



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:28 AM UTC

PDB ID : 7LI3 / pdb_00007li3
EMDB ID : EMD-23359
Title : Structure of the LRRK2 G2019S mutant
Authors : Myasnikov, A.; Zhu, H.; Hixson, P.; Xie, B.; Yu, K.; Pitre, A.; Peng, J.; Sun, J.
Deposited on : 2021-01-26
Resolution : 3.80 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

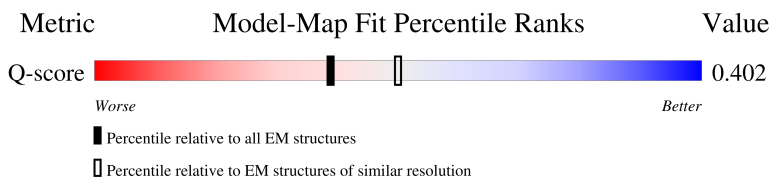
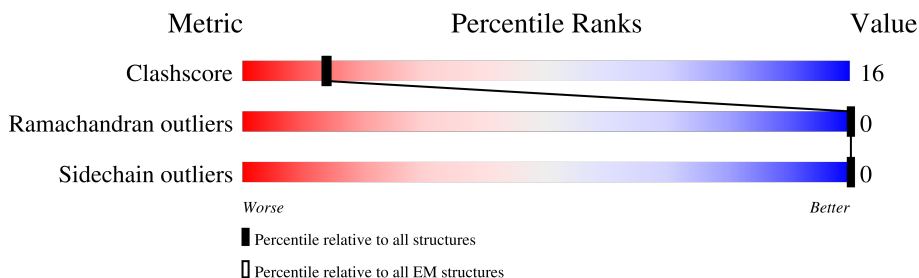
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

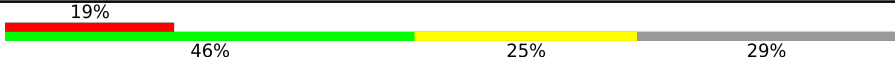
The reported resolution of this entry is 3.80 Å.

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	10198 (3.30 - 4.30)

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 14180 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.

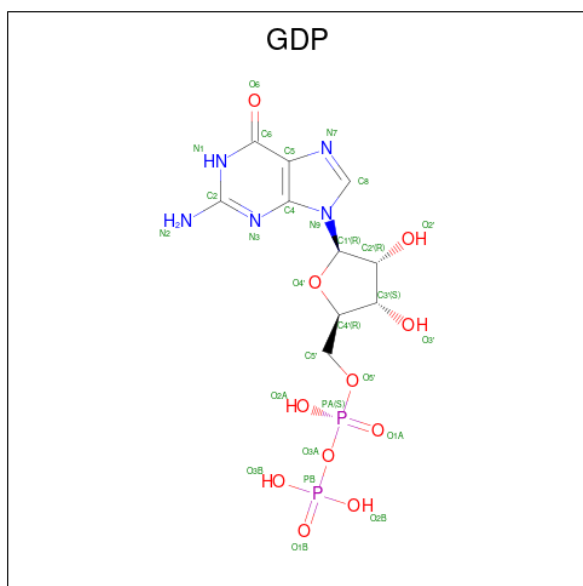
- Molecule 1 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1795	14121	9030	2435	2566	90	0	0

There are 4 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	2019	SER	GLY	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

- # ATP





D1756	D1829	Y1894	M1989	E2075	W2168	R2235	P2299	V2373	D2438	R2522
M1757	L1830	E1899	I1990	Q2076	L2169	H2236	L2300	W2376	L2439	R2523
H1758	M1831	G1900	I1991	L2077	G2172	T2237	M2301	D2377	S2440	T2524
P1759	K1832	E1901	Y1992	K2078	G2173	L2238	C2302	D2378	R2441	S2525
E1760	E1836	V1905	R1993	P2079	T2174	K2240	S2304	K2379	L2443	V2526
L1763	E1837	K1910	D1994	P2080	D2175	M2241	E2305	T2380	L2444	E2527
K1764	D1838	H1911	L1995	N2081	G2176	T2242	T2307	E2381	I2445	
T1765	L1839	T1912	P1996	E2082	Q2177	L2248	N2308	K2382	I2448	
V1767	V1841	R1915	H1997	D2084	Q2178	Y2249	S2309	L2383	Y2449	
P1768	N1842	G1918	H1998	E2085	S2180	C2250	T2310	C2384	N2450	
S1769	P1843	R1919	L2001	L2086	F2181	N2251	E2311	G2385	N2453	
G1770	D1844	Q1918	M2008	E2087	D2182	S2252	R2312	L2386	S2454	
R1771	P1845	V1922	A2016	L2088	D2183	F2253	N2313	C2389	V2455	
G1774	Q1846	V1923	D2017	I2089	T2186	S2254	W2314	V2390	R2456	
I1775	P1847	L1924	Q2022	Q2090	T2190	Q2256	M2315	H2391	Q2462	
L1776	R1847	L1924	Y2023	K2091	S2191	S2257	W2316	F2392	L2463	
L1777	L1848	C1925	R2026	P2095	E2192	K2258	N2328	R2393	G2464	
G1778	L1849	H1926	M2027	V2096	E2193	Q2259	D2329	R2394	S2465	
Q1779	I1850	L1927	GLY	K2097	W2194	K2260	F2330	E2395	L2466	
V1780	P1851	H1928	ILE	E2098	A2195	N2261	T2331	V2396	K2467	
H1781	L1852	L1932	LYS	A2102	D2196	F2262	I2332	T2397	M2468	
D1782	S1853	L1935	T2031	L2110	S2197	L2263	Q2333	V2398	V2472	
H1783	Q1854	I1940	S2032	K2116	T2199	L2264	K2334	E2400	L2473	
I1784	I1855	R1941	E2033	K2125	A2203	G2266	L2335	N2401	N2476	
L1787	I1856	R1942	G2037	Q2120	L2204	T2267	T2338	K2402	R2477	
M1788	I1857	P1943	F2038	E2121	W2205	A2268	R2339	E2403	K2478	
E1789	P1858	M1944	R2039	R2122	H2206	D2269	T2340	S2404	N2479	
E1790	L1859	L1945	P2041	R2122	L2207	G2270	S2341	K2405	T2480	
W1791	I1860	V1946	E2042	S2125	L2207	K2271	Q2342	H2406	E2481	
F1792	L1861	M1947	V2043	A2126	P2208	L2272	L2343	K2407	T2482	
L1795	A1862	E1948	V2043	Q2127	V2209	I2274	L2344	M2408	T2483	
E1797	D1863	D1956	A2044	Q2127	E2210	F2275	S2345	S2409	Q2484	
I1798	L1864	R1957	R2045	F2128	V2209	E2276	Y2346	T2410	K2485	
I1799	P1865	L1958	G2046	W2129	E2211	E2277	A2347	S2411	Q2486	
I1800	N1867	L1959	N2047	D2130	E2212	K2278	E2348	G2412	K2487	
C1801	I1868	Q1960	V2048	I2131	S2213	K2279	P2349	R2413	E2488	
G1802	M1869	N1871	L2049	L2132	W2216	V2280	S2350	L2417	I2489	
E1803	L1870	D1872	I2050	N2133	S2217	K2281	D2351	C2418	Q2490	
E1805	N1873	K1963	N2051	L2146	G2218	L2282	S2352	L2419	S2491	
T1806	E1876	A1964	Q2052	N2149	T2219	Q2283	I2353	Q2420	C2492	
Y1814	Q1879	L1965	Q2058	I2151	Q2220	G2284	I2354	K2421	I2498	
S1815	A1880	T1967	L2063	E2152	S2221	A2285	T2355	N2422	H2502	
F1816	P1881	R1968	Y2064	E2153	G2222	A2286	T2356	T2423	Q2505	
M1817	E1882	T1969	D2065	C2154	T2223	P2287	W2357	A2424	L2511	
D1818	F1883	Q1971	T2069	M2155	L2224	L2288	V2358	L2425	R2514	
G1819	L1884	D1980	G2070	T2159	T2227	K2289	V2359	W2426	I2511	
E1820	L1885	H1986	G2071	H2159	T2229	I2290	D2360	T2427	R2514	
E1821	G1886	T2072	R2072	N2160	E2230	L2291	T2361	G2431	K2519	
H1822	D1887	I2073	I2073	N2161	D2231	N2292	A2362	G2432	F2520	
Q1823	G1888	V2074	V2074	S2162	Q2232	I2293	L2363	H2433	M2521	
K1824	S1889			R2163	Q2234	G2294	T2364	I2434		
I1825	F1890			N2164		N2295	K2233	L2435		
						V2296	K2367	L2436		
						S2297	Q2368	L2437		
						T2298				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	81046	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	1.960	Depositor
Minimum map value	-0.909	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.5	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	0.19	0/14386	0.42	1/19457 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

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	644	ILE	N-CA-C	-5.16	105.80	113.39

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1419	TYR	Peptide

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	14121	0	14407	450	0
2	A	28	0	12	1	0
3	A	31	0	12	2	0
All	All	14180	0	14431	450	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 (450) 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:2462:GLN:HB2	1:A:2467:LYS:HD2	1.62	0.79
1:A:1075:VAL:HG12	1:A:1100:GLU:HG3	1.67	0.76
1:A:1403:SER:O	1:A:1707:ARG:NH1	2.19	0.76
1:A:1869:MET:HE3	1:A:1870:LEU:H	1.50	0.76
1:A:2110:LEU:HD11	1:A:2128:VAL:HG23	1.67	0.76
1:A:1526:CYS:HB3	1:A:1564:LEU:HD11	1.70	0.73
1:A:1402:TYR:HA	1:A:1405:HIS:HD2	1.54	0.73
1:A:1034:LEU:HD11	1:A:1037:LEU:HD22	1.70	0.73
1:A:558:GLY:N	1:A:596:TYR:HH	1.87	0.73
1:A:1935:LEU:HD11	1:A:1945:LEU:HD11	1.71	0.72
1:A:726:GLU:HB2	1:A:760:LEU:HD13	1.72	0.72
1:A:2265:VAL:HB	1:A:2273:ALA:HB3	1.70	0.72
1:A:1693:ARG:NH1	1:A:1829:ASP:OD2	2.23	0.71
1:A:2476:ASN:ND2	1:A:2492:CYS:SG	2.63	0.71
1:A:1341:GLY:HA3	1:A:1347:LYS:HD2	1.73	0.70
1:A:2227:ILE:HD13	1:A:2235:ARG:HB3	1.73	0.69
1:A:2287:PRO:HB2	1:A:2290:ILE:HD11	1.73	0.69
1:A:990:SER:O	1:A:1021:ASN:ND2	2.25	0.69
1:A:1968:ARG:NH2	1:A:1971:GLN:OE1	2.24	0.69
1:A:1701:PRO:HG2	1:A:1704:PHE:HB2	1.74	0.69
1:A:2413:ARG:H	1:A:2430:GLY:H	1.41	0.69
1:A:625:HIS:HB3	1:A:665:LEU:HD23	1.74	0.68
1:A:1512:LYS:HG2	1:A:1515:ASP:HA	1.75	0.68
1:A:2146:LEU:O	1:A:2490:GLN:NE2	2.27	0.68
1:A:1282:ARG:O	1:A:1305:ASN:ND2	2.27	0.68
1:A:2197:SER:HB2	1:A:2220:GLN:HG3	1.76	0.67
1:A:808:PHE:O	1:A:992:ASN:ND2	2.28	0.66
1:A:1557:VAL:HG12	1:A:1562:LEU:HD12	1.77	0.66
1:A:1832:LYS:HZ2	1:A:1859:LEU:HD12	1.61	0.65
1:A:2116:LYS:O	1:A:2122:ARG:NH2	2.26	0.65
1:A:2301:MET:HE1	1:A:2368:GLN:HE21	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1509:LEU:HA	1:A:1519:VAL:HG11	1.79	0.65
1:A:1433:PRO:O	1:A:1437:ASN:ND2	2.30	0.64
1:A:771:VAL:HG13	1:A:790:LEU:HD22	1.80	0.64
1:A:1275:VAL:O	1:A:1278:ASN:ND2	2.31	0.64
1:A:1992:TYR:OH	1:A:2016:ALA:O	2.13	0.64
1:A:1816:PHE:HA	1:A:1850:ILE:HD11	1.80	0.63
1:A:2228:ASN:HD22	1:A:2234:LYS:HD2	1.61	0.63
1:A:638:PHE:O	1:A:645:GLN:NE2	2.31	0.63
1:A:801:ASN:HB3	1:A:984:ILE:HA	1.81	0.63
1:A:2248:LEU:HD23	1:A:2263:LEU:HD21	1.80	0.63
1:A:1991:ILE:HD11	1:A:1993:ARG:HE	1.64	0.63
1:A:2043:VAL:HA	1:A:2050:TYR:HE1	1.64	0.62
1:A:1778:GLY:O	1:A:1918:ARG:NH1	2.31	0.62
1:A:558:GLY:O	1:A:561:LYS:NZ	2.33	0.62
1:A:663:SER:HA	1:A:666:LEU:HD12	1.80	0.62
1:A:1168:MET:HE3	1:A:1171:LEU:HD21	1.81	0.62
1:A:1610:ILE:HG21	1:A:1653:LEU:HD21	1.82	0.62
1:A:2177:GLY:HA3	1:A:2195:ALA:HB3	1.80	0.62
1:A:762:LEU:HD11	1:A:790:LEU:HD23	1.82	0.61
1:A:1493:GLU:OE2	1:A:1501:ARG:NH2	2.21	0.61
1:A:1420:ASP:H	1:A:1452:THR:HG22	1.65	0.61
1:A:810:ILE:H	1:A:992:ASN:HD22	1.49	0.61
1:A:1693:ARG:NH2	1:A:1858:ASP:OD1	2.33	0.61
1:A:1905:VAL:HG12	1:A:1946:VAL:HG22	1.82	0.61
1:A:1959:LEU:HD13	1:A:2070:GLY:HA3	1.83	0.61
1:A:1343:THR:H	1:A:1397:GLY:HA3	1.65	0.60
1:A:1590:LEU:HD22	1:A:1655:LYS:HG3	1.82	0.60
1:A:720:ASN:HD21	1:A:754:SER:HB3	1.65	0.60
1:A:2302:CYS:SG	1:A:2303:LEU:N	2.75	0.60
1:A:1171:LEU:HD13	1:A:1175:MET:HE3	1.82	0.60
1:A:1028:GLN:NE2	1:A:1032:GLU:OE2	2.34	0.60
1:A:1863:ASP:OD2	1:A:1918:ARG:NH2	2.35	0.60
1:A:1437:ASN:OD1	1:A:1702:MET:N	2.34	0.59
1:A:2125:SER:HA	1:A:2128:VAL:HG12	1.85	0.59
1:A:1287:GLU:O	1:A:1290:LYS:NZ	2.35	0.59
1:A:704:MET:SD	1:A:847:GLN:NE2	2.71	0.59
1:A:992:ASN:O	1:A:1021:ASN:ND2	2.36	0.59
1:A:1020:GLN:HA	1:A:1044:SER:HB2	1.85	0.59
1:A:1948:GLU:O	3:A:2602:ATP:N6	2.32	0.59
1:A:1176:THR:HG22	1:A:1177:ILE:HG13	1.85	0.58
1:A:1692:ILE:HG12	1:A:1766:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2304:SER:OG	1:A:2305:GLU:N	2.36	0.58
1:A:2151:ILE:O	1:A:2172:GLY:N	2.36	0.58
1:A:2363:LEU:HB3	1:A:2376:TRP:HB2	1.86	0.58
1:A:2232:GLY:O	1:A:2235:ARG:NH2	2.26	0.58
1:A:667:VAL:HG11	1:A:708:LEU:HD22	1.86	0.58
1:A:2417:LEU:HD12	1:A:2425:LEU:HD11	1.86	0.57
1:A:567:ILE:HA	1:A:570:ILE:HG22	1.86	0.57
1:A:1435:LEU:HD13	1:A:1474:LEU:HD11	1.85	0.57
1:A:1832:LYS:HZ1	1:A:1852:ILE:HG23	1.68	0.57
1:A:1235:LEU:HD23	1:A:1261:PRO:HD2	1.87	0.57
1:A:1940:ILE:HG22	1:A:1941:ARG:H	1.70	0.57
1:A:594:GLN:HE22	1:A:626:LEU:HD11	1.69	0.57
1:A:1316:LYS:HG3	1:A:1320:ARG:HH12	1.69	0.57
1:A:2152:VAL:HG11	1:A:2169:LEU:HD23	1.87	0.57
1:A:2521:MET:O	1:A:2524:THR:OG1	2.22	0.57
1:A:1181:SER:OG	1:A:1182:GLN:OE1	2.16	0.57
1:A:1346:GLY:H	1:A:1452:THR:HG21	1.69	0.57
1:A:1214:PRO:HA	1:A:1217:TRP:HD1	1.69	0.57
1:A:2254:SER:N	1:A:2312:ARG:HH12	2.03	0.57
1:A:1240:LYS:HD2	1:A:1243:LEU:HD11	1.87	0.56
1:A:2213:SER:O	1:A:2229:THR:OG1	2.22	0.56
1:A:1023:LEU:HB2	1:A:1045:ASN:HD22	1.70	0.56
1:A:1529:GLU:O	1:A:1533:ILE:HG12	2.05	0.56
1:A:1840:LEU:HD13	1:A:1849:THR:HG21	1.88	0.56
1:A:1956:ASP:OD1	1:A:1957:ARG:N	2.38	0.56
1:A:2133:ASN:ND2	1:A:2511:ILE:HG13	2.21	0.56
1:A:2355:ILE:N	1:A:2366:ALA:O	2.31	0.56
1:A:1993:ARG:NH2	1:A:2023:TYR:OH	2.34	0.56
1:A:1299:LEU:HD11	1:A:1318:ILE:HD11	1.88	0.56
1:A:812:LYS:NZ	1:A:814:GLU:OE2	2.39	0.56
1:A:1782:ASP:HB2	1:A:1918:ARG:HH11	1.70	0.56
1:A:2205:VAL:HG11	1:A:2263:LEU:HD12	1.88	0.56
1:A:2338:THR:HG22	1:A:2376:TRP:CE2	2.40	0.56
1:A:672:ASP:HA	1:A:675:ILE:HG22	1.88	0.56
1:A:1161:ARG:O	1:A:1163:ASN:ND2	2.38	0.56
1:A:1531:GLU:HB2	1:A:1576:LEU:HD11	1.88	0.56
1:A:1836:GLU:O	1:A:1941:ARG:NH1	2.35	0.56
1:A:2173:HIS:CD2	1:A:2174:THR:HG23	2.41	0.56
1:A:2455:VAL:HG13	1:A:2472:VAL:HG13	1.88	0.55
1:A:1333:ASN:HB3	1:A:1388:LEU:HA	1.87	0.55
1:A:1207:ASP:OD1	1:A:1207:ASP:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1684:HIS:HB3	1:A:1689:GLU:HG3	1.87	0.55
1:A:2153:GLU:HB3	1:A:2456:ARG:HH21	1.70	0.55
1:A:1227:PHE:O	1:A:1230:ASN:ND2	2.40	0.55
1:A:2390:VAL:HA	1:A:2393:LEU:HB2	1.89	0.55
1:A:628:ALA:O	1:A:632:VAL:HG22	2.06	0.55
1:A:1446:PRO:HD3	1:A:1511:PHE:CE1	2.41	0.55
1:A:1342:ASN:ND2	1:A:1427:GLU:OE2	2.40	0.55
1:A:675:ILE:HD11	1:A:699:PHE:HB2	1.89	0.54
1:A:1087:GLN:OE1	1:A:1111:GLN:NE2	2.38	0.54
1:A:1339:ILE:HD11	1:A:1351:LEU:HD13	1.89	0.54
1:A:1888:GLY:HA3	3:A:2602:ATP:H4'	1.89	0.54
1:A:2080:PRO:HA	1:A:2083:PHE:HB3	1.89	0.54
1:A:2438:ASP:HB2	1:A:2445:ILE:HD11	1.89	0.54
1:A:1980:ASP:OD2	1:A:2514:ARG:NH1	2.34	0.54
1:A:1149:LEU:HD22	1:A:1155:VAL:HG21	1.90	0.54
1:A:2159:HIS:HB2	1:A:2462:GLN:HE21	1.73	0.54
1:A:848:MET:O	1:A:852:VAL:HG22	2.08	0.54
1:A:1454:LEU:HD11	1:A:1487:PHE:HB3	1.90	0.54
1:A:1371:ILE:HD12	1:A:1393:TRP:CE3	2.43	0.54
1:A:1788:MET:HG3	1:A:1796:LEU:HD22	1.90	0.54
1:A:753:SER:HB2	1:A:757:LEU:HD23	1.88	0.54
1:A:1512:LYS:HA	1:A:1517:LEU:H	1.72	0.54
1:A:775:LEU:O	1:A:779:ILE:HG12	2.08	0.54
1:A:1411:GLN:OE1	1:A:1444:SER:OG	2.26	0.54
1:A:2468:ASN:HB3	1:A:2498:ILE:HG21	1.88	0.54
1:A:1695:TYR:HB2	1:A:1763:LEU:HB3	1.90	0.53
1:A:2236:HIS:NE2	1:A:2280:VAL:O	2.41	0.53
1:A:1923:VAL:HA	1:A:1926:HIS:HE1	1.72	0.53
1:A:2438:ASP:HB3	1:A:2442:ARG:O	2.08	0.53
1:A:1434:TRP:CZ3	1:A:1702:MET:HE1	2.42	0.53
1:A:1709:ILE:HA	1:A:1738:ILE:HD11	1.91	0.53
1:A:1378:ILE:HD13	1:A:1505:ILE:HD11	1.91	0.53
1:A:701:LYS:HA	1:A:704:MET:HG2	1.90	0.53
1:A:1371:ILE:HD12	1:A:1393:TRP:HE3	1.74	0.53
1:A:1832:LYS:HE2	1:A:1852:ILE:HG12	1.91	0.53
1:A:2039:ARG:NH1	1:A:2084:ASP:OD1	2.41	0.53
1:A:1249:LYS:HE3	1:A:1251:HIS:HE1	1.73	0.52
1:A:1779:GLN:O	1:A:1783:HIS:ND1	2.28	0.52
1:A:650:GLN:HG3	1:A:694:LEU:HD21	1.90	0.52
1:A:1648:GLN:HA	1:A:1651:LYS:HB2	1.92	0.52
1:A:2276:GLU:HB3	1:A:2279:THR:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2477:ARG:HB3	1:A:2489:ILE:HD13	1.90	0.52
1:A:698:CYS:O	1:A:702:VAL:HG23	2.09	0.52
1:A:2223:THR:HA	1:A:2240:LYS:HG3	1.92	0.52
1:A:586:MET:HA	1:A:589:VAL:HG12	1.91	0.52
1:A:2065:ASP:OD2	1:A:2072:ARG:NH2	2.34	0.52
1:A:599:ASP:O	1:A:603:GLN:HG2	2.10	0.52
1:A:738:ALA:HB3	1:A:743:SER:HA	1.90	0.52
1:A:1912:THR:O	1:A:1943:ARG:NH2	2.42	0.52
1:A:2363:LEU:O	1:A:2376:TRP:N	2.38	0.52
1:A:2051:ASN:OD1	1:A:2052:GLN:N	2.37	0.52
1:A:1149:LEU:HB3	1:A:1172:PRO:HD3	1.93	0.51
1:A:2178:GLN:NE2	1:A:2191:SER:HB2	2.25	0.51
1:A:2389:CYS:SG	1:A:2390:VAL:N	2.83	0.51
1:A:1735:ARG:HG2	1:A:1736:GLN:HG3	1.92	0.51
1:A:2267:THR:HG22	1:A:2268:ALA:H	1.74	0.51
1:A:1789:GLU:OE2	1:A:1915:ARG:NH1	2.43	0.51
1:A:2022:GLN:HE21	1:A:2026:ARG:HH11	1.58	0.51
1:A:2043:VAL:HA	1:A:2050:TYR:CE1	2.45	0.51
1:A:1195:LEU:O	1:A:1219:SER:HB3	2.11	0.51
1:A:1305:ASN:ND2	1:A:1516:GLN:HE22	2.08	0.51
1:A:1334:ARG:HG3	1:A:1389:VAL:O	2.11	0.51
1:A:1932:LEU:HD22	1:A:2017:ASP:HB3	1.92	0.51
1:A:2043:VAL:HG22	1:A:2050:TYR:CD1	2.46	0.51
1:A:2350:SER:O	1:A:2367:LYS:NZ	2.38	0.51
1:A:1023:LEU:HB2	1:A:1045:ASN:ND2	2.25	0.51
1:A:1351:LEU:HD11	1:A:1392:VAL:HG21	1.93	0.50
1:A:1788:MET:SD	1:A:1795:LEU:HD12	2.51	0.50
1:A:1601:LYS:HA	1:A:1604:CYS:SG	2.51	0.50
1:A:1734:TRP:CZ2	1:A:1737:GLY:HA3	2.46	0.50
1:A:2168:TRP:HZ2	1:A:2229:THR:HG23	1.74	0.50
1:A:1734:TRP:CD1	1:A:1736:GLN:H	2.29	0.50
1:A:1252:LEU:O	1:A:1255:ASN:ND2	2.45	0.50
1:A:1488:VAL:HG11	1:A:1500:LEU:HD22	1.92	0.50
1:A:2276:GLU:OE1	1:A:2279:THR:N	2.45	0.50
1:A:600:GLN:HG2	1:A:638:PHE:CE1	2.46	0.50
1:A:792:ARG:NH1	1:A:820:PRO:O	2.37	0.50
1:A:1185:PHE:HD2	1:A:1203:MET:HE3	1.76	0.50
1:A:1523:ILE:HD11	1:A:1528:VAL:HG23	1.94	0.50
1:A:1816:PHE:CE1	1:A:1843:PRO:HD3	2.47	0.50
1:A:2261:ASN:N	1:A:2277:ASP:OD2	2.39	0.50
1:A:2397:THR:HB	1:A:2401:ASN:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2085:GLU:O	1:A:2088:ILE:HG22	2.11	0.49
1:A:1057:MET:SD	1:A:1060:ILE:HD12	2.52	0.49
1:A:1997:PRO:HG2	1:A:2073:ILE:HD11	1.93	0.49
1:A:2519:GLU:O	1:A:2523:ARG:HG2	2.12	0.49
1:A:1337:LEU:HD12	1:A:1414:LEU:O	2.12	0.49
1:A:1347:LYS:HD3	2:A:2601:GDP:O3B	2.13	0.49
1:A:1885:LEU:HD12	1:A:1894:TYR:CZ	2.47	0.49
1:A:676:PHE:CD1	1:A:724:MET:HG2	2.48	0.49
1:A:743:SER:OG	1:A:744:LEU:N	2.46	0.49
1:A:1309:LYS:N	1:A:1313:CYS:SG	2.86	0.49
1:A:2377:ASP:HB2	1:A:2384:CYS:SG	2.52	0.49
1:A:2441:THR:O	1:A:2443:ARG:NH2	2.41	0.49
1:A:1051:PRO:HB3	1:A:1053:TYR:CE2	2.48	0.49
1:A:1183:ASN:N	1:A:1206:ASN:HD21	2.11	0.49
1:A:1214:PRO:HB3	1:A:1244:TRP:CD1	2.48	0.49
1:A:2363:LEU:N	1:A:2376:TRP:O	2.31	0.49
1:A:2379:LYS:HG3	1:A:2380:THR:H	1.78	0.49
1:A:1925:CYS:O	1:A:1928:HIS:NE2	2.44	0.49
1:A:742:SER:O	1:A:747:GLN:NE2	2.36	0.49
1:A:2155:MET:HE3	1:A:2473:LEU:HB2	1.95	0.49
1:A:2365:ILE:O	1:A:2373:VAL:HG23	2.13	0.49
1:A:1923:VAL:HA	1:A:1926:HIS:CE1	2.48	0.48
1:A:725:VAL:HG11	1:A:757:LEU:HD13	1.95	0.48
1:A:2022:GLN:HE21	1:A:2026:ARG:NH1	2.11	0.48
1:A:1217:TRP:NE1	1:A:1244:TRP:HZ2	2.11	0.48
1:A:1419:TYR:O	1:A:1427:GLU:HG2	2.14	0.48
1:A:1863:ASP:OD1	1:A:1863:ASP:N	2.44	0.48
1:A:1996:LYS:NZ	1:A:1998:HIS:HB3	2.29	0.48
1:A:672:ASP:HB2	1:A:676:PHE:CE2	2.49	0.48
1:A:2306:SER:OG	1:A:2314:VAL:O	2.29	0.48
1:A:2332:ILE:HD13	1:A:2335:LEU:HD13	1.96	0.48
1:A:2423:THR:HG21	1:A:2502:HIS:CE1	2.49	0.48
1:A:636:TYR:O	1:A:639:LYS:HG3	2.14	0.47
1:A:737:GLN:N	1:A:737:GLN:OE1	2.47	0.47
1:A:1002:GLN:HB2	1:A:1004:CYS:SG	2.54	0.47
1:A:1583:LEU:HD11	1:A:1600:PRO:HB3	1.97	0.47
1:A:2224:LEU:HB3	1:A:2238:LEU:HB2	1.94	0.47
1:A:665:LEU:O	1:A:669:HIS:ND1	2.45	0.47
1:A:2064:TYR:CD2	1:A:2095:PRO:HG3	2.48	0.47
1:A:2484:GLN:N	1:A:2484:GLN:OE1	2.48	0.47
1:A:1342:ASN:OD1	1:A:1342:ASN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2178:GLN:HE21	1:A:2191:SER:HB2	1.79	0.47
1:A:1095:LEU:HD12	1:A:1117:ASN:ND2	2.30	0.47
1:A:1554:LEU:O	1:A:1558:ARG:HG3	2.14	0.47
1:A:2254:SER:H	1:A:2312:ARG:HH12	1.63	0.47
1:A:1120:SER:HA	1:A:1140:HIS:O	2.14	0.47
1:A:1698:PRO:HA	1:A:1760:GLU:OE1	2.15	0.47
1:A:1584:HIS:CE1	1:A:1586:GLN:HG2	2.50	0.47
1:A:1316:LYS:HG3	1:A:1320:ARG:NH1	2.29	0.47
1:A:2276:GLU:CD	1:A:2278:LYS:H	2.22	0.47
1:A:1427:GLU:O	1:A:1431:MET:N	2.49	0.46
1:A:649:PHE:HA	1:A:652:ILE:HD12	1.97	0.46
1:A:1701:PRO:HB2	1:A:1792:PHE:CE2	2.50	0.46
1:A:1858:ASP:OD1	1:A:1858:ASP:N	2.48	0.46
1:A:2153:GLU:HB3	1:A:2456:ARG:NH2	2.30	0.46
1:A:573:PHE:HB2	1:A:574:PRO:HD3	1.97	0.46
1:A:2079:PHE:O	1:A:2083:PHE:N	2.47	0.46
1:A:2053:GLN:NE2	1:A:2122:ARG:O	2.48	0.46
1:A:1321:PHE:HE1	1:A:1527:TYR:HE2	1.63	0.46
1:A:1942:PRO:HD2	1:A:1944:MET:HE3	1.98	0.46
1:A:1968:ARG:HH11	1:A:2102:ALA:HB3	1.80	0.46
1:A:2255:LYS:HB3	1:A:2312:ARG:HH11	1.81	0.46
1:A:2267:THR:HG22	1:A:2268:ALA:N	2.31	0.46
1:A:1957:ARG:O	1:A:1961:GLN:HG2	2.16	0.46
1:A:2413:ARG:O	1:A:2430:GLY:N	2.49	0.46
1:A:608:SER:HB3	1:A:647:LYS:HD3	1.97	0.46
1:A:1339:ILE:HB	1:A:1394:ASP:HA	1.98	0.46
1:A:2427:ILE:HB	1:A:2435:LEU:HB2	1.97	0.46
1:A:791:LEU:HD22	1:A:805:LEU:HD21	1.97	0.46
1:A:1137:SER:HB2	1:A:1161:ARG:HB2	1.98	0.46
1:A:1180:LEU:HB3	1:A:1183:ASN:HD22	1.80	0.46
1:A:1350:LEU:HD12	1:A:1488:VAL:HG21	1.98	0.46
1:A:1545:PHE:CE2	1:A:1547:VAL:HB	2.51	0.46
1:A:1966:LEU:HD12	1:A:2069:THR:HG22	1.98	0.46
1:A:1719:MET:H	1:A:1719:MET:HE2	1.81	0.46
1:A:2437:LEU:HA	1:A:2443:ARG:O	2.15	0.46
1:A:2522:ARG:HH21	1:A:2523:ARG:HD3	1.81	0.46
1:A:703:ALA:HB1	1:A:709:LYS:HG2	1.97	0.46
1:A:1861:LEU:HD12	1:A:1864:LEU:HD12	1.97	0.46
1:A:2146:LEU:HB2	1:A:2491:SER:O	2.16	0.46
1:A:2206:HIS:HA	1:A:2213:SER:HA	1.98	0.46
1:A:2274:ILE:O	1:A:2288:LEU:N	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1832:LYS:NZ	1:A:1859:LEU:HD12	2.28	0.45
1:A:2040:ALA:HB3	1:A:2043:VAL:HG23	1.98	0.45
1:A:2203:ALA:O	1:A:2216:VAL:HG12	2.16	0.45
1:A:1684:HIS:HE1	1:A:1744:PRO:HB2	1.81	0.45
1:A:1707:ARG:HB3	1:A:1787:LEU:HD11	1.98	0.45
1:A:1935:LEU:HD11	1:A:1945:LEU:CD1	2.45	0.45
1:A:2078:LYS:HG3	1:A:2079:PHE:CD2	2.52	0.45
1:A:726:GLU:O	1:A:730:LEU:HG	2.16	0.45
1:A:1265:GLY:HA3	1:A:1290:LYS:NZ	2.31	0.45
1:A:1740:LEU:H	1:A:1740:LEU:HD23	1.81	0.45
1:A:2306:SER:HA	1:A:2359:VAL:HB	1.97	0.45
1:A:1149:LEU:HA	1:A:1149:LEU:HD23	1.82	0.45
1:A:1692:ILE:HA	1:A:1765:ILE:O	2.17	0.45
1:A:2279:THR:HA	1:A:2282:LEU:HD23	1.99	0.45
1:A:1739:TYR:HB2	1:A:1749:LEU:HD13	1.98	0.45
1:A:1841:VAL:O	1:A:1849:THR:OG1	2.22	0.45
1:A:1171:LEU:HD12	1:A:1195:LEU:HD11	1.98	0.45
1:A:1446:PRO:HB3	1:A:1483:ARG:HG3	1.99	0.45
1:A:1687:ASN:OD1	1:A:1815:SER:OG	2.24	0.45
1:A:1337:LEU:HB2	1:A:1390:LEU:HD13	1.99	0.45
1:A:1425:GLN:HG3	1:A:1469:ILE:HG21	1.99	0.45
1:A:1436:PHE:CZ	1:A:1795:LEU:HD21	2.51	0.45
1:A:2001:LEU:HD11	1:A:2016:ALA:HB2	1.99	0.45
1:A:1195:LEU:HD12	1:A:1198:LEU:HD12	1.98	0.45
1:A:1689:GLU:O	1:A:1769:SER:N	2.34	0.45
1:A:1867:ASN:OD1	1:A:1868:ILE:HG23	2.17	0.45
1:A:2390:VAL:HB	1:A:2394:ARG:HG3	1.97	0.45
1:A:641:VAL:HG13	1:A:642:ALA:H	1.81	0.45
1:A:1085:LEU:HD23	1:A:1106:VAL:HG11	1.97	0.45
1:A:1304:LEU:HB2	1:A:1308:PHE:HE2	1.82	0.44
1:A:1621:HIS:HB3	1:A:1625:ILE:HG23	1.99	0.44
1:A:1926:HIS:HA	1:A:1928:HIS:HD2	1.82	0.44
1:A:1308:PHE:HD1	1:A:1309:LYS:HG2	1.80	0.44
1:A:822:PHE:CD1	1:A:984:ILE:HD11	2.53	0.44
1:A:1371:ILE:HD13	1:A:1408:PHE:CD2	2.52	0.44
1:A:1803:GLU:HG2	1:A:1804:GLY:N	2.33	0.44
1:A:2181:PHE:HB3	1:A:2190:THR:HB	1.98	0.44
1:A:601:GLU:HG2	1:A:602:ILE:HG23	2.00	0.44
1:A:2488:GLU:N	1:A:2488:GLU:OE2	2.50	0.44
1:A:990:SER:HB3	1:A:1019:HIS:CE1	2.52	0.44
1:A:1126:LEU:HD23	1:A:1126:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1958:LEU:HD12	1:A:1962:ASP:HB2	2.00	0.44
1:A:1995:LEU:HB3	1:A:2058:SER:OG	2.18	0.44
1:A:2127:GLN:O	1:A:2131:ILE:HG12	2.17	0.44
1:A:2295:ASN:H	1:A:2298:THR:HB	1.83	0.44
1:A:2395:GLU:OE1	1:A:2395:GLU:N	2.50	0.44
1:A:1935:LEU:HA	1:A:1935:LEU:HD12	1.69	0.44
1:A:558:GLY:HA2	1:A:596:TYR:HE2	1.81	0.43
1:A:1090:LEU:HB2	1:A:1114:LEU:HD23	1.99	0.43
1:A:1434:TRP:CE3	1:A:1702:MET:HE1	2.53	0.43
1:A:1781:VAL:HA	1:A:1784:ILE:HG22	2.00	0.43
1:A:1348:THR:HG22	1:A:1394:ASP:OD2	2.17	0.43
1:A:1369:VAL:O	1:A:1605:LYS:NZ	2.51	0.43
1:A:1376:TRP:HE1	1:A:1392:VAL:HG13	1.83	0.43
1:A:2205:VAL:HG12	1:A:2250:CYS:SG	2.58	0.43
1:A:2252:SER:O	1:A:2252:SER:OG	2.34	0.43
1:A:2502:HIS:HA	1:A:2505:GLN:HE21	1.83	0.43
1:A:1709:ILE:O	1:A:1713:LEU:HB2	2.19	0.43
1:A:764:SER:OG	1:A:765:GLY:N	2.51	0.43
1:A:1321:PHE:CE2	1:A:1325:ARG:HD2	2.54	0.43
1:A:1371:ILE:HG12	1:A:1604:CYS:HB2	1.99	0.43
1:A:1483:ARG:NE	1:A:1507:GLU:OE2	2.33	0.43
1:A:2254:SER:HB2	1:A:2258:LYS:O	2.19	0.43
1:A:653:LEU:HD23	1:A:653:LEU:HA	1.80	0.43
1:A:684:MET:SD	1:A:684:MET:N	2.90	0.43
1:A:699:PHE:HZ	1:A:728:LEU:HD21	1.84	0.43
1:A:1449:LEU:O	1:A:1485:TYR:HA	2.18	0.43
1:A:745:ILE:HD12	1:A:745:ILE:H	1.84	0.43
1:A:1466:MET:O	1:A:1469:ILE:HG22	2.19	0.43
1:A:2442:ARG:HA	1:A:2442:ARG:HD2	1.86	0.43
1:A:794:LEU:HA	1:A:794:LEU:HD23	1.79	0.43
1:A:1047:PHE:HB2	1:A:1068:ASN:HB3	2.00	0.43
1:A:1109:LEU:HD21	1:A:1112:LEU:HB2	2.01	0.43
1:A:1183:ASN:H	1:A:1206:ASN:HD21	1.66	0.43
1:A:1832:LYS:NZ	1:A:1852:ILE:HG23	2.33	0.43
1:A:1865:PRO:O	1:A:1868:ILE:HG12	2.19	0.43
1:A:1076:LEU:HD23	1:A:1076:LEU:HA	1.87	0.43
1:A:1225:LEU:HB3	1:A:1227:PHE:HE2	1.84	0.43
1:A:1341:GLY:O	1:A:1434:TRP:NE1	2.52	0.43
1:A:1353:GLN:HB3	1:A:1497:LEU:HD21	2.01	0.43
1:A:1470:THR:O	1:A:1474:LEU:HB3	2.18	0.43
1:A:1742:TRP:CZ3	1:A:1776:LEU:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1427:GLU:HA	1:A:1430:ALA:HB3	2.00	0.43
1:A:2216:VAL:HG11	1:A:2248:LEU:HD22	2.00	0.43
1:A:652:ILE:O	1:A:656:LEU:HG	2.19	0.42
1:A:992:ASN:O	1:A:994:LEU:N	2.51	0.42
1:A:1054:LEU:O	1:A:1057:MET:HG3	2.19	0.42
1:A:1066:SER:HB2	1:A:1091:SER:OG	2.19	0.42
1:A:1337:LEU:HB3	1:A:1392:VAL:HG12	2.01	0.42
1:A:1552:ARG:O	1:A:1556:LEU:HG	2.18	0.42
1:A:2219:THR:HG22	1:A:2223:THR:O	2.19	0.42
1:A:822:PHE:HE2	1:A:1006:ILE:HB	1.85	0.42
1:A:1657:GLN:HB3	1:A:1710:ASN:CG	2.44	0.42
1:A:1840:LEU:HD23	1:A:1851:PRO:HA	2.00	0.42
1:A:2453:ASN:HD22	1:A:2477:ARG:H	1.66	0.42
1:A:1832:LYS:NZ	1:A:1856:ALA:HB3	2.33	0.42
1:A:2302:CYS:SG	1:A:2356:THR:HA	2.60	0.42
1:A:728:LEU:HD23	1:A:728:LEU:HA	1.78	0.42
1:A:1431:MET:HE3	1:A:1431:MET:HB3	1.87	0.42
1:A:1711:ARG:NH1	1:A:1790:GLU:OE1	2.51	0.42
1:A:722:SER:HA	1:A:725:VAL:HG12	2.01	0.42
1:A:1355:MET:HG2	1:A:1376:TRP:CD2	2.54	0.42
1:A:606:GLY:O	1:A:610:ILE:HG12	2.19	0.42
1:A:1013:LEU:HD12	1:A:1013:LEU:HA	1.79	0.42
1:A:1359:LYS:HG3	1:A:1360:SER:N	2.35	0.42
1:A:1739:TYR:HA	1:A:1748:CYS:O	2.20	0.42
1:A:723:ILE:HD12	1:A:836:ALA:HB2	2.01	0.42
1:A:1045:ASN:O	1:A:1068:ASN:ND2	2.50	0.42
1:A:1138:LYS:HA	1:A:1162:MET:HB2	2.02	0.42
1:A:1180:LEU:HB3	1:A:1183:ASN:ND2	2.35	0.42
1:A:1250:LEU:HG	1:A:1252:LEU:HD23	2.01	0.42
1:A:1940:ILE:HG22	1:A:1941:ARG:N	2.33	0.42
1:A:1986:HIS:ND1	1:A:2052:GLN:HB2	2.35	0.42
1:A:2151:ILE:HB	1:A:2173:HIS:N	2.34	0.42
1:A:2293:ILE:HD12	1:A:2332:ILE:HD11	2.02	0.42
1:A:1010:LEU:HD22	1:A:1013:LEU:HD22	2.02	0.41
1:A:1441:ARG:NH2	1:A:1791:TRP:O	2.53	0.41
1:A:1474:LEU:HD12	1:A:1479:PHE:CD2	2.55	0.41
1:A:1573:VAL:HG23	1:A:1582:LEU:HD11	2.00	0.41
1:A:815:PRO:HG3	1:A:1004:CYS:SG	2.60	0.41
1:A:1065:VAL:HG23	1:A:1090:LEU:HD23	2.02	0.41
1:A:2301:MET:HE1	1:A:2368:GLN:NE2	2.33	0.41
1:A:769:GLN:CD	1:A:769:GLN:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1474:LEU:HD12	1:A:1479:PHE:HD2	1.85	0.41
1:A:1565:ASP:OD1	1:A:1565:ASP:N	2.45	0.41
1:A:2110:LEU:HD13	1:A:2131:ILE:HD11	2.02	0.41
1:A:1339:ILE:HG12	1:A:1416:LEU:HD12	2.02	0.41
1:A:1691:ILE:HG13	1:A:1769:SER:HB3	2.02	0.41
1:A:1747:TYR:CE1	1:A:1768:PRO:HD3	2.55	0.41
1:A:1238:SER:HA	1:A:1263:GLU:HG2	2.01	0.41
1:A:1372:ASP:HB2	1:A:1605:LYS:NZ	2.34	0.41
1:A:2228:ASN:OD1	1:A:2229:THR:N	2.49	0.41
1:A:1045:ASN:HB2	1:A:1068:ASN:HD21	1.85	0.41
1:A:1512:LYS:HG3	1:A:1517:LEU:H	1.85	0.41
1:A:1569:LEU:N	1:A:1570:PRO:HD2	2.35	0.41
1:A:2289:LYS:HG2	1:A:2291:LEU:HD11	2.03	0.41
1:A:1419:TYR:HD2	1:A:1421:LEU:HD13	1.86	0.41
1:A:1440:ALA:HB1	1:A:1792:PHE:HB3	2.02	0.41
1:A:1687:ASN:HB3	1:A:1819:GLY:HA2	2.03	0.41
1:A:1712:LEU:HD22	1:A:1780:VAL:HG22	2.03	0.41
1:A:2064:TYR:CE2	1:A:2095:PRO:HG3	2.55	0.41
1:A:561:LYS:O	1:A:565:LYS:HG3	2.20	0.41
1:A:665:LEU:HA	1:A:668:HIS:HB3	2.02	0.41
1:A:997:ILE:HB	1:A:1023:LEU:HD21	2.03	0.41
1:A:1044:SER:H	1:A:1067:ARG:HB2	1.84	0.41
1:A:1263:GLU:OE2	1:A:1263:GLU:N	2.51	0.41
1:A:1338:MET:HE1	1:A:1410:THR:H	1.85	0.41
1:A:1355:MET:HG2	1:A:1376:TRP:CG	2.55	0.41
1:A:1511:PHE:HD2	1:A:1518:VAL:HG11	1.86	0.41
1:A:1652:LEU:HA	1:A:1655:LYS:HB2	2.03	0.41
1:A:2168:TRP:H	1:A:2168:TRP:CD1	2.39	0.41
1:A:2168:TRP:HB3	1:A:2179:LEU:HD21	2.03	0.41
1:A:2363:LEU:HD12	1:A:2363:LEU:HA	1.87	0.41
1:A:2378:LYS:H	1:A:2378:LYS:HG2	1.61	0.41
1:A:2434:ILE:CG2	1:A:2448:ILE:HB	2.51	0.41
1:A:1136:LEU:O	1:A:1139:ASN:ND2	2.54	0.41
1:A:1230:ASN:HD22	1:A:1232:ILE:HD11	1.85	0.41
1:A:1376:TRP:CH2	1:A:1378:ILE:HD11	2.56	0.41
1:A:790:LEU:HD23	1:A:790:LEU:HA	1.90	0.40
1:A:1399:GLU:HA	1:A:1402:TYR:CE1	2.56	0.40
1:A:1695:TYR:OH	1:A:1781:VAL:HG23	2.22	0.40
1:A:1919:GLN:O	1:A:1922:VAL:HG12	2.20	0.40
1:A:1144:LEU:HB2	1:A:1169:PRO:HG3	2.03	0.40
1:A:1208:ILE:HD12	1:A:1230:ASN:ND2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1523:ILE:HD12	1:A:1527:TYR:HB2	2.03	0.40
1:A:2307:THR:HG23	1:A:2308:ASN:OD1	2.21	0.40
1:A:604:CYS:HB2	1:A:647:LYS:HD2	2.03	0.40
1:A:1814:TYR:O	1:A:1825:ILE:N	2.48	0.40
1:A:1967:THR:C	1:A:1969:THR:H	2.29	0.40
1:A:2063:LEU:HD23	1:A:2063:LEU:HA	1.89	0.40
1:A:2433:HIS:CD2	1:A:2449:TYR:HB3	2.56	0.40
1:A:1774:CYS:O	1:A:1775:ILE:C	2.64	0.40
1:A:2037:GLY:HA3	1:A:2083:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1777/2527 (70%)	1563 (88%)	214 (12%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1577/2282 (69%)	1577 (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 (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	594	GLN
1	A	689	GLN
1	A	693	ASN
1	A	720	ASN
1	A	785	GLN
1	A	992	ASN
1	A	1019	HIS
1	A	1021	ASN
1	A	1028	GLN
1	A	1062	ASN
1	A	1068	ASN
1	A	1163	ASN
1	A	1206	ASN
1	A	1216	HIS
1	A	1230	ASN
1	A	1251	HIS
1	A	1254	HIS
1	A	1305	ASN
1	A	1323	GLN
1	A	1405	HIS
1	A	1411	GLN
1	A	1475	ASN
1	A	1486	HIS
1	A	1516	GLN
1	A	1521	GLN
1	A	1571	HIS
1	A	1586	GLN
1	A	1621	HIS
1	A	1684	HIS
1	A	1758	HIS
1	A	1919	GLN
1	A	1926	HIS
1	A	1972	HIS
1	A	2022	GLN
1	A	2081	ASN
1	A	2127	GLN
1	A	2133	ASN
1	A	2149	ASN
1	A	2173	HIS

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Mol	Chain	Res	Type
1	A	2178	GLN
1	A	2368	GLN
1	A	2401	ASN
1	A	2433	HIS
1	A	2462	GLN
1	A	2468	ASN
1	A	2476	ASN
1	A	2502	HIS
1	A	2505	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1.34	5 (15%)	48,52,52	1.72	10 (20%)
2	GDP	A	2601	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	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	-	-	0/22/38/38	0/3/3/3
2	GDP	A	2601	-	-	6/16/32/32	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	4.36	1.46	1.39
2	A	2601	GDP	C5-C4	3.05	1.47	1.38
2	A	2601	GDP	C6-N1	-2.60	1.34	1.38
3	A	2602	ATP	C5-C6	2.56	1.48	1.41
3	A	2602	ATP	C5-N7	-2.38	1.34	1.39
3	A	2602	ATP	C8-N7	2.24	1.36	1.31
3	A	2602	ATP	C4-N9	-2.20	1.33	1.37
2	A	2601	GDP	C5-N7	-2.15	1.34	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2601	GDP	C5-C4-N3	-6.25	118.45	128.39
3	A	2602	ATP	C5-C4-N3	-5.41	119.26	126.72
2	A	2601	GDP	C2-N3-C4	5.09	121.07	112.30
2	A	2601	GDP	N9-C4-N3	4.55	135.05	125.95
3	A	2602	ATP	N3-C4-N9	4.33	134.54	127.17
3	A	2602	ATP	C2-N3-C4	3.53	120.46	111.83
3	A	2602	ATP	C4-C5-N7	-3.33	106.77	110.58
2	A	2601	GDP	C6-C5-N7	3.26	136.22	130.29
3	A	2602	ATP	N3-C2-N1	-3.19	123.76	128.58
3	A	2602	ATP	C4-N9-C8	2.95	108.84	105.74
2	A	2601	GDP	C4-C5-N7	-2.55	106.62	110.67
3	A	2602	ATP	C5-N7-C8	2.43	107.27	103.45
2	A	2601	GDP	C3'-C2'-C1'	2.14	105.50	101.46
3	A	2602	ATP	N9-C8-N7	-2.13	110.92	113.94
2	A	2601	GDP	O6-C6-C5	-2.10	120.98	126.53
3	A	2602	ATP	C6-C5-N7	2.07	136.08	132.09
2	A	2601	GDP	C5-C6-N1	2.02	118.39	113.25
3	A	2602	ATP	C3'-C2'-C1'	2.01	105.27	101.46

There are no chirality outliers.

All (6) torsion outliers are listed below:

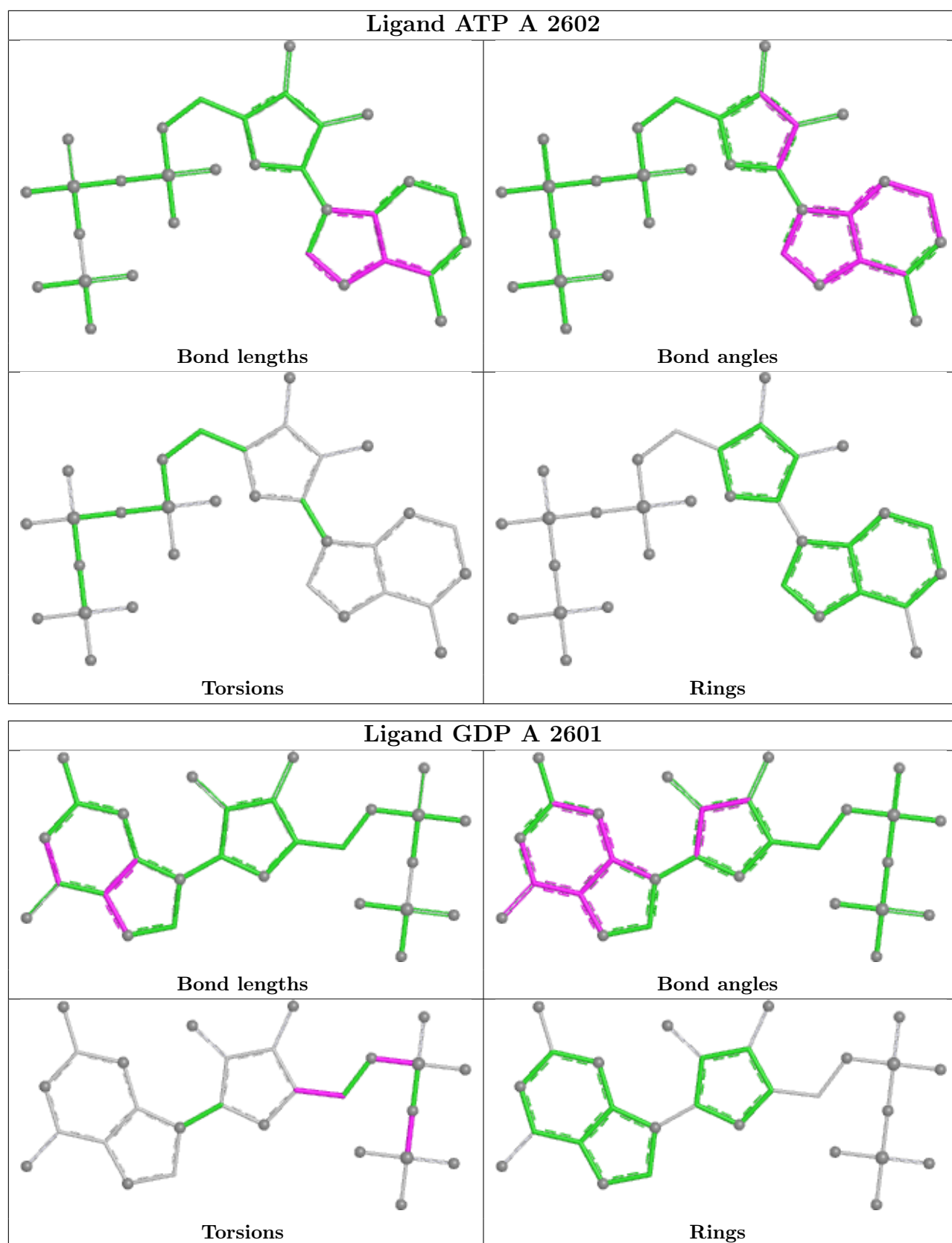
Mol	Chain	Res	Type	Atoms
2	A	2601	GDP	PA-O3A-PB-O2B
2	A	2601	GDP	PA-O3A-PB-O3B
2	A	2601	GDP	C5'-O5'-PA-O3A
2	A	2601	GDP	C5'-O5'-PA-O1A
2	A	2601	GDP	O4'-C4'-C5'-O5'
2	A	2601	GDP	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2602	ATP	2	0
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-23359. These allow visual inspection of the internal detail of the map and identification of artifacts.

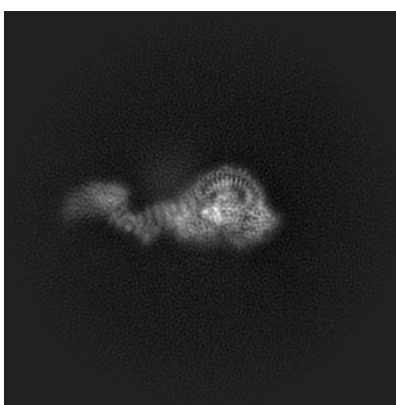
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

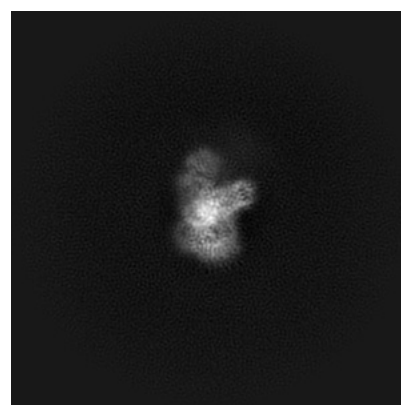
6.1.1 Primary map



X



Y



Z

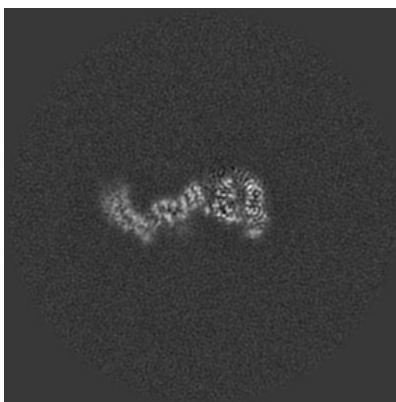
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

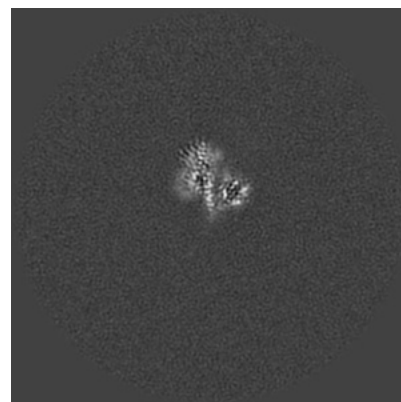
6.2.1 Primary map



X Index: 256



Y Index: 256

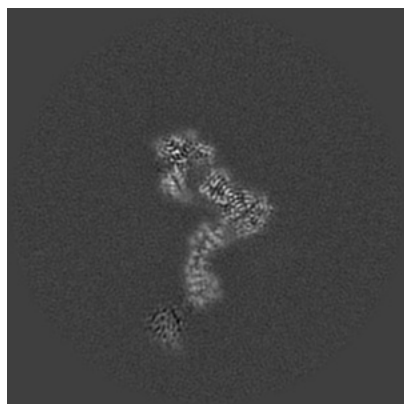


Z Index: 256

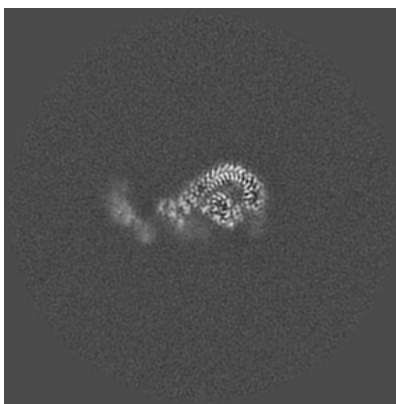
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

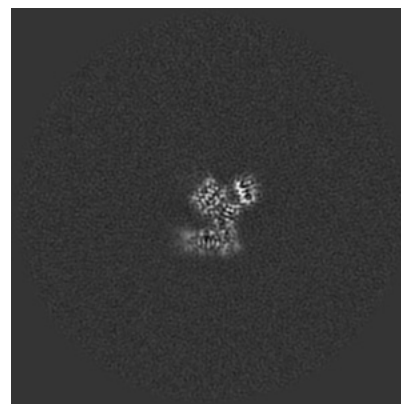
6.3.1 Primary map



X Index: 246



Y Index: 266

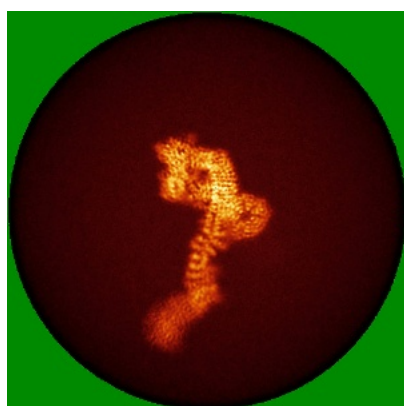


Z Index: 285

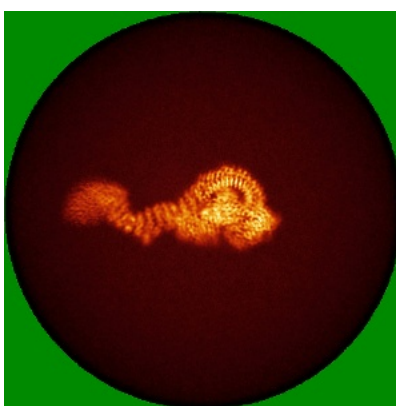
The images above show the largest variance slices of the map in three orthogonal directions.

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

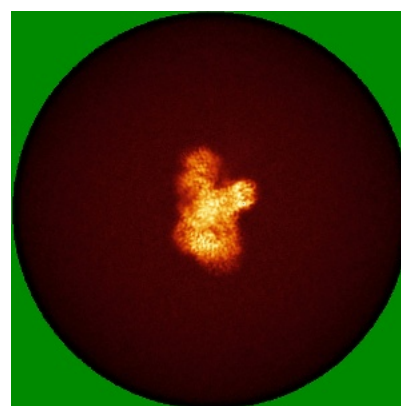
6.4.1 Primary map



X



Y

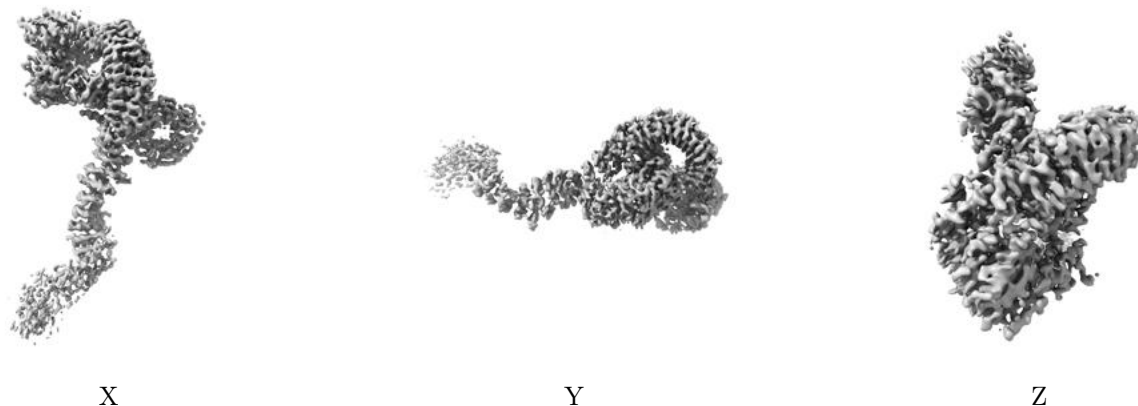


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

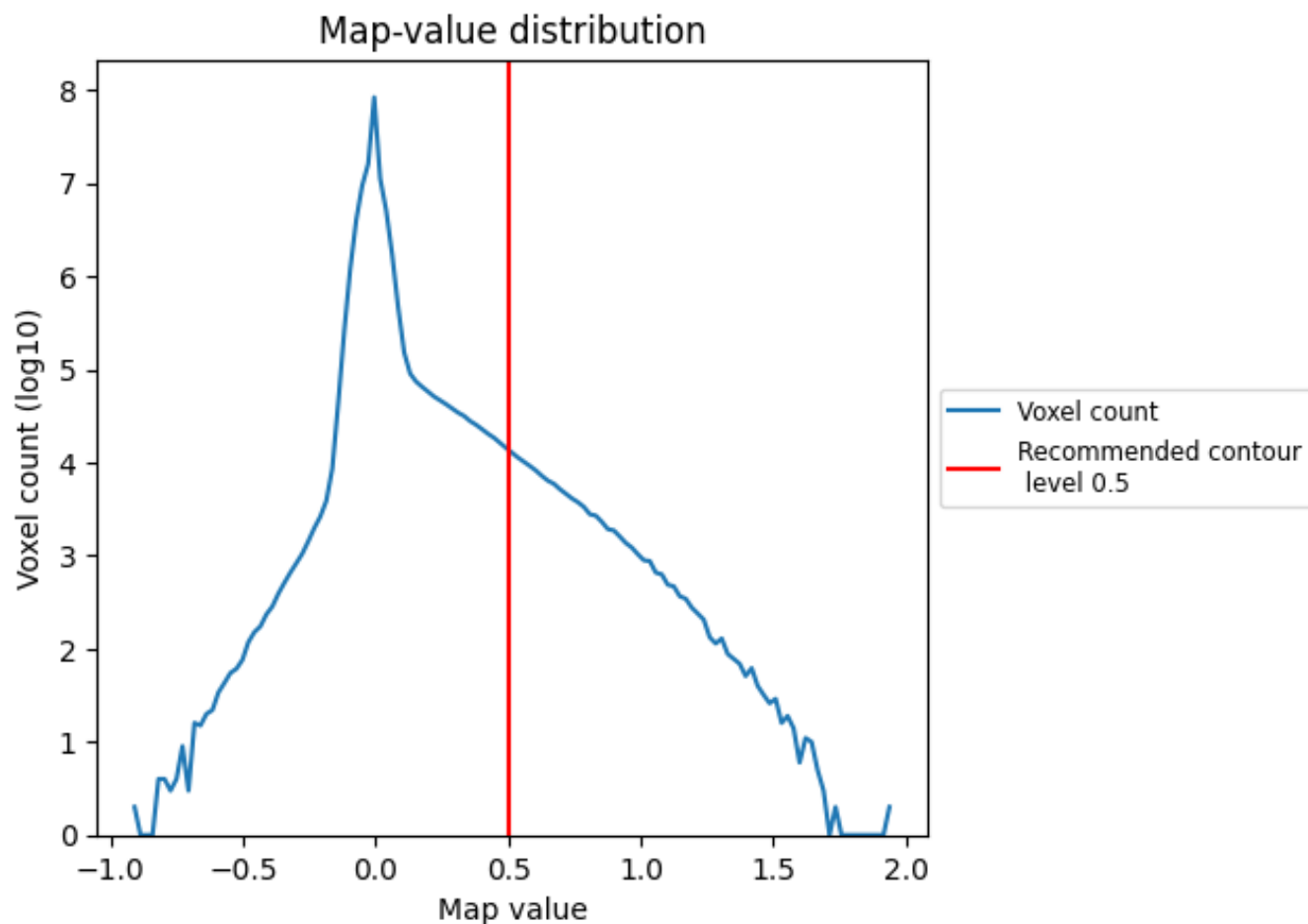
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

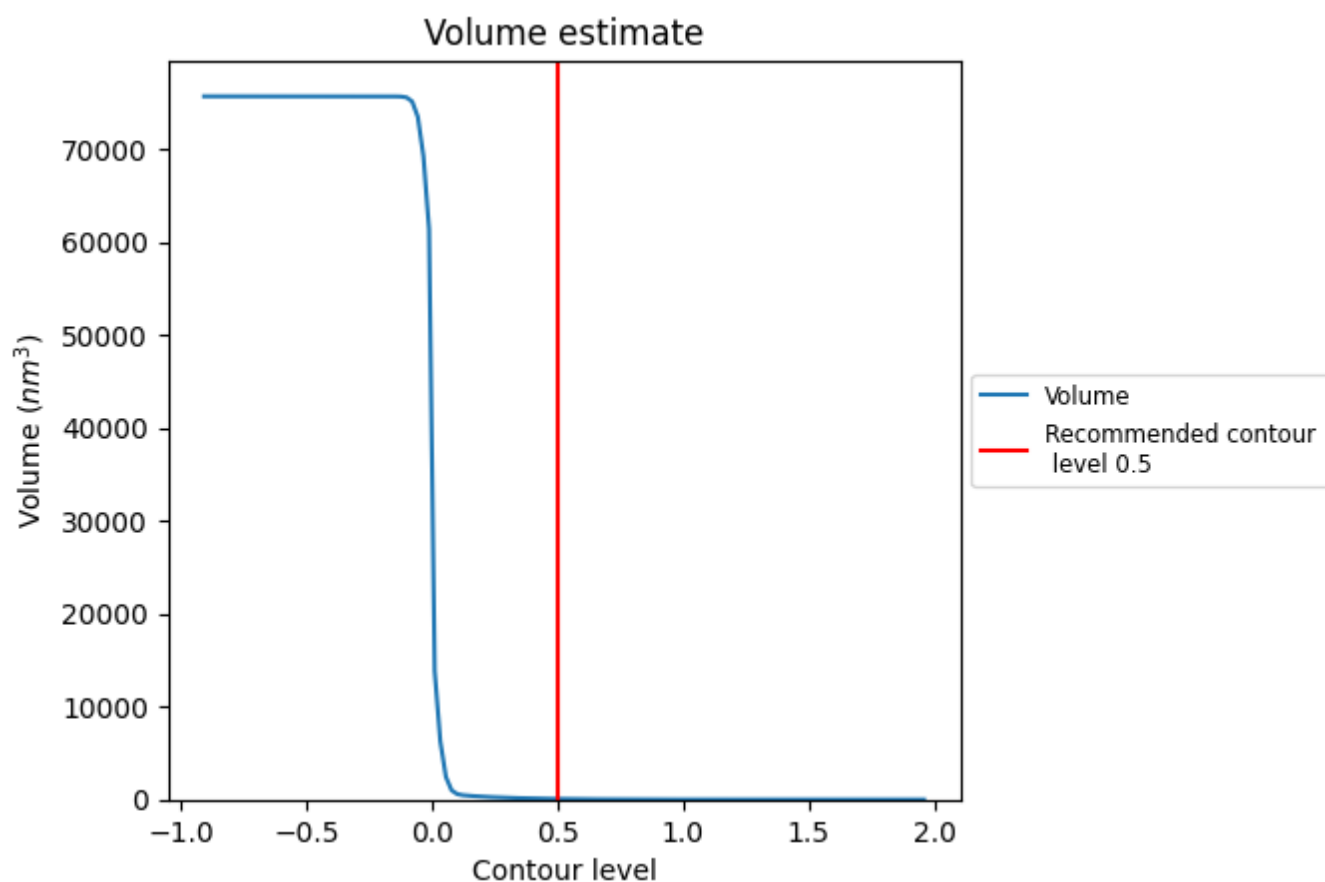
This section contains the results of statistical analysis of the map.

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.

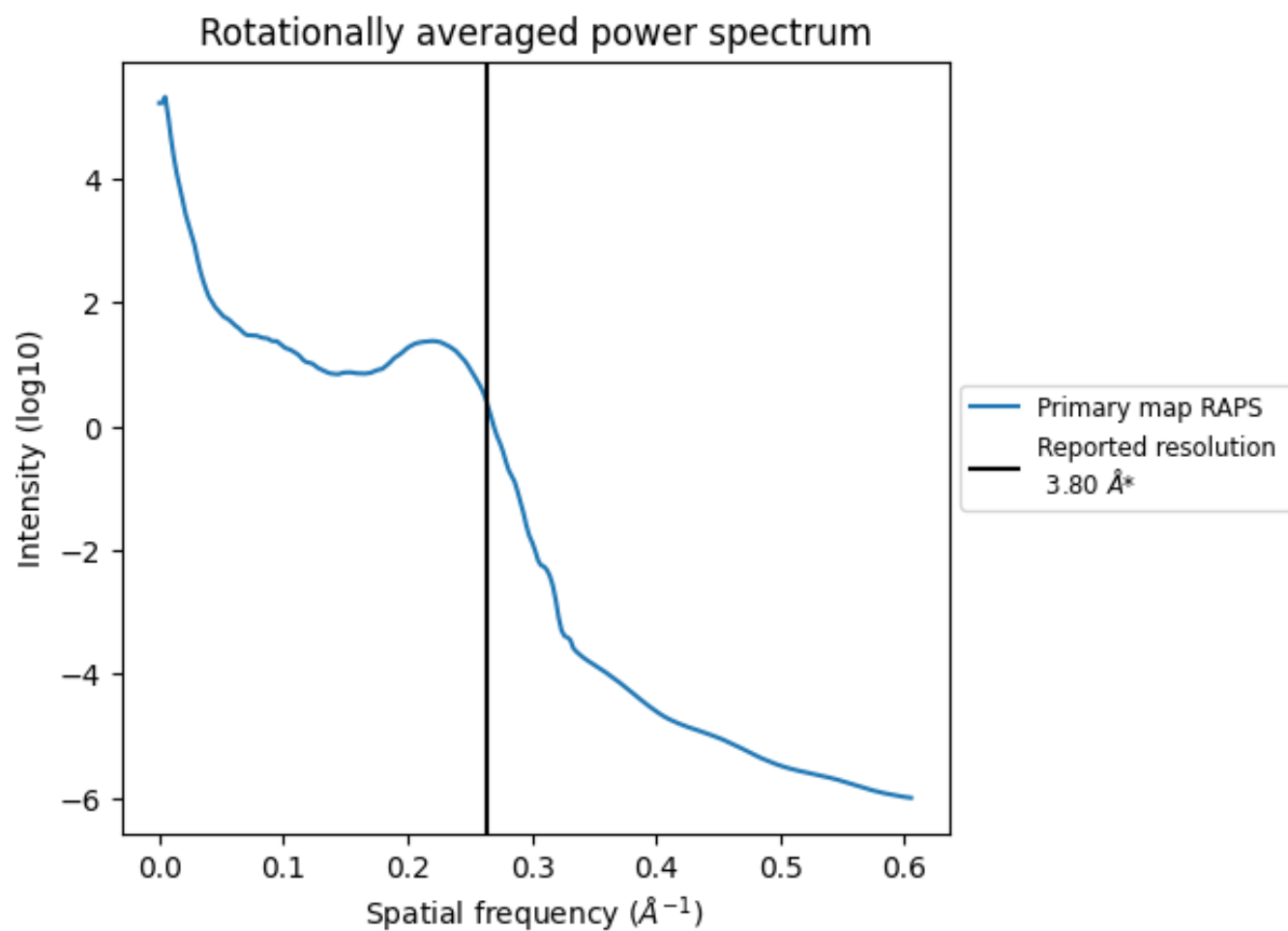
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm³; this corresponds to an approximate mass of 63 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 0.263 Å⁻¹

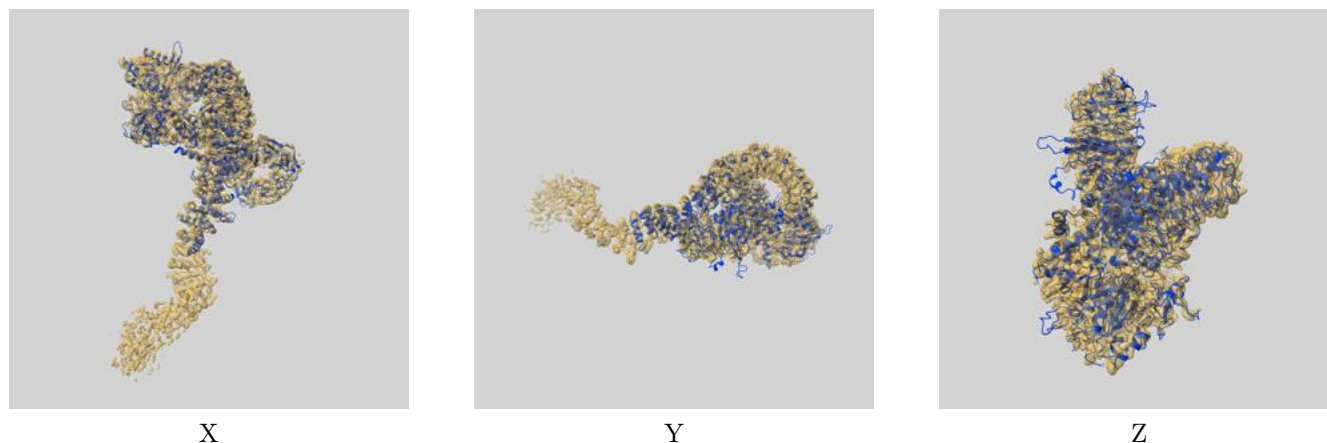
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

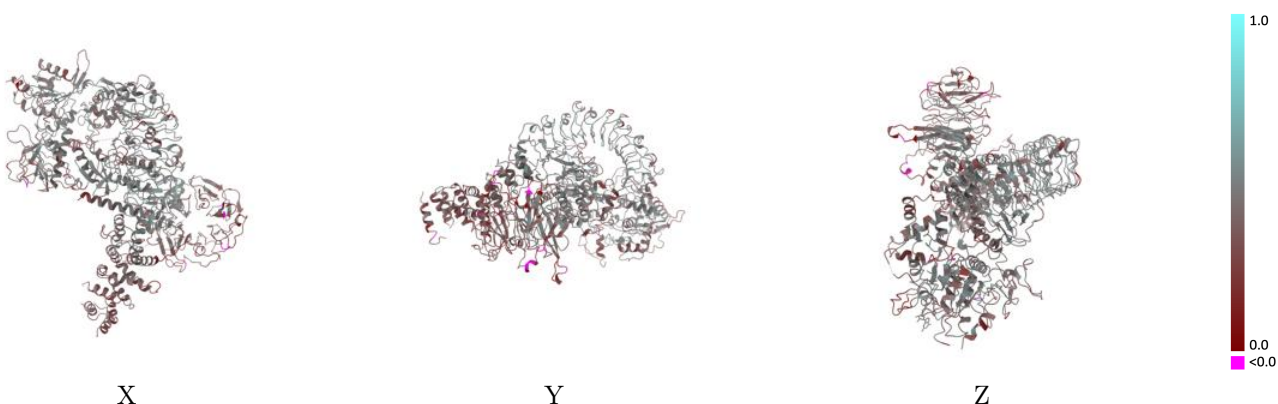
This section contains information regarding the fit between EMDB map EMD-23359 and PDB model 7LI3. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



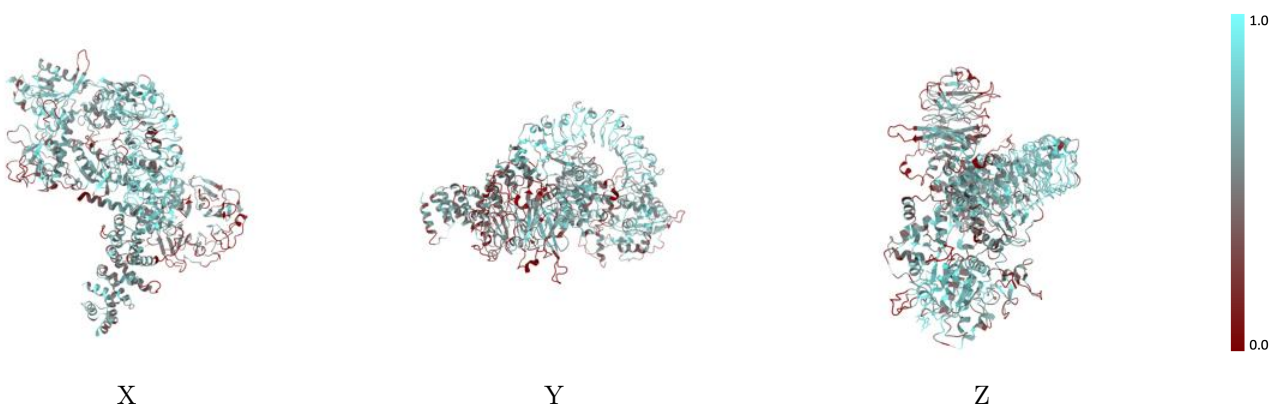
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



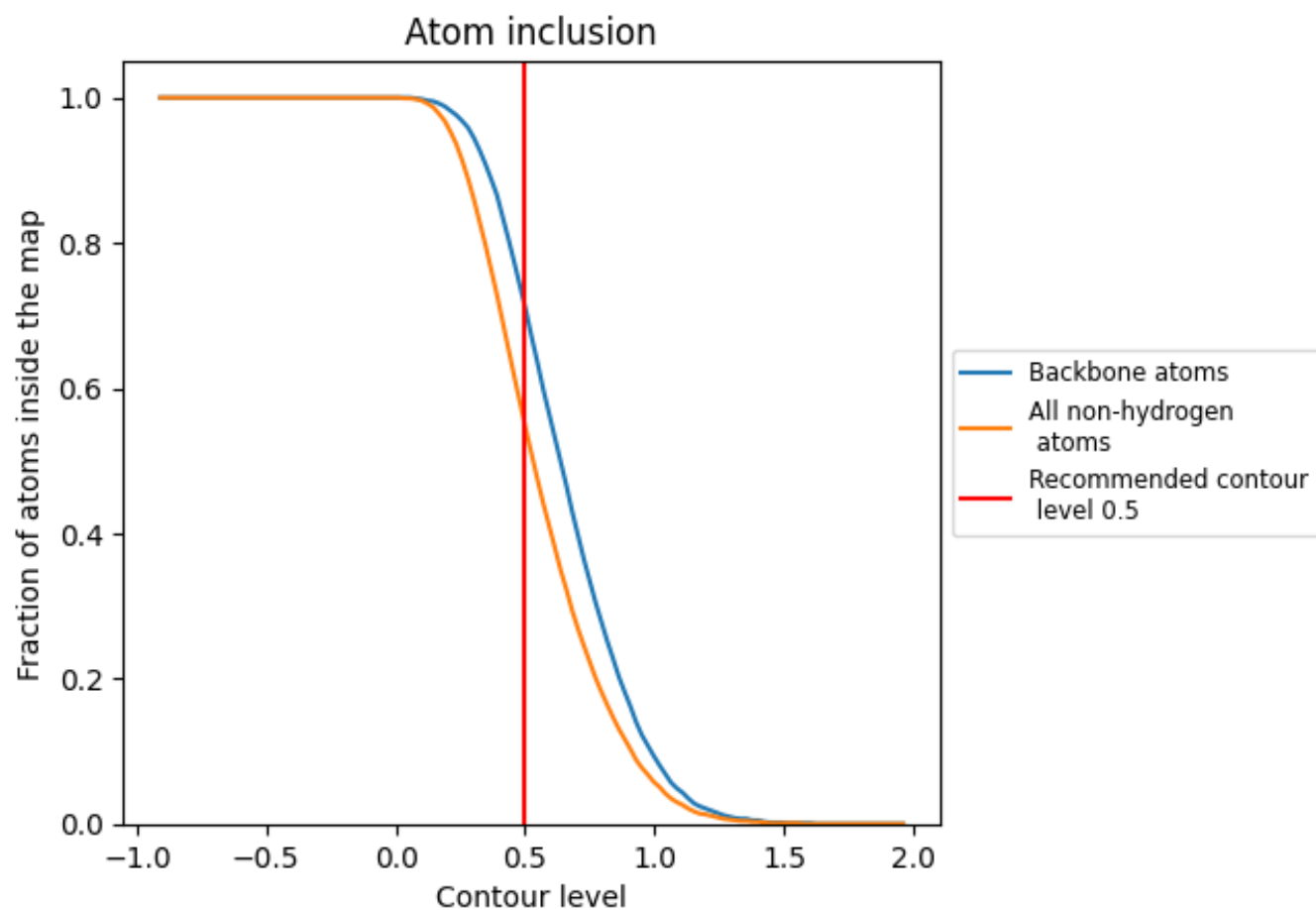
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 55% 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	0.5470	0.4020
A	0.5470	0.4020

