



Full wwPDB EM Validation Report ⓘ

Aug 11, 2026 – 04:35 PM EDT

PDB ID : 9Y68 / pdb_00009y68
EMDB ID : EMD-72556
Title : Full length LRRK2 (G2019S) after symmetry expansion
Authors : Villagran Suarez, A.C.; Bodrug, T.
Deposited on : 2025-09-08
Resolution : 3.25 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.dev133
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) : 2.50

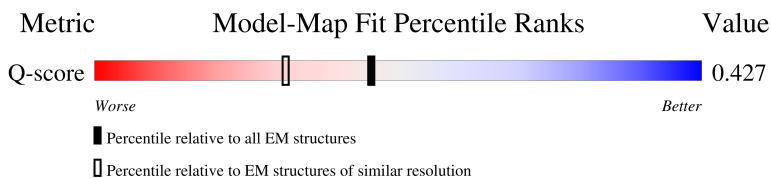
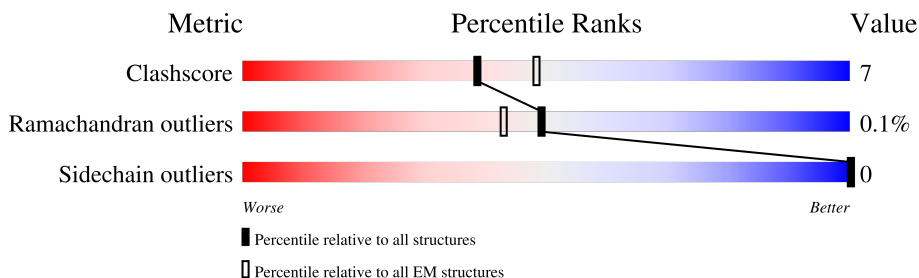
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 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	14599 (2.75 - 3.75)

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 2 unique types of molecules in this entry. The entry contains 13046 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.

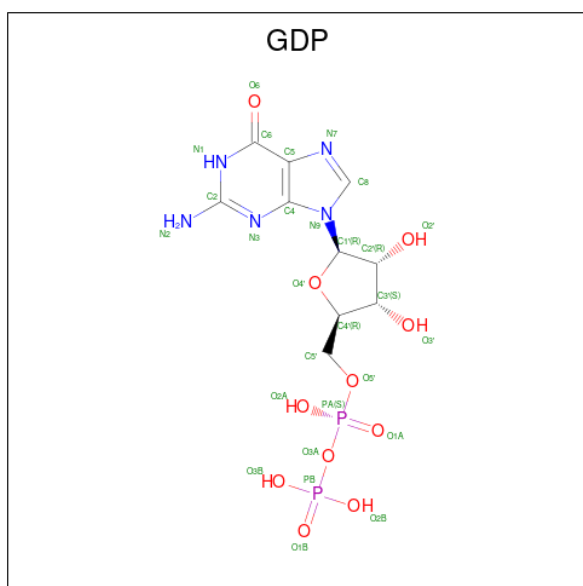
- Molecule 1 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1700	13018	8307	2250	2387	74	1	0

There are 3 discrepancies between the modelled and reference sequences:

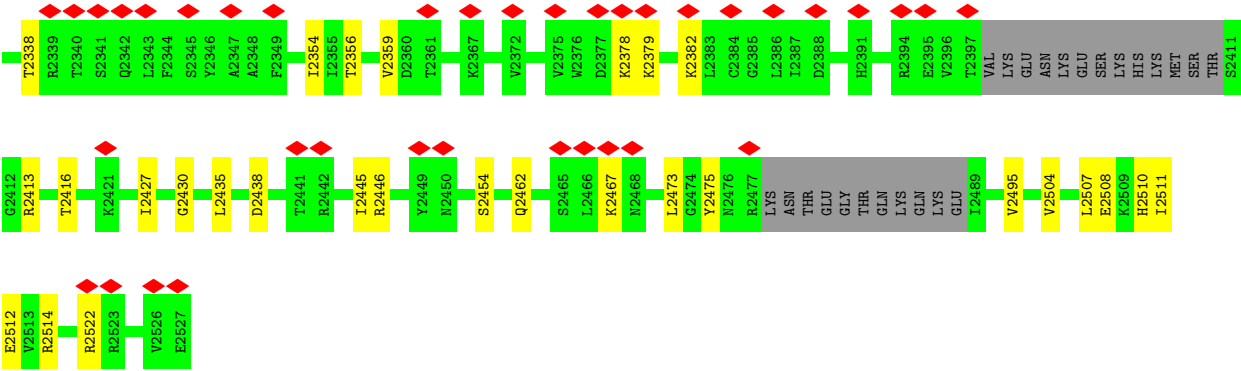
Chain	Residue	Modelled	Actual	Comment	Reference
A	2019	SER	GLY	engineered mutation	UNP Q5S007
A	2397	THR	MET	conflict	UNP Q5S007
A	2410	THR	TYR	conflict	UNP Q5S007

- 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

L2264	A2268	D2269	G2270	K2271	L2272	A2273	L2274	F2275	E2276	D2277	K2278	K2281	L2282	K2283	G2284	A2285	A2286	P2287	L2288	K2289	L2290	L2291	N2292	G2294	N2295	V2296	S2297	L2298	P2299	L2300	N2301	C2302	L2303	S2306	T2307	ASN	SER	THR	E2311	R2312	N2313	W2316	G2317	G2318	C2319	G2320	T2321	N2328	D2329	F2330	T2331	L2332	Q2333			
S2180	F2181	L2182	D2183	T2186	K2078	Y2189	E2193	V2194	A2195	D2196	L2200	A2203	H2206	L2207	PRO	VAL	GLU	LYS	E2212	S2213	L2224	L2225	T2229	E2230	D2231	R2235	L2238	E2239	K2240	M2241	T2242	D2243	S2244	V2245	T2246	C2250	ASN	SER	PHE	SER	LYS	GLN	LYS	GLY	ASN	ALA	S2166	C2171	G2172	H2173	G2174	D2175	Q2178	L2179		
K2078	N2081	E2082	F2083	D2084	E2085	L2086	E2087	L2088	K2091	K2097	M2106	V2107	E2108	K2109	L2110	K2111	L2112	Q2113	Q2120	E2121	R2122	L2140	T2141	R2142	P2147	K2148	N2149	V2150	L2151	V2152	E2153	V2156	A2157	T2158	HIS	HIS	ASN	SER	ARG	ASN	ALA	S2166	C2171	G2172	H2173	G2174	D2175	Q2178	L2179							
T1967	R1968	I1974	H1977	D1980	Y1984	M1989	D1873	E1874	L1875	E1876	Q1879	A1880	F1881	E1882	F1883	L1884	L1885	G1886	D1887	F1890	G1891	S1892	V1893	Y1894	R1895	E1899	G1900	E1901	K1906	H1911	R1915	H1926	L1927	H1928	S1931	L1932	I1933	I1940	R1941	P1942	E1948	L1959	Q1960	Q1961												
R1723	E1724	R1725	A1726	P1729	R1735	N1741	W1742	S1743	P1744	A1746	N1757	L1763	V1767	L1776	L1777	V1780	W1791	D1799	I1800	C1801	E1802	E1803	G1804	W1811	Y1814	E1820	E1821	L1827	K1832	E1836	G1837	D1838	L1839	L1840	D1844	R1847	L1848	T1849	I1855																	
V1488	T1491	E1492	L1500	T1503	T1504	I1505	K1512	V1518	V1519	T1523	C1526	Y1527	V1528	E1529	L1530	I1533	T1534	L1535	R1538	L1553	L1556	V1557	R1558	Q1561	L1562	Q1563	L1564	E1568	H1571	H1574	F1575	L1576	N1577	V1581	H1584	F1585	Q1586	D1587	P1588	A1589	L1590	Q1591														
K1358	K1359	S1360	D1361	L1362	G1363	M1364	Q1365	I1378	R1381	D1382	K1383	R1384	K1385	V1392	F1401	H1407	R1412	D1420	V1428	P1433	N1437	I1438	K1439	A1440	R1441	T1452	H1453	S1457	ASP	GLU	LYS	GLN	R1462	M1466	L1473	R1477	P1480	D1484	Y1485	H1486	F1487															
C1187	L1198	R1199	S1200	L1201	I1208	N1221	L1222	L1225	H1229	N1230	L1237	H1254	L1267	L1270	H1018	H1019	Q1020	N1021	L1034	L1037	W1295	L1299	D1300	K1046	M1057	I1060	H1310	I1311	G1312	C1313	K1314	A1315	K1316	R1325	L1326	K1327	K1336	L1337	M1338	I1339	V1340	G1346	K1347	T1348	T1349											
THR	ALA	SER	GLY	ASP	GLY	ASN	PHE	ARG	CYS	SER	GLU	VAL	ASP	ASN	LEU	GLN	ARG	HIS	PHE	ASP	GLY	TRP	THR	GLY	PHE	ILE	PRO	ILE	PHE	ASP	SER	HIS	SER	GLU	MET	ASP	SER	LEU	VAL	LEU	GLN	LYS	LYS	HIS	MET	SER	ASN	ARG	HIS	SER	ILE	SER	VAL	GLY	ILE	GLU
R767	D770	K773	I777	G782	L791	R792	R793	N800	N801	L805	F808	C809	I810	L818	G819	P820	L821	D824	K825	T826	S827	N828	L829	R830	K831	Q832	T833	N834	I835	A836	S837	T838	L839	M842	V843	I844	R845	Y846	Q847	M848	K849	S850	A851	V852	E853	E854	GLY									



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	83730	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.293	Depositor
Minimum map value	-0.830	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	374.0, 374.0, 374.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.935, 0.935, 0.935	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

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	0.18	0/13251	0.46	0/17965

There are no bond length outliers.

There are no bond angle outliers.

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	13018	0	12886	188	0
2	A	28	0	12	3	0
All	All	13046	0	12898	188	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 7.

All (188) 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:2036:PRO:HA	1:A:2039:ARG:HE	1.51	0.76
1:A:1208:ILE:HB	1:A:1230:ASN:HD21	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:ARG:NH1	1:A:770:ASP:OD2	2.24	0.70
1:A:1420:ASP:OD1	1:A:1453:HIS:ND1	2.24	0.69
1:A:1729:PRO:HB3	1:A:1742:TRP:HE1	1.61	0.66
1:A:808:PHE:O	1:A:992:ASN:ND2	2.29	0.65
1:A:1526:CYS:HB3	1:A:1564:LEU:HD11	1.80	0.63
1:A:1836:GLU:O	1:A:1941:ARG:NH1	2.31	0.62
1:A:1535:LEU:HD23	1:A:1538:ARG:HE	1.63	0.62
1:A:2356:THR:HG21	1:A:2416:THR:HA	1.81	0.62
1:A:1337:LEU:HD23	1:A:1392:VAL:HG22	1.82	0.62
1:A:2224:LEU:HD23	1:A:2238:LEU:HD12	1.82	0.62
1:A:1412:ARG:HH22	1:A:1519:VAL:HA	1.65	0.61
1:A:990:SER:O	1:A:1021:ASN:ND2	2.33	0.61
1:A:1725:ARG:HH21	1:A:2522:ARG:HH21	1.47	0.61
1:A:800:ASN:HD21	1:A:1967:THR:HG21	1.66	0.61
1:A:1886:GLY:HA2	1:A:1895:ARG:HH21	1.65	0.61
1:A:1720:LEU:HD12	1:A:1722:GLY:H	1.65	0.60
1:A:1980:ASP:OD2	1:A:2514:ARG:NH1	2.34	0.60
1:A:1453:HIS:HD2	2:A:2601:GDP:C5	2.19	0.60
1:A:992:ASN:O	1:A:1021:ASN:ND2	2.33	0.60
1:A:1587:ASP:HB3	1:A:1590:LEU:HB2	1.84	0.59
1:A:2053:GLN:HB3	1:A:2122:ARG:HH21	1.66	0.59
1:A:2438:ASP:HB2	1:A:2445:ILE:HD11	1.83	0.59
1:A:2009:ALA:O	1:A:2510:HIS:NE2	2.35	0.58
1:A:1433:PRO:O	1:A:1437:ASN:ND2	2.37	0.58
1:A:1199:ARG:HH21	1:A:1221:ASN:HD21	1.51	0.57
1:A:1586:GLN:HG2	1:A:1587:ASP:H	1.69	0.57
1:A:1657:GLN:HG3	1:A:1707:ARG:HG3	1.85	0.56
1:A:1340:VAL:HG21	1:A:1438:ILE:HD11	1.87	0.56
1:A:1491:THR:HG23	1:A:1492:GLU:HG2	1.86	0.56
1:A:1933:ILE:HG23	1:A:1948:GLU:HB2	1.87	0.56
1:A:1959:LEU:HD13	1:A:2070:GLY:HA3	1.87	0.56
1:A:1004:CYS:SG	1:A:1005:CYS:N	2.79	0.55
1:A:1720:LEU:HD22	1:A:1725:ARG:HB2	1.88	0.55
1:A:1701:PRO:HG2	1:A:1704:PHE:HB2	1.89	0.55
1:A:2180:SER:HB3	1:A:2189:TYR:HE1	1.72	0.55
1:A:1010:LEU:HD22	1:A:1013:LEU:HD11	1.87	0.55
1:A:2147:PRO:HG2	1:A:2150:VAL:HG21	1.89	0.55
1:A:2318:GLY:HA3	1:A:2354:ILE:HD13	1.89	0.55
1:A:1767:VAL:HG21	1:A:1777:LEU:HB2	1.89	0.55
1:A:1286:ASN:OD1	1:A:1325:ARG:NH2	2.40	0.54
1:A:2427:ILE:HB	1:A:2435:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1530:LEU:HB3	1:A:1576:LEU:HD11	1.89	0.54
1:A:2152:VAL:HG13	1:A:2473:LEU:HD21	1.89	0.54
1:A:1931:SER:HB2	1:A:2514:ARG:HH22	1.72	0.54
1:A:2413:ARG:O	1:A:2430:GLY:N	2.41	0.54
1:A:2293:ILE:HD12	1:A:2332:ILE:HD11	1.88	0.54
1:A:2086:LEU:HA	1:A:2091:LYS:HE2	1.88	0.54
1:A:1723:ARG:HB2	1:A:1725:ARG:HH12	1.73	0.54
1:A:1378:ILE:HD13	1:A:1505:ILE:HD11	1.90	0.54
1:A:2246:THR:OG1	1:A:2300:LEU:O	2.21	0.53
1:A:1428:VAL:HG21	1:A:1466:MET:HG3	1.90	0.53
1:A:1453:HIS:CD2	2:A:2601:GDP:C5	2.97	0.53
1:A:1568:GLU:OE1	1:A:1568:GLU:N	2.41	0.53
1:A:1439:LYS:HB2	1:A:1480:PRO:HD3	1.91	0.52
1:A:1034:LEU:HD11	1:A:1037:LEU:HD22	1.91	0.52
1:A:1441:ARG:NH1	1:A:1791:TRP:O	2.42	0.52
1:A:2081:ASN:OD1	1:A:2082:GLU:N	2.41	0.52
1:A:2225:LEU:HD11	1:A:2235:ARG:HB2	1.92	0.52
1:A:810:ILE:H	1:A:992:ASN:HD22	1.58	0.52
1:A:1187:CYS:HA	1:A:1208:ILE:HG23	1.91	0.52
1:A:1893:VAL:HG22	1:A:1906:LYS:HB2	1.91	0.51
1:A:1906:LYS:NZ	1:A:2018:TYR:O	2.41	0.51
1:A:1959:LEU:HD11	1:A:2073:ILE:HD11	1.92	0.51
1:A:1473:LEU:HA	1:A:1477:ARG:HD2	1.92	0.51
1:A:1590:LEU:HA	1:A:1651:LYS:HE2	1.92	0.51
1:A:2109:LYS:O	1:A:2113:GLN:HG3	2.10	0.51
1:A:1057:MET:HB2	1:A:1060:ILE:HB	1.93	0.51
1:A:1131:LEU:HD21	1:A:1134:LEU:HD13	1.92	0.51
1:A:2299:PRO:HG2	1:A:2301:MET:HE1	1.92	0.51
1:A:1684:HIS:NE2	1:A:1744:PRO:O	2.43	0.50
1:A:1931:SER:OG	1:A:1977:HIS:O	2.27	0.50
1:A:742:SER:O	1:A:747:GLN:NE2	2.43	0.50
1:A:1336:LYS:HE2	1:A:1338:MET:HE2	1.93	0.50
1:A:1553:LEU:HA	1:A:1556:LEU:HB2	1.94	0.50
1:A:2462:GLN:HE22	1:A:2467:LYS:HA	1.76	0.50
1:A:1695:TYR:HB2	1:A:1763:LEU:HB3	1.94	0.50
1:A:792:ARG:NH2	1:A:820:PRO:O	2.45	0.49
1:A:1675:ASP:OD2	1:A:1735:ARG:NH2	2.39	0.49
1:A:1349:THR:OG1	1:A:1365:GLN:NE2	2.45	0.49
1:A:1933:ILE:HD12	1:A:2016:ALA:HA	1.95	0.49
1:A:745:ILE:HA	1:A:748:VAL:HG12	1.95	0.48
1:A:818:LEU:HD23	1:A:821:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2289:LYS:HD3	1:A:2330:PHE:HB2	1.96	0.48
1:A:1412:ARG:NH1	1:A:1518:VAL:HG13	2.28	0.48
1:A:1941:ARG:HB3	1:A:1942:PRO:HD3	1.95	0.48
1:A:2264:LEU:HD22	1:A:2303:LEU:HD11	1.95	0.48
1:A:1719:MET:HE1	1:A:1742:TRP:CZ3	2.48	0.48
1:A:1814:TYR:HB3	1:A:1855:ILE:HG21	1.96	0.48
1:A:1006:ILE:HG12	1:A:1010:LEU:HG	1.95	0.48
1:A:1588:PRO:O	1:A:1591:GLN:NE2	2.40	0.48
1:A:2156:VAL:HG21	1:A:2203:ALA:HA	1.96	0.48
1:A:1884:LEU:HB3	1:A:1895:ARG:HB3	1.96	0.48
1:A:1933:ILE:HD11	1:A:2001:LEU:HD12	1.94	0.48
1:A:1866:ARG:HA	1:A:1869:MET:HE3	1.96	0.47
1:A:2151:ILE:O	1:A:2172:GLY:N	2.47	0.47
1:A:2263:LEU:HB3	1:A:2275:PHE:HB2	1.94	0.47
1:A:2454:SER:HB3	1:A:2475:TYR:HB2	1.96	0.47
1:A:1484:ASP:OD1	1:A:1485:TYR:N	2.48	0.47
1:A:1776:LEU:O	1:A:1780:VAL:HG22	2.14	0.47
1:A:1138:LYS:NZ	1:A:1882:GLU:OE1	2.47	0.47
1:A:1696:GLU:OE1	1:A:1811:TRP:NE1	2.36	0.47
1:A:2504:VAL:O	1:A:2508:GLU:HG3	2.14	0.47
1:A:1046:LYS:HB2	1:A:1046:LYS:HE2	1.73	0.47
1:A:1486:HIS:HE2	1:A:1503:THR:HG21	1.80	0.47
1:A:1960:GLN:HG3	1:A:1961:GLN:HG2	1.96	0.47
1:A:2271:LYS:HD3	1:A:2271:LYS:HA	1.78	0.47
1:A:2510:HIS:CE1	1:A:2514:ARG:HD2	2.49	0.47
1:A:1222:LEU:HB3	1:A:1225:LEU:HD21	1.97	0.47
1:A:1915:ARG:HA	1:A:1915:ARG:HD2	1.77	0.46
1:A:2166:SER:OG	1:A:2182:LEU:O	2.30	0.46
1:A:2507:LEU:O	1:A:2511:ILE:HG12	2.16	0.46
1:A:1346:GLY:H	1:A:1452:THR:HG21	1.80	0.46
1:A:1996:LYS:HE3	1:A:1998:HIS:HB2	1.97	0.46
1:A:2300:LEU:HD13	1:A:2319:CYS:HB2	1.97	0.46
1:A:1571:HIS:HA	1:A:1574:HIS:HB3	1.98	0.46
1:A:1827:LEU:HD23	1:A:1832:LYS:HE3	1.97	0.46
1:A:2262:PHE:HB3	1:A:2274:ILE:HD11	1.98	0.46
1:A:1974:ILE:HD11	1:A:2002:LEU:HD21	1.98	0.45
1:A:1291:LEU:HD23	1:A:1294:ILE:HD11	1.97	0.45
1:A:2446:ARG:HD2	1:A:2504:VAL:HG21	1.97	0.45
1:A:1529:GLU:HB2	1:A:1562:LEU:HD11	1.99	0.45
1:A:1870:LEU:HD11	1:A:1875:LEU:HD13	1.99	0.45
1:A:2175:ASP:OD1	1:A:2175:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:LYS:O	1:A:777:ILE:HG12	2.17	0.45
1:A:2173:HIS:CD2	1:A:2174:THR:HG23	2.52	0.45
1:A:1299:LEU:HB3	1:A:1308:PHE:HB2	1.99	0.44
1:A:2213:SER:O	1:A:2229:THR:OG1	2.30	0.44
1:A:1316:LYS:HE2	1:A:1316:LYS:HB2	1.73	0.44
1:A:2171:CYS:SG	1:A:2178:GLN:N	2.90	0.44
1:A:1407:HIS:NE2	1:A:1656:PHE:HA	2.33	0.44
1:A:1538:ARG:NH2	1:A:1581:VAL:O	2.42	0.44
1:A:1401:PHE:CE1	1:A:1608:ALA:HB1	2.53	0.44
1:A:1654:GLU:HA	1:A:1660:LEU:HB2	2.00	0.44
1:A:1840:LEU:HD23	1:A:1849:THR:HB	1.99	0.44
1:A:2378:LYS:HG3	1:A:2379:LYS:HG2	1.99	0.44
1:A:761:LEU:HD23	1:A:761:LEU:HA	1.82	0.43
1:A:1530:LEU:HD13	1:A:1533:ILE:HD11	1.99	0.43
1:A:2053:GLN:O	1:A:2122:ARG:NH2	2.51	0.43
1:A:1119:ILE:HB	1:A:1139:ASN:HD22	1.83	0.43
1:A:2270:GLY:HA3	1:A:2294:GLY:H	1.82	0.43
1:A:2108:GLU:HA	1:A:2111:ILE:HD12	2.00	0.43
1:A:2180:SER:HB3	1:A:2189:TYR:CE1	2.52	0.43
1:A:1065:VAL:HB	1:A:1068:ASN:HD22	1.83	0.43
1:A:1311:ILE:HG12	1:A:1574:HIS:CE1	2.53	0.43
1:A:1327:LYS:HD3	1:A:1563:GLN:HE21	1.83	0.43
1:A:762:LEU:HB3	1:A:793:ARG:HG3	2.00	0.43
1:A:2076:GLY:HA3	1:A:2083:PHE:CD1	2.54	0.43
1:A:810:ILE:HG12	1:A:992:ASN:ND2	2.33	0.43
1:A:1814:TYR:HE2	1:A:1827:LEU:HB2	1.84	0.43
1:A:2238:LEU:HD22	1:A:2285:ALA:H	1.83	0.43
1:A:1488:VAL:HG21	1:A:1500:LEU:HD22	2.01	0.43
1:A:1523:ILE:HD12	1:A:1527:TYR:HB2	1.99	0.42
1:A:1199:ARG:HH21	1:A:1221:ASN:ND2	2.16	0.42
1:A:1742:TRP:HB2	1:A:1746:ALA:O	2.19	0.42
1:A:1858:ASP:OD1	1:A:1858:ASP:N	2.53	0.42
1:A:989:LEU:HB2	1:A:1018:LEU:HD23	2.02	0.42
1:A:1270:LEU:HD12	1:A:1291:LEU:HD21	2.02	0.42
1:A:710:ASN:OD1	1:A:737:GLN:NE2	2.53	0.42
1:A:1229:HIS:HA	1:A:1254:HIS:HB2	2.02	0.42
1:A:2142:ARG:HG3	1:A:2495:VAL:HB	2.00	0.42
1:A:1876:GLU:N	1:A:1876:GLU:OE1	2.52	0.42
1:A:2289:LYS:HE3	1:A:2291:LEU:HD21	2.02	0.42
1:A:747:GLN:O	1:A:751:LYS:HG2	2.20	0.42
1:A:2321:THR:O	1:A:2338:THR:OG1	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1178:LEU:HD23	1:A:1201:LEU:HD13	2.02	0.41
1:A:1295:TRP:CE2	1:A:2036:PRO:HG3	2.54	0.41
1:A:1571:HIS:O	1:A:1571:HIS:HD2	2.03	0.41
1:A:801:ASN:HA	1:A:984:ILE:HD13	2.02	0.41
1:A:2382:LYS:HB3	1:A:2382:LYS:HE3	1.90	0.41
1:A:1339:ILE:HG22	1:A:1347:LYS:HG3	2.03	0.41
1:A:1860:ILE:HA	1:A:1940:ILE:HD13	2.02	0.41
1:A:1577:ASN:ND2	1:A:1584:HIS:H	2.17	0.41
1:A:1586:GLN:HG2	1:A:1587:ASP:N	2.33	0.41
1:A:1237:LEU:HD21	1:A:1267:LEU:HD11	2.01	0.41
1:A:1927:LEU:O	1:A:1984:TYR:OH	2.32	0.41
1:A:791:LEU:HD13	1:A:805:LEU:HD21	2.03	0.41
1:A:1020:GLN:HA	1:A:1044:SER:HB2	2.02	0.41
1:A:2306:SER:HA	1:A:2359:VAL:HB	2.02	0.41
1:A:1071:GLY:O	1:A:1095:LEU:HA	2.21	0.40
1:A:1347:LYS:HE2	2:A:2601:GDP:O1B	2.21	0.40
1:A:2508:GLU:O	1:A:2512:GLU:HG2	2.22	0.40
1:A:1311:ILE:HG23	1:A:1574:HIS:HE1	1.86	0.40
1:A:2510:HIS:O	1:A:2514:ARG:HG3	2.22	0.40
1:A:2106:MET:HG3	1:A:2140:LEU:HD23	2.03	0.40
1:A:1198:LEU:HD12	1:A:1198:LEU:HA	1.92	0.40
1:A:2061:LEU:HD23	1:A:2061:LEU:HA	1.85	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	1675/2527 (66%)	1515 (90%)	159 (10%)	1 (0%)	48 76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1631	VAL

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	1384/2282 (61%)	1384 (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 (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	763	ASN
1	A	800	ASN
1	A	801	ASN
1	A	992	ASN
1	A	1002	GLN
1	A	1012	HIS
1	A	1021	ASN
1	A	1045	ASN
1	A	1117	ASN
1	A	1379	GLN
1	A	1521	GLN
1	A	1561	GLN
1	A	1577	ASN
1	A	1687	ASN
1	A	2052	GLN
1	A	2292	ASN
1	A	2462	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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GDP	A	2601	-	29,30,30	0.61	0	45,47,47	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	A	2601	-	-	5/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2601	GDP	O4'-C4'-C5'-O5'
2	A	2601	GDP	C3'-C4'-C5'-O5'
2	A	2601	GDP	C4'-C5'-O5'-PA
2	A	2601	GDP	PA-O3A-PB-O1B

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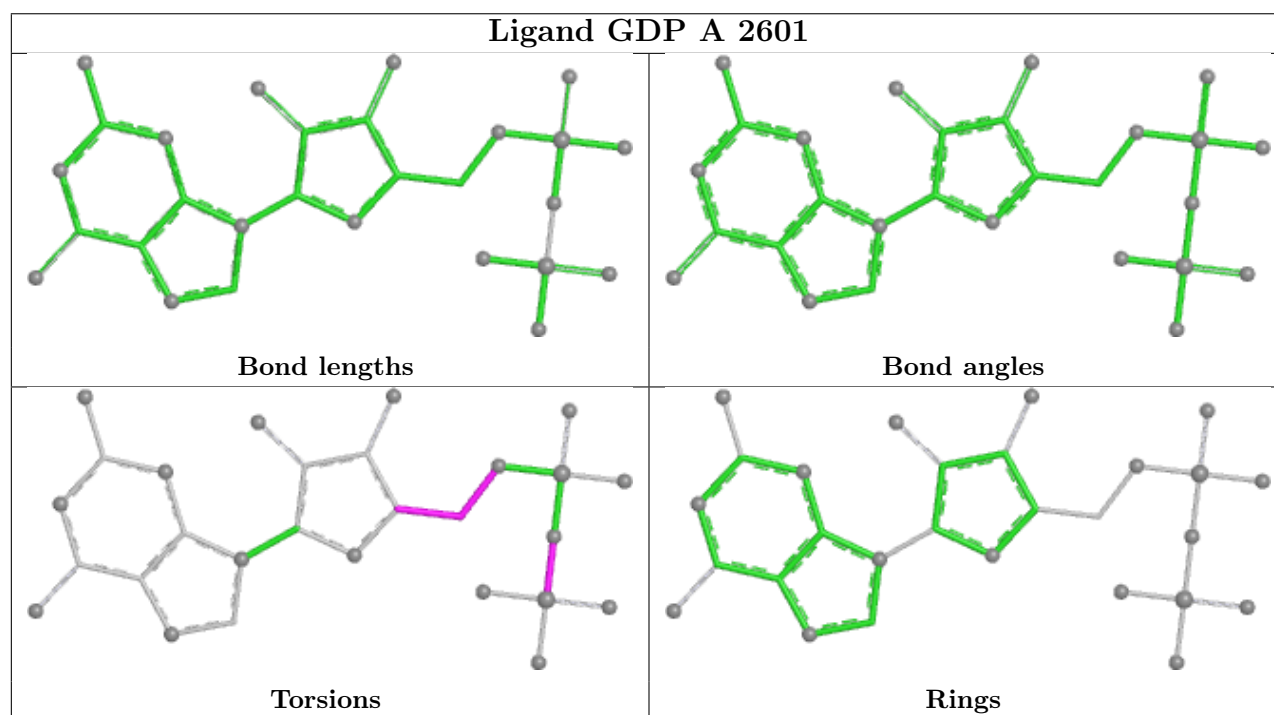
Mol	Chain	Res	Type	Atoms
2	A	2601	GDP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2601	GDP	3	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

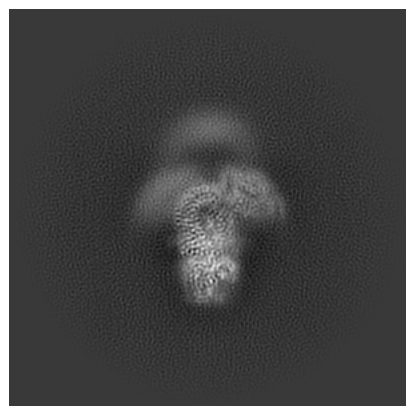
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72556. These allow visual inspection of the internal detail of the map and identification of artifacts.

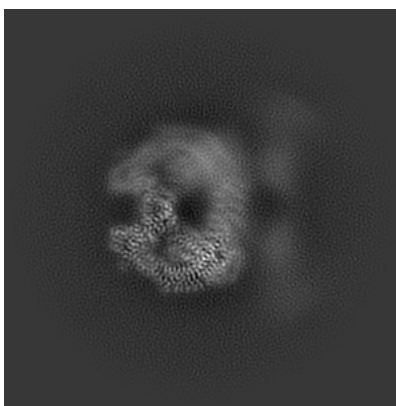
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

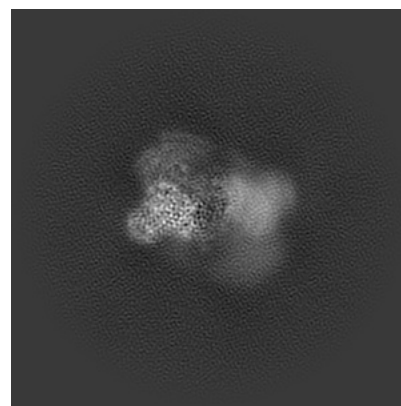
6.1.1 Primary map



X

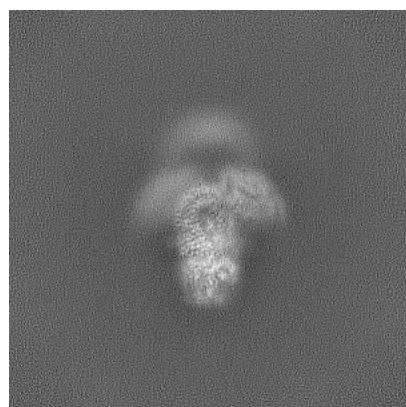


Y

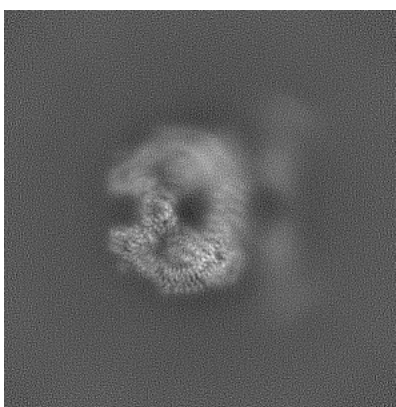


Z

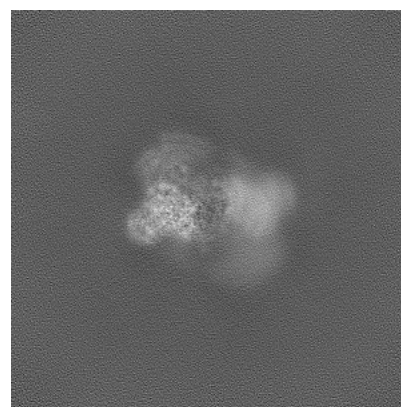
6.1.2 Raw map



X



Y

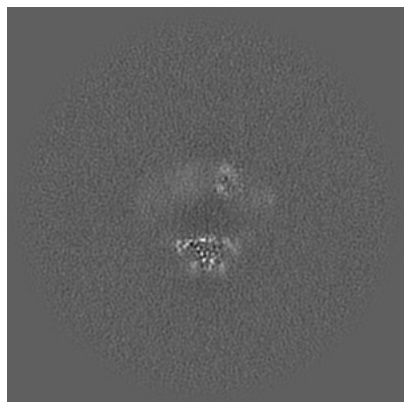


Z

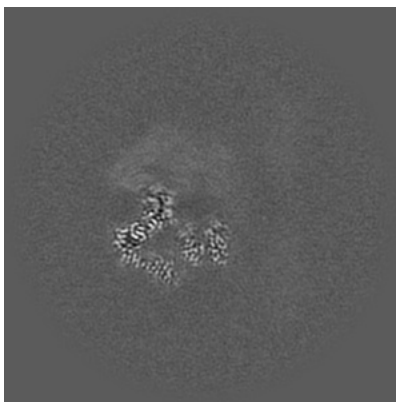
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

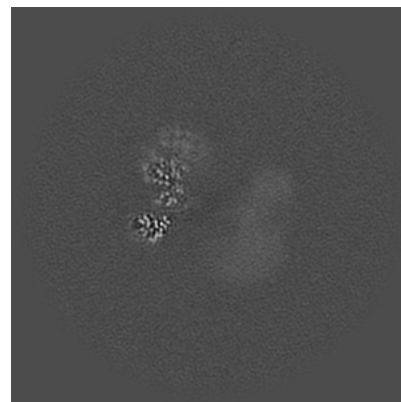
6.2.1 Primary map



X Index: 200



Y Index: 200

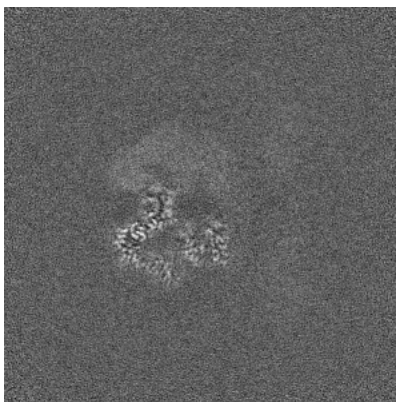


Z Index: 200

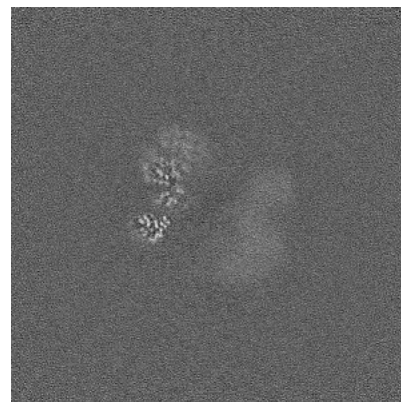
6.2.2 Raw map



X Index: 200



Y Index: 200

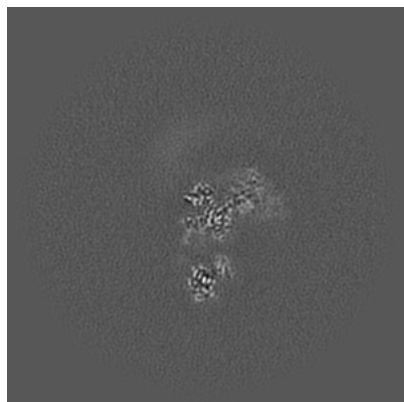


Z Index: 200

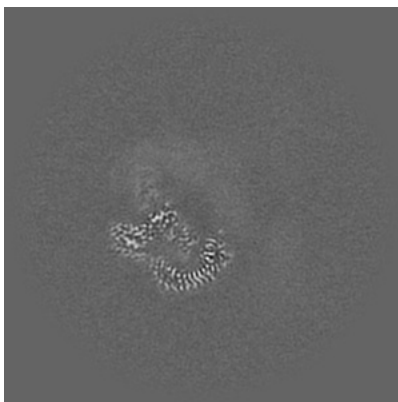
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

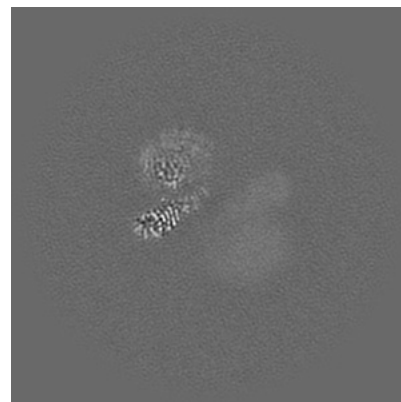
6.3.1 Primary map



X Index: 161

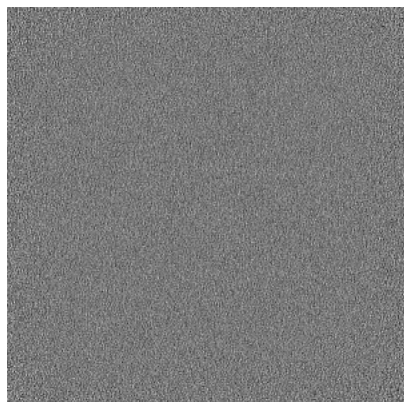


Y Index: 187

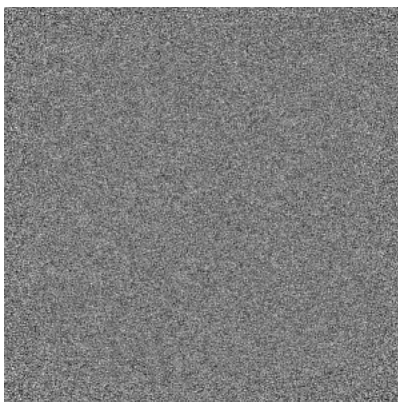


Z Index: 206

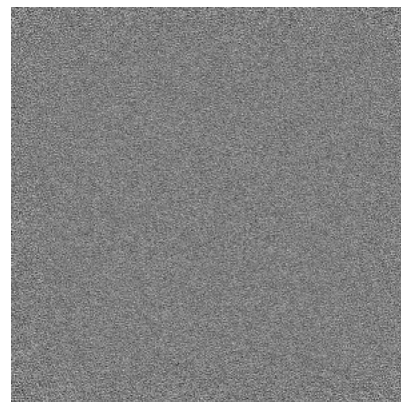
6.3.2 Raw map



X Index: 0



Y Index: 0

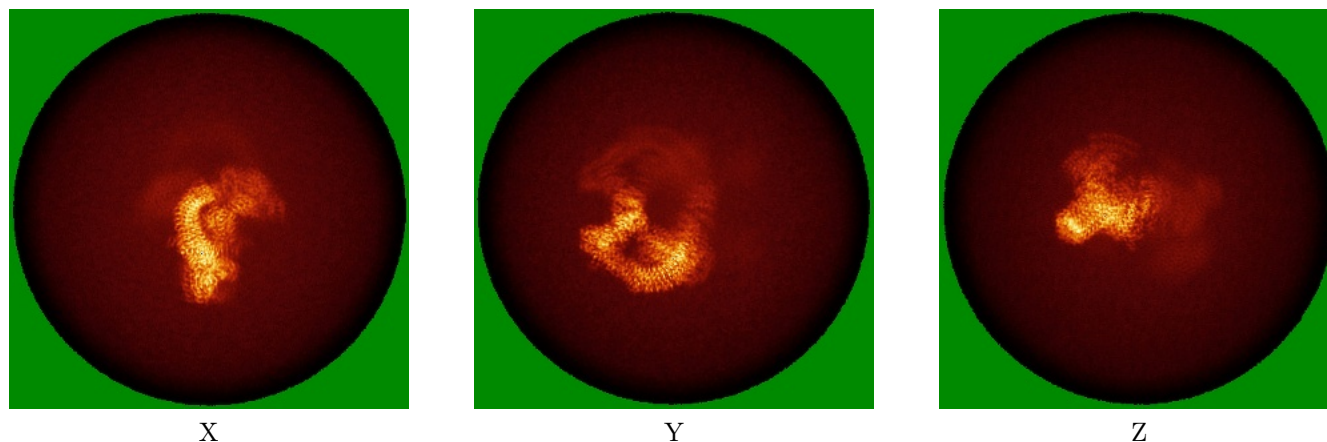


Z Index: 399

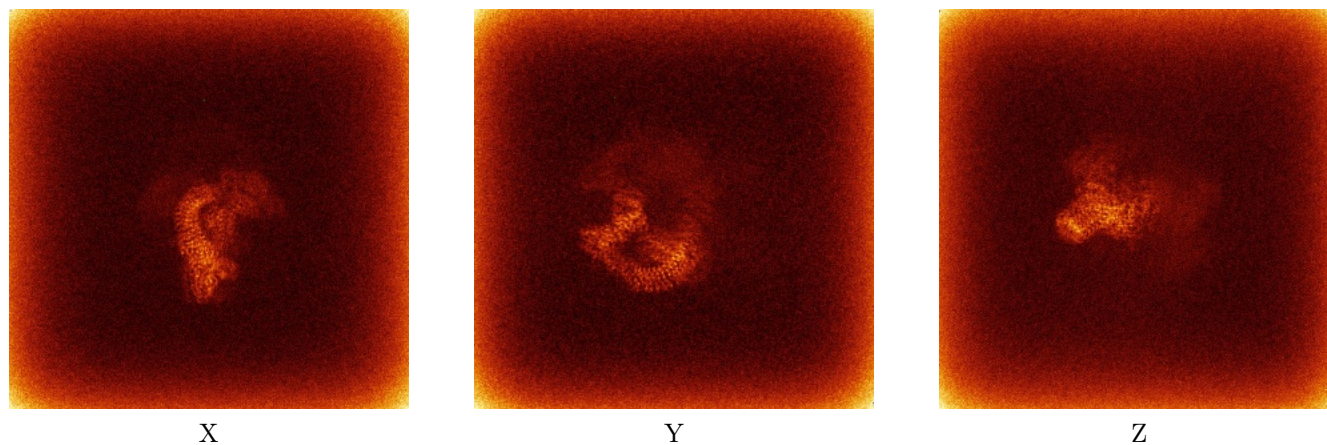
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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.

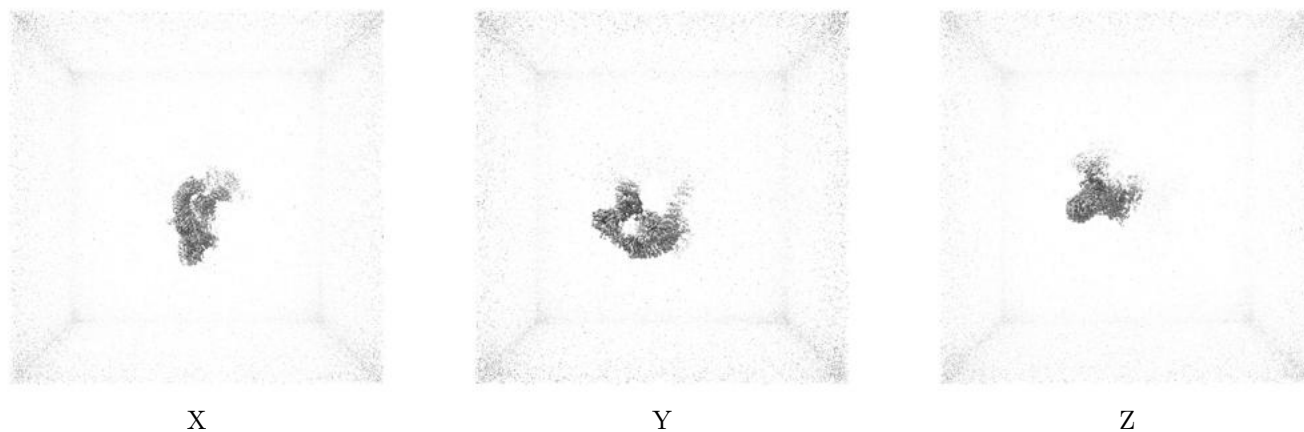
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

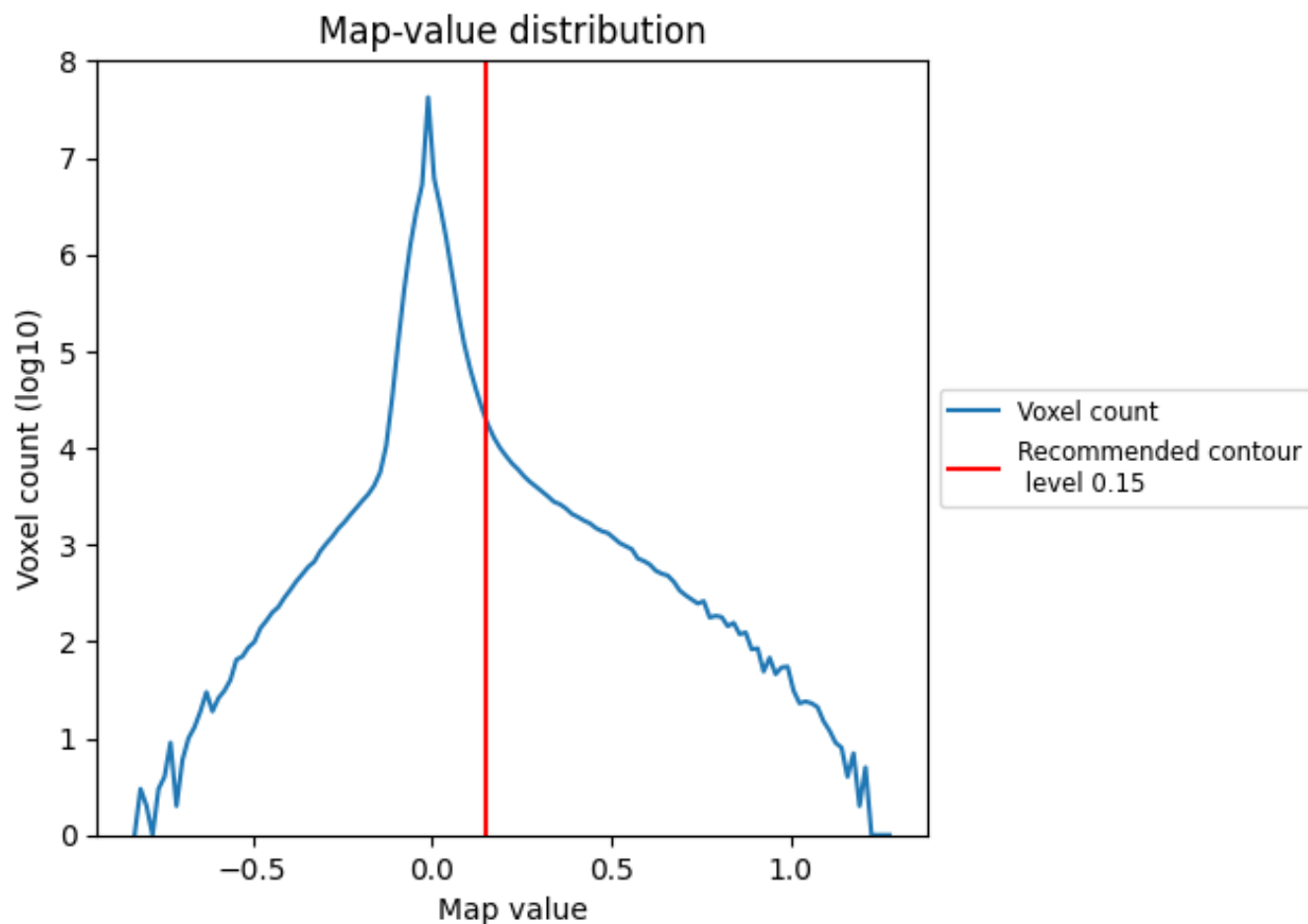
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

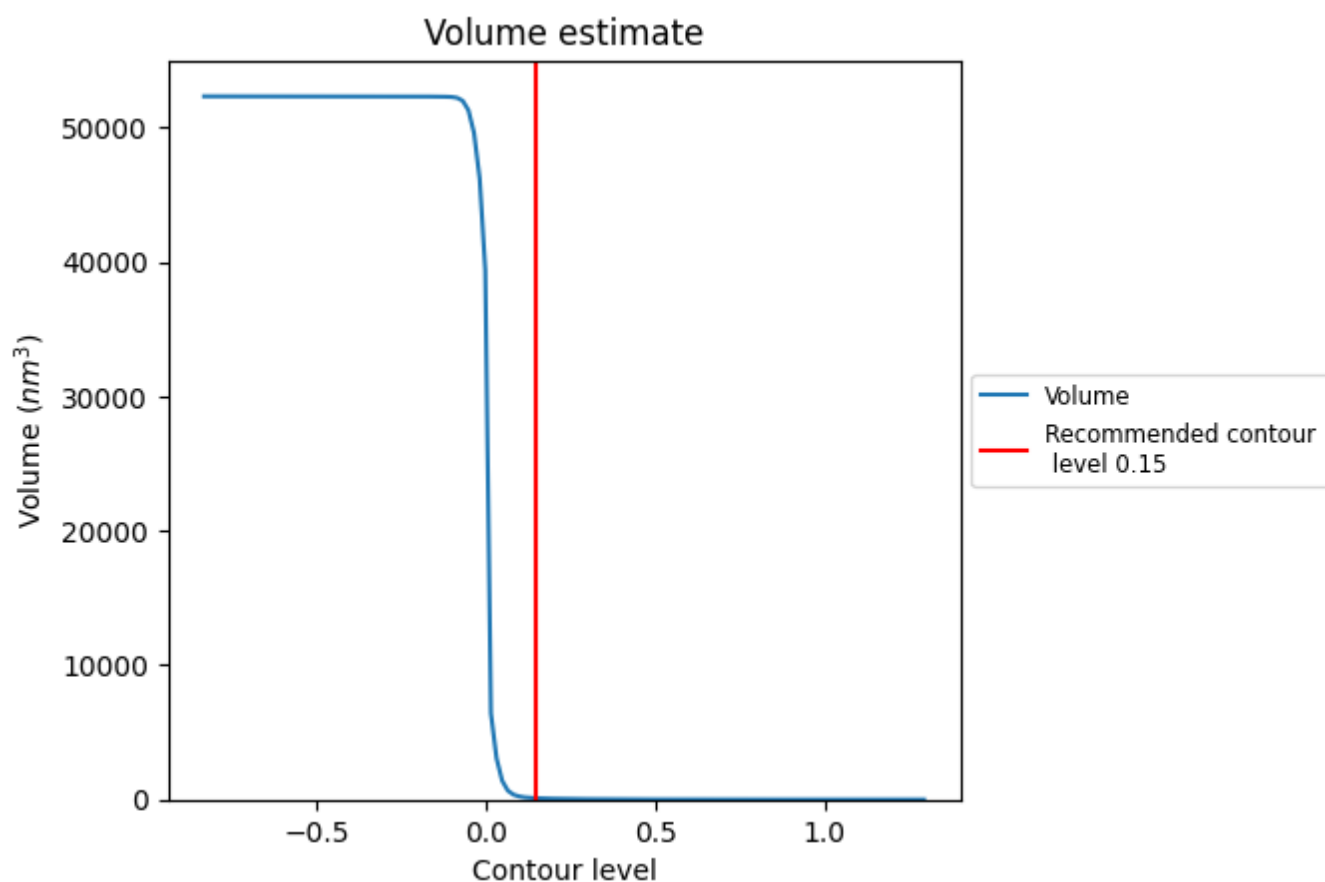
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

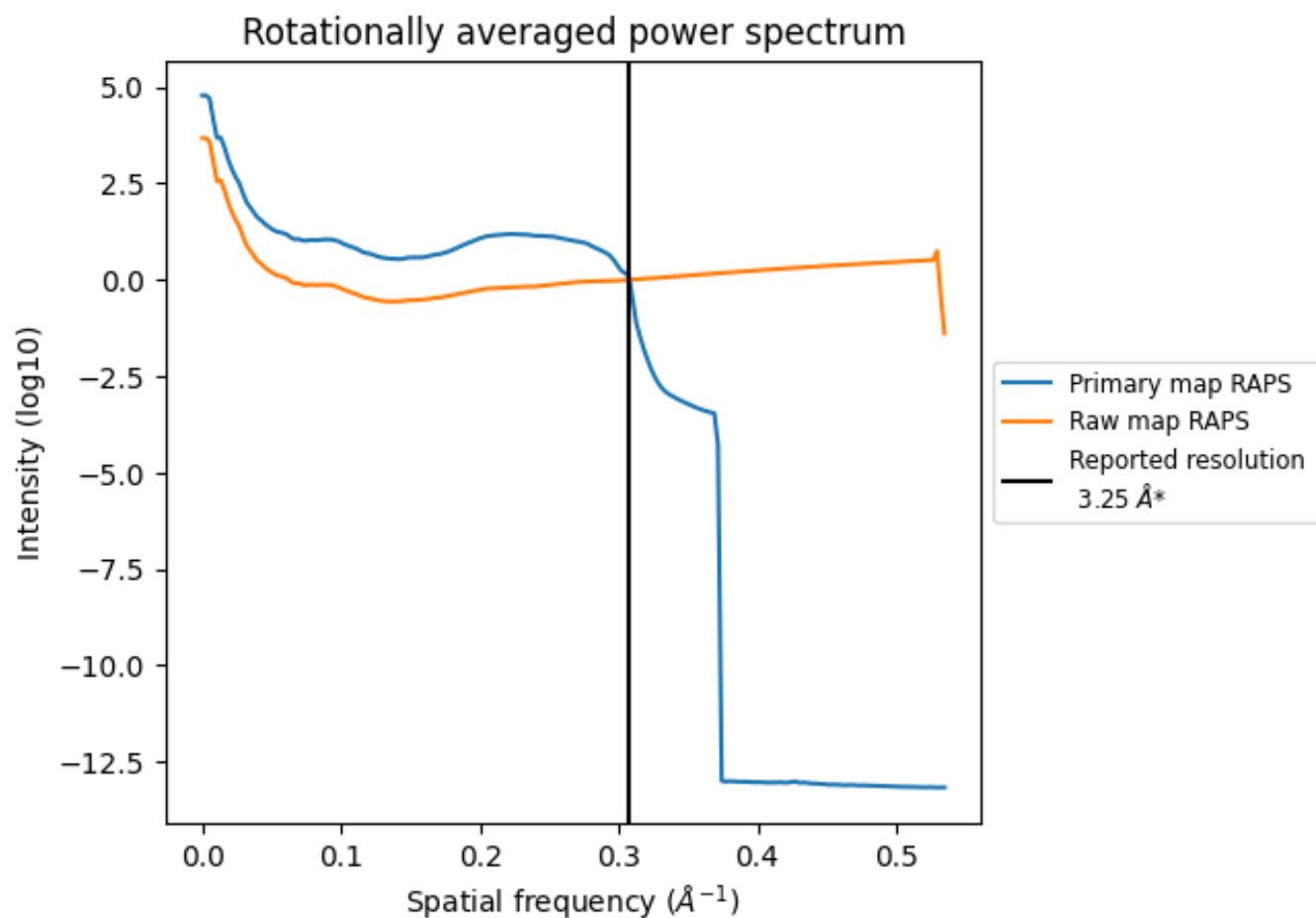
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 99 nm³; this corresponds to an approximate mass of 89 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 ⓘ

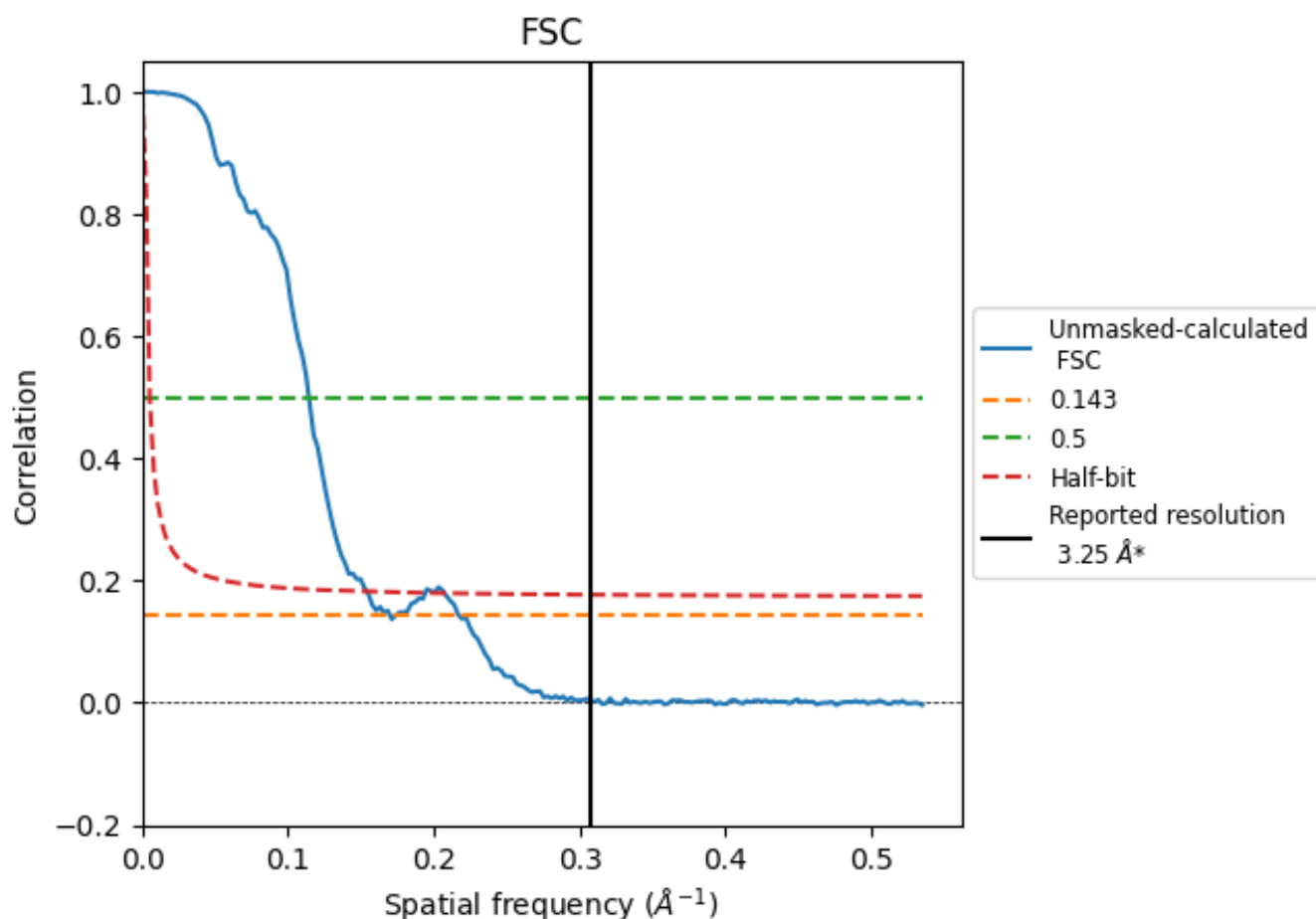


*Reported resolution corresponds to spatial frequency of 0.308 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.308 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

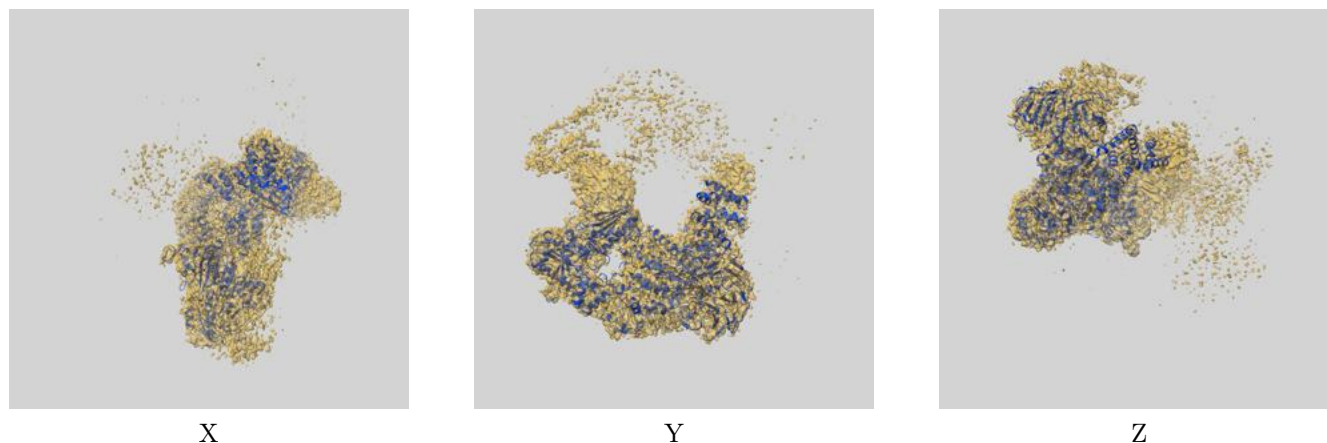
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.89	8.76	6.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.89 differs from the reported value 3.25 by more than 10 %

9 Map-model fit [i](#)

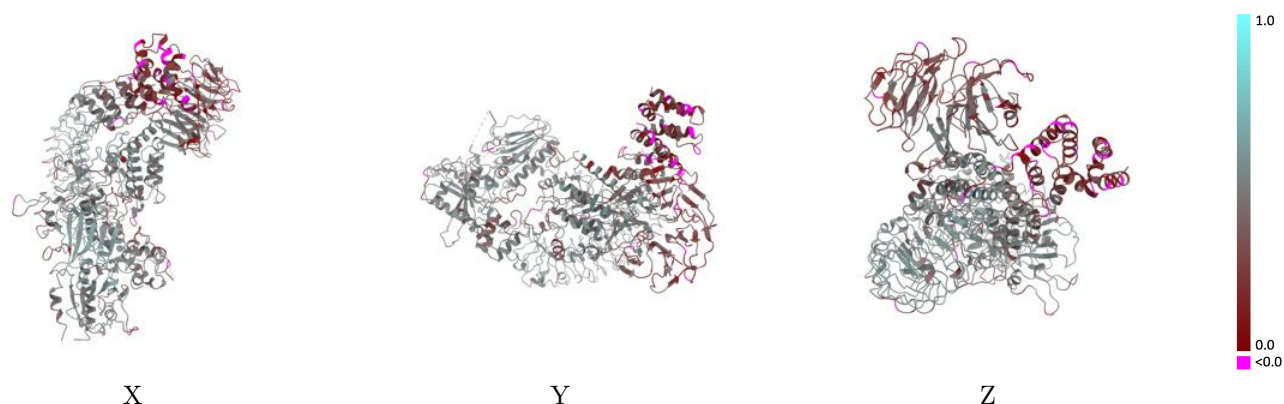
This section contains information regarding the fit between EMDB map EMD-72556 and PDB model 9Y68. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



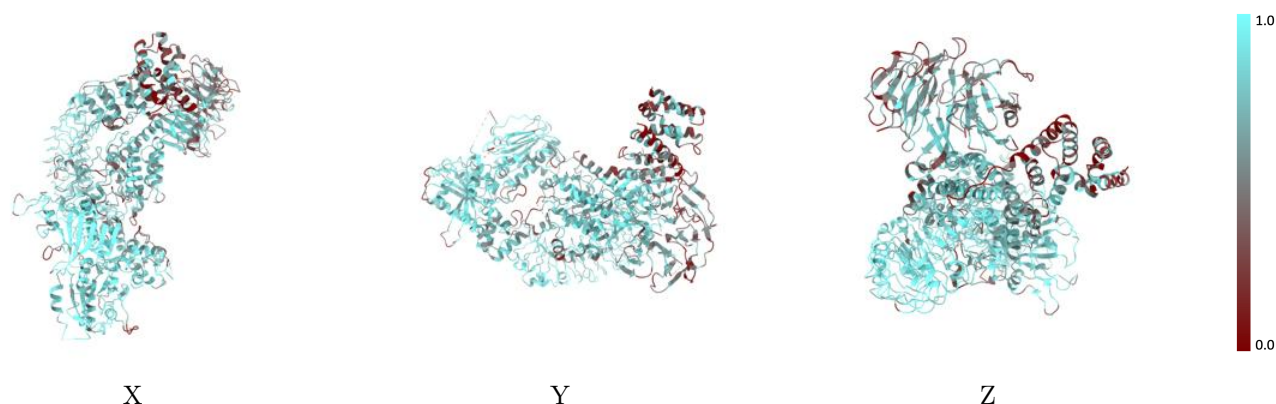
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



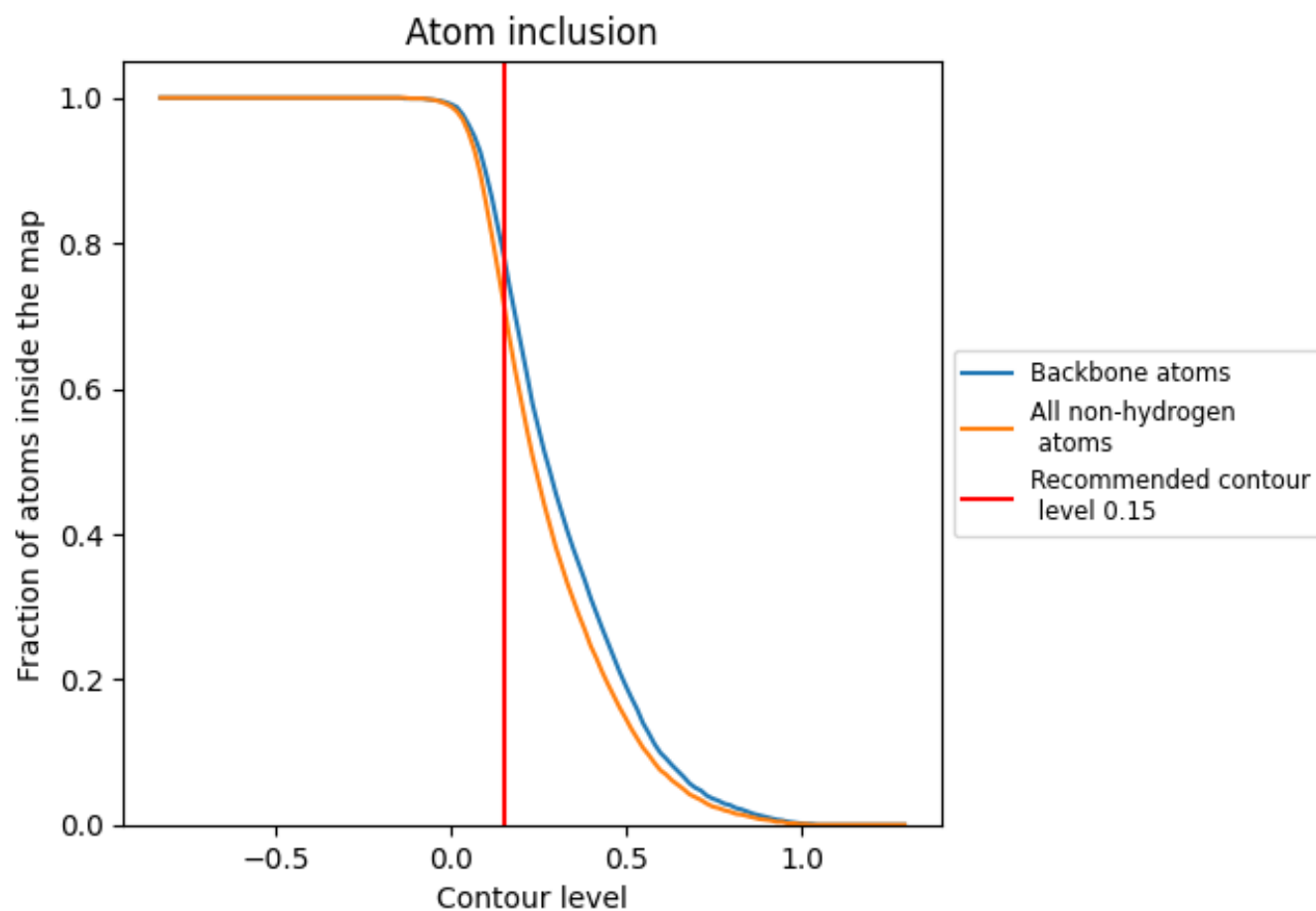
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 72% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7160	0.4270
A	0.7160	0.4270

