



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

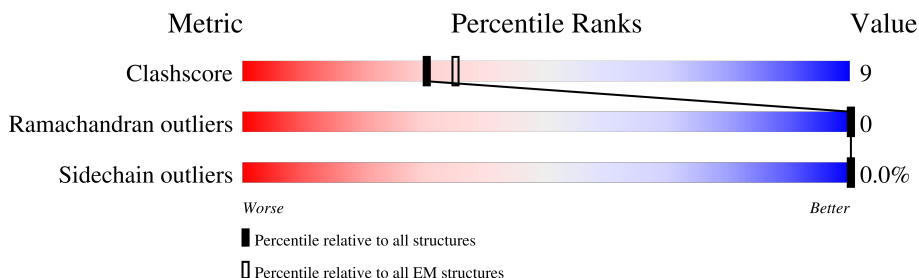
1 Overall quality at a glance

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	<div> <div>9%</div> <div>71%</div> <div>16%</div> <div>12%</div> </div>
1	C	2527	<div> <div>8%</div> <div>72%</div> <div>16%</div> <div>12%</div> </div>
2	B	176	<div> <div>60%</div> <div>75%</div> <div>22%</div> <div>•</div> </div>
2	D	176	<div> <div>64%</div> <div>74%</div> <div>23%</div> <div>•</div> </div>

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
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

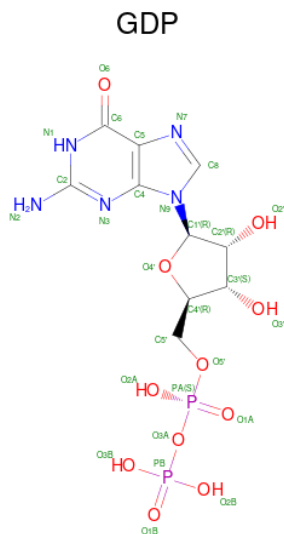
- Molecule 2 is a protein called Ras-related protein Rab-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
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:

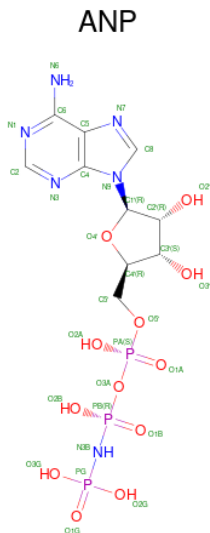
Chain	Residue	Modelled	Actual	Comment	Reference
B	101	LEU	GLN	conflict	UNP Q6IQ22
D	101	LEU	GLN	conflict	UNP Q6IQ22

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



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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$).



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

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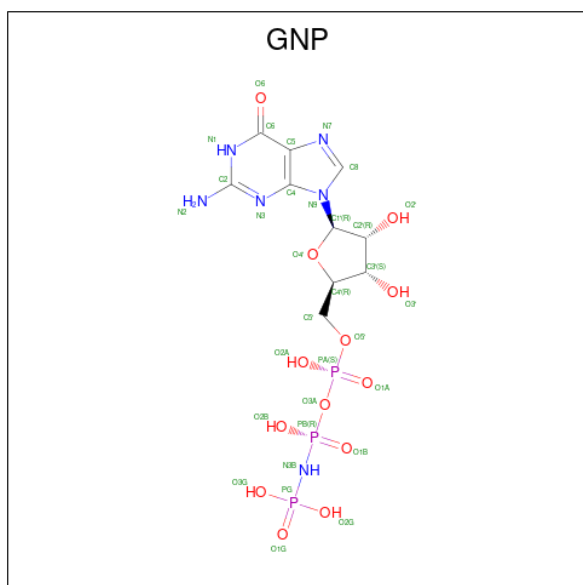
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Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			31	10	6	12	3	

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

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

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

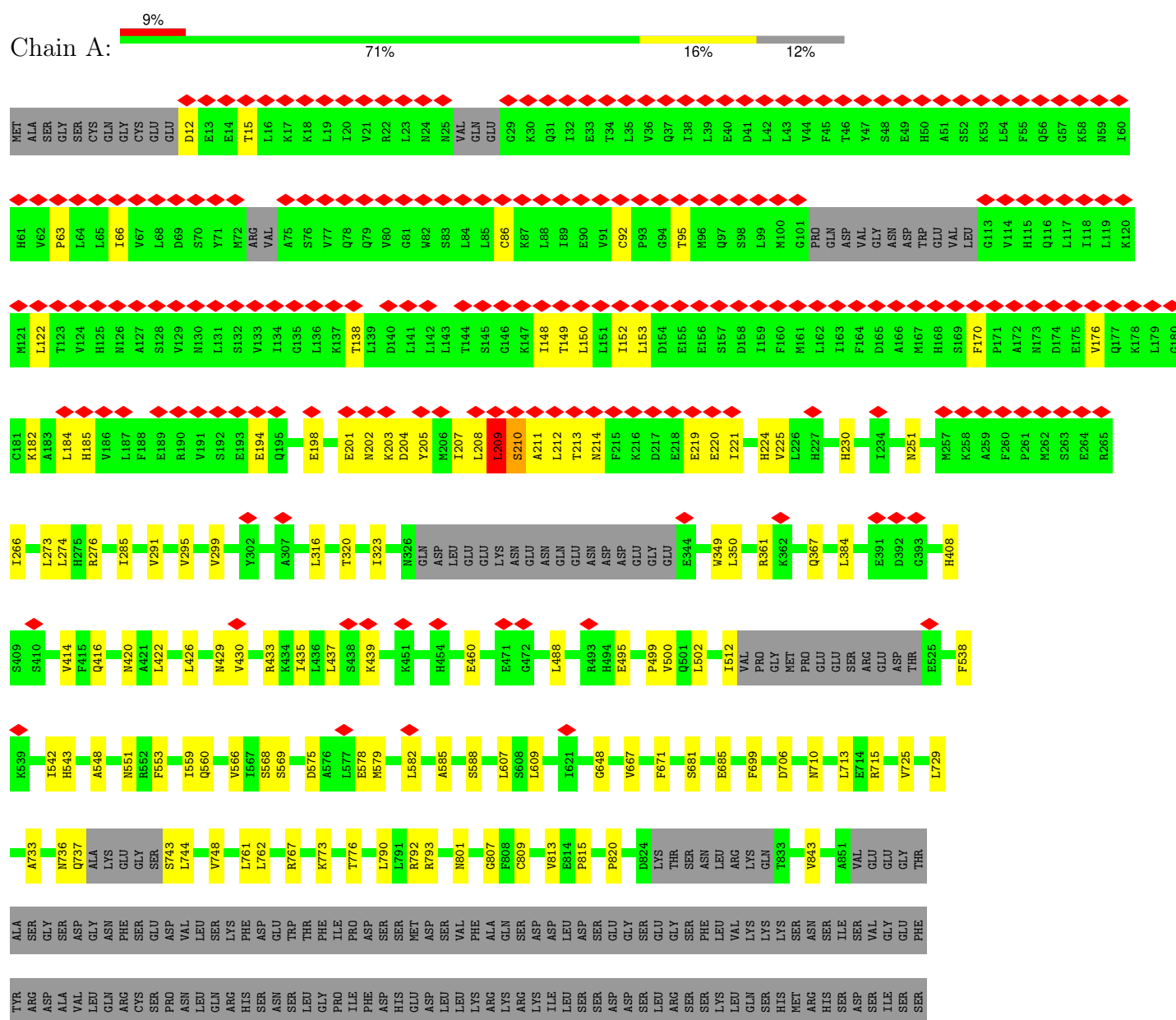


Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			32	10	6	13	3	
6	D	1	Total	C	N	O	P	0
			32	10	6	13	3	

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



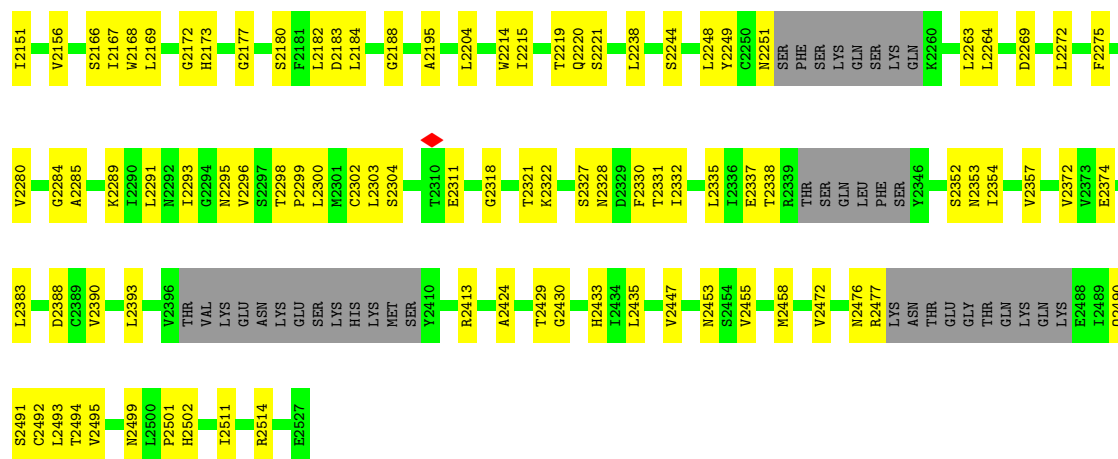
LEU	Q1087	N1305	Y1415	VAL	ARG	D1883	A2040	L2238	N2328	G2430
ALA	L1090	D1317	Y1419	GLU	GLU	L1870	V2043	S2244	D2329	H2433
SER	L1092	L1322	P1433	CYS	ALA	N1872	G2070	V2245	F2330	I2434
ARG	M1093	N1333	W1434	PRO	LEU	N1873	C2101	L2248	I2332	L2435
E982	G1116	L1337	M1437	LYS	ARG	E1882	V2107	V2249	L2335	V2447
Y983	K1138	M1338	P1439	PRO	ARG	F1883	L2110	C2250	E2337	N2453
1984	E1146	V1340	K1441	GLU	LEU	L1884	T2124	S2251	T2338	S2454
T985	N1147	G1341	R1447	VAL	THR	L1885	S2125	PHE	R2339	V2455
S986	P1169	V1342	I1448	GLU	SER	Y1884	A2126	SER	SER	N2458
1987	P1172	N1348	T1452	LYS	GLN	V1905	Q2127	LYS	GLN	V2472
D988	P1176	T1349	D1455	LYS	LYS	N1909	Q2128	GLN	Y2346	N2476
A989	M1175	T1357	V1456	ARG	THR	T1912	L2137	L2263	S2352	R2477
L1000	I1177	LYS	S1457	LYS	LEU	E1920	R2143	L2264	N2353	VAL
C1004	P1189	SER	ASP	PHE	PHE	H1929	L2146	D2269	I2354	GLU
C1005	E1190	ASP	GLY	P1642	ASP	L1932	I2151	L2272	V2357	THR
I1006	A1191	LEU	GLN	A1659	ILE	G1939	V2156	F2275	V2372	GLN
S1007	I1192	GLY	ARG	LEU	CYS	P1942	S2166	V2280	E2374	LYS
L1010	N1193	GLY	K1463	LEU	GLY	R1943	I2167	V2284	L2383	T2488
L1013	L1195	GLY	P1480	LEU	GLY	M1944	V2168	A2285	D2388	Q2490
F1014	L1198	T1368	D1484	TYR	L1787	L1945	L2169	Q2289	C2389	S2491
K1015	R1199	V1369	T1491	LEU	W1791	V1946	G2172	K2289	V2390	L2493
N1021	S1200	K1374	E1492	LEU	I1798	D1956	H2173	L2290	L2393	T2494
F1026	L1225	D1375	I1505	H1684	ASP	L1959	G2177	L2291	V2396	N2499
L1034	F1227	P1377	N1506	E1689	ILE	R1968	S2180	I2293	THR	L2500
L1037	L1237	I1378	M1510	GLY	CYS	F2181	F2181	G2294	VAL	P2501
D1041	H1251	R1381	K1512	L1694	GLY	D1980	D2182	V2295	LYS	H2502
L1042	M1255	LYS	L1517	Y1695	E1805	R1983	D2183	S2297	GLU	R2514
S1043	I1260	L1388	V1518	P1701	W1811	D1994	L2184	T2298	LYS	E2527
N1045	I1267	V1389	V1519	F1704	N1817	P1997	G2188	P2299	GLU	
S1052	D1274	L1390	C1526	R1707	E1820	A2021	A2195	W2301	SER	
Y1053	M1278	N1391	W1541	L1708	K1833	Q2022	L2204	C2302	LYS	
S1058	L1281	V1392	I1548	I1709	T1843	TTR	W2214	L2303	ASN	
C1059	R1282	W1393	F1395	E1714	P1845	CYS	I2215	L2304	GLU	
N1062	S1283	D1394	L1564	ILE	Q1846	ARG	T2219	E2311	LYS	
R1067	M1286	F1398	K1601	PRO	P1846	GLY	Q2220	G2318	THR	
I1070	E1287	R1398	T1612	TYR	R1847	ILE	S2221	T2321	SER	
D1077	K1290	F1408	VAL	LEU	L1848	LYS	G2222	K2322	GLN	
		T1410	LYS	SER	L1859	T2031	T2229	S2327	T2429	

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

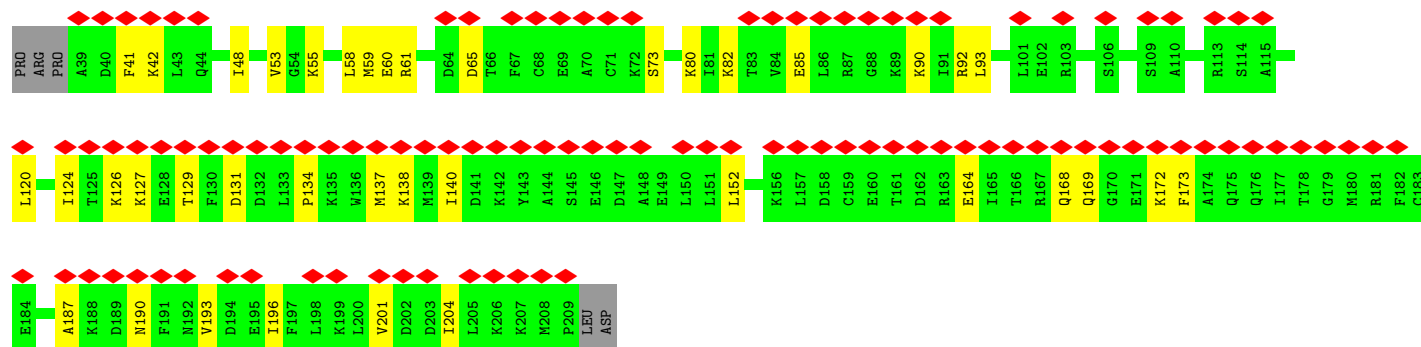
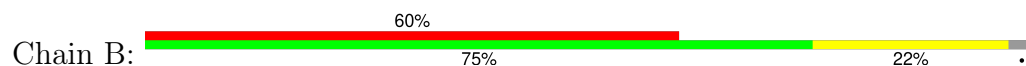


MET	ALA	SER	GLY	SER	CYS	GLN	GLY	CYS	GLU	GLU	D12	E13	E14	T15	L16	K17	K18	L19	L20	L21	R22	L23	L24	R25	VAL	GLN	GLU	G29	K30	K31	I32	I33	E33	T34	L35	V36	I37	L38	L39	E40	D41	L42	L43	V44	F45	T46	Y47	S48	ASP	ASP	TRP	GLU	VAL	VAL	LEU	G113	V114	H115	Q116	L117	I118	L119	K120																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			

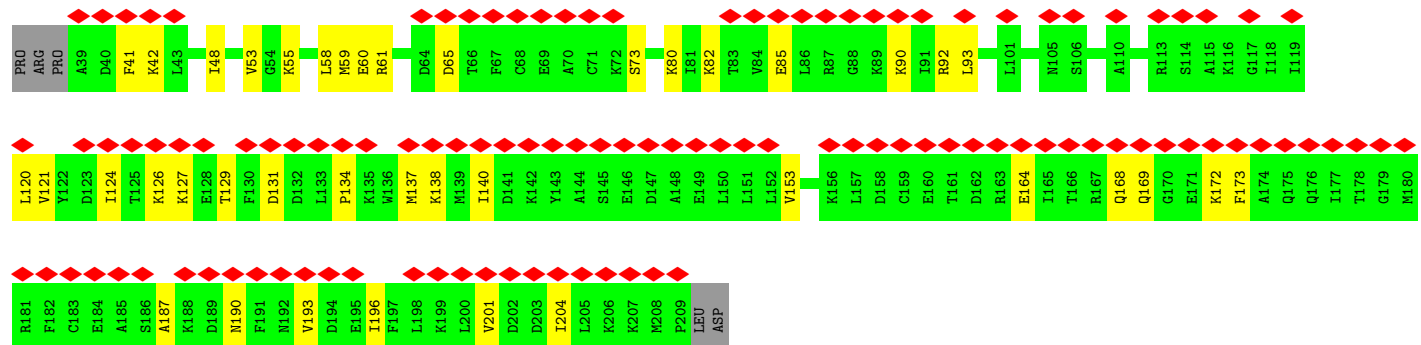
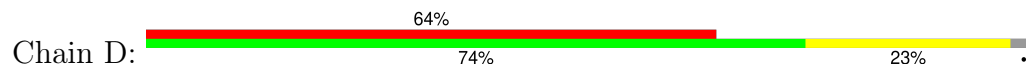
E1920	H1768	P1642	ARG	GLY	P189	A999	TRP	L762	L559	V414	I266	C181	M121
H1929	L1763	A1659	K1463	THR	F189	L1000	THR	R767	Q560	F415	I273	L184	L122
P1930	P1768	LEU	P1480	ILE	A191	S1001	PHE	R772	Q566	Q416	L274	H185	T123
S1931	P1768	ILE	D1484	V1369	I1192	C1004	PRO	R790	V566	N420	H275	H186	V124
L1932	K1772	GLY	T1491	V1373	I1193	C1005	ASP	L791	S563	L426	R276	L187	H125
G1939	I1775	GLU	E1492	K1374	L1195	S1007	SER	R792	S569	N429	I285	R190	N126
P1942	L1787	THR	I1505	W1376	L1198	L1010	MET	R793	D575	V430	V291	V191	S128
R1943	L1787	LEU	N1506	P1377	S1200	L1013	SER	N801	E578	R433	V295	S192	N129
M1944	H1791	L1668	N1506	I1378	S1200	L1013	VAL	S802	M579	R434	V299	E193	N130
V1946	H1684	H1684	N1510	L1225	L1225	N1021	PHE	I803	L582	T435	V299	E194	L131
D1956	A1689	ASP	F1511	R1381	F1227	L1034	ALA	G807	A585	S435	L316	Q195	V133
L1959	L1694	ASP	K1512	ASP	F1227	L1034	GLN	F808	A585	K439	T320	L196	V133
D1980	L1694	LYS	L1517	R1384	H1251	L1037	ASP	C809	S588	H454	I323	T197	I134
R1983	L1694	LYS	V1518	L1388	N1255	D1041	LEU	V813	S588	H454	I323	E198	G135
P1997	L1694	LYS	V1518	V1389	N1255	D1041	ASP	E814	L607	E460	F324	F199	L136
H1998	L1694	LYS	V1518	L1390	I1260	H1043	SER	P815	S608	E460	L325	V200	K137
A2021	L1694	LYS	V1518	N1391	D1274	N1045	GLY	P820	L609	E471	N326	E201	T138
T2022	L1694	LYS	V1518	V1392	D1274	N1045	SER	P820	G648	G472	GLN	N202	L139
CYS	L1694	LYS	V1518	V1393	N1278	S1052	GLY	D824	V667	G472	ASP	K203	D140
ARG	L1694	LYS	V1518	D1394	N1278	S1052	GLY	D824	V667	G472	LEU	D204	L141
MET	L1694	LYS	V1518	F1395	L1281	S1058	SER	LYS	V667	L488	GLU	Y205	L142
ILE	L1694	LYS	V1518	R1398	L1281	S1058	PHE	THR	V667	L488	GLU	M206	L143
LYS	L1694	LYS	V1518	R1398	L1281	S1058	LEU	SER	V667	L488	GLU	L207	T144
T2031	L1694	LYS	V1518	R1398	L1281	S1058	VAL	ASN	F671	E495	ASN	L208	L144
A2040	L1694	LYS	V1518	R1398	L1281	S1058	LYS	LEU	F671	E495	GLU	L209	S145
V2043	L1694	LYS	V1518	R1398	L1281	S1058	GLN	ARG	Q686	P499	ASN	L209	G146
G2070	L1694	LYS	V1518	R1398	L1281	S1058	LYS	GLN	D706	V500	GLN	S210	G147
V2107	L1694	LYS	V1518	R1398	L1281	S1058	ASN	GLN	Y707	Q501	ASN	A211	I148
L2110	L1694	LYS	V1518	R1398	L1281	S1058	SER	ASN	N710	I512	ASP	L212	I149
T2124	L1694	LYS	V1518	R1398	L1281	S1058	ILE	VAL	L713	VAL	ASP	T213	L150
S2125	L1694	LYS	V1518	R1398	L1281	S1058	VAL	GLU	E714	GLY	GLY	N214	L151
A2126	L1694	LYS	V1518	R1398	L1281	S1058	GLY	GLY	R715	GLY	GLY	F215	I152
Q2127	L1694	LYS	V1518	R1398	L1281	S1058	THR	THR	V725	PRO	W349	K216	L153
L2137	L1694	LYS	V1518	R1398	L1281	S1058	ALA	GLY	L729	GLU	L350	D217	D154
T2141	L1694	LYS	V1518	R1398	L1281	S1058	ASP	GLY	A733	SER	R361	E218	E155
R2142	L1694	LYS	V1518	R1398	L1281	S1058	VAL	ASP	L737	ARG	Q367	E219	E156
L2143	L1694	LYS	V1518	R1398	L1281	S1058	LEU	ASP	N736	ASP	I221	E220	S157
L2143	L1694	LYS	V1518	R1398	L1281	S1058	GLN	GLY	Q737	THR	V225	D158	D158
L2143	L1694	LYS	V1518	R1398	L1281	S1058	ARG	PHE	ALA	E525	L384	I159	I159
L2143	L1694	LYS	V1518	R1398	L1281	S1058	CYS	SER	LYS	F538	E391	L229	F160
L2143	L1694	LYS	V1518	R1398	L1281	S1058	SER	GLU	GLU	K339	D392	H230	M161
L2143	L1694	LYS	V1518	R1398	L1281	S1058	PRO	ASP	GLY	E525	G393	I234	L162
L2143	L1694	LYS	V1518	R1398	L1281	S1058	ASN	VAL	SER	E525	G393	I252	I163
L2143	L1694	LYS	V1518	R1398	L1281	S1058	LEU	LEU	S743	H408	S409	I252	F164
L2143	L1694	LYS	V1518	R1398	L1281	S1058	GLN	SER	L744	A548	S410	E255	D165
L2143	L1694	LYS	V1518	R1398	L1281	S1058	ARG	LYS	V748	N551	S411	A256	A166
L2143	L1694	LYS	V1518	R1398	L1281	S1058	HIS	PHE	L761	R552	E264	M167	M167
L2143	L1694	LYS	V1518	R1398	L1281	S1058	SER	ASP	L761	R553	E264	H168	M167
L2143	L1694	LYS	V1518	R1398	L1281	S1058	ASN	GLU	L761	R553	E264	S169	S169
L2143	L1694	LYS	V1518	R1398	L1281	S1058	ASN	GLU	L761	R553	E264	F170	F170
L2143	L1694	LYS	V1518	R1398	L1281	S1058	ASN	GLU	L761	R553	E264	P171	P171
L2143	L1694	LYS	V1518	R1398	L1281	S1058	ASN	GLU	L761	R553	E264	N173	N173
L2143	L1694	LYS	V1518	R1398	L1281	S1058	ASN	GLU	L761	R553	E264	D174	D174
L2143	L1694	LYS	V1518	R1398	L1281	S1058	ASN	GLU	L761	R553	E264	E175	E175
L2143	L1694	LYS	V1518	R1398	L1281	S1058	ASN	GLU	L761	R553	E264	V176	V176
L2143	L1694	LYS	V1518	R1398	L1281	S1058	ASN	GLU	L761	R553	E264	Q177	Q177
L2143	L1694	LYS	V1518	R1398	L1281	S1058	ASN	GLU	L761	R553	E264	K178	K178
L2143	L1694	LYS	V1518	R1398	L1281	S1058	ASN	GLU	L761	R553	E264	L179	L179
L2143	L1694	LYS	V1518	R1398	L1281	S1058	ASN	GLU	L761	R553	E264	G180	G180



• Molecule 2: Ras-related protein Rab-12



• Molecule 2: Ras-related protein Rab-12



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 ⓘ

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:

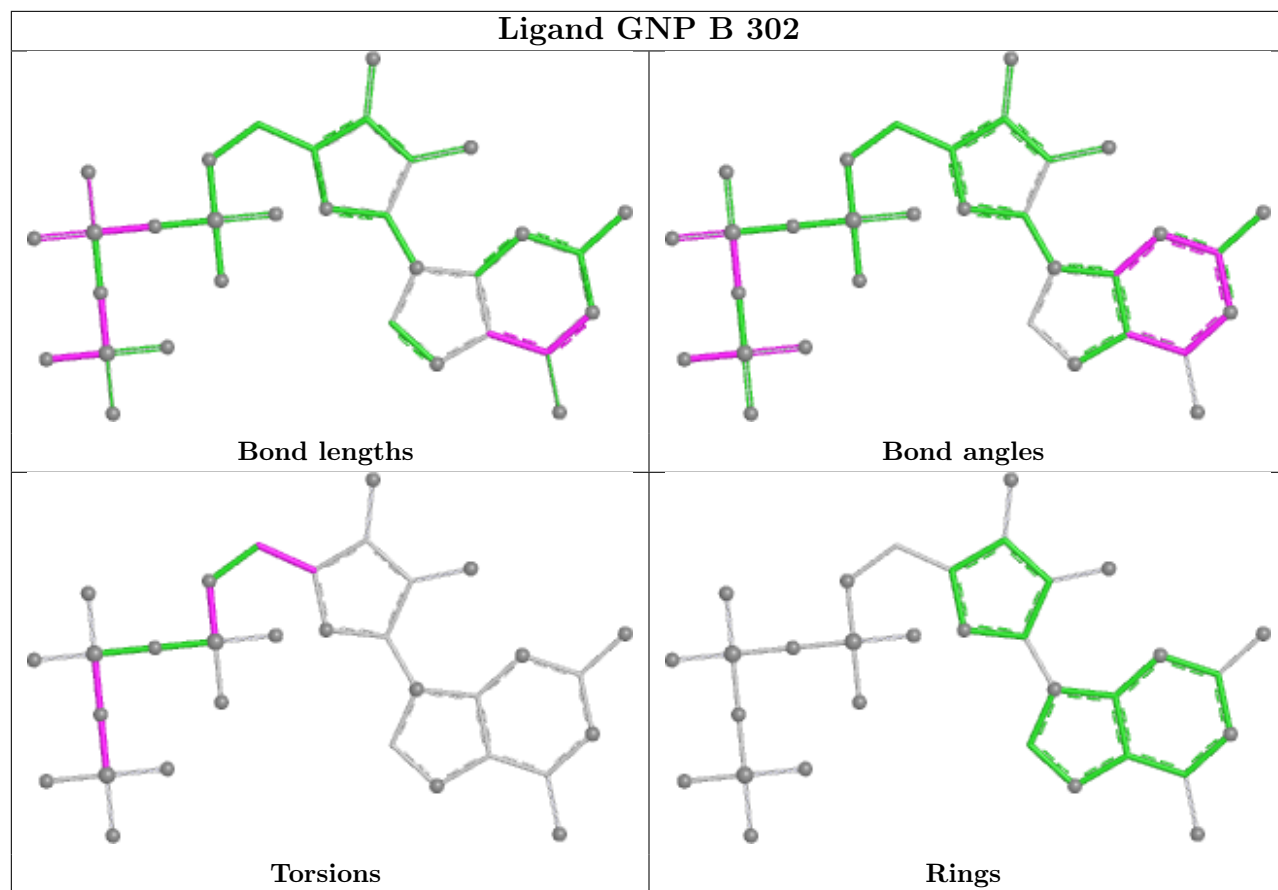
Mol	Chain	Res	Type	Atoms
3	A	2601	GDP	C5'-O5'-PA-O3A
3	A	2601	GDP	C5'-O5'-PA-O1A
3	A	2601	GDP	C5'-O5'-PA-O2A
3	C	2601	GDP	C5'-O5'-PA-O3A
3	C	2601	GDP	C5'-O5'-PA-O1A

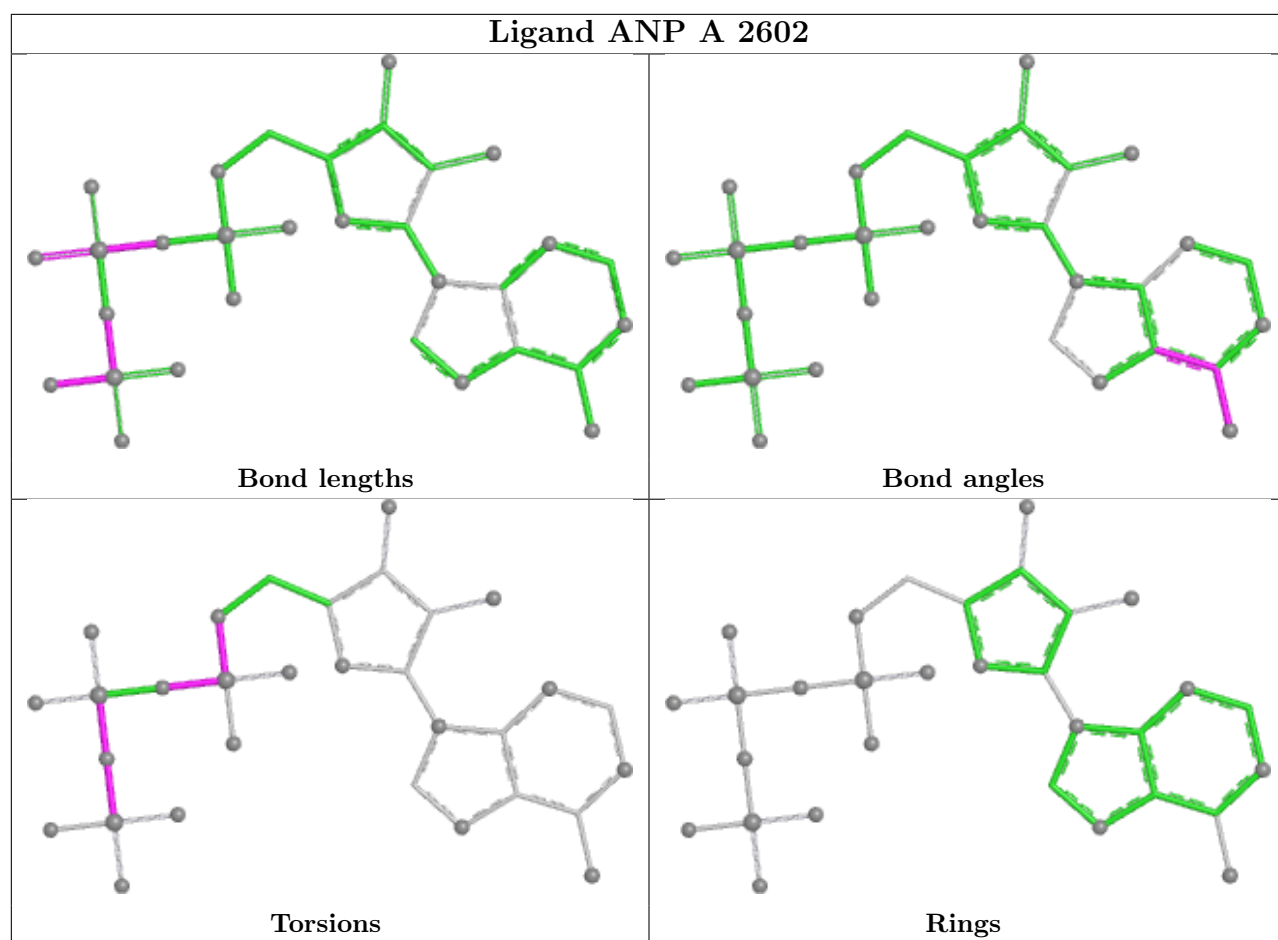
There are no ring outliers.

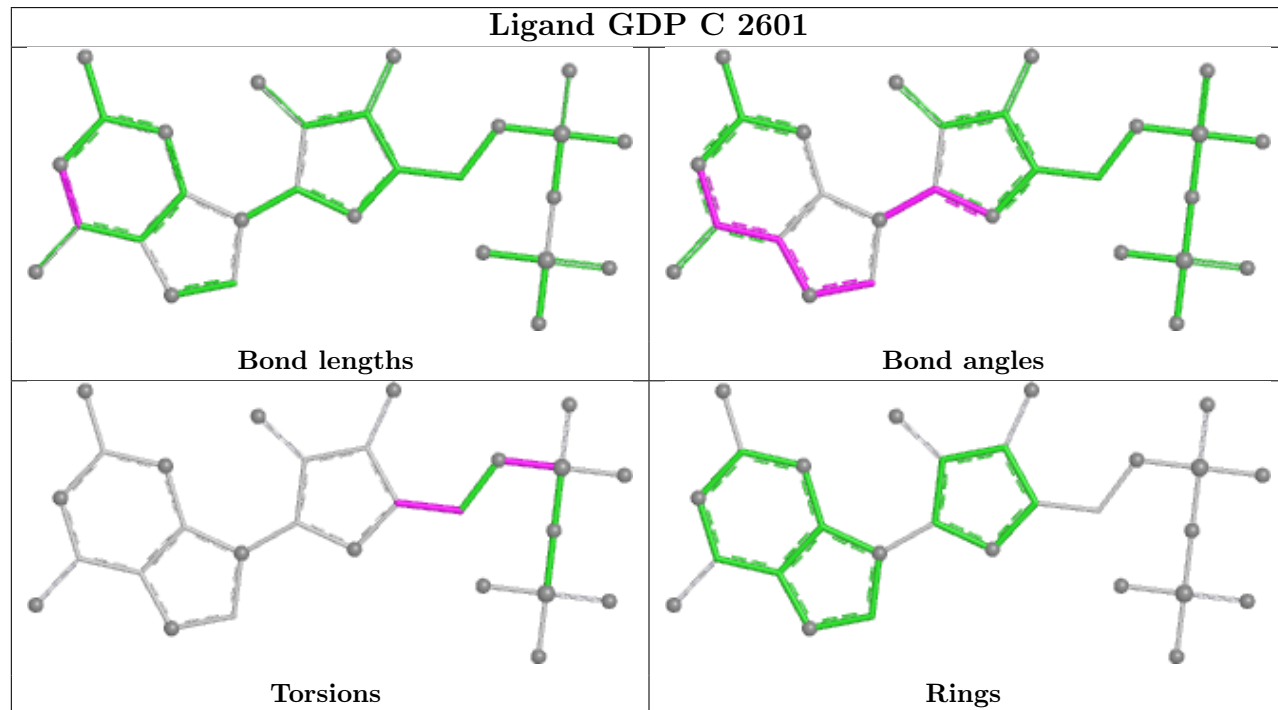
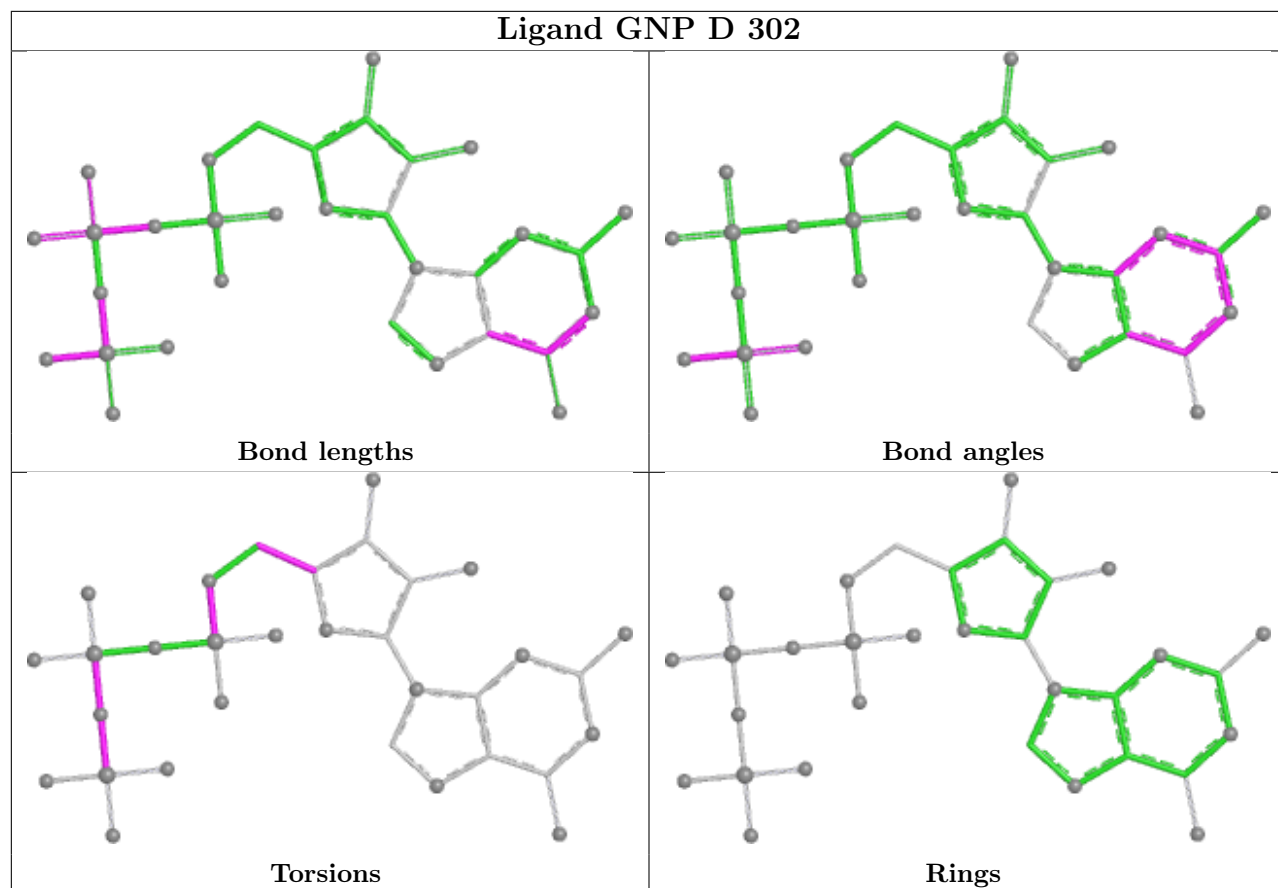
4 monomers are involved in 9 short contacts:

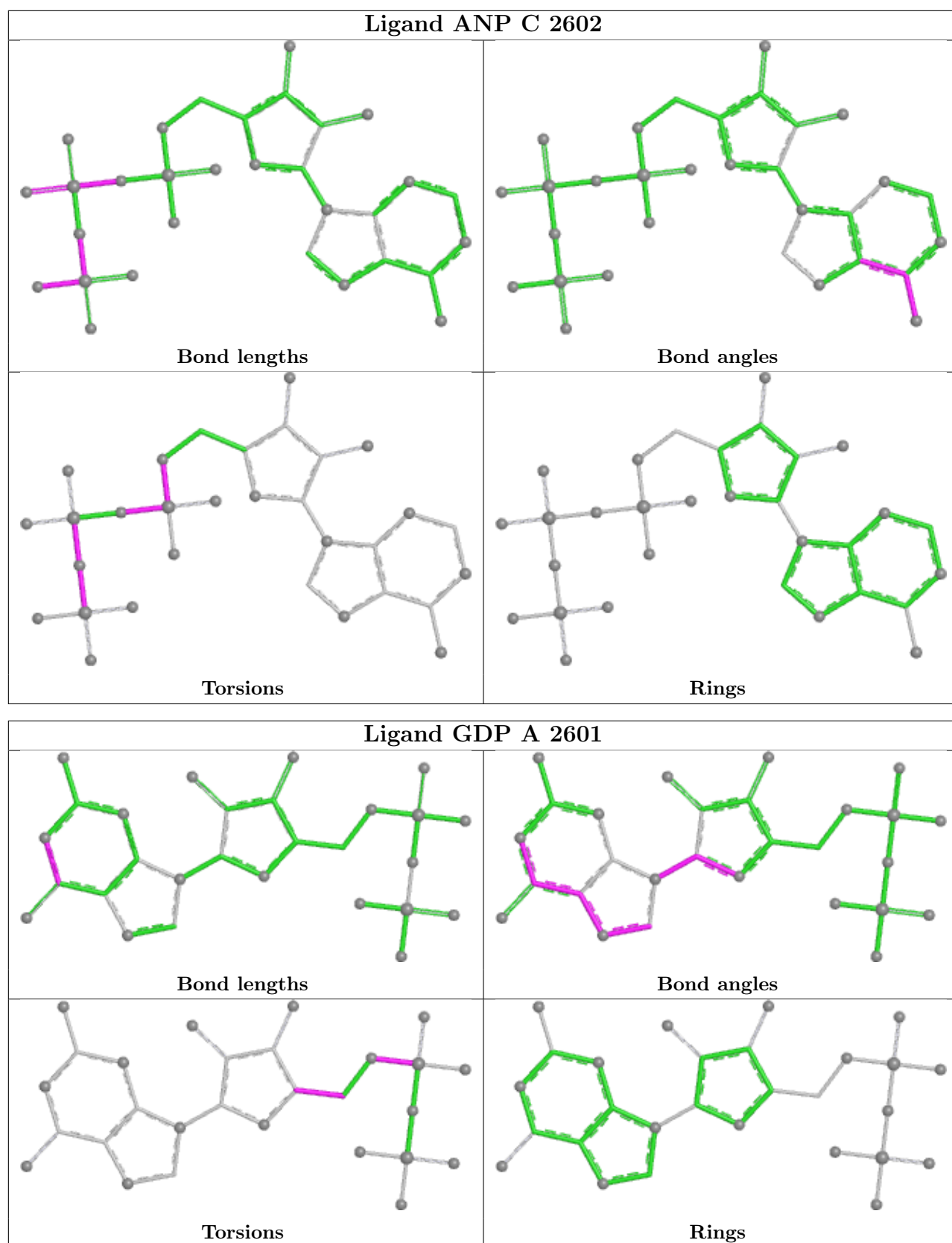
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	302	GNP	3	0
4	A	2602	ANP	1	0
6	D	302	GNP	3	0
4	C	2602	ANP	2	0

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.

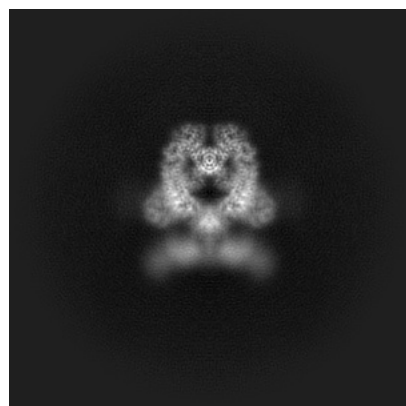
6 Map visualisation [i](#)

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.

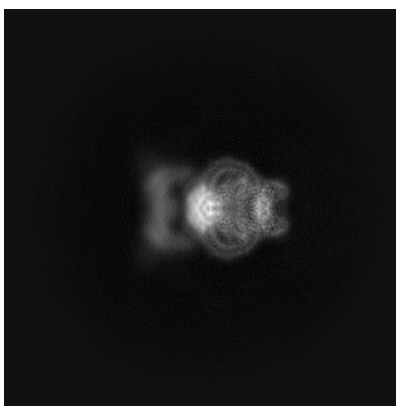
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

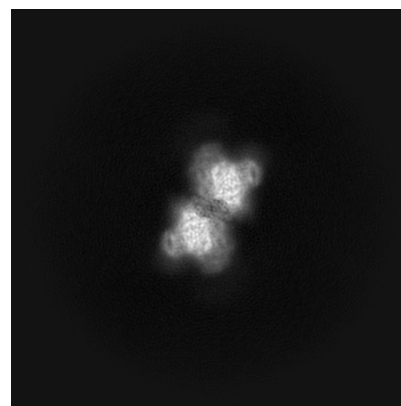
6.1.1 Primary map



X

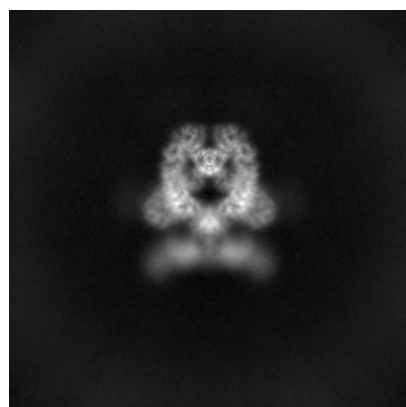


Y

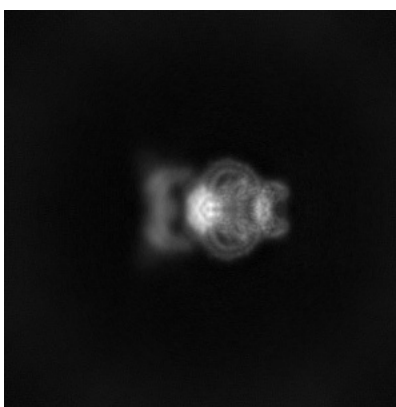


Z

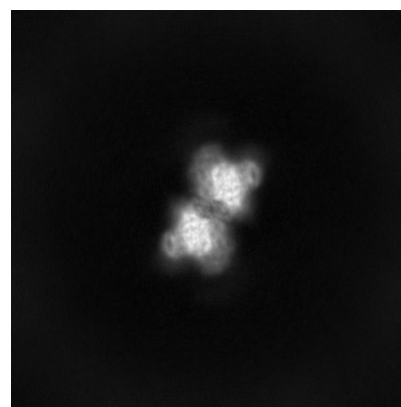
6.1.2 Raw map



X



Y

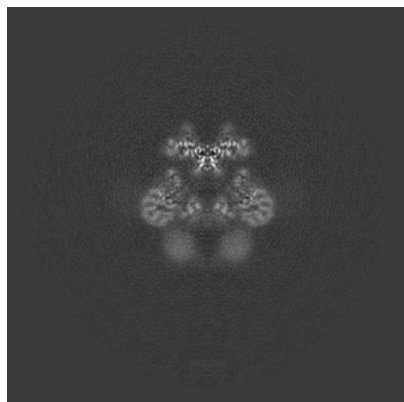


Z

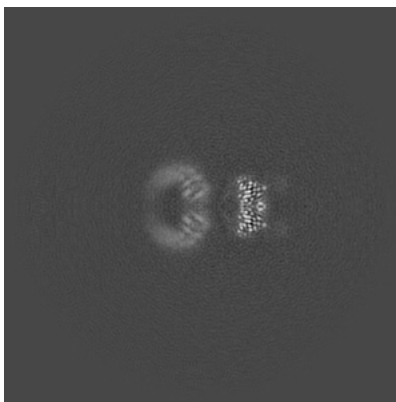
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

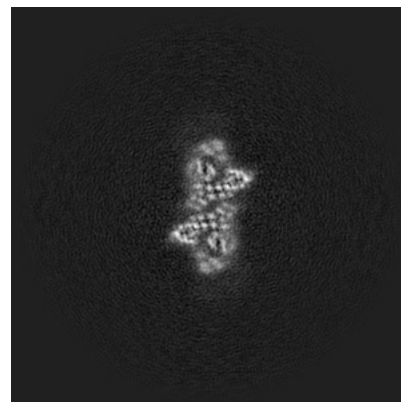
6.2.1 Primary map



X Index: 176

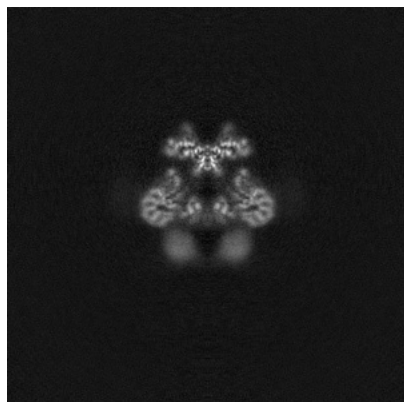


Y Index: 176

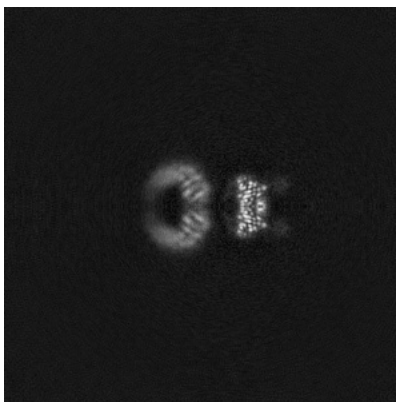


Z Index: 176

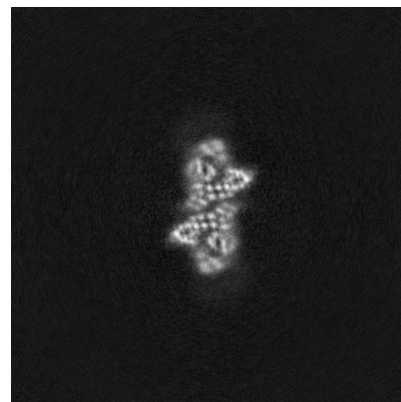
6.2.2 Raw map



X Index: 176



Y Index: 176

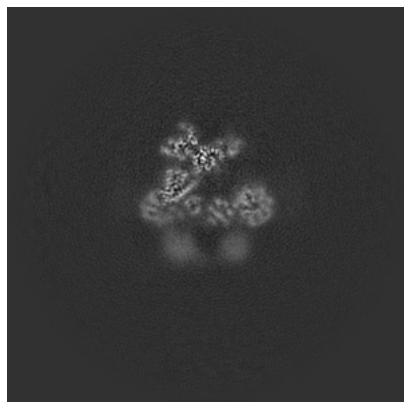


Z Index: 176

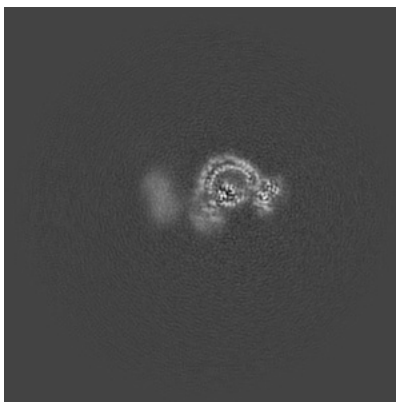
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

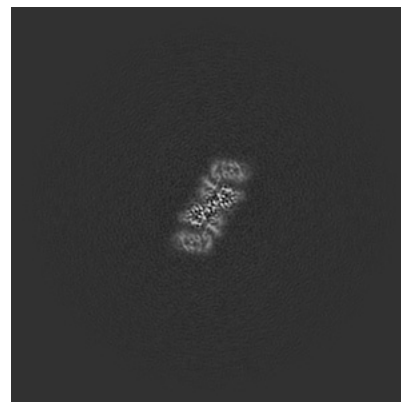
6.3.1 Primary map



X Index: 172

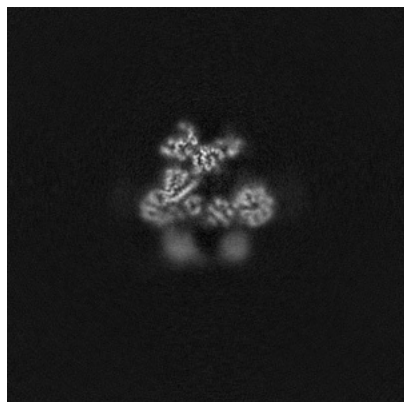


Y Index: 203

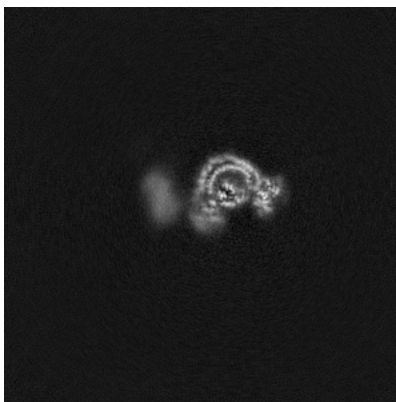


Z Index: 223

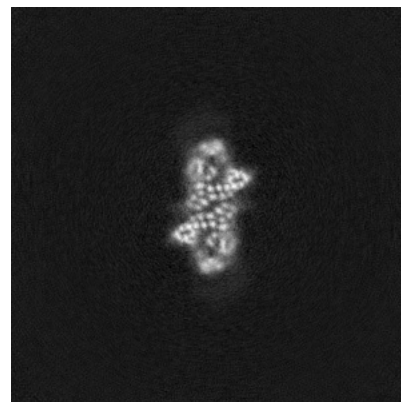
6.3.2 Raw map



X Index: 172



Y Index: 203

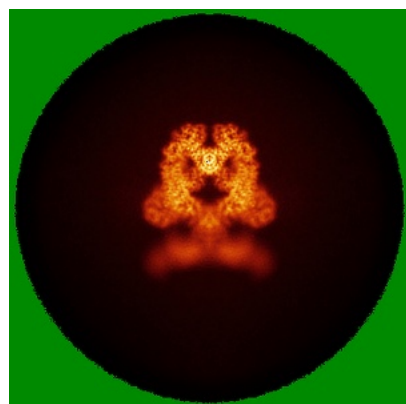


Z Index: 175

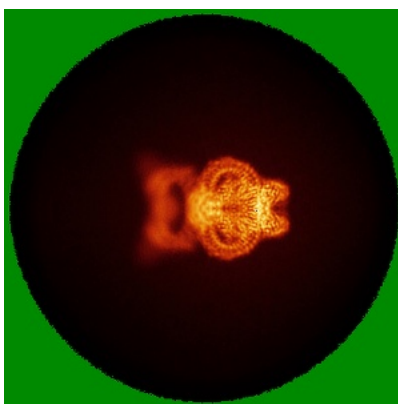
The images above show the largest variance slices of the map in three orthogonal directions.

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

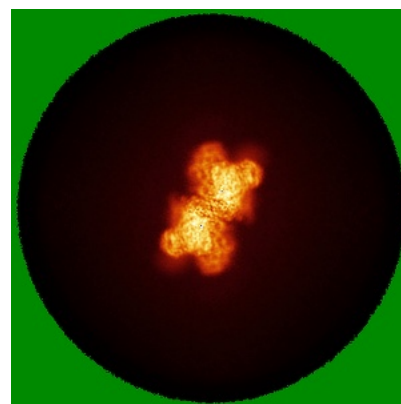
6.4.1 Primary map



X

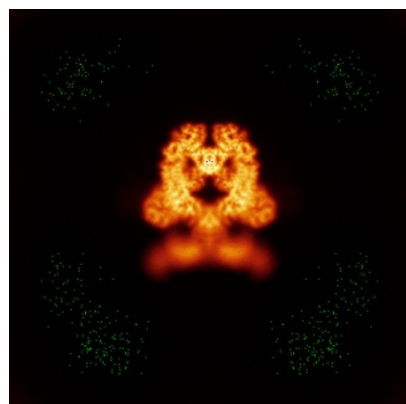


Y

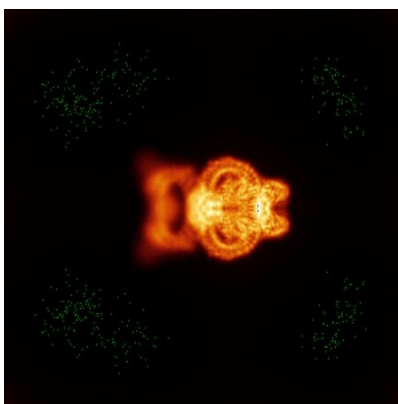


Z

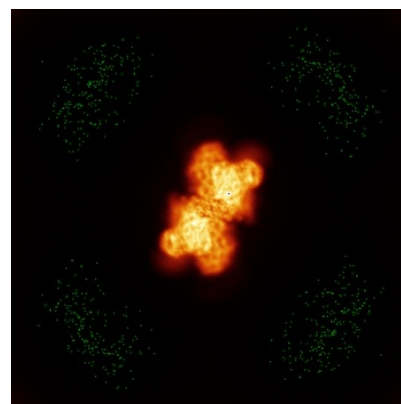
6.4.2 Raw map



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.

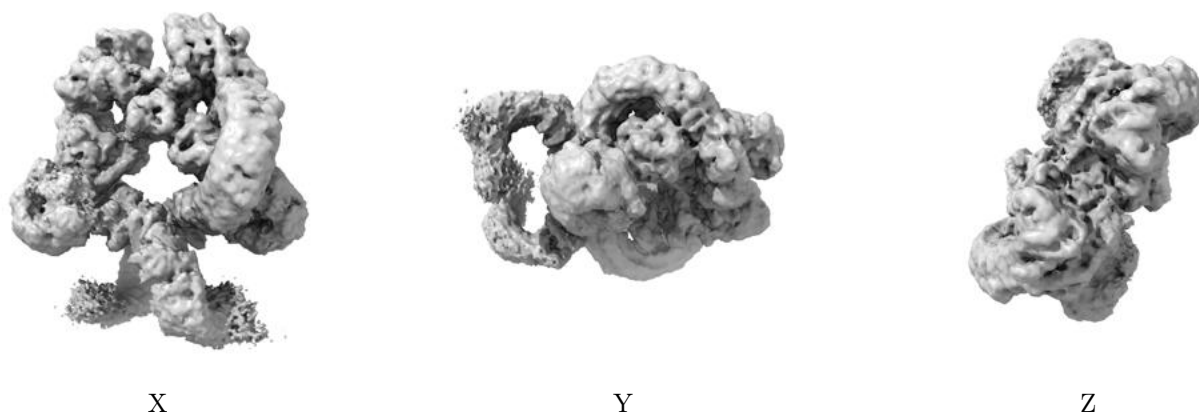
6.5 Orthogonal surface views [i](#)

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.

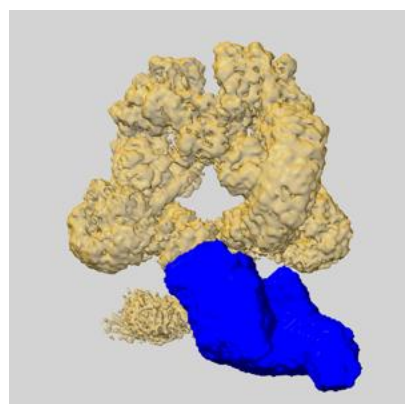
6.6 Mask visualisation [i](#)

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

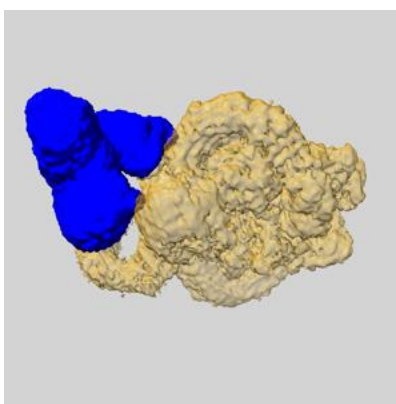
A mask typically either:

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

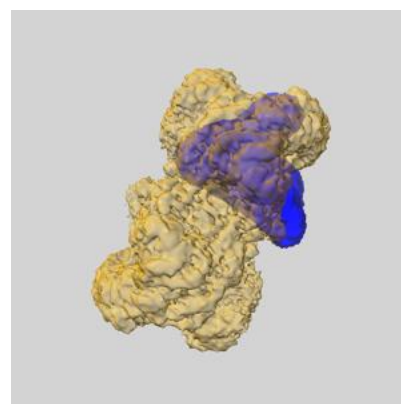
6.6.1 emd_43235_msk_1.map [i](#)



X

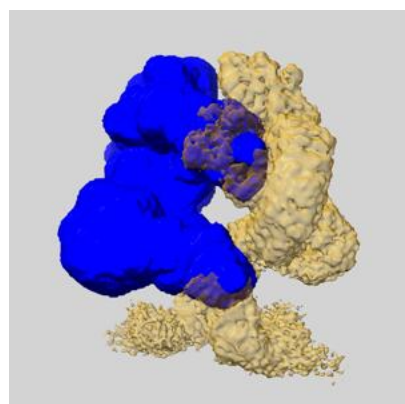


Y

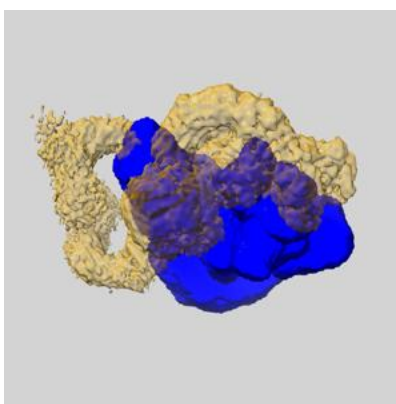


Z

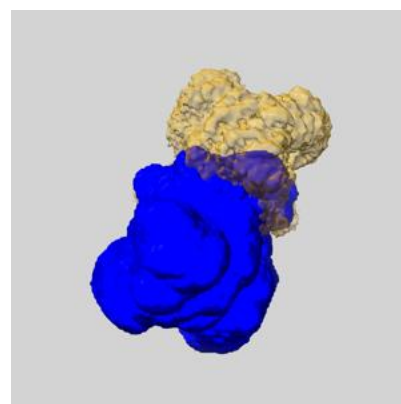
6.6.2 emd_43235_msk_2.map [i](#)



X



Y

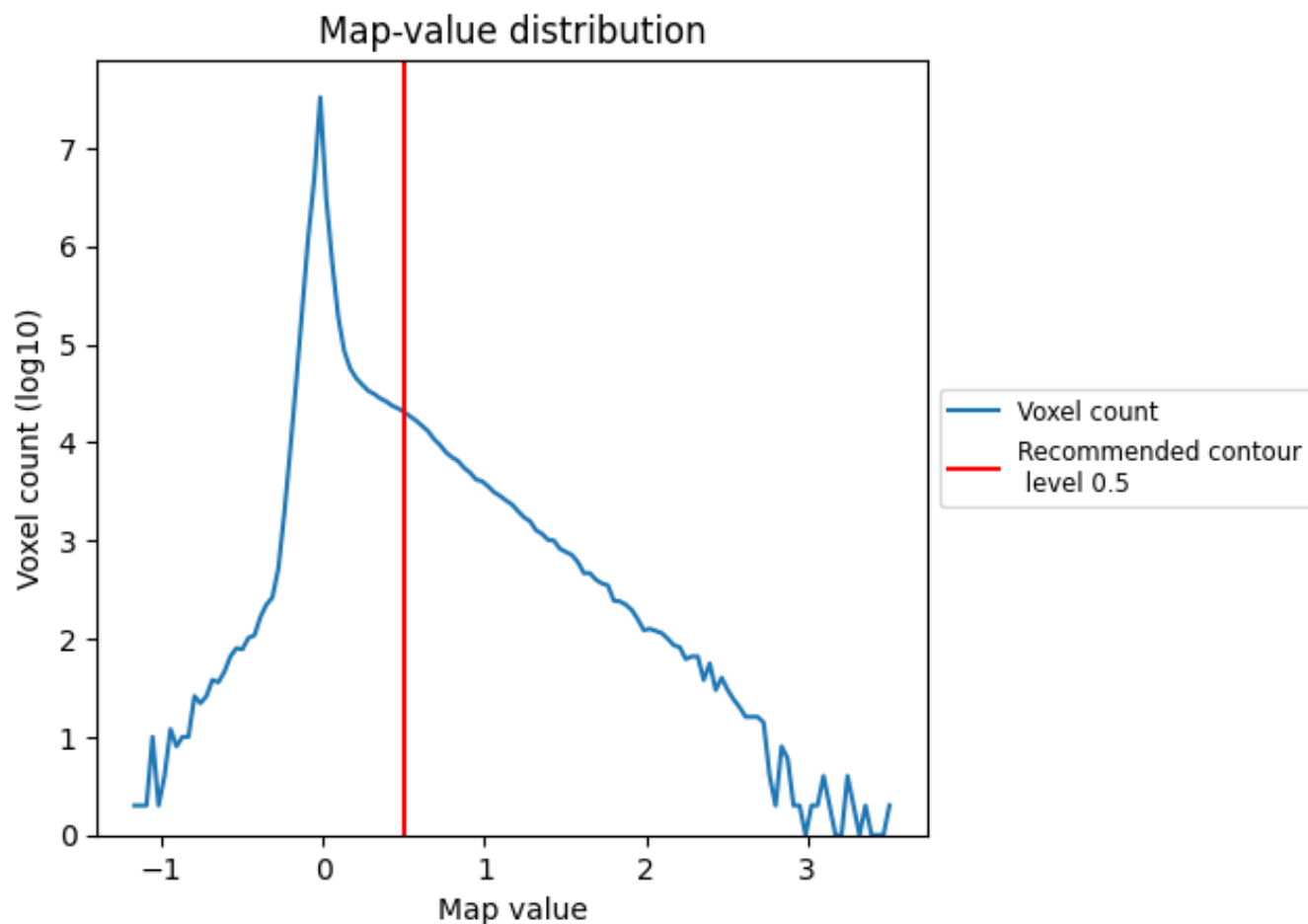


Z

7 Map analysis [i](#)

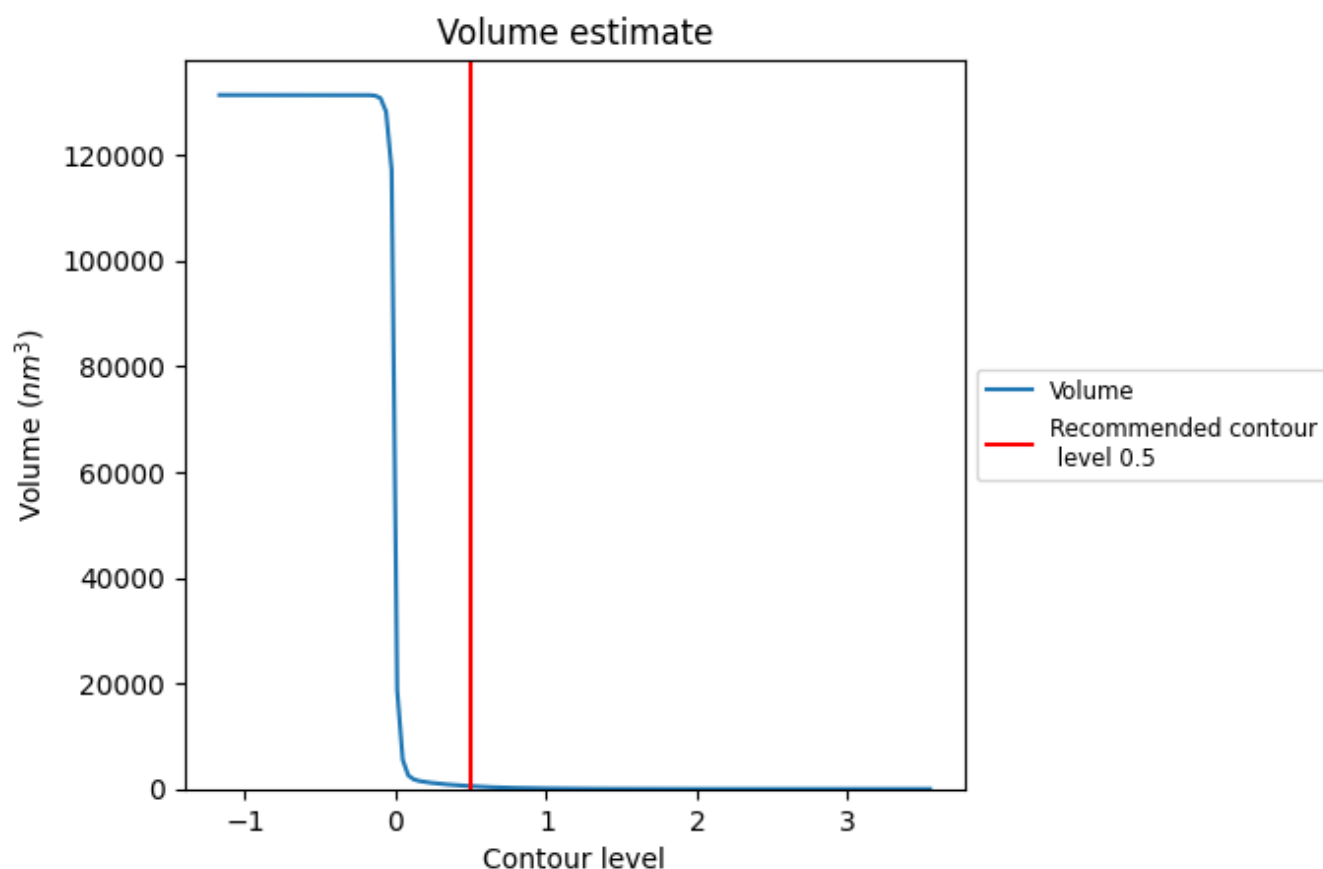
This section contains the results of statistical analysis of the map.

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.

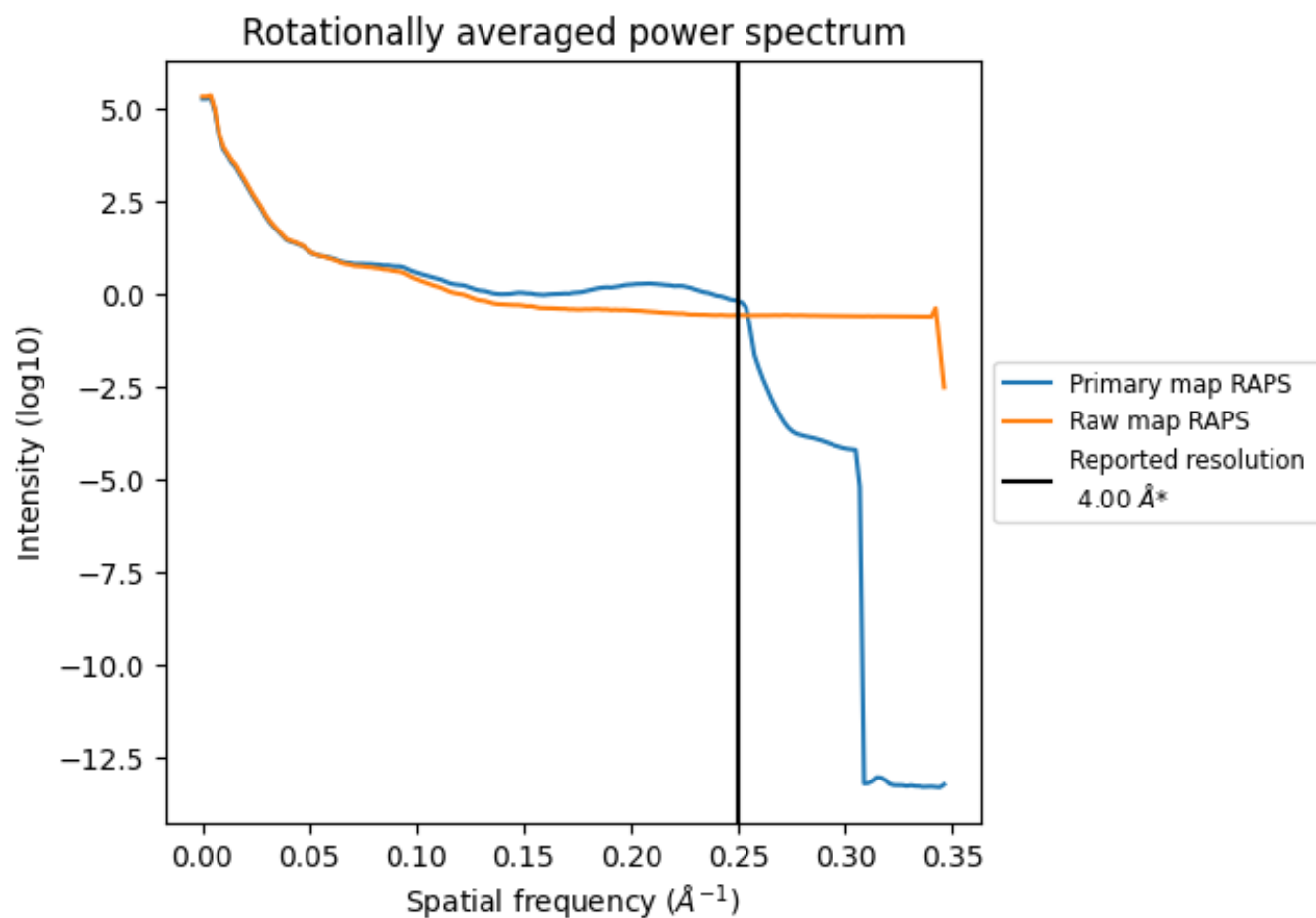
7.2 Volume estimate [i](#)



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 ⓘ

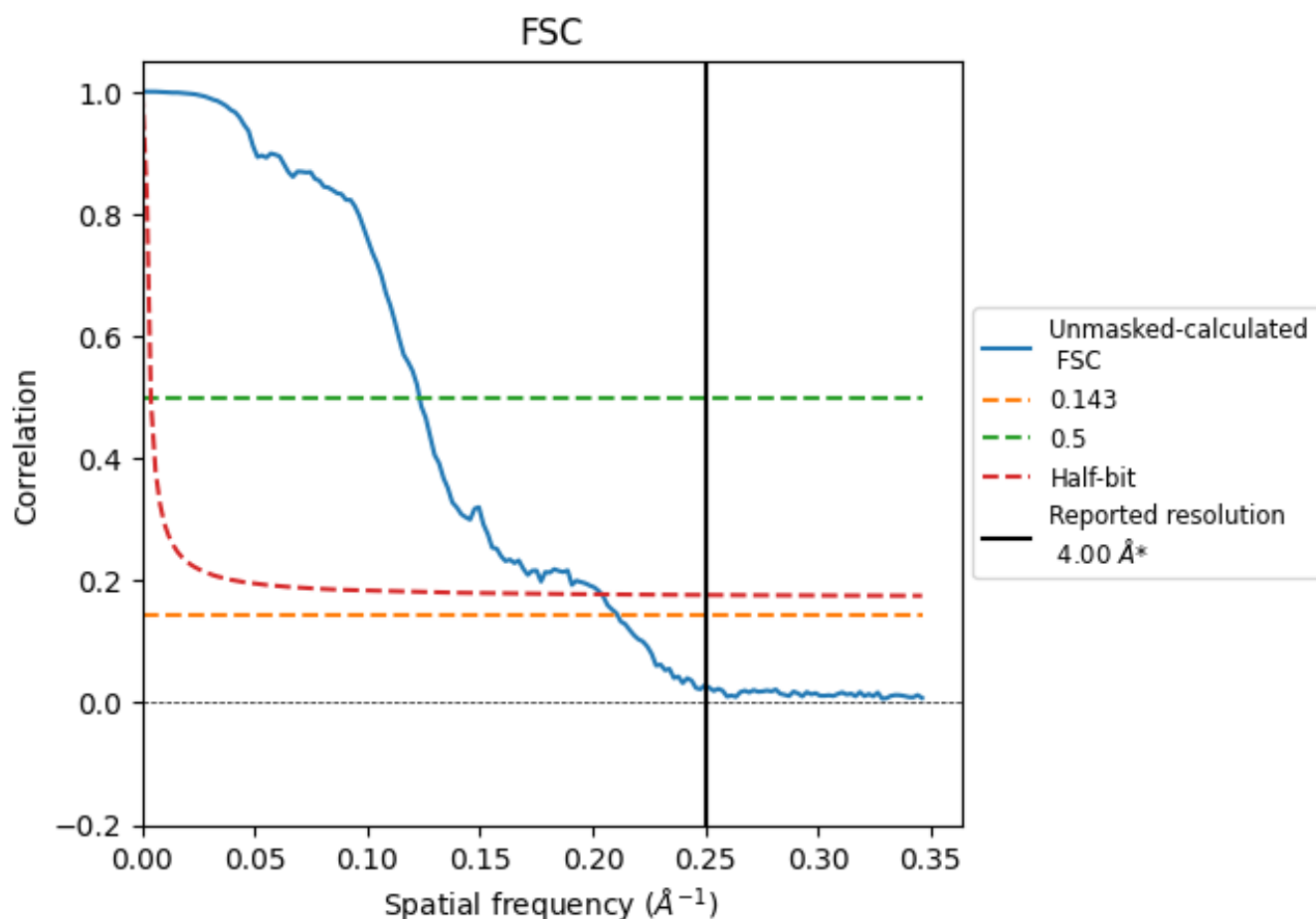


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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](#)

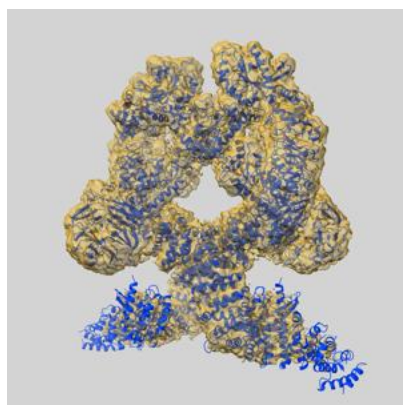
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.74	8.12	4.90

*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 %

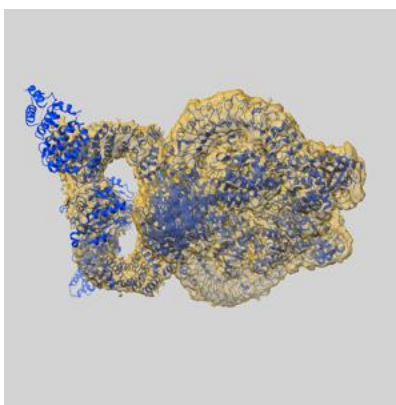
9 Map-model fit [i](#)

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](#).

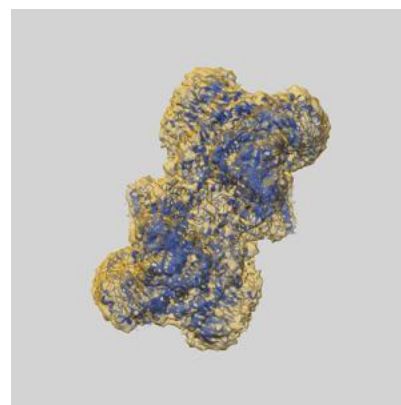
9.1 Map-model overlay [i](#)



X



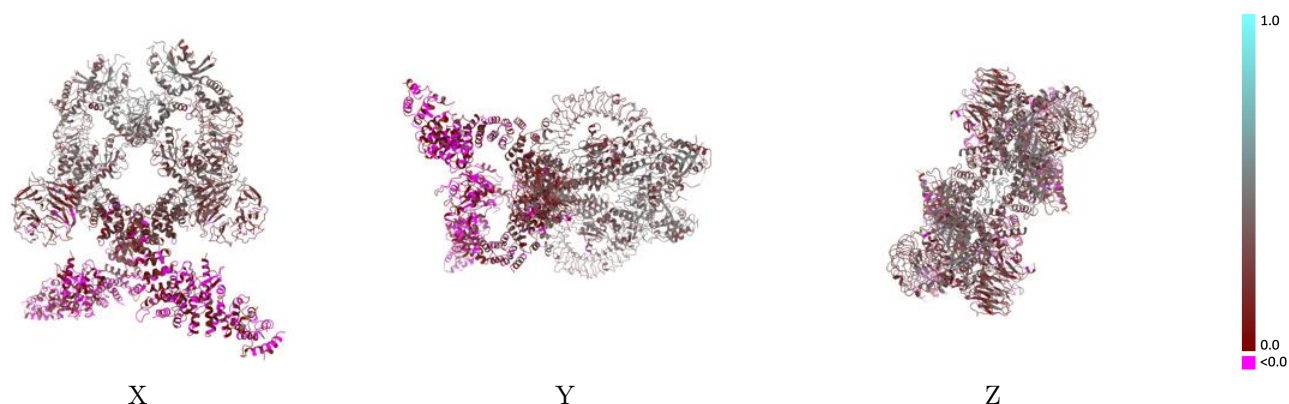
Y



Z

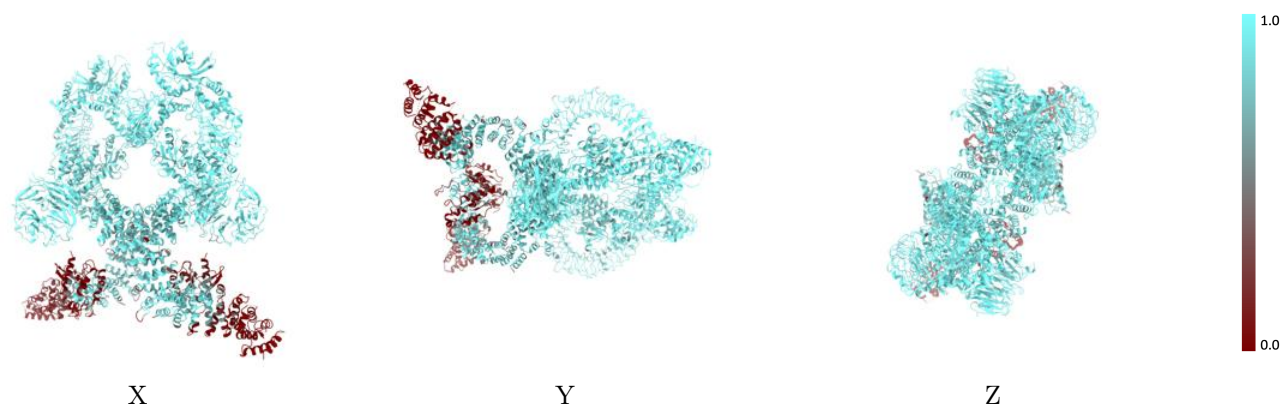
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



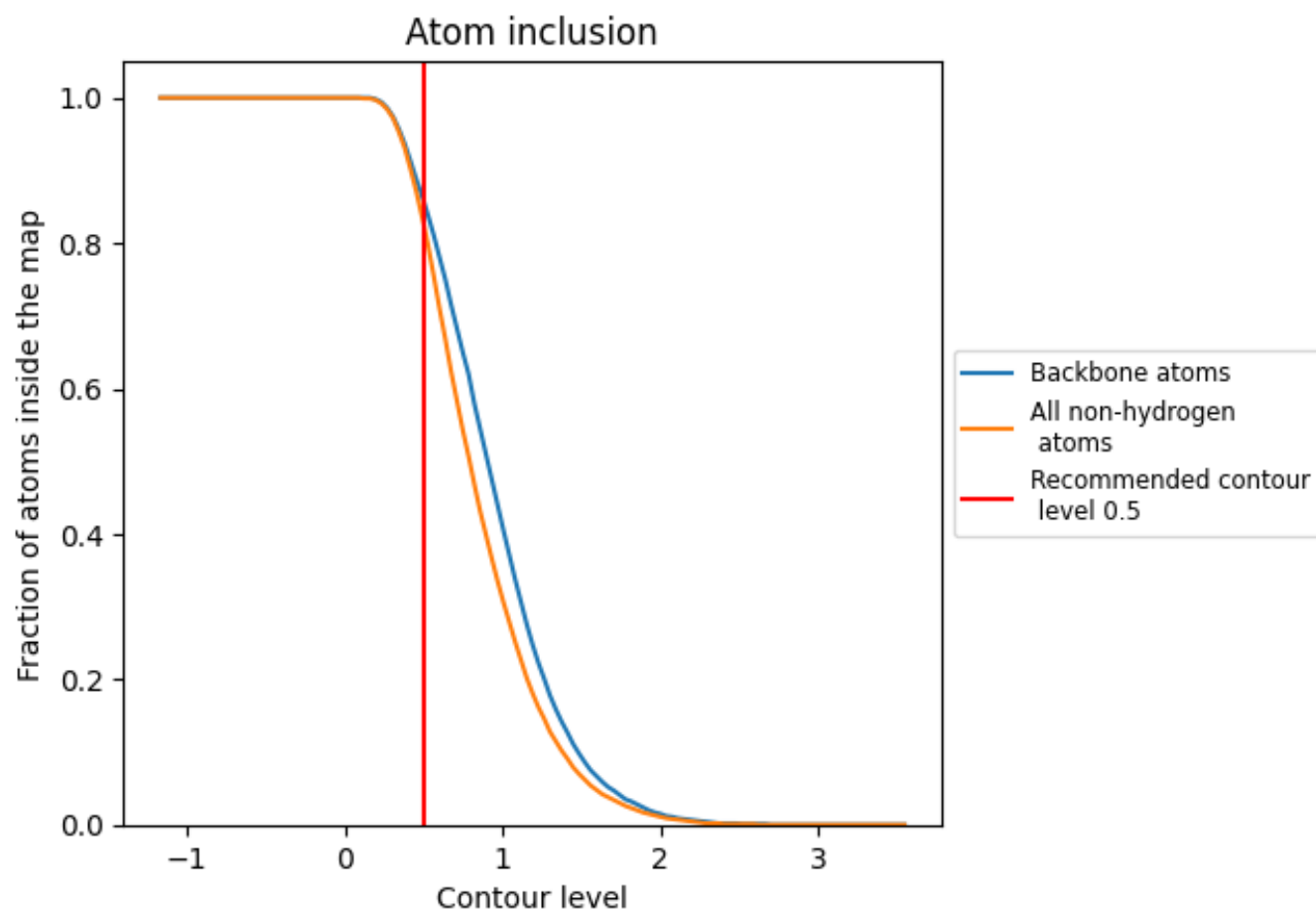
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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	<div></div> 0.8250	<div></div> 0.2480
A	<div></div> 0.8600	<div></div> 0.2600
B	<div></div> 0.3670	<div></div> 0.0350
C	<div></div> 0.8650	<div></div> 0.2690
D	<div></div> 0.3400	<div></div> 0.0440

