



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 12:28 AM UTC

PDB ID : 8RC0 / pdb_00008rc0
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

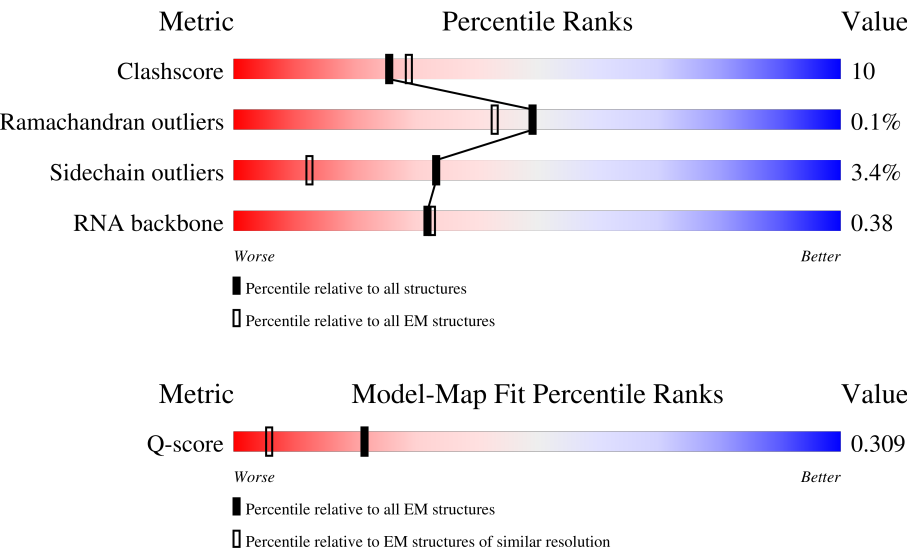
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance 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.



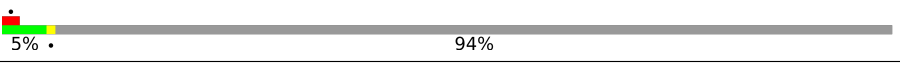
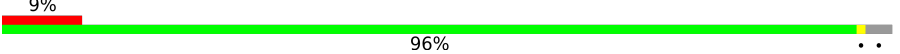
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	F	341	28%13%59%
2	A	2335	23% 65%26%8%
3	5	117	29%47%13%11%

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Mol	Chain	Length	Quality of chain
4	E	941	
5	D	820	
6	G	357	
7	B	2136	
8	i	119	
9	k	126	
10	l	92	
11	m	86	
12	n	76	
13	j	118	
14	h	240	
15	C	972	

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		

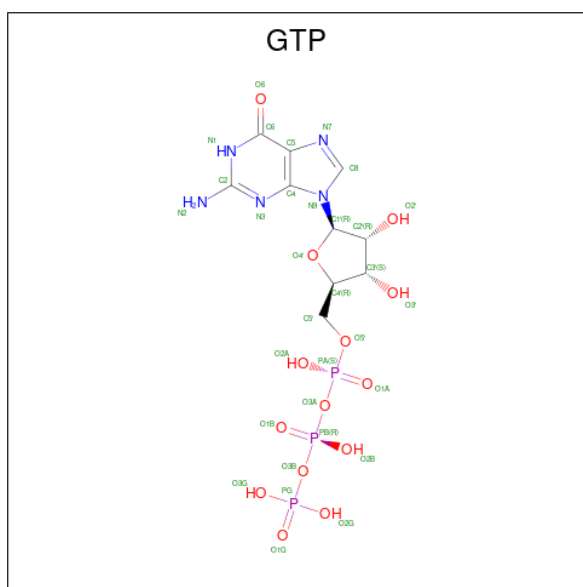
- Molecule 14 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

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		

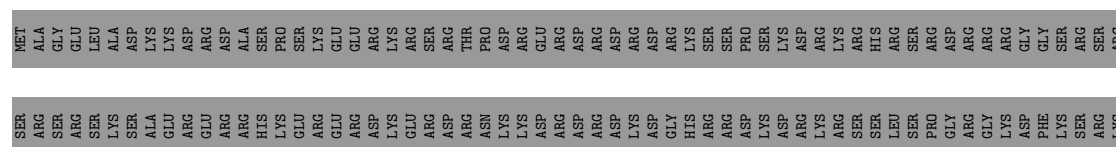
- Molecule 16 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



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

I1809	F1810	M1811	P1812	A1813	T1814	G1815	Q1816	L1817	F1818	L1819	K1820	I1821	I1822	H1823	T1824	S1825	S1826	S1827	A1828	G1829	Q1830	L1831	R1832	L1833	G1834	Q1835	L1836	A1837	K1838	W1839	K1840	T1841	A1842	E1843	F1844	F1845	F1846	F1847	F1848	F1849	F1850	F1851	L1852	P1853	V1854	E1855	E1856	Q1857	P1858	K1859	Q1860	I1861	I1862	V1863	T1864	A1865	K1866	G1867	M1868						
I1747	L1751	Q1752	L1753	Y1754	SER	SER	GLU	PRO	THR	E1760	P1761	L1762	S1764	S1765	L1766	Y1687	S1693	I1694	Y1695	P1696	T1699	G1700	L1701	L1702	I1703	L1706	L1707	L1708	L1709	L1710	K1618	S1619	Y1620	K1621	M1622	M1623	S1624	A1714	Y1715	G1716	N1717	P1720	K1723	P1724	L1725	Q1728	A1729	M1730	A1731	K1732	I1733	R1744	E1745	M1797	L1798	T1799	T1800	K1801	P1802	I1803	N1804	G1805	A1806	I1807	F1808
I1574	Q1575	I1576	F1577	R1578	A1579	H1580	L1581	W1582	Q1583	K1584	I1585	H1586	E1587	S1588	M1589	M1590	M1591	D1592	L1593	E1600	L1601	D1602	I1606	E1607	E1612	H1615	K1618	S1619	Y1620	K1621	M1622	M1623	S1624	A1714	Y1715	G1716	N1717	P1720	K1723	P1724	L1725	Q1728	A1729	M1730	A1731	K1732	I1733	R1744	E1745	M1797	L1798	T1799	T1800	K1801	P1802	I1803	N1804	G1805	A1806	I1807	F1808				
F1502	W1503	E1504	K1505	ALA	SER	GLY	PHE	GLU	GLU	SER	MET	LYS	TRP	LYS	LYS	LEU	K1434	D1435	W1436	R1439	F1440	D1441	F1442	K1443	Q1444	Y1445	Q1446	L1447	L1448	K1449	W1454	W1455	L1456	H1457	Q1458	R1459	H1460	K1463	L1464	W1465	N1466	L1478	E1482	G1483	E1486	H1487	K1491	T1497	W1498	E1499	G1500	L1501	L1508												
G1323	G1324	L1325	G1326	M1327	M1330	L1334	R1341	F1342	S1343	K1344	Q1345	T1346	D1347	V1348	H1352	F1353	R1354	S1355	GLY	MET	SER	HIS	GLU	ASP	Q1363	L1364	F1365	P1366	I1372	W1375	F1379	L1382	Q1383	L1384	V1385	L1391	K1392	R1393	Q1394	E1395	A1396	Q1399	L1403	T1404	D1407	L1408																			
E1223	R1224	T1225	C1228	F1229	L1230	R1231	D1234	R1239	F1240	H1241	N1242	V1244	S1251	T1254	T1255	I1259	N1264	M1271	F1274	R1275	E1276	A1277	V1278	E1283	K1290	K1300	I1301	G1302	L1303	N1304	S1305	P1308	F1311	P1312	F1313	V1314	V1315	F1316	T1317	T1318	F1319	K1320	E1321	L1322																					
R1107	D1108	L1109	T1110	Q1111	E1116	H1117	D1119	E1123	G1127	M1130	R1141	D1146	A1152	P1162	Y1165	W1170	E1171	N1172	S1176	S1179	K1180	D1181	N1182	P1183	N1184	M1188	C1189	E1193	C1194	R1201	E1206	D1211	W1214	N1218	E1219	V1220	T1221	K1222																											
I1017	M1018	Y1019	K1020	D1021	M1022	M1023	H1024	T1025	Y1028	G1029	I1030	I1031	R1032	G1033	F1036	Y1044	V1047	M1048	D1049	L1050	L1051	L1055	M1056	R1057	E1060	G1063	P1064	E1065	Q1066	M1067	D1070	I1077	A1078	F1088	C1089	R1090	Y1091	H1092	D1093	R1094	H1095	I1097	R1100	A1103	A1106																				
K837	L838	L839	I840	L841	E842	L843	R844	R845	Y850	K853	N857	Q860	A870	E876	A877	L878	S879	R880	I881	K882	R883	H884	L885	E886	T887	Q888	R889	A890	F891	K892	E893	V894	G895	I896	E897	F898	M899	D900	L901	Y902	S903	H904	L905	V908	V911	E912	P913	L914	E915	K916	I917														
T918	D919	L922	D923	E929	R933	Y939	D944	T945	E946	L950	L951	K954	N960	L974	N975	A976	S979	F981	E982	F983	H984	Y985	E986	K987	I988	L992	L996	L997	R998	L999	I1000	V1001	D1002	H1003	L1004	I1005	A1006	D1007	M1008	M1009	T1010	A1011	K1012	N1013	V1016																				
SER	H680	L685	D686	G700	C719	A722	N723	K773	L776	L779	T780	R781	L784	K785	A786	E787	Q788	E789	R790	Y794	L795	K796	Y800	E804	E805	A806	V807	A808	V809	T812	H815	W816	L817	E818	S819	R820	F822	S823	P824	I825	Y832	K833	H834	D835	T836																				
V835	M851	Y852	R853	Y854	K855	L608	L611	I612	Y613	N617	V621	A631	A632	R635	V636	W637	M641	T645	L648	E649	R650	W651	L652	L655	L656	A657	ARG	GLN	PHE	GLY	GLY	ARG	HIS	SER	LYS	GLY	VAL	ALA	LYS	THR	VAL	THR	LYS	GLN	ARG	VAL	GLU																		







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	E1489	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	K1498	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
L1566	C1506	Q1446	A1386	P1326	V1266	P1206	K1146	Q1086	M1026	K966	V906	G846
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	E1462	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



F883	S731	H538	L418	E240	H140	GLU
D886	I732	I539	K421	R241	ASP	THR
F887	F735	I559	K422	L242	LYS	ASP
F888	G736			I243	T143	LYS
T889	P737	T562	F430	F145	T144	TYR
H890		A563		V247	TYR	ASP
T891	P742	E573	M433	V255	PRO	GLU
S897	N743			D147	THR	GLU
L898	I744	M603	Q436	C148	ALA	GLY
			H437	K259	ASN	GLY
	D747			I150	GLU	TYR
V907	D748	Y614	P441	R262	VAL	TYR
I916	T749	P615		P155	GLY	ILE
V917	K756	S616	A445	E266	PRO	GLY
I918		L617	K446	E156	PRO	GLU
			P447		GLU	VAL
P925	D764	S624	K448	L298	VAL	LEU
			I449	I299	GLU	ASP
A926	V767	L635		D164	THR	SER
P927	R775	L635	T452	L165	ILE	ASP
H928		D638		G305	VAL	GLU
	L779	R645	G455	Y167	GLN	ASP
R931	C790	M647		N306	GLU	ASP
M934	K788	I651		T168	GLU	ASP
I935	F789	V659	P473	Q313	ASP	GLU
R938	K790	V660	T478	L173	GLU	GLU
	I808	V666	T479	L320	THR	LEU
K941	S818		M465	R177	GLY	GLY
S944	E945				ARG	GLY
D946	M822	S670	P473	S1326	GLU	GLU
V947				Y327	PRO	GLU
				A328	THR	THR
				V186	LYS	LYS
				G332	GLU	ASP
				D333	LEU	ASP
				T192	ILE	ASP
				T193	ILE	ASP
				N335	LYS	GLU
				M203	MET	ASP
				D204	PRO	ASP
				T205	VAL	ASP
					LYS	ASP
				W344	THR	ASP
				F211	LYS	ASP
				S212	LYS	ASP
				D213	PHE	ASP
				T357	THR	ASP
				K358	THR	ASP
				V215	ASP	VAL
				T216	LEU	VAL
				M105	GLY	GLY
				L219	ASP	ASP
				Q365	HIS	ASP
				Q366	F110	ASP
				V225	V111	ASP
				V370	T112	ASP
				F228	HIS	ASP
				L1229	LYS	ASP
				D230	L119	PRO
				E375	M123	GLY
				V388	M131	MET
				E233	N131	GLU
				M236	V132	VAL
				L412	T133	VAL
				V386	L237	LEU
				L416	N238	LEU
				E415	H137	LEU

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	0.18	0/898	0.50	0/1227
2	A	0.24	0/17137	0.44	5/23327 (0.0%)
3	5	0.16	0/2444	0.33	0/3798
4	E	0.11	0/519	0.31	0/688
5	D	0.14	0/2955	0.41	0/3773
6	G	0.12	0/1506	0.40	0/2091
7	B	0.10	0/6990	0.35	0/8734
8	i	0.08	0/323	0.23	0/402
9	k	0.12	0/335	0.33	0/417
10	l	0.09	0/307	0.27	0/382
11	m	0.09	0/291	0.22	0/362
12	n	0.08	0/296	0.23	0/367
13	j	0.08	0/390	0.28	0/484
14	h	0.08	0/290	0.29	0/359
15	C	0.33	1/6777 (0.0%)	0.51	6/9214 (0.1%)
All	All	0.22	1/41458 (0.0%)	0.42	11/55625 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	144	CYS	C-O	-5.34	1.16	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	145	PHE	N-CA-C	-7.76	102.52	110.97
15	C	144	CYS	CA-C-N	-6.56	111.99	120.65
15	C	144	CYS	C-N-CA	-6.56	111.99	120.65
2	A	333	HIS	CA-C-N	6.01	133.11	122.48
2	A	333	HIS	C-N-CA	6.01	133.11	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	784	LEU	CA-CB-CG	5.80	136.59	116.30
2	A	1119	ASP	CB-CA-C	5.77	118.21	110.13
15	C	148	CYS	N-CA-C	-5.59	105.28	111.71
15	C	144	CYS	N-CA-CB	5.51	120.12	110.42
2	A	821	ARG	CA-CB-CG	5.17	124.45	114.10
15	C	927	PRO	CA-N-CD	-5.09	104.88	112.00

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	38	0
2	A	16709	0	15543	468	0
3	5	2192	0	1111	43	0
4	E	516	0	501	10	0
5	D	2941	0	1555	42	0
6	G	1507	0	682	9	0
7	B	6992	0	1835	13	0
8	i	324	0	85	0	0
9	k	336	0	95	1	0
10	l	308	0	83	1	0
11	m	292	0	86	0	0
12	n	297	0	84	1	0
13	j	392	0	98	0	0
14	h	292	0	78	1	0
15	C	6629	0	6607	140	0
16	C	32	0	12	1	0
All	All	40648	0	29176	721	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 (721) 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:2149:PRO:HB2	2:A:2292:MET:HE1	1.62	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
4:E:112:MET:HE3	4:E:112:MET:HA	1.68	0.75
1:F:168:ARG:H	1:F:222:ARG:HD2	1.52	0.74
2:A:899:MET:HE2	2:A:908:VAL:HG21	1.69	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:209:MET:HE3	1:F:209:MET:O	1.95	0.66
2:A:1499:GLU:N	2:A:1499:GLU:OE1	2.27	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
2:A:1579:ALA:O	2:A:1584:LYS:NZ	2.29	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
15:C:473:PRO:O	15:C:498:SER:OG	2.13	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:1067:MET:HA	2:A:1067:MET:HE2	1.80	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
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:213:ASP:OD2	15:C:616:SER:OG	2.17	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
3:5:57:G:O2'	3:5:58:U:O5'	2.19	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:2200:MET:HE1	2:A:2206:TRP:HB3	1.84	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:1384:ARG:HD2	2:A:1384:ARG:C	2.27	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:1271:MET:HE3	2:A:1330:MET:HG3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
15:C:144:CYS:HA	15:C:147:ASP:CG	2.31	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
2:A:1222:LYS:NZ	2:A:2088:ASN:O	2.39	0.56
15:C:110:PRO:HD2	15:C:537:TYR:CE2	2.41	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
15:C:166:CYS:C	15:C:168:THR:H	2.13	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
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
15:C:727:LEU:O	15:C:731:SER:OG	2.17	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
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
2:A:1455:TRP:H	2:A:1455:TRP:CD1	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:VAL:HG23	2:A:1575:GLN:HB2	1.89	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
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: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:1454:TRP:H	2:A:1454:TRP:CD1	2.27	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
2:A:1703:ILE:HG21	2:A:1730:MET:HE2	1.90	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
3:5:89:U:O2	12:n:65:ASN:N	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:150:MET:HE3	2:A:193:LEU:HA	1.92	0.51
2:A:231:THR:H	2:A:234:MET:HE2	1.75	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
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:150:MET:HE2	2:A:193:LEU:HD12	1.93	0.51
2:A:982:GLU:OE2	2:A:1172:ASN:ND2	2.44	0.51
15:C:934:MET:HE3	15:C:938:ARG:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:A:899:MET:HE1	2:A:1448:LEU:HA	1.93	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:1620:TYR:HA	2:A:1622:MET:HE1	1.94	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
2:A:1404:THR:OG1	2:A:1407:ASP:OD2	2.24	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
1:F:175:LEU:HD13	2:A:61:MET:HE1	1.94	0.49
2:A:312:TYR:OH	15:C:886:ASP:OD1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:A:1188:ASN:C	2:A:1188:ASN:HD22	2.21	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
2:A:1047:VAL:HG12	2:A:1048:MET:HE3	1.96	0.48
15:C:144:CYS:HA	15:C:147:ASP:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:C:724:TRP:CZ3	15:C:732:ILE:HD11	2.49	0.48
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:1591:MET:HE2	2:A:1591:MET:C	2.39	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
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
10:I:31:ILE:N	10:I:45:GLY:O	2.47	0.46
15:C:647:MET:HE3	15:C:647:MET:HB2	1.77	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:850:TYR:HA	2:A:853:LYS:HZ1	1.81	0.46
2:A:1487:HIS:HB3	2:A:1541:THR:HB	1.98	0.46
2:A:1576:ILE:HD11	2:A:1746:ARG:C	2.40	0.46
15:C:421:LYS:HE3	15:C:421:LYS:HB2	1.58	0.46
2:A:902:TYR:HB2	2:A:1242:ASN:CG	2.40	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
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
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
2:A:1618:LYS:HZ2	2:A:1628:ASP:CG	2.23	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
15:C:764:ASP:C	15:C:764:ASP:OD1	2.59	0.45
2:A:271:MET:HE1	2:A:313:LYS:HD3	1.99	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:C:144:CYS:O	15:C:145:PHE:C	2.58	0.44
2:A:308:ILE:HD12	2:A:320:TYR:HE1	1.81	0.44
2:A:883:ARG:O	2:A:887:THR:OG1	2.34	0.44
2:A:1271:MET:HE1	2:A:1278:VAL:HG11	1.99	0.44
2:A:1426:ASP:OD1	2:A:1429:THR:HB	2.17	0.44
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
2:A:641:MET:HE2	2:A:641:MET:HB3	1.66	0.44
2:A:1708:ALA:C	2:A:1709:TYR:HD1	2.26	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1048:MET:HA	2:A:1048:MET:HE2	2.00	0.44
2:A:1416:ILE:HD13	2:A:1416:ILE:HA	1.87	0.44
2:A:1436:TRP:CD1	2:A:1436:TRP:H	2.36	0.44
2:A:1621:LYS:C	2:A:1622:MET:HE3	2.43	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:1271:MET:HB2	2:A:1271:MET:HE2	1.56	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:976:MET:HE1	2:A:1096:HIS:HB3	2.00	0.43
2:A:1008:TYR:CD1	2:A:1008:TYR:C	2.94	0.43
2:A:1116:GLU:HG2	2:A:1117:HIS:CD2	2.53	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:C:183:SER:CB	15:C:203:MET:HE2	2.48	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:1223:GLU:HA	2:A:1224:ARG:NH2	2.33	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:1459:ARG:HG3	2:A:1459:ARG:HH11	1.83	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
2:A:1537:TRP:CD1	2:A:1537:TRP:C	2.97	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1384:ARG:NE	2:A:1385:VAL:HG23	2.33	0.42
2:A:1633:ALA:O	2:A:1634:SER:OG	2.31	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:773:LYS:HD2	2:A:773:LYS:C	2.44	0.42
2:A:1070:ASP:OD1	2:A:1070:ASP:C	2.61	0.42
2:A:1414:ARG:NH1	2:A:1414:ARG:HG3	2.33	0.42
15:C:449:ILE:HD12	15:C:465:MET:HE3	2.02	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
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:1501:LEU:HD12	2:A:1754:TYR:C	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:E:112:MET:HA	4:E:112:MET:CE	2.46	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
2:A:2115:ILE:O	2:A:2118:SER:OG	2.36	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:2261:MET:HE2	2:A:2261:MET:HB2	1.92	0.41
2:A:1612:GLU:HB2	2:A:1630:LEU:HD21	2.02	0.41
3:5:37:G:N7	3:5:38:C:O2'	2.44	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
1:F:209:MET:HE2	1:F:217:VAL:HG22	2.02	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:2093:SER:HB3	2:A:2258:ARG:NH2	2.36	0.41
6:G:58:PRO:C	6:G:60:MET:H	2.28	0.41
6:G:58:PRO:O	6:G:60:MET:N	2.53	0.41
14:h:42:LEU:O	14:h:70:VAL:N	2.35	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
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:919:ASP:OD2	2:A:1012:LYS:NZ	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:D:316:GLN:CD	5:D:318:ARG:H	2.22	0.41
9:k:48:VAL:N	9:k:56:ALA:O	2.43	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:192:ASP:CG	15:C:193:THR:N	2.79	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:919:ASP:OD1	2:A:919:ASP:N	2.52	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:854:ARG:NE	15:C:879:ASP:OD2	2.49	0.41
15:C:860:ASP:OD1	15:C:860:ASP:C	2.63	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
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:503:MET:HE2	2:A:503:MET:HB3	1.76	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:1530:PRO:O	2:A:1531:ASN:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1543:ASN:O	2:A:1563:HIS:ND1	2.51	0.40
2:A:987:LYS:HA	2:A:1028:TYR:CE2	2.57	0.40
2:A:1640:SER:C	2:A:1653:ASP:HB2	2.46	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:170:ASP:OD1	2:A:170:ASP:C	2.65	0.40
2:A:999:LEU:HD23	2:A:999:LEU:C	2.46	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:1077:ILE:HD12	2:A:1077:ILE:C	2.46	0.40
2:A:1466:ASN:OD1	2:A:1466:ASN:C	2.63	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: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%)	18 52
2	A	2137/2335 (92%)	2045 (96%)	91 (4%)	1 (0%)	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	18	52
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%)	49	79

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%)	55 (93%)	4 (7%)	14	46
2	A	1626/2108 (77%)	1574 (97%)	52 (3%)	34	65
4	E	55/792 (7%)	55 (100%)	0	100	100
5	D	115/721 (16%)	111 (96%)	4 (4%)	32	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	C	737/866 (85%)	708 (96%)	29 (4%)	28	62
All	All	2592/4768 (54%)	2503 (97%)	89 (3%)	33	64

All (89) 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	208	GLN
2	A	87	VAL
2	A	97	HIS
2	A	176	LEU
2	A	221	ASN
2	A	227	ARG
2	A	310	THR
2	A	346	ASP
2	A	374	ASP
2	A	390	ASP
2	A	422	LEU
2	A	485	THR
2	A	506	LEU
2	A	513	LEU
2	A	593	ARG
2	A	611	LEU
2	A	621	VAL
2	A	645	THR
2	A	809	VAL
2	A	886	LEU
2	A	944	ASP
2	A	951	LEU
2	A	984	MET
2	A	1023	ASN
2	A	1055	LEU
2	A	1089	CYS
2	A	1165	VAL
2	A	1176	SER
2	A	1184	ASN
2	A	1193	GLU
2	A	1194	CYS
2	A	1211	ASP
2	A	1234	ASP

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Mol	Chain	Res	Type
2	A	1244	VAL
2	A	1255	THR
2	A	1301	ILE
2	A	1334	LEU
2	A	1365	ILE
2	A	1372	ILE
2	A	1385	VAL
2	A	1440	THR
2	A	1441	ASP
2	A	1448	LEU
2	A	1482	GLU
2	A	1502	PHE
2	A	1539	SER
2	A	1553	VAL
2	A	1560	ILE
2	A	1574	ILE
2	A	1615	HIS
2	A	1667	ARG
2	A	1710	ASN
2	A	2273	VAL
5	D	280	GLU
5	D	282	THR
5	D	284	ILE
5	D	322	ASP
15	C	109	LEU
15	C	112	THR
15	C	193	THR
15	C	225	VAL
15	C	243	ILE
15	C	247	VAL
15	C	255	VAL
15	C	298	LEU
15	C	334	ILE
15	C	357	THR
15	C	365	SER
15	C	388	VAL
15	C	416	LEU
15	C	452	THR
15	C	478	THR
15	C	498	SER
15	C	509	VAL
15	C	525	CYS

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Mol	Chain	Res	Type
15	C	660	VAL
15	C	666	VAL
15	C	735	PHE
15	C	767	VAL
15	C	790	LYS
15	C	834	VAL
15	C	856	HIS
15	C	889	THR
15	C	907	VAL
15	C	917	VAL
15	C	944	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	300	ASN
2	A	563	GLN
2	A	869	GLN
2	A	1023	ASN
2	A	1035	GLN
2	A	1042	GLN
2	A	1159	ASN
2	A	1182	ASN
2	A	1188	ASN
2	A	1241	HIS
2	A	1246	GLN
2	A	1282	GLN
2	A	1296	GLN
2	A	1458	GLN
2	A	1460	HIS
2	A	1554	GLN
2	A	1615	HIS
2	A	1727	GLN
5	D	287	ASN
5	D	297	GLN
15	C	451	HIS
15	C	502	HIS
15	C	786	ASN
15	C	837	GLN

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	-	33,34,34	0.61	0	50,54,54	0.60	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	-	-	2/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

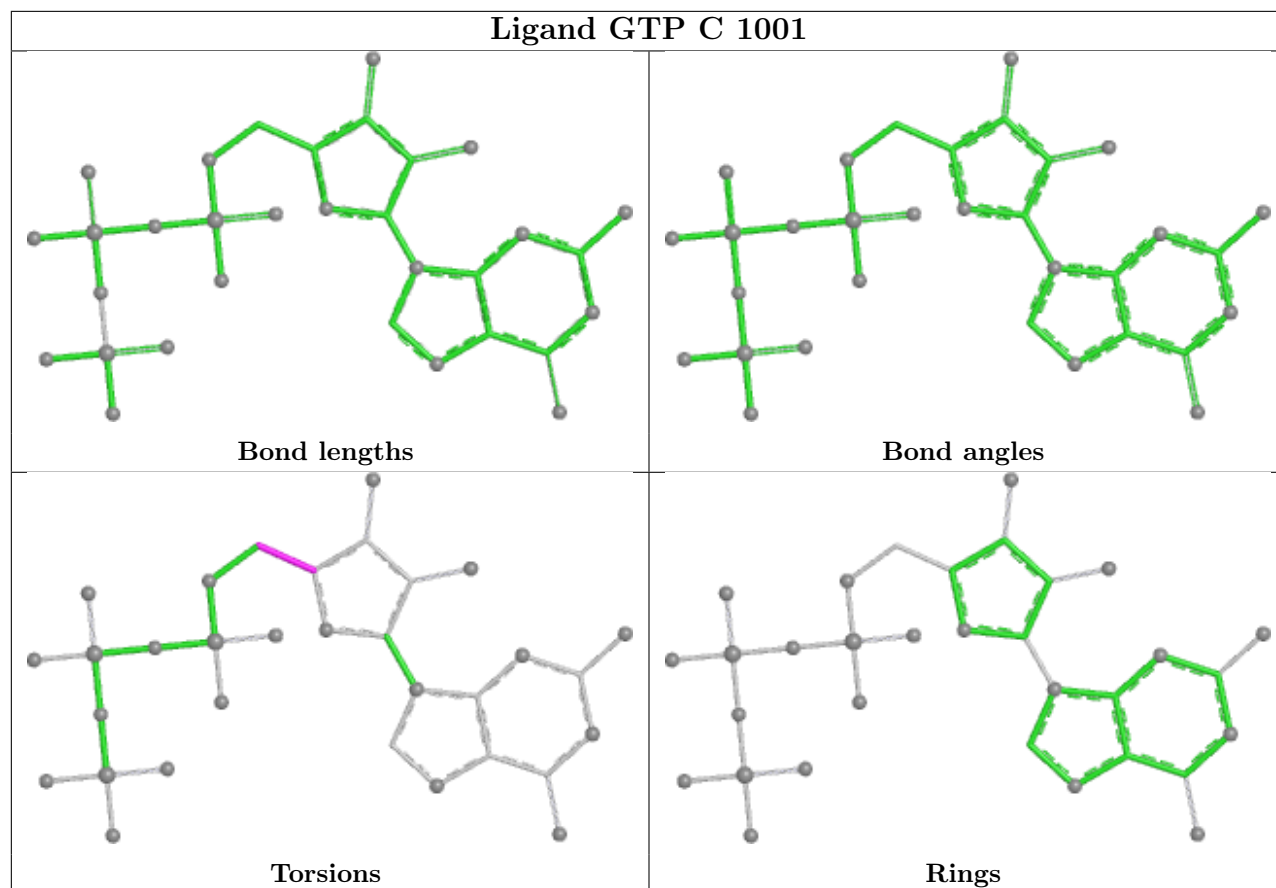
Mol	Chain	Res	Type	Atoms
16	C	1001	GTP	O4'-C4'-C5'-O5'
16	C	1001	GTP	C3'-C4'-C5'-O5'

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.

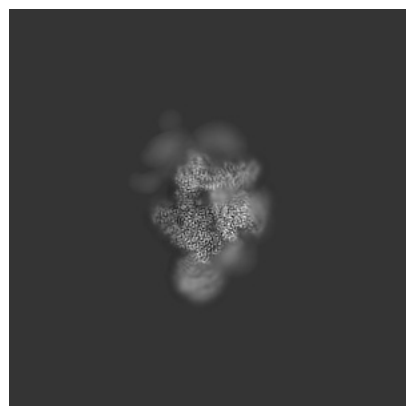
6 Map visualisation [i](#)

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.

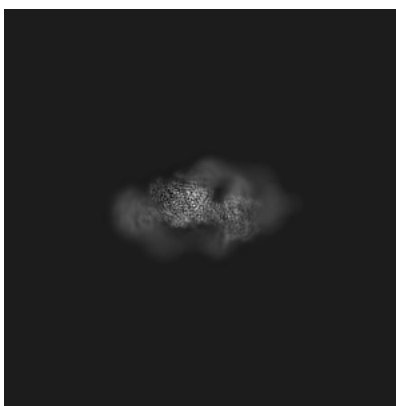
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

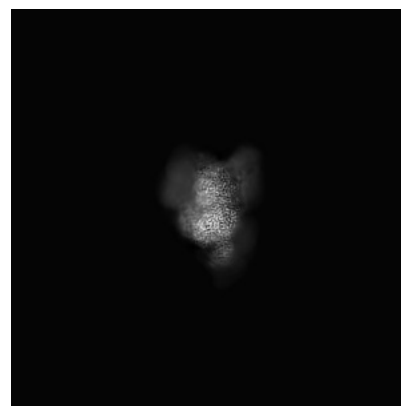
6.1.1 Primary map



X

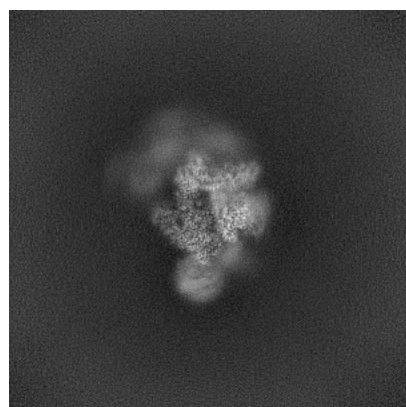


Y

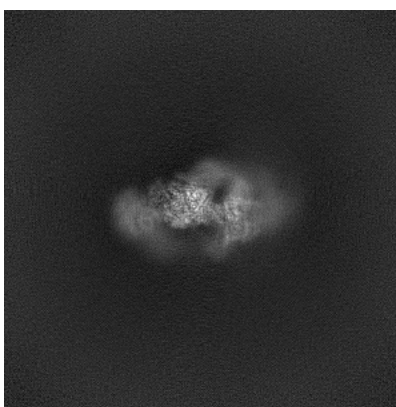


Z

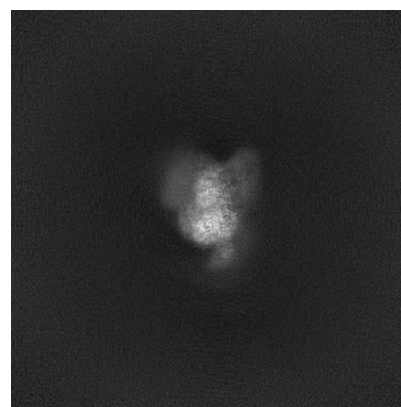
6.1.2 Raw map



X



Y

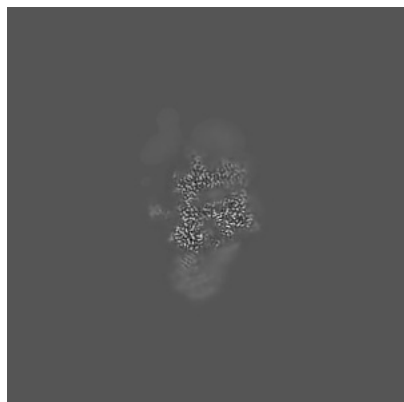


Z

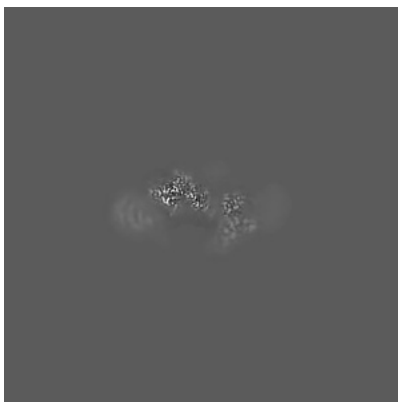
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

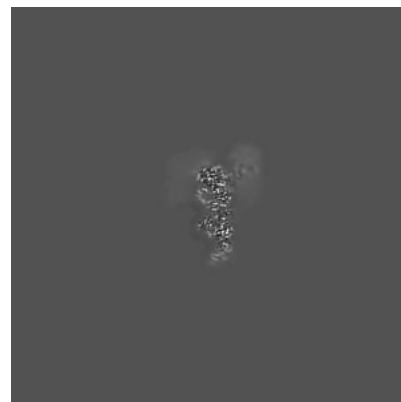
6.2.1 Primary map



X Index: 252

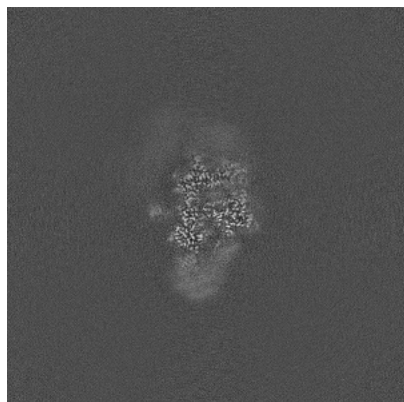


Y Index: 252

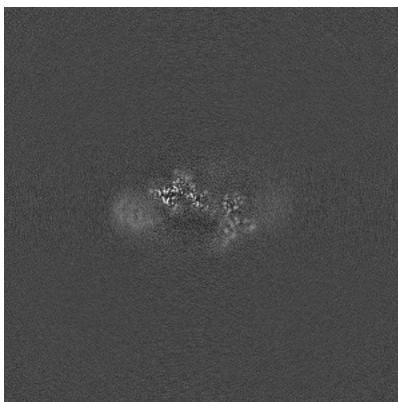


Z Index: 252

6.2.2 Raw map



X Index: 252



Y Index: 252

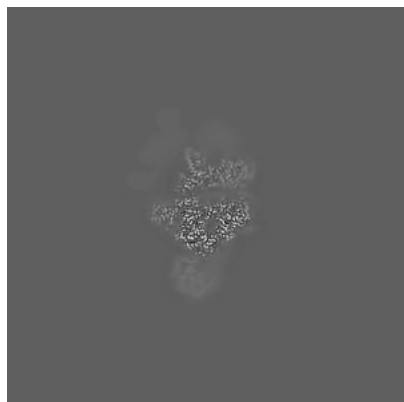


Z Index: 252

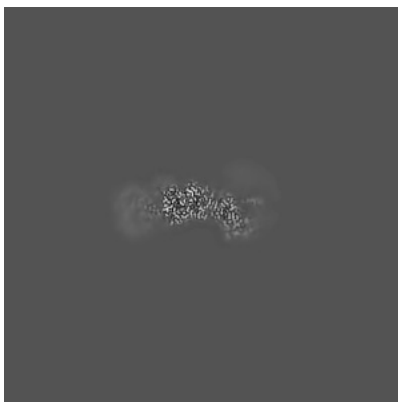
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

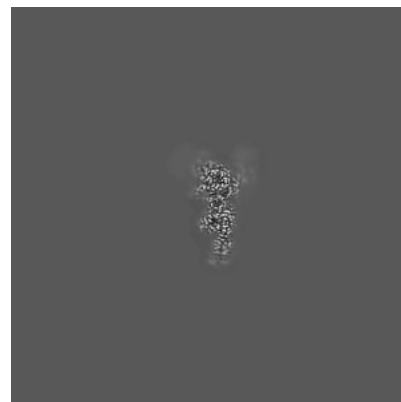
6.3.1 Primary map



X Index: 260

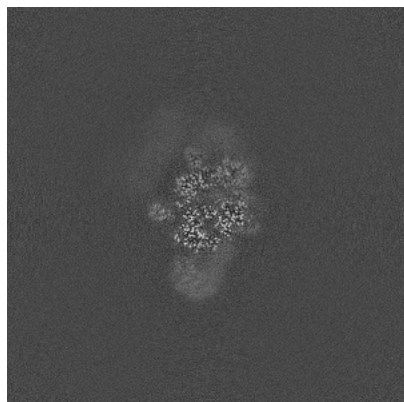


Y Index: 228

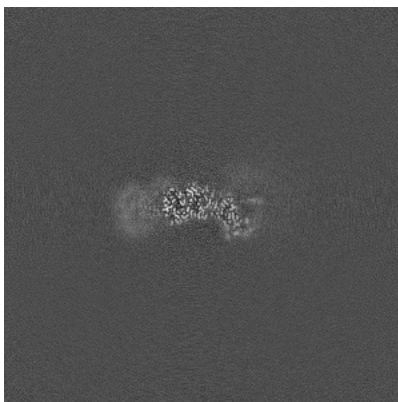


Z Index: 241

6.3.2 Raw map



X Index: 256



Y Index: 228

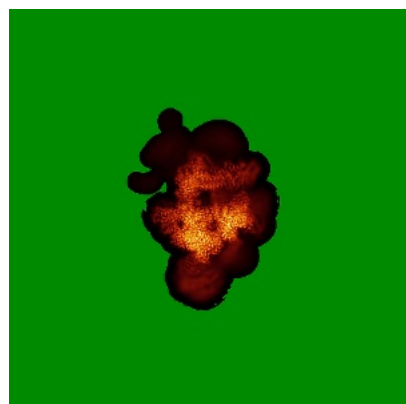


Z Index: 241

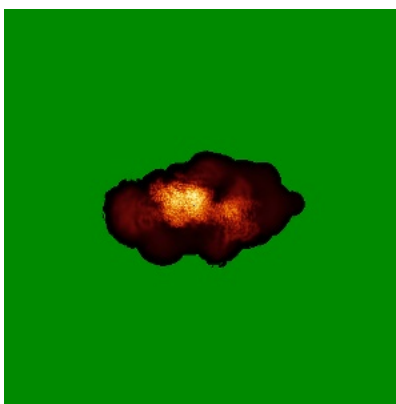
The images above show the largest variance slices of the map in three orthogonal directions.

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

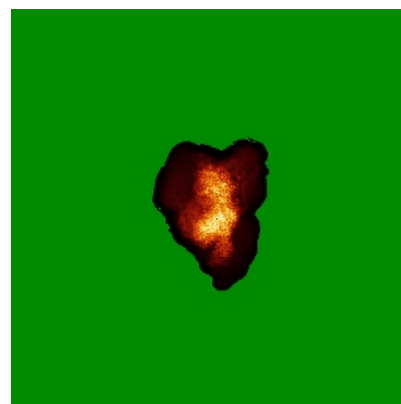
6.4.1 Primary map



X

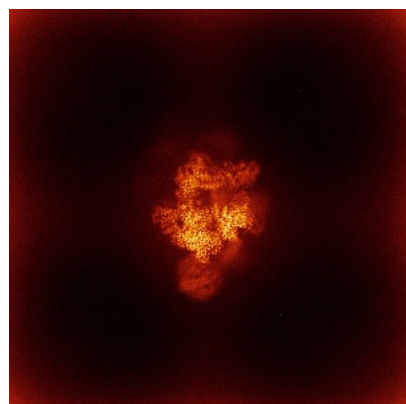


Y

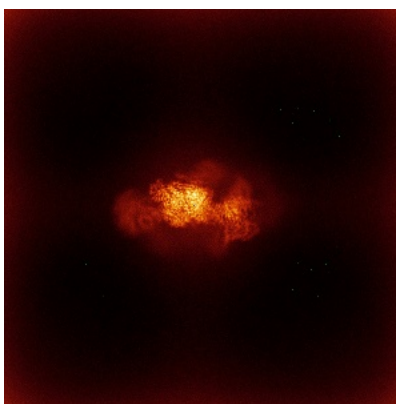


Z

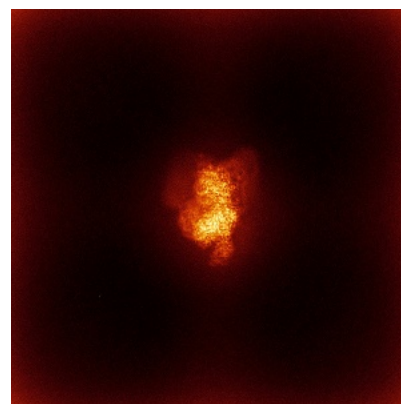
6.4.2 Raw map



X



Y

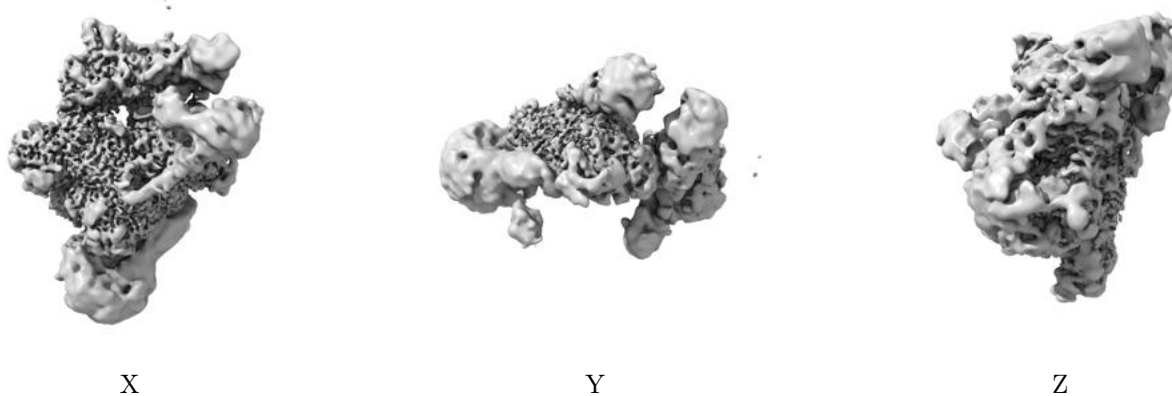


Z

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.

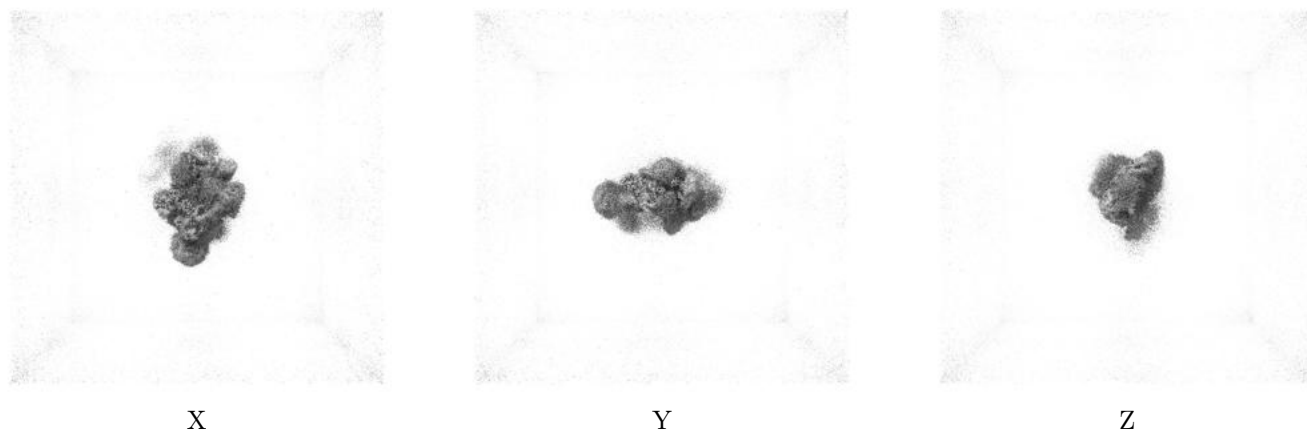
6.5 Orthogonal surface views [i](#)

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.

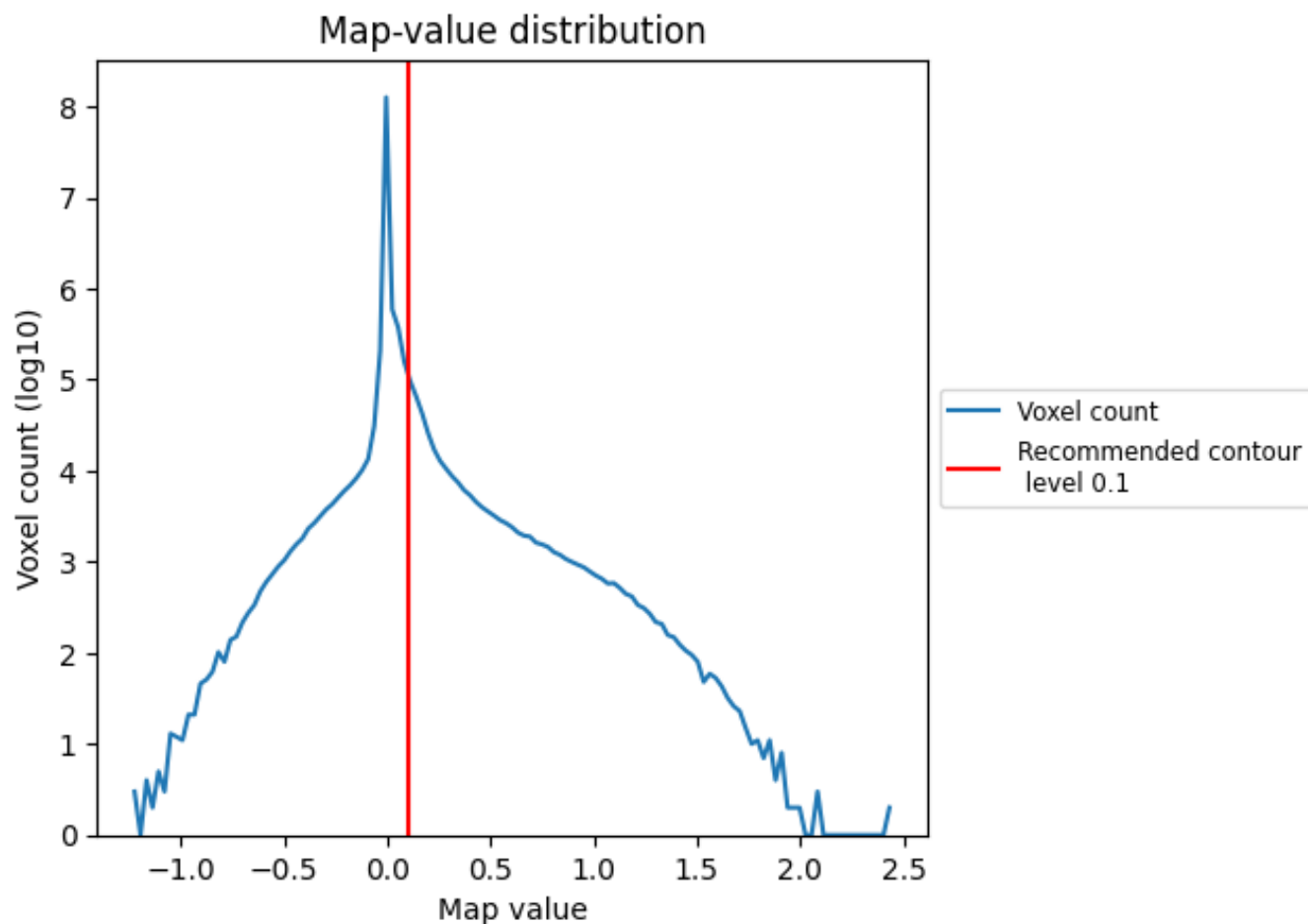
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

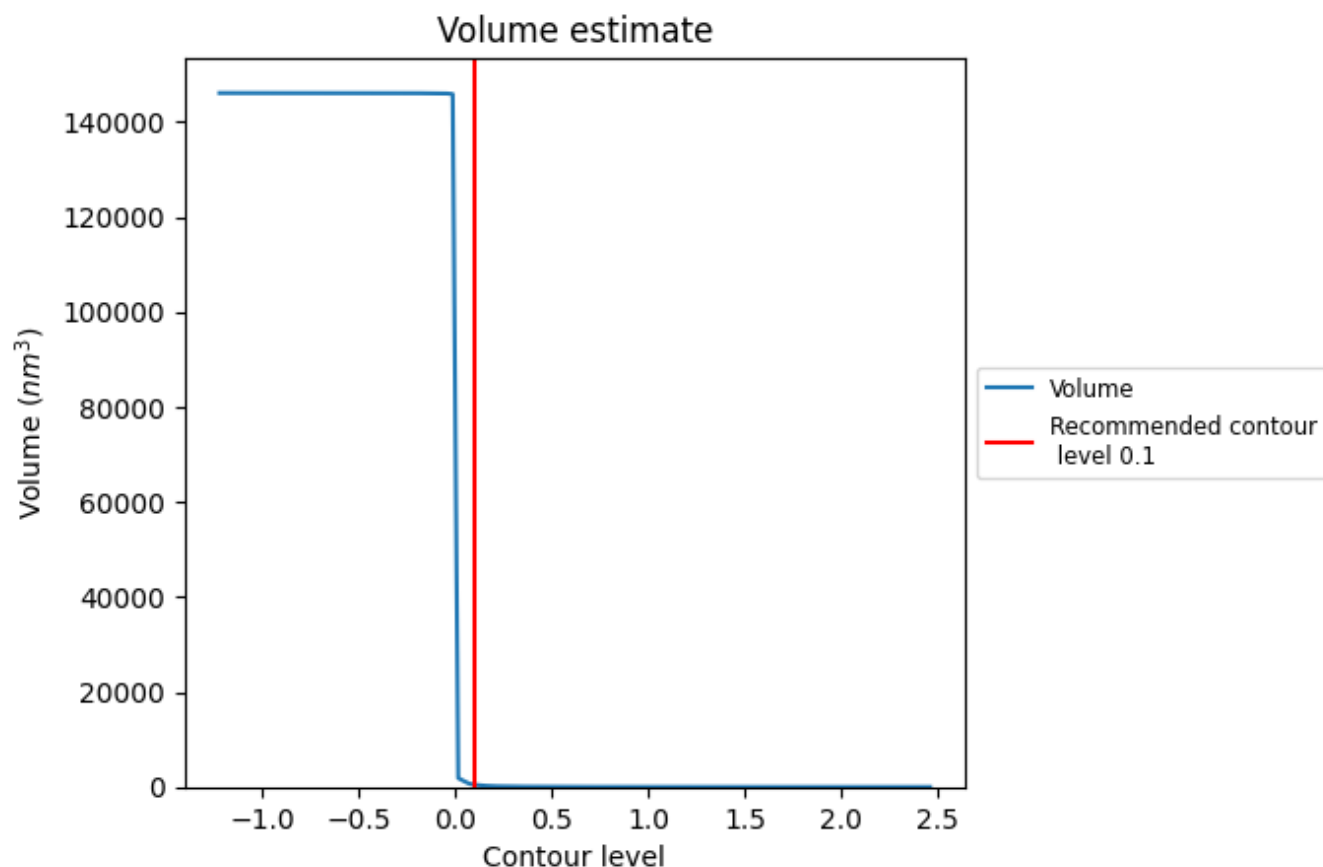
This section contains the results of statistical analysis of the map.

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.

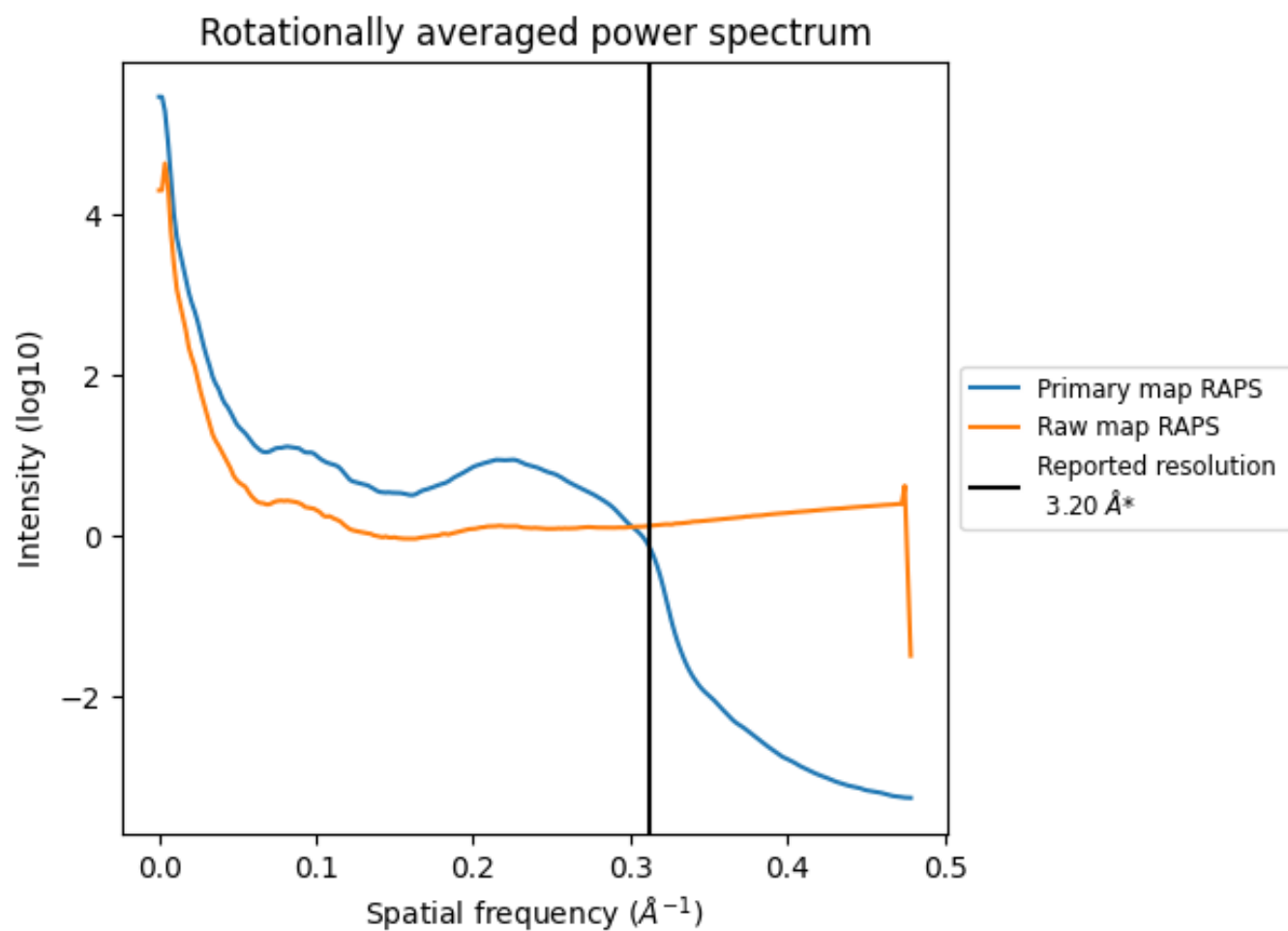
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 456 nm^3 ; 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 ⓘ

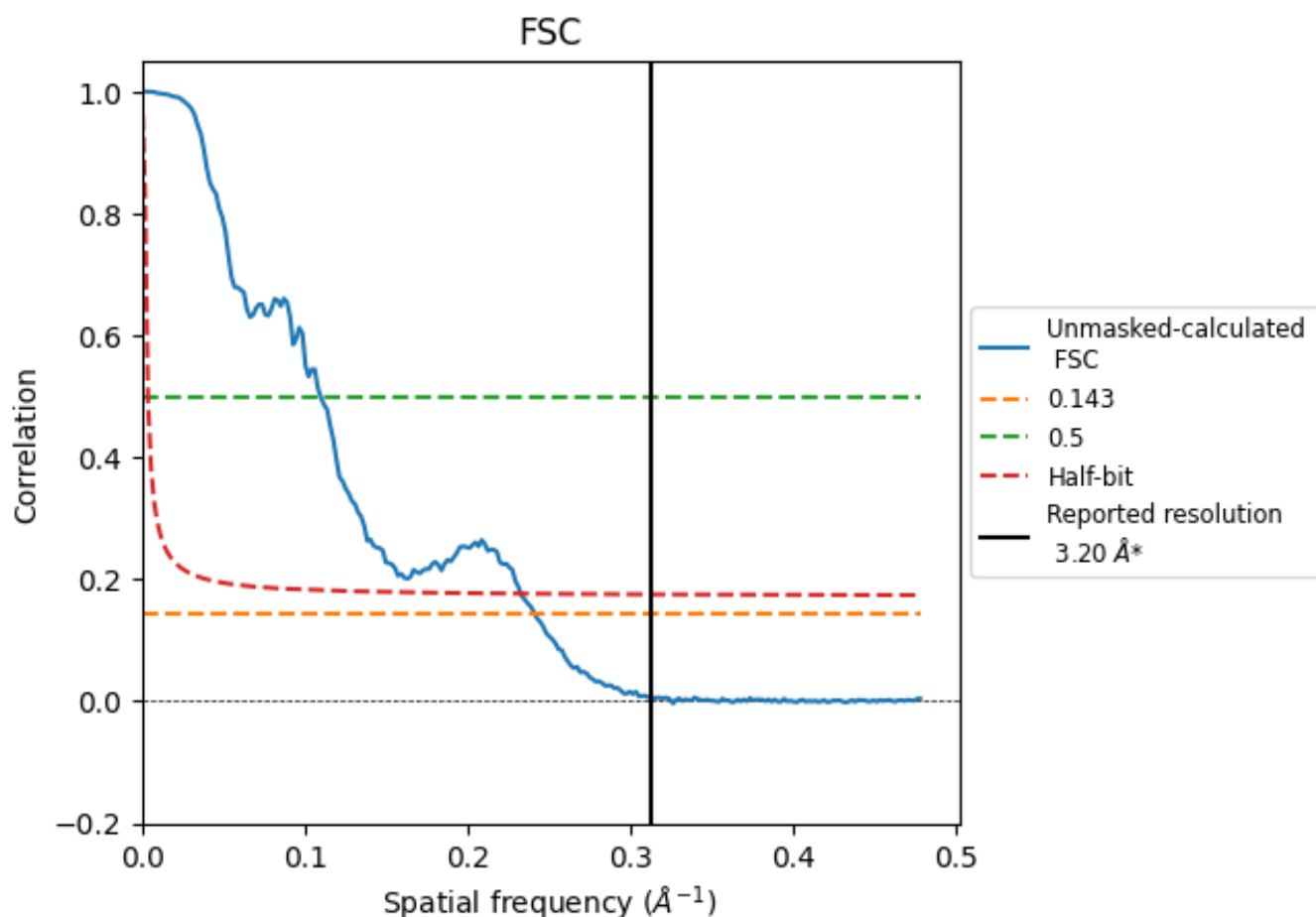


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

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 Å⁻¹

8.2 Resolution estimates [i](#)

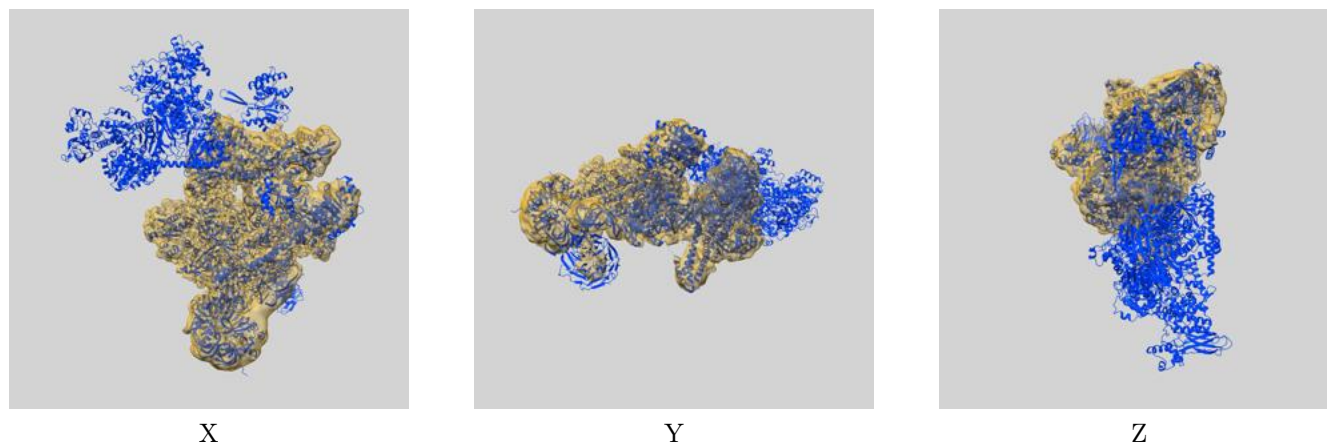
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	9.11	4.29

*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](#)

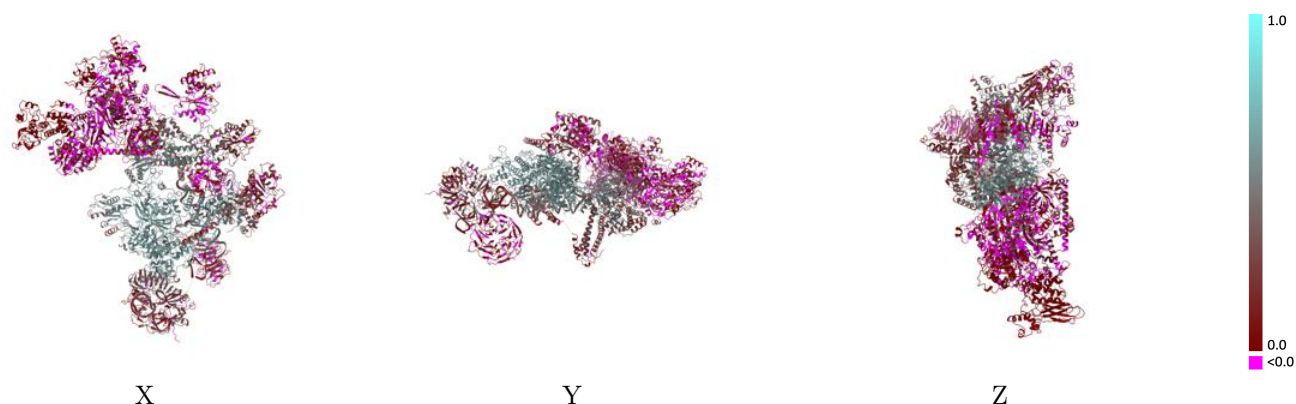
This section contains information regarding the fit between EMDB map EMD-19041 and PDB model 8RC0. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



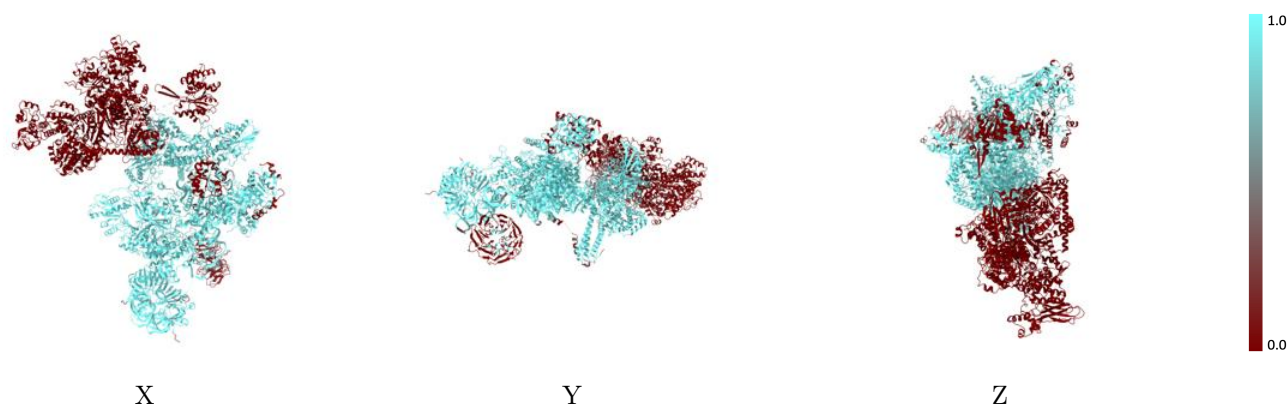
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



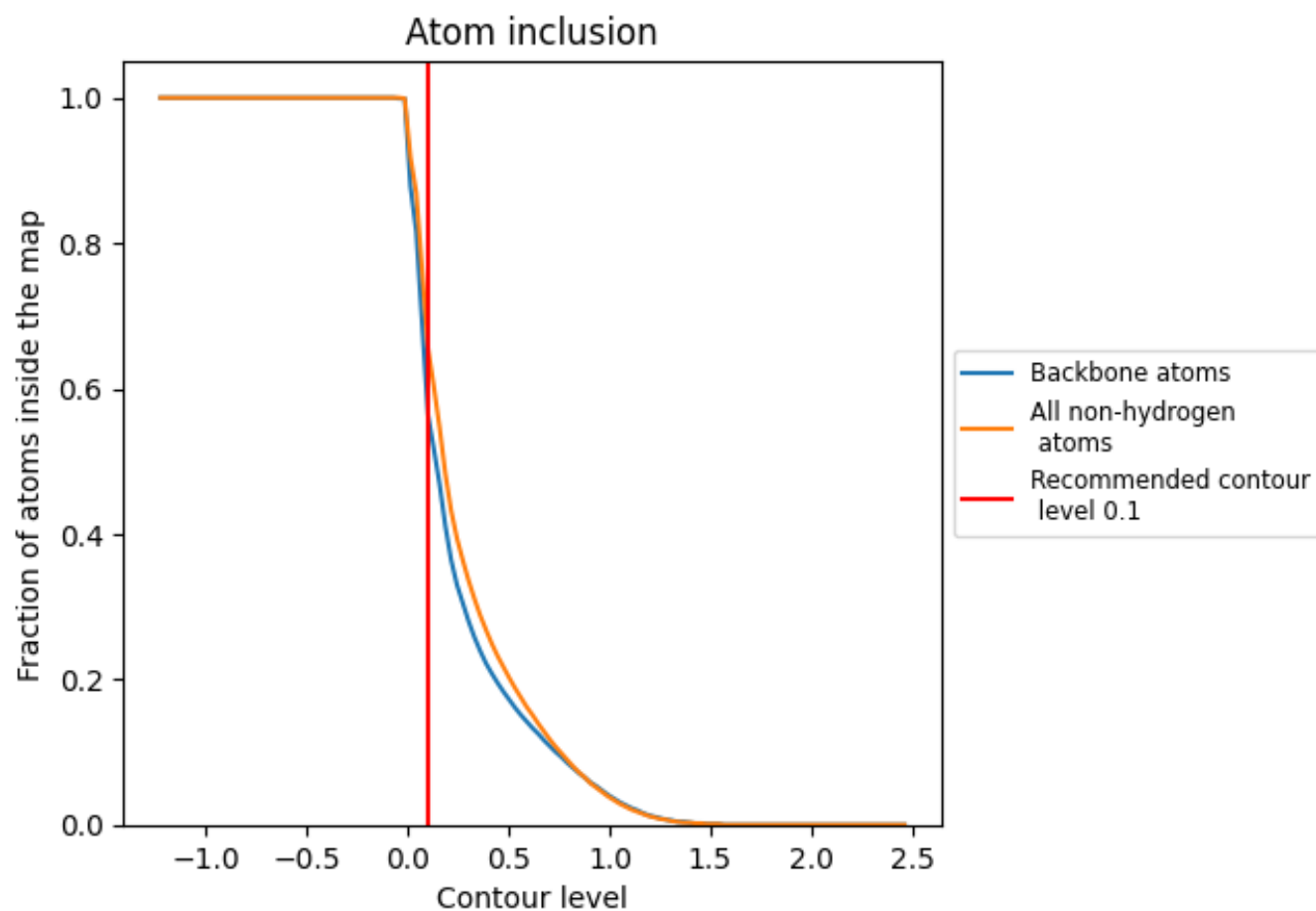
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

