	PHE
15	C	342	ARG
15	C	357	THR
15	C	358	LYS
15	C	359	LYS
15	C	365	SER
15	C	388	VAL
15	C	409	LYS
15	C	416	LEU
15	C	417	ARG
15	C	433	MET
15	C	446	LYS
15	C	478	THR
15	C	498	SER
15	C	525	CYS
15	C	536	ARG
15	C	543	ARG
15	C	660	VAL
15	C	673	LYS
15	C	694	LYS
15	C	735	PHE
15	C	764	ASP
15	C	770	PHE
15	C	775	ARG
15	C	856	HIS
15	C	907	VAL
15	C	914	LYS
15	C	917	VAL
15	C	944	SER

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

Mol	Chain	Res	Type
2	A	994	ASN
2	A	1026	ASN
2	A	1182	ASN
2	A	1188	ASN
2	A	1460	HIS
2	A	1615	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	5	101/117 (86%)	35 (34%)	4 (3%)

All (35) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	5	4	C
3	5	5	U
3	5	9	G
3	5	20	G
3	5	21	A
3	5	22	U
3	5	23	C
3	5	24	G
3	5	25	C
3	5	26	A
3	5	28	A
3	5	36	C
3	5	38	C
3	5	47	A
3	5	48	A
3	5	55	C
3	5	56	C
3	5	57	G
3	5	58	U
3	5	59	G
3	5	66	A
3	5	67	A
3	5	69	A
3	5	71	C
3	5	75	G
3	5	78	U
3	5	86	C
3	5	94	U
3	5	95	G
3	5	97	G
3	5	98	G
3	5	105	U
3	5	106	U
3	5	107	U
3	5	108	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	5	57	G
3	5	58	U
3	5	96	A
3	5	105	U

## 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](#)

1 ligand is 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	$\# Z  > 2$
16	GTP	C	1001	-	26,34,34	1.06	3 (11%)	32,54,54	0.74	0

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
16	GTP	C	1001	-	-	2/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	1001	GTP	C5-C6	-2.71	1.41	1.47
16	C	1001	GTP	C8-N7	-2.18	1.31	1.35
16	C	1001	GTP	C5-C4	-2.01	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

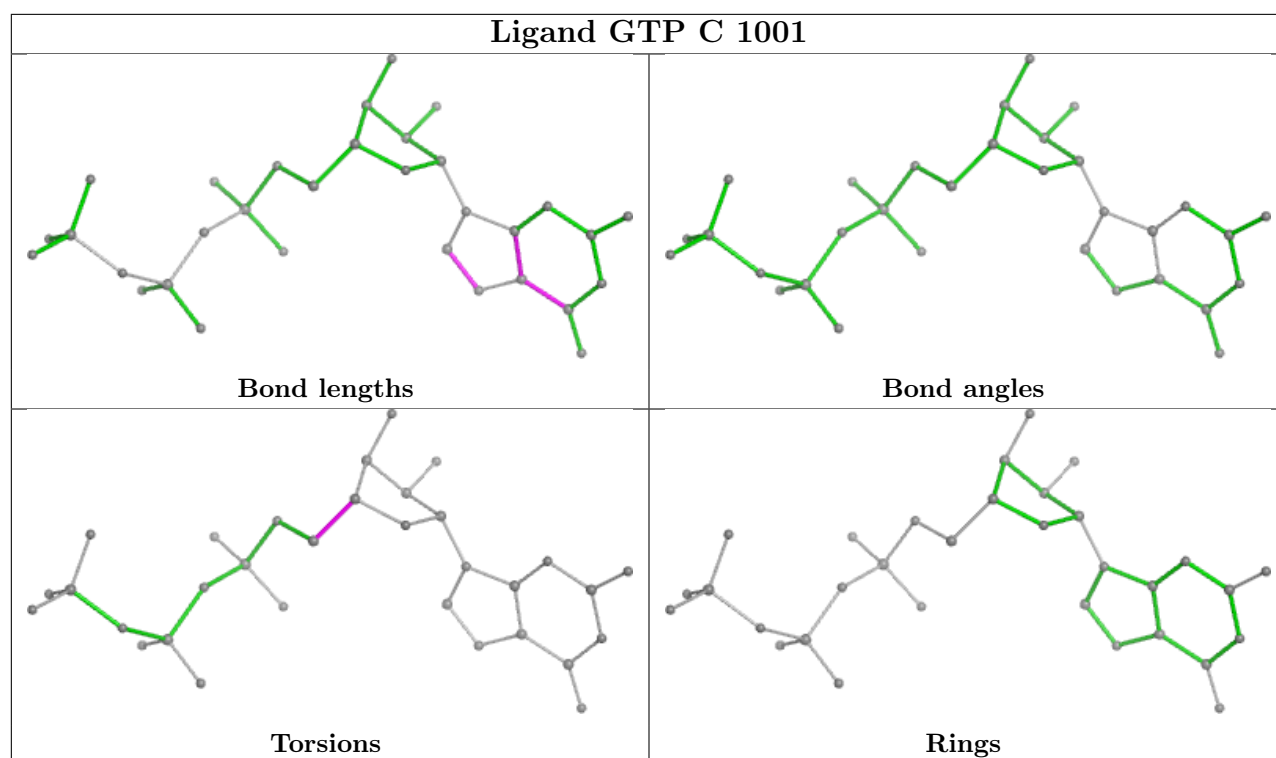
Mol	Chain	Res	Type	Atoms
16	C	1001	GTP	O4'-C4'-C5'-O5'
16	C	1001	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	C	1001	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

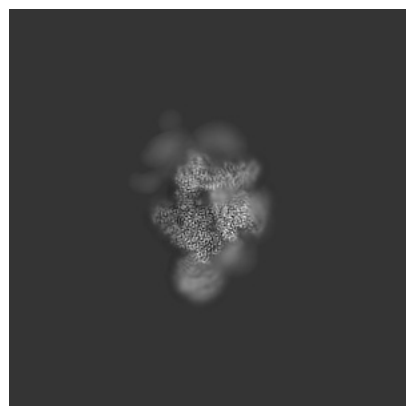
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19041. These allow visual inspection of the internal detail of the map and identification of artifacts.

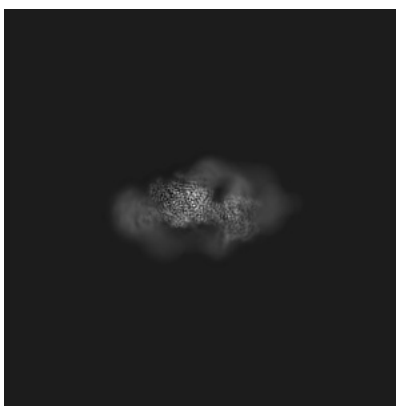
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

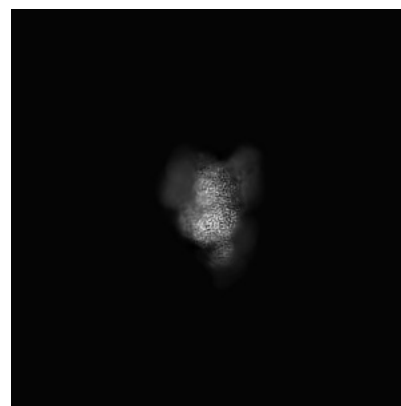
#### 6.1.1 Primary map



X

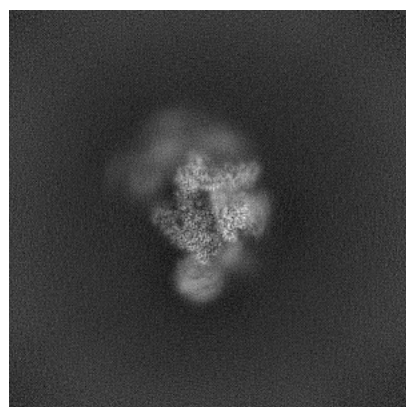


Y

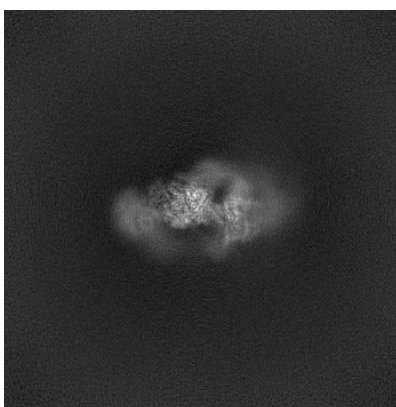


Z

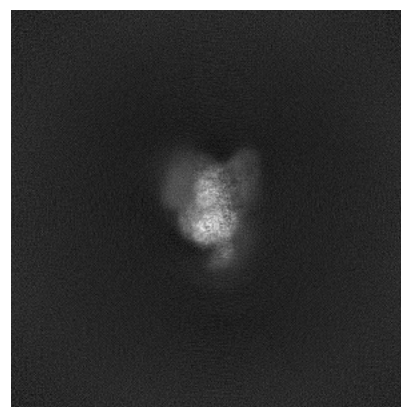
#### 6.1.2 Raw map



X



Y

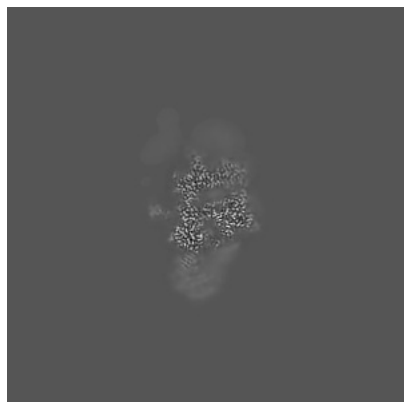


Z

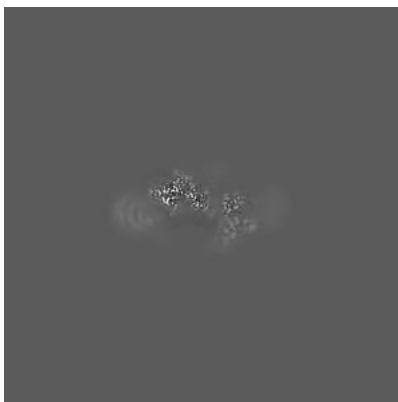
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

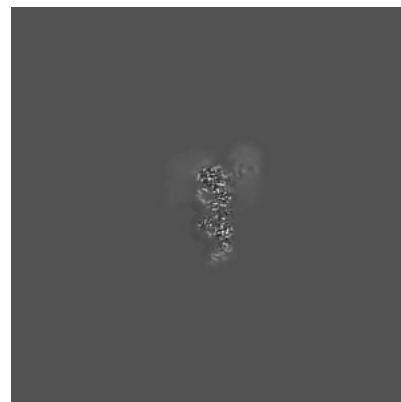
### 6.2.1 Primary map



X Index: 252

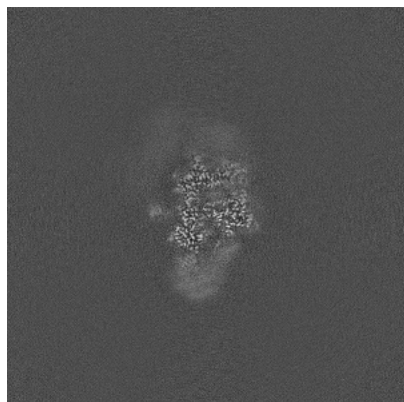


Y Index: 252

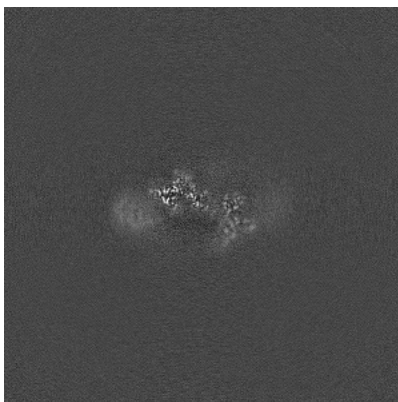


Z Index: 252

### 6.2.2 Raw map



X Index: 252



Y Index: 252

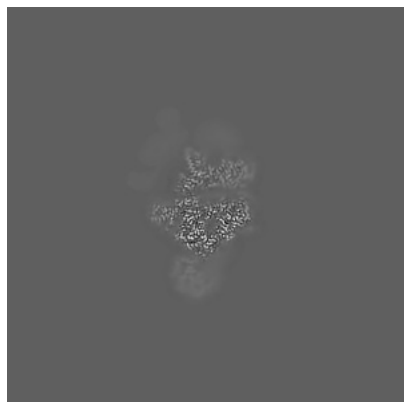


Z Index: 252

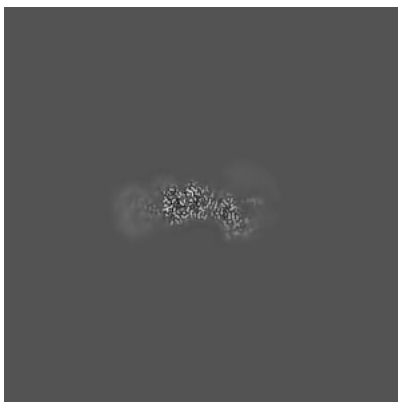
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

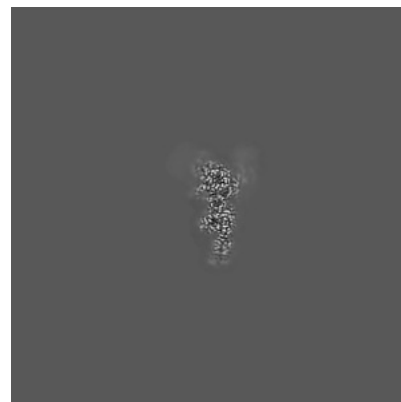
### 6.3.1 Primary map



X Index: 260

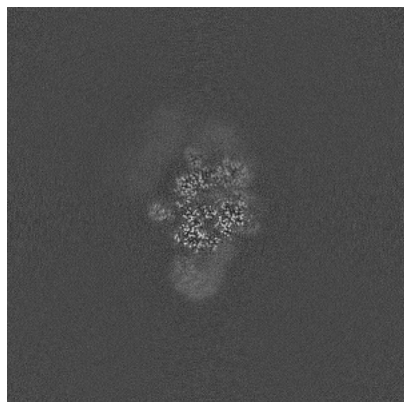


Y Index: 228

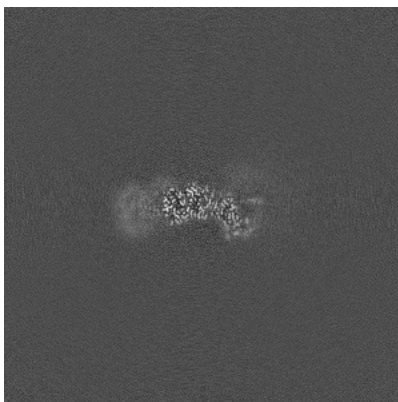


Z Index: 241

### 6.3.2 Raw map



X Index: 256



Y Index: 228



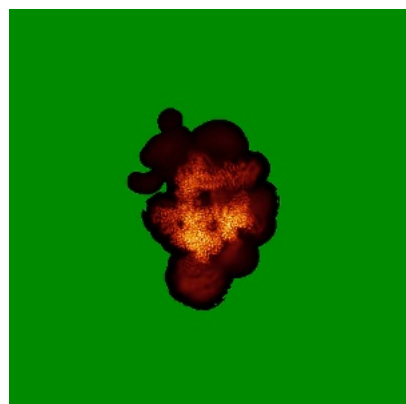
Z Index: 241

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

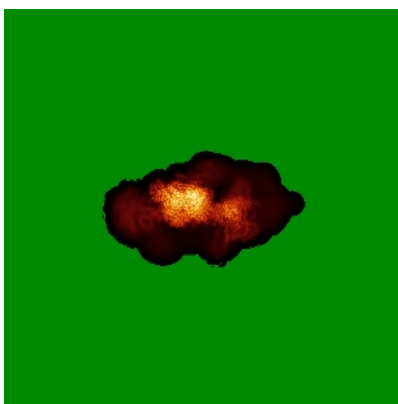


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

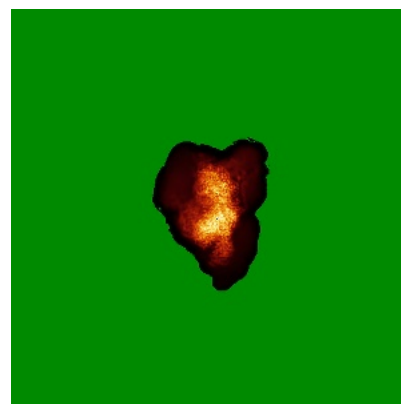
### 6.4.1 Primary map



X

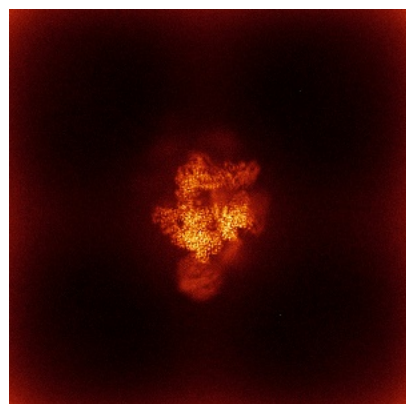


Y

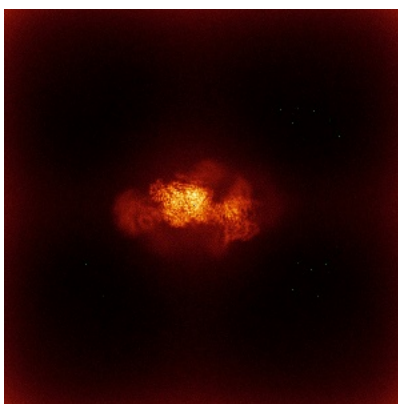


Z

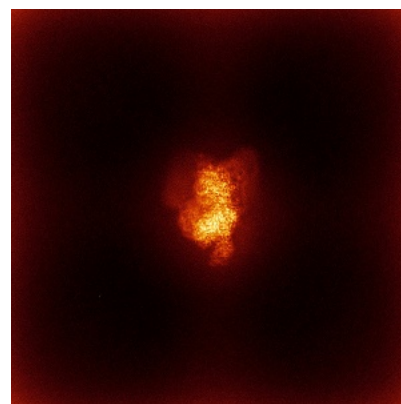
### 6.4.2 Raw map



X



Y

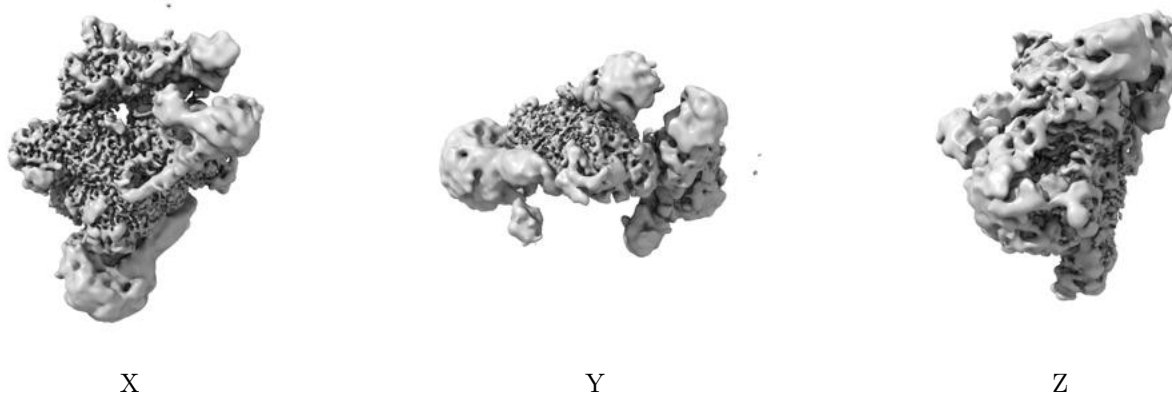


Z

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.

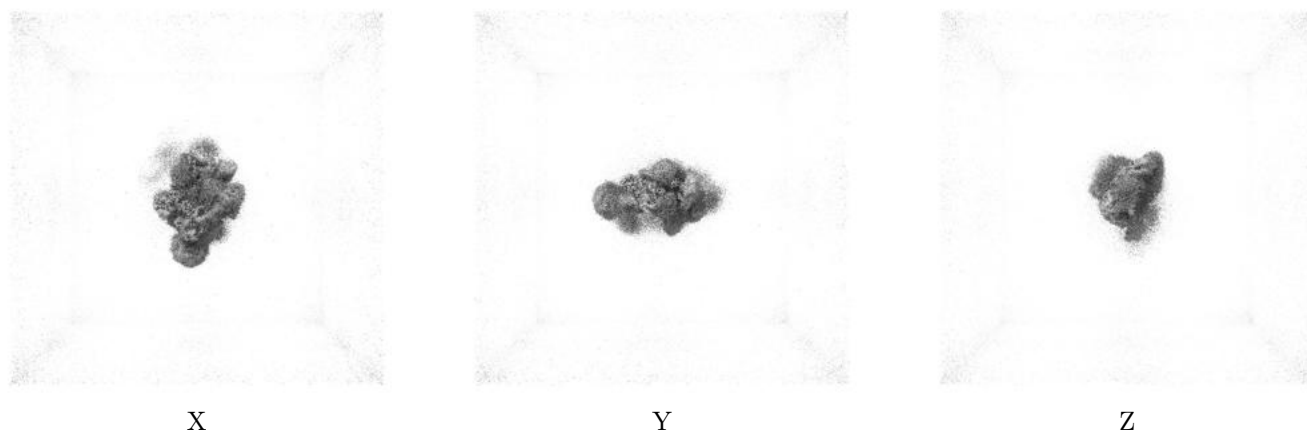
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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



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.

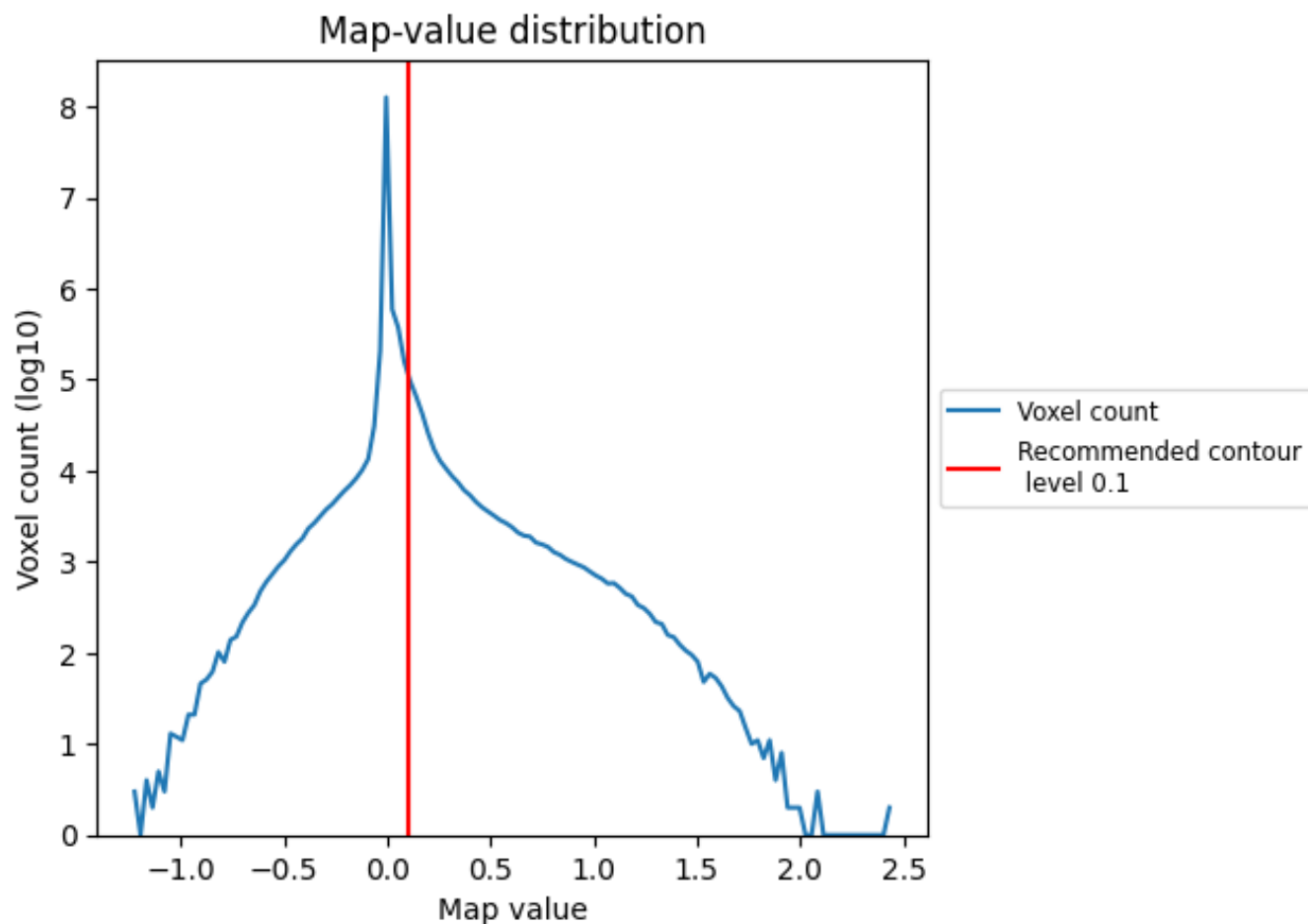
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

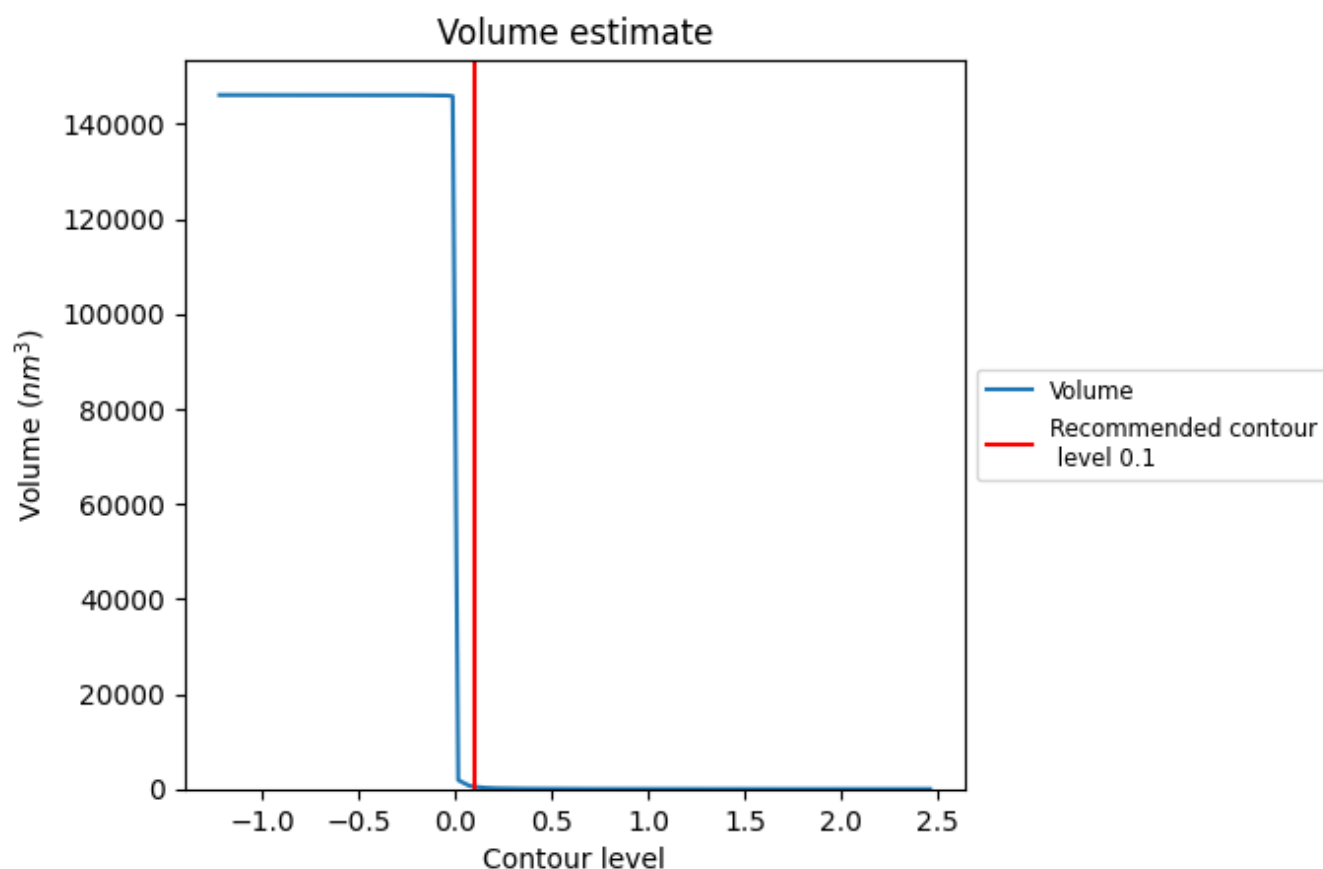
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

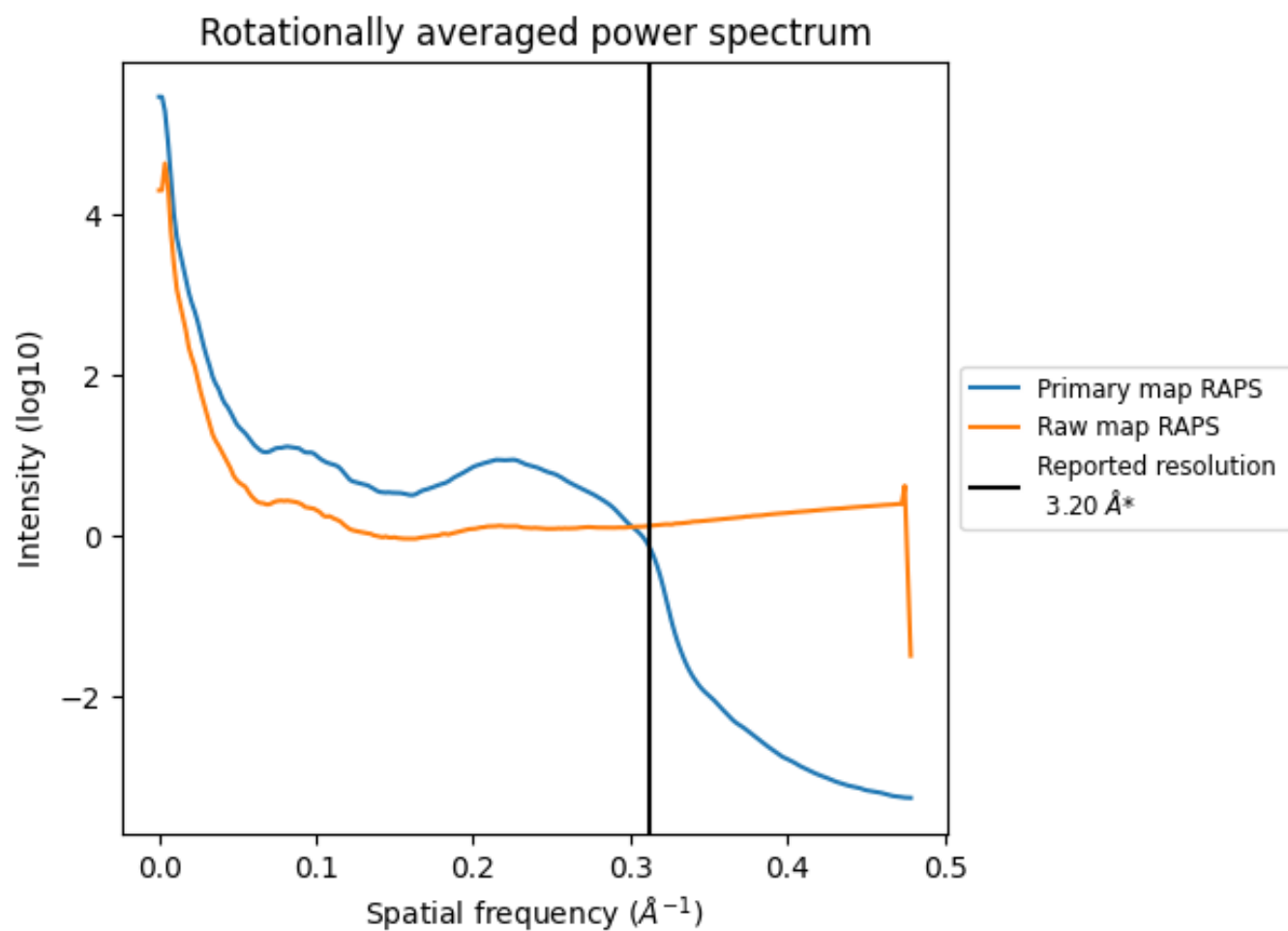
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 456 nm<sup>3</sup>; this corresponds to an approximate mass of 412 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 ⓘ

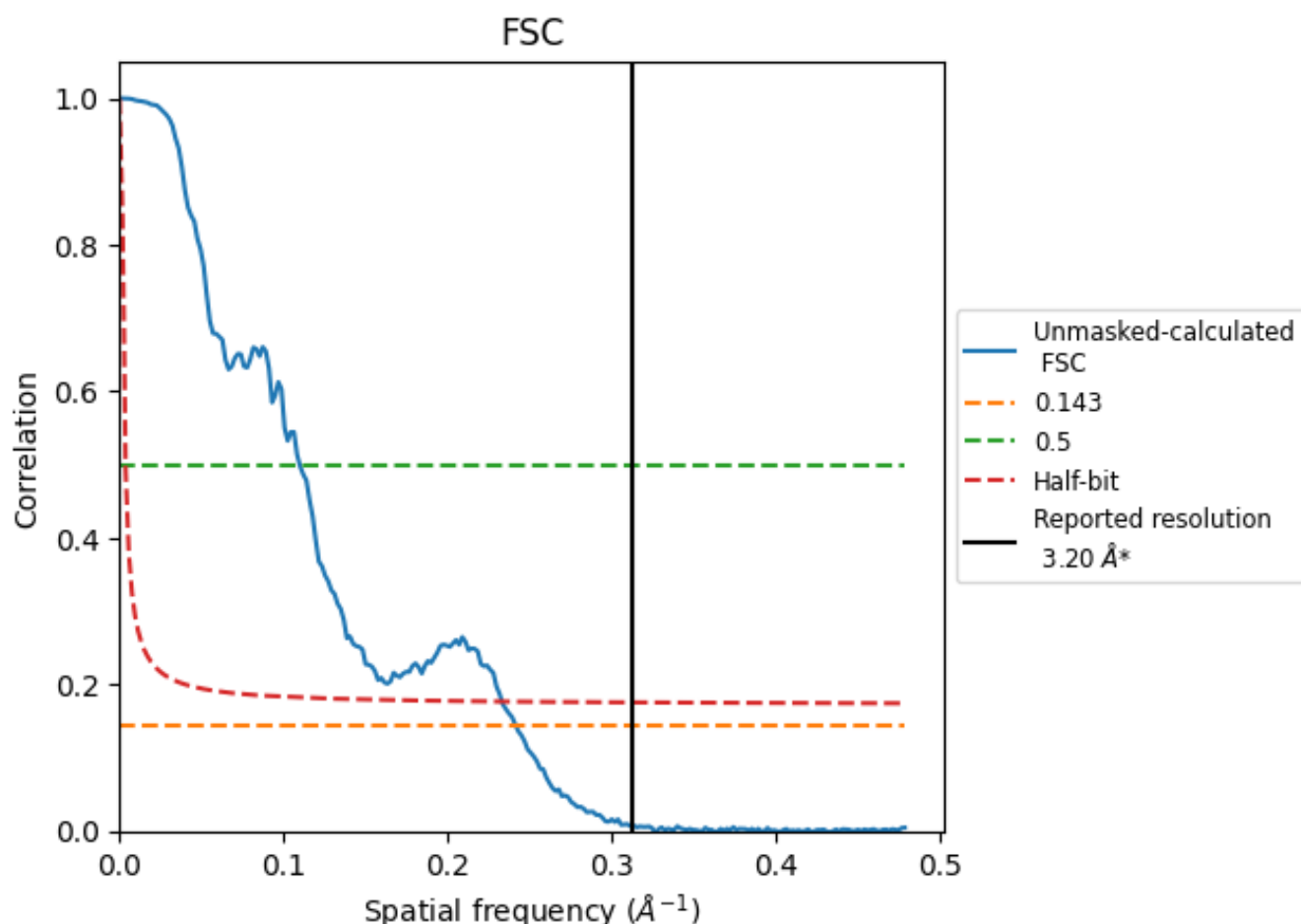


\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

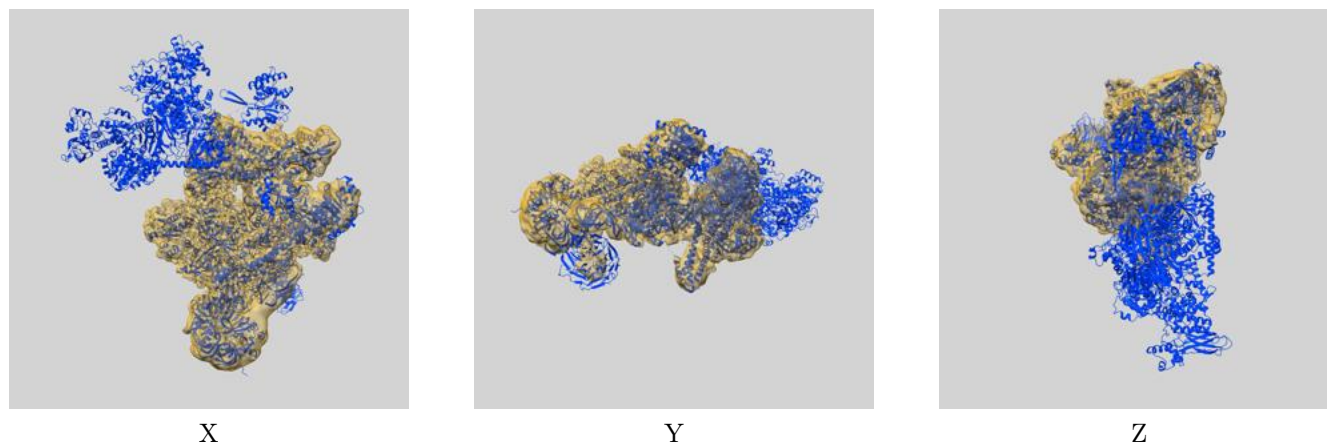
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	9.11	4.29

\*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 4.14 differs from the reported value 3.2 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19041 and PDB model 8RC0. Per-residue inclusion information can be found in section [3](#) on page [7](#).

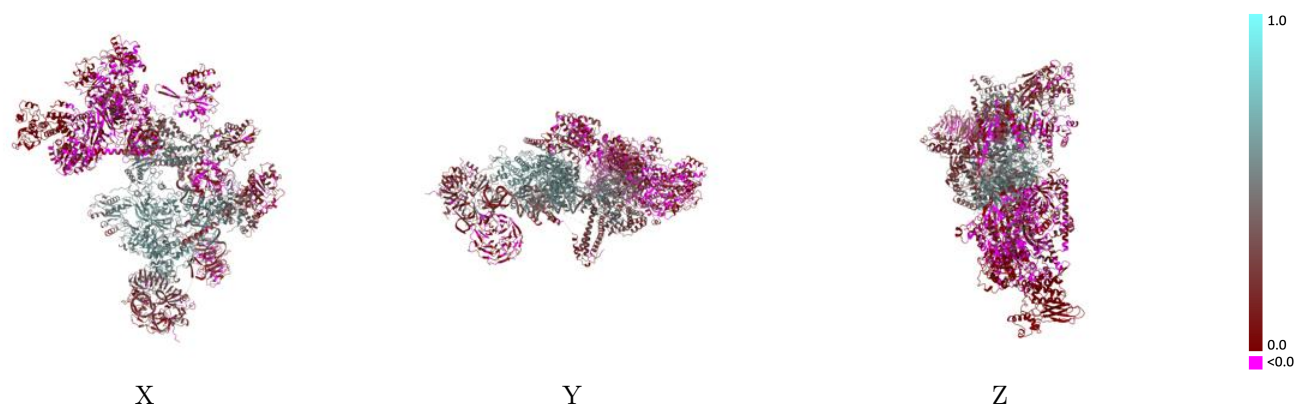
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

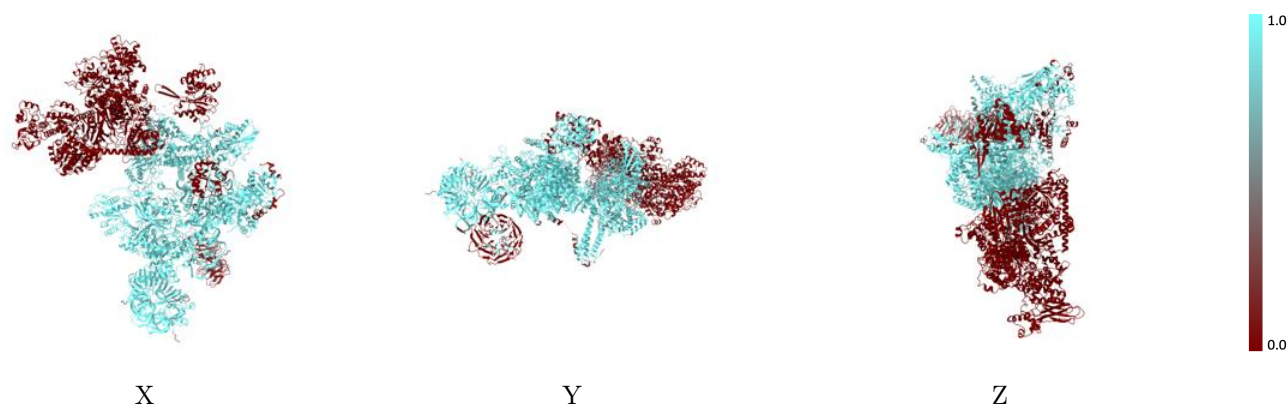


## 9.2 Q-score mapped to coordinate model [i](#)



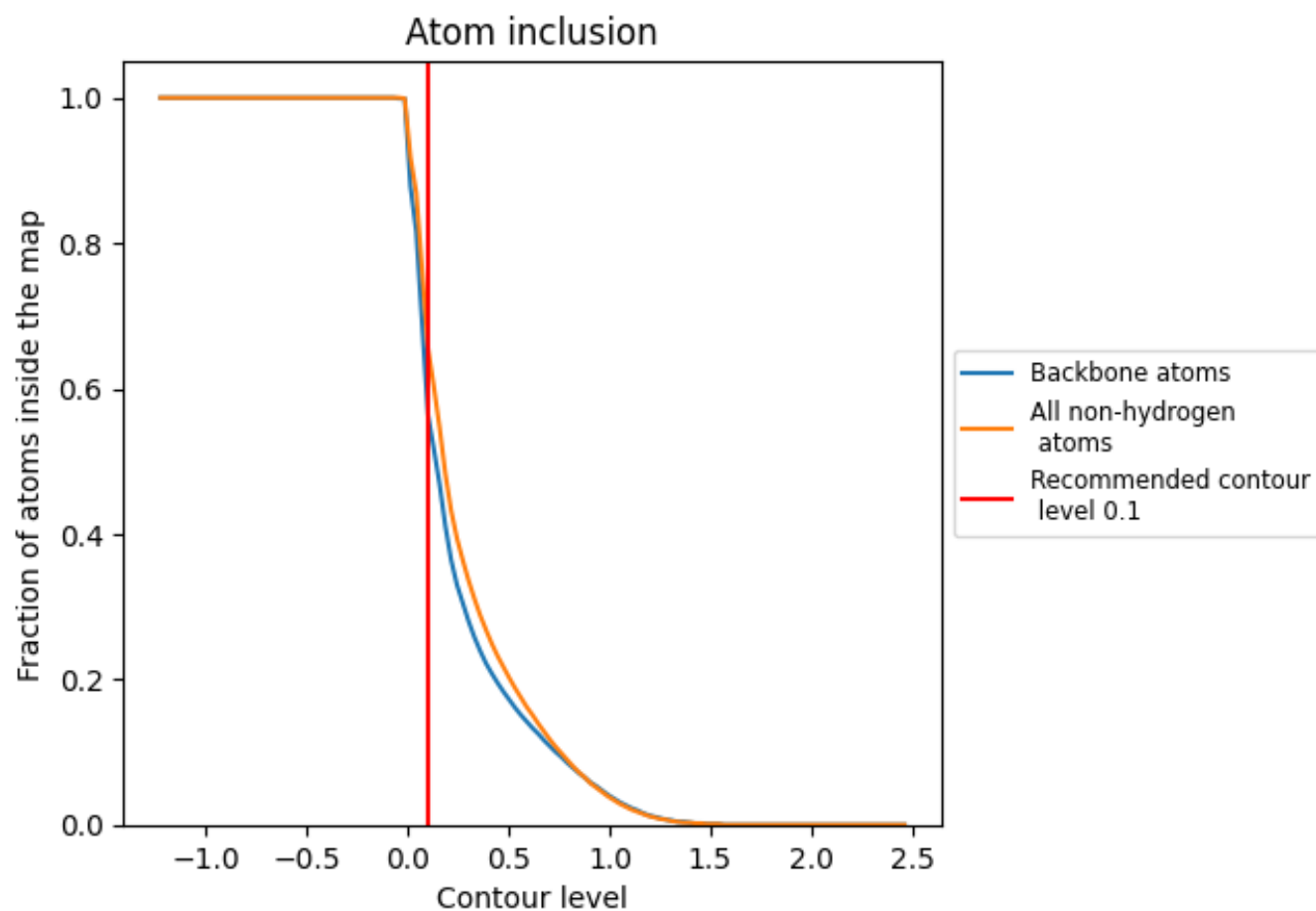
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.1).

































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 66% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6570	 0.3090
5	 0.9510	 0.2970
A	 0.7610	 0.3710
B	 0.0150	 0.0280
C	 0.9810	 0.5600
D	 0.6320	 0.2220
E	 0.5840	 0.1820
F	 0.9410	 0.3760
G	 0.1360	 0.0540
h	 0.9760	 0.3080
i	 0.9970	 0.2900
j	 0.8800	 0.1940
k	 0.9760	 0.4080
l	 1.0000	 0.2280
m	 0.9760	 0.1970
n	 0.8990	 0.3060

