



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:34 AM UTC

PDB ID : 7LHW / pdb_00007lhw
EMDB ID : EMD-23352
Title : Structure of the LRRK2 monomer
Authors : Myasnikov, A.; Zhu, H.; Hixson, P.; Xie, B.; Yu, K.; Pitre, A.; Peng, J.; Sun, J.
Deposited on : 2021-01-26
Resolution : 3.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

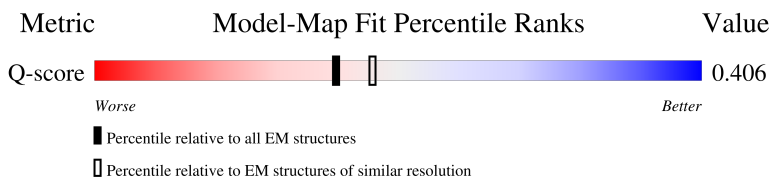
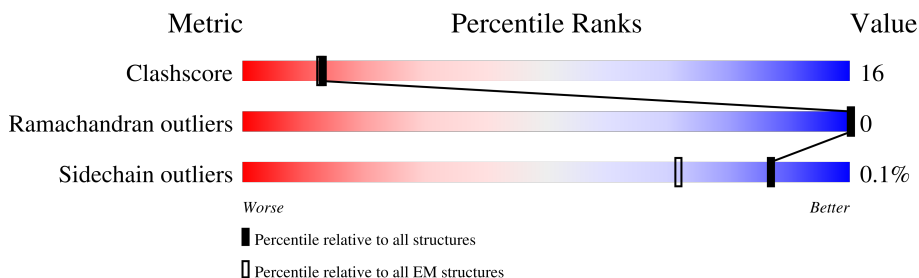
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

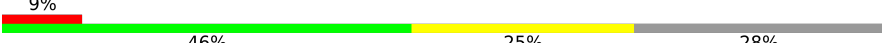
The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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 $\leq 5\%$. 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	A	2527	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14306 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.

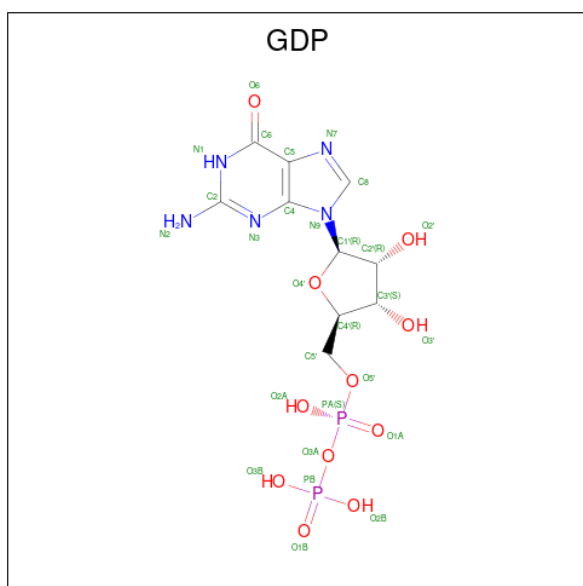
- Molecule 1 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1813	14247	9112	2458	2587	90	0	0

There are 3 discrepancies between the modelled and reference sequences:

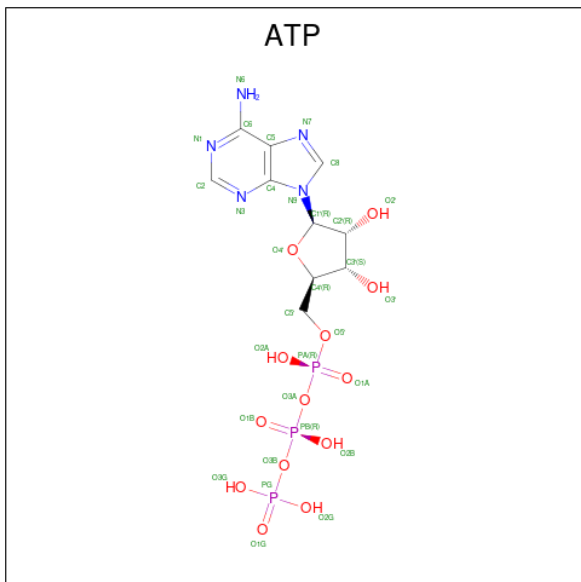
Chain	Residue	Modelled	Actual	Comment	Reference
A	50	HIS	ARG	variant	UNP Q5S007
A	1647	THR	SER	variant	UNP Q5S007
A	2397	THR	MET	variant	UNP Q5S007

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	28	10	5	11	2	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

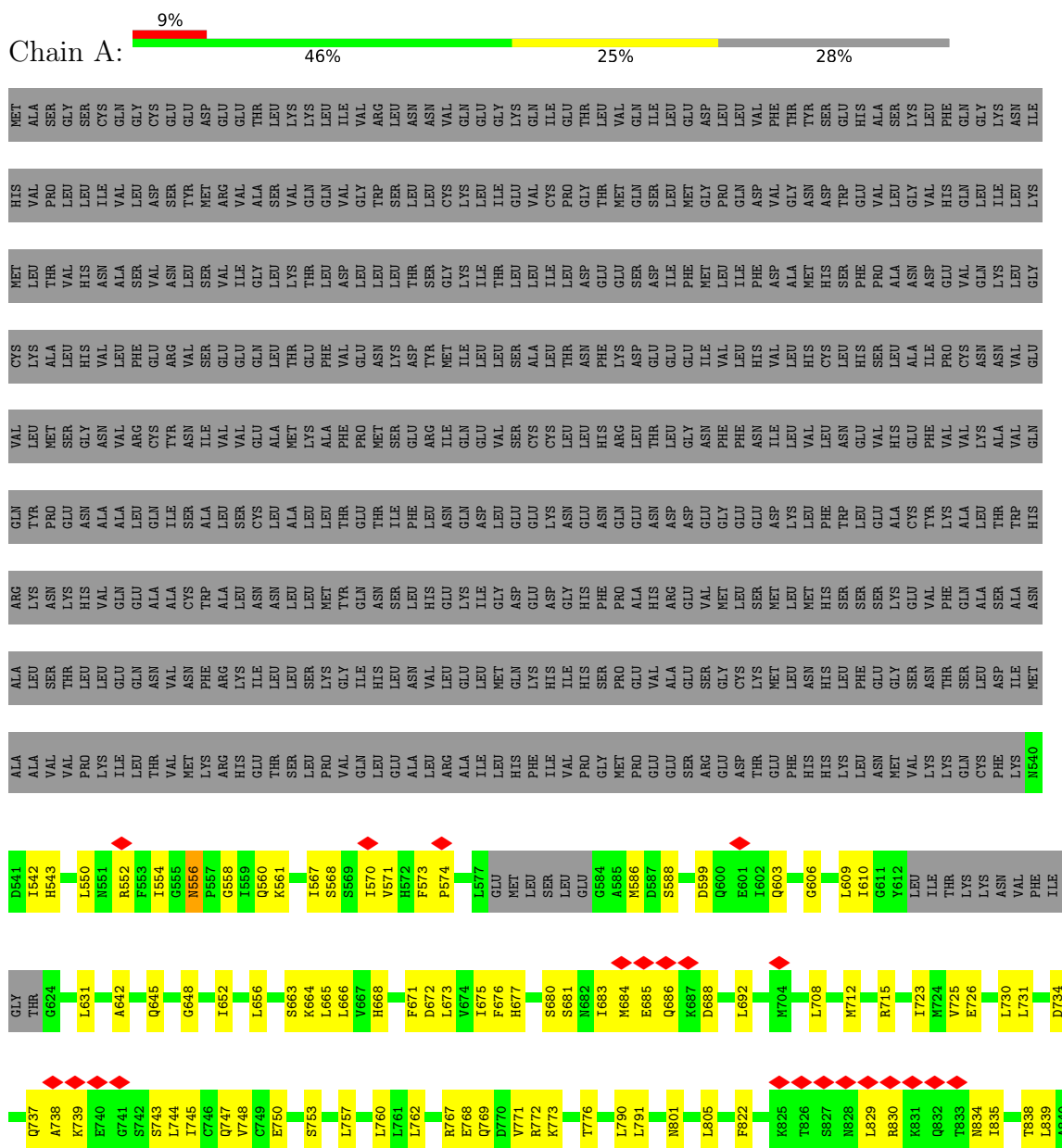


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	31	10	5	13	3	0

3 Residue-property plots

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

- Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2



P1865	R1866	M1867	I1868	L1870	L1875	E1876	F1877	E1878	Q1879	A1880	F1883	S1889	F1890	Y1894	A1897	Y1898	E1899	G1900	V1905	K1906	I1907	K1910	H1911	T1912	R1918	Q1919	E1920	C1925	H1928	S1931	A1937	A1938	G1939	I1940	R1941	I1942	P1943	M1944	L1945	V1946	L1955	D1956	L1959																				
Q1648	F1649	F1650	K1651	L1652	L1653	E1654	K1655	F1656	Q1657	I1658	A1659	LEU	PRO	I1661	L1662	V1663	P1664	L1665	S1666	C1667	E1668	L1669	G1670	L1671	S1672	C1673	L1674	C1675	K1676	L1677	E1678	L1679	F1680	E1681	P1682	H1683	N1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	L1695															
D1799	I1800	C1801	G1802	E1803	G1804	E1805	T1806	L1807	L1808	K1809	K1810	W1811	A1812	L1813	F1816	M1817	D1818	G1819	E1820	E1821	H1822	Q1823	L1824	L1825	L1826	D1827	K1828	L1829	K1830	K1831	E1832	L1833	E1834	G1835	L1836	I1837	L1838	L1839	L1840	V1841	D1842	Q1843	P1844	R1845	R1846	L1847	L1848	I1849	I1850	P1851	I1852	Q1853	M1854	L1855	A1856	F1857	L1858	L1859	D1860	L1861	D1862	L1863	L1864
Y1718	M1719	L1720	SER	GLY	ARG	GLU	ARG	GLU	GLU	A1726	L1727	M1728	P1729	W1734	R1735	Q1736	G1737	Y1738	Y1739	L1740	M1741	W1742	S1743	P1744	E1745	C1748	L1749	V1750	G1751	S1752	M1757	E1760	L1763	T1766	R1771	K1772	C1773	G1774	I1775	Q1779	V1780	V1781	D1782	H1783	I1784	M1788	E1789	W1790	W1791	L1796													
F1575	L1576	V1581	L1582	L1583	F1584	H1585	Q1586	D1587	P1588	A1589	L1590	Q1591	L1592	S1593	D1594	G1595	L1596	F1597	V1598	E1599	P1600	K1601	V1602	L1603	C1604	K1605	I1606	Q1609	V1613	L1614	V1615	E1616	G1617	C1618	P1619	L1620	H1621	P1622	K1623	G1624	I1625	D1630	VAL	GLU	LYS	PHE	LEU	SER	LYS	LYS	ARG	LYS	PHE	K1642	L1643								
R1483	D1484	Y1485	V1488	E1493	S1494	D1495	A1496	L1497	R1501	K1502	I1505	M1506	E1507	S1508	L1509	M1510	F1511	K1512	I1513	L1514	L1517	V1518	C1526	E1531	E1537	F1545	P1546	V1547	I1548	L1554	V1557	R1558	E1559	M1560	Q1561	L1562	Q1563	L1564	D1565	E1566	L1569	P1570	H1571	A1572	V1573	H1574																	
I1378	R1381	D1382	K1383	R1384	K1385	V1389	V1392	W1393	R1398	Y1402	H1407	F1408	M1409	T1410	Q1411	R1412	V1418	Y1419	E1427	M1431	K1432	P1433	W1434	N1437	R1441	P1446	L1449	V1450	D1455	V1456	S1457	GLU	LYS	GLN	ARG	K1463	K1468	E1472	K1476	R1477																							
M1286	K1290	P1298	L1299	H1303	D1307	F1308	K1309	H1310	I1311	G1312	C1313	K1314	D1317	R1320	R1325	R1334	L1337	I1339	V1340	G1341	M1342	K1347	T1348	T1349	L1350	L1351	L1354	M1355	K1358	K1359	S1360	D1361	L1362	G1363	M1364	T1368	I1371	D1372	V1373	K1374	D1375	W1376	P1377																				
L1180	S1181	Q1182	N1183	I1188	P1189	E1190	L1193	N1194	L1195	L1198	M1203	P1212	G1213	P1214	S1219	L1220	N1221	L1222	R1223	E1224	L1225	L1226	F1227	N1230	S1238	L1243	W1244	S1245	K1249	H1251	L1252	N1255	K1256	L1257	I1260	E1263	N1269	V1275	N1278	L1281	R1282																						
S1066	R1067	N1068	V1075	L1085	L1090	S1091	Y1092	M1093	E1100	V1106	E1107	K1108	L1109	L1112	I1113	L1114	S1120	G1121	I1122	L1128	L1131	S1137	K1138	W1139	H1140	L1144	L1149	S1157	F1158	R1161	M1162	N1163	M1168	P1169	F1170	L1171	P1172	M1175	T1176	L1177	L1178	K1179																					
LYS	LYS	ASN	SER	ILE	SER	VAL	GLY	GLU	TVR	PHE	ALA	ARG	ASP	ALA	VAL	GLY	ASP	GLN	ASN	VAL	GLN	ARG	HIS	LYS	SER	PHE	ASN	ASP	GLU	ASP	LEU	LEU	LYS	ARG	ALA	GLN	LYS	LYS	ILE	ASP	LEU	ASP	SER	GLY	SER	GLY	ASP	GLN															
V843	I844	M848	A851	V852	E853	E854	GLY	THR	ALA	SER	GLY	SER	ASP	VAL	ASP	E981	E982	Y883	I984	S990	A991	N992	E993	L994	R995	D996	I997	D998	S1001	K1002	K1003	E1011	H1012	L1013	N1021	T1024	C1031	L1034	K1035	S1036	L1037	T1038	H1039	F1047	P1051	S1052	Y1053	M1057	L1060														

D1962	K1963	A1964	S1965	L1966	T1967	R1968	T1969	L1970	Q1971	H1977	R1983	H1986	M1989	I1990	I1991	Y1992	R1993	A2009	B2017	T2020	A2021	Q2022	Y2023	C2024	C2025	R2026	W2027	GLY	ILE	LYS	T2031	S2032	A2040	V2043	A2044	G2045	G2046	W2047	Y2050	W2051	Q2052	D2055	Y2064	T2069	E2075										
F2079	P2080	N2081	E2082	F2083	D2084	E2085	L2086	E2087	I2088	Q2089	K2091	L2092	P2093	D2094	P2095	V2096	K2097	E2098	A2102	P2103	W2104	P2105	M2106	L2110	K2116	E2117	N2118	E2121	R2122	S2125	A2126	Q2127	V2128	I2131	L2132	A2135	E2136	L2137	L2140	T2141	R2142	K2148	I2151	V2152	E2153	H2159									
H2160	N2161	S2162	R2163	N2164	L2169	G2170	C2171	G2172	H2173	T2174	D2175	Q2178	L2179	S2180	F2181	D2182	D2183	L2184	E2187	G2188	Y2189	T2190	L2200	L2204	V2205	H2206	E2211	L2207	P2208	V2209	E2210	K2211	E2212	S2213	W2214	I2215	V2216	S2217	G2218	T2219	Q2220	S2221	G2222	T2223	V2226	L2227	N2228	T2229	E2230	D2231	G2232	K2233	K2234	R2235	
L2238	E2239	K2240	N2241	T2242	D2243	S2244	V2245	L2248	N2251	S2252	F2253	S2254	K2255	Q2256	S2257	K2258	Q2259	K2260	N2261	F2262	L2263	L2264	V2265	G2266	T2267	A2268	D2269	G2270	K2271	L2272	A2273	I2274	F2275	E2276	D2277	K2278	K2281	L2282	K2283	G2284	A2285	A2286	P2287	L2288	K2289	L2290	L2291	N2292	T2293	G2294	N2295	V2296	S2297	T2298	F2299
L2300	M2301	C2302	L2303	S2304	E2305	S2306	T2307	N2308	S2309	T2310	E2311	R2312	N2313	V2314	K2315	W2316	G2317	G2318	C2319	T2320	T2321	K2322	L2323	F2324	N2328	D2329	F2330	T2331	L2332	I2336	E2337	T2338	R2339	T2340	S2341	Q2342	L2343	F2344	S2345	Y2346	A2347	A2348	D2351	I2354	I2355	T2356	V2357	V2358	V2359	D2360	L2363	Y2364	I2365		
N2369	V2375	W2376	D2377	K2378	K2379	T2380	D2388	C2389	V2390	H2391	F2392	L2393	R2394	E2395	V2398	K2399	E2400	N2401	K2402	E2403	S2404	K2405	H2406	K2407	W2408	S2409	R2413	L2417	C2418	L2419	Q2420	K2421	N2422	A2423	A2424	L2425	V2426	G2427	T2429	G2430	H2433	T2434	L2435	L2436	L2437	D2438	T2441	R2442	R2443	L2444	I2445				
N2450	R2456	V2457	M2458	Q2462	L2463	G2464	S2465	L2466	K2467	N2468	L2471	V2472	L2473	G2474	Y2475	K2478	N2479	T2480	E2481	Q2482	T2483	Q2484	K2485	Q2486	K2487	E2488	V2495	I2498	H2502	L2507	H2510	R2514	A2518	R2522	R2523	T2524	S2525	V2526	E2527																

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	129744	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 ($e^-/\text{\AA}^2$)	81	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.440	Depositor
Minimum map value	-1.328	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	396.47998, 396.47998, 396.47998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	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: ATP, GDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/14514	0.42	1/19633 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	556	ASN	N-CA-C	6.62	124.43	109.81

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	14247	0	14531	469	0
2	A	28	0	12	1	0
3	A	31	0	12	0	0
All	All	14306	0	14555	469	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 16.

All (469) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2200:LEU:CD1	1:A:2220:GLN:HG3	1.48	1.41
1:A:2200:LEU:HD11	1:A:2220:GLN:CG	1.70	1.20
1:A:2200:LEU:CD1	1:A:2220:GLN:CG	2.26	1.12
1:A:2200:LEU:HD13	1:A:2220:GLN:HG3	1.31	1.06
1:A:2200:LEU:HD11	1:A:2220:GLN:HG3	1.23	1.04
1:A:631:LEU:HD21	1:A:652:ILE:HD11	1.60	0.83
1:A:1719:MET:HG3	1:A:1772:LYS:HD2	1.62	0.81
1:A:665:LEU:O	1:A:668:HIS:HB3	1.81	0.79
1:A:1354:LEU:O	1:A:1501:ARG:NH1	2.17	0.78
1:A:1869:MET:HE3	1:A:1870:LEU:H	1.48	0.77
1:A:990:SER:O	1:A:1021:ASN:ND2	2.18	0.77
1:A:2080:PRO:HA	1:A:2083:PHE:HB3	1.68	0.76
1:A:2355:ILE:HG22	1:A:2356:THR:HG23	1.69	0.75
1:A:2369:ASN:HA	1:A:2413:ARG:HG3	1.69	0.73
1:A:1870:LEU:HD11	1:A:1944:MET:HE2	1.70	0.73
1:A:1172:PRO:HD2	1:A:1175:MET:HE3	1.70	0.72
1:A:2200:LEU:HD11	1:A:2220:GLN:CD	2.13	0.72
1:A:2043:VAL:HA	1:A:2050:TYR:HE1	1.55	0.72
1:A:1968:ARG:NH2	1:A:1971:GLN:OE1	2.23	0.72
1:A:1034:LEU:HD11	1:A:1037:LEU:HD22	1.73	0.71
1:A:2110:LEU:HD11	1:A:2128:VAL:HG23	1.71	0.71
1:A:762:LEU:HD11	1:A:790:LEU:HD23	1.71	0.70
1:A:1338:MET:HE1	1:A:1410:THR:H	1.57	0.70
1:A:1739:TYR:HA	1:A:1748:CYS:O	1.92	0.69
1:A:1171:LEU:HD22	1:A:1175:MET:HE1	1.73	0.69
1:A:2272:LEU:HB2	1:A:2291:LEU:HB2	1.75	0.69
1:A:801:ASN:HB3	1:A:984:ILE:HA	1.74	0.69
1:A:992:ASN:O	1:A:1021:ASN:ND2	2.26	0.69
1:A:2183:ASP:OD1	1:A:2184:LEU:N	2.25	0.69
1:A:1512:LYS:HA	1:A:1517:LEU:H	1.57	0.68
1:A:1694:LEU:HB2	1:A:1811:TRP:HB2	1.74	0.68
1:A:2417:LEU:HD12	1:A:2425:LEU:HD11	1.74	0.68
1:A:1993:ARG:HH21	1:A:2050:TYR:HB2	1.56	0.68
1:A:1260:ILE:HG12	1:A:1281:LEU:HD11	1.74	0.68
1:A:1670:PRO:HB3	1:A:1709:ILE:HD11	1.75	0.68
1:A:2227:ILE:HD13	1:A:2235:ARG:HB3	1.76	0.68
1:A:1431:MET:HE1	1:A:1449:LEU:HD22	1.76	0.68
1:A:2390:VAL:HB	1:A:2394:ARG:HG3	1.77	0.67
1:A:1275:VAL:O	1:A:1278:ASN:ND2	2.28	0.67
1:A:2270:GLY:HA2	1:A:2300:LEU:HB2	1.76	0.67
1:A:2271:LYS:HE3	1:A:2292:ASN:HB2	1.76	0.66
1:A:1701:PRO:HG2	1:A:1704:PHE:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2471:LEU:HD22	1:A:2495:VAL:HG22	1.76	0.66
1:A:664:LYS:HG3	1:A:708:LEU:HD21	1.77	0.66
1:A:2213:SER:O	1:A:2229:THR:OG1	2.12	0.66
1:A:2462:GLN:HB2	1:A:2467:LYS:HD2	1.78	0.66
1:A:1195:LEU:O	1:A:1219:SER:OG	2.12	0.66
1:A:2321:THR:HG21	1:A:2339:ARG:HG3	1.77	0.66
1:A:2365:ILE:HD13	1:A:2376:TRP:HD1	1.59	0.66
1:A:1180:LEU:O	1:A:1183:ASN:ND2	2.29	0.65
1:A:1317:ASP:OD1	1:A:1320:ARG:NH1	2.29	0.65
1:A:2200:LEU:HD13	1:A:2220:GLN:CG	2.07	0.65
1:A:2314:VAL:HG13	1:A:2316:TRP:HE1	1.59	0.65
1:A:1614:LYS:HE3	1:A:1614:LYS:HA	1.79	0.65
1:A:556:ASN:HA	1:A:560:GLN:HE22	1.61	0.65
1:A:2478:LYS:HB2	1:A:2488:GLU:HB2	1.78	0.65
1:A:2132:LEU:HA	1:A:2137:LEU:HD21	1.79	0.64
1:A:1583:LEU:HD13	1:A:1600:PRO:HB3	1.78	0.64
1:A:1741:ASN:HD22	1:A:1741:ASN:H	1.44	0.64
1:A:2438:ASP:HB2	1:A:2445:ILE:HD11	1.78	0.64
1:A:2363:LEU:HB3	1:A:2365:ILE:HD11	1.80	0.64
1:A:1011:GLU:OE2	1:A:1035:LYS:NZ	2.31	0.64
1:A:2293:ILE:HD12	1:A:2332:ILE:HD11	1.80	0.63
1:A:2318:GLY:HA3	1:A:2354:ILE:HD13	1.79	0.63
1:A:2211:LYS:HE3	1:A:2211:LYS:HA	1.80	0.63
1:A:981:ARG:HG3	1:A:982:GLU:HG2	1.80	0.63
1:A:556:ASN:HA	1:A:560:GLN:NE2	2.14	0.63
1:A:1337:LEU:HD22	1:A:1392:VAL:HG12	1.81	0.63
1:A:2392:PHE:HB3	1:A:2444:LEU:HD12	1.81	0.63
1:A:1905:VAL:HG12	1:A:1946:VAL:HG22	1.81	0.62
1:A:1433:PRO:O	1:A:1437:ASN:ND2	2.32	0.62
1:A:1446:PRO:HD3	1:A:1511:PHE:CE1	2.34	0.62
1:A:838:THR:HG22	1:A:841:ARG:HH11	1.64	0.62
1:A:1195:LEU:HD12	1:A:1198:LEU:HD12	1.80	0.61
1:A:1472:GLU:O	1:A:1477:ARG:NH2	2.33	0.61
1:A:1334:ARG:O	1:A:1412:ARG:NH1	2.32	0.61
1:A:1484:ASP:OD1	1:A:1485:TYR:N	2.33	0.61
1:A:1509:LEU:HA	1:A:1519:VAL:HG11	1.81	0.61
1:A:2093:PRO:HB2	1:A:2098:GLU:HG3	1.83	0.61
1:A:684:MET:O	1:A:685:GLU:HG2	2.00	0.60
1:A:1526:CYS:HB3	1:A:1564:LEU:HD11	1.83	0.60
1:A:1303:HIS:HB3	1:A:1514:ARG:HD2	1.84	0.60
1:A:2125:SER:HA	1:A:2128:VAL:HG12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2245:VAL:HA	1:A:2267:THR:HA	1.83	0.59
1:A:648:GLY:O	1:A:652:ILE:HD12	2.03	0.59
1:A:1833:LYS:HD3	1:A:1859:LEU:HD22	1.83	0.59
1:A:2173:HIS:CD2	1:A:2174:THR:HG23	2.36	0.59
1:A:1813:LEU:HD21	1:A:1826:LEU:HD23	1.85	0.59
1:A:2216:VAL:HG21	1:A:2263:LEU:HD11	1.84	0.59
1:A:683:ILE:HG21	1:A:692:LEU:HD13	1.86	0.58
1:A:1816:PHE:HA	1:A:1850:ILE:HD11	1.85	0.58
1:A:1986:HIS:CE1	1:A:2052:GLN:HB3	2.39	0.58
1:A:672:ASP:HA	1:A:675:ILE:HG22	1.85	0.58
1:A:1468:LYS:O	1:A:1472:GLU:N	2.36	0.58
1:A:2151:ILE:O	1:A:2172:GLY:N	2.33	0.58
1:A:1168:MET:HE2	1:A:1180:LEU:HD11	1.86	0.57
1:A:2510:HIS:CE1	1:A:2514:ARG:HD2	2.39	0.57
1:A:672:ASP:HB2	1:A:676:PHE:CE2	2.38	0.57
1:A:1227:PHE:O	1:A:1230:ASN:ND2	2.37	0.57
1:A:1695:TYR:HB2	1:A:1763:LEU:HB3	1.85	0.57
1:A:1845:GLN:OE1	1:A:1847:ARG:HG2	2.03	0.57
1:A:2104:TRP:NE1	1:A:2137:LEU:O	2.29	0.57
1:A:1836:GLU:O	1:A:1941:ARG:NH1	2.37	0.57
1:A:1760:GLU:OE2	1:A:1760:GLU:N	2.38	0.57
1:A:1779:GLN:O	1:A:1783:HIS:ND1	2.32	0.57
1:A:753:SER:HB2	1:A:757:LEU:HD23	1.86	0.57
1:A:1557:VAL:HG12	1:A:1562:LEU:HD12	1.87	0.57
1:A:1692:ILE:HG12	1:A:1766:THR:HG22	1.87	0.57
1:A:2118:ASN:HB3	1:A:2121:GLU:HB2	1.87	0.56
1:A:1031:CYS:HG	1:A:1053:TYR:HD1	1.53	0.56
1:A:1488:VAL:HG21	1:A:1497:LEU:HD13	1.87	0.56
1:A:676:PHE:HZ	1:A:712:MET:HG2	1.71	0.56
1:A:1224:GLU:HG2	1:A:1249:LYS:HD3	1.87	0.56
1:A:1584:HIS:ND1	1:A:1586:GLN:OE1	2.38	0.56
1:A:2441:THR:O	1:A:2443:ARG:NH2	2.39	0.56
1:A:2040:ALA:HB3	1:A:2043:VAL:HG23	1.86	0.56
1:A:2339:ARG:HG2	1:A:2351:ASP:HA	1.89	0.55
1:A:1068:ASN:O	1:A:1093:ASN:ND2	2.39	0.55
1:A:2270:GLY:HA3	1:A:2294:GLY:H	1.71	0.55
1:A:1708:LEU:HD11	1:A:1784:ILE:HG12	1.89	0.55
1:A:1225:LEU:HD22	1:A:1227:PHE:HE2	1.72	0.55
1:A:1176:THR:HG22	1:A:1177:ILE:HG13	1.89	0.55
1:A:666:LEU:HG	1:A:671:PHE:HB2	1.87	0.55
1:A:2159:HIS:O	1:A:2162:SER:OG	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1437:ASN:OD1	1:A:1702:MET:N	2.40	0.54
1:A:2206:HIS:HA	1:A:2213:SER:HA	1.89	0.54
1:A:1342:ASN:ND2	1:A:1427:GLU:OE2	2.41	0.54
1:A:2009:ALA:O	1:A:2510:HIS:NE2	2.39	0.54
1:A:1161:ARG:O	1:A:1163:ASN:ND2	2.41	0.54
1:A:1531:GLU:HB2	1:A:1576:LEU:HD11	1.90	0.54
1:A:1838:ASP:O	1:A:1941:ARG:NH1	2.40	0.54
1:A:1075:VAL:HG12	1:A:1100:GLU:HB2	1.89	0.54
1:A:606:GLY:O	1:A:610:ILE:HG12	2.07	0.54
1:A:2082:GLU:HA	1:A:2085:GLU:HG2	1.90	0.54
1:A:1925:CYS:O	1:A:1928:HIS:NE2	2.40	0.54
1:A:672:ASP:OD1	1:A:673:LEU:HD12	2.07	0.53
1:A:998:ASP:O	1:A:1001:SER:OG	2.25	0.53
1:A:1252:LEU:O	1:A:1255:ASN:ND2	2.41	0.53
1:A:1190:GLU:HA	1:A:1193:LEU:HD13	1.90	0.53
1:A:1038:THR:HG23	1:A:1039:HIS:ND1	2.23	0.53
1:A:1741:ASN:HD22	1:A:1741:ASN:N	2.02	0.53
1:A:672:ASP:OD1	1:A:673:LEU:N	2.42	0.53
1:A:1734:TRP:CZ2	1:A:1737:GLY:HA3	2.42	0.53
1:A:1992:TYR:N	1:A:2055:ASP:OD2	2.41	0.53
1:A:2221:SER:HG	1:A:2223:THR:HG1	1.56	0.53
1:A:2348:ALA:HA	1:A:2351:ASP:HB3	1.90	0.53
1:A:1983:ARG:HG3	1:A:2126:ALA:HA	1.91	0.53
1:A:2152:VAL:HG21	1:A:2169:LEU:HB3	1.91	0.53
1:A:2311:GLU:HG3	1:A:2314:VAL:HG12	1.91	0.53
1:A:1493:GLU:OE2	1:A:1501:ARG:NH2	2.40	0.53
1:A:2116:LYS:O	1:A:2122:ARG:NH2	2.32	0.53
1:A:1092:TYR:CG	1:A:1883:PHE:HB3	2.43	0.52
1:A:1221:ASN:OD1	1:A:1223:ARG:NE	2.31	0.52
1:A:1734:TRP:CD1	1:A:1736:GLN:H	2.27	0.52
1:A:2151:ILE:HG12	1:A:2173:HIS:HB3	1.91	0.52
1:A:2153:GLU:N	1:A:2153:GLU:OE1	2.42	0.52
1:A:1090:LEU:HB2	1:A:1114:LEU:HD23	1.91	0.52
1:A:567:ILE:HA	1:A:570:ILE:HG22	1.91	0.52
1:A:1800:ILE:H	1:A:1800:ILE:HD12	1.74	0.52
1:A:2356:THR:OG1	1:A:2417:LEU:HD23	2.10	0.52
1:A:1392:VAL:C	1:A:1393:TRP:HD1	2.17	0.52
1:A:2043:VAL:HA	1:A:2050:TYR:CE1	2.40	0.52
1:A:2106:MET:HB2	1:A:2140:LEU:HD23	1.90	0.52
1:A:2142:ARG:NH2	1:A:2187:GLU:OE2	2.33	0.52
1:A:1841:VAL:O	1:A:1849:THR:OG1	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1966:LEU:HB3	1:A:1971:GLN:HE21	1.75	0.52
1:A:676:PHE:CZ	1:A:712:MET:HG2	2.44	0.52
1:A:1149:LEU:HB3	1:A:1172:PRO:HD3	1.93	0.51
1:A:731:LEU:HD21	1:A:843:VAL:HG11	1.92	0.51
1:A:1341:GLY:O	1:A:1434:TRP:NE1	2.43	0.51
1:A:2289:LYS:HE3	1:A:2291:LEU:HD21	1.90	0.51
1:A:848:MET:O	1:A:852:VAL:HG22	2.10	0.51
1:A:2200:LEU:HD11	1:A:2220:GLN:NE2	2.25	0.51
1:A:2437:LEU:HA	1:A:2443:ARG:O	2.10	0.51
1:A:738:ALA:HB3	1:A:743:SER:HA	1.92	0.51
1:A:835:ILE:O	1:A:839:LEU:HG	2.10	0.51
1:A:2302:CYS:SG	1:A:2303:LEU:N	2.84	0.51
1:A:726:GLU:HB2	1:A:760:LEU:HD13	1.91	0.51
1:A:2329:ASP:OD2	1:A:2331:THR:OG1	2.26	0.51
1:A:2514:ARG:O	1:A:2518:ALA:N	2.43	0.51
1:A:684:MET:HG3	1:A:835:ILE:HD13	1.92	0.51
1:A:996:ASP:OD1	1:A:997:ILE:N	2.42	0.51
1:A:2163:ARG:HG3	1:A:2164:ASN:H	1.74	0.51
1:A:1441:ARG:NH2	1:A:1791:TRP:O	2.43	0.51
1:A:1569:LEU:HA	1:A:1572:ALA:HB3	1.93	0.51
1:A:2043:VAL:HG13	1:A:2050:TYR:CE1	2.46	0.51
1:A:1037:LEU:HD23	1:A:1057:MET:HE1	1.93	0.51
1:A:2017:ASP:O	1:A:2020:ILE:HG12	2.11	0.50
1:A:2204:LEU:HA	1:A:2215:ILE:HD12	1.92	0.50
1:A:2306:SER:HA	1:A:2359:VAL:HG11	1.93	0.50
1:A:2271:LYS:HA	1:A:2292:ASN:HA	1.92	0.50
1:A:2312:ARG:O	1:A:2312:ARG:HG3	2.11	0.50
1:A:791:LEU:HD22	1:A:805:LEU:HD21	1.92	0.50
1:A:1310:HIS:HB3	1:A:1574:HIS:CE1	2.46	0.50
1:A:1351:LEU:HD11	1:A:1392:VAL:HG11	1.94	0.50
1:A:2468:ASN:ND2	1:A:2498:ILE:HG21	2.26	0.50
1:A:2244:SER:O	1:A:2268:ALA:N	2.45	0.50
1:A:1774:CYS:SG	1:A:1863:ASP:HA	2.52	0.50
1:A:2481:GLU:OE1	1:A:2484:GLN:NE2	2.45	0.50
1:A:2302:CYS:SG	1:A:2357:VAL:HG12	2.52	0.49
1:A:1648:GLN:HA	1:A:1651:LYS:HB2	1.94	0.49
1:A:1739:TYR:HB2	1:A:1749:LEU:HD13	1.93	0.49
1:A:2079:PHE:HB3	1:A:2082:GLU:OE1	2.11	0.49
1:A:2413:ARG:O	1:A:2430:GLY:N	2.34	0.49
1:A:734:ASP:OD1	1:A:734:ASP:N	2.45	0.49
1:A:745:ILE:HD12	1:A:745:ILE:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2346:TYR:HE2	1:A:2348:ALA:HB3	1.77	0.49
1:A:1709:ILE:HB	1:A:1738:ILE:HD11	1.93	0.49
1:A:2319:CYS:HB2	1:A:2324:PHE:CE2	2.48	0.49
1:A:838:THR:O	1:A:842:MET:HG3	2.12	0.49
1:A:1670:PRO:HA	1:A:1673:LEU:HD22	1.94	0.49
1:A:2207:LEU:HD13	1:A:2214:TRP:HD1	1.78	0.49
1:A:1308:PHE:HD1	1:A:1309:LYS:HG3	1.78	0.49
1:A:1347:LYS:HG3	1:A:1418:VAL:HG21	1.94	0.48
1:A:2105:PRO:HG3	1:A:2142:ARG:HA	1.94	0.48
1:A:2304:SER:OG	1:A:2305:GLU:N	2.46	0.48
1:A:2238:LEU:HD22	1:A:2285:ALA:H	1.77	0.48
1:A:1476:LYS:C	1:A:1477:ARG:HD3	2.38	0.48
1:A:1286:ASN:OD1	1:A:1325:ARG:NE	2.26	0.48
1:A:1652:LEU:O	1:A:1656:PHE:N	2.43	0.48
1:A:1870:LEU:HA	1:A:1937:ALA:HB1	1.95	0.48
1:A:1368:THR:O	1:A:1398:ARG:NH2	2.45	0.48
1:A:2478:LYS:N	1:A:2488:GLU:O	2.36	0.48
1:A:1307:ASP:O	1:A:1310:HIS:NE2	2.46	0.48
1:A:1782:ASP:HB2	1:A:1918:ARG:HH22	1.78	0.48
1:A:2264:LEU:HG	1:A:2274:ILE:HD12	1.96	0.48
1:A:1011:GLU:HA	1:A:1034:LEU:HA	1.96	0.48
1:A:1047:PHE:HB2	1:A:1068:ASN:HB3	1.95	0.48
1:A:1188:ILE:HD12	1:A:1212:PRO:HD2	1.96	0.48
1:A:2266:GLY:HA2	1:A:2300:LEU:HD23	1.94	0.48
1:A:1695:TYR:OH	1:A:1781:VAL:HG23	2.14	0.48
1:A:2085:GLU:O	1:A:2088:ILE:HG22	2.14	0.48
1:A:1509:LEU:HD23	1:A:1519:VAL:HG21	1.95	0.47
1:A:1576:LEU:HD12	1:A:1581:VAL:HG21	1.96	0.47
1:A:2135:ALA:HB2	1:A:2507:LEU:HD23	1.96	0.47
1:A:542:ILE:HG22	1:A:543:HIS:N	2.29	0.47
1:A:2514:ARG:HB3	1:A:2514:ARG:NH1	2.29	0.47
1:A:672:ASP:OD2	1:A:715:ARG:NE	2.47	0.47
1:A:1238:SER:HA	1:A:1263:GLU:HG2	1.95	0.47
1:A:1376:TRP:CH2	1:A:1378:ILE:HD11	2.49	0.47
1:A:1920:GLU:HB3	1:A:2021:ALA:HB1	1.96	0.47
1:A:2151:ILE:H	1:A:2173:HIS:HB3	1.78	0.47
1:A:550:LEU:O	1:A:554:ILE:HG13	2.15	0.47
1:A:1085:LEU:HD23	1:A:1106:VAL:HG11	1.96	0.47
1:A:1181:SER:HG	1:A:1182:GLN:CD	2.21	0.47
1:A:1573:VAL:HG21	1:A:1596:TYR:CE2	2.50	0.47
1:A:1709:ILE:O	1:A:1713:LEU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:LEU:HD21	1:A:1212:PRO:HG2	1.95	0.47
1:A:1962:ASP:OD2	1:A:1965:SER:OG	2.27	0.47
1:A:1851:PRO:HG2	1:A:1854:GLN:HB2	1.97	0.47
1:A:2241:MET:HG3	1:A:2242:THR:H	1.80	0.47
1:A:1434:TRP:CZ3	1:A:1702:MET:HE3	2.50	0.47
1:A:1810:LYS:O	1:A:1829:ASP:HB2	2.15	0.47
1:A:1703:GLY:HA3	1:A:1707:ARG:NH2	2.29	0.46
1:A:2306:SER:OG	1:A:2313:ASN:HA	2.15	0.46
1:A:568:SER:HB3	1:A:609:LEU:HD11	1.97	0.46
1:A:773:LYS:O	1:A:776:THR:OG1	2.27	0.46
1:A:1548:ILE:HD12	1:A:1598:VAL:HG21	1.97	0.46
1:A:767:ARG:O	1:A:771:VAL:HG23	2.16	0.46
1:A:1601:LYS:HA	1:A:1604:CYS:SG	2.55	0.46
1:A:2323:ILE:HG23	1:A:2336:ILE:HB	1.96	0.46
1:A:1605:LYS:HB2	1:A:1605:LYS:HE2	1.68	0.46
1:A:2300:LEU:HD12	1:A:2318:GLY:O	2.15	0.46
1:A:1545:PHE:CE2	1:A:1547:VAL:HB	2.51	0.46
1:A:1651:LYS:O	1:A:1655:LYS:HD3	2.16	0.46
1:A:1977:HIS:HD2	1:A:2514:ARG:HH21	1.63	0.46
1:A:586:MET:HE2	1:A:586:MET:HA	1.96	0.46
1:A:1592:LEU:HD11	1:A:1652:LEU:HD13	1.98	0.46
1:A:1597:PHE:HE1	1:A:1602:TRP:HZ3	1.63	0.46
1:A:1650:PHE:O	1:A:1654:GLU:HG3	2.15	0.46
1:A:1729:PRO:HB3	1:A:1742:TRP:CD2	2.51	0.46
1:A:1729:PRO:HG3	1:A:1740:LEU:HD12	1.96	0.46
1:A:2180:SER:HB2	1:A:2189:TYR:CE2	2.51	0.46
1:A:1350:LEU:HD11	1:A:1450:VAL:HG11	1.97	0.46
1:A:1373:VAL:HG22	1:A:1393:TRP:CG	2.50	0.46
1:A:1879:GLN:HG2	1:A:1894:TYR:CE2	2.51	0.46
1:A:2316:TRP:CE3	1:A:2363:LEU:HD21	2.51	0.46
1:A:747:GLN:HA	1:A:750:GLU:HB2	1.97	0.46
1:A:1590:LEU:HG	1:A:1655:LYS:HB3	1.98	0.46
1:A:829:LEU:HD23	1:A:830:ARG:O	2.16	0.45
1:A:1359:LYS:HG3	1:A:1360:SER:H	1.81	0.45
1:A:2128:VAL:HA	1:A:2131:ILE:HG22	1.97	0.45
1:A:2458:MET:HE3	1:A:2458:MET:HB2	1.81	0.45
1:A:652:ILE:O	1:A:656:LEU:HG	2.16	0.45
1:A:684:MET:HE2	1:A:835:ILE:HG21	1.98	0.45
1:A:992:ASN:O	1:A:994:LEU:N	2.46	0.45
1:A:1214:PRO:O	1:A:1243:LEU:HD23	2.16	0.45
1:A:1371:ILE:HD13	1:A:1408:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2218:GLY:HA3	1:A:2245:VAL:HG11	1.98	0.45
1:A:2228:ASN:OD1	1:A:2229:THR:N	2.48	0.45
1:A:2295:ASN:H	1:A:2298:THR:HG1	1.60	0.45
1:A:768:GLU:OE2	1:A:772:ARG:NH1	2.49	0.45
1:A:1912:THR:O	1:A:1943:ARG:NH2	2.49	0.45
1:A:2181:PHE:HB3	1:A:2190:THR:OG1	2.16	0.45
1:A:599:ASP:O	1:A:603:GLN:HG2	2.16	0.45
1:A:744:LEU:O	1:A:748:VAL:HG23	2.17	0.45
1:A:1687:ASN:HB3	1:A:1819:GLY:HA2	1.97	0.45
1:A:2089:GLN:O	1:A:2091:LYS:N	2.44	0.45
1:A:2256:GLN:HG2	1:A:2260:LYS:HD2	1.98	0.45
1:A:1225:LEU:HD23	1:A:1225:LEU:HA	1.89	0.45
1:A:1282:ARG:NH2	1:A:1303:HIS:H	2.14	0.45
1:A:2267:THR:HG22	1:A:2268:ALA:N	2.32	0.45
1:A:2287:PRO:HB2	1:A:2290:ILE:HG12	1.98	0.45
1:A:2395:GLU:OE1	1:A:2395:GLU:N	2.49	0.45
1:A:1788:MET:HE2	1:A:1788:MET:HB2	1.76	0.45
1:A:1931:SER:HB3	1:A:2514:ARG:HH22	1.81	0.45
1:A:2064:TYR:CE2	1:A:2095:PRO:HG3	2.52	0.45
1:A:2377:ASP:OD1	1:A:2379:LYS:N	2.50	0.45
1:A:2419:LEU:HG	1:A:2420:GLN:O	2.17	0.45
1:A:2429:THR:HG21	1:A:2433:HIS:HB2	1.98	0.45
1:A:2175:ASP:OD1	1:A:2175:ASP:N	2.47	0.45
1:A:726:GLU:O	1:A:730:LEU:HG	2.16	0.44
1:A:1109:LEU:HD21	1:A:1112:LEU:HB2	1.97	0.44
1:A:1263:GLU:OE2	1:A:1263:GLU:N	2.42	0.44
1:A:1372:ASP:OD2	1:A:1374:LYS:NZ	2.50	0.44
1:A:1875:LEU:HD12	1:A:1898:TYR:HB2	1.99	0.44
1:A:1993:ARG:NH1	1:A:2023:TYR:OH	2.50	0.44
1:A:2171:CYS:SG	1:A:2178:GLN:N	2.90	0.44
1:A:2522:ARG:O	1:A:2525:SER:OG	2.34	0.44
1:A:737:GLN:N	1:A:737:GLN:OE1	2.51	0.44
1:A:2295:ASN:N	1:A:2298:THR:OG1	2.36	0.44
1:A:738:ALA:C	1:A:739:LYS:HD2	2.43	0.44
1:A:1137:SER:OG	1:A:1138:LYS:HG3	2.17	0.44
1:A:2347:ALA:O	1:A:2351:ASP:N	2.45	0.44
1:A:1789:GLU:HB3	1:A:1796:LEU:HD21	2.00	0.44
1:A:2241:MET:HG3	1:A:2242:THR:N	2.33	0.44
1:A:1051:PRO:C	1:A:1053:TYR:H	2.24	0.44
1:A:1120:SER:HA	1:A:1140:HIS:O	2.18	0.44
1:A:1940:ILE:HG22	1:A:1941:ARG:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1967:THR:HG23	1:A:1969:THR:HG22	1.99	0.44
1:A:2254:SER:HA	1:A:2260:LYS:HB3	1.97	0.44
1:A:1689:GLU:OE1	1:A:1689:GLU:N	2.49	0.44
1:A:1741:ASN:N	1:A:1741:ASN:ND2	2.64	0.44
1:A:2456:ARG:HG3	1:A:2475:TYR:CZ	2.53	0.44
1:A:686:GLN:O	1:A:688:ASP:N	2.49	0.44
1:A:2152:VAL:HG13	1:A:2473:LEU:HD11	1.99	0.44
1:A:558:GLY:HA2	1:A:561:LYS:NZ	2.33	0.44
1:A:1361:ASP:N	1:A:1361:ASP:OD1	2.50	0.43
1:A:2088:ILE:HD12	1:A:2088:ILE:HA	1.83	0.43
1:A:2218:GLY:HA3	1:A:2248:LEU:HD11	2.00	0.43
1:A:1282:ARG:HA	1:A:1303:HIS:O	2.18	0.43
1:A:1505:ILE:O	1:A:1509:LEU:HG	2.17	0.43
1:A:573:PHE:HB2	1:A:574:PRO:HD2	2.00	0.43
1:A:683:ILE:HD13	1:A:683:ILE:HA	1.87	0.43
1:A:1832:LYS:HZ1	1:A:1856:ALA:HB3	1.84	0.43
1:A:1845:GLN:HA	1:A:1846:PRO:HD3	1.88	0.43
1:A:1956:ASP:N	1:A:1956:ASP:OD1	2.49	0.43
1:A:2232:GLY:O	1:A:2235:ARG:NH2	2.51	0.43
1:A:568:SER:O	1:A:571:VAL:HG12	2.18	0.43
1:A:993:GLU:H	1:A:993:GLU:CD	2.25	0.43
1:A:1705:TRP:CZ3	1:A:1708:LEU:HD23	2.53	0.43
1:A:1832:LYS:NZ	1:A:1859:LEU:HD12	2.33	0.43
1:A:1355:MET:HG2	1:A:1376:TRP:CD2	2.53	0.43
1:A:1735:ARG:HE	1:A:1735:ARG:HB2	1.60	0.43
1:A:1829:ASP:OD1	1:A:1859:LEU:HD11	2.18	0.43
1:A:1339:ILE:HD12	1:A:1351:LEU:HD13	2.01	0.43
1:A:1729:PRO:HB3	1:A:1742:TRP:CE2	2.53	0.43
1:A:1796:LEU:O	1:A:1796:LEU:HD12	2.19	0.43
1:A:1865:PRO:HG2	1:A:1925:CYS:SG	2.59	0.43
1:A:2337:GLU:OE2	1:A:2339:ARG:HB2	2.19	0.43
1:A:1341:GLY:N	1:A:1347:LYS:HD3	2.34	0.43
1:A:1351:LEU:HD21	1:A:1392:VAL:HG21	2.01	0.43
1:A:1554:LEU:HA	1:A:1557:VAL:HG22	2.00	0.43
1:A:1683:PRO:HG3	1:A:1744:PRO:HA	2.01	0.43
1:A:1858:ASP:OD1	1:A:1858:ASP:N	2.51	0.43
1:A:2221:SER:OG	1:A:2223:THR:OG1	2.31	0.43
1:A:642:ALA:O	1:A:645:GLN:NE2	2.52	0.43
1:A:1348:THR:OG1	2:A:2601:GDP:O1A	2.30	0.43
1:A:1705:TRP:CZ2	1:A:1752:SER:HB2	2.54	0.43
1:A:2025:CYS:SG	1:A:2026:ARG:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2321:THR:HG22	1:A:2321:THR:O	2.18	0.43
1:A:1775:ILE:HG12	1:A:1863:ASP:O	2.19	0.43
1:A:2364:TYR:CD2	1:A:2375:VAL:HG22	2.54	0.43
1:A:744:LEU:HA	1:A:747:GLN:NE2	2.34	0.43
1:A:769:GLN:CD	1:A:769:GLN:H	2.27	0.43
1:A:1510:ASN:HB3	1:A:1512:LYS:HE2	2.01	0.43
1:A:1621:HIS:HB3	1:A:1625:ILE:HG23	2.01	0.43
1:A:1806:THR:C	1:A:1808:LEU:H	2.27	0.43
1:A:1389:VAL:HG23	1:A:1389:VAL:O	2.19	0.42
1:A:1702:MET:HE2	1:A:1702:MET:HB2	1.74	0.42
1:A:1879:GLN:HG2	1:A:1894:TYR:HE2	1.84	0.42
1:A:1737:GLY:HA2	1:A:1750:VAL:O	2.18	0.42
1:A:1250:LEU:HG	1:A:1252:LEU:HD23	2.01	0.42
1:A:1446:PRO:HD3	1:A:1511:PHE:HE1	1.81	0.42
1:A:1569:LEU:O	1:A:1573:VAL:HG12	2.18	0.42
1:A:1870:LEU:HB2	1:A:1939:GLY:HA3	2.01	0.42
1:A:1003:LYS:HD3	1:A:1003:LYS:HA	1.84	0.42
1:A:1128:LEU:HD23	1:A:1128:LEU:HA	1.83	0.42
1:A:2200:LEU:CD1	1:A:2220:GLN:HG2	2.35	0.42
1:A:656:LEU:HD22	1:A:663:SER:HB2	2.00	0.42
1:A:723:ILE:H	1:A:723:ILE:HD12	1.84	0.42
1:A:737:GLN:HE22	1:A:744:LEU:HD21	1.83	0.42
1:A:1108:LYS:HA	1:A:1108:LYS:HD3	1.85	0.42
1:A:1907:ILE:HD13	1:A:1907:ILE:HA	1.92	0.42
1:A:2233:LYS:HB3	1:A:2233:LYS:HE2	1.80	0.42
1:A:822:PHE:CD1	1:A:984:ILE:HD11	2.55	0.42
1:A:1483:ARG:HE	1:A:1507:GLU:CD	2.27	0.42
1:A:1963:LYS:HE3	1:A:2069:THR:OG1	2.20	0.42
1:A:2438:ASP:HB3	1:A:2442:ARG:O	2.20	0.42
1:A:1066:SER:HB2	1:A:1091:SER:HB2	2.02	0.42
1:A:1377:PRO:HA	1:A:1389:VAL:HG12	2.02	0.42
1:A:1569:LEU:N	1:A:1570:PRO:HD2	2.35	0.42
1:A:1657:GLN:HB2	1:A:1710:ASN:CG	2.43	0.42
1:A:1877:PHE:CE1	1:A:1905:VAL:HG21	2.55	0.42
1:A:2140:LEU:HD12	1:A:2141:THR:H	1.85	0.42
1:A:1158:PHE:O	1:A:1178:LEU:HD12	2.19	0.42
1:A:2267:THR:HG22	1:A:2268:ALA:H	1.85	0.42
1:A:2301:MET:O	1:A:2301:MET:HG3	2.19	0.42
1:A:2346:TYR:CE2	1:A:2348:ALA:HB3	2.54	0.42
1:A:1220:LEU:HD23	1:A:1220:LEU:HA	1.94	0.42
1:A:2388:ASP:OD1	1:A:2390:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ASN:C	1:A:560:GLN:HE22	2.27	0.41
1:A:1257:LEU:HD23	1:A:1257:LEU:HA	1.80	0.41
1:A:1989:MET:HE2	1:A:1989:MET:HA	2.01	0.41
1:A:2216:VAL:HG12	1:A:2226:VAL:HG22	2.02	0.41
1:A:2478:LYS:HA	1:A:2478:LYS:HD3	1.84	0.41
1:A:568:SER:HB3	1:A:609:LEU:HD21	2.00	0.41
1:A:684:MET:SD	1:A:684:MET:N	2.92	0.41
1:A:1359:LYS:HG3	1:A:1360:SER:N	2.35	0.41
1:A:1402:TYR:O	1:A:1702:MET:HG3	2.20	0.41
1:A:1419:TYR:O	1:A:1427:GLU:HG2	2.20	0.41
1:A:1990:ILE:HD11	1:A:2020:ILE:HB	2.02	0.41
1:A:1090:LEU:HA	1:A:1090:LEU:HD23	1.86	0.41
1:A:1157:SER:HA	1:A:1177:ILE:O	2.19	0.41
1:A:2319:CYS:HB2	1:A:2324:PHE:HE2	1.84	0.41
1:A:2427:ILE:HB	1:A:2435:LEU:HB2	2.03	0.41
1:A:1013:LEU:HD12	1:A:1013:LEU:HA	1.76	0.41
1:A:1955:LEU:HG	1:A:1959:LEU:HD23	2.02	0.41
1:A:2322:LYS:HG2	1:A:2337:GLU:HG2	2.02	0.41
1:A:1860:ILE:O	1:A:1862:ALA:N	2.51	0.41
1:A:1170:PHE:O	1:A:1170:PHE:CG	2.73	0.41
1:A:1832:LYS:HZ3	1:A:1852:ILE:HG23	1.85	0.41
1:A:2423:THR:HG21	1:A:2502:HIS:CE1	2.55	0.41
1:A:2464:GLY:C	1:A:2466:LEU:H	2.29	0.41
1:A:677:HIS:O	1:A:681:SER:N	2.54	0.41
1:A:834:ASN:OD1	1:A:834:ASN:N	2.53	0.41
1:A:1968:ARG:HE	1:A:2102:ALA:HB3	1.85	0.41
1:A:2488:GLU:OE2	1:A:2488:GLU:N	2.54	0.41
1:A:1057:MET:SD	1:A:1060:ILE:HD12	2.61	0.41
1:A:1131:LEU:HD23	1:A:1131:LEU:HA	1.88	0.41
1:A:1144:LEU:HB2	1:A:1169:PRO:HG3	2.03	0.41
1:A:1203:MET:HE2	1:A:1203:MET:HB3	1.95	0.41
1:A:1799:ASP:OD1	1:A:1799:ASP:N	2.50	0.41
1:A:2148:LYS:NZ	1:A:2488:GLU:HB3	2.35	0.41
1:A:844:ILE:O	1:A:848:MET:HG3	2.21	0.41
1:A:853:GLU:HG2	1:A:854:GLU:CD	2.46	0.41
1:A:1606:ILE:HA	1:A:1609:GLN:HG2	2.02	0.41
1:A:2301:MET:HE2	1:A:2301:MET:HB2	1.94	0.41
1:A:552:ARG:NH2	1:A:588:SER:HB2	2.36	0.40
1:A:725:VAL:HG11	1:A:757:LEU:HD12	2.02	0.40
1:A:1024:THR:HA	1:A:1047:PHE:CD1	2.56	0.40
1:A:1334:ARG:HG3	1:A:1389:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1407:HIS:CE1	1:A:1791:TRP:HH2	2.39	0.40
1:A:680:SER:O	1:A:680:SER:OG	2.39	0.40
1:A:1876:GLU:HB2	1:A:1897:ALA:HB3	2.03	0.40
1:A:2043:VAL:HG22	1:A:2050:TYR:HD1	1.86	0.40
1:A:2261:ASN:O	1:A:2277:ASP:HB2	2.22	0.40
1:A:1609:GLN:O	1:A:1613:VAL:HG13	2.21	0.40
1:A:1806:THR:O	1:A:1808:LEU:N	2.54	0.40
1:A:2302:CYS:C	1:A:2303:LEU:HD12	2.46	0.40
1:A:2311:GLU:OE1	1:A:2311:GLU:N	2.49	0.40
1:A:1311:ILE:HD13	1:A:1586:GLN:HE21	1.87	0.40
1:A:1537:GLU:CD	1:A:1548:ILE:HD11	2.47	0.40
1:A:1674:SER:O	1:A:1734:TRP:HB2	2.21	0.40
1:A:725:VAL:HG11	1:A:757:LEU:CD1	2.52	0.40
1:A:1245:SER:O	1:A:1269:ASN:HB2	2.22	0.40
1:A:1298:PRO:O	1:A:1299:LEU:HD23	2.21	0.40
1:A:1623:LYS:O	1:A:1673:LEU:HD12	2.21	0.40
1:A:1805:GLU:C	1:A:1807:LEU:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1795/2527 (71%)	1597 (89%)	198 (11%)	0	100	100

There are no Ramachandran outliers to report.

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	A	1588/2281 (70%)	1587 (100%)	1 (0%)	88 88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1741	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	594	GLN
1	A	1183	ASN
1	A	1230	ASN
1	A	1365	GLN
1	A	1379	GLN
1	A	1407	HIS
1	A	1648	GLN
1	A	1741	ASN
1	A	1854	GLN
1	A	1872	ASN
1	A	2173	HIS
1	A	2433	HIS
1	A	2450	ASN
1	A	2468	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	A	2602	-	32,33,33	1.35	4 (12%)	48,52,52	1.75	10 (20%)
2	GDP	A	2601	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)

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
3	ATP	A	2602	-	-	1/22/38/38	0/3/3/3
2	GDP	A	2601	-	-	2/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2602	ATP	C5-C4	3.77	1.45	1.39
2	A	2601	GDP	C5-C4	3.07	1.47	1.38
3	A	2602	ATP	C5-N7	-2.87	1.33	1.39
3	A	2602	ATP	C4-N9	-2.73	1.32	1.37
2	A	2601	GDP	C6-N1	-2.57	1.34	1.38
2	A	2601	GDP	C5-N7	-2.16	1.34	1.39
3	A	2602	ATP	C8-N7	2.07	1.35	1.31

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2601	GDP	C5-C4-N3	-6.11	118.66	128.39
3	A	2602	ATP	C5-C4-N3	-5.06	119.75	126.72
2	A	2601	GDP	C2-N3-C4	5.02	120.94	112.30
2	A	2601	GDP	N9-C4-N3	4.51	134.97	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2602	ATP	N3-C4-N9	4.27	134.43	127.17
3	A	2602	ATP	C2-N3-C4	3.39	120.12	111.83
3	A	2602	ATP	N3-C2-N1	-3.35	123.51	128.58
3	A	2602	ATP	C4-N9-C8	3.25	109.16	105.74
2	A	2601	GDP	C6-C5-N7	3.24	136.18	130.29
3	A	2602	ATP	C2'-C1'-N9	-2.94	106.00	113.30
3	A	2602	ATP	C4-C5-N7	-2.65	107.55	110.58
2	A	2601	GDP	C4-C5-N7	-2.51	106.70	110.67
3	A	2602	ATP	N9-C8-N7	-2.25	110.74	113.94
2	A	2601	GDP	C3'-C2'-C1'	2.21	105.65	101.46
2	A	2601	GDP	O6-C6-C5	-2.10	121.00	126.53
3	A	2602	ATP	C5-N7-C8	2.09	106.74	103.45
3	A	2602	ATP	O3'-C3'-C2'	-2.00	105.40	111.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

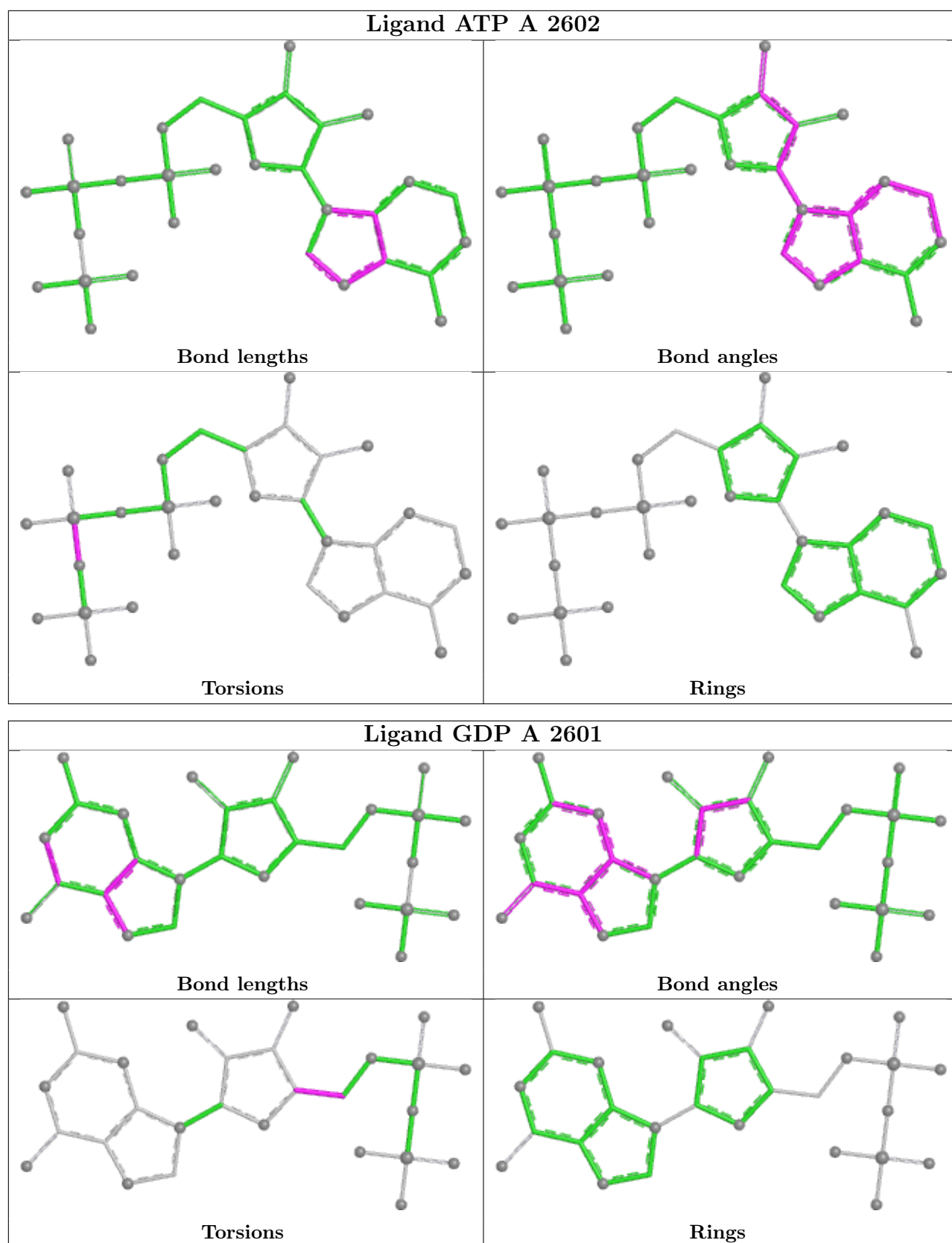
Mol	Chain	Res	Type	Atoms
2	A	2601	GDP	C3'-C4'-C5'-O5'
2	A	2601	GDP	O4'-C4'-C5'-O5'
3	A	2602	ATP	PG-O3B-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2601	GDP	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.

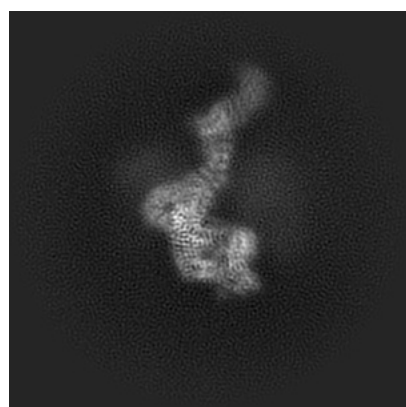
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23352. These allow visual inspection of the internal detail of the map and identification of artifacts.

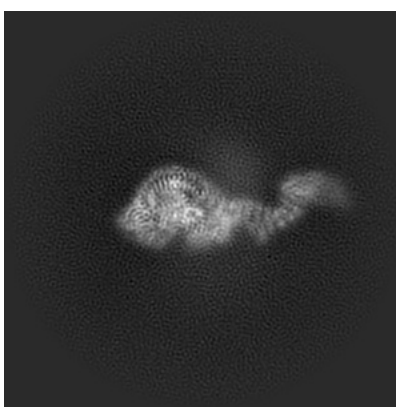
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

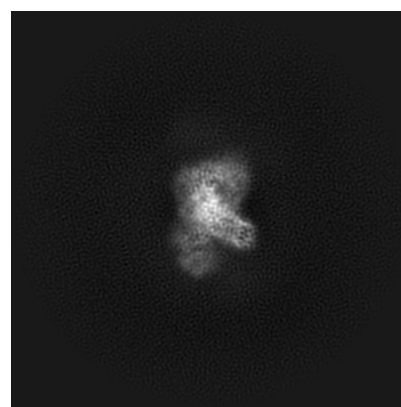
6.1.1 Primary map



X



Y

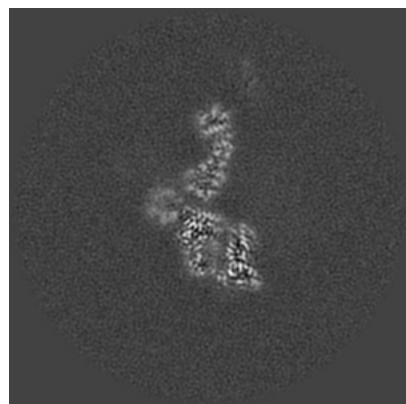


Z

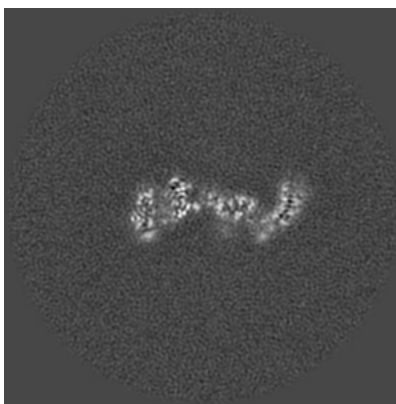
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

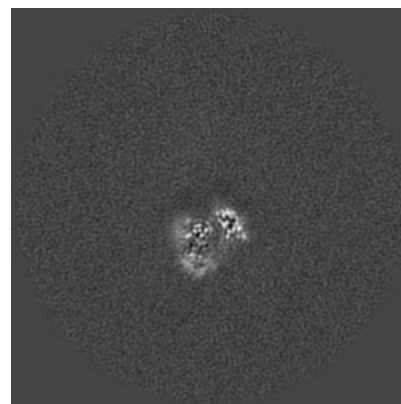
6.2.1 Primary map



X Index: 240



Y Index: 240

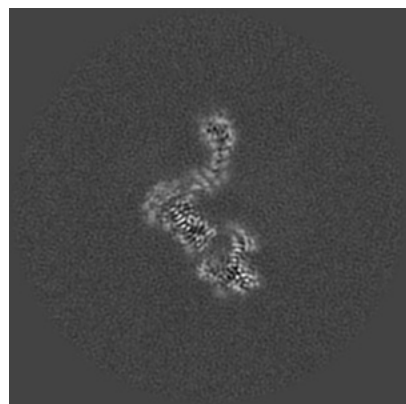


Z Index: 240

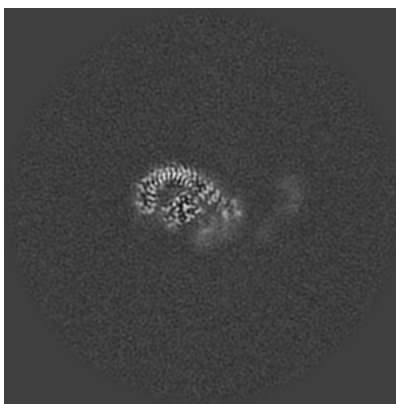
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

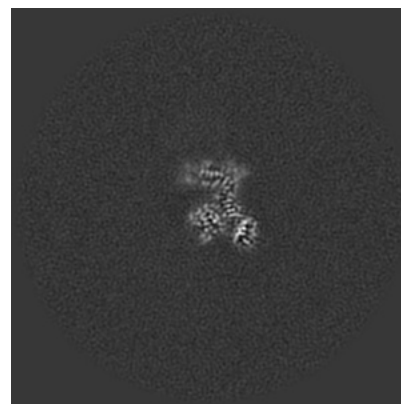
6.3.1 Primary map



X Index: 230



Y Index: 223

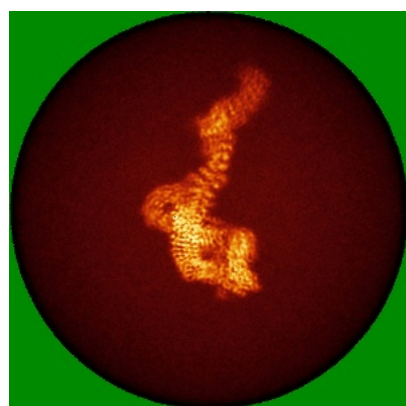


Z Index: 204

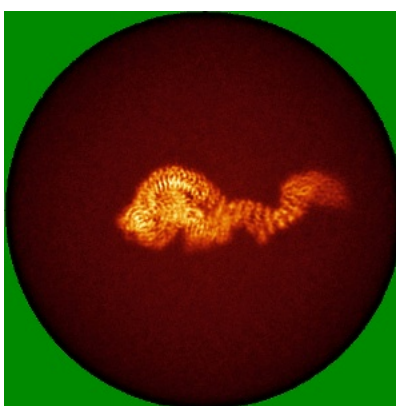
The images above show the largest variance slices of the map in three orthogonal directions.

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

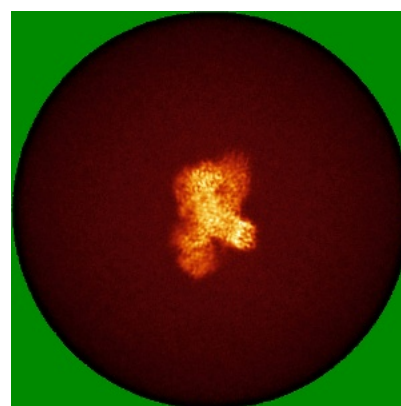
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

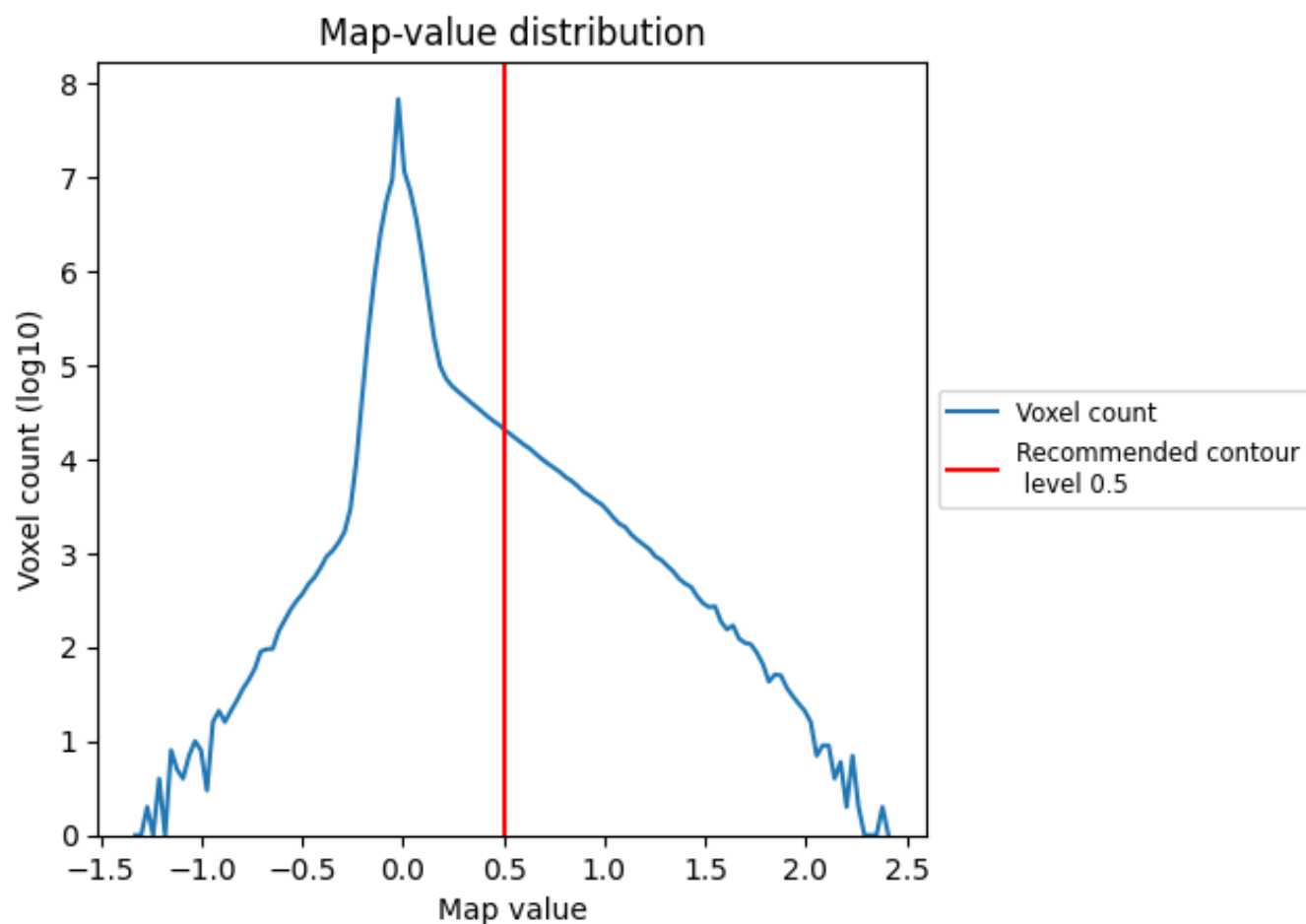
6.6 Mask visualisation

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

7 Map analysis [i](#)

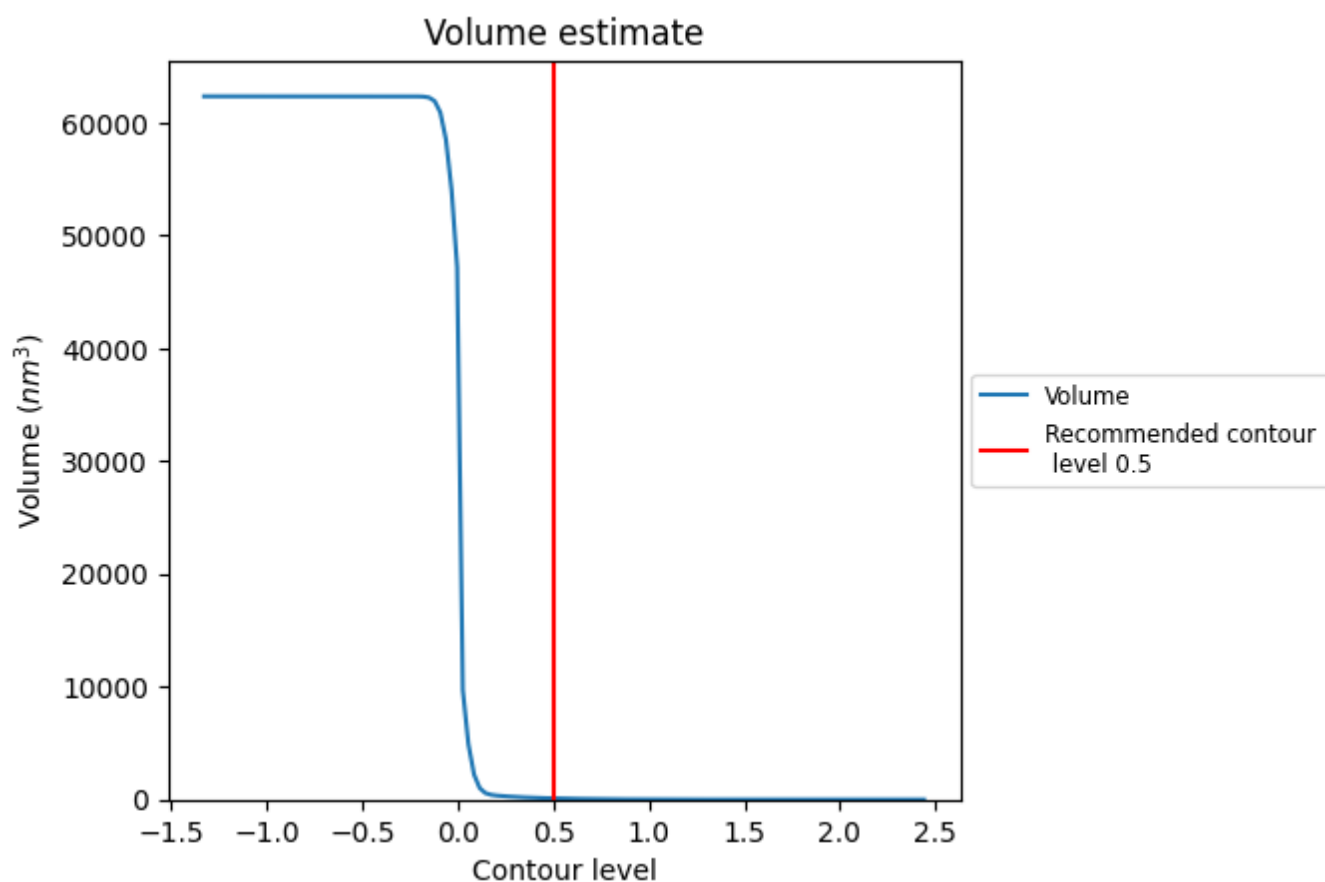
This section contains the results of statistical analysis of the map.

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.

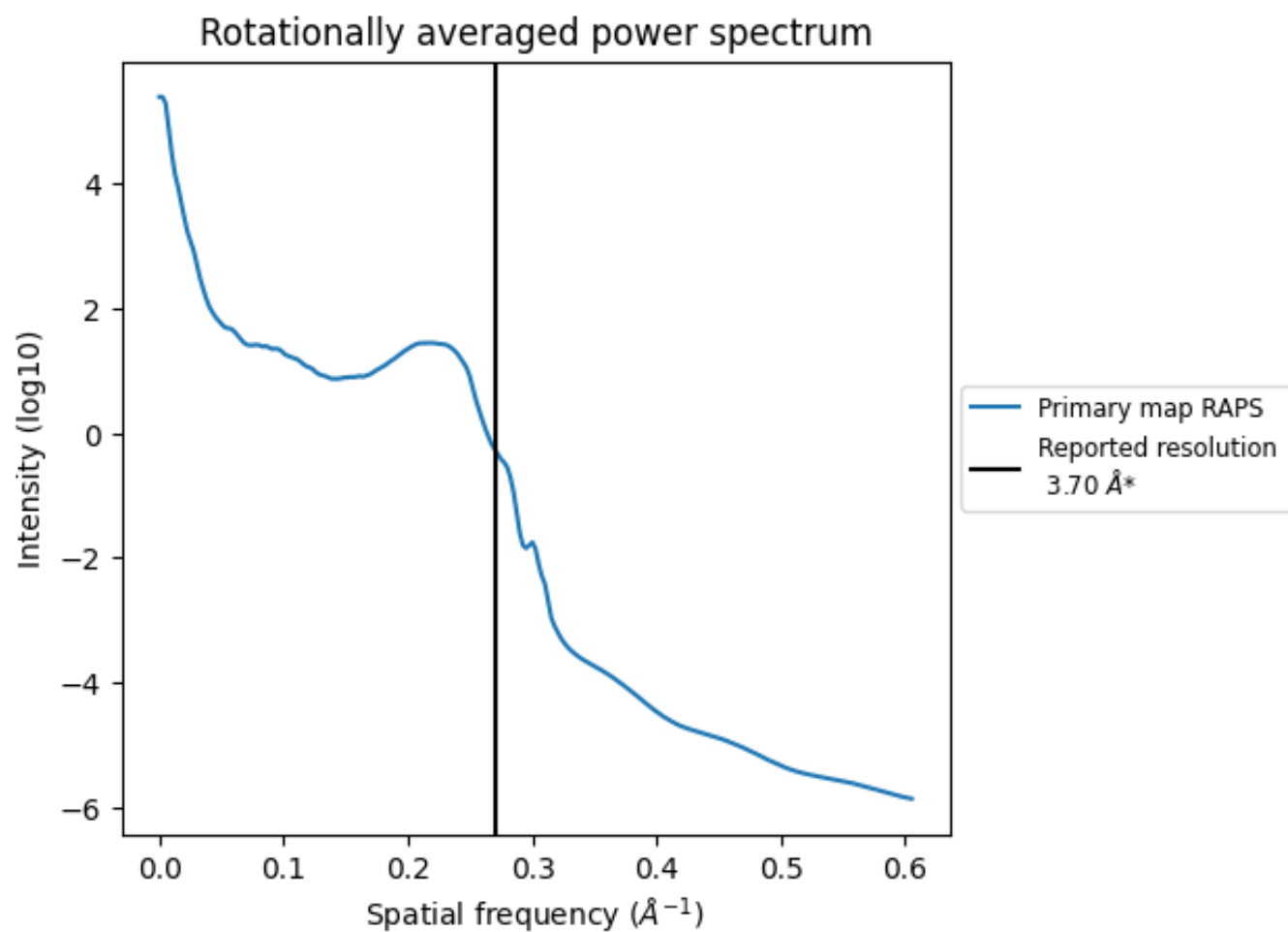
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 107 nm³; this corresponds to an approximate mass of 96 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 0.270 Å⁻¹

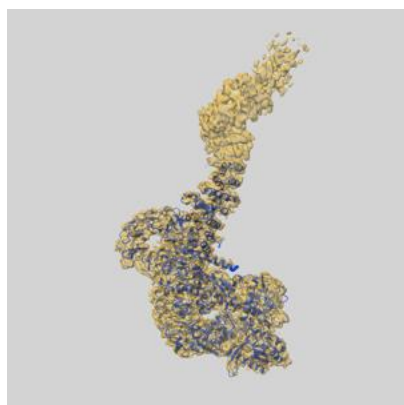
8 Fourier-Shell correlation ⓘ

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

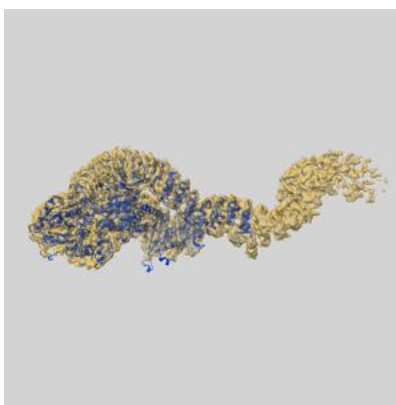
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23352 and PDB model 7LHW. Per-residue inclusion information can be found in section [3](#) on page [5](#).

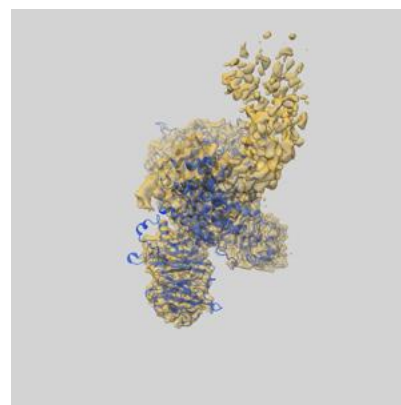
9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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](#)

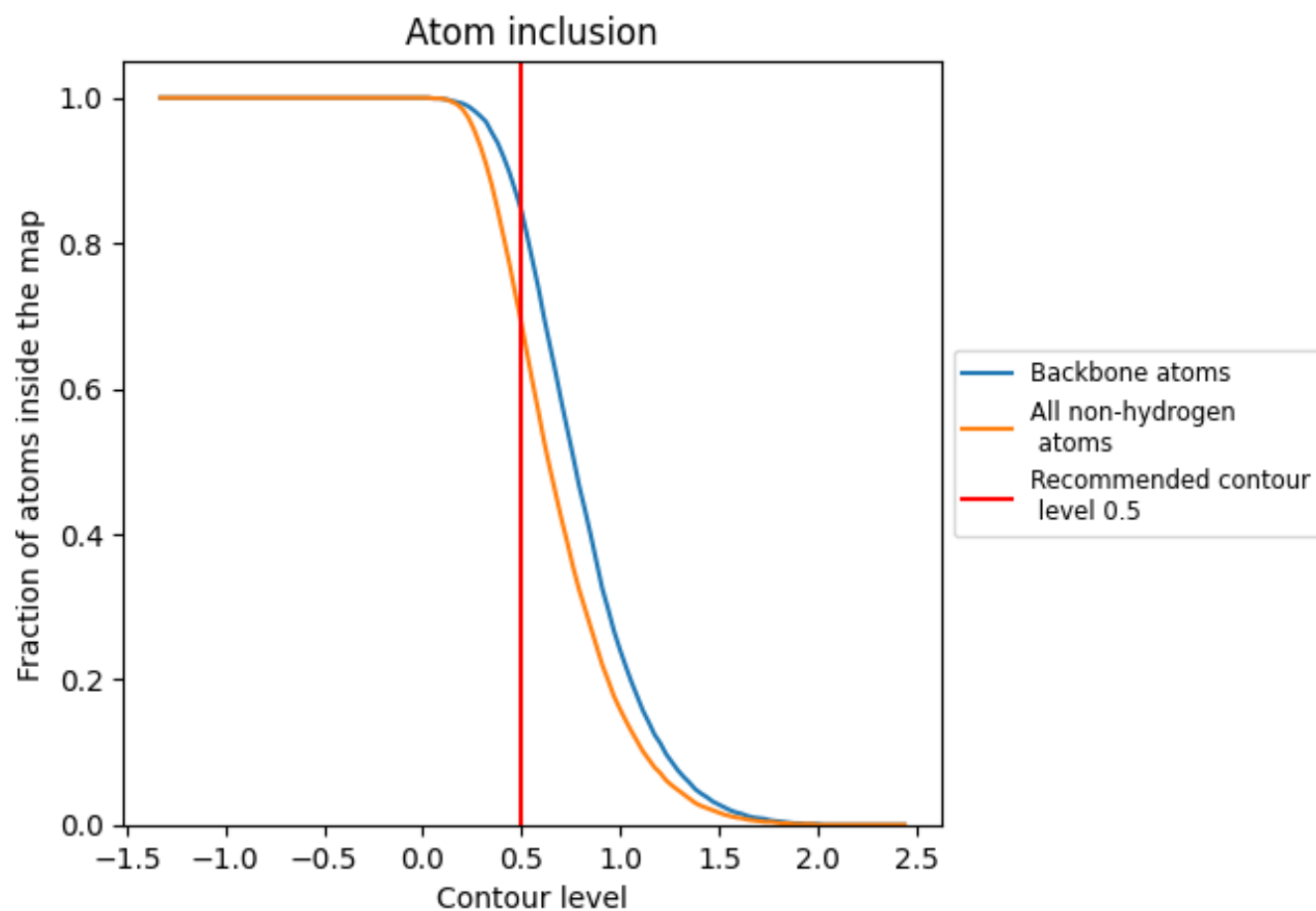


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 69% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6890	0.4060
A	0.6890	0.4060

