



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 04:21 AM UTC

PDB ID : 7LI4 / pdb_00007li4
EMDB ID : EMD-23360
Title : Structure of LRRK2 after symmetry expansion
Authors : Myasnikov, A.; Zhu, H.; Hixson, P.; Xie, B.; Yu, K.; Pitre, A.; Peng, J.; Sun, J.
Deposited on : 2021-01-26
Resolution : 3.10 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

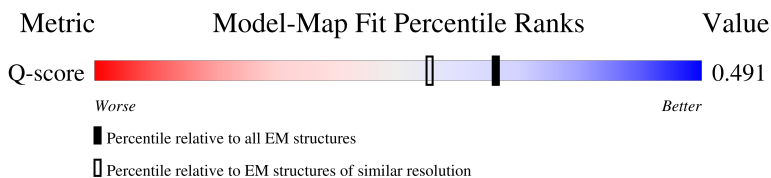
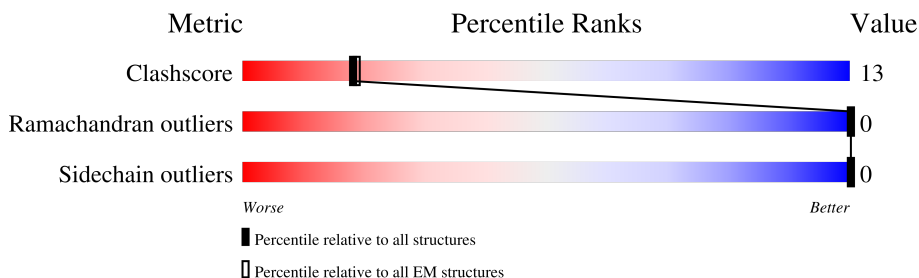
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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 14169 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.

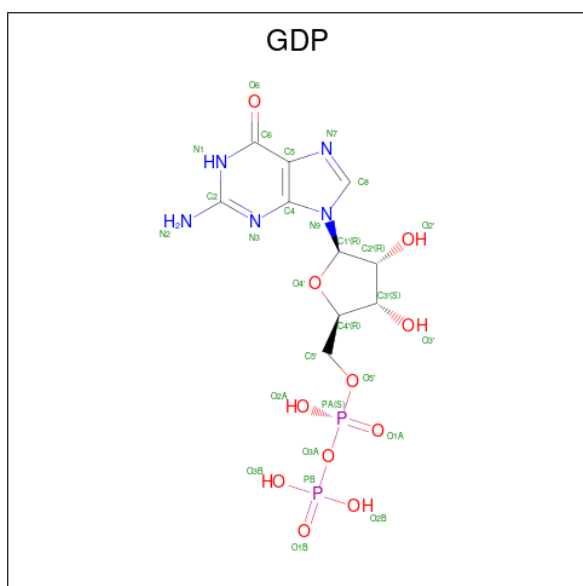
- Molecule 1 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1795	14110	9023	2433	2563	91	0	0

There are 3 discrepancies between the modelled and reference sequences:

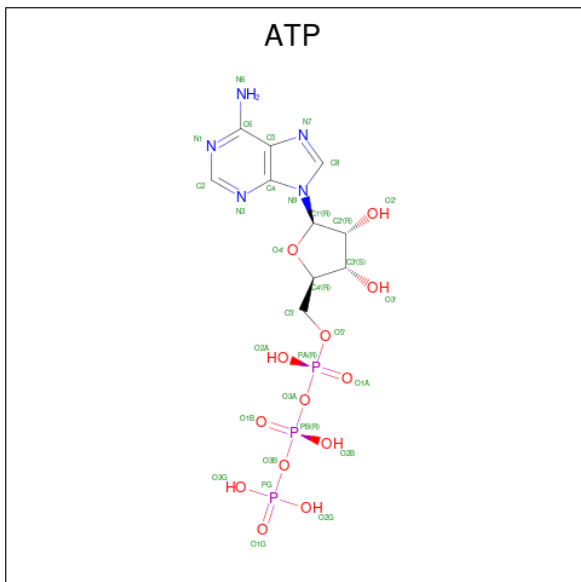
Chain	Residue	Modelled	Actual	Comment	Reference
A	50	HIS	ARG	variant	UNP Q5S007
A	1647	THR	SER	variant	UNP Q5S007
A	2397	THR	MET	variant	UNP Q5S007

- 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).



L2146	L2147	I2151	V2152	E2153	H2159	H2160	H2161	S2162	E2163	C2171	G2172	H2173	T2174	D2175	R2176	G2177	Q2178	L2179	S2180	D2183	L2184	E2187	G2188	Y2189	V2194	A2195	D2196	S2197	L2204	V2205	H2206	L2207	E2210	K2211	E2212	S2213	V2216	Q2220	L2224	L2225	V2226	L2227	N2228	T2229	G2232	K2233				
ILE	LYS	T2031	A2040	V2043	N2047	Y2050	Q2053	A2054	D2055	Y2064	T2068	T2069	G2070	I2073	E2082	E2085	Q2089	G2090	K2091	P2095	V2096	K2097	E2098	Y2099	A2102	P2105	M2106	L2110	R2122	V2128	F2129	D2130	I2131	A2135	E2136	L2137	V2138	C2139	L2140	T2141	R2142									
W1791	F1792	G1793	L1795	L1796	I1800	C1801	G1802	E1803	K1810	L1813	F1816	H1822	Q1823	K1824	L1825	L1826	D1829	L1830	M1831	K1832	E1836	G1837	D1838	L1839	D1844	L1848	T1849	I1850	Q1854	L1859	R1866	L1870	L1875	E1876	F1877	A1880	L1885	G1886	D1887	G1888	S1889	F1890								
E1689	I1692	Y1695	P1701	M1702	G1703	F1704	W1705	S1706	R1707	R1711	L1712	L1713	E1714	I1715	S1716	P1717	Y1718	M1719	L1720	SER	GLY	ARG	GLU	ARG	A1726	P1729	W1734	R1735	G1736	I1737	Y1738	Y1739	L1740	W1741	W1742	L1749	E1753	L1763	K1764	S1769	V1781	D1782	H1783	I1784	L1787					
Q1586	D1587	P1588	A1589	L1590	Q1591	Y1596	F1597	V1598	K1614	V1615	E1616	G1617	C1618	P1619	K1620	I1626	R1629	D1630	VAL	GLU	LYS	PHE	LEU	SER	LYS	LYS	ARG	LYS	PHE	P1642	Y1645	Y1649	F1650	A1651	L1652	L1653	E1654	L1655	F1656	Q1657	I1658	A1659	LEU	PRO	ILE	GLY	GLU	TYR	LEU	S1672
A1481	I1482	R1483	D1484	Y1485	H1486	F1487	V1488	A1489	T1491	R1501	L1509	N1510	F1511	K1512	Q1516	L1517	V1518	V1519	I1523	C1526	E1531	E1537	R1538	V1547	I1548	K1551	R1552	Q1555	L1556	V1557	Q1561	L1562	Q1563	L1564	N1567	V1573	H1574	F1575	L1576	V1581	L1582	L1583	H1584	F1585						
R1381	D1382	K1383	R1386	N1391	V1392	L1304	N1305	F1306	D1307	F1308	K1309	H1310	H1311	G1312	D1317	R1320	F1321	R1325	Y1332	N1333	R1334	L1337	M1338	I1339	V1340	G1341	N1342	T1343	G1346	K1347	L1351	M1355	K1356	K1359	H1361	L1362	G1363	M1364	D1372	V1373	K1374	D1375	W1376	T1380						
P1285	M1288	P1298	L1302	H1303	L1304	N1305	F1306	D1307	F1308	K1309	H1310	H1311	G1312	D1317	R1320	F1321	R1325	Y1332	N1333	R1334	L1337	M1338	I1339	G1341	N1342	T1343	G1346	K1347	L1351	M1355	K1356	K1359	H1361	L1362	G1363	M1364	D1372	V1373	K1374	D1375	W1376	T1380								
V1075	L1085	P1099	E1100	N1101	L1102	V1106	S1120	S1137	K1138	L1139	H1140	L1149	V1155	P1169	F1170	L1171	M1175	T1176	I1177	F1185	L1195	L1198	N1206	L1220	L1226	N1230	L1243	K1249	L1250	H1251	L1252	S1253	L1257	D1274	V1275	S1276	N1277													
HIS	SER	ASP	ILE	SER	LEU	ALA	SER	GLY	R981	I984	L989	N1139	A991	N992	D996	I997	D998	S1001	Q1002	K1003	C1004	L1018	H1019	Q1020	N1021	P1027	L1030	L1034	L1037	T1038	H1039	L1040	S1044	P1051	S1052	Y1053	L1054	M1057	N1062	V1065	N1068									
SER	ILE	SER	VAL	GLY	PHE	TYR	ASP	ALA	VAL	LEU	GLN	ARG	CYS	SER	PRO	ASN	LEU	GLN	SER	HIS	PHE	ASN	SER	GLU	TRP	THR	ILE	PRO	ILE	PHE	ASP	HIS	GLU	ASP	LEU	LYS	ARG	LYS	ARG	GLN	SER	VAL	LYS	LYS	SER	MET	SER	ASN		
Q847	V852	E953	E954	GLY	THR	ALA	SER	GLY	SER	ASP	GLY	ASN	PHE	SER	GLU	ASP	VAL	LEU	SER	LYS	PHE	ASN	SER	GLU	TRP	THR	ILE	PRO	ILE	PHE	ASP	HIS	GLU	ASP	LEU	LYS	ARG	LYS	ARG	GLN	SER	VAL	LYS	LYS	SER	MET	SER	ASN		

K2234	R2235	T2237	L2238	D2243	S2244	N2251	S2252	F2253	S2254	K2255	Q2256	S2257	K2258	Q2259	K2260	N2261	F2262	T2267	A2268	D2269	Q2270	K2271	L2272	A2273	E2276	D2277	K2278	T2279	V2280	A2285	A2286	P2287	L2288	K2289	I2293	S2297	L2300	K2301	C2302	L2303	S2304	E2305	S2306	T2307	N2308	S2309	T2310	E2311	R2312	N2313																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
V2314	M2315	W2316	G2317	G2318	C2319	G2320	F2324	S2325	F2326	S2327	N2328	D2329	F2330	T2331	I2332	T2338	R2339	T2340	S2341	Q2342	L2343	F2344	S2345	Y2346	A2347	F2349	S2350	D2351	I2354	I2355	T2356	D2360	Y2364	K2367	S2370	V2375	W2376	D2377	K2378	K2382	L2383	C2384	D2388	C2389	V2390	H2391	R2394																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
E2395	V2396	T2397	V2398	K2399	E2400	N2401	K2402	E2403	S2404	K2405	H2406	K2407	N2408	S2409	Y2410	S2411	Q2412	R2413	L2417	K2421	N2422	L2425	W2426	I2427	Q2430	I2434	L2435	L2436	L2437	D2438	T2441	R2442	R2443	L2444	I2445	I2448	Y2449	Q2462	L2463	Q2464	S2465	L2466	K2467	N2468	L2473	K2478	N2479	T2480	E2481																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
Q2482	T2483	Q2484	K2485	Q2486	K2487	E2488	I2489	Q2490	W2496	D2497	I2498	N2499	L2500	P2501	V2504	L2507	H2510	R2514	S2525	V2526	E2527																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	231875	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	0.068	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	422.912, 422.912, 422.912	wwPDB
Map dimensions	512, 512, 512	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: GDP, ATP

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	0.21	0/14375	0.45	6/19443 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1171	LEU	CA-C-N	-6.87	113.31	120.38
1	A	1171	LEU	C-N-CA	-6.87	113.31	120.38
1	A	1342	ASN	N-CA-C	5.95	117.14	107.32
1	A	1372	ASP	N-CA-C	5.40	118.85	111.39
1	A	741	GLY	N-CA-C	-5.40	106.25	112.73
1	A	1854	GLN	N-CA-C	5.03	116.77	111.28

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	14110	0	14392	377	0
2	A	28	0	12	0	0
3	A	31	0	12	2	0
All	All	14169	0	14416	377	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 13.

All (377) 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:2106:MET:CB	1:A:2137:LEU:CD1	1.77	1.59
1:A:2106:MET:HB3	1:A:2137:LEU:CD1	1.11	1.54
1:A:2136:GLU:CD	1:A:2448:ILE:CG2	1.95	1.40
1:A:2106:MET:CB	1:A:2137:LEU:HD12	1.35	1.39
1:A:2136:GLU:CD	1:A:2448:ILE:HG23	1.51	1.32
1:A:2136:GLU:OE2	1:A:2448:ILE:CG2	1.81	1.29
1:A:2136:GLU:OE1	1:A:2448:ILE:HG23	1.15	1.29
1:A:2106:MET:C	1:A:2137:LEU:HD11	1.56	1.29
1:A:1454:LEU:HD11	1:A:1487:PHE:O	1.08	1.23
1:A:638:PHE:CD2	1:A:641:VAL:HG21	1.72	1.22
1:A:1454:LEU:CD1	1:A:1487:PHE:O	1.88	1.19
1:A:2136:GLU:HG3	1:A:2496:TRP:CZ3	1.86	1.09
1:A:2136:GLU:CD	1:A:2448:ILE:HG21	1.77	1.09
1:A:2136:GLU:OE2	1:A:2448:ILE:HG21	1.50	1.02
1:A:2106:MET:HB2	1:A:2137:LEU:HD12	1.02	1.00
1:A:636:TYR:O	1:A:639:LYS:HG3	1.61	0.99
1:A:2106:MET:C	1:A:2137:LEU:CD1	2.36	0.97
1:A:2136:GLU:OE2	1:A:2496:TRP:CH2	2.18	0.97
1:A:2136:GLU:OE2	1:A:2496:TRP:HH2	1.48	0.96
1:A:2136:GLU:HG3	1:A:2496:TRP:HZ3	1.28	0.94
1:A:638:PHE:HD2	1:A:641:VAL:HG21	1.10	0.92
1:A:2106:MET:O	1:A:2137:LEU:HD11	1.69	0.92
1:A:2106:MET:CA	1:A:2137:LEU:CD1	2.52	0.88
1:A:2136:GLU:CG	1:A:2496:TRP:CZ3	2.55	0.88
1:A:1885:LEU:HD12	1:A:1894:TYR:CZ	2.09	0.88
1:A:1343:THR:HG22	1:A:1343:THR:O	1.77	0.85
1:A:2136:GLU:OE1	1:A:2448:ILE:CG2	2.07	0.84
1:A:586:MET:HE3	1:A:610:ILE:HG23	1.60	0.82
1:A:2136:GLU:OE2	1:A:2448:ILE:HG22	1.81	0.81
1:A:2136:GLU:CG	1:A:2496:TRP:CH2	2.63	0.81
1:A:2302:CYS:SG	1:A:2303:LEU:N	2.55	0.80
1:A:2106:MET:CB	1:A:2137:LEU:HD13	1.71	0.79
1:A:990:SER:O	1:A:1021:ASN:ND2	2.18	0.76
1:A:2106:MET:O	1:A:2137:LEU:CD1	2.33	0.76
1:A:1403:SER:O	1:A:1707:ARG:NH1	2.20	0.75
1:A:636:TYR:CE2	1:A:639:LYS:CE	2.69	0.75
1:A:2106:MET:HB3	1:A:2137:LEU:HD13	0.75	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2438:ASP:HB2	1:A:2445:ILE:HD11	1.68	0.74
1:A:638:PHE:CG	1:A:641:VAL:HG21	2.23	0.73
1:A:2236:HIS:NE2	1:A:2280:VAL:O	2.22	0.73
1:A:1973:ARG:O	1:A:1977:HIS:ND1	2.22	0.73
1:A:1454:LEU:HD21	1:A:1487:PHE:HB3	1.69	0.72
1:A:2136:GLU:CG	1:A:2496:TRP:HZ3	1.98	0.71
1:A:2110:LEU:HD13	1:A:2131:ILE:HD11	1.72	0.70
1:A:638:PHE:HD2	1:A:641:VAL:CG2	1.98	0.69
1:A:1707:ARG:HB3	1:A:1787:LEU:HD11	1.74	0.69
1:A:801:ASN:HB3	1:A:984:ILE:HA	1.74	0.69
1:A:1512:LYS:HA	1:A:1517:LEU:H	1.57	0.69
1:A:1341:GLY:O	1:A:1434:TRP:NE1	2.25	0.68
1:A:667:VAL:HG11	1:A:708:LEU:HD22	1.74	0.68
1:A:808:PHE:O	1:A:992:ASN:ND2	2.26	0.68
1:A:1339:ILE:HB	1:A:1394:ASP:HA	1.77	0.67
1:A:2106:MET:HG3	1:A:2140:LEU:HD23	1.76	0.67
1:A:2110:LEU:HD11	1:A:2128:VAL:HG23	1.77	0.66
1:A:2136:GLU:CD	1:A:2496:TRP:HH2	2.02	0.66
1:A:1305:ASN:HA	1:A:1516:GLN:NE2	2.12	0.65
1:A:1433:PRO:O	1:A:1437:ASN:ND2	2.30	0.65
1:A:638:PHE:CA	1:A:641:VAL:HG23	2.27	0.65
1:A:2462:GLN:HB2	1:A:2467:LYS:HD2	1.78	0.65
1:A:1037:LEU:HD21	1:A:1040:LEU:HB2	1.78	0.64
1:A:1816:PHE:HA	1:A:1850:ILE:HD11	1.79	0.64
1:A:1996:LYS:HG3	1:A:1998:HIS:H	1.63	0.64
1:A:638:PHE:HA	1:A:641:VAL:HG23	1.79	0.64
1:A:636:TYR:CE2	1:A:639:LYS:HE2	2.33	0.63
1:A:775:LEU:O	1:A:779:ILE:N	2.31	0.63
1:A:1813:LEU:HD21	1:A:1826:LEU:HD23	1.79	0.63
1:A:2251:ASN:HD21	1:A:2262:PHE:HB2	1.63	0.63
1:A:1439:LYS:HB2	1:A:1480:PRO:HD3	1.81	0.62
1:A:2213:SER:O	1:A:2229:THR:OG1	2.16	0.62
1:A:1308:PHE:HD1	1:A:1309:LYS:HG3	1.64	0.62
1:A:1220:LEU:CD2	1:A:1243:LEU:HD22	2.29	0.62
1:A:2413:ARG:O	1:A:2430:GLY:N	2.31	0.62
1:A:2293:ILE:HD12	1:A:2332:ILE:HD11	1.80	0.62
1:A:638:PHE:CB	1:A:641:VAL:HG21	2.30	0.61
1:A:1912:THR:O	1:A:1943:ARG:NH2	2.33	0.61
1:A:2106:MET:HE2	1:A:2137:LEU:HD13	1.82	0.61
1:A:1380:ILE:HD11	1:A:1386:ARG:HG3	1.82	0.61
1:A:992:ASN:O	1:A:1021:ASN:ND2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2238:LEU:HD12	1:A:2285:ALA:H	1.63	0.61
1:A:1075:VAL:HG12	1:A:1100:GLU:HB2	1.83	0.61
1:A:638:PHE:HB3	1:A:641:VAL:CG2	2.30	0.61
1:A:1701:PRO:HG2	1:A:1704:PHE:HB2	1.83	0.60
1:A:2151:ILE:HG12	1:A:2173:HIS:HB3	1.84	0.60
1:A:701:LYS:HA	1:A:704:MET:HG2	1.84	0.60
1:A:2136:GLU:CD	1:A:2496:TRP:CH2	2.76	0.60
1:A:818:LEU:HA	1:A:821:LEU:HD12	1.84	0.60
1:A:2427:ILE:HB	1:A:2435:LEU:HB2	1.84	0.60
1:A:1410:THR:O	1:A:1415:TYR:OH	2.19	0.60
1:A:1885:LEU:HD12	1:A:1894:TYR:CE2	2.36	0.60
1:A:2138:VAL:O	1:A:2138:VAL:HG22	2.02	0.60
1:A:2174:THR:OG1	1:A:2176:ARG:O	2.19	0.60
1:A:586:MET:HE2	1:A:627:LEU:HD22	1.84	0.59
1:A:1739:TYR:HB2	1:A:1749:LEU:HD13	1.84	0.59
1:A:1885:LEU:HD23	1:A:1885:LEU:O	2.02	0.59
1:A:1992:TYR:N	1:A:2055:ASP:OD2	2.33	0.59
1:A:709:LYS:HB3	1:A:733:ALA:HB2	1.84	0.59
1:A:1304:LEU:HB2	1:A:1308:PHE:HE2	1.65	0.59
1:A:1305:ASN:HA	1:A:1516:GLN:HE22	1.68	0.59
1:A:1836:GLU:O	1:A:1941:ARG:NH1	2.34	0.59
1:A:1905:VAL:HG12	1:A:1946:VAL:HG22	1.85	0.59
1:A:2136:GLU:CG	1:A:2496:TRP:HH2	2.14	0.59
1:A:1446:PRO:HD3	1:A:1511:PHE:HE1	1.68	0.59
1:A:738:ALA:HB3	1:A:743:SER:HA	1.85	0.58
1:A:2254:SER:N	1:A:2312:ARG:HH12	2.00	0.58
1:A:636:TYR:CD2	1:A:639:LYS:HE2	2.38	0.58
1:A:638:PHE:CB	1:A:641:VAL:CG2	2.81	0.58
1:A:810:ILE:H	1:A:992:ASN:HD22	1.52	0.58
1:A:2146:LEU:O	1:A:2490:GLN:NE2	2.32	0.58
1:A:1980:ASP:OD2	1:A:2514:ARG:NH1	2.36	0.58
1:A:772:ARG:HH21	1:A:808:PHE:HE1	1.50	0.58
1:A:1557:VAL:HG12	1:A:1562:LEU:HD12	1.84	0.58
1:A:1959:LEU:HD13	1:A:2070:GLY:HA3	1.86	0.58
1:A:1454:LEU:CG	1:A:1487:PHE:O	2.52	0.57
1:A:1796:LEU:HD23	1:A:1796:LEU:H	1.70	0.57
1:A:1672:SER:HA	1:A:1735:ARG:HH21	1.70	0.57
1:A:1039:HIS:CD2	1:A:1062:ASN:HD22	2.23	0.57
1:A:2151:ILE:O	1:A:2172:GLY:N	2.37	0.57
1:A:1351:LEU:HG	1:A:1355:MET:HE2	1.86	0.57
1:A:1509:LEU:HA	1:A:1519:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1703:GLY:O	1:A:1707:ARG:HD3	2.04	0.57
1:A:2272:LEU:HD11	1:A:2300:LEU:HD13	1.86	0.57
1:A:1039:HIS:HD2	1:A:1062:ASN:HD22	1.51	0.57
1:A:2304:SER:OG	1:A:2305:GLU:N	2.37	0.57
1:A:1275:VAL:O	1:A:1278:ASN:ND2	2.36	0.56
1:A:1446:PRO:HD3	1:A:1511:PHE:CE1	2.40	0.56
1:A:1137:SER:O	1:A:1139:ASN:ND2	2.38	0.56
1:A:1839:LEU:HD13	1:A:1941:ARG:HH22	1.70	0.56
1:A:586:MET:CE	1:A:610:ILE:HG23	2.32	0.56
1:A:1484:ASP:OD2	1:A:1486:HIS:NE2	2.35	0.56
1:A:1531:GLU:HB2	1:A:1576:LEU:HD11	1.88	0.56
1:A:2318:GLY:HA3	1:A:2354:ILE:HD13	1.88	0.56
1:A:2227:ILE:HD13	1:A:2235:ARG:HE	1.70	0.55
1:A:1431:MET:HE1	1:A:1449:LEU:HD22	1.87	0.55
1:A:2243:ASP:HB3	1:A:2268:ALA:HB3	1.88	0.55
1:A:1002:GLN:HB2	1:A:1004:CYS:SG	2.47	0.55
1:A:1940:ILE:HG22	1:A:1941:ARG:H	1.71	0.55
1:A:1099:PRO:HB2	1:A:1102:LEU:HD21	1.89	0.55
1:A:1343:THR:O	1:A:1343:THR:CG2	2.50	0.55
1:A:558:GLY:O	1:A:561:LYS:NZ	2.40	0.54
1:A:1195:LEU:HD12	1:A:1198:LEU:HD12	1.89	0.54
1:A:1441:ARG:NH2	1:A:1791:TRP:O	2.41	0.54
1:A:1928:HIS:ND1	1:A:2525:SER:OG	2.38	0.54
1:A:2510:HIS:CE1	1:A:2514:ARG:HD2	2.42	0.54
1:A:1343:THR:H	1:A:1397:GLY:HA3	1.73	0.54
1:A:2197:SER:HB2	1:A:2220:GLN:HG3	1.90	0.54
1:A:1956:ASP:OD1	1:A:1957:ARG:N	2.40	0.54
1:A:990:SER:OG	1:A:991:ALA:N	2.41	0.54
1:A:1695:TYR:HB2	1:A:1763:LEU:HB3	1.90	0.54
1:A:764:SER:OG	1:A:765:GLY:N	2.40	0.54
1:A:1992:TYR:OH	1:A:2016:ALA:O	2.12	0.54
1:A:1416:LEU:HD23	1:A:1448:ILE:HB	1.91	0.53
1:A:2417:LEU:HD12	1:A:2425:LEU:HD11	1.89	0.53
1:A:2377:ASP:HB2	1:A:2384:CYS:SG	2.48	0.53
1:A:691:PHE:CD1	1:A:691:PHE:C	2.85	0.53
1:A:1034:LEU:HD11	1:A:1037:LEU:HD22	1.91	0.53
1:A:1526:CYS:HB3	1:A:1564:LEU:HD11	1.90	0.53
1:A:1692:ILE:HD13	1:A:1764:LYS:HE3	1.91	0.53
1:A:1888:GLY:HA3	3:A:2602:ATP:H4'	1.90	0.53
1:A:2243:ASP:HB2	1:A:2267:THR:HG22	1.89	0.53
1:A:1054:LEU:HD23	1:A:1057:MET:CE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:ILE:HD12	1:A:745:ILE:H	1.73	0.52
1:A:1341:GLY:N	1:A:1347:LYS:HD3	2.24	0.52
1:A:1711:ARG:HD2	1:A:1787:LEU:HD12	1.91	0.52
1:A:1175:MET:HB2	1:A:1195:LEU:HD13	1.91	0.52
1:A:2436:LEU:HD12	1:A:2501:PRO:HB3	1.92	0.52
1:A:2390:VAL:HB	1:A:2394:ARG:HG3	1.91	0.51
1:A:1051:PRO:HB3	1:A:1053:TYR:CZ	2.45	0.51
1:A:1455:ASP:OD1	1:A:1455:ASP:N	2.43	0.51
1:A:638:PHE:HA	1:A:641:VAL:CG2	2.41	0.51
1:A:631:LEU:HD13	1:A:652:ILE:HG12	1.93	0.51
1:A:1552:ARG:NH1	1:A:1555:GLN:OE1	2.44	0.51
1:A:1689:GLU:O	1:A:1769:SER:N	2.38	0.50
1:A:1692:ILE:HD12	1:A:1824:LYS:HE2	1.94	0.50
1:A:1885:LEU:CD1	1:A:1894:TYR:CZ	2.90	0.50
1:A:1149:LEU:HD12	1:A:1155:VAL:HG21	1.93	0.50
1:A:636:TYR:CZ	1:A:639:LYS:CE	2.94	0.50
1:A:736:ASN:HB2	1:A:767:ARG:HE	1.77	0.50
1:A:1942:PRO:HD2	1:A:1944:MET:HE2	1.94	0.50
1:A:610:ILE:HG21	1:A:627:LEU:HD11	1.94	0.50
1:A:2302:CYS:HB2	1:A:2355:ILE:O	2.12	0.50
1:A:1020:GLN:HA	1:A:1044:SER:HB2	1.93	0.49
1:A:2364:TYR:HE1	1:A:2375:VAL:HG13	1.78	0.49
1:A:1343:THR:OG1	1:A:1398:ARG:HA	2.12	0.49
1:A:1436:PHE:HZ	1:A:1795:LEU:HD21	1.77	0.49
1:A:1285:PRO:HG2	1:A:1288:MET:HG3	1.94	0.49
1:A:1436:PHE:CZ	1:A:1795:LEU:HD21	2.48	0.49
1:A:2255:LYS:HB3	1:A:2312:ARG:HH11	1.76	0.49
1:A:2354:ILE:HA	1:A:2367:LYS:HD3	1.94	0.49
1:A:2468:ASN:HB3	1:A:2498:ILE:HG21	1.93	0.49
1:A:1650:PHE:HA	1:A:1653:LEU:HB2	1.93	0.49
1:A:1870:LEU:HD11	1:A:1875:LEU:HD13	1.93	0.49
1:A:1885:LEU:HD12	1:A:1894:TYR:CE1	2.46	0.49
1:A:2269:ASP:OD1	1:A:2271:LYS:HG3	2.12	0.49
1:A:1339:ILE:HD11	1:A:1351:LEU:HD13	1.95	0.49
1:A:1885:LEU:HB2	1:A:1894:TYR:CE2	2.47	0.49
1:A:2152:VAL:HG13	1:A:2473:LEU:HD21	1.94	0.49
1:A:2327:SER:OG	1:A:2328:ASN:N	2.45	0.49
1:A:1332:TYR:HB2	1:A:1523:ILE:HG12	1.94	0.49
1:A:1417:ALA:O	1:A:1450:VAL:N	2.44	0.49
1:A:2438:ASP:HB3	1:A:2442:ARG:O	2.13	0.48
1:A:586:MET:CE	1:A:627:LEU:HD22	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2142:ARG:NH2	1:A:2187:GLU:OE2	2.45	0.48
1:A:2338:THR:HG22	1:A:2376:TRP:CE2	2.48	0.48
1:A:635:LEU:HB2	1:A:674:VAL:HG21	1.95	0.48
1:A:1923:VAL:HA	1:A:1926:HIS:CE1	2.48	0.48
1:A:2043:VAL:HG23	1:A:2050:TYR:CE1	2.49	0.48
1:A:1437:ASN:OD1	1:A:1702:MET:N	2.46	0.48
1:A:740:GLU:HA	1:A:767:ARG:HH22	1.78	0.48
1:A:1705:TRP:CD1	1:A:1736:GLN:HG2	2.49	0.48
1:A:636:TYR:CE2	1:A:639:LYS:NZ	2.82	0.48
1:A:1583:LEU:HB2	1:A:1597:PHE:HB2	1.96	0.48
1:A:1716:SER:OG	1:A:1717:PRO:HD3	2.13	0.48
1:A:1740:LEU:H	1:A:1740:LEU:HD23	1.78	0.47
1:A:636:TYR:CZ	1:A:639:LYS:NZ	2.80	0.47
1:A:1120:SER:HA	1:A:1140:HIS:O	2.14	0.47
1:A:1584:HIS:ND1	1:A:1586:GLN:OE1	2.38	0.47
1:A:1729:PRO:HG3	1:A:1742:TRP:CZ2	2.50	0.47
1:A:1956:ASP:N	1:A:1997:PRO:O	2.48	0.47
1:A:636:TYR:CD2	1:A:639:LYS:CE	2.97	0.47
1:A:1931:SER:OG	1:A:1931:SER:O	2.31	0.47
1:A:1375:ASP:HA	1:A:1391:ASN:HA	1.97	0.47
1:A:638:PHE:HB3	1:A:641:VAL:HG21	1.94	0.47
1:A:771:VAL:HG13	1:A:790:LEU:HD22	1.97	0.47
1:A:1355:MET:HG2	1:A:1376:TRP:CG	2.50	0.47
1:A:1782:ASP:HB2	1:A:1918:ARG:HH11	1.80	0.47
1:A:2162:SER:O	1:A:2464:GLY:HA2	2.15	0.47
1:A:2171:CYS:SG	1:A:2178:GLN:N	2.88	0.46
1:A:2273:ALA:HB1	1:A:2287:PRO:HB3	1.97	0.46
1:A:725:VAL:HG11	1:A:757:LEU:HD13	1.98	0.46
1:A:2105:PRO:HG3	1:A:2142:ARG:HA	1.97	0.46
1:A:1253:SER:HB3	1:A:1274:ASP:OD1	2.14	0.46
1:A:2233:LYS:HE2	1:A:2233:LYS:HB3	1.71	0.46
1:A:2324:PHE:HE1	1:A:2326:PHE:HE2	1.63	0.46
1:A:2339:ARG:NE	1:A:2351:ASP:OD2	2.49	0.46
1:A:1449:LEU:O	1:A:1485:TYR:HA	2.15	0.46
1:A:1695:TYR:HE2	1:A:1784:ILE:HG21	1.80	0.46
1:A:1374:LYS:O	1:A:1392:VAL:N	2.48	0.46
1:A:1652:LEU:HA	1:A:1655:LYS:HB2	1.98	0.46
1:A:675:ILE:HD11	1:A:699:PHE:HB2	1.97	0.46
1:A:2136:GLU:HG3	1:A:2496:TRP:CH2	2.30	0.46
1:A:2178:GLN:NE2	1:A:2179:LEU:O	2.46	0.46
1:A:1305:ASN:ND2	1:A:1516:GLN:HE22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1781:VAL:HA	1:A:1784:ILE:HG22	1.98	0.46
1:A:744:LEU:O	1:A:748:VAL:HG23	2.16	0.45
1:A:752:GLU:HG3	1:A:752:GLU:O	2.16	0.45
1:A:2136:GLU:HG2	1:A:2496:TRP:CH2	2.47	0.45
1:A:2183:ASP:OD1	1:A:2184:LEU:N	2.40	0.45
1:A:2272:LEU:HD11	1:A:2300:LEU:CD1	2.46	0.45
1:A:2302:CYS:SG	1:A:2356:THR:HA	2.55	0.45
1:A:2510:HIS:HE1	1:A:2514:ARG:HD2	1.81	0.45
1:A:1257:LEU:HB2	1:A:1278:ASN:OD1	2.16	0.45
1:A:1626:ILE:HD11	1:A:1629:ARG:HD3	1.98	0.45
1:A:636:TYR:CZ	1:A:639:LYS:HE3	2.52	0.45
1:A:1065:VAL:HG23	1:A:1068:ASN:ND2	2.32	0.45
1:A:704:MET:SD	1:A:847:GLN:NE2	2.87	0.45
1:A:1304:LEU:HB2	1:A:1308:PHE:CE2	2.50	0.45
1:A:1652:LEU:O	1:A:1656:PHE:N	2.42	0.45
1:A:1511:PHE:HD2	1:A:1518:VAL:HB	1.81	0.45
1:A:1832:LYS:NZ	1:A:1859:LEU:HD12	2.32	0.45
1:A:2388:ASP:OD1	1:A:2389:CYS:N	2.50	0.45
1:A:2426:TRP:HE3	1:A:2434:ILE:HD11	1.81	0.45
1:A:1391:ASN:ND2	1:A:1393:TRP:HE1	2.15	0.45
1:A:1455:ASP:HB3	1:A:1489:ASN:HD21	1.81	0.45
1:A:2040:ALA:HB3	1:A:2043:VAL:HG12	1.99	0.45
1:A:2488:GLU:N	1:A:2488:GLU:OE2	2.49	0.45
1:A:679:MET:HE2	1:A:839:LEU:HD13	1.99	0.45
1:A:1479:PHE:HB3	1:A:1480:PRO:HD2	1.98	0.45
1:A:2437:LEU:HA	1:A:2443:ARG:O	2.16	0.45
1:A:2402:LYS:HE3	1:A:2402:LYS:HB3	1.87	0.44
1:A:1288:MET:HE2	1:A:1288:MET:HB3	1.87	0.44
1:A:1719:MET:H	1:A:1719:MET:HE2	1.82	0.44
1:A:1967:THR:C	1:A:1969:THR:H	2.26	0.44
1:A:2043:VAL:HG23	1:A:2050:TYR:CZ	2.52	0.44
1:A:2089:GLN:O	1:A:2091:LYS:N	2.50	0.44
1:A:1919:GLN:HG3	1:A:2025:CYS:SG	2.57	0.44
1:A:1085:LEU:HD23	1:A:1106:VAL:HG11	1.99	0.44
1:A:1562:LEU:HD23	1:A:1562:LEU:HA	1.82	0.44
1:A:1718:TYR:HB2	1:A:1742:TRP:CZ2	2.52	0.44
1:A:656:LEU:HD13	1:A:701:LYS:HB2	2.00	0.44
1:A:2178:GLN:NE2	1:A:2180:SER:OG	2.50	0.44
1:A:1185:PHE:HB2	1:A:1206:ASN:HB3	2.00	0.44
1:A:1334:ARG:O	1:A:1412:ARG:NH1	2.49	0.44
1:A:1712:LEU:HD12	1:A:1738:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1753:GLU:OE1	1:A:1753:GLU:N	2.50	0.43
1:A:1968:ARG:NH1	1:A:2102:ALA:HB3	2.33	0.43
1:A:1573:VAL:HG21	1:A:1596:TYR:CE2	2.53	0.43
1:A:1308:PHE:CE1	1:A:1309:LYS:HE3	2.53	0.43
1:A:2262:PHE:CE2	1:A:2330:PHE:HZ	2.36	0.43
1:A:2135:ALA:HB2	1:A:2507:LEU:HD23	2.00	0.43
1:A:2220:GLN:HA	1:A:2244:SER:HB3	2.00	0.43
1:A:1027:PRO:HG2	1:A:1030:LEU:HB3	2.01	0.43
1:A:1489:ASN:OD1	1:A:1491:THR:OG1	2.34	0.43
1:A:1893:VAL:HG12	3:A:2602:ATP:H5'1	2.01	0.43
1:A:2082:GLU:HA	1:A:2085:GLU:HG2	2.00	0.43
1:A:2136:GLU:HG2	1:A:2496:TRP:CZ3	2.46	0.43
1:A:638:PHE:CA	1:A:641:VAL:CG2	2.95	0.43
1:A:691:PHE:O	1:A:694:LEU:HB3	2.18	0.43
1:A:1838:ASP:OD1	1:A:1838:ASP:N	2.42	0.43
1:A:1848:LEU:HD23	1:A:1848:LEU:H	1.83	0.43
1:A:2464:GLY:C	1:A:2466:LEU:H	2.26	0.43
1:A:1406:PRO:HG3	1:A:1702:MET:HB3	2.00	0.43
1:A:1935:LEU:HG	1:A:1945:LEU:HD11	2.01	0.43
1:A:2300:LEU:HA	1:A:2319:CYS:HA	2.01	0.43
1:A:676:PHE:CE1	1:A:724:MET:HG2	2.54	0.43
1:A:1226:LEU:HD11	1:A:1249:LYS:HE2	2.01	0.43
1:A:1405:HIS:HD2	1:A:1434:TRP:HH2	1.67	0.43
1:A:1551:LYS:HA	1:A:1551:LYS:HD3	1.96	0.43
1:A:2064:TYR:CE2	1:A:2095:PRO:HG3	2.54	0.43
1:A:2135:ALA:CB	1:A:2504:VAL:HA	2.48	0.42
1:A:1317:ASP:OD1	1:A:1320:ARG:NH1	2.52	0.42
1:A:2364:TYR:CE1	1:A:2375:VAL:HG13	2.53	0.42
1:A:692:LEU:HD21	1:A:842:MET:SD	2.59	0.42
1:A:998:ASP:O	1:A:1001:SER:OG	2.37	0.42
1:A:1996:LYS:HD2	1:A:1998:HIS:HB3	2.01	0.42
1:A:2276:GLU:CD	1:A:2278:LYS:H	2.26	0.42
1:A:1276:SER:HA	1:A:1302:LEU:HD22	2.01	0.42
1:A:1340:VAL:HG13	1:A:1434:TRP:CD2	2.55	0.42
1:A:1689:GLU:OE2	1:A:1689:GLU:N	2.52	0.42
1:A:2306:SER:OG	1:A:2308:ASN:O	2.37	0.42
1:A:2303:LEU:HD21	1:A:2315:MET:SD	2.60	0.42
1:A:779:ILE:HD13	1:A:787:ILE:HD13	2.02	0.42
1:A:841:ARG:O	1:A:845:ARG:N	2.44	0.42
1:A:1169:PRO:O	1:A:1170:PHE:C	2.63	0.42
1:A:1176:THR:HG22	1:A:1177:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1206:ASN:O	1:A:1230:ASN:HA	2.19	0.42
1:A:2367:LYS:HB2	1:A:2370:SER:HB3	2.02	0.42
1:A:566:VAL:O	1:A:569:SER:OG	2.32	0.42
1:A:1695:TYR:OH	1:A:1781:VAL:HG13	2.19	0.42
1:A:1795:LEU:HD23	1:A:1795:LEU:HA	1.80	0.42
1:A:2175:ASP:OD1	1:A:2175:ASP:N	2.51	0.42
1:A:2228:ASN:OD1	1:A:2229:THR:N	2.53	0.42
1:A:827:SER:O	1:A:828:ASN:OD1	2.37	0.41
1:A:1538:ARG:NH1	1:A:1581:VAL:O	2.53	0.41
1:A:1810:LYS:O	1:A:1829:ASP:HB2	2.20	0.41
1:A:676:PHE:CD1	1:A:724:MET:HG2	2.55	0.41
1:A:1476:LYS:HE3	1:A:1476:LYS:HB3	1.86	0.41
1:A:1537:GLU:CD	1:A:1548:ILE:HD11	2.45	0.41
1:A:1548:ILE:HD12	1:A:1598:VAL:HG21	2.03	0.41
1:A:1791:TRP:O	1:A:1793:PRO:HD3	2.19	0.41
1:A:1932:LEU:HD23	1:A:2015:ILE:HG13	2.02	0.41
1:A:2216:VAL:HG12	1:A:2226:VAL:HG22	2.03	0.41
1:A:1356:LYS:HG3	1:A:1501:ARG:NH1	2.35	0.41
1:A:1547:VAL:HG22	1:A:1597:PHE:CD1	2.55	0.41
1:A:2147:PRO:HG2	1:A:2189:TYR:CD1	2.55	0.41
1:A:794:LEU:HD23	1:A:794:LEU:HA	1.91	0.41
1:A:1250:LEU:HG	1:A:1252:LEU:HD23	2.02	0.41
1:A:1523:ILE:HD13	1:A:1575:PHE:HE2	1.85	0.41
1:A:2153:GLU:N	1:A:2153:GLU:OE1	2.53	0.41
1:A:2448:ILE:HD13	1:A:2500:LEU:HD21	2.02	0.41
1:A:996:ASP:OD1	1:A:997:ILE:N	2.53	0.41
1:A:1359:LYS:HG3	1:A:1360:SER:H	1.85	0.41
1:A:671:PHE:CE2	1:A:702:VAL:HG21	2.55	0.41
1:A:1734:TRP:CZ2	1:A:1737:GLY:HA3	2.56	0.41
1:A:2382:LYS:HE3	1:A:2382:LYS:HB3	1.94	0.41
1:A:1717:PRO:HB3	1:A:1720:LEU:HD13	2.03	0.41
1:A:671:PHE:HE2	1:A:702:VAL:HG21	1.86	0.41
1:A:989:LEU:HB2	1:A:1018:LEU:HD23	2.03	0.41
1:A:2068:THR:HG21	1:A:2099:TYR:HD2	1.86	0.41
1:A:2267:THR:HG22	1:A:2268:ALA:N	2.35	0.41
1:A:564:LEU:HD22	1:A:589:VAL:HG23	2.02	0.41
1:A:699:PHE:HE1	1:A:712:MET:HE2	1.86	0.41
1:A:2224:LEU:HD23	1:A:2238:LEU:HB2	2.03	0.41
1:A:2267:THR:HG22	1:A:2268:ALA:H	1.85	0.41
1:A:2478:LYS:HD3	1:A:2478:LYS:HA	1.85	0.41
1:A:1337:LEU:HD23	1:A:1392:VAL:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1645:TYR:O	1:A:1649:TYR:N	2.54	0.40
1:A:835:ILE:O	1:A:838:THR:OG1	2.36	0.40
1:A:1274:ASP:OD2	1:A:1298:PRO:HG2	2.22	0.40
1:A:1351:LEU:HD21	1:A:1392:VAL:HG21	2.02	0.40
1:A:1480:PRO:O	1:A:1482:ILE:HD12	2.21	0.40
1:A:2367:LYS:HD3	1:A:2367:LYS:HA	1.93	0.40
1:A:1997:PRO:HG2	1:A:2073:ILE:HD11	2.04	0.40
1:A:2338:THR:HG22	1:A:2376:TRP:CZ2	2.57	0.40
1:A:1321:PHE:HE2	1:A:1325:ARG:HH21	1.70	0.40
1:A:1406:PRO:HG2	1:A:1703:GLY:H	1.87	0.40
1:A:1877:PHE:CE2	1:A:1907:ILE:HD11	2.57	0.40
1:A:2053:GLN:NE2	1:A:2122:ARG:O	2.54	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	1777/2527 (70%)	1561 (88%)	216 (12%)	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	1575/2281 (69%)	1575 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	591	HIS
1	A	992	ASN
1	A	1021	ASN
1	A	1043	HIS
1	A	1045	ASN
1	A	1062	ASN
1	A	1163	ASN
1	A	1206	ASN
1	A	1251	HIS
1	A	1305	ASN
1	A	1333	ASN
1	A	1453	HIS
1	A	1516	GLN
1	A	1644	ASN
1	A	1871	ASN
1	A	1926	HIS
1	A	2053	GLN
1	A	2133	ASN
1	A	2160	HIS
1	A	2433	HIS
1	A	2462	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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	1.36	5 (15%)	48,52,52	1.73	10 (20%)
2	GDP	A	2601	-	29,30,30	1.18	3 (10%)	45,47,47	1.80	8 (17%)

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	-	-	5/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2602	ATP	C5-C4	4.38	1.46	1.39
2	A	2601	GDP	C5-C4	3.10	1.47	1.38
2	A	2601	GDP	C6-N1	-2.54	1.34	1.38
3	A	2602	ATP	C5-C6	2.53	1.48	1.41
3	A	2602	ATP	C5-N7	-2.48	1.34	1.39
3	A	2602	ATP	C8-N7	2.27	1.36	1.31
2	A	2601	GDP	C5-N7	-2.15	1.34	1.39
3	A	2602	ATP	C4-N9	-2.13	1.33	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2601	GDP	C5-C4-N3	-6.18	118.56	128.39
3	A	2602	ATP	C5-C4-N3	-5.66	118.92	126.72
2	A	2601	GDP	C2-N3-C4	5.04	120.98	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2601	GDP	N9-C4-N3	4.69	135.34	125.95
3	A	2602	ATP	N3-C4-N9	4.39	134.64	127.17
3	A	2602	ATP	C2-N3-C4	3.60	120.62	111.83
3	A	2602	ATP	C4-C5-N7	-3.44	106.65	110.58
3	A	2602	ATP	N3-C2-N1	-3.16	123.79	128.58
2	A	2601	GDP	C6-C5-N7	3.11	135.94	130.29
3	A	2602	ATP	C4-N9-C8	2.64	108.51	105.74
3	A	2602	ATP	C5-N7-C8	2.47	107.33	103.45
2	A	2601	GDP	C4-C5-N7	-2.34	106.96	110.67
2	A	2601	GDP	O6-C6-C5	-2.28	120.51	126.53
2	A	2601	GDP	C3'-C2'-C1'	2.28	105.78	101.46
3	A	2602	ATP	C6-C5-N7	2.06	136.05	132.09
2	A	2601	GDP	C5-C6-N1	2.02	118.40	113.25
3	A	2602	ATP	N9-C8-N7	-2.01	111.08	113.94
3	A	2602	ATP	C3'-C2'-C1'	2.01	105.26	101.46

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2601	GDP	C5'-O5'-PA-O3A
2	A	2601	GDP	C5'-O5'-PA-O1A
3	A	2602	ATP	C5'-O5'-PA-O2A
2	A	2601	GDP	C3'-C4'-C5'-O5'
2	A	2601	GDP	O4'-C4'-C5'-O5'
2	A	2601	GDP	C4'-C5'-O5'-PA

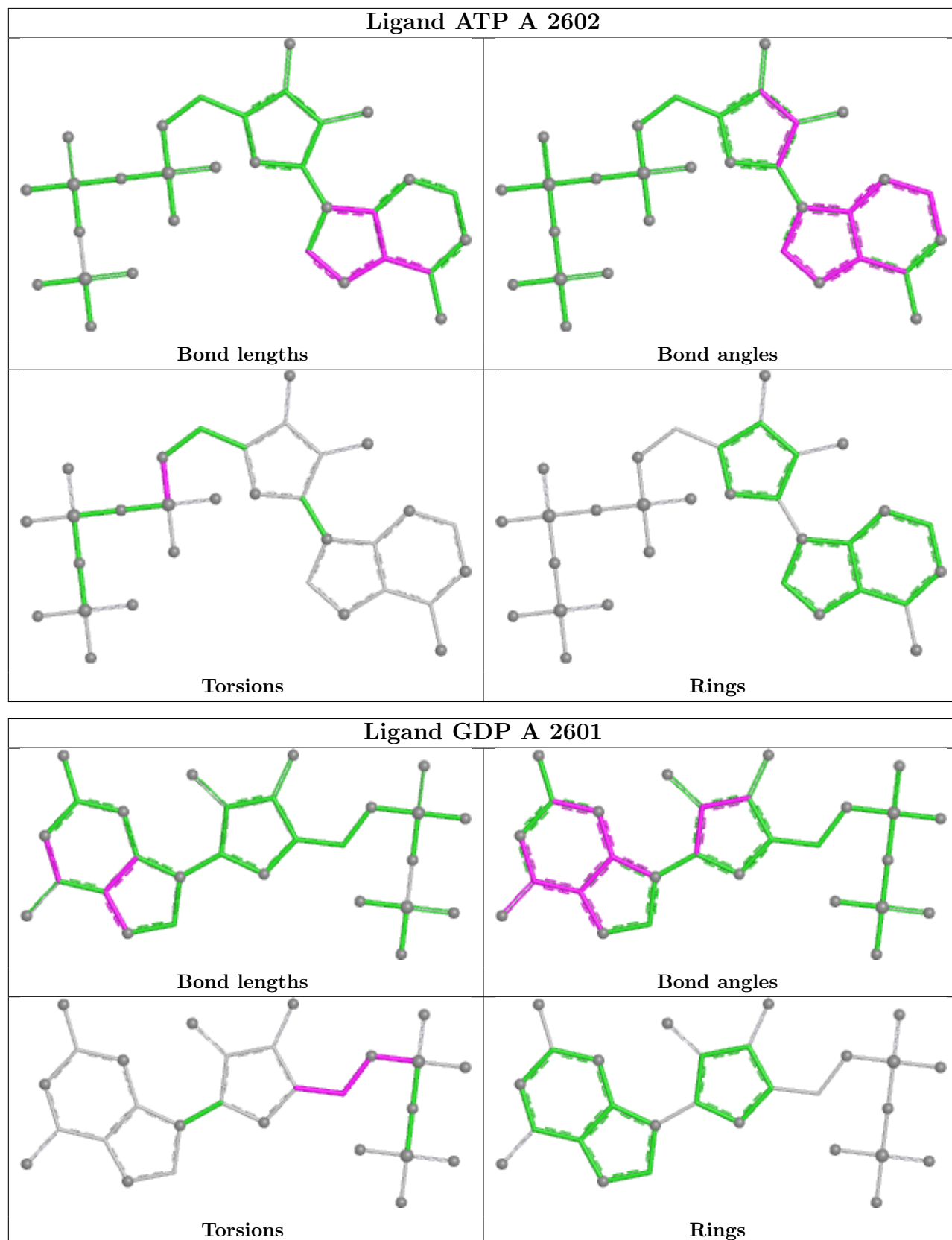
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2602	ATP	2	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.

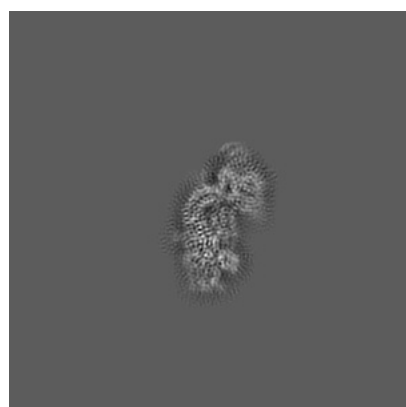
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23360. These allow visual inspection of the internal detail of the map and identification of artifacts.

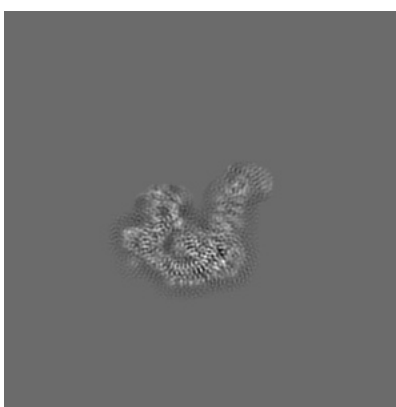
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

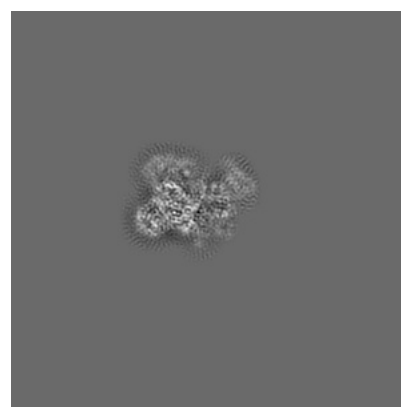
6.1.1 Primary map



X



Y

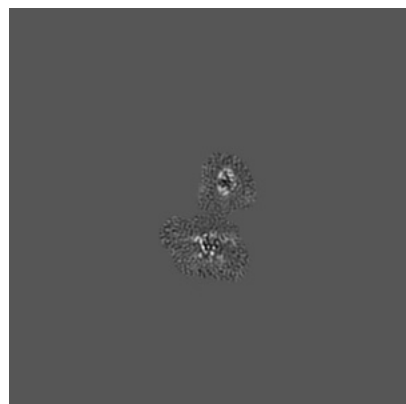


Z

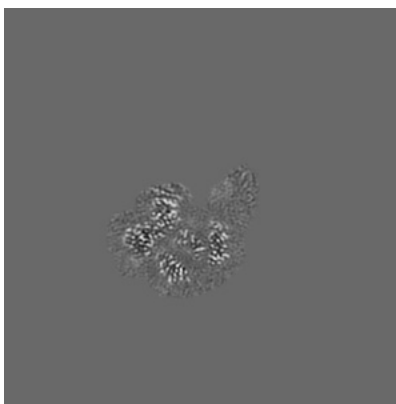
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

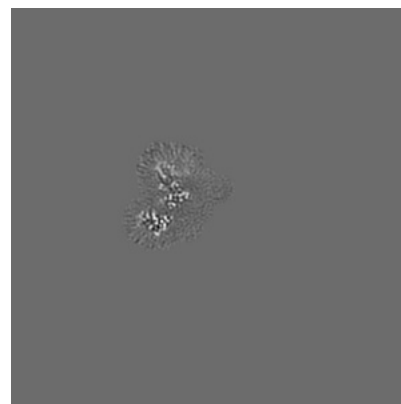
6.2.1 Primary map



X Index: 256



Y Index: 256

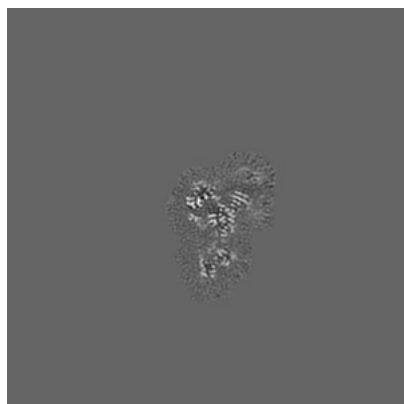


Z Index: 256

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

6.3 Largest variance slices [i](#)

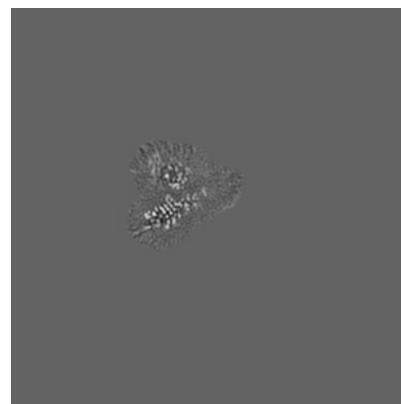
6.3.1 Primary map



X Index: 200



Y Index: 250

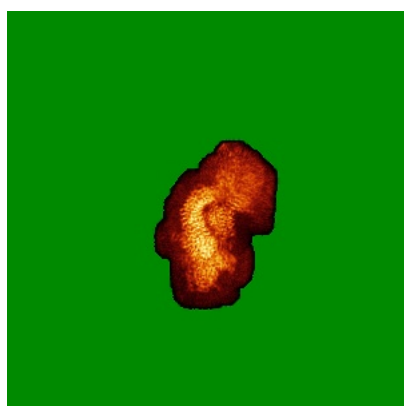


Z Index: 268

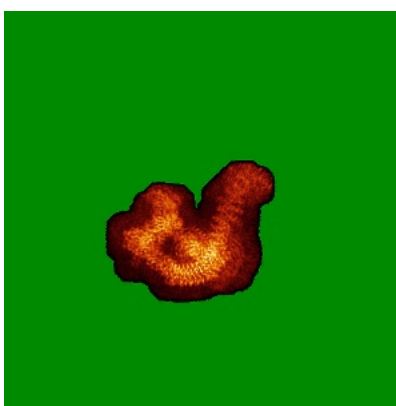
The images above show the largest variance slices of the map in three orthogonal directions.

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

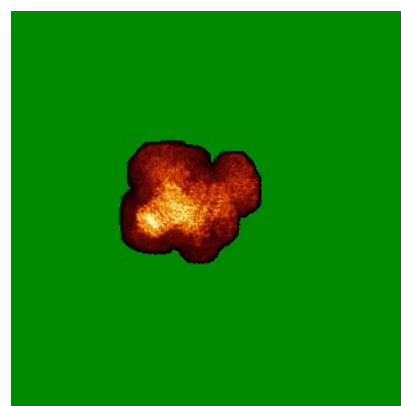
6.4.1 Primary map



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 [i](#)

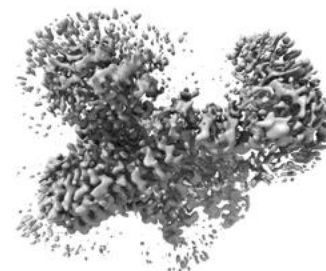
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

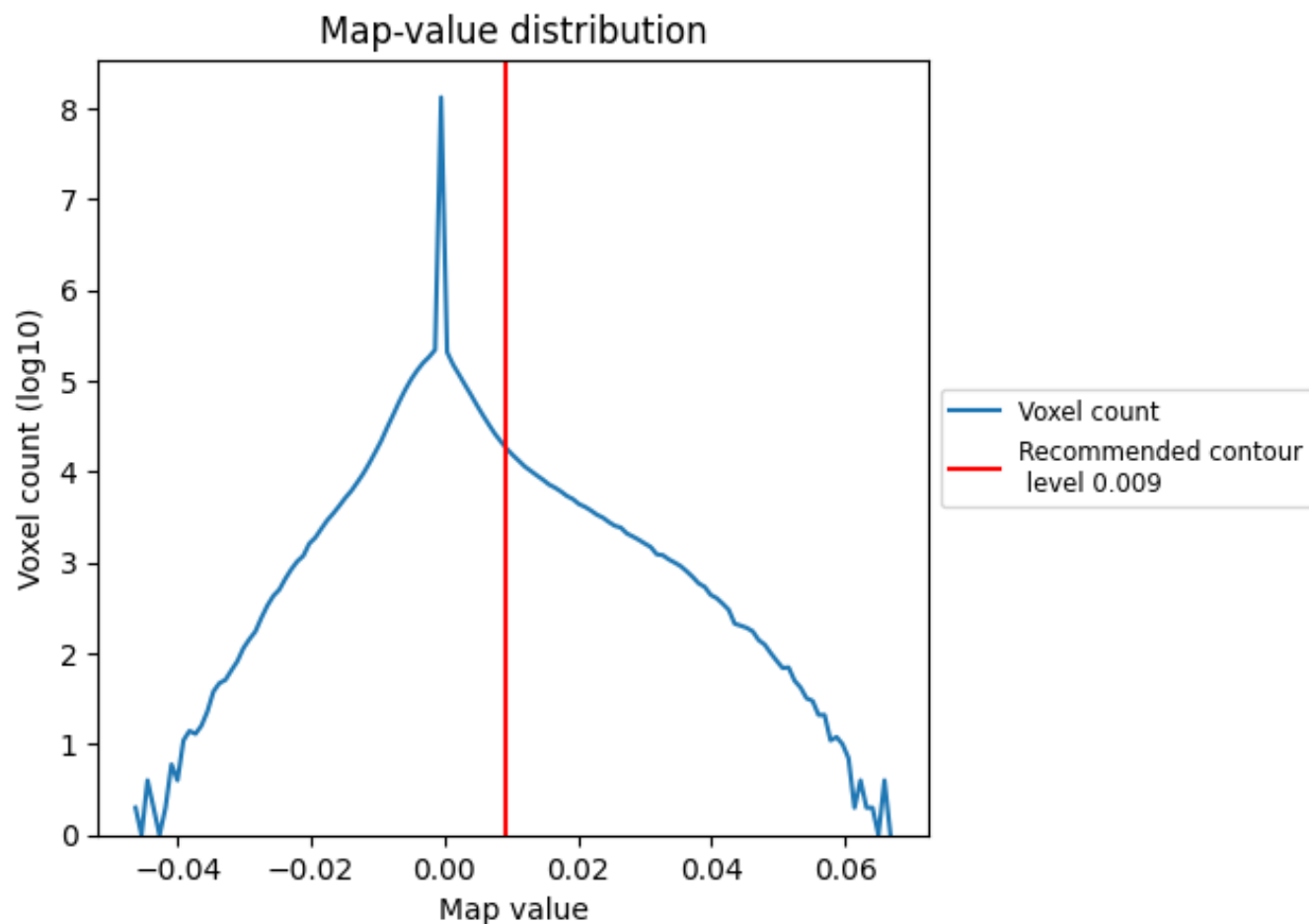
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

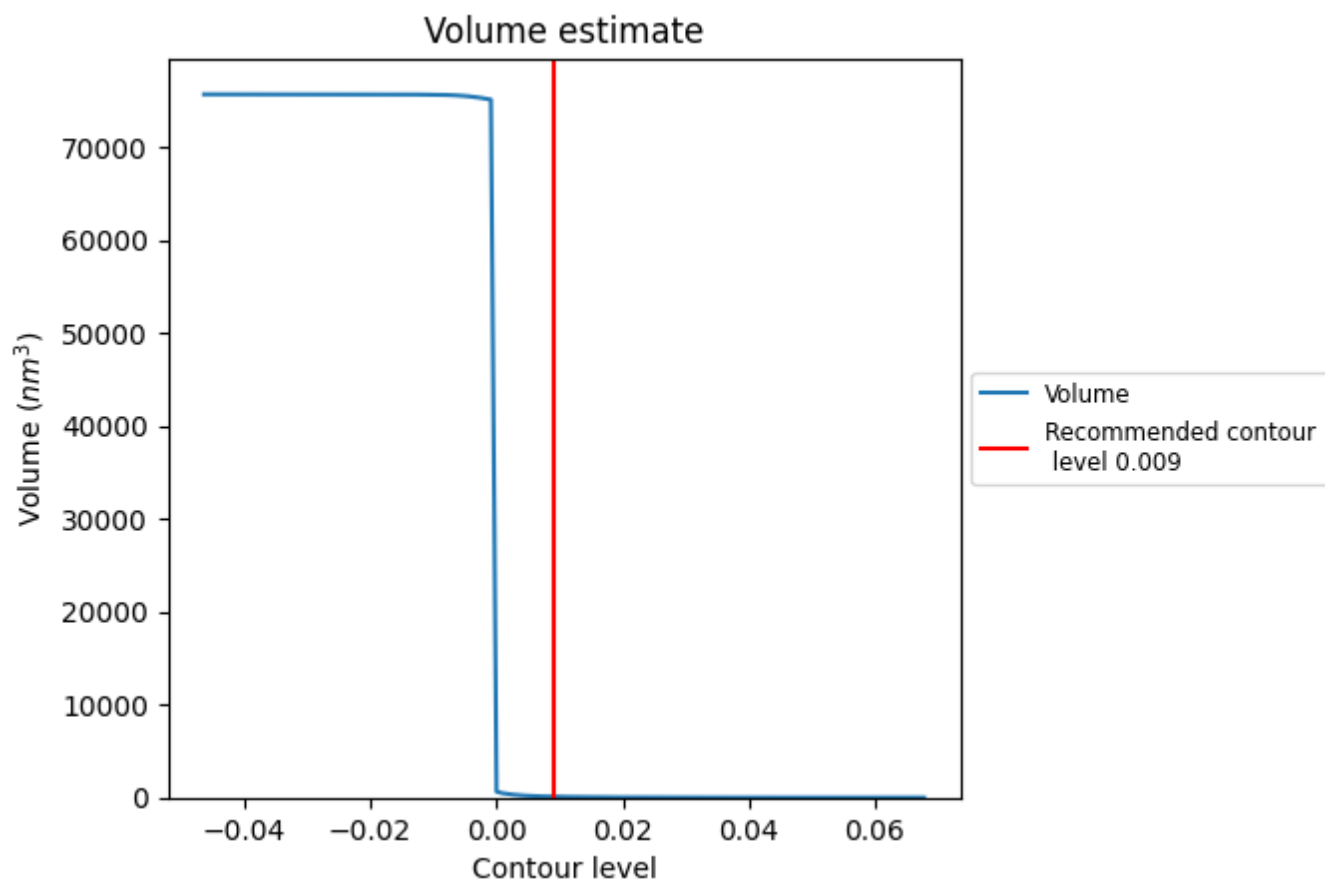
This section contains the results of statistical analysis of the map.

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.

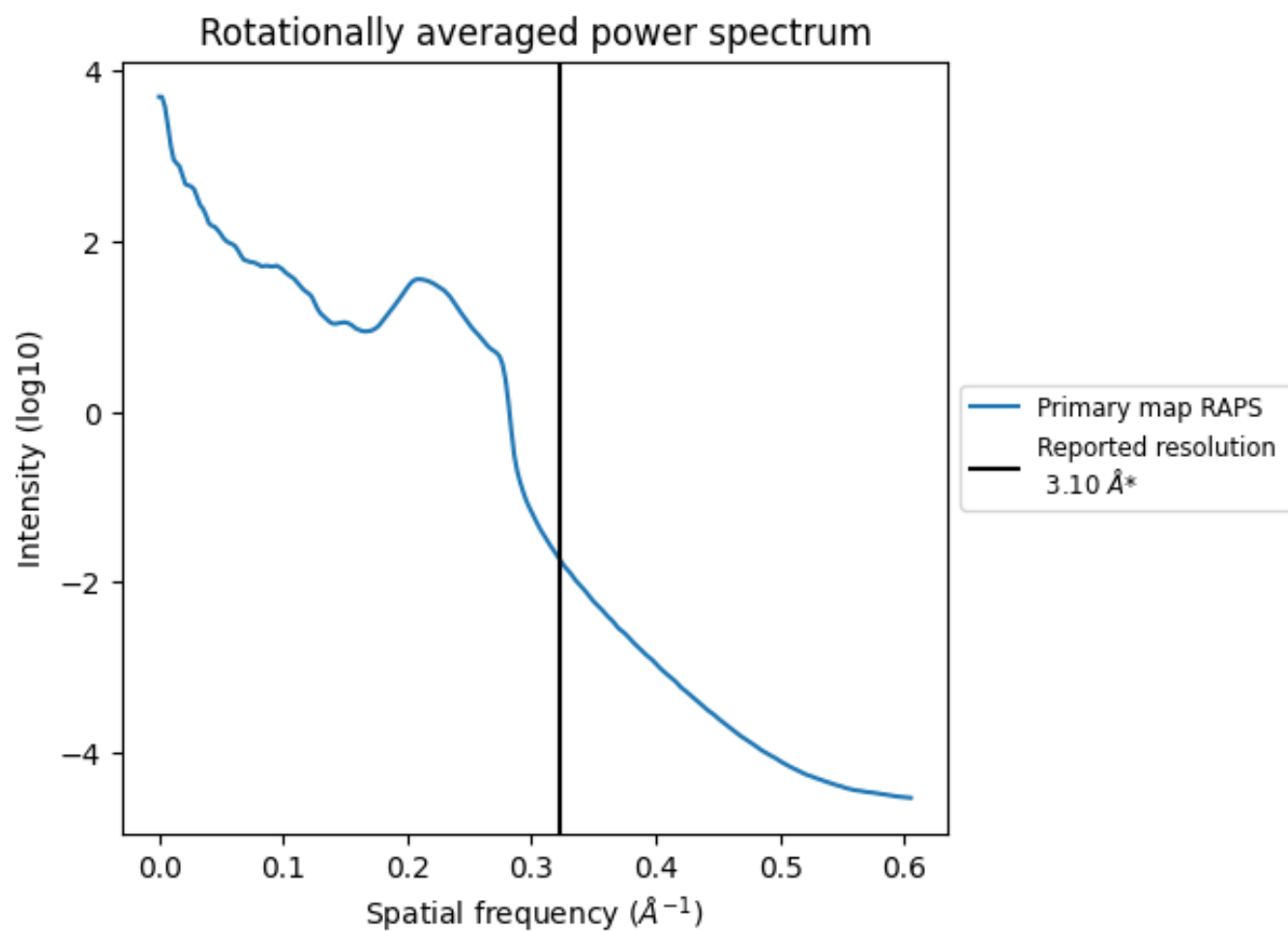
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 96 nm³; this corresponds to an approximate mass of 86 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 0.323 Å⁻¹

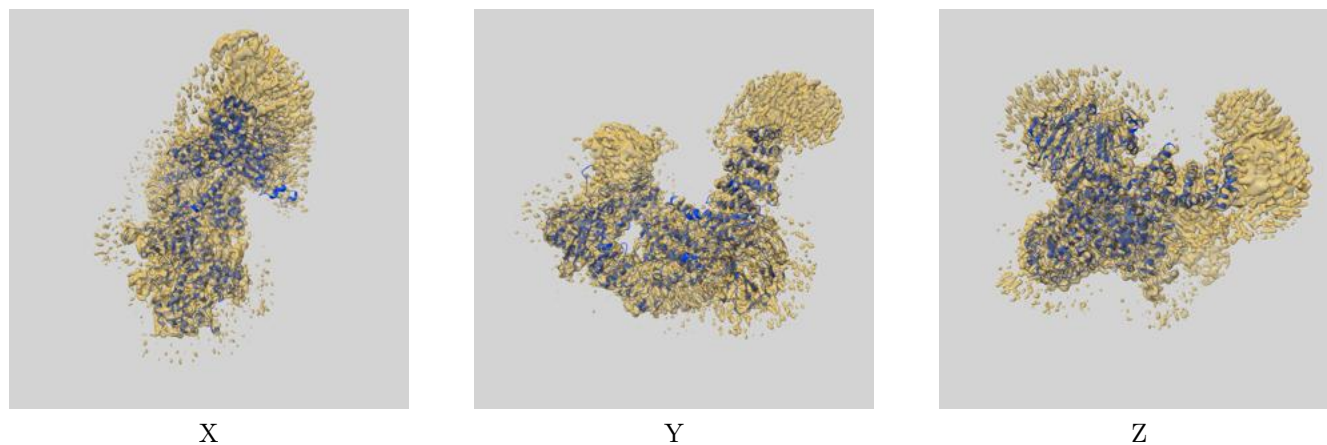
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

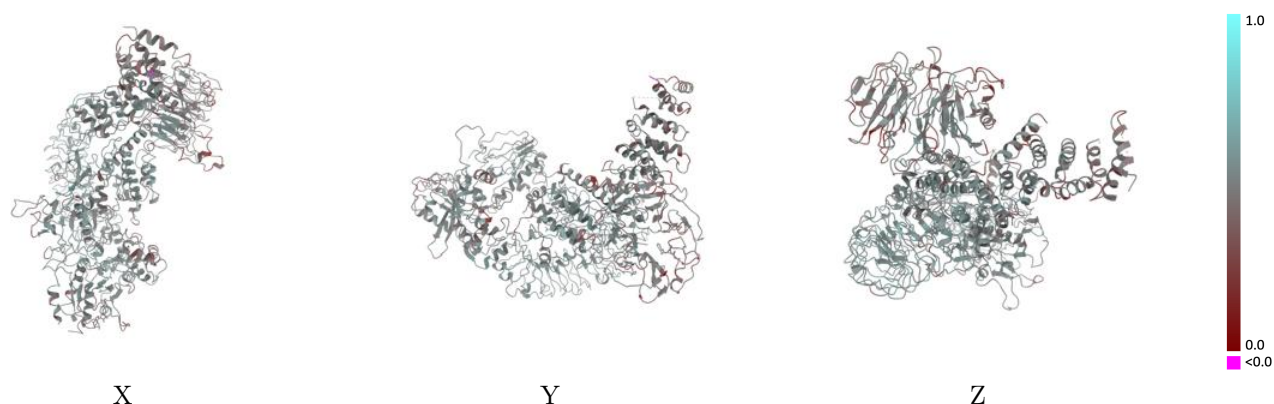
This section contains information regarding the fit between EMDB map EMD-23360 and PDB model 7LI4. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



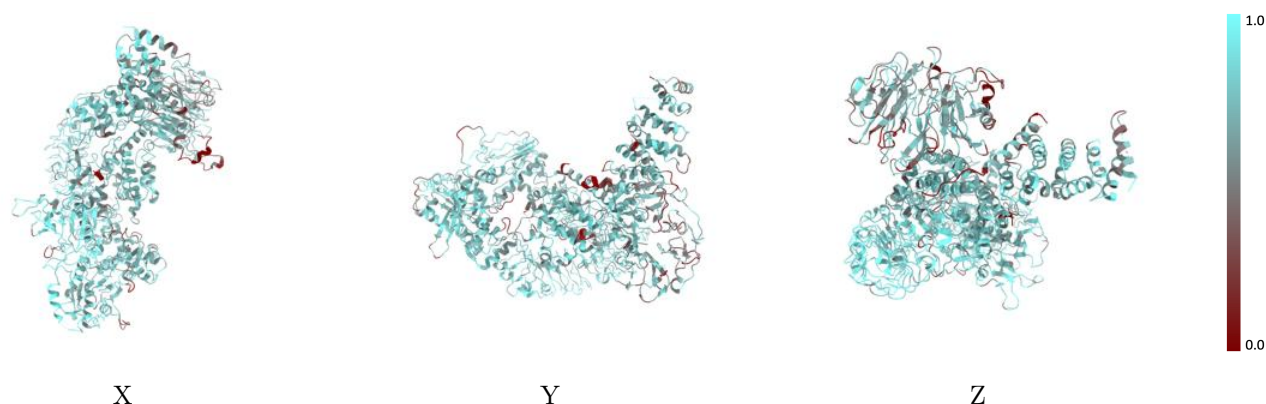
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



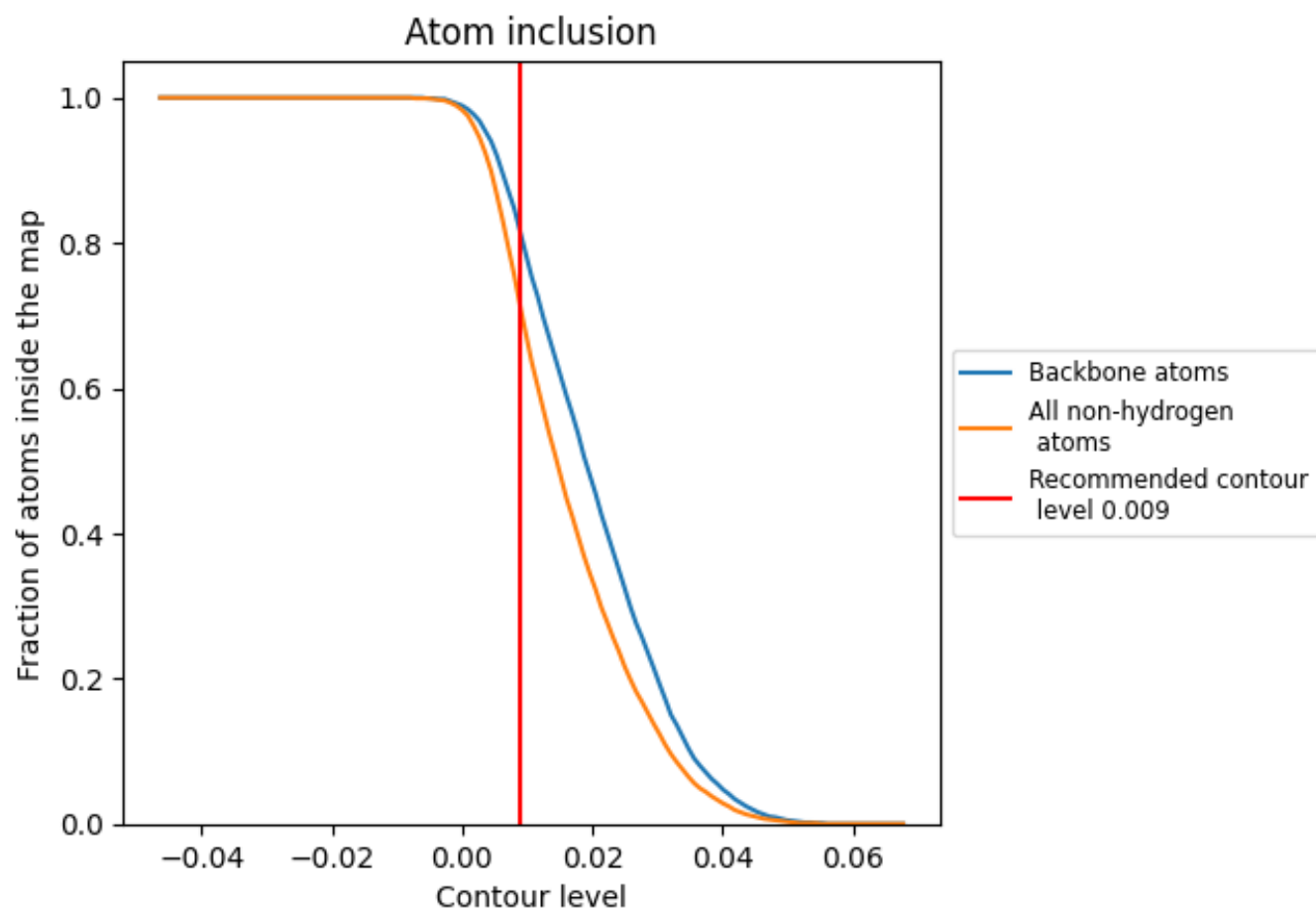
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 71% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7100	0.4910
A	0.7100	0.4910

