



wwPDB EM Validation Summary Report ⓘ

May 19, 2025 – 12:41 AM EDT

PDB ID : 8VH5 / pdb_00008vh5
EMDB ID : EMD-43235
Title : Cryo-EM structure of Rab12-LRRK2 complex in the LRRK2 dimer state
Authors : Zhu, H.; Sun, J.
Deposited on : 2023-12-30
Resolution : 4.00 Å (reported)

This is a wwPDB EM Validation Summary 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

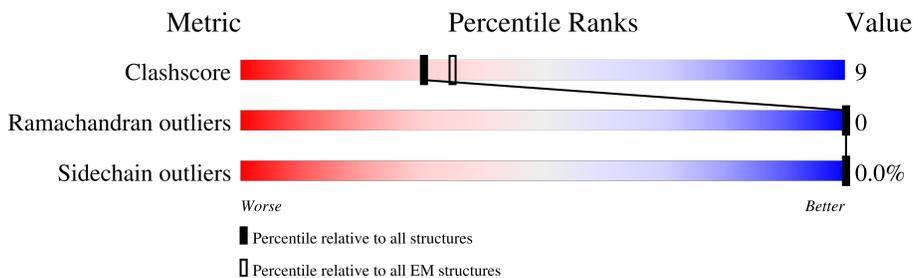
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	
1	C	2527	
2	B	176	
2	D	176	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33744 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	2221	Total	C	N	O	S	0	0
			15573	10054	2651	2783	85		
1	C	2221	Total	C	N	O	S	0	0
			15587	10060	2655	2787	85		

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Ras-related protein Rab-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	171	Total	C	N	O	S	0	0
			1200	775	199	220	6		
2	D	171	Total	C	N	O	S	0	0
			1200	775	199	220	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	101	LEU	GLN	conflict	UNP Q6IQ22
D	101	LEU	GLN	conflict	UNP Q6IQ22

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

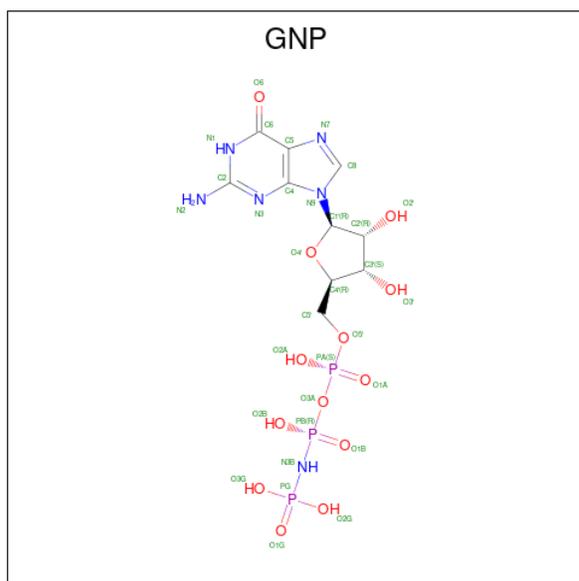
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	C	1	31	10	6	12	3	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	B	1	1	1	0
5	D	1	1	1	0

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

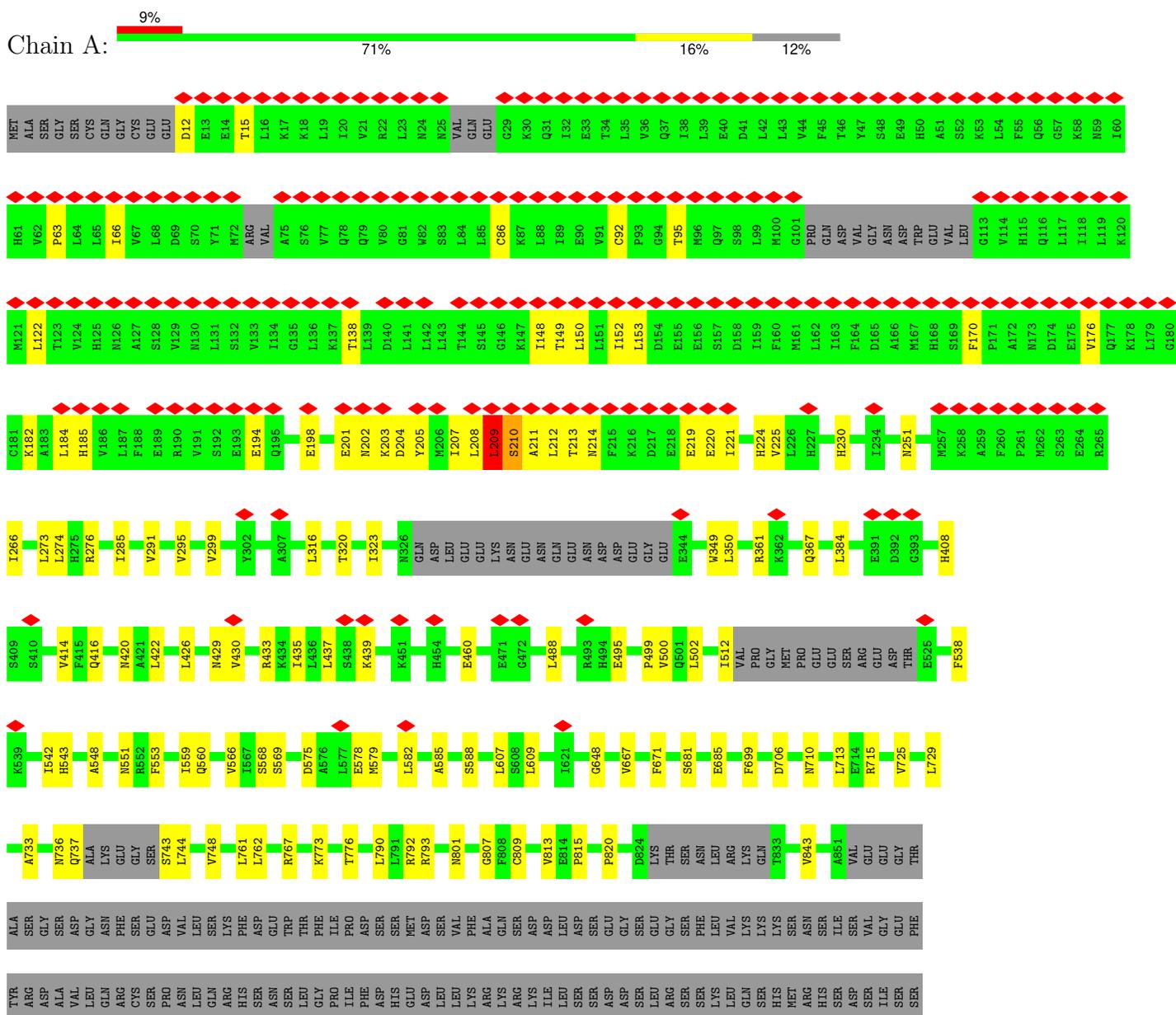


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	B	1	32	10	6	13	3	0
6	D	1	32	10	6	13	3	0

3 Residue-property plots

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

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



LEU	Q1087	M1305	Y1415	VAL	ARG	D1883	A2040	L2238	N2328	G2430
ALA	L1090	D1317	Y1419	GLU	GLU	L1870	V2043	S2244	D2329	H2433
SER	L1092	L1322	P1433	CYS	ALA	M1871	G2070	V2245	F2330	I2434
ARG	M1093	M1333	P1434	PRO	LEU	N1872	C2101	L2248	I2332	L2435
E982	G1116	L1337	M1437	HTS	P1622	D1873	L2110	L2249	L2335	V2447
Y983	K1138	M1338	I1438	P1626	Y1733	E1882	T2124	C2250	I2336	N2453
1984	E1146	M1339	K1439	I1630	W1734	F1883	S2125	R2251	E2337	I2454
1985	M1147	V1340	A1440	VAL	R1735	L1884	Q2127	SER	R2338	S2454
1986	P1169	G1346	R1441	GLU	Q1736	L1885	L2128	PHE	THR	V2455
1987	P1172	K1347	V1447	GLY	G1737	Y1889	L2137	SER	SER	N2458
1988	P1175	T1348	I1448	LEU	I1738	V1905	R2143	LYS	GLN	V2472
1989	M1176	T1349	G1451	PHE	Y1747	M1909	R2146	L2263	L2264	N2476
1991	I1177	Q1365	T1452	LYS	C1748	M1912	L2146	L2265	L2266	R2477
1992	I1192	T1368	D1455	ARG	L1749	T1912	L2151	D2269	S2352	LYS
1993	L1199	V1369	V1456	LEU	L1755	E1920	V2156	L2272	N2353	ASN
1994	L1199	V1370	S1457	ASP	H1758	E1929	V2166	F2275	I2354	THR
1995	L1199	T1371	GLN	LYS	L1763	H1929	S2166	L2277	I2354	GLU
1996	L1199	Q1372	ARG	PHE	P1768	L1932	L2169	L2278	V2357	GLY
1997	L1199	T1373	ARG	LEU	K1772	L1939	G2172	F2275	V2372	THR
1998	L1199	T1374	GLN	LEU	I1775	G1939	H2173	L2290	E2374	GLN
1999	L1199	T1375	ARG	LEU	L1787	P1942	S2166	L2291	V2374	LYS
2000	L1199	T1376	ARG	LEU	L1787	R1943	L2167	L2292	E2374	LYS
2001	L1199	T1377	ARG	LEU	L1787	M1944	L2168	L2293	V2383	GLN
2002	L1199	T1378	ARG	LEU	L1787	L1945	L2169	L2294	D2388	GLN
2003	L1199	T1379	ARG	LEU	L1787	V1946	G2172	L2295	C2389	GLN
2004	L1199	T1380	ARG	LEU	L1787	V1946	H2173	L2296	V2390	GLN
2005	L1199	T1381	ARG	LEU	L1787	V1946	G2172	L2297	L2393	GLN
2006	L1199	T1382	ARG	LEU	L1787	V1946	H2173	L2298	V2396	GLN
2007	L1199	T1383	ARG	LEU	L1787	V1946	G2172	L2299	THR	THR
2008	L1199	T1384	ARG	LEU	L1787	V1946	H2173	L2300	VAL	VAL
2009	L1199	T1385	ARG	LEU	L1787	V1946	G2172	L2301	LYS	LYS
2010	L1199	T1386	ARG	LEU	L1787	V1946	H2173	L2302	GLU	GLU
2011	L1199	T1387	ARG	LEU	L1787	V1946	G2172	L2303	ASN	ASN
2012	L1199	T1388	ARG	LEU	L1787	V1946	H2173	L2304	LYS	LYS
2013	L1199	T1389	ARG	LEU	L1787	V1946	G2172	L2305	GLU	GLU
2014	L1199	T1390	ARG	LEU	L1787	V1946	H2173	L2306	SER	SER
2015	L1199	T1391	ARG	LEU	L1787	V1946	G2172	L2307	THR	THR
2016	L1199	T1392	ARG	LEU	L1787	V1946	H2173	L2308	VAL	VAL
2017	L1199	T1393	ARG	LEU	L1787	V1946	G2172	L2309	GLN	GLN
2018	L1199	T1394	ARG	LEU	L1787	V1946	H2173	L2310	GLU	GLU
2019	L1199	T1395	ARG	LEU	L1787	V1946	G2172	L2311	K30	K30
2020	L1199	T1396	ARG	LEU	L1787	V1946	H2173	L2312	Q31	Q31
2021	L1199	T1397	ARG	LEU	L1787	V1946	G2172	L2313	I32	I32
2022	L1199	T1398	ARG	LEU	L1787	V1946	H2173	L2314	E33	E33
2023	L1199	T1399	ARG	LEU	L1787	V1946	G2172	L2315	F34	F34
2024	L1199	T1400	ARG	LEU	L1787	V1946	H2173	L2316	L35	L35
2025	L1199	T1401	ARG	LEU	L1787	V1946	G2172	L2317	V36	V36
2026	L1199	T1402	ARG	LEU	L1787	V1946	H2173	L2318	I38	I38
2027	L1199	T1403	ARG	LEU	L1787	V1946	G2172	L2319	L39	L39
2028	L1199	T1404	ARG	LEU	L1787	V1946	H2173	L2320	E40	E40
2029	L1199	T1405	ARG	LEU	L1787	V1946	G2172	L2321	D41	D41
2030	L1199	T1406	ARG	LEU	L1787	V1946	H2173	L2322	L42	L42
2031	L1199	T1407	ARG	LEU	L1787	V1946	G2172	L2323	L43	L43
2032	L1199	T1408	ARG	LEU	L1787	V1946	H2173	L2324	V44	V44
2033	L1199	T1409	ARG	LEU	L1787	V1946	G2172	L2325	F45	F45
2034	L1199	T1410	ARG	LEU	L1787	V1946	H2173	L2326	T46	T46
2035	L1199	T1411	ARG	LEU	L1787	V1946	G2172	L2327	V47	V47
2036	L1199	T1412	ARG	LEU	L1787	V1946	H2173	L2328	S48	S48
2037	L1199	T1413	ARG	LEU	L1787	V1946	G2172	L2329	E49	E49
2038	L1199	T1414	ARG	LEU	L1787	V1946	H2173	L2330	H50	H50
2039	L1199	T1415	ARG	LEU	L1787	V1946	G2172	L2331	V51	V51
2040	L1199	T1416	ARG	LEU	L1787	V1946	H2173	L2332	S52	S52
2041	L1199	T1417	ARG	LEU	L1787	V1946	G2172	L2333	K53	K53
2042	L1199	T1418	ARG	LEU	L1787	V1946	H2173	L2334	L54	L54
2043	L1199	T1419	ARG	LEU	L1787	V1946	G2172	L2335	F55	F55
2044	L1199	T1420	ARG	LEU	L1787	V1946	H2173	L2336	Q56	Q56
2045	L1199	T1421	ARG	LEU	L1787	V1946	G2172	L2337	G57	G57
2046	L1199	T1422	ARG	LEU	L1787	V1946	H2173	L2338	K58	K58
2047	L1199	T1423	ARG	LEU	L1787	V1946	G2172	L2339	N59	N59
2048	L1199	T1424	ARG	LEU	L1787	V1946	H2173	L2340	I60	I60
2049	L1199	T1425	ARG	LEU	L1787	V1946	G2172	L2341	H61	H61
2050	L1199	T1426	ARG	LEU	L1787	V1946	H2173	L2342	V62	V62
2051	L1199	T1427	ARG	LEU	L1787	V1946	G2172	L2343	P63	P63
2052	L1199	T1428	ARG	LEU	L1787	V1946	H2173	L2344	L64	L64
2053	L1199	T1429	ARG	LEU	L1787	V1946	G2172	L2345	M65	M65
2054	L1199	T1430	ARG	LEU	L1787	V1946	H2173	L2346	I66	I66
2055	L1199	T1431	ARG	LEU	L1787	V1946	G2172	L2347	V67	V67
2056	L1199	T1432	ARG	LEU	L1787	V1946	H2173	L2348	L68	L68
2057	L1199	T1433	ARG	LEU	L1787	V1946	G2172	L2349	D69	D69
2058	L1199	T1434	ARG	LEU	L1787	V1946	H2173	L2350	S70	S70
2059	L1199	T1435	ARG	LEU	L1787	V1946	G2172	L2351	Y71	Y71
2060	L1199	T1436	ARG	LEU	L1787	V1946	H2173	L2352	M72	M72
2061	L1199	T1437	ARG	LEU	L1787	V1946	G2172	L2353	ARG	ARG
2062	L1199	T1438	ARG	LEU	L1787	V1946	H2173	L2354	VAL	VAL
2063	L1199	T1439	ARG	LEU	L1787	V1946	G2172	L2355	A75	A75
2064	L1199	T1440	ARG	LEU	L1787	V1946	H2173	L2356	K18	K18
2065	L1199	T1441	ARG	LEU	L1787	V1946	G2172	L2357	V76	V76
2066	L1199	T1442	ARG	LEU	L1787	V1946	H2173	L2358	T77	T77
2067	L1199	T1443	ARG	LEU	L1787	V1946	G2172	L2359	Q78	Q78
2068	L1199	T1444	ARG	LEU	L1787	V1946	H2173	L2360	R79	R79
2069	L1199	T1445	ARG	LEU	L1787	V1946	G2172	L2361	V80	V80
2070	L1199	T1446	ARG	LEU	L1787	V1946	H2173	L2362	G81	G81
2071	L1199	T1447	ARG	LEU	L1787	V1946	G2172	L2363	L82	L82
2072	L1199	T1448	ARG	LEU	L1787	V1946	H2173	L2364	S83	S83
2073	L1199	T1449	ARG	LEU	L1787	V1946	G2172	L2365	L84	L84
2074	L1199	T1450	ARG	LEU	L1787	V1946	H2173	L2366	L85	L85
2075	L1199	T1451	ARG	LEU	L1787	V1946	G2172	L2367	C86	C86
2076	L1199	T1452	ARG	LEU	L1787	V1946	H2173	L2368	K87	K87
2077	L1199	T1453	ARG	LEU	L1787	V1946	G2172	L2369	L88	L88
2078	L1199	T1454	ARG	LEU	L1787	V1946	H2173	L2370	I89	I89
2079	L1199	T1455	ARG	LEU	L1787	V1946	G2172	L2371	E90	E90
2080	L1199	T1456	ARG	LEU	L1787	V1946	H2173	L2372	V91	V91
2081	L1199	T1457	ARG	LEU	L1787	V1946	G2172	L2373	C92	C92
2082	L1199	T1458	ARG	LEU	L1787	V1946	H2173	L2374	P93	P93
2083	L1199	T1459	ARG	LEU	L1787	V1946	G2172	L2375	Q94	Q94
2084	L1199	T1460	ARG	LEU	L1787	V1946	H2173	L2376	T95	T95
2085	L1199	T1461	ARG	LEU	L1787	V1946	G2172	L2377	M96	M96
2086	L1199	T1462	ARG	LEU	L1787	V1946	H2173	L2378	L97	L97
2087	L1199	T1463	ARG	LEU	L1787	V1946	G2172	L2379	S98	S98
2088	L1199	T1464	ARG	LEU	L1787	V1946	H2173	L2380	L99	L99
2089	L1199	T1465	ARG	LEU	L1787	V1946	G2172	L2381	M100	M100
2090	L1199	T1466	ARG	LEU	L1787	V1946	H2173	L2382	P101	P101
2091	L1199	T1467	ARG	LEU	L1787	V1946	G2172	L2383	PRO	PRO
2092	L1199	T1468	ARG	LEU	L1787	V1946	H2173	L2384	GLN	GLN
2093	L1199	T1469	ARG	LEU	L1787	V1946	G2172	L2385	ASP	ASP
2094	L1199	T1470	ARG	LEU	L1787	V1946	H2173	L2386	VAL	VAL
2095	L1199	T1471	ARG	LEU	L1787	V1946	G2172	L2387	GLY	GLY
2096	L1199	T1472	ARG	LEU	L1787	V1946	H2173	L2388	ASN	ASN
2097	L1199	T1473	ARG	LEU	L1787	V1946	G2172	L2389	TRP	TRP
2098	L1199	T1474	ARG	LEU	L1787	V1946	H2173	L2390	GLU	GLU
2099	L1199	T1475	ARG	LEU	L1787	V1946	G2172	L2391	VAL	VAL
2100	L1199	T1476	ARG	LEU	L1787	V1946	H2173	L2392	LEU	LEU
2101	L1199	T1477	ARG	LEU	L1787	V1946	G2172	L2393	G113	G113
2102	L1199	T1478	ARG	LEU	L1787	V1946	H2173	L2394	V114	V114
2103	L1199	T1479	ARG	LEU	L1787	V1946	G2172	L2395	H115	H115
2104	L1199	T1480	ARG	LEU	L1787	V1946	H2173	L2396	Q116	Q116
2105	L1199	T1481	ARG	LEU	L1787	V1946	G2172	L2397	L117	L117
2106	L1199	T1482	ARG	LEU	L1787	V1946	H21			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	77265	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 ($e^-/\text{\AA}^2$)	77.6	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.547	Depositor
Minimum map value	-1.169	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	508.288, 508.288, 508.288	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.444, 1.444, 1.444	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, GNP, ANP, MG

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	0.30	1/15858 (0.0%)	0.52	9/21732 (0.0%)
1	C	0.29	0/15871	0.50	7/21745 (0.0%)
2	B	0.25	0/1219	0.42	0/1662
2	D	0.25	0/1219	0.42	0/1662
All	All	0.29	1/34167 (0.0%)	0.51	16/46801 (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	2
1	C	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	THR	C-O	5.33	1.30	1.24

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	THR	CA-C-N	-9.31	105.17	120.72
1	A	213	THR	C-N-CA	-9.31	105.17	120.72
1	C	210	SER	CA-C-N	-7.65	108.22	122.60
1	C	210	SER	C-N-CA	-7.65	108.22	122.60
1	C	179	LEU	N-CA-C	-7.30	104.34	113.18

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	LEU	Mainchain
1	A	986	SER	Peptide
1	C	172	ALA	Mainchain
1	C	986	SER	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	15573	0	14262	254	0
1	C	15587	0	14299	263	0
2	B	1200	0	1080	25	0
2	D	1200	0	1080	25	0
3	A	28	0	12	0	0
3	C	28	0	12	0	0
4	A	31	0	13	1	0
4	C	31	0	13	2	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	32	0	13	3	0
6	D	32	0	13	3	0
All	All	33744	0	30797	569	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 9.

The worst 5 of 569 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:C:173:ASN:ND2	1:C:176:VAL:HG23	1.25	1.48
1:C:173:ASN:ND2	1:C:176:VAL:CG2	1.92	1.32
1:C:173:ASN:HD22	1:C:176:VAL:CG2	1.61	1.05
1:C:133:VAL:HG12	1:C:176:VAL:HG22	1.52	0.89
1:A:813:VAL:HG21	1:A:989:LEU:HD21	1.55	0.87

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	2177/2527 (86%)	1966 (90%)	211 (10%)	0	100	100
1	C	2177/2527 (86%)	1968 (90%)	209 (10%)	0	100	100
2	B	169/176 (96%)	154 (91%)	15 (9%)	0	100	100
2	D	169/176 (96%)	154 (91%)	15 (9%)	0	100	100
All	All	4692/5406 (87%)	4242 (90%)	450 (10%)	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	1423/2281 (62%)	1422 (100%)	1 (0%)	92	94
1	C	1428/2281 (63%)	1428 (100%)	0	100	100
2	B	104/156 (67%)	104 (100%)	0	100	100
2	D	104/156 (67%)	104 (100%)	0	100	100
All	All	3059/4874 (63%)	3058 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	A	1349	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	192	ASN
1	C	2220	GLN
1	C	551	ASN
1	C	2053	GLN
1	C	1510	ASN

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](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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$
6	GNP	B	302	5	29,34,34	1.50	7 (24%)	33,54,54	2.20	6 (18%)
4	ANP	A	2602	-	29,33,33	1.16	4 (13%)	31,52,52	0.81	1 (3%)
6	GNP	D	302	5	29,34,34	1.50	7 (24%)	33,54,54	2.19	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GDP	C	2601	-	25,30,30	0.99	1 (4%)	30,47,47	1.17	3 (10%)
4	ANP	C	2602	-	29,33,33	1.15	4 (13%)	31,52,52	0.81	1 (3%)
3	GDP	A	2601	-	25,30,30	0.98	1 (4%)	30,47,47	1.17	3 (10%)

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
6	GNP	B	302	5	-	7/14/38/38	0/3/3/3
4	ANP	A	2602	-	-	8/14/38/38	0/3/3/3
6	GNP	D	302	5	-	7/14/38/38	0/3/3/3
3	GDP	C	2601	-	-	4/12/32/32	0/3/3/3
4	ANP	C	2602	-	-	8/14/38/38	0/3/3/3
3	GDP	A	2601	-	-	4/12/32/32	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	302	GNP	PB-O3A	3.49	1.63	1.59
6	B	302	GNP	PB-O3A	3.44	1.63	1.59
6	D	302	GNP	C6-N1	3.06	1.38	1.33
6	B	302	GNP	C6-N1	3.02	1.38	1.33
3	C	2601	GDP	C6-N1	-2.93	1.33	1.37

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	302	GNP	C5-C6-N1	-8.63	111.88	123.42
6	D	302	GNP	C5-C6-N1	-8.63	111.88	123.42
6	B	302	GNP	C2-N1-C6	6.64	125.19	115.96
6	D	302	GNP	C2-N1-C6	6.62	125.17	115.96
3	C	2601	GDP	C8-N7-C5	2.93	107.53	102.55

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

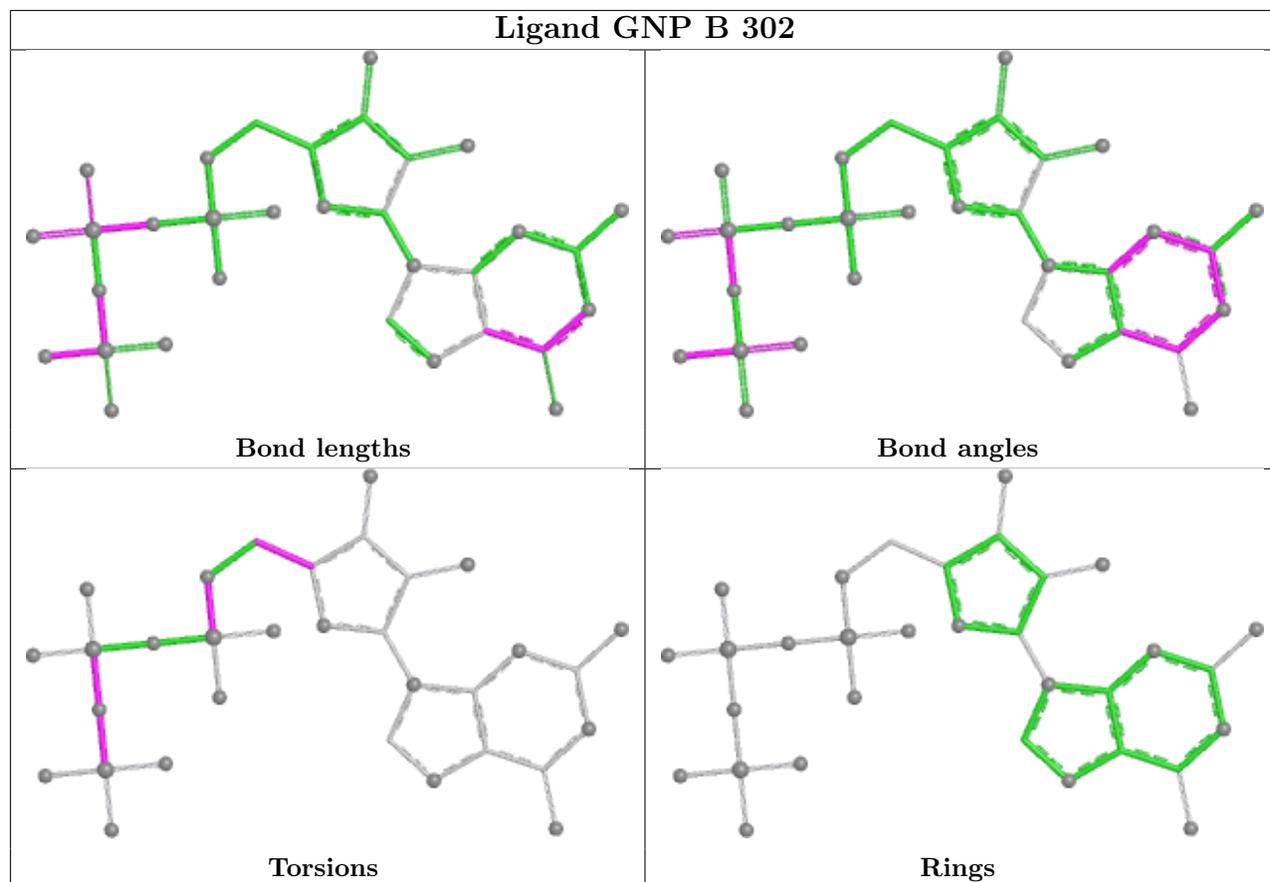
Mol	Chain	Res	Type	Atoms
3	A	2601	GDP	C5'-O5'-PA-O3A
3	A	2601	GDP	C5'-O5'-PA-O1A
3	A	2601	GDP	C5'-O5'-PA-O2A
3	C	2601	GDP	C5'-O5'-PA-O3A
3	C	2601	GDP	C5'-O5'-PA-O1A

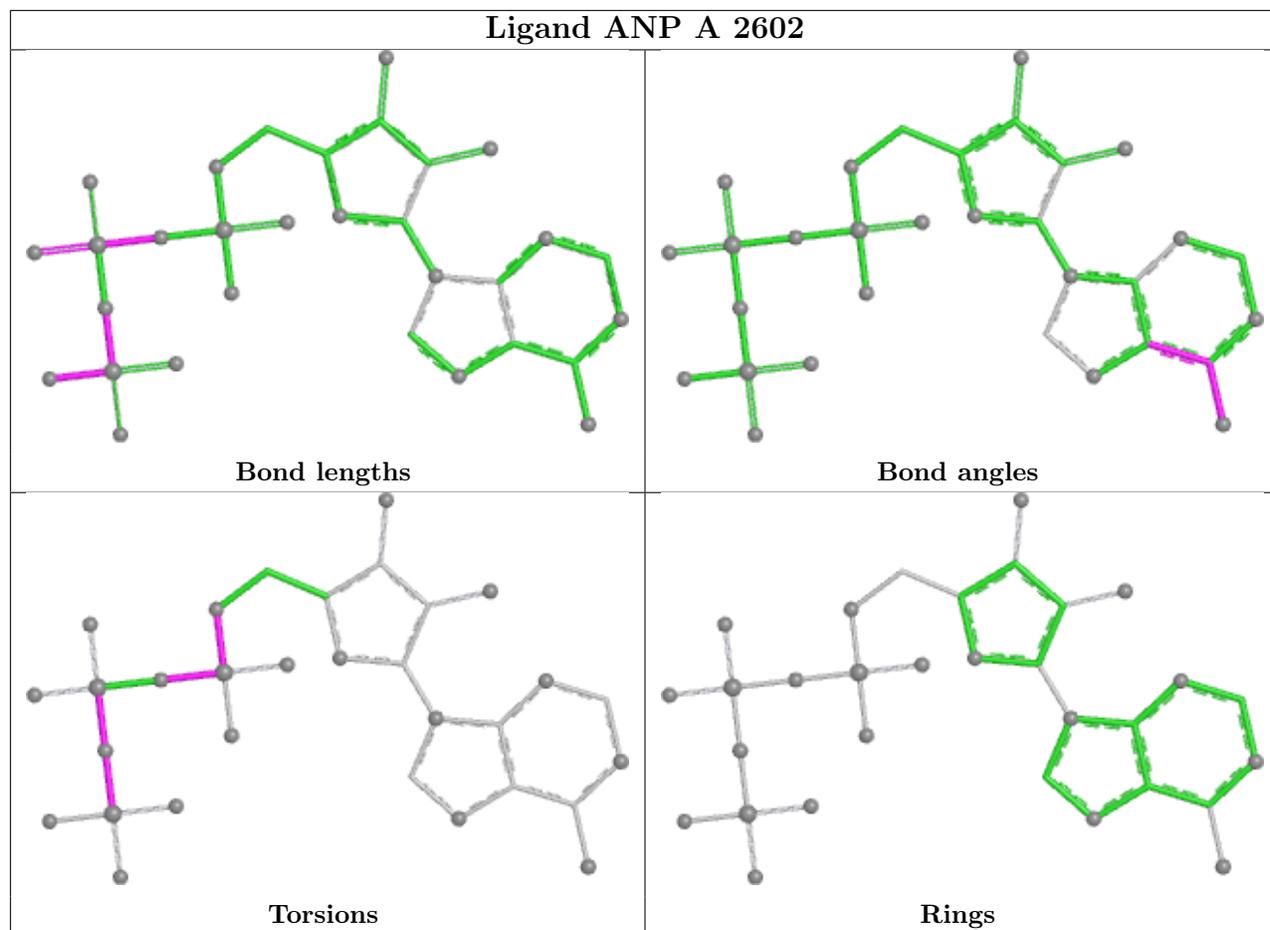
There are no ring outliers.

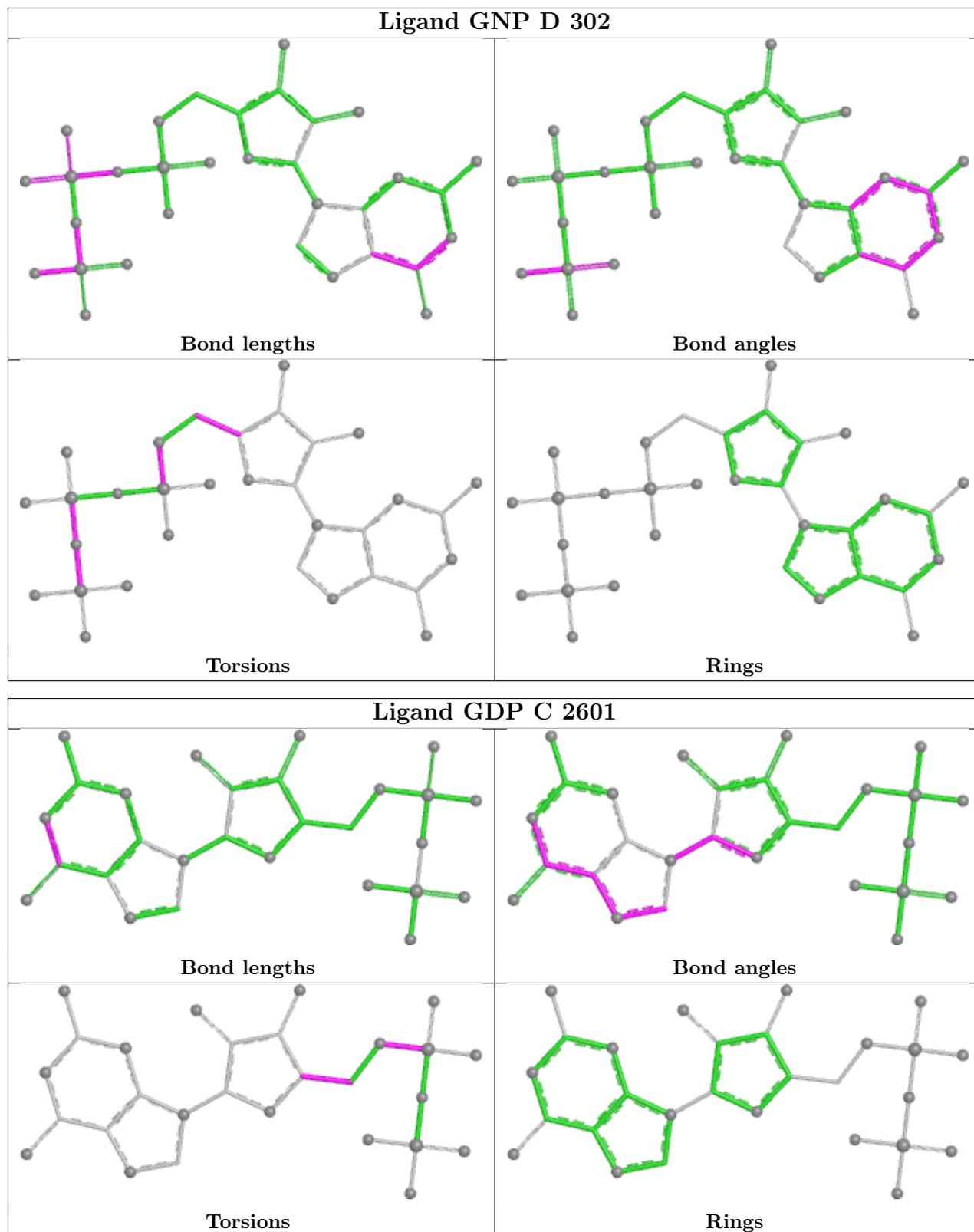
4 monomers are involved in 9 short contacts:

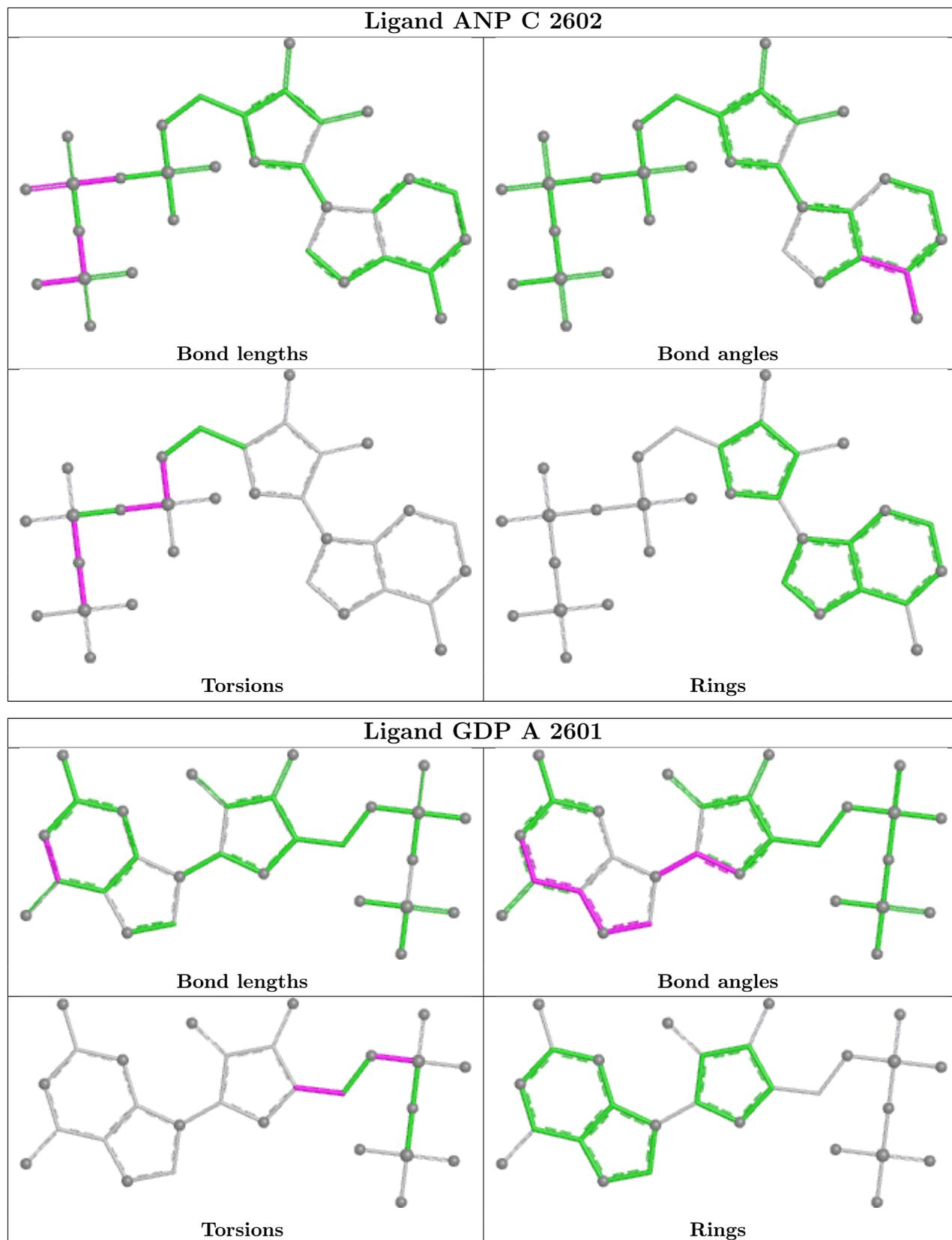
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	302	GNP	3	0
4	A	2602	ANP	1	0
6	D	302	GNP	3	0
4	C	2602	ANP	2	0

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.

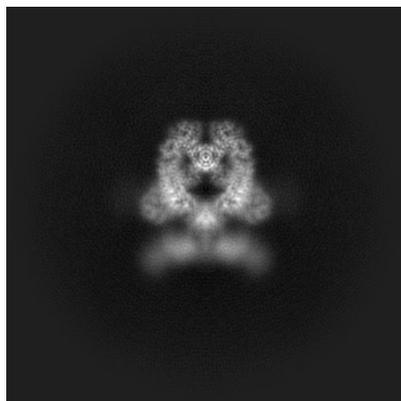
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43235. These allow visual inspection of the internal detail of the map and identification of artifacts.

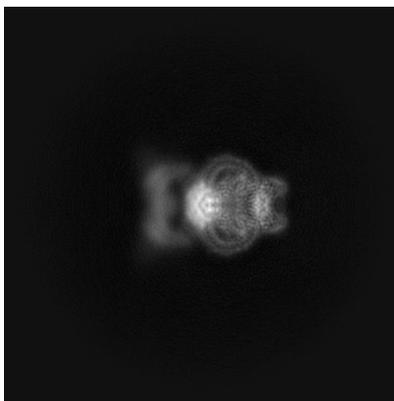
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

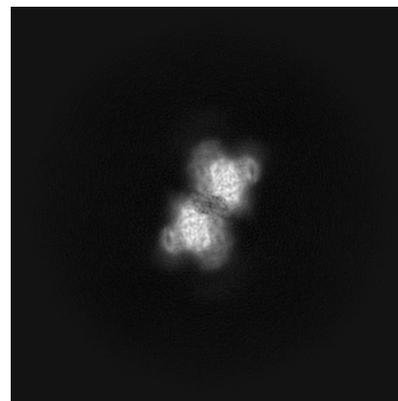
6.1.1 Primary map



X

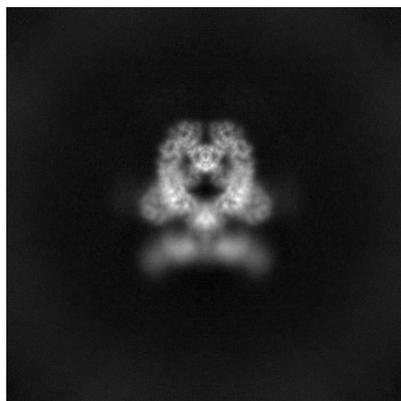


Y

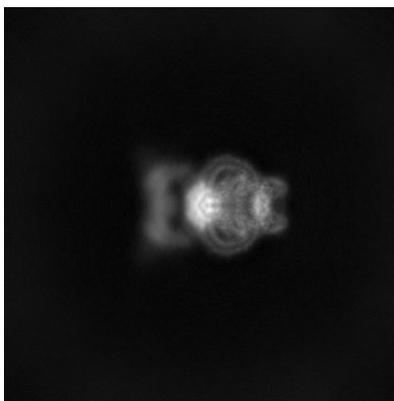


Z

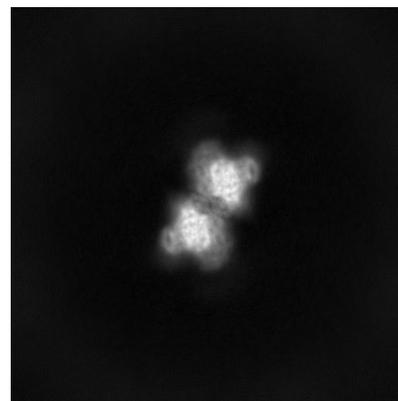
6.1.2 Raw map



X



Y

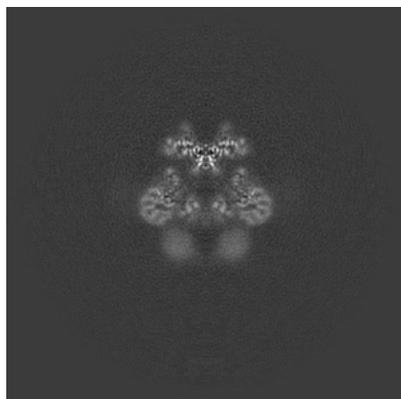


Z

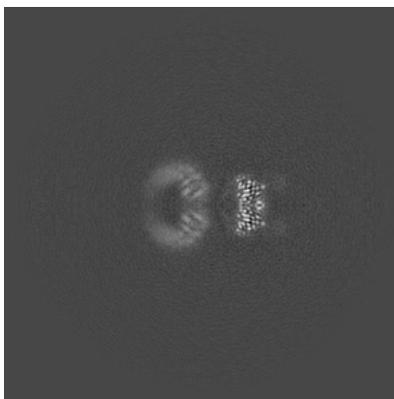
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

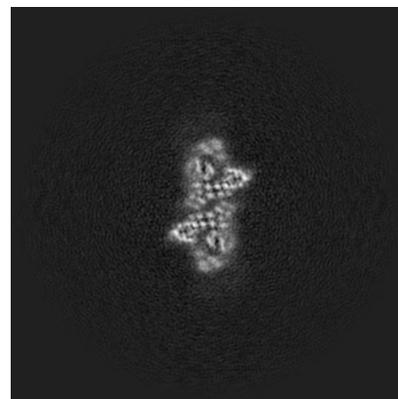
6.2.1 Primary map



X Index: 176

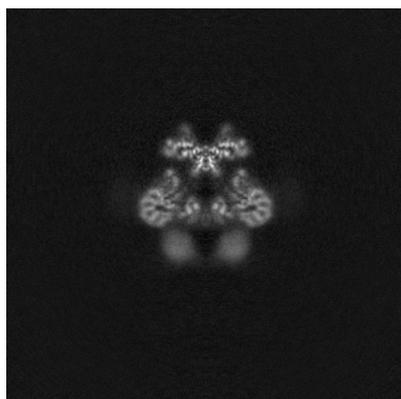


Y Index: 176

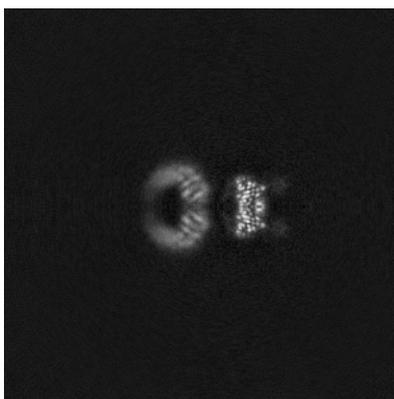


Z Index: 176

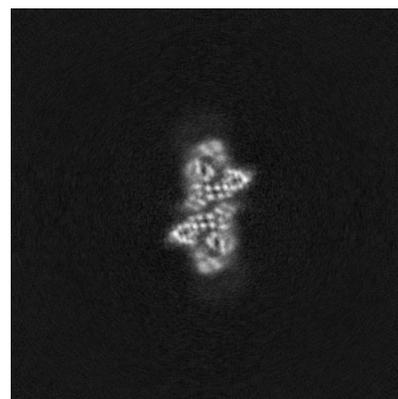
6.2.2 Raw map



X Index: 176



Y Index: 176

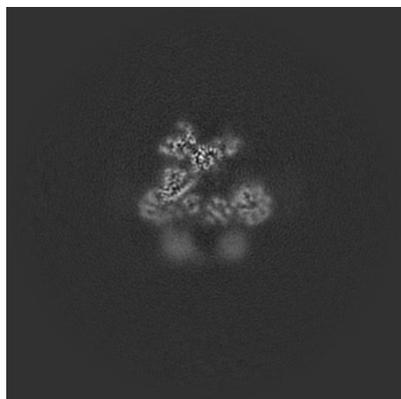


Z Index: 176

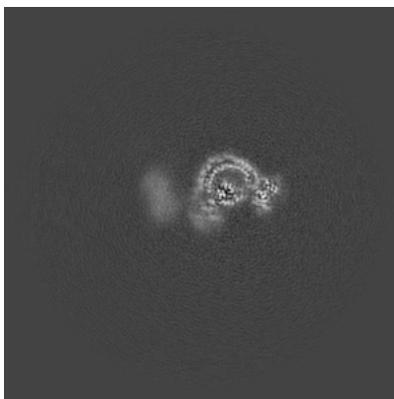
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

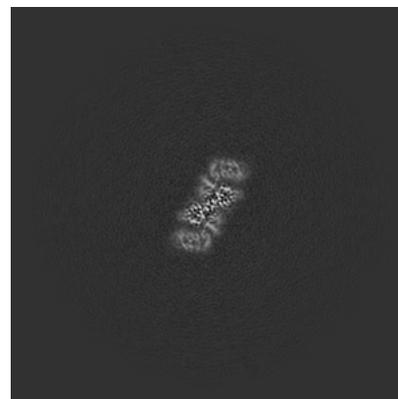
6.3.1 Primary map



X Index: 172

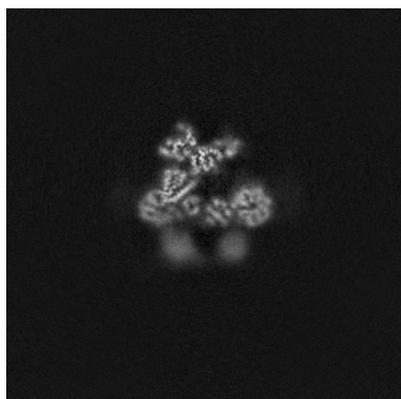


Y Index: 203

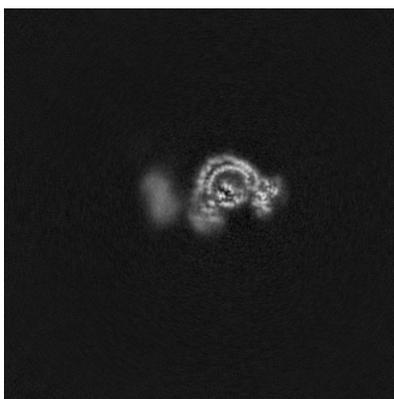


Z Index: 223

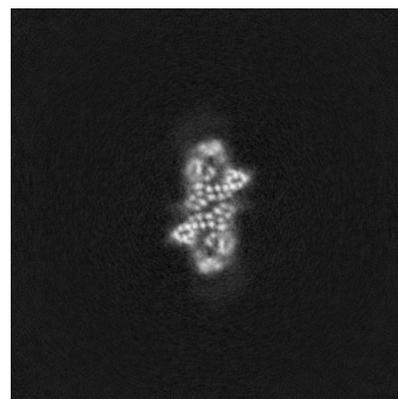
6.3.2 Raw map



X Index: 172



Y Index: 203

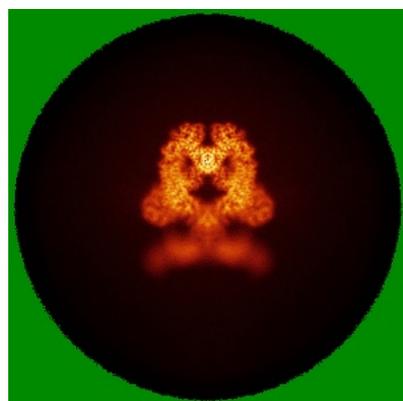


Z Index: 175

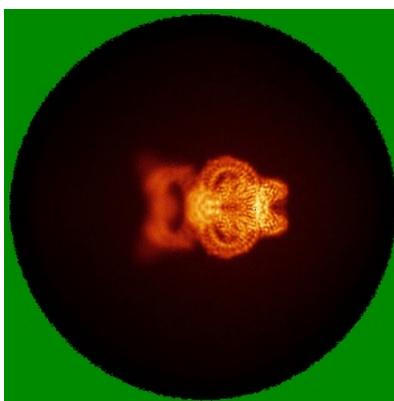
The images above show the largest variance slices of the map in three orthogonal directions.

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

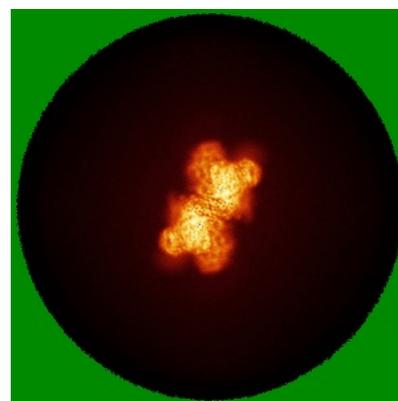
6.4.1 Primary map



X

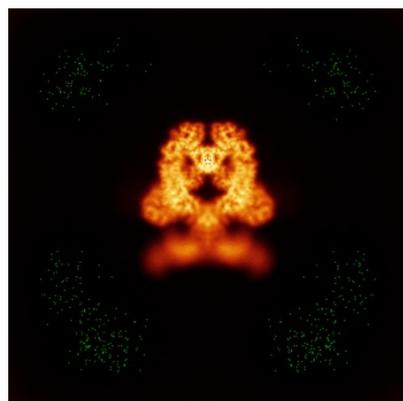


Y

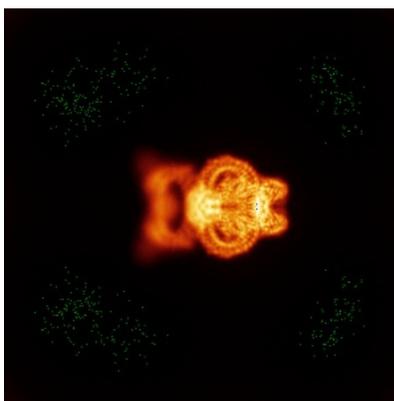


Z

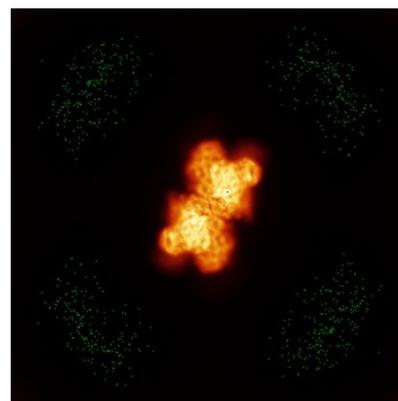
6.4.2 Raw map



X



Y



Z

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

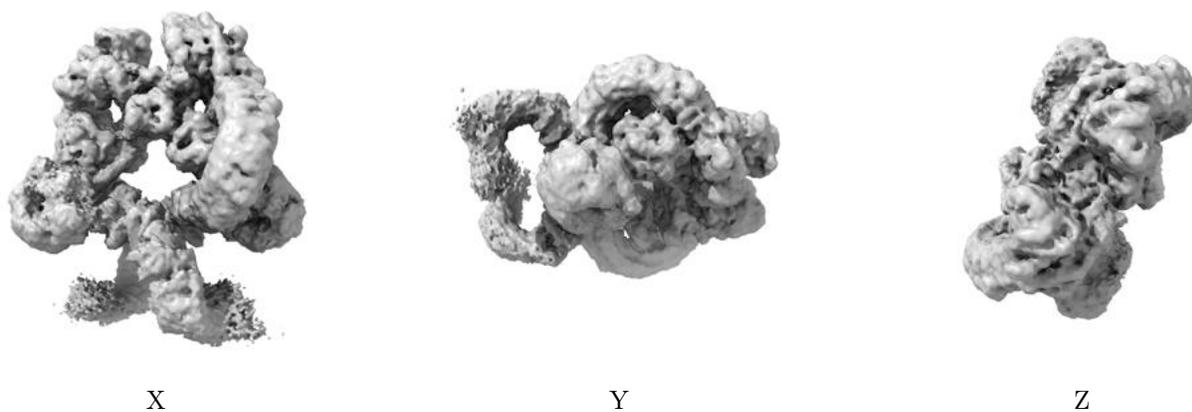
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

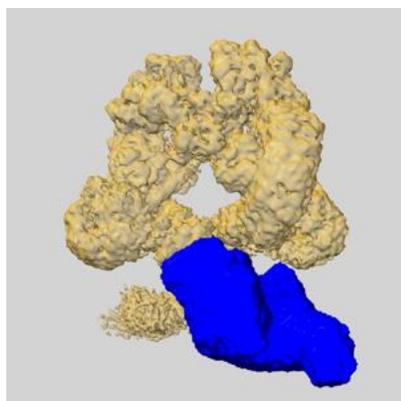
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

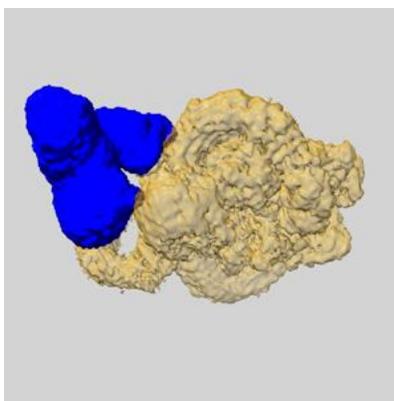
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

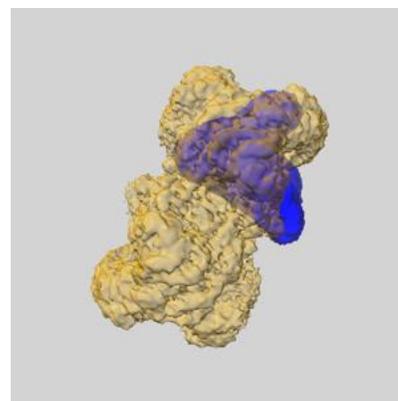
6.6.1 emd_43235_msk_1.map [i](#)



X

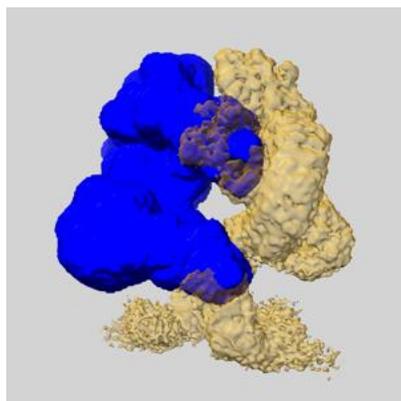


Y

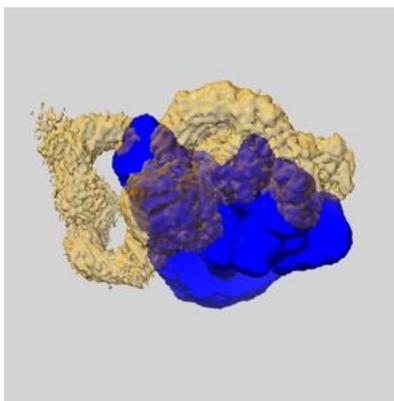


Z

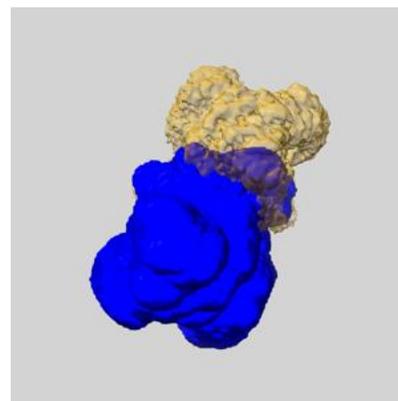
6.6.2 emd_43235_msk_2.map [i](#)



X



Y

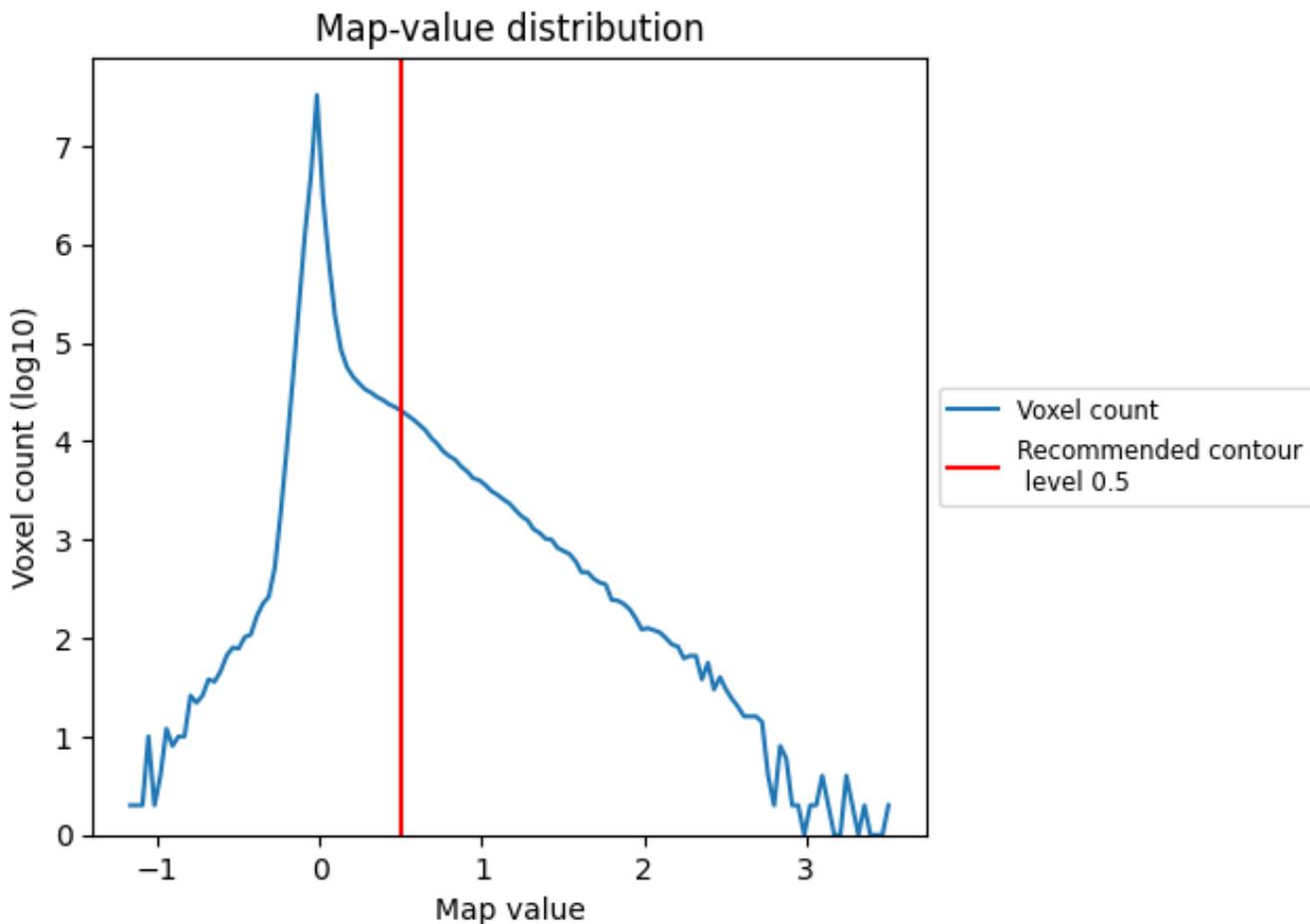


Z

7 Map analysis [i](#)

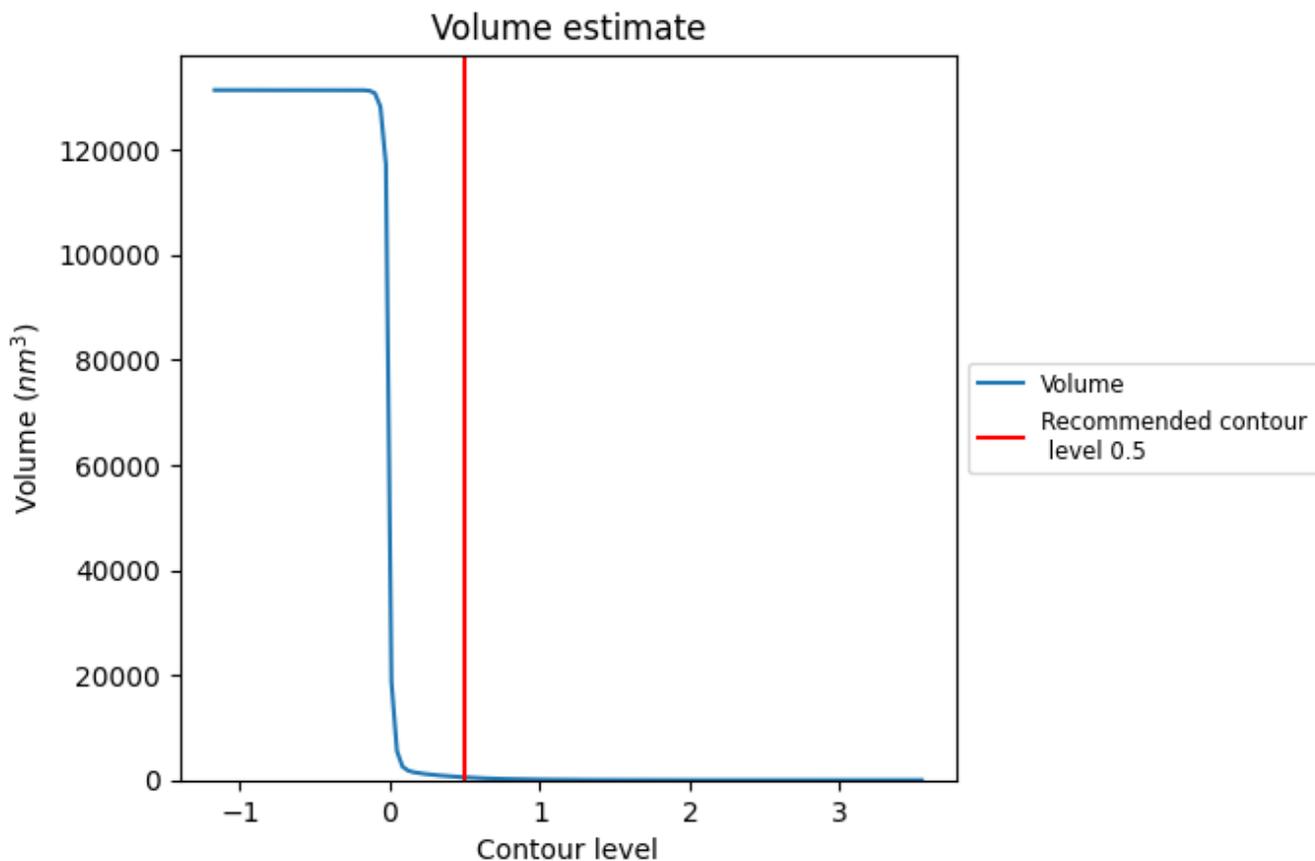
This section contains the results of statistical analysis of the map.

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.

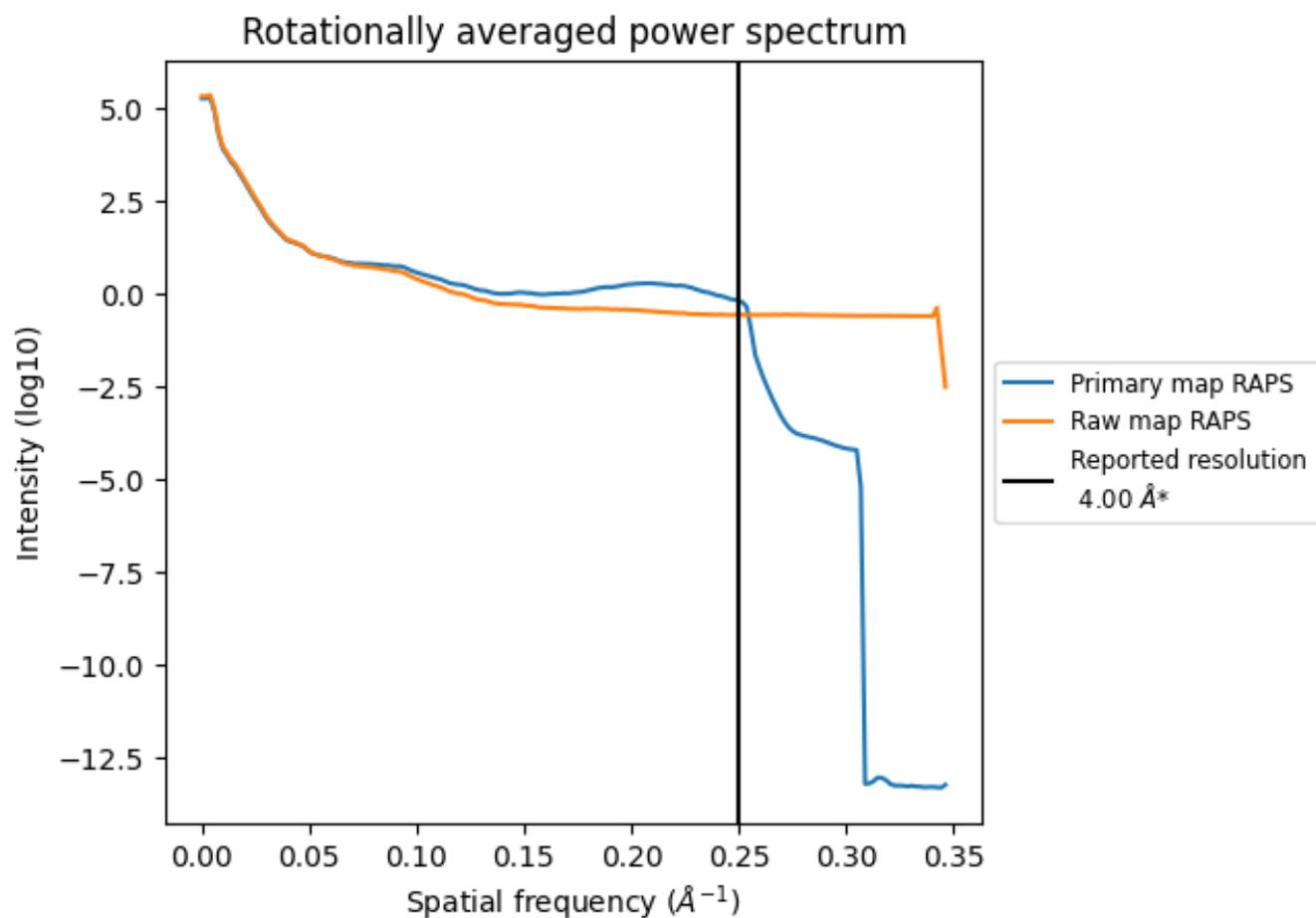
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 530 nm^3 ; this corresponds to an approximate mass of 479 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 i

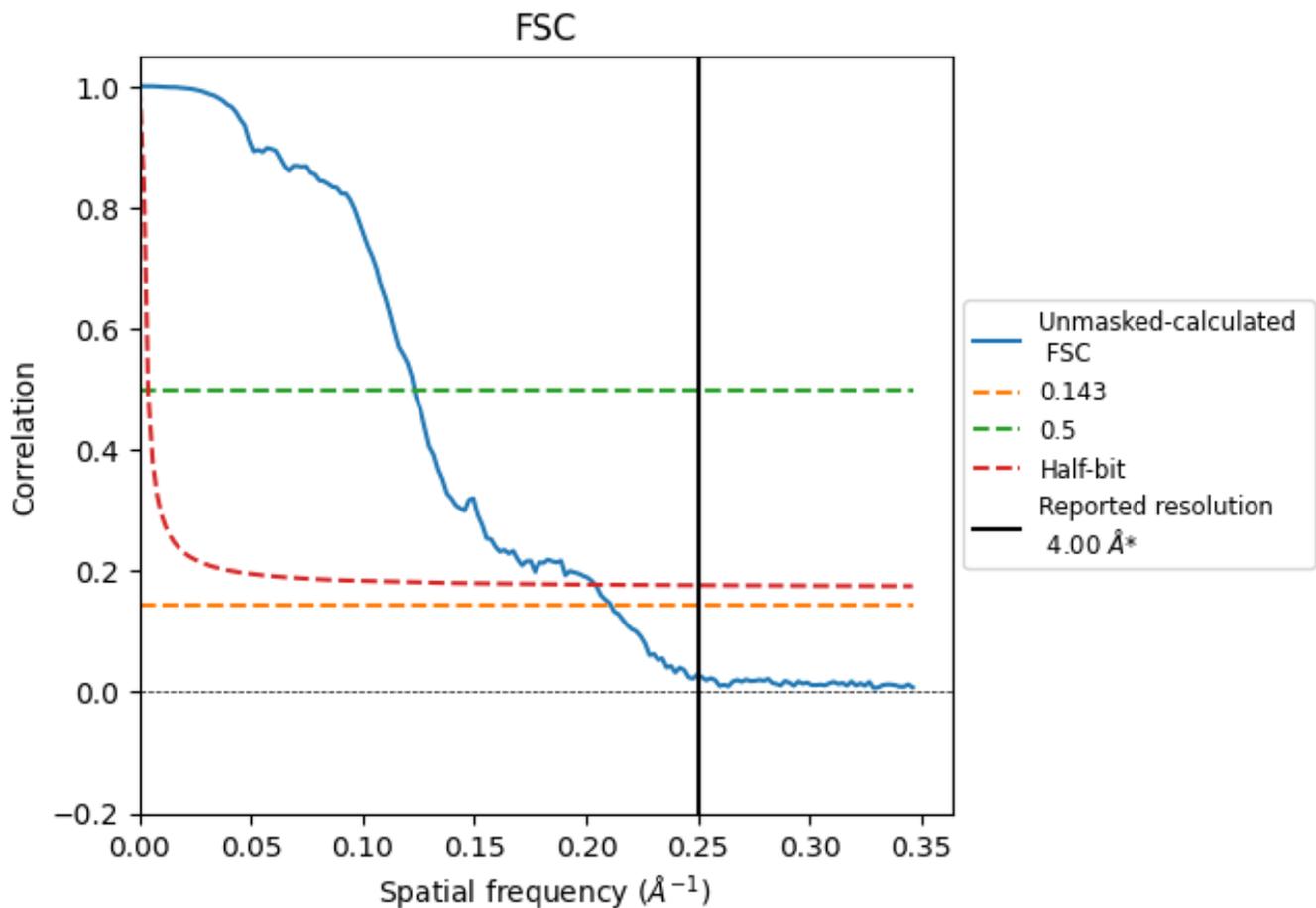


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

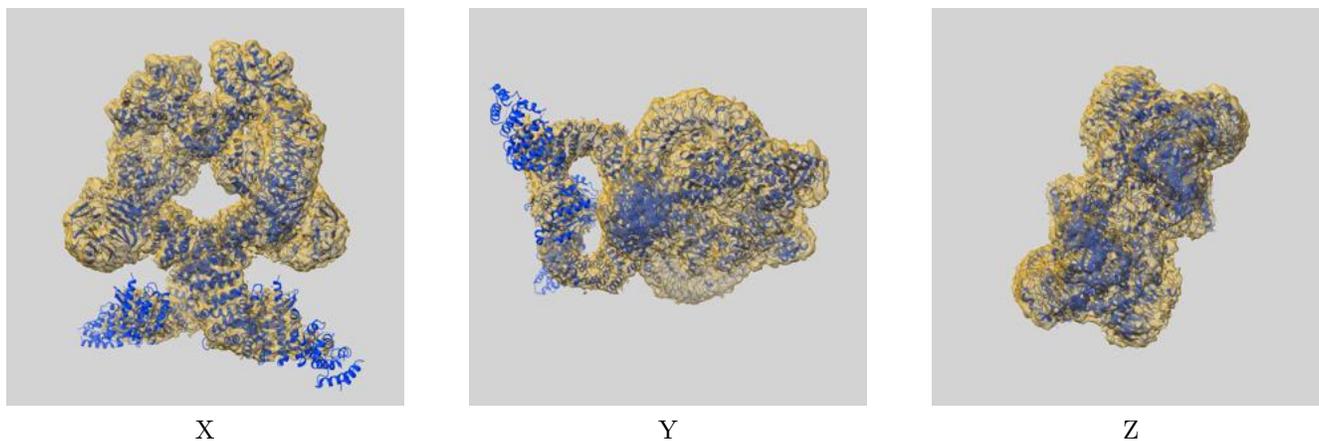
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.74	8.12	4.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.74 differs from the reported value 4.0 by more than 10 %

9 Map-model fit [i](#)

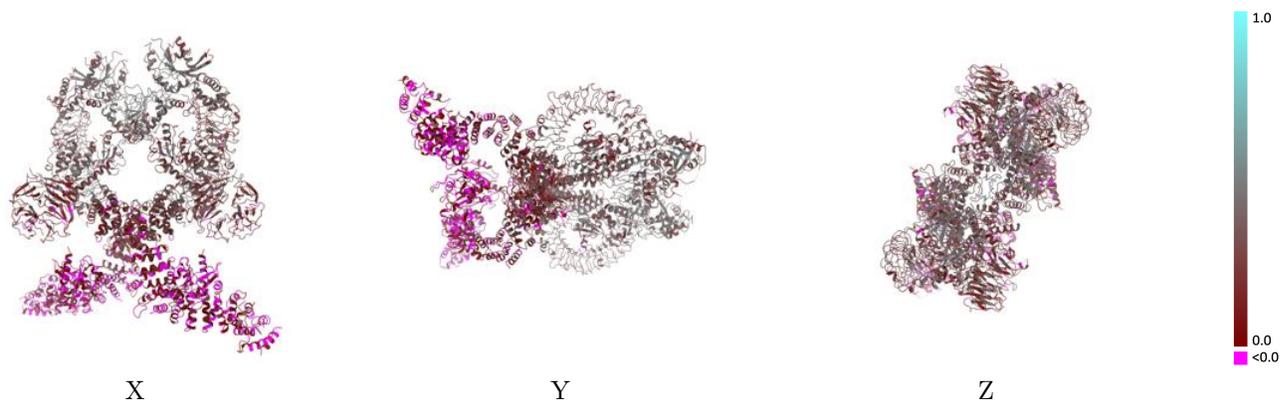
This section contains information regarding the fit between EMDB map EMD-43235 and PDB model 8VH5. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



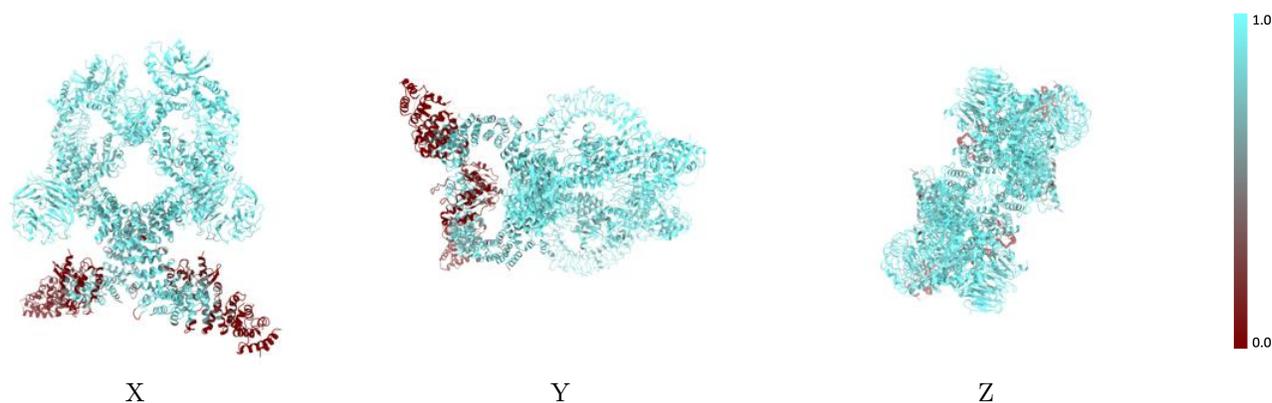
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



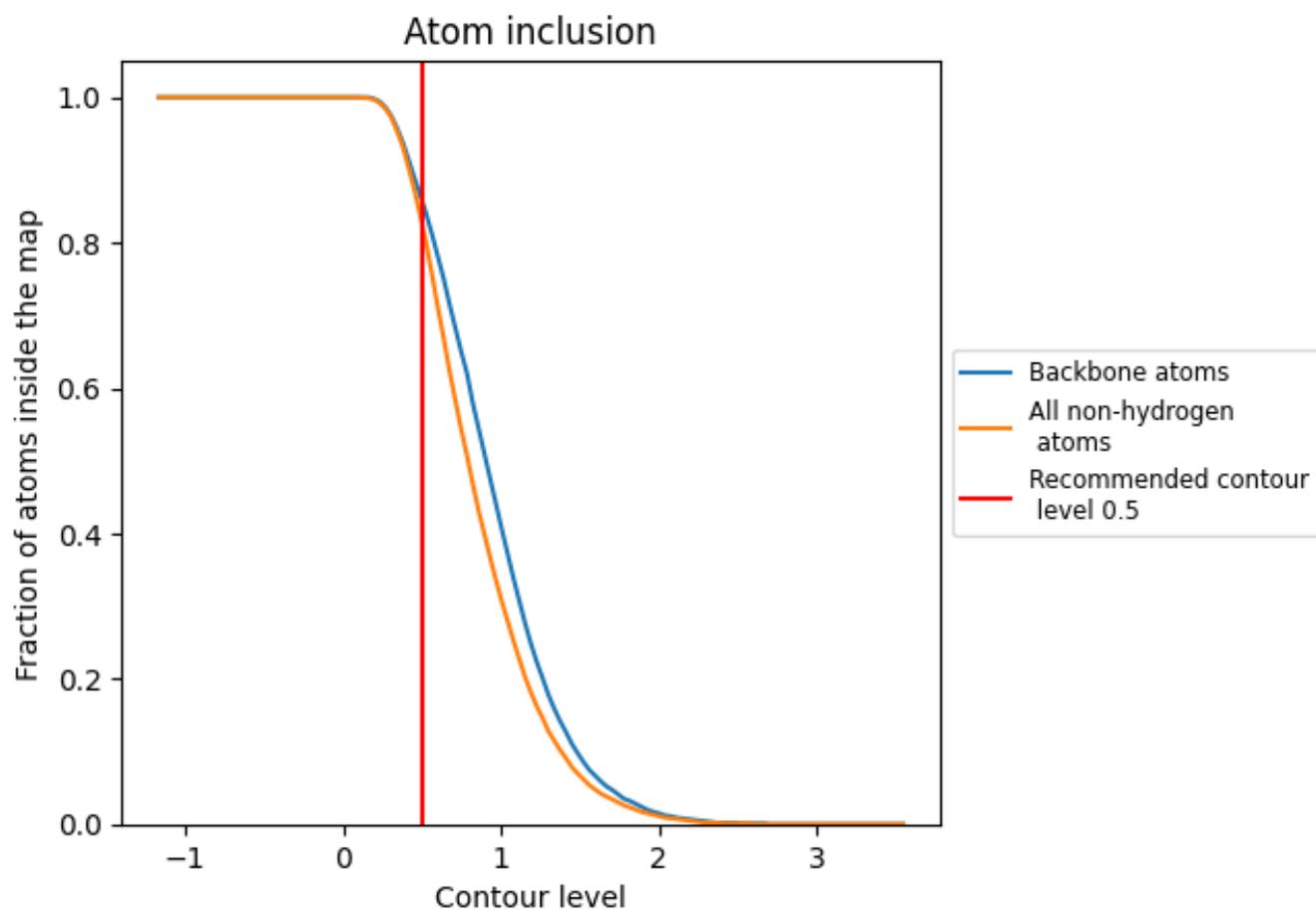
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 86% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

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	 0.8250	 0.2480
A	 0.8600	 0.2600
B	 0.3670	 0.0350
C	 0.8650	 0.2690
D	 0.3400	 0.0440

